

Study of the metabolite changes in *Ganoderma lucidum* under pineapple leaf residue stress via LC-MS/MS coupled with a non-targeted metabolomics approach

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Table S1. Identification information of metabolite in *G.lucidum* under pineapple leaf residue stress

	Average Rt(min)	Average Mz	Metabolite name	Adduct type	Reference m/z	Formula	Ontology	INCHIKEY	SMILES
1	0.161	259.96069	N-acetyl-O-methyltyrosine	[M+H] ⁺	259.96497	C12H15N04	Phenylalanine and derivatives	HRUASHPCEMXOMR-UHFFFAOYSA-N	O=C(O)C(N=C(O)C)CC1=CC=C(OC)C=C1
2	0.168	204.9659	PYROGALLIN	[M+H] ⁺	204.96191	C11H8O4	Tropolones	OLSYHLURTGEIBH-UHFFFAOYSA-N	O=C1C(O)=CC=CC=CC(=O)C=C1O
3	0.172	283.26163	(9Z)-9-octadecenoic acid	[M+H] ⁺	283.26001	C18H34O2	Long-chain fatty acids	ZAPPMIVWEC5IRJ-KTKRT1GZSA-N	O=C(O)CCCCCCCC=CCCCCCCC
4	0.194	111.03909	Butyric acid	[M+H] ⁺	111.04	C4H8O2	Straight chain fatty acids	FERIUCNNQQJTQY-UHFFFAOYSA-N	O=C(O)CCC
5	0.322	118.08617	Betaine	[M+H] ⁺	118.08626	C5H11NO2	Alpha amino acids	KWUHFFTVRNATP-UHFFFAOYSA-N	C[N+](C)(C)CC(=O)[O-]
6	0.333	191.96115	Clopyralid	[M+H] ⁺	191.96136	C6H3Cl2NO2	Pyridinecarboxylic acids	HUBANNPOLNYSAD-UHFFFAOYSA-N	C1=CC(Cl)=NC(=C1Cl)C(=O)O
7	0.34	271.26318	Heptadecanoic acid	[M+H] ⁺	271.26315	C17H34O2	Long-chain fatty acids	KEMQGTRYUADPNZ-UHFFFAOYSA-N	O=C(O)CCCCCCCCCCCCCCC
8	0.352	186.01845	O-PHOSPHO-L-SERINE	[M+H] ⁺	186.02	C3H8NO6P	Alpha amino acids	BZQFWGGLXLEPQ-UHFFFAOYSA-N	O=C(O)C(N)COP(=O)(O)O
9	0.367	171.03514	2-(2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)acetic acid	[M+H] ⁺	171.03999	C6H6N2O4	Alpha amino acids and derivatives	ZFNQFXDDQAEAFI-UHFFFAOYSA-N	O=C1C=CN(C(=O)N1)CC(=O)O
10	0.4	176.01422	1-Methylsulfinybutenyl isothiocyanate	[M+H] ⁺	176.01984	C6H9NOS2	Glucosinolate breakdown metabolites	KQGJFQMGPDVOQE-UHFFFAOYNA-N	CS(=O)C=CCN=C=S
11	0.428	163.05971	3-Hydroxy-3-methylglutaric acid	[M+H] ⁺	163.0601	C6H10O5	Hydroxy fatty acids	NPOAOTPXWNWTSB-UHFFFAOYSA-N	CC(O)(CC(O)=O)CC(O)=O
12	0.438	199.17021	3,7-dimethyl-6-octenyl acetate	[M+H] ⁺	199.17	C12H22O2	Fatty alcohol esters	JOZKFWLHCDGJA-LLVKDONJSA-N	O=C(OCCCC)CCC=C(C)C
13	0.439	96.96992	Phosphoric acid	[M-H] ⁻	96.96962	H3O4P	Non-metal phosphates	NB1LXXVUZAPLBC-UHFFFAOYSA-N	O=P(O)(O)O
14	0.442	285.27829	stearic acid	[M+H] ⁺	285.28	C18H36O2	Long-chain fatty acids	Q1QXTHQIDYTFRIH-UHFFFAOYSA-N	O=C(O)CCCCCCCCCCCCCCC
15	0.464	391.28308	Di(2-ethylhexyl)phthalate (DEHP)	[M+H] ⁺	391.28427	C24H38O4	Benzoic acid esters	BJQHLKABXJIVAM-UHFFFAOYNA-N	CCCCC(CC)COC(C1=CC=CC=C1C(=O)OCC(CC)CCCC)=O
16	0.482	109.02829	p-Benzoquinone	[M+H] ⁺	109.0284	C6H4O2	p-benzoquinones	AZQWKYJCGOJGHM-UHFFFAOYSA-N	O=C1C=CC(=O)C=C1
17	0.487	201.99016	Cysteine-S-sulfate	[M+H] ⁺	201.98384	C3H7NO5S2	S-sulfo-L-cysteines	NOKPBJYHPHWAN-REOHCLBISA-N	C([C-H](C(=O)O)N)SS(=O)=O
18	0.508	132.10263	Isoleucine (not validated)	[M+H] ⁺	132.1028	C6H13NO2	Amino acids	AGPKZVBTJJNPAG-UHFFFAOYNA-N	O=C(O)C(N)C(C)CC
19	0.509	102.12761	Hexylamine	[M+H] ⁺	102.12772	C6H15N	Monoalkylamines	BMVXCPBGZKUPN-UHFFFAOYSA-N	CCCCCCN
20	0.542	186.01791	O-Phosphoserine	[M+H] ⁺	186.0162	C3H8NO6P	L-alpha-amino acids	BZQFWGGLXLEPQ-UHFFFAOYNA-N	O=C(O)C(N)COP(=O)(O)O
21	0.553	232.16878	Alpha-pyrrolidinovalerophenone	[M+H] ⁺	232.17	C15H21NO	Alkyl-phenylketones	YD1DRWHPFMLGR-UHFFFAOYSA-N	O=C(C(=CC=CC=C1)C(N2CCCC2)CCC
22	0.563	297.99988	(E)-2-(hydroxymethyl)-3-(3-oxo-5-propan-2-yl-4,5,6,7-tetrahydro-1H-2-benzofuran-4-yl)propan-2-enoic acid	[M+H] ⁺	298.00226	C15H20O5	Terpene lactones	YVASZTJGPFKRMW-BJMGVGYQSA-N	O=C(O)C(=CC1=CC(=O)OCC2CCC1C(C)C)CO
23	0.597	155.14288	Linalool	[M+H] ⁺	155.14304	C10H18O	Acyclic monoterpenoids	CDOSHSSSFJOMGT-UHFFFAOYNA-N	OC(C=C)C(C)CCC=C(C)C
24	0.606	113.06019	1,2-Cyclohexanedione	[M+H] ⁺	113.05971	C6H8O2	Cyclic ketones	O1LA1QEIWYQPH-UHFFFAOYSA-N	O=C1C(=O)CCCC1
25	0.696	168.02489	Quinolinic Acid	[M+H] ⁺	168.02502	C7H5NO4	Pyridinecarboxylic acids	GJAWHXHKYXBSV-UHFFFAOYSA-N	O=C(O)C1=NC=CC=C1C(=O)O
26	0.7	255.93947	Triclopyr	[M+H] ⁺	255.93295	C7H4Cl3NO3	Polyhalopyridines	REEQLXGVDJJSQ-UHFFFAOYSA-N	OC(=O)COC1=C(Cl)C=C(Cl)C(Cl)=N1
27	0.701	303.02585	4-hydroxy-3-[4-(4-hydroxy-6-methyl-2-oxopyran-3-yl)methyl]-6-methylpyran-2-one	[M+H] ⁺	303.02655	C13H12O6	Pyranones and derivatives	DVLLGHPGJPEUHA-UHFFFAOYSA-N	O=C1OC(=CC(O)=C1CC=CC(=O)OC(=CC2O)C)C
28	0.704	251.16005	Nardosinone	[M+H] ⁺	251.16	C15H22O3	Sesquiterpenoids	KXGHISIMRWPVQM-JWPUOXDNSA-N	O=C1C2=CCCC(C)C2(C)C3C(OC3(C)C)C1
29	0.704	148.94887	Trifluoromethanesulfonic acid	[M-H] ⁻	148.95258	CHF3O3S	PFSA	ITMCEJHCFYS1IV-UHFFFAOYSA-N	O=S(=O)(O)C(F)(F)F
30	0.705	278.94257	5-Chloro-perfluoropentanoic acid	[M-H] ⁻	278.94647	C5HClF8O2	PFSA	VQKMXAMQVPHHB-UHFFFAOYSA-N	O=C(O)C(F)(F)C(F)(F)C(F)C(F)C(F)Cl
31	0.707	147.97292	PFSM-perfluorooalkyl_sulfonamide	[M-H] ⁻	147.96855	ClF2F3NO2S	PFSA	KAKQVSNHTBLJCH-UHFFFAOYSA-N	O=S(=O)(N)C(F)(F)F
32	0.709	370.94284	PFFCA-pentafluorosulfide	[M-H] ⁻	370.94168	C5HF13O2S	PFSA	NDS1RS11HKJNN-UHFFFAOYSA-N	O=C(O)C(F)(F)C(F)(F)C(F)(F)S(F)(F)(F)F
33	0.71	226.05573	Synephrine hydrochloride	[M+H] ⁺	226.06	C9H14ClNO2	1-hydroxy-2-unsubstituted benzenoids	COTCEGYSNTWJQV-UHFFFAOYSA-N	Cl.CC1=CC=C(C=C1)C(O)CNC
34	0.711	385.87479	[4-acetyloxy-2,5-dihydroxy-6-(hydroxymethyl)oxan-3-yl] (E)-3-(4-hydroxyphenyl)propan-2-enoate	[M+H] ⁺	385.87271	C17H20O9	Coumaric acid esters	QXRDLAXUJONPD-QPJXXVBHSA-N	O=C(OC1C(O)OC(CO)C(O)C1OC(=O)C)CC2=CC=C(O)C=C2
35	0.711	236.03975	Carnitine (Dl) Hydrochloride	[M+H] ⁺	236.04503	C7H16ClNO3	Carnitines	JXXCENBLGFBQJM-UHFFFAOYSA-N	Cl.O=C([O-])CC(O)C[N+](C)(C)C
36	0.714	189.02379	6,7-dihydroxybenzofuran-3(2H)-one	[M+H] ⁺	189.02	C8H6O4	Benzofurans	ZDHCVQNRWDINX-UHFFFAOYSA-N	O=C1C2=CC=C(O)C(=O)C=C2O1
37	0.714	308.25049	Pentadecanoyl Ethanolamide	[M+2H] ²⁺	308.25	C17H35NO2	N-acyl ethanolamines	UHPXXKLACDXGS-UHFFFAOYSA-N	O=C(NC(=O)CCCCCCCCCCCCCCC
38	0.715	231.03406	3,4-Dimethoxycinnamic Acid	[M+H] ⁺	231.03662	C11H12O4	Coumaric acids and derivatives	HJWBJAPBAGSQPR-GQCTYL1ASA-N	O=C(O)C=CC1=CC=C(OC)C(OC)=C1
39	0.716	284.01968	Procymidone	[M+H] ⁺	284.02396	C13H11Cl2NO2	Phenylpiperidines	YQKJBPAVAHBARF-UHFFFAOYNA-N	CC12CC2(C)C(N(C3=CC(=CC(=C3)C1)C1)=O)=O
40	0.717	247.02939	columbianetin	[M+H] ⁺	247.03241	C14H14O4	Angular furanocoumarins	XQAQEMCYCSSHJG-UHFFFAOYSA-N	O=C1OC2=C(C=C1)C=CC=CC(C2)C(O)C
41	0.718	233.03185	MUCIC ACID	[M+H] ⁺	233.02678	C6H10O8	Glucuronic acid derivatives	DSLZVSRTYRFBF-DUHHBMHGSA-N	O=C(O)C(O)C(O)C(O)C(=O)O

42	0. 721	283. 02527	1, 3, 5, 8-Tetrahydroxyxanthone	[M+H] ⁺	283. 01999	C13H8O6	Xanthenes	MPXAWSABMVLBU-UHFFFAOYSA-N	O=C1C=2C(O)=CC(O)=CC2OC=3C(O)=CC=C(O)C13
43	0. 722	123. 03981	2-methylcyclohexa-2, 5-diene-1, 4-dione	[M+H] ⁺	123. 04	C7H6O2	P-benzoquinones	VTWDKFNVLAEJH-UHFFFAOYSA-N	O=C1C=CC(=O)C(=C1)C
44	0. 722	165. 03516	Allicin + 2H (not validated, isomer of 328)	[M+H] ⁺	165. 03999	C6H12OS2	Allicin derivatives	XLVMWOFYTFNDKM-UHFFFAOYNA-N	O=S(CCC)SC=CC
45	0. 722	360. 93964	PFSA-unsaturated	[M-H] ⁻	360. 93979	C6HF11O3S	PFSA	WNQXBVFTFYMUUCU-UHFFFAOYSA-N	O=S(=O)(O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F
46	0. 722	212. 03979	PHOSPHOCREATINE	[M+H] ⁺	212. 03999	C4H10N3O5P	Alpha amino acids and derivatives	DRBBFCLWYRJSJZ-UHFFFAOYSA-N	O=C(O)CN(C(=NP(=O)(O)O)N)C
47	0. 723	143. 04996	5-(hydroxymethyl)pyrimidine-2, 4-diol	[M+H] ⁺	143. 05	C5H6N2O3	Pyrimidones	JDBGXEHEITGOBU-UHFFFAOYSA-N	OC1=NC=C(C(O)=N1)CO
48	0. 723	125. 03749	N,N-Dimethylsulfamide	[M+H] ⁺	125. 03793	C2H8N2O2S	Sulfuric acid diamides	QMIAHUAQAJVBIW-UHFFFAOYSA-N	CN(C)S(N)(=O)=O
49	0. 724	167. 01352	3-hydroxy-4-methoxy-2, 3-dihydropyran-6-one	[M+H] ⁺	167. 01662	C6H8O4	Dihydropyranones	PBEXSRJMCVDBFK-UHFFFAOYSA-N	O=C1OCC(O)C(OC)=C1
50	0. 724	146. 1647	Spermidine	[M+H] ⁺	146. 16518	C7H19N3	Dialkylamines	ATHGHQPGPGMSJY-UHFFFAOYSA-N	NCCCNCCCN
51	0. 725	267. 01202	Bauerine C	[M+H] ⁺	267. 01599	C12H8C12N2O	Beta carbolines	JFESWTBLTUPGK-UHFFFAOYSA-N	O=C1NC=CC=2C3=CC=C(C1)C(C1)=C3N(C12)C
52	0. 726	329. 98038	(E)-N-[2-hydroxy-2-(4-hydroxyphenyl)ethyl]-3-(4-hydroxy-3-methoxyphenyl)propan-2-enamide	[M+H] ⁺	329. 98386	C18H19NO5	Hydroxycinnamic acids and derivatives	VJSCHQMOTSXKB-YCRREMBSA-N	OC(=NCC(O)C1=CC=C(O)C=C1)C(=CC2=CC=C(O)C(OC)=C2
53	0. 727	103. 04988	(R)-4-aminoisoxazolidin-3-one	[M+2H] ²⁺	103. 05	C3H6N2O2	Alpha amino acids and derivatives	DYDCUQKUCUJJBH-UWTATZPHSA-N	O=C1NOC1N
54	0. 728	356. 97989	4-[1-(1,3-benzodioxol-5-yl)propan-2-yl]-4,5-dimethoxy-2-prop-2-enylcyclohexa-2,5-dien-1-one	[M+H] ⁺	356. 98035	C21H24O5	Bicyclic monoterpenoids	SMOHLDESHACKE-UHFFFAOYSA-N	O=C1C=C(OC)C(OC)(C=C1CC=C)C(C)CC2=CC=C3OCC3=C2
55	0. 728	160. 97531	OPFC-perfluoroalkyl_sulfate	[M-H] ⁻	160. 97256	C2H4F2O4S	PFSA	LACMPONGXCPPKO-UHFFFAOYSA-N	O=S(=O)(O)OCC(F)F
56	0. 728	221. 04977	Pesticide2_Thiazuron_C9H8N4OS_1-Phenyl-3-(1,2,3-thiadiazol-5-yl)urea	[M+H] ⁺	221. 049	C9H8N4OS	N-phenylureas	HFCYZXMHIUHQI-UHFFFAOYSA-N	OC(=NC1=CC=CC=C1)NC(=S)N=C2
57	0. 729	281. 10614	Huperzine A	[M+H] ⁺	281. 10507	C15H18N2O	Quinolones and derivatives	ZRJBJHW1HUMBLCN-UHFFFAOYSA-N	OC=1N=C2C(=CC1)C3(N)C(=CC)C(C=C(C)C3)C2
58	0. 73	280. 99149	methyl 5,6-diacetyloxy-10-hydroxy-2,4b,7,10a,12a-hexamethyl-12-methylidene-1,4,8-trioxo-da,5,6,6a,9,10,10b,11-octahydronaphthal-1,2-	[M+H] ⁺	280. 99219	C30H40O11	Oxosteroids	FFXYBQSGDXRLHS-UHFFFAOYSA-N	O=C(OC1C(OC(=O)C)C2(C)C3C(=O)OC(C(=O)C)(C(=O)C3(C(=C)C2)C4(C)C(OC(=O)C)=O)C(C1)C1)C1C
59	0. 732	265. 11029	Thiamine	[M+H] ⁺	265. 11121	C12H17N4O5	Thiamines	JJRWGCRZTMMZEH-UHFFFAOYSA-N	CC1=C(COC)SC(=[N+])CC1=CN=C(C)NC1=N
60	0. 741	189. 13409	Homoarginine	[M+H] ⁺	189. 1346	C7H16N4O2	Alpha amino acids	QUOGSRFPZMMIT-UHFFFAOYNA-N	O=C(O)C(N)CCCCNC(=N)N
61	0. 743	188. 17538	N8-Acetylspermidine	[M+H] ⁺	188. 17574	C9H21N3O	Carboximidic acids	FON1WJDLJEJTL-UHFFFAOYSA-N	OC(=NCCCCCCCN)C
62	0. 744	329. 07806	8-(2-hydroxy-1-methoxy-3-methylbut-3-enyl)-7-methoxychromen-2-one	[M+H] ⁺	329. 07858	C16H18O5	Coumarins and derivatives	DBPWCIPOCMUFT-UHFFFAOYSA-N	O=C1OC2=C(C=C1)C(=CC(OC)=C2C(OC)C(O)C(=C)C
63	0. 744	133. 09662	Ornithine	[M+H] ⁺	133. 09715	C5H12N2O3	Alpha amino acids	AHLPHDHMVZTML-UHFFFAOYSA-N	O=C(O)C(N)CCCN
64	0. 745	359. 04245	3-O-acetylpadmatin	[M-H] ⁻	359. 04004	C18H16O8	7-O-methylated flavonoids	WWYQJKYSCMPCP-MSOLQXFSA-N	O=C(OC1C(=O)C2=C(O)C(=O)C=C2OC1C3=CC=C(C(O)C(=O)C3)C
65	0. 748	311. 06683	Cefditoren pivoxil	[M+H] ⁺	311. 06699	C25H28N6O7S3	Cephalosporins	AFZPFLVORLEPPO-OUOWMNRXSA-N	O=C(OCOC(=O)C(C)C(C)C1C(=C(C=C2SC=NC2)CSC3NC(=O)C3N(C(=O)C(=NOC1)C=AN=C(=C4)N
66	0. 75	352. 09363	feruloyltyramine	[M+H] ⁺	352. 09457	C18H19NO4	Methoxyphenols	NPNKMSXYRADT-WEVVXLNSA-N	OC(=NCCC1=CC=C(O)C=C1)C(=CC2=CC=C(O)C(OC)=C2
67	0. 758	175. 11835	Arginine	[M+H] ⁺	175. 119	C6H14N4O2	Arginine and derivatives	ODKSFYDXXFIFQN-UHFFFAOYSA-N	O=C(O)C(N)CCCN=C(N)N
68	0. 758	371. 04456	Norstictic acid	[M-H] ⁻	371. 03799	C18H12O9	Diarylethers	IEVVSJFLBYOUCJ-UHFFFAOYSA-N	O=CC1=C(O)C=C(C(=2C(=O)OC3=C(OC12)C4=C(C(=O)OC4)C(O)=C3C
69	0. 774	189. 1604	NEPSILON, NEPSILON, NEPSILON-TRIMETHYLLYSINE	[M+H] ⁺	189. 16	C9H20N2O2	Alpha amino acids	MXNRLFUSPKVQSK-UHFFFAOYSA-N	O=C([O-])C(N)CCCC[N-]C(C)C
70	0. 778	353. 20703	Hydroxyprogesterone	[M+H] ⁺	353. 2052	C21H30O3	Gluco/mineralocorticoids, progestogens and	DBPWSSGDRRHUNT-UHFFFAOYSA-N	O=C1C=C2CCC3(CCC4(C)C3CCC4(O)C(=O)C)C2(C)CC1
71	0. 783	341. 02631	Pesticide4_Pyrimethanil_C12H13N3_2-Pyrimidinamine, 4,6-dimethyl-	[M-H] ⁻	341. 026	C6H9N3	Aminopyrimidines and derivatives	IDQNBVFPZMCDN-UHFFFAOYSA-N	N=C1N=C(C=C(N1)C)C
72	0. 786	429. 23834	Irbesartan	[M+H] ⁺	429. 23975	C25H28N6O	Biphenyls and derivatives	YOSHYTLCDANDAN-UHFFFAOYSA-N	CCCCC1=NC2(CCCC2)C(N1CC3=CC=C(C=C3)C4=CC=CC=C4C5=NN=N5)=O
73	0. 787	469. 13022	Galapagin	[M-H] ⁻	469. 129	C20H24O10	Phenolic glycosides	NJRLDXGREKHGV-IVABAYMNSA-N	O=C(OC1OC(OC=2C(=C(O)C=3C(=O)C=C(OC32C)C)C(O)C(O)C1O)C
74	0. 787	257. 06497	ONONETIN	[M-H] ⁻	257. 06015	C15H14O4	Stilbenes	XHBZOAYMBBUURD-UHFFFAOYSA-N	O=C(C1=CC=C(O)C=C1O)CC2=CC=C(OC)C=C2
75	0. 789	426. 98535	(Perfluorohexyl)ethanoic acid	[M-H] ⁻	426. 98209	C9H3F15O2	PFSA	WSEBQIVQARAMW-UHFFFAOYSA-N	O=C(O)CC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F
76	0. 79	266. 15857	"Mirtazapine (Remeron, Avanza)"	[M+H] ⁺	266. 16501	C17H19N3	Piperazinoazepines	RONZAEMNMQARA-UHFFFAOYSA-N	N=1C=CC=C2C1N3CCN(C)CC3C=4C=CC=CC4C2
77	0. 79	173. 10349	L-(+)-Arginine	[M-H] ⁻	173. 1044	C6H14N4O2	L-alpha-amino acids	ODKSFYDXXFIFQN-BYPYZUCNSA-N	N[C@H](CCCC(N)=N)C(O)=O
78	0. 794	740. 6745	Glyceryl trimyristate	[M+H] ⁺	740. 677	C45H86O6	Triacylglycerols	DUXYWXYOBRMGIN-UHFFFAOYSA-N	O=C(OC(OC(=O)CCCCCCCCCCCCC)OC(=O)CCCCCCCCCCCCC)CCCCCCCCCCCC
79	0. 795	319. 01706	Medicagol	[M+H] ⁺	319. 01999	C16H8O6	Coumestans	UDMYEUAUWUQHON-UHFFFAOYSA-N	O=C1OC=2C(O)C=CC2=3OC4=CC=5OCC5C=C4C13
80	0. 796	307. 14911	Vincandine	[M-H] ⁻	307. 1452	C19H20N2O2	Alkaloids	JDOFCMASVRMYJU-UHFFFAOYNA-N	CC=C1CN2CC3C4C2C1C(C=O)=C3NC1=C4C=CC=C1O
81	0. 797	216. 01375	2-amino-3-prop-2-enylsulfinylpropanoic acid	[M+H] ⁺	216. 00912	C6H11NO3S	Alpha amino acids	XUHLJQGRKRUPH-UHFFFAOYSA-N	O=C(O)C(N)CS(=O)CC=C
82	0. 797	292. 96927	Daidzein	[M+H] ⁺	292. 96872	C15H10O4	Isoflavones	ZQS1JRDFPHDXIC-UHFFFAOYSA-N	O=C1C(=COC2=CC(O)=CC=C12)C=3C=CC(O)=CC3
83	0. 797	320. 03976	Epalrestat	[M+H] ⁺	320. 04099	C15H13NO3S2	Alpha amino acids and derivatives	CHNUOJQWGUOLD-NFZZJPOKSA-N	O=C(O)CN1C(=S)SC(=CC(=CC2=CC(=CC2)C)C1=O
84	0. 797	420. 95001	Fipronil-sulfide	[M+H] ⁺	420. 95108	C12H4Cl2F6N4S	Phenylpyrazoles	FQXWEKADCSXVOC-UHFFFAOYSA-N	NC1=C(SC(F)(F)C(F)=NN1C1=C(C1)C=C(C=C1)C(F)(F)F)C#N

[illegible]

128	0.854	189.0867	"LL-2, 6-DIAMINOHEPTANEDIOATE"	[M-H] ⁻	189.088	C7H14N2O4	Alpha amino acids	GMKMEZVLHJARHF-UHFFFAOYSA-N	O=C(O)C(N)CCCC(N)C(=O)O
129	0.854	307.11316	5,13,15-trihydroxy-9-methyl-10-oxabicyclo[10.4.0]hexadeca-1(12),13,15-triene-3,11-dione	[M-H] ⁻	307.11871	C16H20O6	Macrolides and analogues	TXFYVWIRTECTR-UHFFFAOYSA-N	O=C1OC(C)CC(C)CC(=O)CC(=O)CC=CC(=O)C=C(O)C12
130	0.854	457.16702	7-O-Ethylmorrisonide	[M+H] ⁺	457.16901	C19H30O11	O-glycosyl compounds	IRKPOLIBQADK-LEYIKRXSA-N	O=C(OC)C1=CC(OC2OC(CO)C(O)C(O)C2O)C3C(OC(OC)CC13)C
131	0.854	293.09772	cyclopenin	[M-H] ⁻	293.09317	C17H14N2O3	1,4-benzodiazepines	APLKWASYUZSLB-PBH1CJAKSA-N	O=C1C=C=CC=CC2N=C(O)C3(OC3C=4C=CC=4)N1C
132	0.854	365.10464	Melibiose	[M+Na] ⁺	365.10544	C12H22O11	O-glycosyl compounds	DLRVLDZNNYCB-ABXIMFFYSA-N	OC1OC(OC22OC(O)C(O)C(O)C2O)C(O)C(O)C1O
133	0.854	250.09183	Muramic acid	[M-H] ⁻	250.09323	C9H17N O7	Sugar acids and derivatives	MSFSPUZXLOGRHJ-UHFFFAOYNA-N	O=C(O)C(OC1C(O)C(OC(O)C1N)CO)C
134	0.854	229.08705	Xanthyletin	[M+H] ⁺	229.086	C14H12O3	Linear pyranocoumarins	QOTBQVNVUBKJMS-UHFFFAOYSA-N	O=C1OC=2C=C3OC(C=CC3=CC2=C1)C)C
135	0.855	385.12561	[(3aS,4S,5S,6E,10Z,11aR)-6-formyl-5-hydroxy-10-(hydroxymethyl)-3-methylidene-2-oxo-3a,4,5,8,9,11a-hexahydrocyclohexa[1,1-f]furan-4-yl]-2-	[M+H] ⁺	385.12576	C19H22O7	Germacranolides and derivatives	HQPSNGXRJBMAL-JVWKVRNCSA-N	O=CC1=CCCC(=CC2OC(=O)C(=O)C2C(OC(=O)C(=O)C)C1O)CO
136	0.855	88.03969	L-ALANINE	[M-H] ⁻	88.0399	C3H7NO2	Alanine and derivatives	QNA5BMKLOCYPGJ-UWTATZPHSA-N	O=C(O)C(N)C
137	0.855	164.03775	Methioninesulfoxide	[M-H] ⁻	164.03868	C5H11NO3S	Alpha amino acids	QEFRNWLZKMPFJ-UHFFFAOYNA-N	O=C(O)C(N)CCS(=O)C
138	0.856	220.08148	N-Acetylglucosamine	[M-H] ⁻	220.08266	C8H15NO6	N-acyl-alpha-hexosamines	OVRNDRQMDRJTHS-UHFFFAOYNA-N	OC(=NC1C(O)CC(CO)C(O)C1O)C
139	0.857	172.07118	Metronidazole	[M+H] ⁺	172.07167	C6H9N3O3	Nitroimidazoles	VAOCPAMSLNLGC-UHFFFAOYSA-N	O=N(=O)C1=CN=C(N1CCO)C
140	0.858	527.15503	Flavone base + 3O, 2MeO, O-guaiacylglycerol	[M+H] ⁺	527.15509	C27H26O11	Flavone O-glycosides	WXNJNHFYWEHL-UHFFFAOYNA-N	O=C1C=C(OC2=CC(O)=CC(O)=C12)C=4C=C(OC)C(OC(CO)C(O)C=3C=CC(O)=C(OC)C=3)=C(OC)C=4
141	0.858	321.12939	Indole-3-acetyl-L-phenylalanine	[M-H] ⁻	321.12448	C19H18N2O3	Amino acids	BUGQHORRADGONS-UHFFFAOYNA-N	OC(CC1=CNC2=CC=CC=C12)=NC(C1=CC=CC=C1)C(O)=O
142	0.858	106.04941	L-Serine	[M+H] ⁺	106.04987	C3H7NO3	Serine and derivatives	MTCFGRXJLQNBG-REOHCLBISA-N	C([C-H](C(=O)O)N)O
143	0.859	312.16492	Xanthinol	[M+H] ⁺	312.16663	C13H21N5O4	Xanthines	DSFGXPJYDCSWTA-UHFFFAOYNA-N	O=C1C2=C(N=CN2CC(O)CN(C)CO)N(C(=O)N1C)O
144	0.86	156.04173	2-amino-4-hydroxypyrimidine-5-carboxylic acid	[M+H] ⁺	156.03999	C5H5N3O3	Pyrimidinecarboxylic acids	GBADBFAXAWZGHM-UHFFFAOYSA-N	O=C(O)C1=CN=C(N=C1O)N
145	0.86	368.11847	2-Chloro-N6-cyclopentyladenosine	[M-H] ⁻	368.1131	C15H20C1N5O4	Purine nucleosides	XSMYYQVWPWIZ-UHFFFAOYNA-N	C1C=1N=C(NC2CCCC2)C=3N=CN(C3N1)C4OC(CO)C(O)C4O
146	0.86	147.07611	Glutamine	[M+H] ⁺	147.07642	C5H10N2O3	Alpha amino acids	ZDXPYRJPDNMRX-UHFFFAOYNA-N	NC(OC(C)=N)C(O)=O
147	0.861	190.07031	N-ACETYL-DL-GLUTAMIC ACID	[M+H] ⁺	190.07001	C7H11N O5	Glutamic acid and derivatives	RFMMVMVDNIPURG-YFKPBYRYSA-N	O=C(O)CCC(NC(=O)C)C(=O)O
148	0.862	412.1445	(S,R)-Nosapine	[M-H] ⁻	412.14017	C22H23N O7	Phthalide isoquinolines	AKNNEGZIBPJZJG-MSOLQXFVSA-N	O=C1OC(C2=CC=C(OC)C(OC)=C12)C3C4C(OC)C=5OCOC5C=C4CCN3C
149	0.862	132.02942	Aspartic acid	[M-H] ⁻	132.03023	C4H7NO4	Aspartic acid and derivatives	CKLJMWIZIZZRS-UHFFFAOYNA-N	O=C(O)CC(N)C(=O)O
150	0.862	298.10217	Erythraline	[M+H] ⁺	298.10001	C18H19NO3	Erythrianes	YOFUERNMZTRYM-UHFFFAOYSA-N	O1C=2C=C3C(=CC2OC1)C4C(C=CC(OC)C4)=OCN5CC3
151	0.863	265.09296	5,9-dihydroxy-5,7,7-trimethyl-4,5a,6,8,8a,9-hexahydro-1H-azuleno[5,6-c]furan-3-one	[M-H] ⁻	265.09396	C15H22O4	Terpene lactones	UIZWJQAQYBHAA-UHFFFAOYSA-N	O=C1OC2=C1CC(O)(C)C3CC(C)(C)CC3C2O
152	0.864	110.05975	4-Aminophenol	[M+H] ⁺	110.06004	C6H7NO	Aniline and substituted anilines	PLIKAWJENQZMHA-UHFFFAOYSA-N	c1cc(ccc1N)O
153	0.865	85.04746	3-Amino-1,2,4-triazole	[M+H] ⁺	85.05087	C2H4N4	Triazoles	KL5JNVNTNUIYHOU-UHFFFAOYSA-N	C1=NC(=N)NN1
154	0.867	517.13977	5,7-dihydroxy-6-[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]-8-[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxychromen-2-one	[M-H] ⁻	517.13855	C21H26O15	Coumarin glycosides	YRVGYJMSCQFOCA-UHFFFAOYSA-N	O=C1OC=2C(OC3OC(CO)C(O)C(O)C3O)=C(O)C(=C(O)C(=O)C2O=C1)C4OC(CO)C(O)C4O
155	0.867	173.09402	N-alpha-Acetyl-L-ornithine	[M-H] ⁻	173.09317	C7H14N2O3	N-acyl-L-alpha-amino acids	JRLGPAXAGHMOL-LURJTMIESA-N	CC(O)=N[C=H](CCCN)C(O)=O
156	0.868	222.09625	N-Acetyl-D-glucosamine	[M+H] ⁺	222.09721	C8H15NO6	N-acyl-alpha-hexosamines	OVRNDRQMDRJTHS-RTRLPJTCSA-N	CC(=N[C-H]1[C=H]([C=H]([C=H](CO)OC1O)O)O)O
157	0.868	168.06749	Norepinephrine	[M-H] ⁻	168.06662	C8H11NO3	Catechols	SFLSHLFXELFJZ-UHFFFAOYNA-N	OC1=CC=C(C=C1O)C(O)CN
158	0.869	527.20825	[(1aR,1bS,2S,5aS,6R,6aS)-5a-hydroxy-1a-methyl-2-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy-1b,2,6,6a-2-amino-5-[2-[[[(3S)-2,3-dihydroxy-2-[(1S)-1-hydroxyethyl]butanoyl]oxymethyl]anilinol-5-oxononanoic acid	[M+H] ⁺	527.21338	C25H36O12	Terpene glycosides	PRWWZJHOHQKQD-SYDQWUJBSA-N	O=C(OC1C2OC2(C)C3C(OC=CC13O)OC4OC(CO)C(O)C4O)C(=CC(OC)C(=C)C)C
159	0.869	399.07019	hydroxyethylbutanoyloxymethylanilinol-5-oxononanoic acid	[M+H] ⁺	399.06964	C18H26N2O8	Glutamine and derivatives	NFINSJKQBJWEB-WAQLSPKVS-N	O=C(O)C(N)CCC(O)=NC(=O)C=CC1COC(=O)C(O)(C)C(O)C(O)C
160	0.869	369.18729	Gardnerine	[M-H] ⁻	369.18198	C20H24N2O2	Alkaloids	RBALJEFQJCAPLN-UHFFFAOYNA-N	COC1=CC=C2C(NC3=C2CC2C(CO)C4CC3N2CC4=CC)=C1
161	0.869	383.16586	Hydroxygardnutine	[M-H] ⁻	383.16125	C20H22N2O3	Alkaloids	OUONWR1EOZMSQ-UHFFFAOYNA-N	COC1=CC=C2C(NC3=C2C2OCC4C2N2CC(=COO)C4CC32)=C1
162	0.869	329.10806	Pesticide1_halofenozide_C18H19ClN2O2_N-Benzoyl-4-chloro-N'-(2-methyl-2-propanoyl)benzohydrazide	[M-H] ⁻	329.10699	C18H19ClN2O2	4-halobenzoic acids and derivatives	CNKHSLKYRMDNQ-UHFFFAOYSA-N	O=C(NN(C)C(=O)C=CC=CC1)C(C)C(O)C2=CC=C(C1)C=C2
163	0.87	477.14401	Isorhamnetin-3-galactoside	[M-H] ⁻	477.14212	C22H22O12	Flavonoid-3-O-glycosides	COLRUI1RRYHYS-UHFFFAOYSA-N	O=C1C(OC2OC(CO)C(O)C(O)C2O)=C(OC=3C(=O)C(=O)C13)C=4C=CC(OC)C=4
164	0.871	263.17041	Oxysphocarpine	[M+H] ⁺	263.17001	C15H22N2O2	Matrine alkaloids	QMGGMESMCJABO-LHDUFFHYS-N	O=C1C=CCC2N1CC3CCC(N+14)[(O-)]CCCC2C34
165	0.871	440.17328	Quinadoline_B_130007	[M+H] ⁺	440.173	C25H21N5O3	Pyridopyrimidines	GACSRZKZGCRJX-PVDOLRBSA-N	O=C1C=2C=CC=CC3N=C3N1C4C(=O)NC3C5(C=6C=CC=CC6N7C(=O)C8N(CCC8)C75)C4
166	0.872	173.09155	Glycyl-L-proline	[M+H] ⁺	173.09207	C7H12N2O3	Dipeptides	KZCNQNBZMBJQJO-YFKPBYRYSA-N	NCC(=O)N1CCCC[C=H]1C(O)=O
167	0.872	292.14835	PiperlotineC	[M+H] ⁺	292.14999	C16H21NO4	Cinnamic acids and derivatives	TYFKYDTUENTUNY-VOTSOKGWSA-N	O=C(C=C1C(=O)CC(=O)C(OC)C(OC)=C1)N2CCCC2
168	0.872	309.13043	Toddalolactone	[M+H] ⁺	309.13	C16H20O6	Coumarins and derivatives	GLWPLQBQHWYKRK-CYBMUJFWSA-N	O=C1OC2=CC(OC)=C(C(OC)=C2C=C1)CC(O)C(O)C(O)C
169	0.873	234.09596	1-Isothiocyanato-8-(methylsulfinyl)-octane	[M+H] ⁺	234.09808	C10H19NO2S	Sulfoxides	BCRXKQWQVFKZAG-UHFFFAOYNA-N	CS(=O)CCCCCCCC=C=S
170	0.873	146.09209	4-Guanidinobutyric acid	[M+H] ⁺	146.09241	C5H11N3O2	Gamma amino acids and derivatives	TUHVJAJXIMEOSA-UHFFFAOYSA-N	O=C(O)CCNC(=O)N

171	0.874	283.10229	Glycitein	[M-H] ⁻	283.10272	C16H1205	Isoflavones	DXUYAIFZCFRPTH-UHFFFAOYSA-N	O=C1C(=COC2=CC(O)=C(OC)C=C12)C=3C(OC(O)=CC3
172	0.875	537.16602	Selaginpulvinin K	[M-H] ⁻	537.16901	C36H2605	Fluorenes	UTTATNZ1WSODLT-UHFFFAOYSA-N	O=CC1=CC=C2C=3C(OC(O)=CC3C(4=C4C(OC)C=C4)(C5=CC=C(OC)C=C5)C2=C1C=C6C=C(C(OC)C=C6
173	0.875	349.13431	Torseimide (Demadex)	[M+H] ⁺	349.133	C16H20N4O3S	Pyridinesulfonamides	NGBFQHQLJINZ-UHFFFAOYSA-N	O=C(NC(C)C)NS(=O)(=O)C1=C=NC=C1NC2=CC=CC(=O)C2
174	0.876	191.10188	2,6-diaminopimelic acid	[M+H] ⁺	191.10265	C7H14N2O4	Alpha amino acids	GMRKEZVLHJARHF-UHFFFAOYSA-N	C(CC(C(=O)O)N)CC(C(=O)O)N
175	0.876	289.18607	4-((1R,3S,5r,7r)-5,7-dimethyl-1,3-diazaadamantan-2-yl)-2-methoxyphenol	[M+H] ⁺	289.19	C17H24N2O2	Methoxyphenols	LATQZYGIAROHX-UHFFFAOYSA-N	OC1=CC=C(C(=C1OC)C2N3CC4(C)CN2CC(C)C3)C4
176	0.877	346.05377	2'-DEOXYGUANOSINE 5'-MONOPHOSPHATE	[M-H] ⁻	346.05499	C10H14N5O7P	Purine 2'-deoxyribonucleoside	LTFMZDNNPPEGNG-UHFFFAOYSA-N	O=C1N=C(N)NC2=C1N=CN2C3OC(COP(=O)(O)O)C(O)C3
177	0.877	346.12225	Omeprazole (Prilosec)	[M+H] ⁺	346.12201	C17H19N3O3S	Sulfinylbenzimidazoles	SUBDBMMJDZJVOS-UHFFFAOYSA-N	O=S(C1=NC=2C=C(OC)C=C2N1)CC3=NC=C(C(OC)=C3)C
178	0.877	288.11932	OPHTHALMIC ACID	[M-H] ⁻	288.12	C11H19N3O6	Peptoid-peptide hybrids	SPLUHYDIQKURQW-UHFFFAOYSA-N	O=C(O)CN(C(=O)CCC(N(=O)O)C(=O)C(=O)C(N)CC
179	0.877	138.05437	Trigonelline	[M+H] ⁺	138.05499	C7H7N02	Alkaloids and derivatives	WWNZCCKKKDOPX-UHFFFAOYSA-N	O=C([O-])C1=CC=C[N+](=C1)C
180	0.878	398.1691	Lipothiazole A	[M+H] ⁺	398.17401	C18H27N3O5S	Peptides	XSLDIFFYKBCQGW-VFNNOXTSA-N	O=C(O)C(N=C(O)CN=C(O)C=CC=IN=C(SC1)CCCCC)CO
181	0.878	247.175	Santonin	[M+H] ⁺	247.17221	C15H18O3	Endemanolides, sesquiterpenolides and Estrogens and derivatives	XJHDMJURBVLE-BOCCBSBMSA-N	O=C1C=CC2(C(=C1C)C3OC(=O)C(C)C3CC2)C
182	0.879	273.19333	d-estradiol	[M+H] ⁺	273.19	C18H24O2	Estrogens and derivatives	VOXZDWNVPJITMN-ZBRFXRBCSA-N	OC1=CC=C2C(=C1)CCC3C2CC4(C)C(O)CCC34
183	0.883	231.09755	(+)-Dihydrokavain	[M-H] ⁻	231.10266	C14H16O3	Kavalactones	VOOYTQRREPYRIW-LBPRGRKZSA-N	O=C1OC(CC(OC)=C1)CCC=2C=CC=CC2
184	0.883	353.15369	1,4a-dimethyl-9-oxo-7-propan-2-yl-3,4,10,10a-tetrahydro-2H-phenanthrene-1-carboxylic acid	[M+H] ⁺	353.15134	C20H26O3	Diterpenoids	MSWJSDLPCCSSNW-UHFFFAOYSA-N	O=C(O)C1(C)CCCC2(C3=CC=C(C(=C3C(=O)C12)C(C)C)C
185	0.883	179.05479	9-Fluorenone	[M-H] ⁻	179.05023	C13H8O	Fluorenes	YLQWCDQCJODRMT-UHFFFAOYSA-N	O=C1C=2C=CC=CC2C=3C=CC=CC13
186	0.883	195.05017	Gluconate	[M-H] ⁻	195.05103	C6H12O7	Medium-chain hydroxy acids and derivatives	RGINJXZEOKUKBD-SQOUGZDYSA-N	OC[C@H](O)[C@H](O)[C@H](O)[C@H](O)C(O)=O
187	0.883	329.1813	Guaiacin	[M+H] ⁺	329.17999	C20H24O4	Aryltetralin lignans	TZAAUYCUP1YQBR-JGRMJRGVSA-N	OC1=CC=C(C(=C1OC)C2C=CC(O)=C(OC)C=C3CC(C)C2C
188	0.883	187.10748	NALPHA-ACETYL-L-LYSINE	[M-H] ⁻	187.108	C8H16N2O3	N-acyl-alpha amino acids	VEYYWZYIYDQJM-ZETCQVMHSA-N	O=C(NC(C(=O)O)CCCC)C
189	0.884	459.13342	(-)-Podophyllotoxin	[M-H] ⁻	459.12967	C22H22O8	Lignols	YJGVLMPVUAXIQN-UHFFFAOYNA-N	COC1=CC(=CC(OC)=C1OC)C1C2C(COC2=O)C(O)C2=C1C1OCOC1=C2
190	0.884	428.21259	2-amino-3-[[[6E,9E]-5-hydroxy-8-methoxy-5,9,13,14-tetramethyl-2-oxo-1-oxacyclotetradeca-6,9-dien-4-yl]sulfinyl]propanoic acid	[M-H] ⁻	428.21121	C21H35NO6S	Macrolides and analogues	XBLHNZXAORYAC-KHQWPHVHSA-N	O=C(O)C(N)CCC1C(=O)OC(C)C(C)CCC=C(C)C(OC)C=CC1(O)C
191	0.884	253.05511	7,2'-Dihydroxyflavone	[M-H] ⁻	253.05063	C15H10O4	Flavones	NUGPQXQICGTVNA-UHFFFAOYSA-N	O=C1C=C(OC2=CC(O)=CC=C12)C=3C=CC=CC3O
192	0.885	311.09625	Seppanone A Dimethyl Ether	[M-H] ⁻	311.09595	C18H16O5	Homoisoflavonoids	VCNDHJFYRZQMHX-KPKJPENVSA-N	O=C1C2=CC=C(OC)C=C2OCC1=CC3=CC=C(OC)C(C)O=C3
193	0.886	113.02359	FT-OH	[M-H] ⁻	113.02197	C3H5F3O	PFSA	HDBGTBNNPRCYND-UHFFFAOYSA-N	FC(F)(F)CO
194	0.886	112.0864	Histamine	[M+H] ⁺	112.08692	C5H9N3	2-arylethylamines	NTYJJOPFLAHURM-UHFFFAOYSA-N	N1=CN=C(C1)CCN
195	0.886	124.03897	Isonicotinic acid	[M+H] ⁺	124.03931	C6H5NO2	Pyridinecarboxylic acids	TWBYWODOCUKOW-UHFFFAOYSA-N	OC(=O)C1=CC=NC=C1
196	0.886	465.10007	Myricitrin	[M+H] ⁺	465.10001	C21H20O12	Flavonoid-3-O-glycosides	DCYOADKABEMIQ-OMMUPTOHS-N	O=C1C(OC2OC(C)C(O)C(O)C2O)=C(OC=3C=C(C)C(=O)C13)C=4C=C(C)C(O)=C(C)C4
197	0.886	186.10512	Norharman	[M+H] ⁺	186.10257	C11H8N2	Beta carbolines	A1PRHYZBTHREPW-UHFFFAOYSA-N	N1=C=CC2=C(C1)NC=3C=CC=CC2
198	0.887	310.11353	N2, N2-Dimethylguanosine	[M-H] ⁻	310.11569	C12H17N5O5	Purine nucleosides	RSPURTUNRHNVG-UHFFFAOYNA-N	OC1=NC(=NC2=C1N=CN2C3OC(C)C(O)C3O)N(C)C
199	0.887	245.11237	palythine	[M+H] ⁺	245.10899	C10H16N2O5	Alpha amino acids and derivatives	KYCB1RYKYQCBFO-UHFFFAOYSA-N	O=C(O)CN=C(C(OC)=C(N)CC(O)CO)C1
200	0.888	212.05486	(+)-Baclofen	[M-H] ⁻	212.04839	C10H12ClNO2	Gamma amino acids and derivatives	KPYSYIEGFHWSV-UHFFFAOYNA-N	NCC(CC(O)=O)C1=CC=C(C1)C=C1
201	0.888	144.10252	(2R)-6-methylpiperidine-2-carboxylic acid	[M+H] ⁺	144.10001	C7H13NO2	L-alpha-amino acids	IHLDCUQIFBWSJU-PRJD1BJQSA-N	O=C(O)C1NC(C)CCC1
202	0.888	363.14069	Gibberellin A8	[M-H] ⁻	363.14493	C19H24O7	C19-gibberellin 6-carboxylic acids	WZRRJZYYGQOHRU-UQJXHNCSA-N	C[C@]12[C@H]3[C@H](C(O)=O)[C@]1(C)C4[C@]2(C)[C@H](C=C1)C(=O)C(=O)C4
203	0.888	134.08087	N-Methylthreonine	[M+H] ⁺	134.08118	C5H11NO3	L-alpha-amino acids	CCAI1PMIAFGKSI-UHFFFAOYNA-N	O=C(O)C(NC)C(O)C
204	0.888	283.06604	Xanthosine (Not validated)	[M-H] ⁻	283.0679	C10H12N4O6	Nucleosides	UBORTCNDUKBEOP-UHFFFAOYNA-N	OC=IN=C(O)C(=N)=CN=C(=N1)C3OC(CO)C(O)C3(O)
205	0.889	290.12292	Arbutin	[M+H] ⁺	290.12341	C12H16O7	Phenolic glycosides	BJRNKVDFOYLUG-RMPHRYRLSA-N	OC1=CC=C(OC2OC(CO)C(O)C(O)C2O)C=C1
206	0.889	315.08136	Eriodictyol 7,3'-dimethyl ether	[M-H] ⁻	315.07901	C17H16O6	7-O-methylated flavonoids	QZJVBGZOLNHWG-AWEZNCQLSA-N	O=C1C2=C(O)C=C(OC)C=C2OC(C3=CC=C(C)C(OC)=C3)C1
207	0.889	322.11252	Pesticide4 Flutolanil_C17H16F3N02_Benzamide, N-[3-(1-methylethoxy)phenyl]-2-(trifluoromethyl)-	[M-H] ⁻	322.10599	C17H16F3NO2	Benzanilides	PTCGDEVHUXTMP-UHFFFAOYSA-N	FC(F)(F)C=C1C=CC=CC1(O)=NC2=CC=CC(OC)C=C2
208	0.889	226.10651	triacanthine	[M+H] ⁺	226.11	C10H13N5	6-aminopurines	BEPGTHDUORHIM-UHFFFAOYSA-N	N1=CN=C2C1=C(N=CN2CC=C(C)C)N
209	0.891	352.15793	9-(beta-d-ribofuranosyl)zeatin	[M+H] ⁺	352.16	C15H21N5O5	Purine nucleosides	GOSWTRUMMSCNCW-GPTCUSJASA-N	CCC(=CN=C1NC=NC2=C1N=CN2C3OC(CO)C(O)C3O)C
210	0.891	479.23477	Dehydrolicudenic acid A, 20(21)-	[M+H] ⁺	479.23999	C27H36O6	11-oxosteroids	APM1CFQMLNFRZ-UHFFFAOYSA-N	O=C(O)CCC(=C)C1CC(=O)C2(C3=C(C(=O)C12)C4(C)CCC(=O)C(C1)C4)C3O
211	0.892	409.18039	2-(5-methoxy-4,8,8-trimethyl-2-oxo-2,8,9,10-tetrahydropyrano[2,3-f]chromen-3-yl)-N-(pyridin-2-yl)acetamide	[M+H] ⁺	409.17999	C23H24N2O5	Angular pyranocoumarins	XBYYUUMUOFZSRJ-UHFFFAOYSA-N	O=C1OC2=C(C)C(OC)=CC=3OC(C)(C)CC32)C(=C1CC(=O)NC4=NC=CC=C4)C
212	0.892	331.1601	Cinchonine hydrochloride	[M+H] ⁺	331.16	C19H23ClN2O	Cinchona alkaloids	IMUHLVEEYGMBC-PAAXXVDQSA-N	C1, OC(C=1C=CN=C2C=CC=CC21)C3N4CCC(C3)C(C=C)C4
213	0.892	410.16357	FucGlcNAcGA	[M+H] ⁺	410.16568	C16H27N011	N-acyl-alpha-hexosamines	ZMHFWGFDQCSHY-GEHFNBAWSA-N	C[C@H]1O[C@H](O)[C@H]2[C@H](O)[C@H](CO)O[C@H](OCC=O)[C@H]2N=C(C)O1[C@H](O)[C@H](O)[C@H]1O

214	0.892	249.10724	Glu-Thr	[M+H] ⁺	249.10811	C9H16N2O6	Dipeptides	JSIQVR1XMINMTA-UHFFFAOYNA-N	O=C(O)CCC(N)C(O)=NC(C(=O)O)C(O)C
215	0.892	337.15906	Lotusine	[M+H] ⁺	337.16	C19H24NO3+	Benzylisoquinolines	ZKTM_LINF1QCERN-QGZVFWFLSA-O	OC1=CC=C(C=C1)CC2C3=CC(=O)C(O)=C(C)=C3OC[N+](=C)C(C)C
216	0.892	235.11823	Mepirizole	[M+H] ⁺	235.11896	C11H14N4O2	Alkyl aryl ethers	RHAXSHUQ1EUEY-UHFFFAOYSA-N	N=IC(=NC(=CC1OC)C)N2N=C(C=C2OC)C
217	0.892	303.2019	Quercetin	[M+H] ⁺	303.20657	C15H10O7	Flavonols	REFJWTPEDVJJY-UHFFFAOYSA-N	O=C1C(O)=C(OC=2C=C(O)C=C(O)C12)C=3C=CC(O)=C(O)C3
218	0.892	457.11777	Raltitrexed	[M-H] ⁻	457.11874	C21H22N4O6S	Glutamic acid and derivatives	IVTVGXNLFDRM-UHFFFAOYNA-N	O=C(O)CCC(NC(=O)C=ISC(=CC1)N(C)CC=2C=CC3=NC(=NC(O)=C3C2)C(C)=O
219	0.893	372.12805	(1r,3R,4S,5S)-4-[(2E)-3-(3,4-Dihydroxyphenyl)-2-propenoyl]oxy-1,3,5-trihydroxycyclohexanecarboxylic acid	[M+H] ⁺	372.12891	C16H18O9	Quinic acids and derivatives	GYFFKZYTFACFR-UCEFYARBSA-N	O=C(O)C1(O)CC(O)C(OC(=O)C=CC2=CC(O)C(O)=C2)C(O)C1
220	0.893	271.12787	3-(4-hydroxy-5-oxo-3-phenyl-2H-furan-2-yl)propanoic acid	[M+H] ⁺	271.12769	C13H12O5	Butenolides	PPZVSYNLXFYAD-UHFFFAOYSA-N	O=C(O)CCC1OC(=O)C(O)=C1C=2C=CC=CC2
221	0.893	291.15372	Androsterone	[M+H] ⁺	291.15656	C19H30O2	Androgens and derivatives	QXBXDMJGAMFCBF-HLUDHZFRSA-N	O=C1CCC2C3CCC4CC(O)CCC4(O)C3CCC12C
222	0.893	116.07078	L-VALINE	[M-H] ⁻	116.071	C5H11NO2	Valine and derivatives	KZSNJWFQEVHDMF-UHFFFAOYSA-N	O=C(O)C(N)C(C)C
223	0.893	251.1671	Lychnopholic acid	[M+H] ⁺	251.16901	C15H22O3	Sesquiterpenoids	LMJMJHGFJXZGDE-WKMLJHOTSAN	O=C(O)C1=CCCC(=C)C2CC(C)C(C)C2(O)C1
224	0.893	341.0383	Pesticide2_Thiophanate-methyl_C12H14N4O4S2_	[M-H] ⁻	341.039	C12H14N4O4S2	Benzene and substituted derivatives	QGHREAKMXNCOA-UHFFFAOYSA-N	O=C(OC)NC(=S)NC=1C=CC=CC1NC(=S)NC(=O)OC
225	0.893	168.06474	Pyridoxal	[M+H] ⁺	168.065	C8H9NO3	Pyridoxals and derivatives	RADKZDMFGJYCB-UHFFFAOYSA-N	O=CC1=C(O)C(=NC=C1CO)C
226	0.894	231.13382	Kainic Acid	[M+H] ⁺	231.13393	C10H15NO4	Kainoids	VLSMHGEGTFMBEZ-OOZYFLPDSA-N	O=C(O)CC1C(NCC1C(=O)C)C(=O)O
227	0.894	380.16791	Kasugamycin	[M+H] ⁺	380.16635	C14H25N3O9	Aminocyclitol glycosides	PVTHJAPFENJVCN-UQTMRZPGSA-N	O=C(O)C(=CC1NC(N)C(OC1C)OC2C(O)C(O)C(O)C(O)C2O)N
228	0.894	257.19839	Sparteine	[M+H] ⁺	257.20001	C15H26N2	Sparteine, lupanine, and related alkaloids	SLRCWJSBJZBV-ZQDZILKHSAN	N12CCCCC1C3NC4CCCCC4C(C2)C3
229	0.894	335.14423	Thymol-beta-D-glucoside	[M+H] ⁺	335.14648	C16H24O6	Terpene glycosides	GKQG1QVSMCHAFX-1BEHDNSVSA-N	OC1OC(OC2=CC(=CC=C2C(C)C)C(O)C(O)C1O)C1O
230	0.895	490.19086	[(2R,3S,4S,5S)-4-hydroxy-2,5-bis(hydroxymethyl)-5-[(2R,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxoxolan-3-yl]-(E)-3-phenylpropan-2-yl]propanamido]propanoyl]nineridine-4-carboxylic acid	[M+H] ⁺	490.19189	C21H28O12	Cinnamic acid esters	AKARZAXADNXORH-WQVLSBKSAN	O=C(OC1C(O)C(OC2OC(CO)C(O)C(O)C2O)(OC1CO)CO)C=CC=3C=CC=C3
231	0.895	278.12198	3-methoxy-6-methyl-6,7-dihydro-5h-dibenzo[c,e]azepin-2-ol	[M+H] ⁺	278.12	C16H17NO2	Benzazepines	GJHXLJRGWNKP-UHFFFAOYSA-N	OC=1C=C2C=3C=CC=C3CN(C)CC2=CC1OC
232	0.895	286.17496	Dendrobine	[M+H] ⁺	286.17001	C16H23NO2	Indoles and derivatives	YCWJWJWRMHVMZ-JSYFJIKASAN	O=C1OC234N(C)CC5CC(C13C2C(C)C)C45C
233	0.895	362.08304	Fenoxaprop-P-ethyl	[M+H] ⁺	362.07898	C18H16ClNO5	2-phenoxypropionic acid esters	PQRBPHEKWERGT-UHFFFAOYNA-N	O=C(OC)C(OC1=CC=C(OC2=NC=3C=CC(=O)C1=CC3O2)C=C1)C
234	0.896	202.10716	(E)-1-(4-methylquinazolin-2(1H)-ylidene)guanidine	[M+H] ⁺	202.11	C10H11N5	Quinazolinamines	ONQSKDLYYDFLL-UHFFFAOYSA-N	N=C(N=C1N=C(C=2C=CC=CC2N1)C)N
235	0.896	392.16251	(S)-methyl 2-(3-(6,7-dimethoxy-4-oxoquinazolin-3(4H)-yl)propanamido)-3-methylbutanoate	[M+H] ⁺	392.16	C19H25N3O6	Hybrid peptides	WLJIRKJXQCBEF-KRWDBZBQSA-N	O=C(OC)C(NC(=O)CCN1C=NC=2C=C(OC)C(OC)=CC2C1=O)C(C)C
236	0.896	312.19	17-hydroxy-3-oxo-, (17??)-19-Norpregna-5(10),9(11)-diene-21-nitrile	[M+H] ⁺	312.19	C20H25NO2	Oxosteroids	VUQMQSOWZOUJR-FUMNGEBSAN	N#CCC1(O)CCC2C3C(=CCC21C)C4=C(CC(=O)O)CC4CC3
237	0.896	579.17517	5,7-dihydroxy-2-(4-hydroxyphenyl)-3-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-[[[(2S,3R,4S,5S)-3,4,5-trihydroxyoxan-2-yl]oxymethyl]oxan-2-yl]oxy]chromen-1-[(S)-2-[(S)-2-(2-hydroxy-4-oxoquinazolin-3(4H)-yl)-3-(1H-indol-3-yl)propanamido]propanoyl]nineridine-4-carboxylic acid	[M-H] ⁻	579.17218	C26H28O15	Flavonoid-3-O-glycosides	YJPZVZYVHLEDNA-KSPKLRDJSA-N	O=C1C(OC2OC(COC3OCC(O)C(O)C3O)C(O)C(O)C2O)=C(OC=4C=C(O)C=C(O)C14)C=C5C=C(CO)C=C5
238	0.897	554.20581	1-[(S)-2-[(S)-2-(2-hydroxy-4-oxoquinazolin-3(4H)-yl)-3-(1H-indol-3-yl)propanamido]propanoyl]nineridine-4-carboxylic acid	[M+H] ⁺	554.20001	C28H29N5O6	N-acyl-alpha amino acids and derivatives	NXJYJHDQJUYBZ-HJPUHRCSSAN	O=C(O)C1CCN(C(=O)O)C(NC(=O)C(N2C(=O)C=3C=CC(=O)C2)CC4=C(NC=5C=CC(=O)C)C1C4
239	0.897	185.12793	2-hydroxy-1-isopentyl-4-methyl-1H-imidazol-5(4H)-one	[M+H] ⁺	185.13	C9H16N2O2	Hydantoins	CEHHMFMAIPKGU-UHFFFAOYSA-N	O=C1N(C(O)=NC1O)CCC(C)C
240	0.897	365.15567	GlcNAcThrNAc	[M+H] ⁺	365.15546	C14H24N2O9	N-acyl-alpha-hexosamines	CUSVSKYUCVKGOL-UYHBOPCKSAN	CC(O)=N[C(H)](CO)[C(H)](O)[C(H)]1O[C(H)](CO)[C(H)](O)[C(H)](O)Y[C(H)]1N=C(O)C=O
241	0.897	385.25507	Ibutilide fumarate	[M+H] ⁺	385.25201	C44H76N4O10S2	Phenylbutylamines	PCIORQNIRWFMV-WXXKFALUSAN	O=C(O)C=CC(=O)O.O=S(=O)(NC1=CC=C(C=C1)C(O)CCN(C)CCCC(C)C.O=S(=O)(NC1=CC=C(C=C1)C(O)CCN(C)CCCC(C)C)C
242	0.897	263.10114	N6-benzyl-7H-purine-2,6-diamine	[M+H] ⁺	263.10001	C12H12N6	6-alkylaminopurines	XSSREOLCRTWEPI-UHFFFAOYSA-N	N1=CNC2=C1N=C(N=C2NCC=3C=CC=CC3)N
243	0.897	279.1254	Pesticide4_Oxadixyl_C14H18N2O4_	[M+H] ⁺	279.134	C14H18N2O4	Anilides	UWVQ1ROCKJWDKL-UHFFFAOYSA-N	O=C1OCCN1N(C(=O)CO)C=2C(=CC=CC2)C
244	0.897	288.10703	Rutaecarpine	[M+H] ⁺	288.10999	C18H13N3O	Beta carbolines	ACGVGWSKVRYFRP-UHFFFAOYSA-N	O=C1C=2C=CC=CC2N=C3C=4NC=5C=CC=CC54CCN13
245	0.898	472.22598	[(2R,3S,4S,5R,6R)-3,4,5-trihydroxy-6-[2-(4-hydroxyphenyl)ethoxy]oxan-2-yl]methyl 2-[2-oxo-1,3-dihydroindol-3-yl]acetate	[M+H] ⁺	472.22751	C24H27N9O	Saccharolipids	YOTVUKXJYRTAR-NAJYVHOLSA-N	O=C(OC1OC(OC2C=CC(=O)C(=O)C(O)C1O)C13C(O)=NC=4C=C(C)C43
246	0.898	257.07693	1-Methylpseudouridine	[M-H] ⁻	257.07791	C10H14N2O6	Nucleoside and nucleotide analogues	UVBYMV0UBXYSFY-UHFFFAOYNA-N	O=C1N=C(O)C(C)=C(N1C)C2OC(CO)C(O)C2O
247	0.898	204.12234	Acetylcarnitine	[M] ⁺	204.12248	C9H18NO4	Acyl carnitines	RDHQFKQ1GNGIED-UHFFFAOYNA-O	O=C(OC(CC(=O)O)C[N+](C)C)C(C)C
248	0.898	347.14291	alboecycline	[M+H] ⁺	347.1416	C18H28O4	Macrolides and analogues	BYWNDLJLWPPJP-REXWONOSSAN	O=C1OC(C)C(C)CCC=C(C)C(OC)C=CC(O)(C=C1)C
249	0.898	354.17535	Dihydrozeatin riboside	[M+H] ⁺	354.17719	C15H22N5O5	Purine nucleosides	DBVYQDG1JAUFAZ-XXYADJKSSAN	CC(CO)CCN1C2=CN(=CN([C@H]3O[C@H](CO)[C@H](O)[C@H]3O)C2=NC=N1
250	0.898	319.14841	Erianin	[M+H] ⁺	319.14999	C18H22O5	Stilbenes	UXDFUVFNIAJEGM-UHFFFAOYSA-N	OC1=CC(=CC=C1OC)CCC2=CC(OC)=C(OC)C(OC)=C2
251	0.899	241.1541	(4R,4aS,6R)-6-isopropenyl-4,4a-dimethyl-4,4a,5,6,7,8-hexahydro-2(3H)-naphthalenone	[M+H] ⁺	241.16	C15H22O	Eremophilane, 8,9-secoeremophilane and	WTOYNNKBUVYIKC-JMSVASOKSAN	O=C1C=C2CCC(C(=O)C)CC2(C)C(C)C1
252	0.899	371.18024	2-(furan-3-yl)-7,8-dihydroxy-6a,7,10b-trimethyl-octahydro-1H-naphthol[2,1-c]naphran-4-one	[M+H] ⁺	371.17999	C20H28O5	Diterpene lactones	RBEATXBLJUTDQZ-UHFFFAOYSA-N	O=C1OC(C=2C=CC(C3(C)C1CCC4(C)C3OCC(O)C4)O)C(O)C
253	0.899	185.05571	2,3-Dihydroxybiphenyl	[M-H] ⁻	185.06081	C12H10O2	Biphenyls and derivatives	YKQAAJBYBTSBS-UHFFFAOYSA-N	C1=CC=C(C=C1)C=2C=CC=C(C2O)O
254	0.899	623.20239	3-[(2S,3R,4S,5S,6R)-4,5-dihydroxy-6-(hydroxymethyl)-3-[(2S,3R,4S,5R,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxoxan-2-yl]oxy-5-hydroxy-2-yl]propanamido]propanoyl]nineridine-4-carboxylic acid	[M-H] ⁻	623.20544	C28H32O16	Flavonoid-3-O-glycosides	PNBEMXOTFKPQL-PVZBESAUSAN	O=C1C(OC2OC(CO)C(O)C(O)C2OC3OC(CO)C(O)C(O)C3O)=C(OC4=C(C)OC)=CC(O)=C14)C=C5C=CC(O)=C5
255	0.899	299.15945	Auraptene	[M+H] ⁺	299.16	C19H22O3	Terpene lactones	RSDDHGSKLOSQFK-RVDMUPIBSAN	O=C1OC=2C=C(OC=C(C)CCC=C(C)C)C=CC2=C1
256	0.899	251.1013	Dehydroeffusol	[M+H] ⁺	251.10001	C17H14O2	Phenanthrois	GSSPKCPIRDPBQE-UHFFFAOYSA-N	OC=1C=C(C=C)C=2C(=CC=C3C2=CC(O)=C3)C1

257	0.899	304.14941	evodiamine	[M+H] ⁺	304.14999	C19H17N3O	Beta carbolines	TXDUTHBFYKGSAB-UHFFFAOYSA-N	O=C1C=2C=C=CC2N(C)C3C=4NC=5C=CC=CC54CCN13
258	0.899	347.17996	Isorosmanol	[M+H] ⁺	347.17999	C20H26O5	Diterpene lactones	UXVPWKTDIRJELA-CLWJZODNSA-N	O=C1OC2C3=CC(=C(O)C(O)=C3C14CCCC(C)C)C4C2O)C(C)C
259	0.899	397.15878	Myrsilignan	[M+H] ⁺	397.16	C21H26O6	Lignans, neolignans and related compounds	ULZFTGWWPHYLG1-UHFFFAOYSA-N	OC1=CC=C(C=C1OC)C(O)C(OC2=C(OC)C=C(C=C2OC)CC)=C
260	0.899	189.12294	N-epsilon-Acetyllysine	[M+H] ⁺	189.12337	C8H16N2O3	D-alpha-amino acids	DTERQVGMUDWYAZ-UHFFFAOYNA-N	O=C(O)C(N)CCCCN=C(O)C
261	0.899	237.12297	Pesticide1_Cymoxanil_C7H10N4O3_(2E)-2-Cyano-N-(ethylcarbamoyl)-2-(methoxymino)acetamide	[M+H] ⁺	237.123	C7H10N4O3	Oxime ethers	XERJKGBORTKEO-VZUCSPMQSA-N	N#CC(=NOC)C(O)=NC(O)=NCC
262	0.899	209.12801	Pilocarpine	[M+H] ⁺	209.12801	C11H16N2O2	Alkaloids and derivatives	QCCHTSOMWOSFDM-UHFFFAOYSA-N	O=C1OCC(C2=C=CN2C)C1CC
263	0.9	355.19733	14-deoxy-11,12-dihydroandrographolide	[M+H] ⁺	355.20001	C20H28O4	Diterpene lactones	GQPOXOPEDHHRQT-CRBRZBIVSA-N	O=C1OCC(C=CC2C(=C)CC3C(C)(CO)C(O)CCC23C)=C1
264	0.9	327.15308	Acepromazine	[M+H] ⁺	327.15256	C19H22N2O5	Phenothiazines	NOSIYYJFMPDDSA-UHFFFAOYSA-N	CN(C)CCCN1C2=CC=C(C=C2)C2C1C=C(C=C2)C(C)=O
265	0.9	152.05614	Guanine	[M+H] ⁺	152.05669	C5H5N5O	Purines and purine derivatives	UYTPUPDQBNUYG-UHFFFAOYSA-N	c1nc2c([nH]c1)[nH]c(=N)nc2O
266	0.9	292.13849	N-Fructosyl isoleucine	[M+H] ⁺	292.1391	C12H23N2O7	N-Fructosyl amino acids	VYGRYVGPYFYCA-UHFFFAOYNA-N	O=C(O)C(NCC1(O)(OC(CO)C(O)C1))C(C)CC
267	0.901	317.17029	[6]-Gingerol	[M+H] ⁺	317.17001	C17H26O4	Gingerols	NLDDIKRKFEXWB-AWEZNCQLSA-N	O=C(CCC1=CC=C(O)C(OC)=C1)CC(O)CCCC
268	0.901	251.07591	2'-Deoxyinosine	[M+H] ⁺	251.07858	C10H12N4O4	Purine 2'-deoxyribonucleosides	VGONTNSXDCQUGY-RRKRQDMSA-N	OC[C@H]1O[C@H](C[C@H]1O)N1C=NC2=C1N=CN=C2O
269	0.901	256.09259	2'-O-Methylcytidine	[M+H] ⁺	256.0939	C10H15N3O5	Pyrimidine nucleosides	RFCQJGFZUQYRF-UHFFFAOYNA-N	N=C1N=C(O)N(C=C1)C2OC(CO)C(C)C2OC
270	0.901	237.08633	3,4-dihydro-2,2-dimethyl-indeno[1,2-b]-pyran-5(2H)-one	[M+H] ⁺	237.08501	C14H14O2	Indenes and isoenindenes	ICNOFNFXLJFTLZ-UHFFFAOYSA-N	O=C1C=2C=CC(=C2)C3=C(C)C(C)C(C)C3
271	0.901	442.19034	butyrolactone i	[M+H] ⁺	442.186	C24H24O7	Fatty acid esters	NGOLMNMWQHWKEU-XMMP1XPASA-N	O=C1OC(C(=O)OC)(C=C1O)C2C=CC(O)=CC2CC3=CC=C(O)C(C=C3)CC=C(C)C
272	0.901	260.15964	Isoleucylglutamine	[M+H] ⁺	260.16	C11H21N3O4	Dipeptides	CNPNGHRMBQHBZ-UHFFFAOYNA-N	O=C(O)C(NC(=O)C(N)C(C)C)CCC(=O)N
273	0.901	188.05731	N-Acetylglutamic acid	[M+H] ⁺	188.05644	C7H11N2O5	Glutamic acid and derivatives	RPMVMVDN1PUKGG-UHFFFAOYNA-N	O=C(O)CCC(N=C(O)C)C(=O)O
274	0.901	194.11696	Pesticide2_Isopropcarb_C1H15N2O2_2-Isopropylphenyl methylcarbamate	[M+H] ⁺	194.117	C11H15N2O2	Cumenes	QBSJMK1UKICUGNG-UHFFFAOYSA-N	OC(=NC)OC1=C=CC=CC1C(C)C
275	0.901	303.03775	Thymidine-3',5'-cyclic monophosphate sodium salt	[M+H] ⁺	303.03876	C10H13N2O7P	Pyrimidones	QSJFDQVQZVUQ6-UHFFFAOYNA-N	CC1=CN(C2CC3OP(O)(=O)CC3OC2)C(=O)NC1=O
276	0.902	382.16867	Azelastine	[M+H] ⁺	382.16806	C22H24ClN3O	Phthalazinones	MBUVEWMHONZEDQ-UHFFFAOYNA-N	CN1CCCC(C1)N2C(C3=C=CC=C3C(C4=CC=C(C=C4)C1)=N2)=O
277	0.902	627.14978	Baimeside	[M+H] ⁺	627.15002	C27H30O17	Flavonoid-3-O-glycosides	RDUAJ1JVNHTQ-UJEXCLDQSA-N	O=C1C(OC2OC(CO)C(O)C(=O)C2OC3OC(CO)C(C)C3O)=CC(=OC)=4C=C(CO)C=C(CO)C14C=5C=C(CO)=C(CO)C5
278	0.902	255.09207	Chrysin	[M+H] ⁺	255.09	C15H10O4	Flavones	RT1XKCRFFJGDFG-UHFFFAOYSA-N	O=C1C=C(OC2=C(O)C=C(C)C2)C=C3C=CC=CC3
279	0.902	300.10641	Erysovine	[M+H] ⁺	300.10001	C18H21N3O3	Erythrinanes	IHPMURIXWRKED-UHFFFAOYSA-N	OC=1C=C2C(=CC1OC)CCN3CC=C4C=CC(OC)CC423
280	0.902	164.07068	Phenylalanine (Not validated)	[M+H] ⁺	164.0708	C9H11N2O2	Amino acids	COLNVLDHWKLR1-UHFFFAOYNA-N	O=C(O)C(N)CC1=CC=CC=C1
281	0.903	454.19165	3,7,21-trihydroxy-17,17-dimethyl-14-(3-methylbut-2-en-1-yl)-10,12,16-trioxapentacyclo[11.8.0.02,22.02,2,022,22]henicosane	[M+H] ⁺	454.186	C25H24O7	8-prenylated isoflavanones	DQNIISLSDHTEPL-UHFFFAOYSA-N	O=C1C2=C(O)C=3C=CC(OC3C(=C2OC4OC5=CC(O)=CC=C5C4)CC=C(C)C(C)C
282	0.903	271.09088	Alloimperatorin	[M+H] ⁺	271.09	C16H14O4	8-hydroxypsoralens	KDXVZYMSYLWJMA-UHFFFAOYSA-N	O=C1OC=2C(O)=C3OC=CC3C(C2C=C1)CC=C(C)C

300	0. 908	161. 10692	Tryptamine	[M+H] ⁺	161. 10699	C10H12N2	Tryptamines and derivatives	APJYDQYAXCRM-UHFFFAOYSA-N	NCCC1=CN=C-2C=CC=C21
301	0. 909	525. 1203	(2S, 3R, 4aS, 12bR)-2, 3, 4a, 8-tetrahydroxy-12b-(5-hydroxy-6-methyloxan-2-yl)oxy-3-methyl-2, 4-dihydrobenzofalanthracene-1, 7, 12-trione	[M+H] ⁺	525. 11572	C25H26O10	Anthraquinone glycosides	CKZMKYSFWSICZ-GTJLABFSSA-N	O=C1C=2C=CC3(O)CC(O)(C)C(O)C(=O)C3(O)C4OC(C)C(O)CC4)C2C(=O)C=5C=C(C(=O)C)C15
302	0. 909	421. 17996	15-Acetoxyeremantholide B	[M+H] ⁺	421. 17999	C22H28O8	Furofurans	UNFGPCUYMXWDG-OOQPEQBPSA-N	O=C(OC(C1=CC2OC(=O)C3(C)C2C(OC3(O)C(C)C)CC4(OC1=CC4=O)C)C
303	0. 909	409. 10858	5, 7-dihydroxy-2-(4-hydroxy-3-methoxyphenyl)-6-(3-methylbut-2-enyl)-2, 3-dihydrochromen-4-one	[M+H] ⁺	409. 1048	C21H22O6	6-prenylated flavanones	GWGVAPNTKLROZ-UHFFFAOYSA-N	O=C1C2=C(O)C(=C(O)C=C2OC(C3=CC=C(O)C(OC)=C3)C1)CC=C(C)C
304	0. 909	133. 01364	D-(+)-Malic acid	[M-H] ⁻	133. 01425	C4H6O5	Beta hydroxy acids and derivatives	BJEPYKJPYRNKOW-UWTATZPHSA-N	O[C=H](CC(O)=O)C(O)=O
305	0. 909	305. 06287	Flavanol base + 50	[M-H] ⁻	305. 06491	C15H14O7	Flavanol O-glycosides	XMOCLSLCDHWHP-UHFFFAOYNA-N	OC3=CC(O)=C2C(OC(C1=CC(O)=C(O)C(O)=C1)C(O)C2)=C3
306	0. 91	291. 08328	Epicatechin	[M+H] ⁺	291. 08401	C15H14O6	Catechins	PFTAWBLQPZVEMU-UKRRQHQSNA-N	OC=C(C(O)C2=C(OC(C3=CC=C(O)C(O)=C3)C(O)C2)C1
307	0. 91	327. 11667	Eucalyptin	[M+H] ⁺	327. 116	C19H18O5	7-O-methylated flavonoids	NHMMAMIRMITGRD-UHFFFAOYSA-N	O=C1C=C(OC2=C1C(O)=C(C(OC)=C2)C)C=C3=CC(OC)=CC3
308	0. 91	137. 04549	Hypoxanthine	[M+H] ⁺	137. 04579	C5H4N4O	Hypoxanthines	FDQGSTZJBFJUBT-UHFFFAOYSA-N	c1nc2c([nH]1)ncnc20
309	0. 91	328. 13754	N-Fructosyl phenylalanine	[M+H] ⁺	328. 13879	C15H21N07	N-Fructosyl amino acids	FAVRCIXPIVJIPN-UHFFFAOYNA-N	O=C(O)C(NCC1(O)(OC(CO)C(O)C1(O)))CC2=CC=CC=C2
310	0. 911	173. 05659	1-naphthalenecarboxaldehyde, 2-hydroxy	[M+H] ⁺	173. 05971	C11H8O2	Naphthols and derivatives	NTCCNERMXRIPTR-UHFFFAOYSA-N	C1=CC=C2C(=C1)C=CC(=C2C)=O
311	0. 911	115. 00303	Maleic acid	[M-H] ⁻	115. 00368	C4H4O4	Dicarboxylic acids and derivatives	VZCYOOQTPCHOFL-UHRSURJSA-N	OC(=O)C=C(C(O)=O)
312	0. 911	245. 185	N-L-Leucyl-L-leucine	[M+H] ⁺	245. 18597	C12H24N2O3	Peptides	LCPYQJ1KPJDLB-UHFFFAOYSA-N	O=C(O)C(NC(=O)C(N)CC(C)C)CC(C)C
313	0. 912	452. 22025	(3, 5, 14-trihydroxy-13-methyl-17-(5-oxo-2, 5-dihydrofuran-3-yl)hexadecahydro-1H-cyclopenta[al]phenanthren-10-yl)methyl nitrate	[M+H] ⁺	452. 22	C23H33N08	Cardenolides and derivatives	HCEPYGKCFDOPJ-UHFFFAOYSA-N	O=C1OCC(=C1)C2CC3(C)CC4CC5(O)CC(O)CC5(CO[N+](=O)[O-])C4OC23C
314	0. 912	132. 10138	Isoleucine	[M+H] ⁺	132. 1019	C6H13N02	Isoleucine and derivatives	AGPKZVBTJJNPAG-UHFFFAOYNA-N	CCC(C)C(N)C(O)=O
315	0. 912	585. 30957	lappaconitine	[M+H] ⁺	585. 31	C32H44N2O8	Lappaconitine-type diterpenoid alkaloids	NBWCXBPKTTZNQ-GSAAXPBRSA-N	O=C(OC12CN(C)C3C4CC1C3(C(OC)CC2)C5C6C(OC)CC4(O)C5(O)C6OC)C=C7C=CC=C7N(C)=O)C
316	0. 912	163. 02548	Lumazine	[M-H] ⁻	163. 02615	C6H4N4O2	Pteridines and derivatives	UYEUXMDVNYCAM-UHFFFAOYSA-N	OC=1N=C(O)C2=NC=CN=C2N1
317	0. 912	154. 04941	Mesalazine	[M+H] ⁺	154. 04987	C7H7N03	Aminobenzoic acids	KBOPZPXVLCULAV-UHFFFAOYSA-N	C1=CC(=C(C=C1N)C(=O)O)O
318	0. 912	303. 08398	N-Acetylaspartylglutamic acid	[M-H] ⁻	303. 08337	C11H16N2O8	Dipeptides	OPVPKGADVGKTG-UHFFFAOYNA-N	O=C(O)CCC(N(=O)C)C(N=C(O)C)CC(=O)C(O)C(=O)O
319	0. 913	220. 11786	Pantothenic acid	[M+H] ⁺	220. 11795	C9H17N05	Secondary alcohols	GHOXGWTUJEAQD-UHFFFAOYSA-N	CC(C)(CO)C(C(=NCCC(=O)O)O)O
320	0. 913	153. 07565	Ribitol	[M+H] ⁺	153. 07574	C5H12O5	Sugar alcohols	HEBKCHPVOIAGTA-ZXFHETHRNA-N	OC[C=H](O)[C-](H)(O)[C-](H)(O)CO
321	0. 914	370. 20917	allocryptopine	[M+H] ⁺	370. 21036	C21H23N05	Protopine alkaloids	HYBRYAPKQCZIAE-UHFFFAOYSA-N	O=C1C2=CC=3OCOC3C=C2CC(N)CC4=C(OC)C(C)C(OC)=CC=C4C1
322	0. 915	159. 02898	2-OXOADIPATE	[M-H] ⁻	159. 02901	C6H8O5	Medium-chain keto acids and derivatives	FGSBNBHOZHUBO-UHFFFAOYSA-N	O=C(O)C(=O)CCCC(=O)O
323	0. 916	495. 10931	Flavonol base + 40, 1Me0, 0-Hex	[M+H] ⁺	495. 11292	C22H22O13	Flavonol O-glycosides	AFCDXKGLUDDCK-UHFFFAOYNA-N	O=C2C(O)=C(OC=3C=C(OC1OC(C)C(O)C1(O)C1(O)C(OC)=C(O)C2=3)C4=C(C=C(O)C)C=C4
324	0. 916	301. 10318	Haematoxilin	[M-H] ⁻	301. 10031	C16H14O6	1-benzopyrans	WZUVPKKBWHMQCE-UHFFFAOYSA-N	OC1=CC=C2C(OC(C)CC4=CC(O)=C(O)C=C4C23)=C1O
325	0. 916	335. 05991	Pachyrrhizin	[M-H] ⁻	335. 05612	C19H12O6	Isoflav-3-enones	PENSQRMNZZWMGV-UHFFFAOYSA-N	O=C1OC2=CC=3OC=CC3C=C2C=C1C=4C=C5OCOC5=CC4OC
326	0. 918	204. 08644	7-Methylsulfonylheptyl isothiocyanate	[M+H] ⁺	204. 08752	C9H17NS2	Glucosinolate breakdown metabolites	LDIRGNDMTGVRB-UHFFFAOYSA-N	CSCCCCCCCNC=S
327	0. 918	103. 03886	ACETOACETATE	[M+H] ⁺	103. 04	C4H6O3	Short-chain keto acids and derivatives	WDJHALXBUFZDSR-UHFFFAOYSA-N	O=C(O)CC(=O)C
328	0. 918	117. 05432	Ketoisovaleric acid	[M+H] ⁺	117. 05462	C5H8O3	Short-chain keto acids and derivatives	QHKABHOEWYVLI-UHFFFAOYSA-N	O=C(O)C(=O)C(C)C
329	0. 918	273. 03693	Phenylbenzimidazole sulfonic acid	[M-H] ⁻	273. 03394	C13H10N2O3S	Phenylbenzimidazoles	UVCJGUGAGLPAA-UHFFFAOYSA-N	C1=CC=C(C=C1)C2=NC=3C=CC(=CC3N2)S(O)(=O)=O
330	0. 918	523. 10327	Protopseudohypericin	[M+H] ⁺	523. 09998	C30H18O9	Perylenequinones	QFAPJWSQKUFHAP-UHFFFAOYSA-N	O=C1C2=C(O)C=C(C=C2C3=4C=5C=C(C=C(O)C5C(=O)C6=C(O)C=C(O)C(=C7C(O)=CC(O)=C1C73)=C64)O)C
331	0. 921	425. 10352	[3-hydroxy-3-methyl-1-(7-oxofuro[3, 2-g]chromen-9-yl)oxybutan-2-yl] (Z)-2-methylbut-2-enoate	[M+H] ⁺	425. 10196	C21H22O7	Psoralens	VJVXQSFKVUEFY-XG1CHPGQSA-N	O=C1OC2=C(OC(C(OC(=O)C(=CC)C(O)(C)C)C=3OC=CC3C=C2C=C1
332	0. 922	406. 10947	8-(azepan-1-ium-1-ylmethyl)-3-(4-chlorophenyl)-4-oxo-4H-chromen-7-olate	[M+H] ⁺	406. 10999	C22H22ClN03	Isoflavones	LUXRPLCGZWQEC-UHFFFAOYSA-N	O=C1C(=COC=C2C1=CC=C(C(=O)C2C1N)13CCCCC3)C=C4C=CC(C1)=CC4
333	0. 922	285. 10693	8-hydroxy-5, 8a-dimethyl-3-methylidene-3a, 4, 4a, 8, 9, 9a-hexahydrobenzo[f[1]l]benzofuran-2, 7-dione	[M+H] ⁺	285. 10971	C15H18O4	Eudesmanolides, sesquidesmanolides, and p-Hydroxybenzoic acid alkyl esters	XAFJ1JZCMNHLRS-UHFFFAOYSA-N	O=C1OC2CC3(C)C(O)C(=O)C=C(C)C3CC2C1=C
334	0. 923	453. 09949	1-(2R, 3S, 4S, 5R, 6S)-6-(3, 4-dihydroxybenzoyl)oxy-3, 4, 5-trihydroxyoxan-2-yl)methyl 3, 4-dihydroxybenzoate	[M+H] ⁺	453. 10275	C20H20O12	19-gibberellin 6-carboxylic acids	VNQNUOLCMXPFER-XDCWJTEKSA-N	O=C(OC1OC(OC(=O)C2=CC=C(O)C(O)=C2)C(O)C(O)C1O)C3=CC=C(O)C(O)C=C3
335	0. 924	369. 18414	Gibberellin A4A7	[M+H] ⁺	369. 18405	C19H22O5	Dicarboxylic acids and derivatives	SEEGHKWBVBQTF-UKJRIFTCSA-N	O=C(O)C1C2C3(OC(=O)C2(C)C(O)C=C3)C4CCCC(C)C(C)C1C45
336	0. 927	103. 00303	MALONATE	[M-H] ⁻	103. 003	C3H4O4	Dicarboxylic acids and derivatives	OFQBLEULBTSOW-UHFFFAOYSA-N	O=C(O)CC(=O)O
337	0. 929	222. 01904	5-Aminonaphthalene-2-sulfonic acid	[M-H] ⁻	222. 02304	C10H9NO3S	2-naphthalene sulfonates	OPBJYQVRSWYIGZ-UHFFFAOYSA-N	C1=CC2=CC(=CC(=C2C(=C1)N)S(O)(=O)=O
338	0. 933	209. 02934	GALACTARATE	[M-H] ⁻	209. 03	C6H10O8	Glucuronic acid derivatives	DSLZVSRJTYRBFB-UHFFFAOYSA-N	O=C(O)C(O)C(O)C(O)C(O)C(=O)O
339	0. 934	400. 14264	9-[[3-methyl-3-[(4-methyl-5-oxo-2H-furan-2-yl)methyl]oxiran-2-yl)methoxyl]furo[3, 2-g]chromen-7-one	[M+H] ⁺	400. 13907	C21H18O7	Psoralens	C1SFAPDYRQPRCZ-UHFFFAOYSA-N	O=C1OC2=C(OC(C3OC3(C)CC4OC(=O)C(=C4)C)C=5OC=CC5C=C2C=C1
340	0. 935	573. 1394	methyl 8, 11, 15, 20, 22-pentahydroxy-24-methyl-13, 18, 27-trioxo-6-oxahentacyclo[15. 10. 2. 02. 22. 02. 22. 02. 22. 02. 22]nonacosane	[M+H] ⁺	573. 13916	C31H24O11	Xanthones	K1WTYJVARRBPR-UHFFFAOYSA-N	O=C1C=2C(O)=C3C(=CC2OC4(C(=O)OC)C1=C(O)CC4O)CC56C=CC3(C(=O)C6=C(O)C=C7C(O)=CC(=CC7C5=O)C
341	0. 935	351. 08566	Pinastic acid	[M-H] ⁻	351. 086	C20H16O6	Anisoles	KXQKSBAQMGQSN-FBMGVBCBSA-N	O=C1OC(C(O)=C1C=2C=CC(OC)=CC2)C(C(=O)OC)C=C3C=CC=CC3
342	0. 936	202. 06985	2-((2H-pyrazolo[3, 4-d]pyrimidin-4-yl)amino)ethanol	[M+H] ⁺	202. 07001	C7H9N5O	Pyrazolo[3, 4-d]pyrimidines	LCOTUPXIQXPIPA-UHFFFAOYSA-N	OCCNC1=NC=NC=C2N1C=C2

[illegible]

386	0.968	258.1091	sn-Glycero-3-phosphocholine	[M] ⁺	258.10956	C8H21N06P	Glycerophosphocholines	SUHQVVVLYNQK-MRVFVSSYA-O	C[N+](C)(C)CCOP(O)=O)OC[C-H](O)CO
387	0.969	388.14377	methyl 3-(4-hydroxyphenyl)-2-[(4-hydroxyphenyl)methyl]-4-methoxy-5-oxofuran-2-carboxylate	[M+H] ⁺	388.13907	C20H18O7	Fatty acid esters	DYMDWEI1IXYN-UHFFFAOYSA-N	O=C1OC(C=O)OC(C(C=2C=CC(=O)C2)=C1OC-CC3=CC=C(O)C=C3
388	0.97	80.04919	Pyridine	[M+H] ⁺	80.04948	C5H5N	Pyridines and derivatives	JUJWRO01HBZHM-UHFFFAOYSA-N	C1=CC=NC=C1
389	0.971	212.05444	Imidacloprid-urea	[M+H] ⁺	212.05852	C9H10ClN3O	2-halopyridines	ADWTYURAFSWSU-UHFFFAOYSA-N	OC1=NCCN1C1=CN=C(C1)C=C1
390	0.974	367.06216	Dracorhodin perchlorate	[M+H] ⁺	367.06	C17H15ClO7	5-O-methylated Flavonoids	KRTYZFUODYMZG-UHFFFAOYSA-N	[O-]([C1+3]([O-])([O-])([O-])1O-1,OC=1C=C2([O-])1=C(C=C2C=CC(C(C2)C1)C=C3C=CC=CC3
391	0.975	649.21802	(S)-2-((((S)-7-acetamido-1,2,3-trimethoxy-9-oxo-5,6,7,9-tetrahydrobenzo[ah]n[1,2-b:4,5-b']oxazol-10-yl)amino)-N-(benzo[d]thiazol-2-yl)-4-	[M+H] ⁺	649.21997	C38H36N4O6S2	Methionine and derivatives	RU1FGEPTYTTFK-DHLKGQNSA-N	O=C1C=C2C=C(C=C1C=C(C(=O)N)C3=NC=4C=CC=C4S)CCSC)C5=C(O)C(C)C(OC)=C(OC)C=C5COC2NC(=O)C
392	0.976	282.08313	Guanosine (Not validated)	[M-H] ⁻	282.0834	C10H13N5O5	Nucleosides	NHYBQMYSK1UIF-UHFFFAOYNA-N	O=C3C(=NC1=C3(=N)C1C2OC(CO)C(C)C2(O))N
393	0.977	300.0481	2-Chloroadenosine	[M-H] ⁻	300.05051	C10H12ClN5O4	Purine nucleosides	B1XYZ1J1J1XVW-UHFFFAOYNA-N	C1C=1N=C(N)C=2N=C(C2N1)C3OC(CO)C(O)C3O
394	0.977	214.03406	3-Chlorotyrosine	[M-H] ⁻	214.02765	C9H10ClN3O3	Tyrosine and derivatives	ACWBAGYTKWBCD-UHFFFAOYNA-N	O=C(O)C(N)CC1=CC=C(O)C(C1)=C1
395	0.977	218.10289	Pesticide4 Pymetrozine, C10H11N5O, (E)-4,5-Dihydro-6-methyl-4-[(3-pyridinylmethylene)amino]-1,2,4-triazin-3(2H)-one	[M+H] ⁺	218.103	C10H11N5O	1,2,4-triazines	QHMTXANCGJZRX-WUXMJOGZSA-N	OC1=NN=C(C)CN1N=CC=CC=NC=CC2
396	0.977	292.07083	PFSM-ammonio	[M-H] ⁻	292.07101	[C8H16F3N2O4S] ⁺	PFSA	ODUULAMNNKMD-UHFFFAOYSA-O	O=C(O)C([N+](C)C)CCN3(=O)C(=O)C(F)F
397	0.98	332.15433	Deoxysappanone B 7,3'-Dimethyl Ether	[M+H] ⁺	332.14923	C18H18O5	Homoisoflavanones	OFAYBXSZCUARK-UHFFFAOYSA-N	O=C1C2=CC=C(OC)C=C2OCC1C3=CC=C(O)C(OC)=C3
398	0.981	343.12183	2-alpha-Mannobiose	[M+H] ⁺	343.12347	C12H22O11	O-glycosyl compounds	HTWPGMGAMJNRG-UHFFFAOYNA-N	OC1OC(O)C(OC2OC(CO)C(C)C2O)C(CO)C1O
399	0.986	395.05588	bisdethiobis(methylthio)gliotoxin	[M+H] ⁺	395.0564	C15H20N2O4S2	Alpha amino acids and derivatives	OVRBAGMLZLXSBN-UOVKNHLSA-N	O=C1N(C)C(SC)C(C=O)N2C3C(=CC=CC3)C12SC)CO
400	0.986	325.11331	Disaccharide (Hex-Hex)	[M+H] ⁺	325.11371	C12H22O11	Sugars	PVXPJ1JGRGXGY-UHFFFAOYNA-N	OC2OC(OC1OC(O)C(CO)C1(O)C(O)C(O)C2(O)
401	0.986	505.17514	Raffinose	[M+H] ⁺	505.1763	C18H32O16	Oligosaccharides	MUPFEKTMRGPLJ-UHFFFAOYNA-N	OC1OC(OC2OC(OC3(OC(CO)C(CO)C3O)C(CO)C2O)C(CO)C1O
402	0.988	277.17801	NP1EC (TENTATIVE)	[M-H] ⁻	277.18091	C17H26O3	Phenoxyacetic acid derivatives	N1SAHDHKGWBEM-UHFFFAOYSA-N	CCCCCCCCC1=CC=C(C=C1)OCC(=O)C
403	0.989	249.03647	Diphenyl phosphate	[M-H] ⁻	249.03223	C12H11O4P	Aryl phosphodieters	ASMOGLCHMWQK-UHFFFAOYSA-N	C1=CC=C(C=C1)OP(O)C(=O)C2=CC=CC=C2
404	0.99	227.07306	4-methoxy-9H-xanthen-9-one	[M+H] ⁺	227.071	C14H10O3	Xanthenes	SYEHMRXODULBY-UHFFFAOYSA-N	O=C1C=C2C=C(CC2OC=3C(OC)=CC=CC13
405	0.99	319.04898	Flavanone base + 60	[M-H] ⁻	319.0459	C15H12O8	Flavanone O-glycosides	KJXSIXMJHKAJOD-UHFFFAOYNA-N	O=C2C3=C(O)C=C(O)C3(OC(C1=CC(O)C(O)C1)=C1)C2(O))
406	0.991	148.02434	3-Hydroxyaspartic acid	[M-H] ⁻	148.02515	C4H7NO5	Aspartic acid and derivatives	YYLQUHNPNCGKJQ-UHFFFAOYNA-N	O=C(O)C(O)C(C)=O
407	0.991	263.01627	4:2 Fluorotelomer alcohol	[M-H] ⁻	263.01239	C6H5F9O	PFSA	JCMNMOBHVONLD-UHFFFAOYSA-N	FC(F)(F)C(F)C(F)C(F)C(F)C(F)CO
408	0.991	305.13574	5,9-dihydroxy-7-(hydroxymethyl)-5,7-dimethyl-4,5a,6,8,8a,9-hexahydro-1H-azuleno[5,6-c]furan-3-one	[M+H] ⁺	305.13593	C15H22O5	Terpene lactones	DBK1EMOKQWYZO-UHFFFAOYSA-N	O=C1OC2=C1CC(O)C(C)C3CC(C)(CO)CC3C2O
409	0.992	177.09456	Canavanine	[M+H] ⁺	177.09821	C5H12N4O3	L-alpha-amino acids	FSB1GDSMBEYOFN-VKHMVHEASA-N	O=C(O)C(N)CCON(=O)N
410	0.994	306.1171	2-methyl-3-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxopropan-4-one	[M+H] ⁺	306.11835	C12H16O8	O-glycosyl compounds	YGS1RXHFAPUEJG-GPTQWHSKA-N	O=C1C=CC(C=C1OC2OC(CO)C(O)C2O)C
411	0.994	275.01581	6-PHOSPHOGLUCONIC ACID	[M-H] ⁻	275.017	C6H13O10P	Monosaccharide phosphates	BRISGZKFKLSJQ-UHFFFAOYSA-N	O=C(O)C(C)C(O)C(C)C(O)COP(=O)(O)O
412	0.994	199.96814	Cysteine S-sulfate	[M-H] ⁻	199.96928	C3H7NO5S2	S-sulfo-L-cysteines	NOKPB1JYHPHWAN-REOHLBLSA-N	[N-](C)C(SS(O)=O)C(O)C=O
413	0.995	323.0274	URIDINE-5-MONOPHOSPHATE	[M-H] ⁻	323.02802	C9H13N2O9P	Pyrimidine ribonucleoside	D1JCFXVJDGTHFX-UHFFFAOYSA-N	O=C1C=CN(C(=O)N1)C2OC(COP(=O)(O)O)C(CO)C2O
414	0.996	333.05783	(2S,3S)-3,5,7-trihydroxy-6-methyl-2-(3,4,5-trihydroxyphenyl)-2,3-dihydrochromen-4-one	[M-H] ⁻	333.06158	C16H14O8	Epigallocatechins	NZRL0DDQFPZTPM-CVEARBZSA-N	O=C1C2=C(O)C=C(O)C=C2OC(C3=CC(O)C(O)C3)=C1O(C)=C3)C1O(C
415	0.996	553.11426	Biflavonoid-flavone base + 30 and flavanone base + 20 + 1MeO	[M-H] ⁻	553.11218	C31H22O10	Biflavonoids	XMFL1YCNQLOLA-CYLJNIGPNA-N	O=C1C=C(OC2=C1C(O)=CC(O)C(CO)C3O)=C(O)C=C2OC4=CC(O)C4OC=5C(C(=O)C4)C6=CC=C(C(=O)C6=C6
416	0.997	167.99599	Cysteic Acid	[M-H] ⁻	167.99722	C3H7NO5S	Alpha amino acids	XVOYSCVBGLYSOL-UHFFFAOYNA-N	O=C(O)C(N)CS(=O)C(=O)O
417	0.997	413.10254	Deacetylasperulosidic acid	[M+H] ⁺	413.10001	C16H22O11	Iridoid O-glycosides	ZYXWFTVHEWJOU-YYGDFGFSNA-N	O=C(O)C1=CC(OC2OC(CO)C(O)C2O)C2OC(=CC(O)C13)CO
418	0.997	317.0563	Myricetin	[M-H] ⁻	317.05789	C15H10O8	Flavonols	IKMDFBPZJNCSN-UHFFFAOYSA-N	O=C1C(O)=C(OC=2C=C(O)C=C(O)C12)C=3C=C(O)C(O)=C(O)C3
419	0.998	171.00551	Glycerophosphate(2)	[M-H] ⁻	171.00639	C3H9O6P	Glycerophosphates	AVUCVROLDV1AJX-GSVOUTGSA-N	OC[C-H](O)COP(O)(O)=O
420	0.999	233.0287	(2R)-5-methoxy-2-methyl-2,3,8,9-tetrahydrofuro[2,3-h]chromen-4-one	[M-H] ⁻	233.02577	C13H14O4	Chromones	BCRDBKZKSRLMH-SSDOT75WSA-N	O=C1C2=C(OC)C=C3OCC3=C2OC(C)C1
421	0.999	192.08609	Shikimic Acid	[M+H] ⁺	192.08664	C7H10O5	Shikimic acids and derivatives	JXOHHGKNMLTUB-HSUXUTPPSA-N	O=C(O)C1=CC(O)C(O)C(CO)C1
422	1.002	259.02078	D-Mannose-6-phosphate	[M-H] ⁻	259.02243	C6H13O9P	Hexose phosphates	NBSCHQZLSJFNG-QTVWNMPRSA-N	OC1O[C-H]COP(O)(O)=O)[C-H](O)[C-H](O)[C-H]1O
423	1.002	585.14142	Neomangiferin	[M+H] ⁺	585.14001	C25H28O16	Xanthenes	VUWGVXVRYBSGI-IRXABLMPSA-N	O=C1C2=CC(OC3OC(CO)C(CO)C3O)=C(O)C=C2OC4=CC(O)C4OC=5C(C(=O)C4)C6=CC=C(C(=O)C6=C6
424	1.003	274.0907	Pentose + Proline	[M+H] ⁺	274.0932	C11H15N3O7	Amino acids	VMOJEEZNLOLYBG-UHFFFAOYNA-N	O=C(O)C1N(C(=O)CC1)CC2(O)CC(CO)C(CO)C2(O)
425	1.003	273.02631	Simonyellin	[M-H] ⁻	273.03	C14H10O6	Isocoumarins and derivatives	GJSCVPZGPZ1BMU-UHFFFAOYSA-N	O=C1OC=C2C(OC)=C(O)C(=O)C3=C2C1=C(O)C=C3C
426	1.005	183.08548	D-Sorbitol	[M+H] ⁺	183.08632	C6H14O6	Sugar alcohols	FBPPTZCFMRRESA-FBXPSONDNA-N	OC[C-H](O)[C-H](O)[C-H](O)[C-H](O)CO
427	1.006	393.07874	Hexose + C5H10O3, 1phosphate	[M-H] ⁻	393.07819	C11H23O13P	Organic acids	HJZBAIMJDQCPL-UHFFFAOYNA-N	C(C1C(C(C(C(O1)OC(COP(=O)(O)O)C(CO)O)O)O)O)O)O
428	1.006	279.04669	Piscidic Acid	[M+H] ⁺	279.04749	C11H12O7	Phenylpropanoic acids	TUODPMGCCJSJRH-UHFFFAOYSA-N	O=C(O)C(C)C(O)C(C(=O)O)CC1=CC=C(O)C=C1

429	1.007	241.01073	33FTA	[M-H] ⁻	241.0105	C6H5F7O2	Medium-chain fatty acids	ISFSKSWQWIRDNC-UHFFFAOYSA-N	OC(=O)CCC(F)(F)C(F)(F)C(F)(F)F
430	1.007	261.03696	D-Sorbitol 6-phosphate	[M-H] ⁻	261.03809	C6H15O9P	Monosaccharide phosphates	GACTWZ2MVUMRG-SLPGGIOYSA-N	OC[C@H](O)[C@H](O)[C@H](O)[C@H](O)COP(=O)(O)=O
431	1.007	373.17044	Phillygenin	[M+H] ⁺	373.17001	C21H24O6	Furanoid lignans	CPJKWDCUOOTEW-YJXPFGSGSA-N	OC1=CC=C(C=C1OC)C2OC3C(OC23)C4=CC=C(OC)C(OC)=C4
432	1.008	337.12189	Pesticide6_Fenbuconazole_C19H17C1N4_4-(4-Chlorophenyl)-2-phenyl-2-((1H-1,2,4-triazol-1-ylmethyl)butanenitrile	[M+H] ⁺	337.121	C19H17C1N4	Linear 1,3-diarylpropanoids	RQD1ADAK1FFEKU-UHFFFAOYSA-N	N#CC(C=C1=CC=CC1)(CN2N=CN=C2)CCC3=CC=C(C1)C=C3
433	1.009	603.15314	[(2R,3S,4S,5R,6S)-6-[2,3-dihydroxy-4-[(6)-3-(4-hydroxyphenyl)prop-2-enoyl]phenoxy]-3,4,5-trihydroxyoxan-2-yl]methyl (E)-3-(4-	[M+H] ⁺	603.14728	C30H28O12	Flavonoid O-glycosides	MXL1DYXRCRYPL-SVQBVAIGSA-N	O=C(OC1OC(OC2=CC=C(C(=O)C=C3=CC=C(C(=O)C=C3)C(=O)=C2O)C(=O)C(=O)C1O)C=CC4=CC=C(O)C=C4
434	1.009	123.05582	2-Acetylpyrazine	[M+H] ⁺	123.0553	C6H6N2O	Aryl alkyl ketones	DBZAKQWXICEWN-UHFFFAOYSA-N	CC(=O)c1cncn1
435	1.009	229.01082	D-RIBOSE 5-PHOSPHATE	[M-H] ⁻	229.011	C5H11O8P	Pentose phosphates	PPQRONHOSHZGFQ-UHFFFAOYSA-N	O=CC(O)C(O)C(O)COP(=O)(O)O
436	1.009	237.01511	Methazolamide	[M+H] ⁺	237.013	C5H8N4O3S2	Thiadiazole sulfonamides	FLOSMHQXBMRNHR-UHFFFAOYSA-N	O=C(N=C1SC(=NN1C)S(=O)(=O)N)C
437	1.011	207.01566	2-Naphthalene sulfonic acid	[M-H] ⁻	207.01215	C10H8O3S	2-naphthalene sulfonates	KVBGVZZKJNLXJU-UHFFFAOYSA-N	C1=CC=C2C=C(C(=CC2=C1)S(=O)(=O)=O
438	1.011	241.03622	4,6,8-trihydroxy-7-methoxy-3-methyl-3,4-dihydroisochromen-1-one	[M+H] ⁺	241.03632	C11H12O6	Hydroxybenzoic acid derivatives	ZLLQKQ1TRWKTU-UHFFFAOYSA-N	O=C1OC(C)C(O)C2=C(C(=O)C)=C(OC)C(O)=C12
439	1.011	218.06564	O-Succinylhomoserine	[M-H] ⁻	218.06702	C8H13NO6	L-alpha-amino acids	GNISQJGXJDKDJ-UHFFFAOYNA-N	O=C(O)CCC(=O)OCCC(N)C(=O)O
440	1.011	275.04526	Ursinoic Acid	[M-H] ⁻	275.04794	C15H16O5	2,2-dimethyl-1-benzoyltrans	XUXBOSSCMLZGTA-UHFFFAOYSA-N	O=C(O)CC(=O)C1=CC=C(OC)C2=CC=CC(OC21)C(C
441	1.014	765.20166	5-hydroxy-3-[(2S,3R,4R,5S)-3-hydroxy-5-(hydroxymethyl)-4-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy]-6-(hydroxymethyl)tetrahydro-2H-pyran-3,4,5-triol	[M+H] ⁺	765.20203	C32H38O19	Flavonoid 7-O glycosides	LKV1DBLGZHMPCV-HLAATANNSA-N	O=C1C(OC2OC(CO)C(OC3OC(CO)C(O)C(O)C3O)C2O)=C(OC4=CC(OC5OC(C)C(O)C(O)C5O)=CC(O)=C14)C=6C=CC(O)=C6
442	1.014	329.00366	Furosenide	[M-H] ⁻	329.00046	C12H11ClN2O5S	Aminobenzenesulfonamides	ZZUPCTLCJWQSV-UHFFFAOYSA-N	C=1C-C(CNC2=CC(=C(C=C2C(=O)O)S(N)(=O)=O)Cl)OC1
443	1.016	173.02065	sn-Glycerol 3-phosphate	[M+H] ⁺	173.02095	C3H9O6P	Glycerophosphates	AVUCVRLDVIAXJ-GSVOUGTGS-N	OC[C@H](O)COP(=O)(O)O
444	1.018	236.11203	N-(9-oxodecyl)acetamide	[M+H] ⁺	236.11226	C12H23NO2	Acetamides	JRJBWJJIQGLDP-UHFFFAOYSA-N	O=C(C)CCCCCCCNC(=O)C
445	1.018	257.00549	PPCA-H	[M-H] ⁻	257.0054	C6H5F7O3	PFSA	NYXWTWRATMQVGT-UHFFFAOYSA-N	O=C(O)C(=O)C(F)(F)C(F)(F)C(F)(F)F
446	1.019	94.98025	Methanesulfonate	[M-H] ⁻	94.98083	CH4O3S	Organosulfonic acids	AFVFIQVMOAPDHO-UHFFFAOYSA-N	CS(=O)(=O)=O
447	1.02	407.16507	(2R,3R,4S,6R)-2-((5-hydroxy-2,2-dimethyl-3,4-dihydro-2H-benzo[h]chromen-6-yl)oxy)-6-(hydroxymethyl)tetrahydro-2H-pyran-3,4,5-triol	[M+H] ⁺	407.16599	C21H26O8	Phenolic glycosides	WVILKFLAZPSRT-MEUAUJKLSA-N	OC1=C(OC2OC(CO)C(O)C(O)C2O)C3=CC=CC3C=4OC(C)C(OC)CC14
448	1.02	183.00534	2,4-Dinitrophenol	[M-H] ⁻	183.00475	C6H4N2O5	Dinitrophenols	UFBJCMHMOXMKC-UHFFFAOYSA-N	C1=CC(=C(C=C1N(=O)=O)N(=O)=O)O
449	1.02	218.03207	Ornidazole	[M-H] ⁻	218.0338	C7H10ClN3O3	Nitroimidazoles	IPWKIXLWTCNBKN-UHFFFAOYNA-N	O=N(=O)C1=CN=C(N1CC(=O)CC1)C
450	1.021	329.00134	iodinated analogue of makaluvone	[M+H] ⁺	329	[C11H10IN2O2] ⁺	Pyrolo[4,3,2-de]nolines	NXSZMSHNYDJLD-UHFFFAOYSA-O	O=C1C(=O)C2=C3C(=CN2C)CC[NH2-]C3=C11
451	1.021	140.99435	Phosphonoacetic acid	[M+H] ⁺	140.99474	C2H5O5P	Organic phosphonic acids	NWJLQHKOGNDPB-UHFFFAOYSA-N	O=C(O)CP(=O)(O)O
452	1.023	239.03094	Sphondin	[M+H] ⁺	239.03046	C12H8O4	Angular furanocoumarins	DLJCNIRLOSJKQW-UHFFFAOYSA-N	O=C1OC=2C(C=C1)=CC(OC)=C3OC=CC32
453	1.027	338.98691	"FRUCTOSE 1,6-BIPHOSPHATE"	[M-H] ⁻	338.98801	C6H14O12P2	Hexose phosphates	XPYBS1WDXQFNMH-UYFOZJQFSA-N	O=C(COP(=O)(O)C(O)C(O)C(O)COP(=O)(O)O
454	1.031	277.05878	3-(5,7-dimethoxy-4-oxochromen-2-yl)propanoic acid	[M-H] ⁻	277.0603	C14H14O6	Chromones	AKJLPZYHXYQVJT-UHFFFAOYSA-N	O=C(O)CCC=1OC2=CC(OC)=CC(OC)=C2C(=O)C1
455	1.033	319.04214	Disulfiram	[M+H] ⁺	319.04099	C10H20N2S4	Thiuram disulfides	AUZONCFQVSMFAP-UHFFFAOYSA-N	S=C(SSC(=S)N(C)CC)N(C)CC
456	1.033	233.04124	Quebrachitol	[M+H] ⁺	233.04219	C7H14O6	Cyclohexanols	DSCPFYEQKRSV-UHFFFAOYSA-N	OC1C(O)C(O)C(OC)C(O)C1O
457	1.035	608.08636	Uridine-5-diphosphoacetylgalactosamine	[M+H] ⁺	608.08887	C17H27N3O17P2	Pyrimidine nucleotide sugars	LFTYTUAZOPRMMI-UHFFFAOYNA-N	O=C1N=C(O)C=CN1C2OC(COP(=O)(O)OP(=O)(O)OC3OC(CO)C(O)C(=O)C3N=C(O)C(=O)C2O
458	1.036	535.03558	UDP-xylose	[M-H] ⁻	535.03717	C14H22N2O16P2	Pyrimidine ribonucleoside	DQQDLYVHOTLR-OCIMBMBZSA-N	O[C@H]1[C@H](COP(=O)(=O)OP(=O)(=O)O[C@H]2OC[C@H](O)[C@H](O)[C@H]2O)O[C@H](C(=O)C(=O)N1C)C(=O)C(=O)C2O
459	1.039	166.97424	PHOSPHO(ENOL)PYRUVIC ACID	[M-H] ⁻	166.97501	C3H5O6P	Phosphate esters	DTBNBXWJWCWCIK-UHFFFAOYSA-N	O=C(O)C(OP(=O)(O)O)O=C
460	1.04	463.04724	4-Hydroxyglucobrassicin	[M-H] ⁻	463.04868	C16H20N2O10S2	Alkylglucosinolates	CSMYCLLIHFFFLG-UHFFFAOYNA-N	O=S(=O)(O)ON=C(SC1OC(C)C(O)C1O)CC2=CNC=3C=CC=C(O)C2
461	1.045	585.13806	7-[(2S,3R,4R,5R,6S)-3,4,5-trihydroxy-6-methylxan-2-yl]oxy-3-[4-[(2S,3R,4R,5R,6S)-3,4,5-trihydroxy-6-methylxan-2-yl]oxyphenyl]chromen-4-	[M+H] ⁺	585.1369	C27H30O12	Isoflavonoid O-glycosides	RIXHO1PNPVCBZ-WIYOTWCASA-N	O=C1C(=COC2C(OC3OC(CO)C(O)C3O)=CC(=C12)C=4C=CC(OC5OC(C)C(O)C(O)C5O)=CC4
462	1.045	203.14989	Asymmetric dimethylarginine	[M+H] ⁺	203.15025	C8H18N4O2	Arginine and derivatives	YDGMGEXADEMOP-LURJTMIESA-N	CN(C)C(=N)NCCC[C@H](C(=O)O)N
463	1.045	412.96481	Perfluorooctanoic acid	[M-H] ⁻	412.96643	C8HF15O2	Perfluoroalkyl carboxylic acid and Glucosinolate breakdown metabolites	SNRGREZHAYWORS-UHFFFAOYSA-N	C(C(C(C(C(C(C(F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)F)F(=O)O
464	1.046	176.01884	1-Isothiocyanato-4-(methylsulfinyl)-butane	[M-H] ⁻	176.02094	C6H11NO52		SUVMBJBUFCVSAD-UHFFFAOYNA-N	CS(=O)CCCCN=C=S
465	1.047	517.01044	2-(3,4-dihydroxyphenyl)-5,8-dihydroxy-7-methoxy-3-[(2S,3R,4R,5R,6S)-3,4,5-trihydroxy-6-methylxan-2-yl]oxychromen-4-one	[M+H] ⁺	517.01416	C22H22O12	Flavonoid-3-O-glycosides	PTUBUBVQXWVPI-QJCKQCTOSA-N	O=C1C(OC2OC(C)C(O)C2O)=C(OC3=C(C(OC)=CC(O)=C13)C=4C=CC(OC5OC(C)C(O)C(O)C5O)=CC4
466	1.047	259.02002	Carbamazepine	[M+H] ⁺	259.0192	C15H12N2O	Dibenzazepines	FTGPTBGLSHEPO-UHFFFAOYSA-N	N=C(O)N1C=2C=CC=CC2C=CC=3C=CC=CC31
467	1.048	266.9931	Dichlorophen	[M-H] ⁻	266.9985	C13H10Cl2O2	Diphenylmethanes	MDNWOSDZYLHTCG-UHFFFAOYSA-N	C=1C=C(C(=CC2=CC(=C(C=O)C1)=CC1C1)O
468	1.05	149.02304	Phthalic anhydride	[M+H] ⁺	149.02332	C8H4O3	Phthalic anhydrides	LGRFSURHDFAJT-UHFFFAOYSA-N	O=C1OC(=O)C2=CC=CC=C12
469	1.05	189.1597	Propamocarb	[M+H] ⁺	189.15976	C9H20N2O2	Carbamate esters	WZZLXDUDQPOXNW-UHFFFAOYSA-N	CCCOC(=O)NCCN(C)C
470	1.05	325.04221	Uridine 5'-monophosphate	[M+H] ⁺	325.04315	C9H13N2O9P	Pyrimidine ribonucleoside	DJJCXFPVJDGTHFX-UHFFFAOYNA-N	O=C1N=C(O)C=CN1C2OC(COP(=O)(O)O)C(O)C2O
471	1.052	146.11703	Acetylcholine	[M+H] ⁺	146.117	C7H16NO2	Acyl choline	O1PILFWKSMYRGL-UHFFFAOYSA-N	CC(=O)OCC[N+](C)(C)C

472	1.053	357.02502	(E)-1,4-bis(4-hydroxy-3-methoxyphenyl)-2,3-dimethylbut-2-ene-1,4-dione	[M+H] ⁺	357.02454	C20H20O6	Lignans, neolignans and related compounds	ZTNYRNGTBAGY1Z-VAWXSNFSA-N	O=C(C1=CC=C(C(=O)(C(C)=O)C1)C(=C(C(=O)C2=CC=C(C(=O)C)=C2)C)C
473	1.053	225.01572	Xanthotoxol	[M+H] ⁺	225.01601	C11H6O4	8-hydroxy psoralens	JWVYQGERKEAHW-UHFFFAOYSA-N	O=C1OC2=C(O)C=CC3=C2C=C=C1
474	1.074	398.07434	Dysidin	[M+H] ⁺	398.069	C16H22C13N04	N-substituted carboxylic acid imides	PXUALOWHEOKSO-SOXOQJGTS-N	O=C(C=C(C(OC)CC(C)C(C1)C1)C1)N1C(=O)C=C(OC)C1C(C)C
475	1.083	405.00891	Uridine 5'-diphosphate	[M+H] ⁺	405.00946	C9H14N2O12P2	Pyrimidine ribonucleoside	XOCTY1AWTASQJW-XVCMESISA-N	O[C=H]1[C=H](COP(=O)(=O)OP(=O)(O)=O[C=H](1C=H)O)N1C=C(C(=O)=N)C=O
476	1.086	307.04114	Techochrysin	[M+H] ⁺	307.04001	C16H12O4	7-O-methylated flavonoids	IRZVHDLBAYNPT-UHFFFAOYSA-N	O=C1C=C(OC)C2=C(C(OC)C=C(C1)C2)C3=C(C=C)C=C3
477	1.086	565.04608	UDP-D-glucose	[M+H] ⁺	565.04773	C15H24N2O17P2	Pyrimidine nucleotide sugars	HSCJRCJZDFQWQP-JZMIEXBBSA-N	OC[C@H]1O[C@H](OP(=O)(=O)OP(=O)(=O)OC[C@H]2O[C@H](1C=H)(C(=O)N2)N2P(=CC(=O)C(=O)N2)=O)[C@H](O)[C@H](O)[C@H]1O
478	1.088	265.13943	9-hydroxy parthenolide	[M+H] ⁺	265.14001	C15H20O4	Germaconolides and derivatives	RZUCKARTVHQBW-CVZYAWFWSA-N	O=C1OC2C3OC3(C)CCC=C(C)C(O)CC2C1=C
479	1.088	213.02667	Juarezic Acid	[M+H] ⁺	213.03123	C11H10O2	Styrenes	FE1QOMCWGDNMMH-KBXYBYNKSX-N	O=C(O)C=C=C=C1C=CC=C1
480	1.092	185.03188	Glutamine (L)	[M+H] ⁺	185.0323	C5H10N2O3	L-alpha-amino acids	ZDXPYRJPDNTRX-VKHMVHEASA-N	O=C(O)C(N)CCC(=O)O
481	1.094	113.05945	1,4-Cyclohexanedione	[M+H] ⁺	113.0597	C6H8O2	Cyclic ketones	DCZFGQYXRKMVFG-UHFFFAOYSA-N	O=C1CCC(=O)CC1
482	1.095	606.07379	Uridine 5'-diphospho-N-acetylglucosamine	[M+H] ⁺	606.07428	C17H27N3O17P2	Pyrimidine nucleotide sugars	LFTYTUAZOPRMI-CFRASDGFSA-N	CC(=O)N[C@H]1[C@H](OP(=O)(=O)OP(=O)(=O)OC[C@H]2O[C@H](1C=H)(C(=O)N2)N2P(=CC(=O)C(=O)N2)=O)[C@H](O)[C@H](O)[C@H]1O
483	1.096	608.0863	Uridine-5-diphosphoacetylglucosamine	[M+H] ⁺	608.08887	C17H27N3O17P2	Pyrimidine nucleotide sugars	LFTYTUAZOPRMI-UHFFFAOYSA-N	O=C1N=C(O)C=CN1C2OC(COP(=O)(=O)OP(=O)(=O)OC3OC(CO)C(C)C(=O)C3N=C(O)C(C)C(=O)C2O
484	1.1	413.09427	2-amino-5-[2-[[2,3-dihydroxy-2-(1-hydroxyethyl)butanoyl]oxymethyl]-4-hydroxyvanillinol]-5-oxononanoic acid	[M+H] ⁺	413.0943	C18H26N2O9	Glutamine and derivatives	JMRJLJQBHHWY1U-UHFFFAOYSA-N	O=C(O)C(N)CCC(=O)NC1=CC=C(C)C=C1OCC(=O)C(C)C(C)C(C)C(=O)C
485	1.1	127.03925	Dihydro-4,4-dimethyl-2,3-furandione	[M+H] ⁺	127.04007	C6H8O3	Gamma butyrolactones	HRTQFBQOIFEE-UHFFFAOYSA-N	O=C1OCC(C1=O)C(C)C
486	1.101	132.02939	D-ASPARTATE	[M+H] ⁺	132.03	C4H7N04	Aspartic acid and derivatives	CKLJMWTLIZZHCS-UHFFFAOYSA-N	O=C(O)CC(N)C(=O)O
487	1.102	356.08932	Balsalazide	[M+H] ⁺	356.08881	C17H15N3O6	Beta amino acids and derivatives	KONZQJABTUMFX-UHFFFAOYSA-N	O=C(O)C1=CC(=NC2=CC=C(C=C2)C(=O)NCCC(=O)O)C=C1=O
488	1.105	422.1037	(Z)-2-(2-methoxybenzylidene)-9-(pyridin-3-yl)-8,9-dihydro-2H-furo[2,3-f]chromene-3,7-dione	[M+H] ⁺	422.10001	C24H17N05	Aurone flavonoids	FE1HRQSTXZRGQD-JA1QZGSSA-N	O=C1OC2=CC(=C3C(=O)C(OC3=C2C(=C4C=CC(=O)C1)=CC(=O)C=C4)C5=CC=C(C)C=C5
489	1.105	164.09171	N,N-dimethyl-7H-purin-6-amine	[M+H] ⁺	164.09	C7H9N5	6-alkylaminopurines	BV1AQMSVZHOJW-UHFFFAOYSA-N	N1=CN=C(C=NC2=NC12)N(C)C
490	1.106	189.1602	"NEPSILON, NEPSILON, NEPSILON-TRIMETHYL LYSINE"	[M+H] ⁺	189.16	C9H20N2O2	Alpha amino acids	MXNRLFUSFKVQSK-UHFFFAOYSA-N	O=C([O-])C(N)CCCC[N+](C)(C)C(C)C
491	1.106	291.11734	1,2-DIOL	[M+H] ⁺	291.12201	C16H18O5	Diphenylethers	W1OKWEJDRXNVSH-UHFFFAOYSA-N	OC=CC(C(OC)C=C(C1OC=CC(C=C(C(OC)C2O)C)C
492	1.106	723.19165	dimethyl 3,3'-(2,5-dihydroxy-3,6-dioxocyclohexa-1,4-diene-1,4-diyl)bis(3-(3-methoxy-4-(2-methoxy-2-oxoethoxy)phenyl)propanoate)	[M+H] ⁺	723.19	C34H36O16	Dalbergiones	CH1GK1GFBZGFG-UHFFFAOYSA-N	O=C(OC)CCC1=CC=C(C=C1OC)C(C=C2)C(=O)C(=O)C(C2O)C(C3=C(C(=O)C(OC)C(C(OC)=C3)C(C(=O)O)C)C(=O)O
493	1.108	146.11807	DEOXYCARNITINE	[M+H] ⁺	146.12	C7H15N02	Straight chain fatty acids	JHPNVN1EXLNTX-UHFFFAOYSA-N	O=C([O-])CCC[N+](C)(C)C(C)C
494	1.108	382.08154	Metsulfuron-methyl	[M+H] ⁺	382.08157	C14H15N5O6S	Benzoic acid esters	RSMUVRMZCOLBH-UHFFFAOYSA-N	COC(=O)C1=CC=C(C=C1S(=O)(=O)N=C(N)C1=CC=C(C)C(=O)N1C=CC(=O)C=C1S(=O)(=O)N=C(N)C1=CC=C(C)C(=O)N1
495	1.108	139.05795	Salicylic Acid	[M+H] ⁺	139.05215	C2H6H4O9	Medium-chain fatty acids	M1NDH1VHJZYEER-HBBSNRFSA-N	O=C(O)CCCCCCCC(=O)C=C(C

515	1.123	504.18906	1,1'-azanediylibis(3-methyl-2H-naphtho[1,2,3-de]quinoline-2,7(3H)-dione) triacetate	[M+H] ⁺	504.19	C40H33N3O10	Anthracenes	VVA1GFCJFBXWBL-UHFFFAOYSA-N	O=C(O)C, O=C(O)C, O=C(O)C, O=C1C=2C=CC=CC2=C3C(NC=4C(=O)N(C=5C=CC=C6C(=O)C=7C=C(C=C7C4)C65)C1)C(=8C=C(C=C1)C8
516	1.123	251.05205	Perseitol	[M+H] ⁺	251.0528	C7H1607	Sugar alcohols	OXQKEKGBFMQTML-UHFFFAOYSA-N	OC(C)(O)C(C)(O)C(C)(O)CO
517	1.124	483.10959	Parishin E	[M+H] ⁺	483.10999	C19H24013	Phenolic glycosides	XAIUTKLNZBMEG-UHFFFAOYSA-N	O=C(O)CC(O)C(C(=O)O)CC(=O)OCC1=CC=C(C(=O)C(C)(O)C2=O)C=C1
518	1.125	367.13229	(3E,12E)-3,12-dimethyl-8-methylidene-6,18-dioxatricyclo[14.2.1.0 ^{2,9}]nonadeca-3,12,16(19)-triene-7,17-dione	[M+H] ⁺	367.13062	C20H2404	Diterpene lactones	KTYZXFERQUCPX-SPUCVAIDSA-N	O=C1OC2C=C1CCC=C(C)CCC3(C=C(C)O)OC3=C(C)C2
519	1.125	305.08261	5,7-dimethoxy-2-phenyl-4H-chromen-4-one	[M+H] ⁺	305.07999	C17H1404	7-O-methylated flavonoids	JRFZSUMZAHNSL-UHFFFAOYSA-N	O=C1C=C(C(=C2=CC(O)C=CC(=C2)C=3C=CC=CC3
520	1.125	257.08453	Flavan-3-ols + 30	[M+H] ⁺	257.082	C15H1405	Flavanol O-glycosides	RSYUFYQIACJFML-DDOUPSRJNA-N	OC1=CC=C(C=C1)C3OC=2C=C(O)C=C(O)C=2C3(O)
521	1.125	321.05811	fuzhuanin A	[M+H] ⁺	321.05899	C15H1208	1-benzopyrans	QCFAYXITEXFSLB-QMTHXVAHSA-N	O=C(O)C=1OC(=O)C=C(C1)C2OC=3C=C(O)C=C(O)C3CC2O
522	1.125	616.20166	JACAGLABROSIDE B	[M+2H] ²⁺	616.20245	C30H30013	Saccharolipids	A1FVFGWRWAMEB-GSQIIVKLSA-N	O=C1C=CC(O)C(C=C1)CC(=O)OC2OC(OC(=O)CC3(O)C=CC(=O)C=C3)C(OC(=O)C=C4C=CC=C4)C(C)C2O
523	1.127	146.09229	4-Guanidinobutanoic acid	[M+H] ⁺	146.09239	C5H11N302	Gamma amino acids and derivatives	TUHVJAJIMEOSA-UHFFFAOYSA-N	C(CC(=O)O)CNC(=N)N
524	1.127	221.04111	4-hydroxy-3,5-dimethoxybenzoic acid	[M+Na] ⁺	221.03999	C9H1005	Galic acid and derivatives	JMSVCTVWECHDZ-UHFFFAOYSA-N	O=C(O)C1=CC(OC)=C(O)C(OC)=C1
525	1.128	445.1189	baicalin	[M+H] ⁺	445.12244	C21H18011	Flavonoid-7-O-glucuronides	IKTI1ZLYTISPEN-ZFORQUDYSA-N	O=C(O)C1OC(OC=2C=3OC(=CC(=O)C3=C(O)C2O)C=4C=CC=CC4)C(C)(O)C1O
526	1.128	112.05007	Cytosine	[M+H] ⁺	112.05054	C4H5N303	Pyrimidones	OPTASPLRGRNAP-UHFFFAOYSA-N	Clcnc([nH]c1=N)O
527	1.128	604.06958	Guanosine 5'-diphosphate-D-mannose	[M+H] ⁺	604.06989	C16H25N5O16P2	Purine nucleotide sugars	MMVSCBBUIHUTGJ-GDJBKNASNA-N	OC[C@H]1O[C@H](OP(O)(=O)OP(O)(=O)OC[C@H]2O[C@H](C=C1)C(=O)C=C2)N2C=CC3=C2NC(=N)N=C3O[C@H]1O
528	1.128	193.07103	Methyl-beta-galactopyranoside	[M+H] ⁺	193.07176	C7H1406	O-glycosyl compounds	HOVAGTYPOGVJG-UHFFFAOYNA-N	OC[C@H](O)C(C)(O)C1O
529	1.13	522.20026	(2S,3S)-3-hydroxy-2-((S)-2-((S)-2-(2-hydroxy-4-oxoquinazolin-3(4H)-yl)-3-(H-indol-3-yl)propanamido)propanamido)butanoic acid	[M+H] ⁺	522.20001	C26H27N507	Oligopeptides	JZZOGGANLZATZ-1MSL1LBVSA-N	O=C(O)C(NC(=O)C(NC(=O)C(NC(=O)C=2C=CC(=C2)N1)CC3=CN(C=4C=CC=CC4)C1)C1O
530	1.131	380.09595	Atalaphylline	[M+H] ⁺	380.09744	C23H25N04	Acridones	GLXYKTAS1IUSRC-UHFFFAOYSA-N	O=C1C=2C=CC=C(O)C2N3=C1C1(O)=C(C(=O)C=3CC=C(C)C)CC=C(C)C1
531	1.132	462.17926	Morphine_3_Glucuronide	[M+H] ⁺	462.17587	C23H27N09	Morphinans	WAEXKFNHRHFBZ-UHFFFAOYNA-N	CN1CC23C4OC5=C(OC6OC(C)(O)C(O)C6O)C(O)=O=C(OC1C2C=C4O)=C35
532	1.132	151.06015	Xylitol	[M+H] ⁺	151.0612	C5H1205	Sugar alcohols	HEBCKHPVO1AQTA-UHFFFAOYNA-N	OC(C)(O)C(C)(O)CO
533	1.133	253.0808	Osthenol	[M+H] ⁺	253.08	C14H1403	7-hydroxycoumarins	RAKJVIPCCGXHHS-UHFFFAOYSA-N	O=C1OC2=C(C=C1)C=CC(O)=C2OC=C(C)C
534	1.133	219.02779	THEOBROMINE	[M+H] ⁺	219.02788	C7H8N402	Xanthines	YAPQBXVYLJRXSA-UHFFFAOYSA-N	O=C1N=C(O)C2=C(N=CN2)N1C
535	1.133	203.05363	Theophylline	[M+H] ⁺	203.05	C7H8N402	Xanthines	ZFXYPBG1UFBOJW-UHFFFAOYSA-N	O=C1C=2NC=NC2N(C(=O)N1)C
536	1.133	149.04483	Xylose	[M+H] ⁺	149.04555	C5H1005	Pentoses	PYMPYHUWUMLA-VPENIKCSA-N	O=CC(O)C(O)C(O)CO
537	1.134	400.14685	2,6-dihydroxy-3-mesityl-5-(1,2,3,4-tetrahydroisoquinolin-1-yl)pyrimidin-4(3H)-one	[M+H] ⁺	400.14999	C22H23N303	Tetrahydroisoquinolines	IO1BYVJO1SLAKR1-UHFFFAOYSA-N	O=C1C(=C(O)N=C(O)N1C=2C(=CC(=C2)C)C)C3NCCC=4C=CC=CC43
538	1.135	221.06551	Ethyl-beta-glucuronide	[M+H] ⁺	221.06668	C8H1407	O-glucuronides	1WJBMVJWSFZNJH-UHFFFAOYNA-N	O=C(O)C1OC(OC)C(O)C(C)C1O
539	1.136	274.1871	4-hydroxy-2-octylquinoline 1-oxide:Series 4 HAQ C8	[M+H] ⁺	274.18201	C17H23N02	4-hydroxy-2-alkylquinolines	UKKYWOFQJOMYIL-UHFFFAOYSA-N	O=N1C=2C=CC=CC2(C)=CC1CCCCCCC
54									

558	1. 145	275. 12375	L-Saccharopine	[M-H] ⁻	275. 12485	C11H20N2O6	Glutamic acid and derivatives	ZDGJAHTZVHLOT-YUMQZZPRSA-N	N[C-H] (CCCCN[C-H] (CCC(O)=O) C(O)=O) C(O)=O
559	1. 147	317. 11499	Heptelidic acid chlorohydrin 130129	[M+H] ⁺	317. 11499	C15H21ClO5	Terpene lactones	BJGUEPXNQBVBW-RTWAVKEYSA-N	O=C(O) C1=CC2C(C(=O)OC1) C(O) (CC1) CCC2C(C) C
560	1. 152	191. 01877	ISOCITRIC ACID	[M-H] ⁻	191. 019	C6H8O7	Tricarboxylic acids and derivatives	ODBLHEXUDAPZAU-UHFFFAOYSA-N	O=C(O) CC(C(=O)O) C(O) C(=O)O
561	1. 152	208. 1178	Miglitol	[M+H] ⁺	208. 11795	C8H17NO5	Piperidines	IBAQQPQHRJAVAV-UHFFFAOYNA-N	OCCN1CC(O) C(O) C(O) C1CO
562	1. 153	179. 05449	Glucanolactone	[M+H] ⁺	179. 05501	C6H10O6	Glucanolactones	PHQVHQSTUBQKQ-UHFFFAOYNA-N	O=C1OC(O) C(O) C(O) C1O
563	1. 156	163. 05965	1,6-Anhydro-beta-D-glucose	[M+H] ⁺	163. 0601	C6H10O5	Oxepanes	TWN1BLMWSKIRAT-VFUOTHLCSA-N	O[C-H] 1[C-H] 2CO[C-H] (O2) [C-H] (O) [C-H] 1O
564	1. 156	435. 08917	Irisaxanthone	[M-H] ⁻	435. 09329	C20H20O11	Xanthones	MTQVPZUBZBTLNO-HSLVGEKZSA-N	O=C1C2=CC=C(O) C(OC)=C2OC3=CC(O)=C(C(O)=C13) C4OC(CO) C(O) C(O) C4O
565	1. 157	233. 04103	2-pyridin-3-yl-thiazolidine-4-carboxylic acid	[M+H] ⁺	233. 03999	C9H10N2O2S	L-alpha-amino acids	FSNGLHIMQHWTFN-JGVFFNPUSA-N	O=C(O) C1NC(SC1) C=2C=NC=CC2
566	1. 158	180. 08737	Galactosamine	[M+H] ⁺	180. 08665	C6H13NO5	Hexoses	MSWZFWKMSRAUBD-UHFFFAOYNA-N	OCC1OC(O) C(N) C(O) C1O
567	1. 158	97. 02883	Propionic acid	[M+H] ⁺	97. 03	C3H6O2	Carboxylic acids	XBQKXXY1PTUBI-UHFFFAOYSA-N	O=C(O) CC
568	1. 159	184. 05969	4-PYRIDOXATE	[M+H] ⁺	184. 06	C8H9NO4	Pyridinecarboxylic acids	HXACOUQ1XZGNBF-UHFFFAOYSA-N	O=C(O) C1=C(O) C(=NC=C1CO) C
569	1. 161	298. 15143	(3aS,8aR)-1,3a,8-trimethyl-1,2,3,3a,8,8a-hexahydropyrrolo[2,3-b]indol-5-yl methylcarbamate	[M+H] ⁺	298. 14999	C15H21N3O2	Pyrroloindoles	PIJJDFTBXTXHHH-HI FRSDPNSA-N	O=C(OC1=CC=CC(=C1) C3(C) CCN(C) C3N2C) NC
570	1. 161	423. 08878	5-hydroxy-6,8-dimethoxy-7-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxychromen-2-one	[M+H] ⁺	423. 08978	C17H20O11	Coumarin glycosides	KDWYRFBEPULRG-KIZWGMFSA-N	O=C1OC=2C(OC)=C(OC3OC(CO) C(O) C(O) C3O) C(OC)=C(O) C2C=C1
571	1. 162	166. 01382	"PYRIDINE-2,3-DICARBOXYLATE"	[M-H] ⁻	166. 01401	C7H5NO4	Pyridinecarboxylic acids	GJAWHXHKYXBSV-UHFFFAOYSA-N	O=C(O) C1=NC=CC=C1C(=O)O
572	1. 163	256. 08228	Caramboxin	[M+H] ⁺	256. 082	C11H13NO6	Phenylalanine and derivatives	DYJJDGJHOLTGBO-ZETCQYMISA-N	O=C(O) C1=C(O) C=C(OC) C=C1CC(N) C(=O)O
573	1. 164	241. 04602	7,8-dimethylalloxazine (lumichrome)	[M-H] ⁻	241. 04625	C12H10N4O2	Flavins	ZJTJUVIJVLGSP-UHFFFAOYSA-N	OC=1N=C(O) C=2N=C3C=C(C(=CC3=NC2N1) C) C
574	1. 169	170. 10217	ADONITOL	[M+H] ⁺	170. 10229	C5H12O5	Sugar alcohols	HEBKCHPVO1AQTA-UHFFFAOYSA-N	OCC(O) C(O) C(O) CO
575	1. 169	414. 1597	narcotine	[M+H] ⁺	414. 16	C22H23NO7	Phthalide isoquinolines	AKNNEG1BPJZJG-MSOLQXFVSA-N	O=C1OC(C2=CC=C(OC) C(OC)=C12) C3C4=C(OC) C=5OCOC5C=C4CCN3C
576	1. 17	349. 08817	(E)-3-[2-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyphenyl]propan-2-enoic acid	[M+H] ⁺	349. 08939	C15H18O8	Phenolic glycosides	GVRIYIMJGULCZ-ZMKUSUEASA-N	O=C(O) C=C=C1CC=CC(OC1OC2OC(CO) C(O) C(O) C2O
577	1. 171	350. 0845	2-(2,6-dihydroxy-4-methoxycarbonylbenzoyl)-3-hydroxybenzoic acid	[M+H] ⁺	350. 08704	C16H12O8	Benzophenones	QQRQIRHJXTGCW-UHFFFAOYSA-N	O=C(O) C=C1C=CC=C(O) C1C(=O) C2=C(O) C(=O) C(=C2O) C(=O) OC
578	1. 171	330. 0582	3',5'-Cyclic AMP	[M+H] ⁺	330. 05978	C10H12N5O6P	3',5'-cyclic purine nucleotides	IVOMOUHDPKRL-LKQYXXCUSA-N	NC1=C2N=CN([C-H] 3O[C-H] 3O[C-H] 4COP(O)(=O)O[C-H] 4[C-H] 3O) C2=NC(=N) 1
579	1. 171	200. 11229	Pyrimethanil	[M+H] ⁺	200. 11823	C12H13N3	Aniline and substituted anilines	ZLIBICFPKPGIZ-UHFFFAOYSA-N	CC1=CC(C)=CC(=CC=C1C) C(=O)O
580	1. 176	409. 17883	Beclomethasone	[M+H] ⁺	409. 17801	C22H29ClO5	21-hydroxysteroids	NEMKJDKGKEAPL-WOOFSPWISA-N	O=C1C=CC2(C(=C1) CCC3C4CC(C) C(O) C(=O) C4) C(C) CC(O) C3CC21) C
581	1. 178	129. 01866	4-Amino-2-chloropyridine	[M+H] ⁺	129. 02141	C5H5ClN2	Aminopyridines and derivatives	BLBDTBGCPHPLJK-UHFFFAOYSA-N	NC1=CC(C1)=NC=C1
582	1. 178	251. 03645	Bisphenol S	[M+H] ⁺	251. 03726	C12H10O4S	Benzenesulfonyl compounds	VFPWNQTHUCYWMVZ-UHFFFAOYSA-N	C=1C=C(C(=CC1O) S(C2=CC=C(C(=C2)O) (=O)O
583	1. 179	242. 06512	1-(2-((1H-indol-3-yl)ethyl)thiourea	[M+H] ⁺	242. 07001	C11H13N3S	3-alkylindoles	HRBGONPRSGPFMT-UHFFFAOYSA-N	S=C(N) NCCC1=CC=CC=C1C=CC2C1
584	1. 18	243. 09708	beta-lapachone	[M+H] ⁺	243. 097	C15H14O3	Naphthopyranones	QZPQTZNNJUOLS-UHFFFAOYSA-N	O=C1C(=O) C2=C(OC(C) C(O) C2) C=3C=CC=CC13
585	1. 182	248. 11403	1-Isothiocyanato-9-(methylsulfinyl)-nonane	[M+H] ⁺	248. 11374	C11H21NOS2	Sulfoxides	MQFLXLMNOHPTC-UHFFFAOYNA-N	CS(=O) CCCCCCCCCN=C=S
586	1. 183	300. 12726	Lotaustalin	[M+H] ⁺	300. 12491	C11H19NO6	Cyanogenic glycosides	WEWBVMVTOYUPHH-GXUZXPEDSA-N	N#CC(OC1OC(CO) C(O) C(O) C1O) (C) CC
587	1. 185	275. 09473	(2R)-8-ethyl-7-hydroxy-5-methoxy-2-methyl-3,4-dihydrochromen-4-one	[M+H] ⁺	275. 09579	C13H16O4	Chromones	BPTMO1WHAHUBPJ-SSDOTTSWSA-N	O=C1C=2C(OC)=CC(O)=C(C2OC(C) C1) CC
588	1. 185	73. 02811	PROPENOIC ACID	[M+H] ⁺	73. 0284	C3H4O2	Acrylic acids	NIXOWILLQJLNCW-UHFFFAOYSA-N	OC(=O) C=C
589	1. 187	213. 05269	2,4-Dihydroxybenzophenone	[M-H] ⁻	213. 05573	C13H10O3	Benzophenones	ZXDDPOHVAWLBH-UHFFFAOYSA-N	C1=CC=C(C(=C1) C) C=2C=CC(=CC2O) O=O
590	1. 19	318. 12933	ethyl 3-(2,4-dihydroxy-6-methylpyridin-3-yl)-3-(3-hydroxyphenyl)propanoate	[M+H] ⁺	318. 13	C17H19NO5	Pyridinones	YKJXWYJQVADMO-UHFFFAOYSA-N	O=C(OC) CC(C(=1C=CC(O) C1) C2=C(O) N=C(C=2O) C
591	1. 191	244. 12846	Agomelatine	[M+H] ⁺	244. 133	C15H17NO2	N-acetyl-2-arylethylamines	YJYPHIXNFPHND-UHFFFAOYSA-N	O=C(NCCC1=CC=CC2=CC=C(OC) C=C21) C
592	1. 191	320. 14288	Norfloxacin (Norxacin)	[M+H] ⁺	320. 14099	C16H18FN3O3	Quinoline carboxylic acids	OGJPXUAPXNRGGI-UHFFFAOYSA-N	O=C(O) C1=CN(C2=CC(=C(F) C=C2C1=O) N3CCNCC3) CC
593	1. 191	172. 09665	terrein	[M+H] ⁺	172. 09682	C8H10O3	1,2-diols	MHOOPNKRBMHEC-HZIBQTDNSA-N	O=C1C=C(C=CC) C(O) C1O
594	1. 192	231. 02568	3-[(1-Carboxyvinyl)oxy]benzoic acid	[M+H] ⁺	231. 02638	C10H8O5	Phenoxyacetic acid derivatives	HGVAHYJMDVROLE-UHFFFAOYSA-N	O=C(O) C(OC1=CC=CC(=C1) C(=O)O) O=C
595	1. 192	175. 04327	4-Methylumbelliferone	[M-H] ⁻	175. 04201	C10H8O3	7-hydroxycoumarins	HSIN1TRMYLLCV-UHFFFAOYSA-N	O=C1OC=2C=C(O) C=CC2(=C1) C
596	1. 192	217. 11894	5-isopropenyl-2-methyl-2-cyclohexen-1-yl acetate	[M+H] ⁺	217. 12	C12H18O2	Menthane monoterpeneoids	YTHRBOFHYZBZBJ-VXGBAGGSA-N	O=C(OC1C(=O) C(=CC(C(=C) C1) C) C
597	1. 193	333. 04517	Methoxyhaemantosine	[M-H] ⁻	333. 04999	C16H14O8	Isochromanquinones	WPHIVUBMBWBSCK-SPHRHQWCSA-N	O=C1OC(C) C(OC) C2=C(O) C=CC(O) C(OC)=CC(=O) C3C(O) C=C12
598	1. 194	283. 09113	2-(5-formyl-3,4-dihydro-2,2-dimethyl-2H-pyran-6-yl)-Benzoic acid	[M+H] ⁺	283. 091	C15H14O3	Naphthopyranones	QZPQTZNNJUOLS-UHFFFAOYSA-N	O=C1C(=O) C2=C(OC(C) C(O) C2) C=3C=CC=CC13
599	1. 194	150. 05768	Methionine	[M+H] ⁺	150. 058	C5H11NO2S	Methionine and derivatives	FFEARJCKVFRZRR-UHFFFAOYSA-N	O=C(O) C(N) CCSC
600	1. 195	273. 07199	5-Hydroxymethyluridine	[M-H] ⁻	273. 07281	C10H14N2O7	Pyrimidine nucleosides	VQAJJNQKTRZJQ-UHFFFAOYNA-N	O=C1N=C(O) C(=CN1C2OC(CO) C(O) C2O) CO

[illegible]

644	1. 22	269. 15915	sophocarpine	[M+H] ⁺	269. 16	C15H22N2O	Matrine alkaloids	AAGPPTSOPGCNQ-KYEXDWHISA-N	O=C1C=CCC2N1CC3CCCN4CCCC2C43
645	1. 221	213. 12245	Prolylproline	[M+H] ⁺	213. 12489	C10H16N2O3	Dipeptides	RWCOTTLHDJWHRS-UHFFFAOYNA-N	O=C(O)C2N(C(=O)C1NCCC1)CCC2
646	1. 223	344. 03741	"GUANOSINE 3', 5'-CYCLIC MONOPHOSPHATE"	[M-H] ⁻	344. 04001	C10H12N5O7P	3', 5'-cyclic purine nucleotides	ZOOGRGPOEVQX-UOQKFMHZA-N	O=C1N=C(N)NC2=C1N=CN2C3OC4COP(=O)(O)OC4C3O
647	1. 223	247. 05748	Haematomic Acid, Ethyl Ester	[M+H] ⁺	247. 05769	C11H12O5	p-Hydroxybenzoic acid alkyl esters	HUXJGSHUVDWZAM-UHFFFAOYSA-N	O=CC1=C(O)C=C(C(=O)OC)C=C1O
648	1. 225	163. 06049	2-DEOXY-D-GLUCOSE	[M-H] ⁻	163. 061	C6H12O5	Fatty alcohols	VRALKFPQXWPIH-UHFFFAOYSA-N	O=CCC(O)C(O)C(O)CO
649	1. 225	391. 17041	Pseudolaric Acid C	[M+H] ⁺	391. 17001	C21H26O7	Diterpene lactones	RBXVTEUAOTYME-GPGKBOPFSA-N	O=C(O)C(=CC=CC1(OC(=O)C2CCC(=C(C(=O)OC)CCC3(O)C1CC2)C)C
650	1. 226	375. 17523	3-[(E)-3, 4-dihydroxy-3, 5-dimethylhept-1-enyl]-7, 8-dihydroxy-7-methyl-8, 8a-dihydro-1H-isochromen-6-one	[M+H] ⁺	375. 1778	C19H28O6	Azaphilones	ZMOXNUGJSHBRR-VOTSOKGWSA-N	O=C1C=C2C=C(OC2CC(O)C1(C)C)C=CC(O)C(C)C(C)CC
651	1. 226	241. 1554	Alpha Cyperone	[M+Na] ⁺	241. 14999	C15H22O	Eudesmane, isoeudesmane or cycloesudesmane	KUFXJZXMWHNCEH-DOMZBBRYSA-N	O=C1C(=C2CC(C(=C)C)CCC2(C)CC1)C
652	1. 228	308. 09705	N-ACETYLNEURAMINATE	[M-H] ⁻	308. 09799	C11H19NO9	N-acylneuraminic acids	SQVRNKLJHWKZAKO-UHFFFAOYSA-N	O=C(O)C1(O)OC(C(O)C(O)CO)C(NC(=O)C)C(O)C1
653	1. 229	160. 06078	ALPHA-AMINOADIPATE	[M-H] ⁻	160. 061	C6H11NO4	L-alpha-amino acids	OY1FNHCXNCRBQ1-BYPYZUCNSA-N	O=C(O)CCCC(N)C(=O)O
654	1. 229	178. 04991	HIPPURATE	[M-H] ⁻	178. 05	C9H9NO3	Hippuric acids	QIAPMBKCNZACKA-UHFFFAOYSA-N	O=C(O)CNC(=O)C=1C=CC=CC1
655	1. 23	280. 10553	1-Methyladenosine	[M-H] ⁻	280. 10513	C11H15N5O4	Purine nucleosides	GFYLSDSUHVORB-UHFFFAOYNA-N	N=C1C=2N=CN(CN=CN1C)C3OC(CO)C(O)C3O
656	1. 23	306. 08517	PFSM-ammonio_N_CMAmP_FT_FOSA	[M-H] ⁻	306. 08667	[C9H18F3N2O4S] ⁺	PFSA	UBADCKSMADBWHM-UHFFFAOYSA-O	O=C(O)CC[N+](C)(C)CCCN3(=O)(=O)C(F)(F)F
657	1. 231	116. 03471	N-ACETYLGLYCINE	[M-H] ⁻	116. 035	C4H7NO3	N-acyl-alpha amino acids	OKJIRPAQVSHGFK-UHFFFAOYSA-N	O=C(O)CNC(=O)C
658	1. 232	298. 11313	7-Methylguanosine	[M+H] ⁺	298. 11404	C11H16N5O5	Purine nucleosides	OGHAROSJZRT1OK-UHFFFAOYNA-O	N=C1N=C(O)C2=C(N1)N(C=[N+](2C)C3OC(CO)C(O)C3O
659	1. 232	68. 05067	Pyrrol	[M+H] ⁺	68. 04948	C4H5N	Heteroaromatic compounds	KAESVJQAVNADME-UHFFFAOYSA-N	C=1C=CNC1
660	1. 235	321. 04709	THYMIDINE 5'-MONOPHOSPHATE	[M-H] ⁻	321. 04901	C10H15N2O8P	Pyrimidine 2' - deoxynucleoside	GYZOZYVXFNDGLJ-UHFFFAOYSA-N	O=C1NC(=O)N(C=C1C)C2OC(COP(=O)(O)O)C(O)C2
661	1. 237	273. 06055	Pesticide3_Neburon_C12H16C12N2O_Urea_N-butyl-N-(3, 4-dichlorophenyl)-N-methyl-	[M-H] ⁻	273. 05701	C12H16C12N2O	N-phenylureas	CCPGUMWYLI1CGL-UHFFFAOYSA-N	C1C1=CC=C(N=C(O)N(C)CCCC)C=C1C1
662	1. 238	363. 06802	Esculin	[M+H] ⁺	363. 07001	C15H16O9	Coumarin glycosides	XHCADAYNF1FUHF-TVKJYDYSA-N	O=C1OC=2C(O)C(OC3OC(CO)C(O)C(O)C3O)=CC2C=C1
663	1. 239	212. 09132	isoferulic acid	[M+H] ⁺	212. 09174	C10H10O4	Hydroxycinnamic acids	QURCYMIEKCOAJU-HWKANZROSA-N	O=C(O)C=CC1=CC=C(OC)C(O)=C1
664	1. 24	542. 14038	(S, Z)-2-((2-(3, 4-dimethoxybenzylidene)-3-oxo-2, 3-dihydrobenzofuran-6-yl)oxy)acetamido]-3-(4-hydroxyphenyl)propanoic acid	[M+H] ⁺	542. 14001	C28H25NO9	Tyrosine and derivatives	ZOLBQWQZBEHMY-CLVGAISSA-N	O=C(O)C(NC(=O)CC1=CC=C2C(=O)C(OC2=C1)=CC3=CC=C(OC)C(O)C(=C3)CC4=CC=C(O)C=C4
665	1. 24	300. 1174	Octopamine, N-p-coumaroyl-	[M+H] ⁺	300. 12	C17H17NO4	Styrenes	VATOSFCFM0AIX-XCYCLJG0SA-N	O=C(C=CC1=CC=C(O)C=C1)NCC(O)C2=CC=C(O)C=C2
666	1. 242	233. 14844	Threonylleucine (isomer of 925, 926)	[M+H] ⁺	233. 1485	C10H20N2O4	Dipeptides	BQBC1BCLXBKYHW-UHFFFAOYNA-N	O=C(O)C(NC(=O)C(N)C(O)C)CC(C)C
667	1. 243	108. 04404	2-Aminophenol	[M+H] ⁺	108. 04549	C6H7NO	Aniline and substituted anilines	CDAWCLQXVUBKRW-UHFFFAOYSA-N	OC=1C=CC=CC1N
668	1. 243	263. 0542	maclurin	[M+H] ⁺	263. 06	C13H10O6	Benzophenones	XNWPXDGRBWJ1ES-UHFFFAOYSA-N	O=C(C1=CC=C(O)C(O)=C1)C=2C(O)=CC(O)=CC2O
669	1. 244	297. 10928	4-hydroxy-8-methoxy-5-methyl-3-(3-methylbut-2-enyl)chromen-2-one	[M+H] ⁺	297. 10971	C16H18O4	4-hydroxycoumarins	YPKUMLVKFVYOT-UHFFFAOYSA-N	O=C1OC2=C(OC)C=CC(=C2(O)=C1CC=C(C)C)C
670	1. 244	201. 08812	Methyleugenol	[M+H] ⁺	201. 09	C11H14O2	Dimethoxybenzenes	ZYEMGP1YFJGTP-UHFFFAOYSA-N	O(C1=CC=C(C(=1OC)CC=C)C
671	1. 245	133. 04996	DEOXYRIBOSE	[M-H] ⁻	133. 05	C5H10O4	Beta-hydroxy aldehydes	ASJSAQ1RZKANQN-UHFFFAOYSA-N	O=CCC(O)C(O)CO
672	1. 25	171. 02905	3-DEHYDROSHIKIMATE	[M-H] ⁻	171. 02901	C7H8O5	Cyclohexenones	SLWJWJZMPHJJOPI-PHDIDXHISA-N	O=C(O)C1=CC(=O)C(O)C(O)C1
673	1. 25	155. 0811	Cyclo-prolylglycine	[M+H] ⁺	155. 0815	C7H10N2O2	Amino acids	OWOHLURDBZHNGG-UHFFFAOYNA-N	O=C1CNC(=O)C2CCCN12
674	1. 25	215. 10204	LEVODOPA	[M+H] ⁺	215. 10263	C9H11NO4	Tyrosine and derivatives	WTDROQBEARIYVC-LURJTMIESA-N	O=C(O)C(N)CC1=CC=C(O)C(O)=C1
675	1. 25	154. 04971	N-(2, 5-dioxocyclopentyl)acetamide	[M-H] ⁻	154. 049	C7H9NO3	Beta-diketones	QVZXVWBZHYCGL-UHFFFAOYSA-N	O=C1CCC(=O)C1N=C(O)C
676	1. 252	283. 13013	(2S, 8R)-8-hydroxy-2-[(1S)-1-hydroxyheptyl]-2, 3, 4, 6, 7, 8-hexahydrochromen-5-one	[M+H] ⁺	283. 13016	C16H26O4	Benzopyrans	INHVP1PHEJQOP-ZNMIVQWSA-N	O=C1C2=C(OC(C2)C(O)CCCCC)C(O)CC1
677	1. 257	271. 04425	alternariol monomethyl ether	[M-H] ⁻	271. 04236	C15H12O5	Coumarins and derivatives	LCSQDFNUYFTXMT-UHFFFAOYSA-N	O=C1OC2=CC(O)=CC(=C2C3=CC(OC)=CC(O)=C13)C
678	1. 257	411. 09671	Artemitin	[M+H] ⁺	411. 10001	C20H20O8	7-O-methylated flavonoids	RIGYMJVPEJNCKD-UHFFFAOYSA-N	O=C1C(OC)=C(OC=2C=C(OC)C(OC)=C(O)C12)C=3C=CC(OC)=C(OC)C3
679	1. 257	388. 12189	fraxin	[M+H] ⁺	388. 12381	C16H18O10	Coumarin glycosides	CRSFLLTWRCYXNK-QBNNVSCSA-N	O=C1OC=2C(OC3OC(CO)C(O)C(O)C3O)=C(O)C(OC)=CC2C=C1
680	1. 258	229. 03406	Asulam	[M-H] ⁻	229. 02885	C8H10N2O4S	Aminobenzenesulfonamides	VGPYEIKOIGJKV-UHFFFAOYSA-N	OC(O)=NS(=O)(=O)C1=CC=C(N)C=C1
681	1. 264	423. 19849	N-Fructosyl isoleucylglutamate	[M+H] ⁺	423. 1994	C17H30N2O10	N-Fructosyl peptides	OJDUYMYADCXNAN-UHFFFAOYNA-N	O=C(O)CCC(NC(=O)C(NCCT(O)(OC(CO)C(O)C1(O)C)C(C)C)C(=O)O
682	1. 265	274. 05573	Flufenacet ESA	[M-H] ⁻	274. 05548	C11H14FN04S	Anilides	SZCMHDLQVYZYST-UHFFFAOYSA-N	CC(C)N(C(O)CS(O)=(O)=O)C1=CC=C(F)C=C1
683	1. 266	229. 08144	Dihydroresveratrol	[M-H] ⁻	229. 08702	C14H14O3	Stilbene glycosides	H1TJFUSPLYBJPE-UHFFFAOYSA-N	OC1=CC=C(C=C1)CCC2=CC(O)=CC(O)=C2
684	1. 268	403. 1062	2-[3-ethenyl-5-methoxycarbonyl-2-[(2S, 3R, 4S, 5S, 6R)-3, 4, 5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy-3, 4-dihydro-2H-pyran-4-yl]acetic acid	[M-H] ⁻	403. 10376	C17H24O11	Terpene glycosides	MQLSOVRLZHTATK-WNCYHATQSA-N	O=C(O)CC1C=CC(OC2OC(CO)C(O)C(O)C2O)C1C=C(C(O)OC
685	1. 271	453. 13568	bungeiside C	[M+H] ⁺	453. 13672	C19H26O11	Phenolic glycosides	YQOKGDRMWQLQNR-BMWMOQRNSA-N	O=C(C1=CC=C(OC2OC(COC3OC(CO)C(O)C3O)C(O)C(O)C2O)C=C1)C
686	1. 271	303. 0462	Flavanone base + 50	[M-H] ⁻	303. 0498	C15H12O7	Flavanone 0-glycosides	CXQWRCVTOMQVX-UHFFFAOYNA-N	O=C2C3=C(O)C=C(O)C=C3(OC(C1C=CC(O)=C(O)C=C1)C2(O))

[illegible]

730	1.361	425.1936	2-[5-[2-[2-[5-(2-hydroxypropyl)oxolan-2-yl]propanoyloxy]propyl]oxolan-2-yl]propanoic acid	[M+H] ⁺	425.1936	C20H3407	Dicarboxylic acids and derivatives	V1HRKOVWCGJQP-UHFFFAOYSA-N	O=C(O)C(C)C1OC(C(C)C)CC(OC(=O)C(C)C)C2OC(C(C)C)C(C)C
731	1.361	415.17322	6-formyl-10-(hydroxymethyl)-5-methoxy-3-methylidene-2-oxo-2H,3H,3aH,4H,5H,8H,9H,11aH-cyclodecab[h]furan-4-yl 2-methylbutanoate	[M+H] ⁺	415.1727	C21H2807	Germacranolides and derivatives	LOFBWESBEBUNJU-FRYCYAQMISA-N	O=CC1=CCCC(=C2OC(=O)C(=C)C)C2C(OC(=O)C(C)C)C1OC)CO
732	1.361	204.12425	Isopentenyladenine	[M+H] ⁺	204.12437	C10H13N5	6-alkylaminopurines	HYVABZ1GRDEKCD-UHFFFAOYSA-N	N=1C=NC=2C1NC=NC2NCC=C(C)C
733	1.363	331.06491	Gallic acid hexoside	[M-H] ⁻	331.06491	C13H16O10	Phenolic glycosides	GDVRUDXLQBVIKP-UHFFFAOYNA-N	O=C(OC1OC(CO)C(O)C(O)C1(O))C2=CC(O)=C(O)C(O)=C2
734	1.363	261.1459	Glutamylleucine	[M+H] ⁺	261.1459	C11H20N2O5	Dipeptides	MYFMARDICOWMQP-UHFFFAOYNA-N	O=C(O)C(N)CCC(=O)NC(C(=O)O)CC(C)C
735	1.364	282.14529	Pendimethalin	[M+H] ⁺	282.14484	C13H19N3O4	Dinitroanilines	CH1FOSRWNCZCFN-UHFFFAOYSA-N	CCC(CC)NC1=C(C=C(C)C(C)=C1N(=O)=O)N(=O)=O
736	1.369	247.0385	Fludioxonil	[M-H] ⁻	247.03246	C12H6F2N2O2	Benzodioxoles	MUJOIMFYNIEBMC-UHFFFAOYSA-N	FC1(F)OC2=CC=CC(=C2O1)C1=CNC=C1C#N
737	1.371	296.1579	Nuciferine	[M+H] ⁺	296.16	C19H21NO2	Aporphines	JR1VQPIHKOARKV-OAHLLOKOSA-N	O(C=1C=C2C3=C(C1OC)C4=CC=CC=C4CC3N(C)CC2)C
738	1.375	423.19608	5-[(Z)-12-(3,5-dihydroxyphenyl)dodec-8-enyl]benzene-1,3-diol	[M+H] ⁺	423.19321	C24H32O4	Resorcinols	JD1DEXHTJXTVES-HYXAFXHYSA-N	OC=1C=C(O)C=C(C(C)C)CCCC=CCCCCCC=2C(O)C=C(O)C2
739	1.375	366.07083	GALANTHAMINE HYDROBROMIDE	[M-H] ⁻	366.07101	C17H22BrN03	Galanthamine-type amarvilliaceae alkaloids	QORVIGQLPPAFRS-UHFFFAOYSA-N	Br. OC1C=C23C4=C(OC2C1)C(OC)=CC=C4CN(C)CC3
740	1.378	439.08249	(Z)-methyl 4-((9-(furan-2-yl)-3,7-dioxo-3,7,8,9-tetrahydro-2H-furo[2,3-f]chromen-2-ylidene)methyl)benzoate	[M+H] ⁺	439.07999	C24H16O7	Aurone flavonoids	KUN1PLHO1JFHHR-ODLFYWEKSA-N	O=C(OC)C1=CC=C(C=C1)C=C2OC=3C(=CC=C4OC(=O)CC(C=5OC=CC5)C43)C2=O
741	1.378	235.14507	Coumaroyl putrescine	[M+H] ⁺	235.1447	C13H18N2O2	Coumaric acid and derivatives	CJHDBEPXKGBDW-UHFFFAOYSA-N	O=C(C=C(C1=CC=CC(O)C=C1)NCCCC
742	1.378	343.19937	Pesticide3 Iprovalicarb Isomer 1* C18H28N2O3 Isopropyl [(2S)-3-methyl-1-[[1-(4-methylphenyl)ethyl]amino]-1-oxo-2-butan-1-yl]carbamate	[M+H] ⁺	343.19901	C18H28N2O3	Toluenes	NWUWYYSKZY1QAE-WMAAGAKSA-N	OC(=NC(C)C(O)=NC(C1=CC=C(C=C1)C)C(C)C(O)C(C)C
743	1.382	102.02722	Biuret	[M-H] ⁻	102.0309	C2H5N3O2	Isoureas	OHJMTUP1ZMNBFR-UHFFFAOYSA-N	N=C(O)NC(=N)O
744	1.388	131.07187	2-Hydroxy-4-methylpentanoic acid	[M-H] ⁻	131.07137	C6H12O3	Hydroxy fatty acids	LVRFTAZAXQPHI-UHFFFAOYNA-N	O=C(O)C(O)CC(C)C
745	1.388	330.11115	Nizatidine	[M-H] ⁻	330.10638	C12H21N5O2S2	2,4-disubstituted thiazoles	SCXXNSQHWDMGGP-UHFFFAOYSA-N	O=N(=O)C(=O)NC(NCSCC=1N=C(SC1)CN(C)C
746	1.393	154.0139	4-Nitrocatechol	[M-H] ⁻	154.01459	C6H5NO4	Nitrophenols	XJNPXNSISMKQEX-UHFFFAOYSA-N	O=N(=O)C1=CC=C(O)C(C)=C1
747	1.393	182.04498	4-Pyridoxic acid	[M-H] ⁻	182.04588	C8H9NO4	Pyridinecarboxylic acids	HXACOUQ1XZGNBF-UHFFFAOYSA-N	O=C(O)C1=C(O)C(=NC=C1CO)C
748	1.396	387.14172	[(3aR,4S,6R,11aR)-6,9-dihydroxy-6,10-dimethyl-3-methylidene-2,7-dioxo-3a,4,5,8,9,11a-hexahydrocyclodecab[h]furan-4-yl] 2-methylpropanoate	[M+H] ⁺	387.14142	C19H24O7	Germacranolides and derivatives	JGWDBQRL0BLTHU-XHOJJKXOPSA-N	O=C(OC1CC(O)C(=O)CC(OC)C(=CC2OC(=O)C(=C)C21)C(C)C(=C)C
749	1.396	261.0957	3-hydroxyflavone	[M+H] ⁺	261.09534	C15H10O3	Flavonols	HVQAJTFOCKORIN-UHFFFAOYSA-N	O=C1C(O)C(=C(OC=2C=CC=C21)C=3C=CC=CC3
750	1.396	438.24002	Dicoumaroyl Spermidine	[M+H] ⁺	438.23981	C25H31N3O4	Coumaric acid and derivatives	QYBCMVQSCJMSA-UHFFFAOYSA-N	O=C(C=CC1=CC=C(O)C=C1)NCCCNCCCNCC(=O)C=C2C=CC=C(O)C=C2
751	1.396	322.15076	Famciclovir	[M+H] ⁺	322.15097	C14H19N5O4	Purines and purine derivatives	GGXKRWVZWMJTEH-UHFFFAOYSA-N	O=C(OC(COC(=O)C)CCN1C=NC2=CNC(=N)N=C21)C
752	1.396	308.17105	Zolpidem	[M+H] ⁺	308.17575	C19H21N3O	Phenylimidazoles	ZAFYATHCZYHLPB-UHFFFAOYSA-N	O=C(N(C)C)CC1=C(N=C2C=CC(=CN21)C)C3=CC=C(C=C3)C
753	1.4	218.13818	Propionylcarnitine	[M+H] ⁺	218.13869	C10H19NO4	Acyl carnitines	UFAHZZIUPFNSHSL-UHFFFAOYNA-N	O=C([O-])CC(OC(=O)C)C[N-](C)C(C)C
754	1.413	195.11346	Hydroxypyridin + C5H10NO or 6-Hydroxypseudooxynicotine (not validated)	[M+H] ⁺	195.11369	C10H14N2O2	Nicotine and derivatives	UML0UOEDBG0HHR-UHFFFAOYNA-N	O=C(C=C1C(=O)C(=CC1)CCCC
755	1.422	392.11758	S-(2-Carboxypropyl)glutathione	[M-H] ⁻	392.11249	C14H23N3O8S	Peptides	JQWABENXYMJMW-UHFFFAOYNA-N	O=C(O)CNC(=O)C(=O)CNC(=O)CCC(N(C(=O)O)CSCC(C(=O)O)C
756	1.428	254.11336	Triantereene	[M+H] ⁺	254.11501	C12H11N7	Pteridines and derivatives	FNYLWVPVPXG1IP-UHFFFAOYSA-N	N1=C(N=C(N)C2=NC(=C(N=C12)N)C3=CC=CC=C3)N
757	1.432	146.11812	(3R,4S)-3-Amino-4-methylhexanoic acid	[M+H] ⁺	146.11755	C7H15NO2	Beta amino acids and derivatives	JHEDYGILOIBOTL-NTSWFWBYSA-N	CC[C@H](C)C[C@H](N)CC(O)=O
758	1.432	362.11255	Bezafibrate	[M+H] ⁺	362.11536	C19H20ClN04	Phenoxyacetic acid derivatives	11BYAHWJQTYFKB-UHFFFAOYSA-N	CC(C)C(C(=O)O)OC1=CC=C(C=C1)CCNC(C2=CC=C(C=C2)C1)=O
759	1.436	371.08096	Rebamipide	[M+H] ⁺	371.07901	C19H15ClN2O4	Hippuric acids	ALLWOAYDORUJLA-UHFFFAOYSA-N	O=C1C=C(C(=2C=CC=C2N1)CC(NC(=O)C3=CC=C(C1)C=C3)C(=O)O
760	1.439	203.13892	Ala-Ile	[M+H] ⁺	203.13902	C9H18N2O3	Dipeptides	ZSOTCJZJSRWNHX-UHFFFAOYNA-N	O=C(O)C(N=C(O)C(N)C)C(C)CC
761	1.442	341.10834	Trehalose	[M-H] ⁻	341.10895	C12H22O11	O-glycosyl compounds	HDTRYLNUVZCOYI-UHFFFAOYNA-N	OC(C1OC(OC2OC(CO)C(O)C2O)C(O)C1O)C1O
762	1.444	542.1701	PUROMYCIN HYDROCHLORIDE	[M-H] ⁻	542.16907	C22H31ClN27O5	Purine 3'-deoxyribonucleosides	MKSVFGKWLUTTO-FZFAUISWSA-N	Cl.C1.OC(=NC1C(O)C(OC1CO)N2C=NC=3C2=NC=3N(C)C(C)C(C)CC4=CC=C(OC)C=C4
763	1.449	105.07031	"L-2,3-DIAMINOPROPIONIC ACID"	[M+H] ⁺	105.07	C3H8N2O2	Alpha amino acids	PECYZEOJVMXISF-UHFFFAOYSA-N	O=C(O)C(N)CN
764	1.462	258.06073	2-Thiocytidine	[M-H] ⁻	258.05539	C9H13N3O4S	Pyrimidine nucleosides	RHFUOMFWGUKKO-UHFFFAOYNA-N	N=C1N=C(S)N(C=C1)C2OC(CO)C(O)C2O
765	1.464	263.052	Sorbitol-6-phosphate	[M+H] ⁺	263.05264	C6H15O9P	Monosaccharide phosphates	GACTVZZWMVMURNG-UHFFFAOYNA-N	O=P(O)(O)OC(CO)C(O)C(O)C(CO)CO
766	1.468	479.1684	2-[3,4-dihydroxy-2,2-dimethyl-8-(3-methylbut-2-en-1-yl)-3,4-dihydrochromen-6-yl]-5,7-dihydroxy-2,3-dihydrochromen-4-one	[M+H] ⁺	479.16763	C25H28O8	3'-prenylated flavanones	LNFRDRVYARCALE-UHFFFAOYSA-N	O=C1C=2C(O)=CC(O)=CC2OC(C3=CC(OC(=C(C)C)=C4OC(C)C(C)C(O)C4)=C3)C1
767	1.47	282.11804	2'-O-Methyladenosine	[M+H] ⁺	282.11969	C11H15N5O4	Purine nucleosides	PFUGCISOLXNPPC-UHFFFAOYNA-N	OC(C1OC(N2C=NC=3C(=NC32)N(C)CC(C)C1O
768	1.475	144.06543	4-Hydroxy-6-Methylpyran-2-One	[M+H] ⁺	144.06552	C6H6O3	Pyranones and derivatives	NSYSSMYQLSPOD-UHFFFAOYSA-N	O=C1OC(=C)C(=O)C=C1C
769	1.476	432.10999	HMB0A + O-Hex	[M-H] ⁻	432.11371	C16H21NO10	Benzoxazinoids	UOASSFRPBORTCT-UHFFFAOYNA-N	O=C2N(CO)C=C3C=CC(OC)=CC3(OC2(OC1OC(CO)C(O)C1)C1(O))
770	1.481	593.15564	kaempferol 7-neohesperidoside	[M-H] ⁻	593.1579	C27H30O15	Flavonoid-7-O-glycosides	ZEJXENDZTYVXD-CSIJBIPPSA-N	O=C1C(O)=C(OC2=CC(OC3OC(CO)C(O)C3OC4OC(C)C(O)C4O)C(=O)C2=CC(=C12)C=5C=CC(O)=CC5
771	1.483	361.15149	Perivine	[M+H] ⁺	361.14999	C20H22N2O3	Vobasan alkaloids	NKTOURNHXYVXS-XXMLWKDOSAN	O=C(OC)C1C2NCC(=CC1)CC(=O)C=3NC=4C=CC=CC4C3C2
772	1.484	269.02911	3-deoxysappanchalcone	[M-H] ⁻	269.02448	C16H14O4	Cinnamylphenols	PACBGANPNVHGNP-RUTMKATFSA-N	O=C(C(=CC1=CC(=O)C=C1)C2=CC=C(C)C=C2OC

773	1.485	711.21649	Tetrasaccharides (Hex-Hex-Hex-Hex)	[M-H]-	711.21698	C24H42O21	Sugars	UQZ1YBXSHAGNOE-UHFFFAOYNA-N	OCC4OC(OCC3OC(OCC2OC(C1(C(CO(C)C)O)C1O))C(O)C(CO)C(CO)C2O)C(CO)C(CO)C3O)C(CO)C4O)C(CO)C5O)C(CO)C6O)C(CO)C7O)C(CO)C8O)C(CO)C9O)C(CO)C10O)C(CO)C11O)C(CO)C12O)C(CO)C13O)C(CO)C14O)C(CO)C15O)C(CO)C16O)C(CO)C17O)C(CO)C18O)C(CO)C19O)C(CO)C20O)C(CO)C21O)C(CO)C22O)C(CO)C23O)C(CO)C24O)C(CO)C25O)C(CO)C26O)C(CO)C27O)C(CO)C28O)C(CO)C29O)C(CO)C30O)C(CO)C31O)C(CO)C32O)C(CO)C33O)C(CO)C34O)C(CO)C35O)C(CO)C36O)C(CO)C37O)C(CO)C38O)C(CO)C39O)C(CO)C40O)C(CO)C41O)C(CO)C42O)C(CO)C43O)C(CO)C44O)C(CO)C45O)C(CO)C46O)C(CO)C47O)C(CO)C48O)C(CO)C49O)C(CO)C50O)C(CO)C51O)C(CO)C52O)C(CO)C53O)C(CO)C54O)C(CO)C55O)C(CO)C56O)C(CO)C57O)C(CO)C58O)C(CO)C59O)C(CO)C60O)C(CO)C61O)C(CO)C62O)C(CO)C63O)C(CO)C64O)C(CO)C65O)C(CO)C66O)C(CO)C67O)C(CO)C68O)C(CO)C69O)C(CO)C70O)C(CO)C71O)C(CO)C72O)C(CO)C73O)C(CO)C74O)C(CO)C75O)C(CO)C76O)C(CO)C77O)C(CO)C78O)C(CO)C79O)C(CO)C80O)C(CO)C81O)C(CO)C82O)C(CO)C83O)C(CO)C84O)C(CO)C85O)C(CO)C86O)C(CO)C87O)C(CO)C88O)C(CO)C89O)C(CO)C90O)C(CO)C91O)C(CO)C92O)C(CO)C93O)C(CO)C94O)C(CO)C95O)C(CO)C96O)C(CO)C97O)C(CO)C98O)C(CO)C99O)C(CO)C100O)C(CO)C101O)C(CO)C102O)C(CO)C103O)C(CO)C104O)C(CO)C105O)C(CO)C106O)C(CO)C107O)C(CO)C108O)C(CO)C109O)C(CO)C110O)C(CO)C111O)C(CO)C112O)C(CO)C113O)C(CO)C114O)C(CO)C115O)C(CO)C116O)C(CO)C117O)C(CO)C118O)C(CO)C119O)C(CO)C120O)C(CO)C121O)C(CO)C122O)C(CO)C123O)C(CO)C124O)C(CO)C125O)C(CO)C126O)C(CO)C127O)C(CO)C128O)C(CO)C129O)C(CO)C130O)C(CO)C131O)C(CO)C132O)C(CO)C133O)C(CO)C134O)C(CO)C135O)C(CO)C136O)C(CO)C137O)C(CO)C138O)C(CO)C139O)C(CO)C140O)C(CO)C141O)C(CO)C142O)C(CO)C143O)C(CO)C144O)C(CO)C145O)C(CO)C146O)C(CO)C147O)C(CO)C148O)C(CO)C149O)C(CO)C150O)C(CO)C151O)C(CO)C152O)C(CO)C153O)C(CO)C154O)C(CO)C155O)C(CO)C156O)C(CO)C157O)C(CO)C158O)C(CO)C159O)C(CO)C160O)C(CO)C161O)C(CO)C162O)C(CO)C163O)C(CO)C164O)C(CO)C165O)C(CO)C166O)C(CO)C167O)C(CO)C168O)C(CO)C169O)C(CO)C170O)C(CO)C171O)C(CO)C172O)C(CO)C173O)C(CO)C174O)C(CO)C175O)C(CO)C176O)C(CO)C177O)C(CO)C178O)C(CO)C179O)C(CO)C180O)C(CO)C181O)C(CO)C182O)C(CO)C183O)C(CO)C184O)C(CO)C185O)C(CO)C186O)C(CO)C187O)C(CO)C188O)C(CO)C189O)C(CO)C190O)C(CO)C191O)C(CO)C192O)C(CO)C193O)C(CO)C194O)C(CO)C195O)C(CO)C196O)C(CO)C197O)C(CO)C198O)C(CO)C199O)C(CO)C200O)C(CO)C201O)C(CO)C202O)C(CO)C203O)C(CO)C204O)C(CO)C205O)C(CO)C206O)C(CO)C207O)C(CO)C208O)C(CO)C209O)C(CO)C210O)C(CO)C211O)C(CO)C212O)C(CO)C213O)C(CO)C214O)C(CO)C215O)C(CO)C216O)C(CO)C217O)C(CO)C218O)C(CO)C219O)C(CO)C220O)C(CO)C221O)C(CO)C222O)C(CO)C223O)C(CO)C224O)C(CO)C225O)C(CO)C226O)C(CO)C227O)C(CO)C228O)C(CO)C229O)C(CO)C230O)C(CO)C231O)C(CO)C232O)C(CO)C233O)C(CO)C234O)C(CO)C235O)C(CO)C236O)C(CO)C237O)C(CO)C238O)C(CO)C239O)C(CO)C240O)C(CO)C241O)C(CO)C242O)C(CO)C243O)C(CO)C244O)C(CO)C245O)C(CO)C246O)C(CO)C247O)C(CO)C248O)C(CO)C249O)C(CO)C250O)C(CO)C251O)C(CO)C252O)C(CO)C253O)C(CO)C254O)C(CO)C255O)C(CO)C256O)C(CO)C257O)C(CO)C258O)C(CO)C259O)C(CO)C260O)C(CO)C261O)C(CO)C262O)C(CO)C263O)C(CO)C264O)C(CO)C265O)C(CO)C266O)C(CO)C267O)C(CO)C268O)C(CO)C269O)C(CO)C270O)C(CO)C271O)C(CO)C272O)C(CO)C273O)C(CO)C274O)C(CO)C275O)C(CO)C276O)C(CO)C277O)C(CO)C278O)C(CO)C279O)C(CO)C280O)C(CO)C281O)C(CO)C282O)C(CO)C283O)C(CO)C284O)C(CO)C285O)C(CO)C286O)C(CO)C287O)C(CO)C288O)C(CO)C289O)C(CO)C290O)C(CO)C291O)C(CO)C292O)C(CO)C293O)C(CO)C294O)C(CO)C295O)C(CO)C296O)C(CO)C297O)C(CO)C298O)C(CO)C299O)C(CO)C300O)C(CO)C301O)C(CO)C302O)C(CO)C303O)C(CO)C304O)C(CO)C305O)C(CO)C306O)C(CO)C307O)C(CO)C308O)C(CO)C309O)C(CO)C310O)C(CO)C311O)C(CO)C312O)C(CO)C313O)C(CO)C314O)C(CO)C315O)C(CO)C316O)C(CO)C317O)C(CO)C318O)C(CO)C319O)C(CO)C320O)C(CO)C321O)C(CO)C322O)C(CO)C323O)C(CO)C324O)C(CO)C325O)C(CO)C326O)C(CO)C327O)C(CO)C328O)C(CO)C329O)C(CO)C330O)C(CO)C331O)C(CO)C332O)C(CO)C333O)C(CO)C334O)C(CO)C335O)C(CO)C336O)C(CO)C337O)C(CO)C338O)C(CO)C339O)C(CO)C340O)C(CO)C341O)C(CO)C342O)C(CO)C343O)C(CO)C344O)C(CO)C345O)C(CO)C346O)C(CO)C347O)C(CO)C348O)C(CO)C349O)C(CO)C350O)C(CO)C351O)C(CO)C352O)C(CO)C353O)C(CO)C354O)C(CO)C355O)C(CO)C356O)C(CO)C357O)C(CO)C358O)C(CO)C359O)C(CO)C360O)C(CO)C361O)C(CO)C362O)C(CO)C363O)C(CO)C364O)C(CO)C365O)C(CO)C366O)C(CO)C367O)C(CO)C368O)C(CO)C369O)C(CO)C370O)C(CO)C371O)C(CO)C372O)C(CO)C373O)C(CO)C374O)C(CO)C375O)C(CO)C376O)C(CO)C377O)C(CO)C378O)C(CO)C379O)C(CO)C380O)C(CO)C381O)C(CO)C382O)C(CO)C383O)C(CO)C384O)C(CO)C385O)C(CO)C386O)C(CO)C387O)C(CO)C388O)C(CO)C389O)C(CO)C390O)C(CO)C391O)C(CO)C392O)C(CO)C393O)C(CO)C394O)C(CO)C395O)C(CO)C396O)C(CO)C397O)C(CO)C398O)C(CO)C399O)C(CO)C400O)C(CO)C401O)C(CO)C402O)C(CO)C403O)C(CO)C404O)C(CO)C405O)
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[illegible]

859	2. 007	441. 18497	Gomisin H	[M+H] ⁺	441. 189	C23R3007	Hydrolyzable tannins	NLJJSPPKWNBDNS-DAOPMWJZSA-N	OC1=C (OC) C (OC) =CC2=C1C3=C (OC) C (OC) C=C3OC (O) (C) C (C)2
860	2. 008	164. 07065	Phenylalanine	[M-H] ⁻	164. 0717	C9H11N02	Phenylalanine and derivatives	COLNVLDHVKWLRT-UHFFFAOYNA-N	O=C (O) C (N) CC=1C=CC=CC1
861	2. 011	311. 13065	Desloratadine	[M+H] ⁺	311. 13095	C19H19ClN2	Benzocycloheptapyridines	JAU0IFJMECKXRG1-UHFFFAOYSA-N	C1=CC=2CCC3=CC (=CC=C3C (=C4CNCC4) C2N=C1) C1
862	2. 015	361. 97177	1-Pentanesulfonamide, 1, 1, 2, 2, 3, 3, 4, 4, 5, 5, 5-undecafluoro-N-methyl-	[M-H] ⁻	361. 97144	C6H4F11NO2S	PFSA	BKNDZBSSSAGTB-UHFFFAOYSA-N	O=S (=O) (NC) C (F) (F) C (F) (F) C (F) (F) C (F) (F) F
863	2. 022	279. 01834	purpurin	[M+H] ⁺	279. 01999	C23H22O6	8-prenylated flavanones	QLKSLGRVBGPPG-XODARUQUSA-N	O=C (OC1C2C=3C (OC2OC1) C) C=CC=C4C (=O) CC (OC43) C=5C=CC=CC5C
864	2. 027	326. 12341	Acetaminophen glucuronide	[M-H] ⁻	326. 12726	C14H17N08	Phenolic glycosides	IPROLSTVTHAGLE-BYN1DDHOSA-N	O=C (O) C1OC (OC2=CC=C (N=C (O) C) C=C2) C (O) C (O) C1O
865	2. 034	392. 17993	4-methyl-N-(((1S,9aR)-octahydro-1H-quinolizin-1-yl)methyl)-2-phenylthiazole-5-carboxamide	[M+H] ⁺	392. 17999	C21H27N3O5	Quinolizines	CDDYZYIBFIQEGM-ZWKOTPCISA-N	O=C (NCC1CCNCCC(CCC21) C=3SC (=NC3) C=4C=CC=CC4
866	2. 059	115. 00298	FUMARATE	[M-H] ⁻	115. 003	C4H4O4	Dicarboxylic acids and derivatives	VZCYOOQTPQCHFL-UHFFFAOYSA-N	O=C (O) C=CC (=O) O
867	2. 066	319. 98358	PFSM-carboxylic_acid	[M-H] ⁻	319. 98331	C6H6F7N04S	PFSA	QXQNEIFHTSUFRRH-UHFFFAOYSA-N	O=C (O) CN (C) S (=O) (=O) C (F) (F) C (F) (F) F
868	2. 072	100. 07543	2-Piperidone	[M+H] ⁺	100. 0757	C5H9NO	Piperidinones	XUHWAMWETGRKB-UHFFFAOYSA-N	C1CCN=C (C1) O
869	2. 079	311. 12274	gamma-Glutamyltyrosine	[M+H] ⁺	311. 12375	C14H18N2O6	Tyrosine and derivatives	VVLXCVSSLPQDS-UHFFFAOYNA-N	O=C (O) C (N=C (O) CCC (N) C (=O) O) CC1=C=C=C (O) C=C1
870	2. 081	278. 15903	1-(1-hydroxybutyl)-1, 3, 4, 5, 6, 7-hexahydro-2-benzofuran-4, 5, 6, 7-tetrol	[M+H] ⁺	278. 15979	C12H20O6	Isobenzofurans	TWDKEWYUIMHMA-UHFFFAOYSA-N	OC1C2=C (C (O) C (O) C1O) C (OC2) C (O) CCC
871	2. 084	254. 16238	Anabasamine	[M+H] ⁺	254. 16518	C16H19N3	Alkaloids	TZROBHMKTWECOV-UHFFFAOYNA-N	CN1CCCCC1C1=CN=C (C=C1) C1=CN=CC=C1
872	2. 116	443. 19943	pomiferin	[M+H] ⁺	443. 2012	C25H24O6	6-prenylated isoflavonones	GHCZYXUOYFOXP-UHFFFAOYSA-N	O=C1C (=CC=2C=3C=CC (OC3C (=C (O) C12) CC=C (C) C) (C) C) C=4C=C (O) C=C (O) C4
873	2. 118	204. 12241	O-Acetyl-L-carnitine	[M+H] ⁺	204. 12248	C9H18N04	Acyl carnitines	RDHQFKQ1GNGIED-MRVPVSSYSA-O	CC (=O) O [C=H] (CC (O) =O) C [N+] (C) (C) C
874	2. 124	128. 14313	DL-Coniine	[M+H] ⁺	128. 14337	C8H17N	Alkaloids and derivatives	NDNUANOUZGGEPO-UHFFFAOYNA-N	CCCC1CCCCN1
875	2. 133	225. 09425	3-(4-hydroxyphenyl)-1-phenyl-2-propen-1-one	[M+H] ⁺	225. 09	C15H12O2	Retrochalcones	PWCDTYUYPOAUT-DHZZHJOJOSA-N	O=C (C=C=C1=CC=C (O) C=C1) C=2C=CC=CC2
876	2. 136	281. 14859	(5R)-trans-1, 7-diphenyl-5-hydroxy-6-hepten-3-one	[M+H] ⁺	281. 14999	C19H20O2	Linear diarylheptanoids	NEQQOKAPXXESR-YLZCUGDYSA-N	O=C (CCC=1C=C=CC1) CC (O) C=CC=2C=CC=CC2
877	2. 146	174. 02158	Orthanilic acid	[M+H] ⁺	174. 02194	C6H7N03S	Benzenesulfonic acids and derivatives	ZMCHSEMPFKYNSKA-UHFFFAOYSA-N	O=S (=O) (O) C=1C=CC=CC1N
878	2. 163	307. 09982	mollugin	[M+H] ⁺	307. 10001	C17H16O4	Naphthopyrans	VLGATXOTCNBWT-UHFFFAOYSA-N	O=C (OC) C=1C (O) =C2C=CC=CC2=C3OC (C=CC31) (C) C
879	2. 169	342. 13794	Feruloyl O-methyldehydrodopamine	[M+H] ⁺	342. 13489	C19H19N05	Ferulic acid and derivatives	IQGMSXKRPLDGB-CFSCNVPRSA-N	COC1=CC (\C=C\N) C (=O) \C=C\C2=CC=C (O) C (OC) (=C2) =CC=C1O
880	2. 171	196. 09621	Methyltyrosinate	[M+H] ⁺	196. 09682	C10H13N03	Tyrosine and derivatives	MRZPEN1JLWBSY-UHFFFAOYNA-N	O=C (OC) C (N) CC1=CC=C (O) C=C1
881	2. 185	392. 18021	Corydaline	[M+H] ⁺	392. 17999	C22H27N04	Protoberberine alkaloids and derivatives	HRXRLJTYQVQHC-QUXALOBESA-N	O (C1=CC=C2C (=C1OC) CN3CCC4=CC (OC) =C (OC) C=C4C3CC2) C
882	2. 192	323. 12186	Neobavaisoflavone	[M+H] ⁺	323. 12	C20H18O4	Isoflavones	OBGPEBYHGIUFBN-UHFFFAOYSA-N	O=C1C (=CC2=CC (O) =CC=C12) C=3C=CC (O) =C (C3) CC=C (C) C
883	2. 206	261. 0932	FARNESOL	[M+H] ⁺	261. 09418	C15H26O	Sesquiterpenoids	CRDAMVZIKSXFV-YFVJMTDSA-N	CCC=C (C) CCC=C (C) CCC=C (C) C
884	2. 223	422. 21112	(S)-2-(3-(2, 5-dimethyl-1H-pyrrol-1-yl)propanoyl)-6, 7-dimethoxy-N-methyl-1, 2, 3, 4-tetrahydroisoquinoline-3-carboxamide	[M+H] ⁺	422. 20999	C22H29N3O4	Alpha amino acid amides	OAPHWZYGAPFW-SHVURJRSA-N	O=C (NC) C1N (C (=O) CCN2C (=CC=C2) C) CC3=CC (OC) =C (OC) C=C3C1
885	2. 227	539. 28168	MUPIROCIN	[M+H] ⁺	539. 28137	C26H44O9	Medium-chain fatty acids	MINDHHQZYEEK-HBBNESRPSA-N	O=C (O) CCCCCCCCC (=O) C=C (O) CC1CCC (CC2OC2) C (O) C (O) C1O
886	2. 23	453. 19492	(1R,5S)-3-(1-oxo-2-(pyridin-4-ylmethyl)-1, 2-dihydroisoquinoline-4-carbonyl)-3, 4, 5, 6-tetrahydro-1H-1, 5-methanonpyrido[1, 2-a][1, 5]diazocin-	[M+H] ⁺	453. 19	C27H24N4O3	Cytisine and derivatives	HR1XOCFMOJEHEU-UXHICEINSA-N	O=C1C=CC=C2N1CC3CN (C (=O) C4=CN (C (=O) C=5C=CC=CC54) CC=6C=CN=CC6) CC2C3
887	2. 235	395. 20108	brucine	[M+H] ⁺	395. 20001	C23H26N2O4	Strychnos alkaloids	RRKTZK1UPZVBMF-IBTVXLQLSA-N	O=C1CN2C=CC (OC) =C (OC) C=C3C4SCCN6C7=CCOC (C) C (C7CC64) C25
888	2. 242	307. 16434	Epigallocatechin	[M+H] ⁺	307. 16379	C15H14O7	Epigallocatechins	XMOCLSLCDHWDHP-IUODEQHRSA-N	OC=1C=C (O) C2=C (OC (C3=CC (O) =C (O) C (O) =C3) C (O) C2) C1
889	2. 243	240. 17947	Benzphetamine	[M+H] ⁺	240. 17468	C17H21N	Amphetamines and derivatives	YXKTVDFXDRQTKV-UHFFFAOYNA-N	C=1C=CC (=CC1) CN (C) C (C) CC=2C=CC=CC2
890	2. 243	195. 12186	Octyl acetate	[M+H] ⁺	195. 13	C10H20O2	Fatty alcohol esters	YLYBTZ1QSIWLI-UHFFFAOYSA-N	O=C (OCCCCCCC) C
891	2. 247	272. 15967	Napropamid	[M+H] ⁺	272. 16449	C17H21N02	Naphthalenes	WXVAROIGSPCFJ-UHFFFAOYNA-N	CCN (CC) C (=O) C (C) OC1=CC=CC=CC=C12
892	2. 248	368. 09482	6, 10a-dihydroxy-4-(hydroxymethyl)-4, 7, 11b-trimethyl-1, 2, 3, 4a, 5, 6, 6a, 7, 11, 11a-decahydronaphtho[2, 1-f][1]benzofuran-9-one	[M+H] ⁺	368. 09167	C20H30O5	Naphthofurans	LLK1VVHUJOPYIV-UHFFFAOYSA-N	O=C1OC2 (O) C (=C1) C (C) C3C (O) CC4C (CO) CCCC4 (C) C3C2
893	2. 249	420. 17572	4-amino-5-(5-hydroxy-2, 6-dimethyl-5'-prop-1-en-2'-ylspiro[7'-oxabicyclo[4. 1. 0]heptane-3, 1'-cyclooctan]-2-yl)oxy-5-oxononanoic acid	[M+H] ⁺	420. 17828	C20H31N06	Glutamic acid and derivatives	RWFZYEB1QUWPE-UHFFFAOYSA-N	O=C (O) CCC (N) C (=O) OC1C2OC (C) (O) CC13C (C=C) C) CCC3C
894	2. 258	331. 19727	2', 4-Dihydroxy-3, 4', 6' -Triamethoxychalcone	[M+H] ⁺	331. 19855	C18H18O6	2'-Hydroxychalcones	BXXKRESPUMTEI-FNORWQMLSA-N	O=C (C=CC1=CC=C (O) C (OC) =C1) C=2C (O) =CC (OC) =CC2OC
895	2. 258	158. 08086	Acetylproline	[M+H] ⁺	158. 0816	C7H11N03	Amino acids	GMMSLDIYJOSUSW-UHFFFAOYNA-N	O=C (O) C1N (C (=O) C) CCC1
896	2. 264	378. 16501	Droperidol	[M-H] ⁻	378. 16232	C22H22FN3O2	Alkyl-phenylketones	RMEDXOLNCUSCGS-UHFFFAOYSA-N	O=C (C1=CC=C (F) C=C1) CCCN2CC=C (N3C (O) =NC=4C=CC=CC43) CC2
897	2. 269	127. 0396	4-Hydroxy-6-methyl-2-pyrone	[M+H] ⁺	127. 03897	C6H6O3	Pyranones and derivatives	NSYSMSYQPLSPOD-UHFFFAOYSA-N	O=C1OC (=CC1) C
898	2. 271	131. 03413	Glutaric acid	[M-H] ⁻	131. 03499	C5H8O4	Dicarboxylic acids and derivatives	JFCQEDHGNZCLN-UHFFFAOYSA-N	OC (=O) CCCC (O) =O
899	2. 273	218. 10214	D-(+)-Pantothenic acid	[M-H] ⁻	218. 10339	C9H17N05	Secondary alcohols	GHOXGWTUJJEAGQ-ZETCQYMHSA-N	CC (C) (CO) [C=H] (O) C (O) =NCCC (O) =O
900	2. 274	260. 11197	(Z)-2-methyl-4-[(2R, 3R, 4S, 5S, 6R)-3, 4, 5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxybut-2-enenitrile	[M+H] ⁺	260. 11285	C11H17N06	Fatty acyl glycosides of mono- and disaccharides	ZMELG1PFIWPHX-GMLQCYRESA-N	N#CC (=CCOC1OC (CO) C (O) C (O) C1O) C
901	2. 279	267. 133	honokiol	[M+H] ⁺	267. 14001	C18H18O2	Biphenyls and derivatives	FVYX1JYOAQAIQK-UHFFFAOYSA-N	OC1=CC=C (C=C1C2=CC=CC (O) =C (C2) CC=C) CC=C

902	2. 279	290. 17026	Hyoscyamine	[M+] ⁺	290. 17001	C17H23N03	Tropane alkaloids	RKUNBYITZUJHSG-LGGPCSOHSA-N	O=C (OC1CC2N (C) C (CC2) C1) C (C=3C=CC-CC3) CO
903	2. 284	281. 09781	1, 5, 9-trihydroxy-5, 7, 7-trimethyl-4, 5a, 6, 8, 8a, 9-hexahydro-1H-azulenol[5, 6-c]furan-3-one	[M-H] ⁻	281. 09555	C15H22O5	Terpene lactones	MMDNQAVYQDZQ1-UHFFFAOYSA-N	O=C1OC (O) C2=C1CC (O) (C) C3CC (C) (C) CC3C2O
904	2. 29	233. 14841	Threonylleucine (isomer of 809, 926)	[M+] ⁺	233. 151	C10H20N2O4	Dipeptides	BQBCEBCLXBKYHW-UHFFFAOYNA-N	O=C (O) C (NC (=O) C (N) C (O) C) CC (O) C
905	2. 292	378. 9436	7-Chloro-perfluoroheptanoic acid	[M-H] ⁻	378. 94006	C7HClF12O2	PFSA	WMFYUM1VMSLSX-UHFFFAOYSA-N	O=C (O) C (F) (F) C (F) (F) C (F) (F) C (F) C (F) (F) C1
906	2. 292	342. 96674	FT-sulfonic acid	[M-H] ⁻	342. 96921	C6H5F9O4S	PFSA	FVJAERWL1COZSD-UHFFFAOYSA-N	O=S (=O) (O) C (O) CC (F) (F) C (F) (F) C (F) C (F) F
907	2. 299	140. 07011	3-hydroxy-1, 2-dimethylpyridin-4 (1H)-one	[M+] ⁺	140. 07001	C7H9NO2	Methylpyridines	TXKXOCQBNNJULO-UHFFFAOYSA-N	O=C1C=CN (C (=C1O) C) C
908	2. 303	203. 138	Ala-Leu	[M+] ⁺	203. 13902	C9H18N2O3	Peptides	RD1KFPRLVJLMER-UHFFFAOYNA-N	O=C (O) C (N=C (O) C (N) C) CC (O) C
909	2. 303	356. 1192	Duguetine	[M+] ⁺	356. 117	C20H21NO5	Hydroxy-7-aporphines	ZAVWGRCRKSHIMO-OALUTQOASA-N	OC1C2=CC (OC) =C (OC) C=C2C=3C=4OCC4C=C5C3C1N (C) CC5
910	2. 319	189. 12254	Gly-Leu	[M+] ⁺	189. 12337	C8H16N2O3	Peptides	DKEXFJVMVGETOQ-UHFFFAOYNA-N	O=C (O) C (N=C (O) CN) CC (O) C
911	2. 33	393. 11371	(1R, 2E, 8S, 10R, 11S)-10, 11-dihydroxy-6- (methoxymethyl)-1, 10-dimethyl-5-oxo-4, 14-dioxatriazolo[9, 2, 1, 0P, 2]tetradeca-2, 6-dien-8-yl 2-methylpropan-2-ylidene-2-oxo-3-oxo-4-oxo-5-oxo-6-oxo-7-oxo-8-oxo-9-oxo-10-oxo-11-oxo-12-oxo-13-oxo-14-oxo-15-oxo-16-oxo-17-oxo-18-oxo-19-oxo-20-oxo-21-oxo-22-oxo-23-oxo-24-oxo-25-oxo-26-oxo-27-oxo-28-oxo-29-oxo-30-oxo-31-oxo-32-oxo-33-oxo-34-oxo-35-oxo-36-oxo-37-oxo-38-oxo-39-oxo-40-oxo-41-oxo-42-oxo-43-oxo-44-oxo-45-oxo-46-oxo-47-oxo-48-oxo-49-oxo-50-oxo-51-oxo-52-oxo-53-oxo-54-oxo-55-oxo-56-oxo-57-oxo-58-oxo-59-oxo-60-oxo-61-oxo-62-oxo-63-oxo-64-oxo-65-oxo-66-oxo-67-oxo-68-oxo-69-oxo-70-oxo-71-oxo-72-oxo-73-oxo-74-oxo-75-oxo-76-oxo-77-oxo-78-oxo-79-oxo-80-oxo-81-oxo-82-oxo-83-oxo-84-oxo-85-oxo-86-oxo-87-oxo-88-oxo-89-oxo-90-oxo-91-oxo-92-oxo-93-oxo-94-oxo-95-oxo-96-oxo-97-oxo-98-oxo-99-oxo-100-oxo-101-oxo-102-oxo-103-oxo-104-oxo-105-oxo-106-oxo-107-oxo-108-oxo-109-oxo-110-oxo-111-oxo-112-oxo-113-oxo-114-oxo-115-oxo-116-oxo-117-oxo-118-oxo-119-oxo-120-oxo-121-oxo-122-oxo-123-oxo-124-oxo-125-oxo-126-oxo-127-oxo-128-oxo-129-oxo-130-oxo-131-oxo-132-oxo-133-oxo-134-oxo-135-oxo-136-oxo-137-oxo-138-oxo-139-oxo-140-oxo-141-oxo-142-oxo-143-oxo-144-oxo-145-oxo-146-oxo-147-oxo-148-oxo-149-oxo-150-oxo-151-oxo-152-oxo-153-oxo-154-oxo-155-oxo-156-oxo-157-oxo-158-oxo-159-oxo-160-oxo-161-oxo-162-oxo-163-oxo-164-oxo-165-oxo-166-oxo-167-oxo-168-oxo-169-oxo-170-oxo-171-oxo-172-oxo-173-oxo-174-oxo-175-oxo-176-oxo-177-oxo-178-oxo-179-oxo-180-oxo-181-oxo-182-oxo-183-oxo-184-oxo-185-oxo-186-oxo-187-oxo-188-oxo-189-oxo-190-oxo-191-oxo-192-oxo-193-oxo-194-oxo-195-oxo-196-oxo-197-oxo-198-oxo-199-oxo-200-oxo-201-oxo-202-oxo-203-oxo-204-oxo-205-oxo-206-oxo-207-oxo-208-oxo-209-oxo-210-oxo-211-oxo-212-oxo-213-oxo-214-oxo-215-oxo-216-oxo-217-oxo-218-oxo-219-oxo-220-oxo-221-oxo-222-oxo-223-oxo-224-oxo-225-oxo-226-oxo-227-oxo-228-oxo-229-oxo-230-oxo-231-oxo-232-oxo-233-oxo-234-oxo-235-oxo-236-oxo-237-oxo-238-oxo-239-oxo-240-oxo-241-oxo-242-oxo-243-oxo-244-oxo-245-oxo-246-oxo-247-oxo-248-oxo-249-oxo-250-oxo-251-oxo-252-oxo-253-oxo-254-oxo-255-oxo-256-oxo-257-oxo-258-oxo-259-oxo-260-oxo-261-oxo-262-oxo-263-oxo-264-oxo-265-oxo-266-oxo-267-oxo-268-oxo-269-oxo-270-oxo-271-oxo-272-oxo-273-oxo-274-oxo-275-oxo-276-oxo-277-oxo-278-oxo-279-oxo-280-oxo-281-oxo-282-oxo-283-oxo-284-oxo-285-oxo-286-oxo-287-oxo-288-oxo-289-oxo-290-oxo-291-oxo-292-oxo-293-oxo-294-oxo-295-oxo-296-oxo-297-oxo-298-oxo-299-oxo-300-oxo-301-oxo-302-oxo-303-oxo-304-oxo-305-oxo-306-oxo-307-oxo-308-oxo-309-oxo-310-oxo-311-oxo-312-oxo-313-oxo-314-oxo-315-oxo-316-oxo-317-oxo-318-oxo-319-oxo-320-oxo-321-oxo-322-oxo-323-oxo-324-oxo-325-oxo-326-oxo-327-oxo-328-oxo-329-oxo-330-oxo-331-oxo-332-oxo-333-oxo-334-oxo-335-oxo-336-oxo-337-oxo-338-oxo-339-oxo-340-oxo-341-oxo-342-oxo-343-oxo-344-oxo-345-oxo-346-oxo-347-oxo-348-oxo-349-oxo-350-oxo-351-oxo-352-oxo-353-oxo-354-oxo-355-oxo-356-oxo-357-oxo-358-oxo-359-oxo-360-oxo-361-oxo-362-oxo-363-oxo-364-oxo-365-oxo-366-oxo-367-oxo-368-oxo-369-oxo-370-oxo-371-oxo-372-oxo-373-oxo-374-oxo-375-oxo-376-oxo-377-oxo-378-oxo-379-oxo-380-oxo-381-oxo-382-oxo-383-oxo-384-oxo-385-oxo-386-oxo-387-oxo-388-oxo-389-oxo-390-oxo-391-oxo-392-oxo-393-oxo-394-oxo-395-oxo-396-oxo-397-oxo-398-oxo-399-oxo-400-oxo-401-oxo-402-oxo-403-oxo-404-oxo-405-oxo-406-oxo-407-oxo-408-oxo-409-oxo-410-oxo-411-oxo-412-oxo-413-oxo-414-oxo-415-oxo-416-oxo-417-oxo-418-oxo-419-oxo-420-oxo-421-oxo-422-oxo-423-oxo-424-oxo-425-oxo-426-oxo-427-oxo-428-oxo-429-oxo-430-oxo-431-oxo-432-oxo-433-oxo-434-oxo-435-oxo-436-oxo-437-oxo-438-oxo-439-oxo-440-oxo-441-oxo-442-oxo-443-oxo-444-oxo-445-oxo-446-oxo-447-oxo-448-oxo-449-oxo-450-oxo-451-oxo-452-oxo-453-oxo-454-oxo-455-oxo-456-oxo-457-oxo-458-oxo-459-oxo-460-oxo-461-oxo-462-oxo-463-oxo-464-oxo-465-oxo-466-oxo-467-oxo-468-oxo-469-oxo-470-oxo-471-oxo-472-oxo-473-oxo-474-oxo-475-oxo-476-oxo-477-oxo-478-oxo-479-oxo-480-oxo-481-oxo-482-oxo-483-oxo-484-oxo-485-oxo-486-oxo-487-oxo-488-oxo-489-oxo-490-oxo-491-oxo-492-oxo-493-oxo-494-oxo-495-oxo-496-oxo-497-oxo-498-oxo-499-oxo-500-oxo-501-oxo-502-oxo-503-oxo-504-oxo-505-oxo-506-oxo-507-oxo-508-oxo-509-oxo-510-oxo-511-oxo-512-oxo-513-oxo-514-oxo-515-oxo-516-oxo-517-oxo-518-oxo-519-oxo-520-oxo-521-oxo-522-oxo-523-oxo-524-oxo-525-oxo-526-oxo-527-oxo-528-oxo-529-oxo-530-oxo-531-oxo-532-oxo-533-oxo-534-oxo-535-oxo-536-oxo-537-oxo-538-oxo-539-oxo-540-oxo-541-oxo-542-oxo-543-oxo-544-oxo-545-oxo-546-oxo-547-oxo-548-oxo-549-oxo-550-oxo-551-oxo-552-oxo-553-oxo-554-oxo-555-oxo-556-oxo-557-oxo-558-oxo-559-oxo-560-oxo-561-oxo-562-oxo-563-oxo-564-oxo-565-oxo-566-oxo-567-oxo-568-oxo-569-oxo-570-oxo-571-oxo-572-oxo-573-oxo-574-oxo-575-oxo-576-oxo-577-oxo-578-oxo-579-oxo-580-oxo-581-oxo-582-oxo-583-oxo-584-oxo-585-oxo-586-oxo-587-oxo-588-oxo-589-oxo-590-oxo-591-oxo-592-oxo-593-oxo-594-oxo-595-oxo-596-oxo-597-oxo-598-oxo-599-oxo-600-oxo-601-oxo-602-oxo-603-oxo-604-oxo-605-oxo-606-oxo-607-oxo-608-oxo-609-oxo-610-oxo-611-oxo-612-oxo-613-oxo-614-oxo-615-oxo-616-oxo-617-oxo-618-oxo-619-oxo-620-oxo-621-oxo-622-oxo-623-oxo-624-oxo-625-oxo-626-oxo-627-oxo-628-oxo-629-oxo-630-oxo-631-oxo-632-oxo-633-oxo-634-oxo-635-oxo-636-oxo-6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945	2. 511	375. 17459	Cyproterone	[M+H] ⁺	375. 17215	C22H27ClO3	Gluco/mineralocorticoids progestogens and	DU\$HUSLJJDGTE-UHFFFAOYNA-N	CC(C1(CCC2C3C=C(C4=CC(C5CC5C4(C)C3CCC21C)=O)C1)O)=O
946	2. 52	305. 16125	Propentofylline	[M-H] ⁻	305. 1619	C15H22N4O3	Xanthines	RBQQRQRFDPXAGN-UHFFFAOYSA-N	O=C1C2=C(N=CN2CC)N(C(=O)N1CCCC(=O)C)C
947	2. 526	357. 21194	galbulin	[M+H] ⁺	357. 20999	C22H28O4	Aryltetralin lignans	WYBOV1SLCPAJFV-QLEMLULZSA-N	O(C1=CC=C(C=C1OC)C2C3=CC(OC)=C(OC)C=C3CC(C)C2)C
948	2. 534	174. 02164	ANILINE-2-SULFONIC ACID	[M+H] ⁺	174. 02	C6H7N	Aniline and substituted anilines	PAYRUJLWNCNPSJ-UHFFFAOYSA-N	NC=1C=CC=CC1
949	2. 537	125. 05965	Isovaleric acid	[M+H] ⁺	125. 06	C5H10O2	Methyl-branched fatty acids	GWYPCCOPABKNJV-UHFFFAOYSA-N	O=C(O)CC(C)C
950	2. 538	291. 15387	1-(8-methyl-3a,4,5,6-tetrahydro-1H-pyrazino[3,2,1-jk]carbazol-3(2H)-yl)ethanone	[M+H] ⁺	291. 14999	C17H20N2O	Carbazoles	TVYGDGMZPKRPM-UHFFFAOYSA-N	O=C(N1CCN2C3=C(C=C(C3C4=C2C1CCC4)C)C
951	2. 538	340. 14975	Tetrahydroberberine	[M+H] ⁺	340. 14999	C20H21NO4	Protoberberine alkaloids and derivatives	VZTU1EROBZXUFA-MRXNPFDSA-N	O(C1=CC=C2C(=C1OC)CN3CCC4=CC=5OC5C=C4C3C2)C
952	2. 544	285. 17981	Oseltamivir carboxylate	[M+H] ⁺	285. 18088	C14H24N2O4	Gamma amino acids and derivatives	NENPYTRHICXVCS-YNEHK1RBSA-N	CCC(CC)O[C=H]1C=C(C[C=H](N)[C=H]1N=C(C)O)C(O)=O
953	2. 545	385. 15891	(2R,3S,4S,5R,6S)-2-(hydroxymethyl)-6-(3,4,5-trimethoxyphenoxy)oxane-3,4,5-triol	[M+H] ⁺	385. 159	C15H22O9	Phenolic glycosides	NBLLRWANAFOKON-ZHZZCYKASA-N	OC1OC(OC=2C=C(OC)C(OC)=C(OC)C2)C(O)C(O)C1O
954	2. 545	317. 16904	(S)-[6]gingerol	[M+H] ⁺	317. 17001	C17H26O4	Gingerols	NLDDIKRKFEXWBK-CQSZAC1VSA-N	O=C(OC(C1=CC=C(O)C(OC)=C1)CC(O)CCCC
955	2. 554	122. 09717	2,6-Xylidine	[M+H] ⁺	122. 09643	C8H11N	m-Xylenes	UFEBMTHBGFGIHF-UHFFFAOYSA-N	CC=C1C=CC=C(C)C1N
956	2. 557	298. 09607	5'-S-Methylthioadenosine	[M+H] ⁺	298. 09683	C11H15N5O3S	5'-deoxy-5'- thionucleosides	WUUGFSXJNOTRMR-IOSLPCCSA-N	CSC[C=H]10[C=H]([C=H]1)[C=H]10)N1C=NC2(C)N=N=CN=C12
957	2. 557	331. 19568	8-[3-oxo-2-[(E)-pent-2-enyl]cyclopenten-1-yl]octanoic acid	[M+H] ⁺	331. 19421	C18H28O3	Medium-chain fatty acids	RHWQVSLVMXMBR-VXNBXDJSA-N	O=C(O)CCCCCCC1=C(C(=O)CC1)CC=CCC
958	2. 561	447. 112	Cynaroside	[M-H] ⁻	447. 112	C21H20O11	Flavonoid-7-O-glycosides	PEFNSGRTCBGNAN-QNDFKXLGSA-N	O=C1C=C(OC2=CC(OC3OC(C)C(O)C3O)=CC(O)=C12)C4=C(CO)=C(O)C4
959	2. 566	224. 12794	Bufexamac	[M+H] ⁺	224. 12801	C12H17N3O3	Phenylacetamides	MXJWRABVEGLYDG-UHFFFAOYSA-N	O=C(NC)CC1=CC=C(OC(C)C)C=C1
960	2. 567	259. 00827	Bromacil	[M-H] ⁻	259. 00876	C9H13BrN2O2	Halopyrimidines	CTSLUCNDVMDHG-UHFFFAOYNA-N	CCC(C)N1C(O)=NC(=C(Br)C1)=O
961	2. 568	146. 1171	(S)-3-Amino-5-methylhexanoic acid	[M+H] ⁺	146. 11755	C7H15NO2	Beta amino acids and derivatives	MLYMS1KVLAPCAK-LURJTMIESA-N	CC(C)C[C=H](N)CC(O)=O
962	2. 58	247. 1279	desmotroposantonin	[M+H] ⁺	247. 13	C15H18O3	Naphthofurans	ZLKGXNSQJJSAU-PSEJXGSSA-N	O=C1OC2C=3C(C(O)C=C(C3CCC21C)C)C
963	2. 582	208. 0598	7,8-dimethoxy-benzo[d][1,2]oxazin-1-one	[M+H] ⁺	208. 06	C10H9NO4	Benzoxazines	KPEBLJUVHUTNCC-UHFFFAOYSA-N	O=C1ON=CC=2C=CC(OC)=C(OC)C12
964	2. 592	292. 04517	1,8-dinitropyrene	[M-H] ⁻	292. 04895	C16H8N2O4	Pyrenes	BLYYNH1KOMELAP-UHFFFAOYSA-N	C1=CC=2C=CC(=C3C=CC4=C(C=CC1=C4C23)N(=O)=O)N(=O)=O
965	2. 598	319. 15021	[(2R)-1-[(2S)-6-oxo-2,3-dihydropyran-2-yl]propan-2-yl]-3-(3,4-dihydroxyphenyl)propanoate	[M-H] ⁻	319. 14777	C17H20O6	Catechols	DEJPAJWPUCTUPL-YPMHXNCESA-N	O=C1OC(CC=C1)CC(OC(=O)CCC2=CC=C(O)C(=O)=C2)C
966	2. 598	239. 10242	Felbamate	[M+H] ⁺	239. 10263	C11H14N2O4	Benzene and substituted derivatives	WKGXYQOCVYPAC-UHFFFAOYSA-N	N=C(O)OCC(C1=CC=CC=C1)OCC(=N)O
967	2. 598	305. 14777	Miltirone	[M+H] ⁺	305. 14999	C19H22O2	Tanshinones, isotanshinones, and	FEFA1BOZOKSLJR-UHFFFAOYSA-N	O=C1C(=O)C(=CC=2C=CC3=C(C21)CCCC3(C)C)C(C)C
968	2. 598	272. 14792	Pesticide5_Methoprotryne_C11H21N5O5_	[M+H] ⁺	272. 15399	C11H21N5O5	Methylthio-s-triazines	DDU1UBJPQOKOMV-UHFFFAOYSA-N	N=1C(=NC(=NC1CCOC)NC(C)SC
969	2. 602	135. 06491	2-Deoxyribose	[M+H] ⁺	135. 06519	C5H10O4	Beta-hydroxy aldehydes	ASJSAQIRZKANQN-UHFFFAOYNA-N	O=CCC(O)C(O)CO
970	2. 602	283. 16464	ANISOMYCIN	[M+H] ⁺	283. 16522	C14H19NO4	Anisoles	YKJYKKNCCRKFSL-BFHYXJOUA-N	O=C(OC1C(O)CNC1CC2=CC=C(OC)C=C2)C
971	2. 604	488. 25916	deltamine	[M+H] ⁺	488. 26001	C25H39NO7	Aconitane-type diterpenoid alkaloids	GLMPFCVWRKKB-JB-YUAUPFRZA-N	OC1C2C3(C)CN(CO)C4C51OCOC65CC(OC)C7CC(O)(C6C7OC)C42C(O)C1C3
972	2. 617	229. 15366	Leucylproline	[M+H] ⁺	229. 15511	C11H20N2O3	Dipeptides	VTJUN1YRYIAIHF-UHFFFAOYNA-N	O=C(O)C1N(C(=O)C)NC(O)C)CCC1
973	2. 623	373. 17047	2-[2-[(Z)-pent-2-enyl]-3-[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxycyclopentyl]lactic acid	[M-H] ⁻	373. 17352	C18H30O8	Fatty acyl glycosides of mono- and disaccharides	GJZJZRWFRZFTEE-ARJAWSKDSA-N	O=C(O)C1CCC(OC2OC(C)C(O)C(=O)C2O)C1CC=CCC
974	2. 624	192. 97765	PYROCATECHUIC ACID	[M+H] ⁺	192. 98041	C7H6O4	Salicylic acids	GLDQAMYCGOIJDV-UHFFFAOYSA-N	O=C(O)C=1C=CC=C(O)C1O
975	2. 625	234. 16899	(2R)-2-[(2R,5S)-5-[(2S)-2-hydroxybutyl]oxolan-2-yl]propanoic acid	[M+H] ⁺	234. 16997	C11H20O4	Oxolanes	HTCUURQJNZBKIA-XFWSIPNHSA-N	O=C(O)C(C)C1OC(C1)CC(O)CC
976	2. 625	221. 09212	Ethyl 9-D-glucuronide	[M-H] ⁻	221. 09399	C8H14O7	O-glucuronides	1WJBJVMJWSPZQJH-UQGZVRACSA-N	O=C(O)C1OC(OC)C(O)C(O)C1O
977	2. 629	551. 24854	Pseudolaric Acid A-O-beta-D-glucopyranoside	[M+H] ⁺	551. 25	C28H38O11	Diterpene lactones	IYVWRYGMQNDQB-VHJBJYHKS-A-N	O=C(OC1OC(CO)C(O)C1O)C(=CC=CC2(OC(=O)C34CC=C(C)CCC4(OC(=O)C)C2C3)C)C
978	2. 631	277. 11722	1-Pentanone, 3-hydroxy-1,5-diphenyl-	[M+H] ⁺	277. 1199	C17H18O2	Alkyl-phenylketones	QJUWGGININGVSC-UHFFFAOYSA-N	O=C(C(=1C=CC=CC1)CC(O)CCC=2C=CC=CC2
979	2. 64	307. 08417	Clobenpropit	[M-H] ⁻	307. 07898	C14H17ClN4S	Chlorobenzenes	UCA1EVHKDLM1FL-UHFFFAOYSA-N	C1C1=CC=C(C=C1)CNC(=N)SCCCC2=CN=CN2
980	2. 641	145. 04965	Adipic acid	[M-H] ⁻	145. 05063	C6H10O4	Medium-chain fatty acids	WNLRTBRMVRJNCN-UHFFFAOYSA-N	O=C(O)CCCC(=O)O
981	2. 647	352. 18637	Eseroline Fumarate	[M+H] ⁺	352. 18668	C17H22N2O5	Pyrrrolindoles	PBZRBRADJWNBPNY-WLHGVMLRSA-N	O=C(O)C=CC(=O)O.OC1=CC=C2C(=C1)C3(C)CN(C)C3N2C
982	2. 647	263. 15131	phenylacetylglutamine	[M-H] ⁻	263. 15192	C13H16N2O4	N-acyl-alpha amino acids	FLFLIEFSWGNOPJJ-JTQLQ1EISA-N	O=C(O)C(N=C(O)CC=1C=CC=CC1)CCC(=N)O
983	2. 653	159. 09116	1-Benzylimidazole	[M+H] ⁺	159. 09167	C10H10N2	N-substituted imidazoles	KKKDDZZJCRFGSD-UHFFFAOYSA-N	N=1C=CN(C1)CC=2C=CC=CC2
984	2. 673	333. 16385	(5R)-5-hydroxy-1-(4-hydroxy-3-methoxyphenyl)decan-3-one	[M+H] ⁺	333. 16513	C17H26O4	Gingerols	NLDDIKRKFEXWBK-CQSZAC1VSA-N	O=C(OC(C1=CC=C(O)C(OC)=C1)CC(O)CCCC
985	2. 673	263. 14029	Prolylphenylalanine	[M+H] ⁺	263. 14069	C14H18N2O3	Dipeptides	1W1ANZLCJYVEFX-UHFFFAOYNA-N	O=C(O)C(NC(=O)C1NCCC1)CC2=CC=CC=C2
986	2. 673	102. 09207	valeramide	[M+H] ⁺	102. 09134	C5H11NO	Fatty amides	1PWFJLQDVFKJDU-UHFFFAOYSA-N	N=C(O)CCCC
987	2. 675	299. 07574	Benzoic acid + 10, 0-Hex	[M-H] ⁻	299. 07611	C13H16O8	Phenolic glycosides	XSSDY1MYZONMEL-UHFFFAOYNA-N	O=C(O)C2=CC=C(OC1OC(CO)C(O)C1)C(=O)C=C2

988	2.677	293.11203	Climbazole	[M+H] ⁺	293.10513	C15H17C1N2O2	Phenol ethers	OEWGHB0CFMBLFP-UHFFFAOYNA-N	CC(C) C(C) C(N(C=CN(C1) OC2=CC=C(C=C2) C1)=O
989	2.68	196.06087	"3,4-DIHYDROXY-L-PHENYLALANINE"	[M-H] ⁻	196.061	C9H11N04	Tyrosine and derivatives	WTRDRQBEARUVNC-UHFFFAOYSA-N	O=C(O) C(N) CC1=CC=C(O) C(O)=C1
990	2.684	237.12273	Alanylphenylalanine	[M+H] ⁺	237.1254	C12H16N2O3	Dipeptides	OMNVYXHOSHNRUL-UHFFFAOYNA-N	O=C(O) C(NC (=O) C(N) C) CC1=CC=CC=C1
991	2.684	367.15933	Dehydroisoandrosterone sulfate	[M-H] ⁻	367.15848	C19H28O5S	Sulfated steroids	CZWCKZRVVOZZJNW-UHFFFAOYNA-N	O=C1CCC2C3CC=C4CC(OS(=O)(=O) CCC4) C3CCC12C
992	2.69	345.12744	santin	[M+H] ⁺	345.12683	C18H16O7	6-O-methylated flavonoids	DWZAJFEYZIHFO-UHFFFAOYSA-N	O=C1(C) C(=C(OC2=CC(O)=C(C) C(O)=C12) C=3C=CC(OC)=CC3
993	2.692	348.13931	(R)-1-((4,8-dimethoxyfuro[2,3-b]quinolin-7-yl)oxy)-3-methylbutane-2,3-diol	[M+H] ⁺	348.14001	C18H21NO6	Furanoquinolines	PXGMNDHTVJAHL-CYBMJJFWSA-N	OC(COC(=C=CC2=C(N=C3OC=CC3=C2OC) C1OC) C(O) C(C) C
994	2.692	161.10818	Tryptamine (not validated)	[M+H] ⁺	161.108	C10H12N2	Indole and derivatives	APJYDQYYACXCRM-UHFFFAOYSA-N	NCCC=CNC1=CC=CC=C12
995	2.693	387.13974	DL-Praeurtorin A	[M+H] ⁺	387.14001	C21H22O7	Angular pyranocoumarins	XGPBRZDOJDLKOT-IZZDOVSWSA-N	O=C1OC2=C(C=C1) C=CC=3OC(C) C(C) C(OC(=O) C(=CC) C) C(OC(=O) C1) C32
996	2.697	176.07047	3-Indoleacetic acid	[M+H] ⁺	176.0706	C10H9NO2	Indole-3-acetic acid derivatives	SEOVTRFC1GRIMH-UHFFFAOYSA-N	c1ccc2c(c1)c(cc(=O) O) c[nH]2
997	2.697	227.07596	cis-resveratrol	[M-H] ⁻	227.07137	C14H12O3	Stilbenes	LUKBXSAWLPMSZ-UHFFFAOYSA-N	OC1=CC=C(C=CC2=CC(O)=CC(O)=C2) C=C1
998	2.698	204.14201	Crotamiton	[M+H] ⁺	204.13829	C13H17NO	Anilides	DNTGZGPQQTQKF-UHFFFAOYSA-N	CC=CC(N) CC(C1=CC=CC=C1) C=O
999	2.702	369.12857	gibberellic acid	[M+H] ⁺	369.13	C19H22O6	C19-gibberellin 6-carboxylic acids	I XORZMNAPKEEDV-OBDJNFBSA-N	O=C(O) C1C2C3(C(=O) C2) C(C) C(C3) C4CCCC(O) C(=C) C(C1) C45
1000	2.705	571.29352	Khayanathone	[M+H] ⁺	571.29016	C32H42O9	Limonoids	AKPJXLBDLSOFY-YCUUMJCDSA-N	O=C(OC1CC(OC(=O) C2) C(C) C(OC(=O) C) C3(C) C2CCCC4(C) C(C(=O) C5OC543) C6=COC=C6) C1(C) C1C
1001	2.706	288.14313	11,22-dimethyl 6E,17E)-3,14-dioxo-8,19-bis(((2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-ylloxy))-4,9,15,20-	[M+H] ⁺	288.14417	C13H18O6	O-glycosyl compounds	GKHCBYBLTXYEY-UJPAAIJSA-N	OC1OC(OC2=CC=CC2) C(O) C(O) C1O
1002	2.706	186.1485	Chrysanthemic Acid	[M+H] ⁺	186.14885	C10H16O2	Monocyclic monoterpenoids	XLOPRKKSJMMEW-UHFFFAOYSA-N	O=C(O) C1C(C=C(C) C) C1(C) C
1003	2.71	235.10803	Carbetamide	[M-H] ⁻	235.10881	C12H16N2O3	Phenylcarbamic acid esters	AMRXHFHNZFDCU-UHFFFAOYNA-N	CCN=C(O) C(C) C(O) C(=O) N=C1=CC=CC=C1
1004	2.736	561.31152	sodium (E)-2-((4S)-16-acetoxy-3,11-dihydroxy-4,8,10,14-tetramethyldodecahydro-1H-cyclopenta[a]phenanthren-17(2H,10H,14H)-	[M+H] ⁺	561.31	C31H47NaO6	Steroid esters	HJHVQCXHMVGNCZ-LHTWEHRSA-M	[Na ⁺], O=C(1O=1) C(=C1C(OC(=O) C) C2) C(C) C2(C) C1(C) C(C) C(C) C4OCC32
1005	2.741	180.10284	(R)-3-Amino-4-phenylbutyric acid	[M+H] ⁺	180.1019	C10H13NO2	Beta amino acids and derivatives	OFVBKLINTLPEGH-SECBINFHISA-N	N[C-H] (CC(O)=O) CC1=CC=CC=C1
1006	2.745	295.12836	Aspartame	[M+H] ⁺	295.12885	C14H18N2O5	Peptides	IAOZJIPTCAWRG-QWRGIYKSSA-N	COC(=O) [C-H] (Cc1ccccc1) N=C([C-H] (CC(=O) O) N) O
1007	2.746	255.10432	Ketoprofen	[M+H] ⁺	255.10158	C16H14O3	Benzophenones	DKYVVDODHFEZIM-UHFFFAOYNA-N	CC(C(O)=O) C1=CC(=CC(C1) C(=O) C1=CC=CC=C1
1008	2.749	479.16275	Flavin Mononucleotide	[M+H] ⁺	479.16177	C17H21N4O9P	Flavin nucleotides	FVTCRASFAZXNN-SCRCRAPSA-N	O=C1N=C(O) C2=C3N=CC(=C(C=C3N(C2=N1) CC(O) C(C) C(O) COP(=O)(O) O) C
1009	2.759	322.13937	Pesticide1 Pyriproxyfen_C20H19NO3 Pyridine, 2-[1-methyl-2-(4-nhenoxynhenoxylethoxy)-	[M+H] ⁺	322.14301	C20H19NO3	Diphenylethers	NHDHVHZCFYSRB-UHFFFAOYSA-N	N=C1=CC=CC1OC(C) COC2=CC=C(OC(=3C=CC=CC3) C=C2
1010	2.762	425.1907	Kushanol F	[M+H] ⁺	425.19	C25H28O6	8-prenylated flavanones	XRYVAQLDYTHCL-CIQJOMJSA-N	O=C1C2=C(O) C=C(O) C(=C2OC(=3=CC=C(O) C=C3O) C1) CC(C(=C) C) C(=CC(C) C
1011	2.774	316.07977	[2-[(E)-3,4-dihydropent-1-enyl]-6-oxooxan-3-yl] (E)-2-methylbut-2-enoate	[M+H] ⁺	316.07916	C15H22O6	Delta valerolactones	WEDIEMZPFJDNCG-BZNITMXSSA-N	O=C(OC1CCC(=O) OC1C=CC(O) C(O) C) C(=CC) C
1012	2.778	229.11754	Proline-hydroxyproline	[M+H] ⁺	229.11829	C10H16N2O4	Dipeptides	ONPXCLZMDSJLSP-UHFFFAOYNA-N	O=C(O) CIN(C(=O) C2NCCC2) CC(O) C1
1013	2.782	370.1123	kinetin riboside	[M+H] ⁺	370.10999	C15H17N5O5	Purine nucleosides	CAGLGYNQSTUGX-SDBHTRESA-N	OC1OC(N2C=NC(=C(-NC=NC3) NC=4OC=CC4) C1) C(C1O
1014	2.784	480.1701	[(2R,3S,4S,5R,6R)-6-[(2S,3S,4S,5R)-3,4-dihydroxy-2,5-bis(hydroxymethyl)oxolan-2-yl]oxy-3,4,5-trihydroxyoxan-2-yl]methyl 4-[4,5-dihydroxy-3,4-bis(hydroxymethyl)-4a,8,8-trimethyl-5,6,7,8a-tetrahydro-1H-naphthalen-1-yl] hexanoate	[M+H] ⁺	480.17114	C19H26O13	O-glycosyl compounds	CDTMEVVBGLIF-OVUASUJSA-N	O=C(OC1CC(OC2(OC(CO)C(O)C2O)C(C)C(O)C1O)C3=CC=C(CO)C=C3)
1015	2.785	407.24121	2',2'-Difluoro-2'-deoxyuridine	[M+H] ⁺	407.24039	C21H36O6	Fatty acid esters	PBKUHTZGOWKEU-UHFFFAOYSA-N	O=C(OC1C=C(CO)C(O) C(O) C2(C)C(C)C(C)C(C12)OCCCC
1016	2.785	265.06323	2'-2'-Difluoro-2'-deoxyuridine	[M+H] ⁺	265.06305	C9H10F2N2O5	Pyrimidine 2'-deoxyribonucleosides	FIRDBEQ1QERSE-QPPQHFZASA-N	OC[C-H]1O[C-H](N2C=CC(O)=NC2=O)C(F)[C-H]1O
1017	2.787	337.13873	aurapten	[M+H] ⁺	337.13971	C19H22O3	Terpene lactones	RSDHGSKLQSQFK-RYDMVPIBSA-N	O=C1OC=2C=C(OC(C=C)CCC=C(C)C)C=C2C=C1
1018	2.797	265.15353	Feruloyl putrescine (isomer of 1173)	[M+H] ⁺	265.15469	C14H20N2O3	Ferulic acid and derivatives	SFUVCMKSYKHYLD-UHFFFAOYSA-N	O=C(C=CC(=C=CC(O)=C(CO)C)N)NCCCC
1019	2.8	356.13199	(1R,3R,4S,5R)-1,3,4-trihydroxy-5-[(E)-3-(4-hydroxyphenyl)prop-2-enoyl]oxycyclohexane-1-carboxylic acid	[M+H] ⁺	356.13397	C16H18O8	Quinic acids and derivatives	BMSEYFENKXDIS-QHAYPTCMSA-N	O=C(OC1CC(O) C(=O) C(C) C1O) C1OC=CC2=CC(C) C=C2
1020	2.8	361.19592	Prednisolone	[M+H] ⁺	361.20096	C21H28O5	21-hydroxysteroids	OIGXJSKKLXVSL5-VWUMJDOOSA-N	C(=C12C[C-H]1O[C-H]3[C-H](CCC4=CC(=O)C=C(C134C)[C-H]11OC(=C2)C(C)=O)C
1021	2.808	319.12817	Irigenol	[M+H] ⁺	319.1286	C15H10O8	Isoflavones	DFURNQJNFMYTHM-UHFFFAOYSA-N	O=C1C(=COC2=C(O) C(=O) C(O) C=C12) C=3C=C(C) C(O) C(=O) C3
1022	2.808	128.07082	L-PIPECOLIC ACID	[M-H] ⁻	128.071	C6H11NO2	Alpha amino acids	HXEACLLIILLPRG-UHFFFAOYSA-N	O=C(O)C1NCCC1
1023	2.811	413.13992	Loganin	[M+H] ⁺	413.14001	C17H26O10	Iridoid O-glycosides	AMBQHHVBBHTQBF-UOUCRYGSSA-N	O=C(OC)C1=CC(OC2OC(CO)C(O)C(O)C2O)C3C1CC(O)C3C
1024	2.812	347.13058	Aucubin	[M+H] ⁺	347.13	C15H22O9	Iridoid O-glycosides	RJWJHRPNHPIHRYN-FKVJWERZSA-N	OC1=CC(O)C2C=CC(OC3OC(CO)C(O)C(C)C3O)C12
1025	2.819	401.23792	Bisucaberin	[M+H] ⁺	401.23999	C18R32N4O6	Macrolactams	G7ADQMQRQBOJIO-UHFFFAOYSA-N	O=C1N(O)CCCCN=C(O)CCC(=O)N(O)CCCCN=C(O)CC1
1026	2.832	285.12521	Articaïne HCl	[M+H] ⁺	285.12701	C13H21C1N2O3S	Alpha amino acid amides	GWDWBGSGNEMGJ-UHFFFAOYSA-N	C1. O=C(OC) C=1SC=C(C1NC(=O) C(NCCC) C
1027	2.832	110.02074	Hypotaurine	[M+H] ⁺	110.02702	C2H7NO2S	Sulfinic acids	VYIUBCNYACGLLY-UHFFFAOYNA-N	NCS(O)=O
1028	2.837	294.06021	N4-Acetyl sulfamethoxazole	[M-H] ⁻	294.05539	C12H13N3O4S	Benzene sulfonamides	GXP1UNCZALHJVA-UHFFFAOYSA-N	CC(O)=NC1=CC=C(C=C1)S(=O)(=O)NC1=O
1029	2.847	137.05943	2-Hydroxyacetophenone	[M+H] ⁺	137.05971	C8H8O2	Alkyl-phenylketones	ZWVHTXAYIKBMEU-UHFFFAOYSA-N	O=C(C=C1C=CC=CC1)CO
1030	2.854	287.16	2-(1-hydroxy-1-methoxy-3-methylbutyl)-6-methyl-5H-[1,3]dioxolo[4,5-f]chloridin-4-one	[M+H] ⁺	287.16013	C13H19NO5	Pyridinones	VVLWYPUJJAWYBV-UHFFFAOYSA-N	OC=1N=C(C=C2OC(OC12)C(O)C(CO)C(C)C

1031	2. 854	316. 18579	Nordihydrocapsaicin	[M+H] ⁺	316. 17999	C17H27N03	Methoxyphenols	VQEONGKQWIFHMN-UHFFFAOYSA-N	O=C (NCC1=CC=C (O) C (OC)=C1) CCCCC (C) C
1032	2. 855	217. 07097	1-hydroxypyrene	[M-H] ⁻	217. 06589	C16H100	Pyrenes	BJJNHUAPTJVYVQ-UHFFFAOYSA-N	C1=CC=2C=CC=3C=CC (=C4C=CC (=C1) C2C3) 4 0
1033	2. 855	253. 12022	lindenolol	[M+H] ⁺	253. 12	C15H1802	Naphthofurans	XRDJYSGPJZSG-HGUIZDCDSA-N	OC1C2=C (OC=C2C) CC3 (C) C1C (=C) C4CC43
1034	2. 875	421. 2438	3-(3, 4-dihydroxyphenyl)-5, 7-dihydroxy-6, 8-bis (3-methylbut-2-enyl) chromen-4-one	[M-H] ⁻	421. 24014	C25H2606	6-prenylated isoflavonones	OAUIRSVJXOFAOO-UHFFFAOYSA-N	0=C1C (=COC2=C1C (O)=C (C (O) =C2C=C (C) C) CC=C (C) C) C=3C=CC (O)=C (O) C3
1035	2. 882	251. 13829	Caffeoyl putrescin (isomer of 1059)	[M+H] ⁺	251. 1396	C13H18N203	Caffeic acid and derivatives	KTZNZCYTXQEHT-UHFFFAOYSA-N	O=C (C=C=C1C=CC (O) =C (O) C=1) NCCCCN
1036	2. 89	102. 12746	1-Hexylamine	[M+H] ⁺	102. 12772	C6H15N	Monoalkylamines	BMVXCPBGZKUPN-UHFFFAOYSA-N	CCCCCN
1037	2. 898	254. 04308	Kinetin	[M+H] ⁺	254. 04387	C10H9N50	6-alkylaminopurines	QANMHLXAZMSUEX-UHFFFAOYSA-N	N=1C=NC=2C1NC=NC2NCC=3OC=CC3
1038	2. 899	359. 19031	Prednisone	[M+H] ⁺	359. 1853	C21H2605	21-hydroxysteroids	XOFYZVNMUHLCC-UHFFFAOYNA-N	CC12CC (=O) C3C (CCC4=CC (=O) C=CC34C) C1CCC2 (O) C (=O) CO
1039	2. 912	285. 13354	methyl 2-ethyl-4-[[(3R, 4R, 5S)-5-hydroxy-4, 5-dimethyl-2-oxooxolan-3-yl]-2-methyl-3-oxobutanoate	[M-H] ⁻	285. 13437	C14H2206	Annonaceous acetogenins	VOYCJQSSBDMXNQ-YZGKFDMSA-N	O=C1OC (O) (C) C (C) C1CC (=O) C (C (=O) OC) (C) CC
1040	2. 913	428. 24899	Ranolazine (Ranexa)	[M+H] ⁺	428. 254	C24H33N304	Anisoles	XXLMZUWNAPSZ-UHFFFAOYSA-N	O=C (NC=1C (=CC=C1C) C) CN2CC (CC2) CC (O) COC=3C=CC=CC3OC
1041	2. 919	332. 09717	ADRENALINE BITARTRATE	[M-H] ⁻	332. 09869	C13H19N09	Catechols	YLX1PWW10ISBDD-NDAAPVSOSA-N	O=C (O) (C) C (O) C (=O) C. OC1=CC=C (C=1O) C (O) CNC
1042	2. 919	317. 11469	eupomatoid 5	[M+H] ⁺	317. 11481	C19H1803	2-arylbenzofuran flavonoids	HMGCTPMQYVGXSC-SNAWJCMRSA-N	OC=1C=CC (=CC1OC) C=2OC3=CC=C (C=CC) C=C3C2C
1043	2. 919	237. 14984	Gliocladiic acid 130132	[M+H] ⁺	237. 149	C14H2204	Menthane monoterpenoids	SLYSUVFUFJMKCV-URFGDBDFSA-N	O=C (O) C (=CC1C=C (O) C) C1C (C) CO
1044	2. 932	418. 23227	Cilazapril monohydrate (Inhibace)	[M+H] ⁺	418. 23401	C22H33N306	Dipeptides	JQRZBPFGBR1WSN-OKJRKUMDSA-N	0=C (O) C1N2C (=O) C (NC (C (=O) OCC) CCC=3C=CC=CC3) CCCC2CCCC1. 0
1045	2. 936	255. 04359	3-(5-phenylthiophen-2-yl)prop-2-ynyl Acetate	[M-H] ⁻	255. 04852	C15H1202S	2, 5-disubstituted thiophenes	QRLHSFULTXQLE-UHFFFAOYSA-N	O=C (OCC#CC=1SC (=CC1) C=2C=CC=CC2) C
1046	2. 939	263. 138	8-acetyl-5, 7-dimethoxy-2, 2-dimethylchromene	[M+H] ⁺	263. 13	C15H1804	Precocenes	JELWYGQTQBQPH-UHFFFAOYSA-N	O=C (C1=C (OC) C=C (OC) C=2C=CC (OC21) (C) C) C
1047	2. 939	372. 09232	DTMBOA + O-Hex	[M-H] ⁻	372. 0929	C15H19N010	Benzoxazinoids	WTGXAWKYZMQEDA-UHFFFAOYNA-N	0=C2N (O) C=3C=CC (OC) =CC=3 (OC2 (OC1OC (C) C (O) C) C1 (O)))
1048	2. 944	144. 08055	Tryptophanol (not validated)	[M+H-H2O] ⁺	144. 082	C10H11N0	Indole and derivatives	MBBOMCVGYCRMEA-UHFFFAOYSA-N	OCCC2=CN=C1CC=CC=C12
1049	2. 956	265. 1185	Magnolol	[M-H] ⁻	265. 12341	C18H1802	Biphenyls and derivatives	VVOAZFWZEDHOOU-UHFFFAOYSA-N	OC1=C (C=C (CC=C) C=C1) C1=C (C) C=CC (CC=C) =C1
1050	2. 957	305. 07678	Glutamyl-S-(C3H5)-Cysteine sulfoxide	[M-H] ⁻	305. 07999	C11H18N206S	Peptides	LMNDKXWMBGGAL-UHFFFAOYNA-N	O=C (O) C (O) CCC (=O) NC (=O) CS (=O) C=CC
1051	2. 964	205. 14316	3, 5-dihydroxydecanoic acid	[M+H] ⁺	205. 14343	C10H2004	Medium-chain hydroxy acids and derivatives	WQZRAWSNEARGPV-UHFFFAOYSA-N	O=C (O) CC (O) CC (O) CCCCC
1052	2. 983	180. 10143	(S)-3-Amino-4-phenylbutyric acid	[M+H] ⁺	180. 1019	C10H13N02	Beta amino acids and derivatives	OFVBLKINTLPEGH-VIFFVBQESA-N	N[C@H] (CC (O) =O) CC1=CC=CC=C1
1053	2. 986	190. 05339	N-ACETYL-DL-METHIONINE	[M-H] ⁻	190. 054	C7H13N03S	Methionine and derivatives	XUYPXLMDZJIRQH-UHFFFAOYSA-N	O=C (O) C (NC (=O) C) CCSC
1054	2. 988	285. 1077	isosakuranetin	[M-H] ⁻	285. 10324	C16H1405	4'-O-methylated flavonoids	HMUJXQRRKBLVVO-AWEZNCQLSA-N	O=C1C=2C (O) =CC (O) =CC2OC (C3=CC=C (OC) C=C3) C1
1055	2. 99	405. 22357	(E)-Resveratrolside	[M-H] ⁻	405. 2236	C20H2209	Stilbene glycosides	OLCVOESSVCAFGR-CUYWLFDRSA-N	OC=1C=C (O) C=C (CC2=CC=C (OC3OC (C) C (O) C) C3O) C (O) =C2) C1
1056	2. 992	174. 09094	7-methanesulfinylheptanenitrile	[M+H] ⁺	174. 0956	C8H15N0S	Glucosinolate breakdown metabolites	MVGLREOVTAKNK-UHFFFAOYNA-N	N#CCCCCCCCS (=O) C
1057	2. 998	192. 10193	N, N-Diethyl-4-hydroxybenzamide	[M-H] ⁻	192. 103	C11H15N02	Benzamides	WLRVSRJKZYJCJY-UHFFFAOYSA-N	CCN (CC) C (=O) C1=CC=C (O) C=C1
1058	2. 998	190. 08568	synephrine	[M+Na] ⁺	190. 086	C9H13N02	1-hydroxy-2-unsubstituted benzenoids	YRCWQPVGYLSOX-UHFFFAOYSA-N	OC1=CC=C (C=C1) C (O) CNC
1059	3. 002	625. 32233	Dauricine	[M+H] ⁺	625. 32001	C38H44N206	Benzylisoquinolines	AQASRZOCERRGBL-R0JLC1KYSNA-N	OC1=CC=C (C=C1OC2=CC=C (C=C2) CC3C4=CC (OC) =C (OC) C=C4CCN3C) CC5C6=CC (OC) =C (OC) C=C6C7CN5C
1060	3. 003	352. 16083	MITOMYCIN C	[M+H] ⁺	352. 16153	C15H18N405	Mitomycins	NW1BSHFKLJFRCO-WUDYKRTCSA-N	O=C1C2=C (C (=O) C (N) =C1) C (COC (=N) O) C3 (OC) N2CC4NC43
1061	3. 005	329. 17172	(2E)-N-(4-acetamidobutyl)-3-(4-hydroxy-3-methoxyphenyl)prop-2-enamide	[M+H] ⁺	329. 17133	C16H22N204	Hydroxycinnamic acids and derivatives	ZVMGKOAHHB1HLO-SOPGYVHQSA-N	OC (=NCCCCN=C (O) C) C=C1=CC=C (O) C (OC) =C1
1062	3. 008	300. 19998	Dehydroabietamide	[M+H] ⁺	300. 19943	C20H29N0	Diterpenoids	AKKGFKWEDCJQJ-UHFFFAOYSA-N	N=C (O) C1 (C) CCCC2 (C3=CC=C (C=C3CC12) C (C) C) C
1063	3. 012	447. 1604	2-[2-(4-methyl-2-oxo-2h chromen-7-yl)oxy]acetyl]-2, 3, 4, 9-tetrahydro-1h-heta-carboline-3-carboxylic acid methyl ester	[M+H] ⁺	447. 16	C25H22N206	Beta carbolines	WYAYNBDJBJVOP-0AQYLSRUSNA-N	0=C1OC=2C=CC (=O) N3CC=4NC=5C=CC5C4OC3C (=O) OC) C=CC2C=C1C
1064	3. 012	301. 15369	Pesticide3_Bifenazate.C17H20N203.1-Methylethyl 2-(4-methoxybiphenyl-3-yl)hydrazinecarboxylate	[M+H] ⁺	301. 15399	C17H20N203	Biphenyls and derivatives	VHLKTXFWDRIX1LV-UHFFFAOYSA-N	OC (=NCC=1C=C (C=CC1OC) C=2C=CC=CC2) OC (C) C
1065	3. 025	254. 14897	Irgarol	[M+H] ⁺	254. 14339	C11H19N6S	Methylthio-s-triazines	HDHLIWCXDDZUFH-UHFFFAOYSA-N	CC (C) (C) NC1=NC (=NC2CC2) N=C (N1) SC
1066	3. 033	400. 18982	Thiethylperazine	[M+H] ⁺	400. 18756	C22H29N3S2	Phenothiazines	XTCTYLCDETUOIP-UHFFFAOYSA-N	CCSC1=CC2=C (SC3=CC=CC=C3N2CCN2CCN (C) CC2) C=C1
1067	3. 037	284. 0397	CGS 15943	[M-H] ⁻	284. 03445	C13H8C1N50	Quinazolinamines	MSJODEOZODDVGW-UHFFFAOYSA-N	C1C=1C=CC=2NC (=N) N3N=C (N=C3C2C1) C=4OC=CC4
1068	3. 039	312. 1459	7-methoxy-6-(1, 2, 3-trihydroxy-3-methylbutyl)chromen-2-one	[M+H] ⁺	312. 14417	C15H1806	Coumarins and derivatives	PCSZTTAMZGNGNB-UHFFFAOYSA-N	O=C1OC=2C=C (OC) C (=C2C=C1) C (O) C (O) C (O) C
1069	3. 04	245. 18495	Leucylleucine	[M+H] ⁺	245. 187	C12H24N203	Dipeptides	LCPPYQJ1KPJDLBL-UHFFFAOYNA-N	O=C (O) C (NC (=O) C) CC (C) C
1070	3. 041	283. 09219	4-methoxy-9-(2-methylbut-3-en-2-yl) furo[3, 2-g]chromen-7-one	[M-H] ⁻	283. 09756	C17H1604	5-methoxypsoralens	ZPLVEUISKJ1JDT-UHFFFAOYNA-N	O=C1OC2=C (C=C1) C (OC) =C3C=OC3=C2C (=C) (C) C
1071	3. 042	401. 10739	Apodanthoside (Not validated)	[M-H] ⁻	401. 10849	C17H22011	Iridoid glycosides	QXLZMPXGMPPIPW-UHFFFAOYNA-N	0=C (OC) C2=COC (OC1OC (CO) C (O) C) C1 (O)) C3C (=CC23) C (=O) O
1072	3. 045	262. 11789	BIOTIN	[M+H] ⁺	262. 12198	C10H16N203S	Biotin and derivatives	YBJHBARHTGYGT-ZKWXUAAHSA-N	O=C (O) CCCCC1SCC2N=C (O) NC21
1073	3. 046	285. 10678	Epoxy (4, 5A)alpha)-4, 5-Dihydrosantonin	[M+H] ⁺	285. 10971	C15H1804	Eudesmanolides, sesquidesmanolides, and	GTD1WC1TYRGAKM-ORRHJWQCSA-N	O=C1OC2C (CCCC (C=CC (=O) C4 (OC243) C) C) C1C

1074	3. 051	447. 15884	Gefitinib (Iressa)	[M+H] ⁺	447. 159	C22H24ClFN4O3	Quinazolinamines	XGALLCVXEZPNRQ-UHFFFAOYSA-N	FC1=CC=C(C=C1C1)NC=2N-CN=C3C=C(OC)C(OC(CN4COC3C4)=CC32
1075	3. 054	425. 19089	6-Hydroxysumatrol	[M-H] ⁻	425. 19553	C23H22O8	Rotenones	RMAYNNFCPNGTQW-UHFFFAOYSA-N	O=C1C2=C(O)C=C3OC(C=C)C(C3)=C2OC4C(O)OC5=CC(OC)=C(OC)C=C(C14)
1076	3. 054	420. 14963	Chloroaustralasine C	[M+H] ⁺	420. 155	C22H26ClN5O5	Pyranquinolines	XVDZSHAEMKCIW-DBFNBLSLA-N	O=C(OCN1C(=O)C2=C(OC(C)(C)C3CC(O)(C)C(C1)C23)C=C4CC=C(C41)C
1077	3. 056	350. 12189	Voriconazole	[M+H] ⁺	350. 12201	C16H14F3N5O	Phenylpropanes	BCEHBSKCWLPMON-MGPLVRAMSA-N	FC1=CC=C(C(F)=C1)C(O)(CN2N-CN=C2)C(C=3N-CN=CC3F)C
1078	3. 06	311. 0321	Cotarnine Chloride	[M+H] ⁺	311. 0321	[C12H15ClN4] ⁻	Tetrahydroisoquinolines	UONSFNPHCTWRGS-UHFFFAOYSA-M	[C1-]. OC1C2=C(OC)C=3OC3C=C=C2CCN1C
1079	3. 062	283. 10977	2-(4-oxoquinazolin-3(4H)-yl)ethyl isobutyrate	[M+H] ⁺	283. 10999	C14H16N2O3	Quinazolines	DXZNCVCRUZDRWL-UHFFFAOYSA-N	O=C(OCN1C=NC=CC=CC2C1=O)C(C)C
1080	3. 062	237. 07712	Pesticide5_Metribuzin_C8H14N4O5_4-Amino-6-(2-methyl-2-propanyl)-3-(methylsulfanyl)-1,2,4-triazin-5(4H)-one	[M+H] ⁺	237. 078	C8H14N4O5	Aryl thioethers	FOFZRZUHNHCZPX-UHFFFAOYSA-N	O=C1C(=NN=C(SC)N1N)C(C)C(C)C
1081	3. 064	404. 14612	_130050	[M+H] ⁺	404. 147	C22H23N5O5	Phenylquinolines	PJPKEOASXRGMD-SIKLNZKXSA-N	O=C1NC=2C=CC=3C=CC(OC3C2C(O)(C4=CC=C(OC)C=C4)C1OC)(C)C
1082	3. 074	261. 04266	Methyl 7-Deshydroxyprogallin-4-Carboxylate	[M-H] ⁻	261. 04044	C13H10O6	Tropolones	DQWQITLWUFBXON-UHFFFAOYSA-N	O=C(OC)C1=CC(=O)C(O)=C2C(O)=C(C)C=CC2=C1
1083	3. 074	137. 02448	P-HYDROXYBENZOIC ACID	[M-H] ⁻	137. 02441	C7H6O3	Hydroxybenzoic acid derivatives	FJKROLUGYXJWQN-UHFFFAOYSA-N	OC(=O)C1=CC(=O)C(C)=C1
1084	3. 077	216. 08636	N-(2-furylmethyl)-9H-purin-6-amine	[M+H] ⁺	216. 08701	C10H9N5O	6-alkylaminopurines	QANMHLXAZMSUEX-UHFFFAOYSA-N	N=1C=NC(NCC=2OC=CC2)=C3N=CNC13
1085	3. 088	255. 17235	alpha-Estradiol	[M+H] ⁺	255. 17435	C18H24O2	Estrogens and derivatives	VOXZDWNVPJITMN-AWDGRILASA-N	CC12CCC3C(CCC4=CC(O)=CC=C34)C1CC([C@H]2O)
1086	3. 089	317. 11163	Tanshinone IIA	[M+H] ⁺	317. 10999	C19H18O3	Tanshinones, isotanshinones, and 3'-O-methylated flavonoids	HYXITZLLTYIPDF-UHFFFAOYSA-N	O=C1C(=O)C2=C(C=CC3=C2CCCC3(C)C)=C4OC(C(C14)C
1087	3. 093	301. 12839	5, 7-dihydroxy-2-(4-hydroxy-3-methoxyphenyl)-2, 3-dihydrochromen-4-one	[M-H] ⁻	301. 12933	C16H14O6	Flavonoids	FTDDBIPDXTXRG-UHFFFAOYSA-N	O=C1C=C2C(O)=CC(O)=CC2OC(C3=CC=CC(O)C(OC)=C3)C1
1088	3. 093	166. 1223	Hordeanine	[M+H] ⁺	166. 12	C10H15NO	Phenethylamines	KUBCEEMXQZUPDQ-UHFFFAOYSA-N	OC1=CC=C(C=C1)CCN(C)C
1089	3. 097	285. 12268	Prolylphenylalanine	[M+H] ⁺	285. 12094	C14H18N2O3	Dipeptides	IWTANZLCJYVEFX-UHFFFAOYSA-N	O=C(O)C(N=C(O)C1NCCC1)CC=2C=CC=CC2
1090	3. 098	395. 14761	Arctigenin	[M+H] ⁺	395. 147	C21H24O6	Dibenzylbutyrolactone lignans	NOQVSMVKKMHTF-JKSUJKBBSA-N	O=C1OCC(CC2=CC=C(OC)C(OC)=C2)C1CC3=CC=C(C)C(OC)=C3
1091	3. 114	376. 10229	1-(3,4-dihydroxyphenyl)-6,7-dihydroxy-1,2-dihydronaphthalene-2,3-dicarboxylic acid	[M+H] ⁺	376. 10269	C18H14O8	Aryltetralin lignans	WJMFQMBNLYADA-UHFFFAOYSA-N	O=C(O)C1=CC=2C=C(O)C(O)=C2C(C3=CC=C(O)C(O)=C3)C1C(=O)
1092	3. 116	486. 18063	(1S,3R,17S,19S)-3-hydroxy-9,16,16-tetramethyl-8-oxa-14,23,25-triazabentacyclo[7.5.2.0(2,22).0(2,22).0(2,22).0(2,22)hexacos-3aR,3a1S,5S,5aS,10bS)-methyl 6-acetyl-3a-ethyl-2,3,3a,3a1,4,5,5a,6,11,12-decahydro-1H-indolizino[8,1-cd]carbazole-5-carboxylate	[M+H] ⁺	486. 17896	C26H29N3O4	2,2-dimethyl-1-benzopyrans	PYHKDROALAEDE-VKAWXPLSA-N	O=C1N2CCCC3C(O)=NC14C5(O)C6=CC=C(COC7=C6N=C5C(C)(C)C4C3)C1C
1093	3. 119	383. 22815	(3aR,3a1S,5S,5aS,10bS)-methyl 6-acetyl-3a-ethyl-2,3,3a,3a1,4,5,5a,6,11,12-decahydro-1H-indolizino[8,1-cd]carbazole-5-carboxylate	[M+H] ⁺	383. 23001	C23H30N2O3	Aspidospermat-type alkaloids	DHHWJWGDXKXSV-HFOUZZJZSA-N	O=C(OC)C1CC2(CC)CCN3CC4(C=5C=CC=CC5N(C(=O)C)C14)C32
1094	3. 12	274. 12805	phenylglucoside	[M+H] ⁺	274. 12851	C12H16O6	Phenolic glycosides	NEZJDVYDZSTRFS-RMPHRYRLSA-N	OC1OC(OC=2C=CC2)C(O)C(C)C1O
1095	3. 127	343. 18509	4,5-dihydroxy-4,5,6-trimethyl-2,8-dioxo-13-azatricyclo[8.5.1.0(2,22)hexadec-10-ene-3,7-dione	[M+H] ⁺	343. 18634	C16H23NO6	Pyrrrolizines	WOPYGCANEAIOEM-UHFFFAOYSA-N	O=C1OCC2=CCN3CCC(=O)C(=O)C(O)(C)C(O)C(C1)C23
1096	3. 129	317. 1116	6-(2-hydroxyethyl)-6,6a-dihydroisindolo[2,1-a]quinazoline-5,11-dione	[M+H] ⁺	317. 10999	C17H14N2O3	Indoloquinazolines	CWG1HUKKVIQOGZ-UHFFFAOYSA-N	O=C1C=C2C=CC=C2C3N1C=4C=CC=CC4(=O)N3COC
1097	3. 137	253. 16391	Hexazinone	[M+H] ⁺	253. 16591	C12H20N4O2	Dialkylarylaminines	CAXWKEEDBZRFPE-UHFFFAOYSA-N	CN(C)C1=NC(N(C2CCC2)C(N1C)=O)=O
1098	3. 137	286. 13019	Piperine	[M+H] ⁺	286. 14001	C17H19NO3	Alkaloids and derivatives	MXWOMOGUJBK1W-YPYC1CBESA-N	O=C(C=CC=CC1=CC=C2OCC2=C1)N3CCCC3
1099	3. 14	295. 12747	bakuchiol	[M+H] ⁺	295. 12744	C18H24O	Aromatic monoterpenoids	LFYJSSARVMHQJB-QIXNEVBVSA-N	OC1=CC=C(C=C1)C=CC(C=C)C(C)C=C(C)C
1100	3. 145	192. 13791	4-Methylethcathinone	[M+H] ⁺	192. 138	C12H17NO	Alkyl-phenylketones	ZOXZWYWOECBSH-UHFFFAOYSA-N	O=C(C1=CC(=C(C=C1)C)C(NC)C
1101	3. 163	266. 13104	8-acetamido-2-methyl-7-oxononanoic acid	[M+H] ⁺	266. 13626	C12H21NO4	Medium-chain fatty acids	UALLEVOGEQZKXS-UHFFFAOYSA-N	O=C(O)C(C)CCCC(=O)C(N=C(O)C)C
1102	3. 163	682. 36823	S4:19(P3:17/F1:2)	[M+H] ⁺	682. 37207	C31H52O15	Saccharolipids	NNYRMBHXZJRGU-UHFFFAOYNA-N	CCCCC(=O)OC1C(OC2(CO)OC(CO)C(OC(C)=O)C2O)OC(CO)C(OC(=O)CCCC)C1OC(=O)CCCC
1103	3. 169	197. 07062	benzo[b][1,8]naphthyridin-5-ol	[M+H] ⁺	197. 07001	C12H8N2O	Hydroquinolones	DAFMSUZBESPPSV-UHFFFAOYSA-N	OC1=C2C=CC=NC2=NC=3C=CC=CC31
1104	3. 178	299. 15927	6-Shogaol	[M+H] ⁺	299. 16	C17H24O3	Shogaols	OQWKEEDHDMUXEO-BQYQJAHWSA-N	O=C(C=CCCCC)CCC1=CC=C(O)C(OC)=C1
1105	3. 182	318. 20459	Nateglinide (Starlix)	[M+H] ⁺	318. 20599	C19H27NO3	Phenylalanine and derivatives	OELFLUMRDSZNSF-BRWVUGUISA-N	O=C(O)C(NC(=O)C1CCC(C)C(C)C)CC=2C=CC=CC2
1106	3. 186	160. 03951	2, 8-Quinolinediol	[M-H] ⁻	160. 04041	C9H7NO2	Quinolones and derivatives	ZXZKYHTWJHFT-UHFFFAOYSA-N	OC=1N=C2C(O)=CC=CC2=C1
1107	3. 195	476. 22162	1-(9-hydroxy-2-isopropyl-10-(2,3,4-trimethoxyphenyl)pyrrolo[3',4'':6,7]azepino[4,3,2-cd]indol-8(2H,7H,10H)-	[M+H] ⁺	476. 22	C27H29N3O5	Benzazepines	QAPJG1XRNRPRW-UHFFFAOYSA-N	O=C(N1C(O)=C2C(=NC3=CC=CC4=C3C(=CN4(C)C)C2C5=CC=C(OC)C(OC)=C5OC)C1)C
1108	3. 2	341. 16959	Cinanserin	[M+H] ⁺	341. 16821	C20H24N2O5	Cinnamic acid amides	RSUVYMGADVGOU-UHFFFAOYSA-N	OC(=NC1=C=CC1SCCCN(C)C)C=CC=2C=CC=CC2
1109	3. 205	217. 09842	1, 2, 3, 4-tetrahydro-6-methoxy-1-oxo-beta-carboline	[M+H] ⁺	217. 10001	C12H12N2O2	Beta carbolines	PWARHOUWJUADN-UHFFFAOYSA-N	O=C1NCCC=2C=3C=C(OC)C=C3CCN12
1110	3. 205	293. 1235	Glutamylphenylalanine	[M-H] ⁻	293. 12369	C14H18N2O5	Amino acids	XHHOZFPNYFQJL-UHFFFAOYNA-N	O=C(O)C(N)CCC(=O)NC(C(=O)O)CC1=CC=CC=C1
1111	3. 213	337. 17365	Hapalindole D	[M+H] ⁺	337. 17401	C12H14N2S	Bicyclic monoterpenoids	PHWOUZMWNUINO-QAUUQPOASA-N	S=C=NC1C(C2=CNC=3C=CC=CC32)C(C(=C)C)CCC1(C=C)C
1112	3. 22	438. 23776	Lunarine	[M+H] ⁺	438. 23871	C25H31N3O4	Macrolactams	Y1WJEBPTHXHQF-L1ML1WGDASA-N	O=C1CCC23C=CC(O)=NCCC(NCCN=C(O)C)C=CC=4C=CC(OC2C1)=C3C4
1113	3. 222	178. 05336	Cyclamate	[M-H] ⁻	178. 05434	C6H13NO3S	Cyclamates	HCAJEUSONLESMK-UHFFFAOYSA-N	C1OCC(C)NS(O)(=O)=O
1114	3. 222	312. 14291	Domoic acid	[M+H] ⁺	312. 14301	C15H21NO6	Kainoids	VZFRNCSOCOPNDB-ZDUSDAASANA-N	O=C(O)CC1C(NCC1C(=CC=CC(C(=O)O)C)C)C(=O)O
1115	3. 244	269. 04083	(3R)-8-hydroxy-3-(4-methoxyphenyl)-3,4-dihydroisochromen-1-one	[M-H] ⁻	269. 04114	C16H14O4	2-benzopyrans	DEF1JGJJKEYGS-CQSAC1VSA-N	O=C1OC(C2=CC=C(OC)C=C2)CC=3C=CC=C(O)C13
1116	3. 244	187. 18019	Lupinine	[M+H] ⁺	187. 18048	C10H19NO	Lupinine-type alkaloids	HDVAWXJVMJBAR-VHSXEESVSA-N	OC1CCN2CCOCC21

1117	3.244	283.16461	Panaxadiol	[M+H] ⁺	283.16	C17H24O2	Long-chain fatty alcohols	D5VMGWEVREYQ-ODQHUEKSA-N	OC(C#CC#CC(=O)CCCCC)C=C
1118	3.253	138.05614	2-Pyridylacetic acid	[M-H] ⁻	138.05496	C7H7NO2	Pyridines and derivatives	BPSNETAJDFTO-UHFFFAOYSA-N	c1ccnc(c1)CC(=O)O
1119	3.253	359.23135	Ochroposinin	[M+H] ⁺	359.233	C21H30N2O3	Beta carbolines	CMGYMWXDJQLJ-DEYYWGMSA-N	CCCC1CC2C=3NC=4C(OC)C(OC)=CC4C3CN2C1CC
1120	3.255	112.0389	2,3-Dihoxypyridine	[M+H] ⁺	112.03931	C5H5NO2	Pyridinones	GGOZGYRTNRSSA-UHFFFAOYSA-N	c1cc(c(nc1))O=O
1121	3.261	162.05431	Indole-3-carboxylic acid	[M+H] ⁺	162.05496	C9H7NO2	Indolecarboxylic acids and derivatives	KMAKOBLIOCQGJP-UHFFFAOYSA-N	O=C(O)C1=CNC=CC=C2C1=C
1122	3.264	316.18655	Nateglinide	[M-H] ⁻	316.1918	C19H27NO3	Phenylalanine and derivatives	OELFLUMRDSZNSF-UHFFFAOYNA-N	O=C(O)C(N=C(O)C1CCC(C)C(C)C)CC=CC=CC2
1123	3.268	154.04942	5-Aminosalicylic acid	[M+H] ⁺	154.04987	C7H7NO3	Aminobenzoic acids	KBOPZPVLCLAV-UHFFFAOYSA-N	O=C(O)C1=CC(N)=CC=C1O
1124	3.274	167.10629	Pesticide4_Cyromazine_C6H10N6_Vetrazin	[M+H] ⁺	167.104	C6H10N6	N-aliphatic s-triazines	LVDK1WDGRHTE-UHFFFAOYSA-N	N=C1NC(=N)NC(=NC2CC2)N1
1125	3.279	229.09686	Ozagrel	[M+H] ⁺	229.097	C13H12N2O2	Cinnamic acids	SHZKQBHERIJWAO-AATRIKPKSA-N	O=C(O)C(=C1CC=C(C=C1)CN2C=NC=C2
1126	3.281	145.04991	2-Methylglutaric acid	[M-H] ⁻	145.05063	C6H10O4	Methyl-branched fatty acids	AQYCMVICNBXNA-UHFFFAOYNA-N	CC(CCC(O)=O)C(O)=O
1127	3.284	190.04993	5-HYDROXYINDOLEACETATE	[M-H] ⁻	190.05	C10H9NO3	Indole-3-acetic acid derivatives	DUUGKCCEGLZNO-UHFFFAOYSA-N	O=C(O)CC1=CNC=CC(=O)C=C21
1128	3.29	490.2728	Delsoline	[M+H] ⁺	490.26999	C25H41NO7	Aconitane-type diterpenoid alkaloids	JYBLTQQBEQLEY-DIZROMASANA-N	OC1CCC2(COC)CN(CC)C3C4(O)(CO)C2C1C3C5OC6(OC)CC4(O)C5C6O
1129	3.292	263.13879	Delsohexital	[M+H] ⁺	263.13901	C14H18N2O3	Barbituric acid derivatives	NZXKDXXBHYTKP-UHFFFAOYNA-N	O=C1NC(O)C(C(=O)N1C)(CC=C)C(C#CC)C
1130	3.305	352.10245	Parfumine	[M-H] ⁻	352.10706	C20H19NO5	Indanones	AINUBWOYIOHGFN-UHFFFAOYSA-N	O=C1C2=C3COC3C=CC(=O)C1C4C5=CC(O)=C(CO)C=C5OC4C
1131	3.314	198.13458	2-Hydroxyatrazine	[M+H] ⁺	198.13493	C8H15N5O	1,3,5-triazines	NFMIMWNQAWNDU-UHFFFAOYSA-N	CCN=C1NC(=NC(C)C)NC(=N)O
1132	3.315	201.0761	Diethyloxalpropionate	[M-H] ⁻	201.07684	C9H14O5	Gamma-keto acids and derivatives	NGRAIMFUWGAEU-UHFFFAOYSA-N	O=C(OCC)C(=O)CCC(=O)OCC
1133	3.317	554.26862	(12bS)-7-(4-ethylphenyl)-12b-methyl-2-(3,4,5-trimethoxybenzyl)-2,3,6,7-tetrahydronaziridinol ¹ , 2'-yl-2-hydroxy-3,4-dihydro-1,4-dioxo-1,4-dione	[M+H] ⁺	554.27002	C38H35N3O5	Beta carbolines	WNGVOVMNRJJOX-RULBIHMZSA-N	O=C1NC2C(C3=C(C=C3)C(=O)C(=O)C=C5C4C2C(=O)N(C)CC6=C(C(=O)C(=O)C)C(=O)C)C1C
1134	3.319	167.03412	4-Hydroxymandelic acid	[M-H] ⁻	167.03499	C8H8O4	1-hydroxy-2-unsubstituted benzenoids	YHXHKYRLYLQTH-UHFFFAOYNA-N	O=C(O)C(O)C1=C(C=O)C(C)C1
1135	3.326	354.11731	2-(4a,9,10a-trihydroxy-1-methyl-5,10-dioxo-3,4-dihydro-1H-benzof[3,2-b]pyridine-3-yl)acetic acid	[M+H] ⁺	354.11835	C16H16O8	Naphthopyranones	JJKCXJIYNIHOS-UHFFFAOYSA-N	O=C(O)CC1OC(C)C2(O)C(=O)C=CC(=O)C2(O)C1
1136	3.326	435.18414	Artocaprin	[M-H] ⁻	435.1813	C26H28O6	3-prenylated flavones	KRGDFVWQJIMEK-RMKNTFCPSA-N	COc1c(\C=C\C(C)C)C(C)C(=O)C2C(OC(=C(C(C)C)C)C2=O)C2=CC=C(C)C(=O)C2=O
1137	3.327	243.1702	Isoleucylisoleucine	[M-H] ⁻	243.1716	C12H24N2O3	Peptides	BCVIOZZGJNOES-UHFFFAOYNA-N	O=C(O)C(NC(=O)C(N)C(C)CC)C(C)CC
1138	3.338	217.09648	Carboline base + 4H, carboxylic acid	[M+H] ⁺	217.10069	C12H12N2O2	Carbolines	FSCNEEGOMTYKY-UHFFFAOYNA-N	O=C(O)C3NC(=O)C=C(C)C=C1C2=C3
1139	3.34	251.01828	FT-thioether	[M-H] ⁻	251.01706	C7H9FSO2S	PFSA	KVLYLHRZJIPAQE-UHFFFAOYSA-N	O=C(O)C(=O)CCSCC(F)(F)C(F)F
1140	3.348	464.2598	(3S,3'R,3'as,6'S,6aS,6bS,7ar,9R,11bR)-3-hydroxy-3',6',10,11b-tetramethylsino[1,2,3,4,6,6a,6b,7,8,11a-decahydrobenzo[f]fluorene-9,2'-diol	[M+H] ⁺	464.25613	C27H39NO3	Jerveratrume-type alkaloids	CLEXYPLHGJONT-GDMKTYSQSA-N	O=C1C2=C(C)C3(COC4C(C)C(C)C4)CC2C3C(=O)CC6(C)C=C15
1141	3.352	595.16992	5,7-dihydroxy-2-(2-hydroxyphenyl)-3-(1-(2R,3S,4R,5R,6S)-3,4,5-trihydroxy-6-((1-(2R,3S,4S,5S,6S)-3,4,5-trihydroxy-6-methyltetrahydro-2H-pyran-2-ylideneamino)oxy)phenyl)-propan-1-one	[M+H] ⁺	595.16998	C27H30O15	Flavonoid-3-O-glycosides	BJJCXTDXEJUWIC-RGLPMSMOA-N	O=C1C(OC2OC(COC3OC(C)C(O)C3O)C(C)C2O)=C(OC(=O)C(=O)C(C)C1)C=C5C(=O)C=C5O
1142	3.352	489.13254	Agusine	[M+H] ⁺	489.13	C22H26O11	Iridoid O-glycosides	GLAGCTACLKIJX-QNAXTHAFSA-N	O=C(OCC1=CC(O)C2=C=CC(OC3OC(C)C(O)C(C3O)C12)C4=CC=C(O)C=C4
1143	3.356	457.10947	Naringenin-7-O-beta-D-glucoside	[M+H] ⁺	457.10999	C21H20O10	Flavonoid-7-O-glycosides	DLIKSSGEMUFQOK-SFTVRKLSA-N	O=C1C2=C(O)C=C(OC3OC(C)C(O)C3O)C=C2OC(C4=CC=C(O)C=C4)C1
1144	3.357	455.09698	Riboflavin-5'-monophosphate	[M-H] ⁻	455.09735	C17H21N4O9P	Flavin nucleotides	FVTCRASFADXXNN-SCRDCRAPSA-N	CC1=CC2=C(C=C1)N(C[C@H](O)[C@@H](O)[C@H](O)COP(O)(O)=O)C1=NC(=O)N=C(O)C1=N2
1145	3.36	180.0291	DIBOA	[M-H] ⁻	180.02921	C8H7NO4	Benzoxazinoids	COVOPZQCGJUPY-UHFFFAOYNA-N	O=C1N(O)C2=CC=CC(=O)C1(O)
1146	3.362	136.03967	4-AMINO BENZOATE	[M-H] ⁻	136.03999	C7H7NO2	Aminobenzoic acids	ALYNCZND1QEVRU-UHFFFAOYSA-N	O=C(O)C1=CC=C(N)C=C1
1147	3.368	207.14842	Pesticide3_Isoproturon_C12H18N2O_Arelon	[M+H] ⁺	207.149	C12H18N2O	N-phenylureas	PUIYMUZLKQOUZ-UHFFFAOYSA-N	O=C(NC1=CC=C(C=C1)C(C)C)N(C)C
1148	3.371	293.10114	_120106	[M+H] ⁺	293.10101	C15H16O6	2-benzopyrans	MMHTXATDNFMYU-UHFFFAOYSA-N	O=C1OC2(C(=CC(O)C(O)C2)C=3C=C(OC)C=C(O)C13)C
1149	3.375	273.21927	5-beta-Androstan-17-beta-ol-3-one	[M+H] ⁺	273.22128	C19H30O2	Androgens and derivatives	NYKAWKGWV1WPM-NOLKSFPSPA-N	CC12CCC3(C(C[C@H]4CC(=O)CCC43)C1CC[C@H]52O
1150	3.375	436.18503	PHYSTOSTIGMINE SALICYLATE	[M+H] ⁺	436.18427	C22H27N3O5	Pyrroloindoles	HZOTZTANVBDFOP-PBQOUBLSA-N	O=C(O)C1C=CC=CC1O.OC(=NC)OC1=CC=C(C=C1)C3(C)CC(N)C3N2C
1151	3.381	250.09113	(2E,4E)-N-(2-methylpropyl)-6-thiophen-2-ylhexa-2,4-dienamide	[M+H] ⁺	250.09003	C14H19NO5	N-acyl amines	KNGBFMEGLRFVH-PRKJIMSOSA-N	OC(=NC(C)C)C=CC(=O)C=C1C
1152	3.386	353.16858	7-[(2E,5E)-7-hydroxy-3,7-dimethylocta-2,5-dienoxy]chromen-2-one	[M+H] ⁺	353.1683	C19H22O4	Coumarins and derivatives	ZHQPRJMIALLFHX-ATTWORZSA-N	O=C1OC=2C=C(OC)C(C)CC(=O)C(C)C=C2C2=C1
1153	3.388	230.11665	Sebutylazine	[M+H] ⁺	230.1167	C9H16ClN5	1,3,5-triazine-2,4-diamines	BZRUVKZGXNSXMB-UHFFFAOYNA-N	CCN=C1NC(NC(C1)=N)=NC(C)CC
1154	3.397	212.12766	Mescaline	[M+H] ⁺	212.12801	C11H17NO3	Phenethylamines	RHCSKNNOAZULRK-UHFFFAOYSA-N	O(C1C=C(C=C(C(OC)C1OC)CC)C
1155	3.397	187.13246	Royal jelly acid	[M+H] ⁺	187.13	C10H18O3	Medium-chain hydroxy acids and derivatives	QHBZHVUGROELI-SOFGYVWQSA-N	O=C(O)C=CCCCCCC
1156	3.398	425.1954	2-(3,4-dihydroxyphenyl)-5,7-dihydroxy-6,8-dimethoxychromen-4-one	[M+H] ⁺	425.1951	C17H14O8	8-O-methylated flavonoids	QHMWHJFJTURES-UHFFFAOYSA-N	O=C1C=C(OC=2C(OC)=C(O)C(C)C(OC)=C3C=C(OC)C=C(C)C3
1157	3.398	324.11081	Dehydroevodiamine	[M+H] ⁺	324.11099	C19H15N3O	Quinazolinones	VXHSVKJHXSXKM-UHFFFAOYSA-N	O=C1C=2C=C(=CC2N1)(=C3=C4[N-]C=5C(=O)C=C5C4ACN13)C
1158	3.415	188.06987	Desethylatrazine	[M+H] ⁺	188.06975	C6H10ClN5	1,3,5-triazine-2,4-diamines	DFWFIQMSFGDQ-UHFFFAOYSA-N	CC(C)N=C1NC(C1)=NC(=N)N1
1159	3.416	151.039	L-(-)-Mandelic acid	[M-H] ⁻	151.04007	C8H8O3	Benzene and substituted derivatives	1WYDHOAUDTYEUF-SSDOTSWSA-N	O[C@H](O)C(=O)C1=CC=CC=C1

1160	3. 421	226. 10651	6-Benzyladenine	[M+H] ⁺	226. 10899	C12H11N5	6-alkylaminopurines	NWEJYWHLCVSVIJ-UHFFFAOYSA-N	N=1C=NC=2C1NC=NC2NC=3C=C=CC3
1161	3. 426	334. 17429	convolvicine	[M+H] ⁺	334. 17001	C18H23N05	P-methoxybenzoic acids and derivatives	HZE0ENYXYFFIU-QDMKHRRSA-N	O=C (OC) CC2N (C (=O) C) (CC2) C1 C3=C=C=C (OC) C (OC) C=C3
1162	3. 427	359. 12326	9-methoxy-4, 4-dimethyl-13-phenyl-6, 14-dioxatetracyclo[8. 4. 0. 0 ² . 2. 0 ² . 2]tetradeca-1, 7, 9-trien-11-one	[M+H] ⁺	359. 12537	C21H20O4	Pyranoflavonoids	NGRRXMEVSBATO-UHFFFAOYSA-N	O=C1C2=C (OC) C=C3OC4C (C3=C2OC (C=5C=CC=OC5) C1) C4 (C) C
1163	3. 445	154. 06151	L-HISTIDINE	[M-H] ⁻	154. 062	C6H9N3O2	Histidine and derivatives	HNDVDQJC1GZPNO-UHFFFAOYSA-N	O=C (O) C (N) CC1=CN=CN1
1164	3. 45	411. 17828	Gomisin J	[M+H] ⁺	411. 17801	C22H28O6	Hydrolyzable tannins	PICOUNAPKDEPCA-TXEJJXNPSA-N	OC1=CC2=C (C (OC)=C1OC) C3=C (OC) C (OC)=C (O) C=C3CC (C) C (C) C2
1165	3. 45	377. 1488	Vincamine	[M+H] ⁺	377. 14786	C21H26N2O3	Eburnan-type alkaloids	RXPRRQKFXBCSJ-G1VPXCGWSA-N	O=C (OC) C1 (O) N2C=3C=CC=CC34=C2C5N (CC4) CCCC5 (CC) C1
1166	3. 458	305. 12299	(2S, 3S)-2-(3, 4, 5-trihydroxyphenyl)-3, 4-dihydro-2H-chromene-3, 5, 7-triol	[M-H] ⁻	305. 12299	C15H14O7	Epigallocatechins	XMOCLSLCDHWDHP-WFASDCNBSA-N	OC=1C=C (O) C2=C (OC (C3=CC (O) =C (O) C (O) =C3) C (O) C2) C1
1167	3. 464	179. 03427	Caffeic acid	[M-H] ⁻	179. 03499	C9H8O4	Hydroxycinnamic acids	KATPRVGONGVQAS-RQOWECAXSA-N	OC (=O) \C=C/C1=CC (O) =C (O) C=C1
1168	3. 472	251. 14108	Caffeoyl putrescin (isomer of 1060)	[M+H] ⁺	251. 1407	C13H18N2O3	Caffeic acid and derivatives	KTNZCYCTXQYEHT-UHFFFAOYSA-N	O=C (C=CC=1C=CC (O) =C (O) C=1) NCCCCN
1169	3. 476	304. 16455	scopolamine	[M+H] ⁺	304. 16	C17H21NO4	Beta hydroxy acids and derivatives	STECJAGHUSJQJN-KXKVBQCLSA-N	O=C (OC1CC2N (C) C (C1) C3OC32) C (C=4C=CC=CC4) CO
1170	3. 48	188. 07005	4-hydroxy-4-(pyridin-2-yl)butan-2-one	[M+H] ⁺	188. 07001	C9H11NO2	Pyridines and derivatives	NYKHQRHPWDLZTL-UHFFFAOYSA-N	O=C (C) CC (O) C1=NC=CC=C1
1171	3. 48	194. 11719	Salsoline	[M+H] ⁺	194. 11749	C11H15NO2	Tetrahydroisoquinolines	YTPRLBGPZHUPO-UHFFFAOYSA-N	OC=1C=C2C (-CC1OC) C (NCC2) C
1172	3. 481	346. 22156	XLR11 N-(4-HYDROXYPENTYL)	[M+H] ⁺	346. 21701	C21H28FN02	N-alkylindoles	MDPXYRYUGDTVIS-UHFFFAOYSA-N	O=C (C1=CN (C=2C=CC=CC12) CCCC (O) CP) C3C (C) (C) C3 (C) C
1173	3. 483	226. 08589	2'-Deoxycytidine	[M-H] ⁻	226. 08333	C9H13N3O4	Pyrimidine 2'-deoxyribonucleosides	CKTSBUTUHMZGZ-UHFFFAOYNA-N	N=C1N=C (O) N (C=C1) C2OC (CO) C (O) C2
1174	3. 492	73. 06451	ETHYL METHYL KETONE	[M+H] ⁺	73. 06479	C4H8O	Ketones	ZWEHNRKPNVVGH-UHFFFAOYSA-N	CCC (C) =O
1175	3. 497	130. 08614	N-Methyl-L-proline	[M+H] ⁺	130. 08626	C6H11NO2	Proline and derivatives	CWLQUGTUXBTLF-YFKPYBVYSA-N	CN1CCC[C@H]1C (=O) O
1176	3. 498	587. 33295	Anthranoyllycotonine	[M+H] ⁺	587. 3327	C32H46N2O8	Alkaloids	NNDHVDYFEDRMGH-UHFFFAOYNA-N	CCN1CC2 (CC (=O) C3=C (N) C=CC=C3) CCC (OC) C34C5CC6 (OC) C5C (C (OC6O) C (O) C (OC) C23) C14
1177	3. 498	213. 16159	Caryophyllene [T(-)]	[M+H] ⁺	213. 16136	C14H22	Branched unsaturated hydrocarbons	INOSMBKABLJUL-CHWSQXEYSA-N	C=C1CC=C (C) CCC2C1CC2 (C) C
1178	3. 498	441. 22687	Deacetylgedunin	[M+H] ⁺	441. 22714	C26H32O6	Limonoids	HCEYJYMN1GHPK-DXTZDJJUSA-N	O=C1OC (C2=COC=C2) C3 (C) CCC4C5 (C=CC (=O) C (C) C5CC (O) C4 (C) C63OC16) C
1179	3. 498	371. 19586	Splendoline	[M+H] ⁺	371. 19699	C21H26N2O4	Strychnos alkaloids	PUJOYKCYBTUSK-LQOCACJHSA-N	O=C (N1C=2C=CC=CC234CCN5OC6 (CC (C6CC530) C14) C) CO
1180	3. 5	178. 04909	ABOA	[M+H] ⁺	178. 05051	C9H7NO3	Benzoxazinoids	FZAQRVWPQCSGPC-UHFFFAOYSA-N	O=C1OC2=CC=CC (=O) C=C2 (N1)
1181	3. 504	159. 06555	Pinelic acid	[M-H] ⁻	159. 06628	C7H12O4	Medium-chain fatty acids	WLJYNTCWHLRURA-UHFFFAOYSA-N	O=C (O) CCCCC (=O) O
1182	3. 505	154. 08597	Dopamine	[M+H] ⁺	154. 08626	C8H11NO2	Catecholamines and derivatives	VYFYTYLLBUKUHU-UHFFFAOYSA-N	c1cc (c (cc1CCN) O) O
1183	3. 505	297. 18936	Exemestane	[M+H] ⁺	297. 185	C20H24O2	Androgens and derivatives	BFY1ZQONLCFLEV-DAELLWXTSA-N	O=C1C=CC2 (C (=C1) C (=O) CC3CC2C4 (C (=O) CC34) C) C
1184	3. 518	374. 19846	Hetisine	[M-H] ⁻	374. 1973	C20H27NO3	Alkaloids	PI1WJSAMCEMZ1DO-UHFFFAOYNA-N	CC12CN34CC56CC (=C) C7C (O) C5C3C (CC (O) C1) (C24) C6C7O
1185	3. 518	356. 09747	HMBOA + O-Hex	[M-H] ⁻	356. 09811	C15H19NO9	Benzoxazinoids	PMBZSEOA1OYRMW-UHFFFAOYNA-N	O=C2NC3=CC=C (OC) C=C3 (OC2 (OC1OC (CO) C (O) C (O) C1 (O)))
1186	3. 523	487. 19064	2-[1-[4, 5-dihydroxy-3-[(2S, 3R, 4S, 5S, 6R)-3, 4, 5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxovan-2-yl]indol-3-yl]acetic acid	[M+H] ⁺	487. 19223	C21H27NO11	Indole-3-acetic acid derivatives	ISMUGWKRUVABAZ-XRKNWZDJJSA-N	O=C (O) CC1=C=CN (C=2C=CC=CC21) C3OC (O) C (O) C3OC4OC (CO) C (O) C (O) C4O
1187	3. 523	344. 25702	Denudatine	[M+H] ⁺	344. 26001	C22H33NO2	Napelline-type diterpenoid alkaloids	F1AOWYBS1NDVNF-ARX1JESMSA-N	OC1C (=C) C2CC134CC5C6 (C) CN (CC) C4C5 (CCCC) C3CC2O
1188	3. 525	468. 24429	Penigequinolones A and B (diastereomers) _120177	[M+H] ⁺	468. 241	C27H33NO6	Phenylquinolines	CVWJKBJRSXD1W-IUEPNFLLSA-N	O=C1NC2=CC=C (C=CC3 (CCC (C) (C) CC3) C) C (O) =C2C (O) (C4=CC=C (OC) C=C4) C1OC
1189	3. 526	298. 13885	stepharine	[M+H] ⁺	298. 14001	C18H19NO3	Protoporphines	OGJKMZVJJYJWKO-CYBMUJFWSA-N	O=C1C=CC2 (C=C1) C=3C (OC) =C (OC) C=C4C3C (NCC4) C2
1190	3. 527	213. 06482	Harmin	[M+H] ⁺	213. 06572	C13H12N2O	Harmala alkaloids	BXNJHAXVSOCGBA-UHFFFAOYSA-N	N=1C=CC=2C=3C=CC (OC) =CC3NC2C1C
1191	3. 533	355. 14783	Notopterol	[M+H] ⁺	355. 14999	C21H22O5	Terpene lactones	BK1ACVAZUK1SOR-MKMNVTDBSA-N	O=C1OC=2C=C3OC=CC3=C (OCC=C (C) CC (O) C=C (C) C) C2C=C1
1192	3. 535	239. 14024	CMF	[M-H] ⁻	239. 14258	C12H16O5	Furanoid fatty acids	WMQWQXZMV1ETAO-UHFFFAOYSA-N	O=C (O) C1=C (OC (=C1C) CCC) CCC (=O) O
1193	3. 536	319. 97372	PFSM-sulfonic acid	[M-H] ⁻	319. 96912	C5H8F5NO5S2	PFSA	RNRXRAT1QNUKCT-UHFFFAOYSA-N	O=S (=O) (O) CCCCN (=O) (=O) C (F) (F) C (F) (F) F
1194	3. 538	210. 07664	Methoxytyrosine	[M-H] ⁻	210. 0766	C10H13NO4	Amino acids	PPDUKDQEHURQC-UHFFFAOYNA-N	O=C (O) C (N) CC1=CC=C (O) C (OC) =C1
1195	3. 542	285. 1329	Fisetin	[M-H] ⁻	285. 13168	C15H10O6	Flavonols	XHEFD1BZL1XQHF-UHFFFAOYSA-N	O=C1C (O) =C (OC2=CC (O) =CC=C12) C=3C=CC (O) =C (O) C3
1196	3. 543	289. 15344	Indole-3-acetyl-L-isoleucine	[M+H] ⁺	289. 15466	C16H20N2O3	Amino acids	WPTUQMUCTVOFW-UHFFFAOYNA-N	CCC (C) C (N=C (O) CC1=CN2C=CC=CC=C12) C (O) =O
1197	3. 543	425. 16571	Pentose-Hexose + C5H9	[M-H] ⁻	425. 16531	C16H28O10	Terpene glycosides	NYSQJ1JJJAWCE-UHFFFAOYNA-N	OC2OC (OCC1OC (OCC=C (C) C (O) C (O) C1 (O)) C (O) C2 (O))
1198	3. 545	331. 12976	SPECTINOMYCIN	[M-H] ⁻	331. 12915	C14H24N2O7	1, 4-dioxanes	UNFWIHTNXNPBV-WXKVWSESA-N	O=C1CC (OC2OC3C (O) (NC) C (O) (NC) C3OC12O) C
1199	3. 547	302. 10492	Dimechthlor ESA	[M+H] ⁺	302. 10568	C13H19NO5S	Anilides	RVSCDW1KJDBFRS-UHFFFAOYSA-N	COCCN (C (=O) CS (O) (=O) =O) C1=C (C) C=CC=C1C
1200	3. 55	418. 93854	Fipronil sulfide	[M-H] ⁻	418. 93652	C12H4C12F6N4S	Phenylpyrazoles	FQXWEKADCSXYOC-UHFFFAOYSA-N	C1=C (C=C (C (=C1C1) N2C (=C (C (CN) =N2) SC (F) (F) F) N) C1) C (F) (F) F
1201	3. 563	261. 14432	Isoleucylglutamate	[M+H] ⁺	261. 14429	C11H20N2O5	Dipeptides	KTGPOCFYOZQVRJ-UHFFFAOYNA-N	O=C (O) CC (NC (=O) C (N) C (C) C) C (=O) O
1202	3. 564	363. 11801	(4R, 6S, 8S, 9Z, 11E)-16-chloro-17, 19-dihydroxy-4-methyl-3, 7-dioxatricyclo[13. 4. 0. 0 ²]nonadeca-1 (15), 9, 11, 16, 18-pentaene-2, 13-dione	[M-H] ⁻	363. 1167	C18H17ClO6	Hydroxybenzoic acid derivatives	WYZWZEGROGVYHK-RFJJWQTDSA-N	O=C1OC (C) CC2OC2=CC=CC (=O) CC=3C (C1) =C (O) C=C (O) C13

[illegible]

1246	3. 697	584. 33673	Shearinine_F_120146	[M+H] ⁺	584. 33899	C37H45N05	Naphthopyrans	QYRAHJVRFPI1QW-MHXJJHONSA-N	O=C1C=C2C3(OC1C(03)(C)C)CC4(C)C2(0)CCC5C=6C=7C=C8C(=C7)N(C6C54C)C9=C(C8)C(OC(C)C)C9(C)C
1247	3. 697	359. 16888	tabersonine	[M+H] ⁺	359. 17001	C21H24N2O2	Plumeran-type alkaloids	FMGGIPWAZSFRCN-HEMCJLEPSA-N	O=C(OC)C1=C2N=C3C=C=C=CC24CN5C=CC(C1)(CC)C54
1248	3. 708	265. 08093	(S)-3-(4-hydroxyphenyl)chroman-7-ol	[M+H] ⁺	265. 07999	C15H14O3	Isoflavanols	ADFCQWZHKSPAJ-GPCVVEGCSA-N	OC1=CC=C(C=C1)C2OC3=CC(0)=CC=C3C2
1249	3. 71	439. 29025	Ochrolifunaine A	[M+H] ⁺	439. 28601	C29H34N4	Harmala alkaloids	BYHWAEE1GYEBJ-QJTMEEXSA-N	C=1C=CC2=C(1)NC3=C2CCN3CC4CC5C=6N=C=7C=CC=CC76CCN5CC4CC
1250	3. 711	221. 091	2-amino-3-(5-hydroxy-1H-indol-3-yl)propanoic acid	[M+H] ⁺	221. 09	C19H22N2O	Eburnan-type alkaloids	WYJAPUKIYAZSEM-MOPGFXCFSA-N	O=C1NC2=C3C=CC=C3C4=C2C5N(CC4)CCCC5(C1)CC
1251	3. 719	383. 16577	Isolaserpitin	[M+H] ⁺	383. 16812	C19H20O6	Angular pyranocoumarins	KJWF0HVSTFGWZ-YHYXMQVSA-N	O=C1OC2=C(C=C1)C=C=3OC(C)C(OC(=O)C(=CC)C(C)C)C32
1252	3. 719	405. 18011	reserpine	[M+H] ⁺	405. 17999	C22H26N2O4	Yohimbine alkaloids	KXEMQGRZUWJJS-RXR0KKEWSA-N	O=C(OC)C1=COC(C)C2CN3CCC=4C=5C=CC(OC)=CC5NC4C3OC12
1253	3. 72	183. 09167	Harman	[M+H] ⁺	183. 09167	C12H10N2	Harmala alkaloids	PSFDQSOQUJVVGF-UHFFFAOYSA-N	CC1=C2NC3=CC=CC=C3C2=CC=N1
1254	3. 734	227. 07654	aspernigrin A	[M-H] ⁻	227. 0789	C13H12N2O2	Nicotinamides	RIUZDCZRFRLJFC-UHFFFAOYSA-N	O=C1C=C(NC=C1C(=N)O)CC=2C=CC=CC2
1255	3. 735	106. 06487	3-Methylthiopropylamine	[M+H] ⁺	106. 0685	C4H11NS	Dialkylthioethers	KKYSBGWCYXOHA-UHFFFAOYSA-N	S(C)CCCN
1256	3. 736	593. 15002	Apigenin-6-C-glucoside-7-O-glucoside	[M-H] ⁻	593. 15118	C27H30O15	Flavone C, O-glycosides	HGUVPEBGCAVWD-UHFFFAOYNA-N	O=C2C=C(OC=3C=C(OC1OC(CO)C(O)C1(O)C)C(=C(O)C2=3)C4O(C(CO)C(CO)C(C)C4(O)C5=C(C=C(C)C)C=C5
1257	3. 744	152. 07027	Acetaminophen	[M+H] ⁺	152. 0706	C8H9NO2	1-hydroxy-2-unsubstituted benzenoids	RZVJ1NKP0RJJF-UHFFFAOYSA-N	CC(=N)C(=O)O
1258	3. 746	323. 14667	1-[4,5-bis(hydroxymethyl)-3-methoxy-2-methylphenoxy]-3-methylbutane-2,3-diol	[M+H] ⁺	323. 14648	C15H24O6	Benzyl alcohols	MAQMSUGBC1GLJ-UHFFFAOYSA-N	OC1=CC(OC(C)C(C)C)C(OC)=C1OO)C
1259	3. 746	584. 34082	Shearinine_A_120147	[M+H] ⁺	584. 34003	C37H45N05	Naphthopyrans	YAGQ1ZPAJNEIKG-KBCUGRHSA-N	O=C1C=C2C3(OC1C(03)(C)C)CC4(C)C2(0)CCC5C=6C7=C8C(=C7)N(C6C54C)C9=C(C8)C(OC(C)C)C9(C)C
1260	3. 748	421. 24219	(1, 9, 9b-trihydroxy-6, 6, 9a-trimethyl-3, 5, 5a, 7, 8, 9-hexahydro-1H-benzo[el]2[1h]benzofuran-5-yl)-hexanoate	[M+H] ⁺	421. 24319	C21H34O6	Naphthofurans	GFMG0VRF0OAFMN-UHFFFAOYSA-N	O=C(OC1C=C2COC(0)C2(0)C3(C)C(OC)C(C)C13)CCCC
1261	3. 748	317. 15945	(2S, 3S)-2-(3, 4-dihydroxyphenyl)-3, 5, 7-trihydroxy-6-methyl-2, 3-dihydrochromen-4-one	[M-H] ⁻	317. 16092	C16H14O7	Flavanonols	KPCWZLBRHGXPFV-CYEARBPZSA-N	O=C1C2=C(C)C(=C(C)C)C=C2OC(C3=CC=C(C)C(OC)=C3)C1O)C
1262	3. 754	310. 12711	Ketotifen	[M+H] ⁺	310. 12601	C19H19NO5	Cycloheptathiophenes	ZCVMWBYGMWGHF-UHFFFAOYSA-N	O=C1C=C2SC=C2C(C=3C=CC=CC3C1)=C4CCN(C)CC4
1263	3. 756	565. 15277	methyl (2S, 3R, 4S)-3-ethenyl-4-[(2-(3, 4, 5-trihydroxybenzoyl)oxyethyl]-2-[3, 4, 5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy-3, 4-dihydro-2H-pyran-5-11A-Acetoxyprogesterone	[M+H] ⁺	565. 15277	C24H30O14	Terpene glycosides	SMTKSCLXONVGL-FMDXMRPMSA-N	O=C(OC)C1=CC(OC2OC(CO)C(C)C2O)C(C=C(C)C1)CCCC(=O)C3=CC(O)C(C)C3
1264	3. 758	373. 24261	11A-Acetoxyprogesterone	[M+H] ⁺	373. 23734	C23H32O4	Glucoc/mineralocorticoids, progestogens and	IWRPVTXREYVBT-QHXRXISESA-N	O=C(OC1CC2(C)C(C(=O)CCC2C3CCC=CC(=O)CC4(C)C13)C
1265	3. 758	192. 06592	Actrarit	[M-H] ⁻	192. 06662	C10H11NO3	Benzene and substituted derivatives	MROJXXOCABQVEF-UHFFFAOYSA-N	O=C(OC)CC1=CC=C(N=C(C)C)C=C1
1266	3. 759	355. 10211	Feruloyl Hexoside (isomer of 847)	[M-H] ⁻	355. 1022	C16H20O9	Ferulic acid and derivatives	JWRQVQWBNRGPK-UHFFFAOYNA-N	O=C(OC1OC(CO)C(C)C(OC)C1(O)C)C=CC=CC(OC)=C(OC)C=C2
1267	3. 76	358. 24216	diacetylsongorine	[M+H] ⁺	358. 23999	C22H31NO3	Napelline-type diterpenoid alkaloids	CDOSLVQFGANTL-DWPYZRQCSA-N	O=C1CC2C3(CCC1C(C)C3O)C4CC5C6(C)CN(C6)C4C25C(OC)CC6
1268	3. 763	147. 04362	Coumaric acid (isomer of 189, 194)	[M+H2O] ⁺	147. 0443	C9H8O3	Coumaric acid and derivatives	NSWKAQJWESNS-UHFFFAOYSA-N	O=C(C)C=CC1=C(C)C(OC)=C1
1269	3. 763	335. 15857	triptophenolide	[M+H] ⁺	335. 16	C20H24O3	Oxosteroids	KPX1BWGPZSPARK-PXNSMCTSA-N	O=C1OCC2=C1CC3(C4=C=C(C(OC)=C4)CC(C23)C(C)C)C
1270	3. 773	313. 11658	5, 7-dimethoxy-3-(4-methoxyphenyl)-4H-chromen-4-one	[M+H] ⁺	313. 10999	C18H16O5	7-O-methylisoflavones	PVORTURQBPBPF-UHFFFAOYSA-N	O=C1C=C(COC2=CC(OC)=CC(OC)=C2)C=3C=CC(OC)=CC3
1271	3. 778	399. 18561	4-hydroxy-9-(4-hydroxy-3, 6-dimethoxyphenyl)-5a, 6, 8a, 9-tetrahydro-5H-[2]benzofuro[5, 6-f][1, 3]benzodioxol-8-one	[M-H] ⁻	399. 1853	C21H20O8	Lignan lactones	JGGWNGRBJWAOC-UHFFFAOYSA-N	O=C1OCC2CC3(C)C(=O)C4OCOC4=C3C(C5=C(C)C(OC)=C5)C=C12
1272	3. 781	241. 09642	Cyanazine	[M+H] ⁺	241. 0963	C9H13ClN6	Aminotriazines	MZZBPKVEFVLFF-UHFFFAOYSA-N	CCN=C1NC(NC(C)C)C(=N)C(C1)=N1
1273	3. 794	593. 15302	2-(3, 4-dihydroxyphenyl)-5-hydroxy-7-[(2S, 3R, 4S, 5S, 6R)-3, 4, 5-trihydroxy-6-[[[(2R, 3R, 4R, 5R, 6S)-3, 4, 5-trihydroxy-6-methylloxan-2-yl]oxymethyl]loxan-2-	[M-H] ⁻	593. 1524	C27H30O15	Flavonoid-7-O-glycosides	MGYBYJXAXUBTQF-FOBVWLSUSA-N	O=C1C=C(OC2=CC(OC3OC(COC4OC(C)C(OC)C4O)C(OC)C(OC)C3O)=CC(OC)=C12)C=C5C=CC(OC)=C(OC)C5
1274	3. 797	432. 27969	veratramine	[M+H] ⁺	432. 28	C27H39NO2	Fluorenes	MALFOD1CPS1XPO-AZAJSESZSA-N	OC1CC2=CCC3C4=CC=C(C(=C4)CC3C2(C)CC1)C(C)C(C5NCC(C)CC5O
1275	3. 814	373. 16257	4-[2-(2, 6-dimethoxy-4-prop-2-enylphenoxy)-1-hydroxypropyl]-2-methoxyphenol	[M-H] ⁻	373. 16565	C21H26O6	Lignans, neolignans and related compounds	ULZFTGWPHYGLI-UHFFFAOYSA-N	OC1=C=C(C=C1)OC(C)C(OC2=C(C)C(OC)=C(C2OC)CC=C(C)C
1276	3. 815	374. 22787	SH373-1	[M+H] ⁺	374. 229	C17H31N3O6	Peptides	UKFUHWPKCYQQR-UHFFFAOYSA-N	O=C(C)C(N=C(C)C(N=C(C)CCC(N)C(=O)C(C)C)CC(C)C
1277	3. 815	324. 11893	Tetrahydrocoptisine	[M+H] ⁺	324. 12	C19H17NO4	Protoberberine alkaloids and derivatives	UXYJCYXWJGAKQY-OAHLLOKOSA-N	O1C2=CC=C3C(=C2OC1)CN4CC5=CC=6OOC6C=C5C4C3
1278	3. 821	226. 14308	Terbutaline	[M+H] ⁺	226. 14377	C12H19NO3	Resorcinols	XWYYSIMOBUGWOL-UHFFFAOYNA-N	CC(C)C(NCC(OC)C1=CC(OC)=CC(OC)=C1
1279	3. 823	504. 29684	andrastin A	[M+H] ⁺	504. 29556	C28H38O7	Steroid esters	GRBXNADBNJGZRR-GJEDHNSHSA-N	O=CC12CCC(OC(=O)C(C)C(C)C2)CC3(C)C1C=C(C)C4(C(=O)C(C(=O)C43C(=O)OC)C1C
1280	3. 823	362. 21054	Octocrylene	[M+H] ⁺	362. 21146	C24H27NO2	Diphenylmethanes	FMJSMJQBSVNSBF-UHFFFAOYNA-N	CCCC(C)COC(C(C#N)=C(C1=CC=CC=C1)C2=CC=CC=C2)=O
1281	3. 823	223. 15576	Tetraglyme	[M+H] ⁺	223. 15401	C10H22O5	Dialkyl ethers	ZUHZGEOKBGKPSW-UHFFFAOYSA-N	COCOCOCOCOCOCOC
1282	3. 824	506. 23178	3, 15-dibenzyl-1, 4, 12-trimethyl-1, 4, 7, 10, 13-pentazacyclopentadecane-2, 5, 8, 11, 14-pentone	[M-H] ⁻	506. 23819	C27H33N5O5	Macrolactams	MS1MMLAIWYFPLY-UHFFFAOYSA-N	O=C1N(C)C(C(=O)N(C)C(C(OC)=NC(C(OC)=NCC(C)C(OC)=2C=C(C(OC2)C)=3C=C(C)C
1283	3. 826	384. 17468	Quetiapine	[M+H] ⁺	384. 17401	C21H25N3O2S	Dibenzothiazepines	ROKOMYMAXPYNW-UHFFFAOYSA-N	OCOCOCN1CCN(C2=NC=3C=CC=CC3SC=4C=CC=CC42)CC1
1284	3. 827	300. 14331	Metoclopramide	[M+H] ⁺	300. 14734	C14H22ClN3O2	Aminophenyl ethers	TTWJBBZEZQ1CB1-UHFFFAOYSA-N	CCN(CC)CCN(C)C1=C(OC)C=C(N)C(C1)=C1
1285	3. 827	246. 11154	resveratrol	[M+H] ⁺	246. 11246	C14H12O3	Stilbenes	LURKXSALWPMMSZ-OWJBTEDSA-N	OC1=CC=C(C=C1)C=C(C=C1)C=C(C(OC)=C(C)C)C2
1286	3. 828	121. 02873	2-Hydroxybenzaldehyde	[M-H] ⁻	121. 0295	C7H6O2	Hydroxybenzaldehydes	SMQUZDBALYZAC-UHFFFAOYSA-N	O=C=C1C=CC=CC1O
1287	3. 834	299. 12369	angoletin	[M-H] ⁻	299. 12888	C18H20O4	2'-Hydroxy-dihydrochalcones	HBRYKWADRULLHU-UHFFFAOYSA-N	O=C(C(=C(C)C)=C(C)C(OC)C(C)C)CCC=2C=CC=CC2
1288	3. 838	281. 03995	Pseudobaptigenin	[M-H] ⁻	281. 04553	C16H10O5	Isoflavones	KNJNBK1NYHZUGC-UHFFFAOYSA-N	OC1=CC=C2C(=O)C(=C(C2=C1)C1=CC2=C(C(OC2)C)C=C1

1289	3.839	335.11554	(E)-3-hydroxy-6-(4-hydroxy-6-methoxy-7-methyl-3-oxo-1H-2-benzofuran-5-yl)-4-methylhex-4-enoic acid	[M-H] ⁻	335.11362	C17H2007	Phthalides	OGJCZLO1KMTMKF-XBXARRHUSA-N	O=C1OCC2=C1C(O)=C(C(OC)=C2C)CC=C(C(C)O)CC(=O)O
1290	3.84	364.14859	(+)-Corypalmine	[M+H] ⁺	364.14999	C20H23N04	Protoberberine alkaloids and derivatives	BM CZTYDZHNTKPR-MRXNPFEDSA-N	OC1=C2C(=CC1OC)C3N(C4=C(OC)C(OC)=CC=C4C3)CC2
1291	3.84	123.04374	3-Hydroxybenzaldehyde	[M+H] ⁺	123.04405	C7H602	Hydroxybenzaldehydes	IAVREABSGIHHMO-UHFFFAOYSA-N	O=C=O=C=CC(=O)C1
1292	3.845	372.04974	Glucanapin (3-butenylglucosinolate)	[M-H] ⁻	372.05542	C26H4409	Medium-chain fatty acids	MINDHVHHQZYEEK-HBBNESRPSA-N	O=C(O)CCCCCCCC(=O)C=C(C(OC)CC1OCC(C2COC2C(C)O)C(C)O)C1O
1293	3.849	303.19116	Hesperetin	[M+H] ⁺	303.19211	C16H1406	4'-O-methylated flavonoids	A1ONOLUJ1ZLMTK-AWEZNCLSA-N	O=C1C=2C(O)=CC(O)=CC2OC(2C=CC=C(OC)C(O)=C3)C1
1294	3.855	322.10635	methyl 1-oxo-2-(o-tolyl)-1,2,3,6,7,7a-hexahydro-3a,6-epoxyisoindole-7-carboxylate	[M+H] ⁺	322.10501	C17H17N04	Phenylpyrrolidines	NDOPUHIEVZKCTM-UHFFFAOYSA-N	O=C(OC)C1C2OC3(C=C2)CN(C(=O)C13)C=4C=CC=CC4C
1295	3.865	129.05515	Ketoleucine	[M-H] ⁻	129.05573	C6H1003	Short-chain keto acids and derivatives	BKAJNAXTPSGJCU-UHFFFAOYSA-N	O=C(O)C(=O)CC(C)C
1296	3.866	506.26962	(2E,6E,11E)-18-(2,6-dioxopiperidin-4-yl)-9,13-dihydroxy-8-methoxy-10,12,14-trimethyl-15-oxooctadeca-2,6,11-trienoic acid	[M-H] ⁻	506.27161	C27H41N08	Linoleic acids and derivatives	HJCZOTBHYAPUHT-XHOLQ0DBSA-N	O=C(O)C=CCCCC(OC)C(O)C(C=C(C)C)C(C)C(=O)CCCC1CC(=O)N=C(O)C1)C(C
1297	3.866	434.1893	(7,8-dimethoxy-2,2,3-trimethyl-2,3-dihydro-1H-benzodiazepin-4-yl) (3,4-dimethoxyphenyl)methanone	[M+H] ⁺	434.19	C24H29N05	Benzazepines	11NU1ABWYMTUJM-UHFFFAOYSA-N	O=C(C1=CC=C(C(OC)=C1)C2=CC=CC(OC)C(C(OC)=CC3CC(N2C)C)C
1298	3.869	241.11798	Pyrogulutamyl-Isoleucine	[M-H] ⁻	241.11909	C11H18N204	Peptides	MKCVLTRITQNGQJ-UHFFFAOYNA-N	O=C(O)C(NC(=O)C1NC(=O)CC1)C(C)CC
1299	3.881	283.12076	verruculotoxin	[M+H] ⁺	283.12073	C15H20N20	Alpha amino acid amides	CUANCTHYEDWUMU-KBPBESRZSA-N	OC1=NC(CC=2C=CC=CC2)CN3CCCCC13
1300	3.885	197.15053	(2E)-3,7-dimethyl-2,6-octadienyl acetate	[M+H] ⁺	197.14999	C12H2002	Fatty alcohol esters	HIQQPQRQ1QDZMP-DHZHJOJOSA-N	O=C(OC=C(C)CCC=C(C)C)C
1301	3.885	508.28674	deltaline	[M+H] ⁺	508.29001	C27H41N08	Aconitane-type diterpenoid alkaloids	DTTPWCNKMTQTE-TYNNPWLESA-N	O=C(OC1C2C3(C)CN(C)C4C51OOC6SCC(OC)C7OC(O)C6C7OC)C42C(OC)CC3)C
1302	3.885	541.17786	gossypol	[M+H] ⁺	541.17999	C30H3008	Sesquiterpenoids	QBKSWRVYCFDQOT-UHFFFAOYSA-N	O=CC1=C(O)C(O)=C(C2=CC(=C(C)C)=C12)C3=C(O)C4=C(C=O)C(C(O)=C(O)C=C4C3C2)C(C)C(C)C(C
1303	3.885	300.1803	Rinderine	[M+H] ⁺	300.18054	C15H25N05	Alkaloids	SFVVQRJOGUKCEG-UHFFFAOYNA-N	CC(C)C(O)C(C)O)C(=O)CC1=CC2CCC(O)C12
1304	3.887	363.17471	[5-acetyloxy-3-(hydroxymethyl)-2-oxo-6-propan-2-ylcyclohex-3-en-1-yl] 3-methylpentanoate	[M+H] ⁺	363.1778	C18H2806	Menthane monoterpenoids	MPXXS1CHRNCHHK-UHFFFAOYSA-N	O=C(OC1C=C(C(=O)C(OC(=O)CC(C)C)C1C(C)C)O)C
1305	3.892	492.25519	Imatinib	[M-H] ⁻	492.25174	C29H31N70	Benzanilides	KTUFNOKBVMGRW-UHFFFAOYSA-N	O=C(NC1=CC=C(C(=C1)NC=2N=CC(=N2)C3=CN=CC(=C3)C)C4=CC=C(C(=C4)CN5CCN(C)CC5
1306	3.897	311.10065	(3S,3'R)-3'-(3-hydroxyphenyl)-4-methylspiro[1H-1,4-benzodiazepine-3,2'-oxetane]-1,5-dione	[M+H] ⁺	311.10263	C17H14N204	1,4-benzodiazepines	BDDNYDPRCDQJQ-PBHCJAKSA-N	O=C1C=2C=CC=C2N=C(O)C3(OC3=4C=CC=C(O)C4)N1C
1307	3.9	282.16809	judaicin (eudesmane naphthofuran)	[M+H] ⁺	282.16998	C15H2004	Eudesmanolides, secoeudesmanolides, and	NGPDZEAC1WDCX-WUDKMPASANA-N	O=C1OC2C(CCC3(C(=O)C=C(O)C(C)23)C)C1C
1308	3.901	370.17041	N-methylglaucaine	[M+H] ⁺	370.17001	[C22H28N04] ⁺	Aporphines	WKHHFWJ1JRCXHA-INTZCTEOSANA-N	O(C1C=4C=2C=3C(OC)=C(OC)C=C4C3C(C2=CC1OC)[N+](C)(C)CC4)C
1309	3.901	215.05664	Pesticide3 Monolinuron C9H11ClN2O2 Urea, N'-(4-chlorophenyl)-N-methoxy-N-methyl-	[M+H] ⁺	215.058	C9H11ClN202	N-phenylureas	LKJPSUCKSLORMF-UHFFFAOYSA-N	O=C(NC1=CC(=C(C)C)C1)N(OC)C
1310	3.901	265.09973	Peucedanol	[M+H] ⁺	265.10001	C14H1605	7-hydroxycoumarins	WRTWKAQFZYXAEJ-GPCCEGCSANA-N	O=C1OC=2C=C(O)C(=CC2C=C1)CC(O)C(O)C
1311	3.909	256.11725	3,4,5-trimethoxycinnamic acid	[M+H] ⁺	256.11795	C12H1405	Coumaric acids and derivatives	YTFVRYKNXDABI-SNAWJOMRSANA-N	O=C(O)C=CC1=CC(OC)=C(OC)C(OC)=C1
1312	3.909	389.21622	icaraside B5	[M+H] ⁺	389.216	C19H3208	Fatty acyl glycosides of mono- and disaccharides	YTFVRYKNXDABI-SNAWJOMRSANA-N	O=C1C=C(C)C(O)C(CCC(OC2OC(C)C(O)C(C)2)C(C)C(C)C(C)C(C)C1
1313	3.913	290.14923	Antibiotic TAN 1169B	[M+H] ⁺	290.14999	C15H19N303	Pyroloindoles	OXGGVEYZLRHHP-UHFFFAOYNA-N	O=C(OC1=CC=C2NC3N(C(=O)C)CC3(C2=C1)C)NC
1314	3.917	287.07208	licochalcone B	[M+H] ⁺	287.07257	C16H1405	Retrochalcones	DRDRYGIIYOPBZ-XBXARRHUSA-N	O=C(C=CC1=CC=C(O)C(O)=C1OC)C2=CC=C(O)C=C2
1315	3.918	374.14645	Gatifloxacin	[M-H] ⁻	374.14301	C19H22FN304	Quinoline carboxylic acids	XUBOMFCQDBHKN-UHFFFAOYSA-N	O=C(O)C1=CN(C2=C(OC)C(=C(F)C=C2C1O)N3CCNC(C)3)C4CC4
1316	3.924	359.22754	(Z)-5-[(1S,2R,4aR,8aR)-5-(hydroxymethyl)-1,2,4a-trimethyl-2,3,4,7,8,8a-hexahydronaphthalen-1-yl]-3-(hydroxymethyl)pent-2-enoic acid	[M+H] ⁺	359.22626	C20H3204	Colensane and clerodane diterpenoids	LRLROPPFPABQRF-CBYQQG1ISA-N	O=C(O)C=C(C)O)CCC1(C)C(C)CCC2(C(=CCCC21)CO)C
1317	3.939	314.2077	(2E,4E)-N-[2-(4-hydroxyphenyl)ethyl]dodeca-2,4-dienamide	[M-H] ⁻	314.21255	C20H29N02	1-hydroxy-2-unsubstituted benzeneoids	VVRNVAJXAUQHEN-BNFZFUHLSANA-N	OC(=NCCC1=CC=C(C)C=C1)C=CC=CCCCCCC
1318	3.94	179.03389	trans-Caffeic acid	[M-H] ⁻	179.03497	C9H804	Caffeic acid and derivatives	QAIPRVGONGVQAS-UHFFFAOYSA-N	O=C(O)C=CC1=CC=C(O)C(O)=C1
1319	3.943	244.15416	Pinacidil	[M-H] ⁻	244.15677	C13H19N5	Pyridines and derivatives	IVNVZDGDKPTYHK-UHFFFAOYNA-N	N#CN=C(N=C1C=CNC=C1)NC(C)C(C)C
1320	3.944	231.16985	Isoleucylvaline	[M+H] ⁺	231.1707	C11H22N203	Dipeptides	BXBI0NYJCSDF-UHFFFAOYNA-N	O=C(O)C(NC(=O)C(N)C(C)CC)C(C)C
1321	3.95	323.19946	16-Heptadecyne-1,2,4-triol	[M+H] ⁺	323.1983	C17H3203	Long-chain fatty alcohols	OHLQBKXSJYBMK-UHFFFAOYSA-N	C#CCCCCCCCCCCC(O)CC(O)CO
1322	3.95	292.20428	Terbinafine	[M+H] ⁺	292.20596	C21H25N	Naphthalenes	DOMXUEMWDABQBU-UHFFFAOYSA-N	CC(C)C(C)C#CC=CCN(C)CC1=CC=CC2=CC=CC=C2C1
1323	3.951	241.14296	Imiquimod	[M+H] ⁺	241.145	C14H16N4	Imidazoquinolines	DOUYETYNHVLEO-UHFFFAOYSA-N	N1=CN(C2=C1C(=NC=3C=CC(=CC32)N)CC(C)C
1324	3.952	270.16925	(8aR,12S,12aR)-12-hydroxy-4-methyl-4,5,6,7,8,8a,12,12a-octahydro-1H-3-benzoxecine-2,9-dione	[M+H] ⁺	270.16998	C14H2004	Oxocins	WTQWON1IPGERSZ-ROAVRGLVSA-N	O=C1OC(C)CCCCC2C(=O)C=CC(O)C2C1
1325	3.965	151.07516	1-(4-methoxyphenyl)ethanone	[M+H] ⁺	151.08	C9H1002	Alkyl-phenylketones	NTPLXRHDUXRPN-UHFFFAOYSA-N	O=C(C1=CC=C(OC)C=C1)C
1326	3.97	160.09651	N-Isovalerylglycine	[M+H] ⁺	160.09682	C7H13N03	N-acyl-alpha amino acids	ZRXKMKMBMNNQC-UHFFFAOYSA-N	O=C(O)CN=C(O)CC(C)C
1327	3.971	187.09625	2-(1-hydroxyethyl)-4-(2-hydroxypropyl)-2H-furan-5-one	[M+H] ⁺	187.09648	C9H1404	Butenolides	JAAFNWYGLROOGI-UHFFFAOYSA-N	O=C1OC(C=C1CC(O)C)C(O)C
1328	3.976	321.15485	8:1+20 fatty acyl hexoside	[M-H] ⁻	321.1546	C14H2608	Fatty acyl hexosides	YUPLCLHITUNDMAN-UHFFFAOYNA-N	O=C(OC(C)CC(OC1OC(CO)C(O)C(C1)O)C)C
1329	3.978	271.13528	alpinetin	[M+H] ⁺	271.1337	C16H1404	5-O-methylated flavonoids	QQQCWDPMPFUG-UHFFFAOYSA-N	O=C1C=2C(OC)=CC(O)=CC2OC(2C=CC=CC3)C1
1330	3.98	625.15057	3-O-beta-(6''-trans-caffeoyl)-galactopyranosyl quercetin	[M-H] ⁻	625.14801	C30H26015	Flavonoid 3-O-p-coumaroyl glycosides	IHBVMUCQZEAPE-YBDSQCSQSA-N	O=C(OC1OC(OC=2C(=O)C=3C(O)=CC(O)=CC3OC2=4C=CC(O)=C(O)C4)C(C)C(C)O)C1)C=CC=C(C(OC)C(C)C)=C5
1331	3.981	427.18152	[8,8-dimethyl-10-(3-methylbut-2-enyloxy)-2-oxo-9,10-dihydropyrano[2,3-f]chromen-9-yl] 3-methylbutanoate	[M-H] ⁻	427.17621	C24H2807	Angular pyranocoumarins	MYXNO11PWBFPR-UHFFFAOYSA-N	O=C1OC2=C(C=C1)C=CC=3OC(C)C(C)C(OC(=O)CC(C)C)C(OC(=O)C=C(C)C)C32

1332	3.982	257.17389	((6aR,9R,10aR)-7-methyl-4,6,6a,7,8,9,10,10a-octahydroindolo[4,3-f ₂]indolin-9-yl)methanol	[M+H] ⁺	257.17001	C16H20N2O	Clavines and derivatives	UFKTX1XVYGAES-WDBKCZKBSA-N	0CC1CN(C)C2CC3-NC4-CC-CC(=C43)C2C1
1333	3.986	245.1019	Indole-3-acetyl-L-alanine	[M-H] ⁻	245.09317	C13H14N2O3	N-acyl-L-alpha-amino acids	FBDCJLXTUCMLF-UHFFFAOYNA-N	CC(N=C(O)C1=CN=C2-CC-OC(=C12)C(O)=O
1334	3.987	338.12286	barceloneic acid A	[M+H] ⁺	338.12341	C16H16O7	Diphenylethers	ULPVI8VORQAXJB-UHFFFAOYSA-N	O=C(O)C1=C(O)C=C(C=C1OC2=C(O)C=C(OC)C=C2OC)C
1335	3.989	328.23236	UR-144 N(4-hydroxypentyl)	[M+H] ⁺	328.22699	C21H29NO2	N-alkylindoles	YHFRYHZNLEAAP-UHFFFAOYSA-N	O=C(C1=CN(C=2C-CC-CC12)CCCC(O)C)C3C(C)(C)C3(C)C
1336	3.99	190.05022	(2-oxo-2,3-dihydro-1H-indol-3-yl)acetic acid	[M-H] ⁻	190.05096	C10H9NO3	Indolyl carboxylic acids and derivatives	ILGMGHZPRDCCS-UHFFFAOYNA-N	O=C(O)CC1C(O)=NC=2C-CC-CC21
1337	3.994	247.08559	(3Z)-3-butylidene-6,7-dihydroxy-4,5,6,7-tetrahydro-2-benzofuran-1-one	[M+H] ⁺	247.09	C12H16O4	Isobenzofurans	DQNCMIQSXNGHOA-WTKPLQERSA-N	O=C1OC(=CCCC)C2=C1(C)(O)CC2
1338	4.001	408.19009	3-(2-((7H-purin-6-yl)amino)ethyl)-2-methyl-4-oxo-3,4,5,6-tetrahydro-2H-2,6-methanobenzo[<i>c</i>]1,3loxazocine-5-carboxamide	[M+H] ⁺	408.19	C20H21N7O3	6-alkylaminopurines	MMJORIFFCDBAA-UHFFFAOYSA-N	O=C(N)C1C(=O)N(CCNC2=NC=NC=3C=NC32)C4(OC=5C=CC-CC5C1C41C
1339	4.001	390.14249	Taldalafil	[M+H] ⁺	390.14484	C22H19N3O4	Beta carbolines	WOXKDGUGVFFRN-UHFFFAOYNA-N	O=C1N2C(C3=CC=C4OC(C4=C3)C=5NC=6C-CC-CC65CC2C(=O)N(C)C1
1340	4.002	251.17474	Rivastigmine tartrate (Exelon)	[M+H] ⁺	251.175	C18H28N2O8	Phenoxy compounds	GWGHUAUXRMOT-MBANBLQSA-N	O=C(O)C(O)C(O)C(=O)O, O=C(OC1=CC-CC(=C1)C(N(C)C)C(N)C)C
1341	4.004	313.11664	2-(3,4-dimethoxyphenyl)-7-methoxy-4H-chromen-4-one	[M+H] ⁺	313.10999	C18H16O5	7-O-methylated flavonoids	VSEFYCZPDWYSYS-UHFFFAOYSA-N	O=C1C=C(OC2=CC(OC)=CC(=C12)C=3C=CC(OC)=C(C)OC3
1342	4.009	434.22311	Valsartan	[M-H] ⁻	434.21976	C24H29N5O3	Valine and derivatives	ACWBPQMZXGDQFX-UHFFFAOYNA-N	CCCCC(N(C(=C(C=C(C1)C2=CC-CC=C2C3=NNN=N3)C(C)C(C)C(=O)O)=O
1343	4.01	309.08609	Gastrodin	[M+H] ⁺	309.09	C13H18O7	Phenolic glycosides	PIQSUZTXKPLAPR-UJPOAAIJSAN	0CC1=CC=C(OC2OC(CO)C(O)C2O)C=C1
1344	4.01	386.2088	Uncarine c	[M+H] ⁺	386.20743	C21H24N2O4	Indolizidines	JMIAZDVHNCPPDM-UHFFFAOYSA-N	O=C(OC)C1=CC(C)C2CN3CCC4(C)=NC=5C-CC=C54)C3CC12
1345	4.031	332.9382	PFAP-diPAP	[M-H] ⁻	332.93799	C4HF10O4P	PFSA	HJLWRXZHQHRZCH-UHFFFAOYSA-N	O=P(O)(OC(F)(F)F)OC(F)(F)C(F)(F)F
1346	4.04	257.14899	Isocurcumenol	[M+H] ⁺	257.14999	C15H22O2	Guianes	DEBDFZGNZTYMF-NZBPQADJSA-N	OC12OC3(C=C1C(C)C(C)C(C)C2)CCC3C
1347	4.041	165.05421	P-Coumaric acid	[M+H] ⁺	165.05499	C9H8O3	Hydroxycinnamic acids	NGSWKAQJJWESNS-ZXXKWIFPSA-N	O=C(O)C=CC1=CC=C(O)C=C1
1348	4.042	579.12897	quercetin-3-O-deoxyhexosyl(1-2)pentoside	[M-H] ⁻	579.13397	C26H28O15	Flavonoid-3-O-glycosides	WRLBR1WXGBKHQ-UHFFFAOYSA-N	O=C1C(OC2OC(C)C(O)C2OC3OC(C)C(O)C3O)=C(OC=4C=C(O)C=C(C)C14)=5C=C(C)C(=O)C5
1349	4.043	474.27902	Chasmanine	[M+H] ⁺	474.28	C25H41N06	Aconitane-type diterpenoid alkaloids	DBODJJZKZFBZD-XXYVQWTJSA-N	OC1C2C3CC1C(O)(CC2OC)C4C(OC)C5C6(OC)CN(OC)4C35C(OC)C6
1350	4.045	506.30612	2-(((4R)-4-((3R,5S,7R,8R,9S,12S,14S,17R)-3,7,12-trihydroxy-10,13-dimethylhexadecahydro-1H-cyclopenta[<i>a</i>]phenanthren-17-yl))pentanamido)acetic	[M+H] ⁺	506.31	C26H45N07	Glycinated bile acids and derivatives	WDKPFRHOCMLKPR-SSBNMFHASA-N	O=C(O)CNC(=O)CCC(C)C1CC2C3C(O)CC4C(O)CC4(C)C3CC(O)C12C
1351	4.049	152.01614	2-Hydroxybenzothiazole	[M+H] ⁺	152.01646	C7H5N05	Benzothiazoles	YEDIAINPPJYDJZ-UHFFFAOYSA-N	C1=CC=C2C(=C1)N=C(O)S2
1352	4.061	239.12686	7-Hydroxyflavone	[M+H] ⁺	239.12721	C15H10O3	Flavones	MQGPGSCMMJKNHQ-UHFFFAOYSA-N	O=C1C=C(OC2=CC(O)=CC=C12)C=3C=CC=C3
1353	4.073	613.17047	Safflomin A	[M+H] ⁺	613.16998	C27H32O16	C-glycosyl compounds	IABVBSVCVHLRGE-UXEKTNMQSA-N	O=C1C(=C(O)C=CC2=CC(C)(C=C2)C(O)=C(C(=O)C1)C3OC(CO)C(O)C(O)C3O)C4OC(CO)C(O)C4O
1354	4.08	373.11234	(2S,3S,4S,5R,6R)-6-(3-benzoyloxy-2-hydroxypropoxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	[M+H] ⁺	373.11292	C16H20O10	0-glucuronides	DLZMKPZOEYXKHQ-MQCRQNCBSA-N	O=C(O)C1OC(OC(C)COC(=O)C=2C=CC=CC2)C(O)C(O)C1O
1355	4.08	395.09357	[(E)-3-acetyloxy-7-hydroxy-7-(6-oxo-2,3-dihydropyran-2-yl)hept-4-en-2-yl] acetate	[M+H] ⁺	395.09351	C17H24O8	Tricarboxylic acids and derivatives	STNNWPKHREBGMQ-CHDGQBGSA-N	O=C1OC(C=C1)C(O)C(OC)C=CC(OC(=O)C)C(OC(=O)C)C

1375	4. 184	625. 17059	Isorhamnetin 3-O-neohesperoside	[M+H] ⁺	625. 16998	C28H32O16	Flavonoid-3-O-glycosides	QHLKSZBF1JJREC-SPSUIZEHSA-N	O=C1C(OC2OC(CO)C(O)C(CO)C2OC3OC(C)C(O)C(CO)C3O)=C(OC=C=C(O)C=C(O)C14)C=C5C=CC(O)=C(OC)C5
1376	4. 191	180. 10138	N-acetyltyramine	[M+H] ⁺	180. 1019	C10H13NO2	1-hydroxy-2- unsubstituted benzenoids	ATDWJOOPFDQZNK-UHFFFAOYSA-N	OC1=CC=C(C=C1)CCN=C(O)C
1377	4. 196	171. 13741	gamma-Decalactone	[M+H] ⁺	171. 13795	C10H18O2	Gamma butyrolactones	IFYYFLINQYPWGJ-UHFFFAOYNA-N	CCCCCCC1CCC(=O)O1
1378	4. 201	333. 10757	Isopongaflavone	[M+H] ⁻	333. 11322	C21H18O4	Pyranoflavonoids	DPAGRPSAFDXQDN-UHFFFAOYSA-N	O=C1C=C(OC2=C3C=CC(OC3=CC(OC)=C12)(C)C)C=C4C=CC=CC4
1379	4. 211	327. 20206	hydroquinidine	[M+H] ⁺	327. 20001	C20H26N2O2	Cinchona alkaloids	LJQQZACKSYWCH-NIHZBZNOSA-N	OC(C=1C=CN=C2C=CC(OC)=CC21)C3M4CC(C3)C(C4)CC
1380	4. 214	434. 20047	(2R,3S,4S,5R,6R)-2-[[[(2S,3R,4R)-3,4-dihydroxy-4-(hydroxymethyl)oxolan-2-yl]oxymethyl]-6-(2-phenylethoxy)oxane-3,4,5-triol]	[M+NH4] ⁺	434. 20206	C19H28O10	0-glycosyl compounds	GZSQKQFXMZDKPV-DERWZJFJSA-N	OC(C1)COC(OC2COC(OCCC=3C=CC=C3)C(O)C(O)C2O)C1O
1381	4. 222	407. 14322	Amlodipine	[M+H] ⁻	407. 13791	C20H25ClN2O5	Dihydropyridinecarboxylic acids and derivatives	HTIQEAQVCTYUB-UHFFFAOYNA-N	O=C(OC)C1=C(NC(C=C1)C(=O)OCC)C1C=C2CC=CC2C1)COCN)C
1382	4. 229	327. 08633	5-hydroxy-3,7-dimethoxy-2-(4-methoxyphenyl)-4H-chromen-4-one	[M+H] ⁻	327. 086	C18H16O6	7-O-methylated flavonoids	WSQWAMGRHLQANC-UHFFFAOYSA-N	O=C1C(OC)=C(OC=C2C(OC)C=C(O)C12)C=C3CC(OC)=CC3
1383	4. 233	153. 05418	Vanillin	[M+H] ⁺	153. 05463	C8H8O3	Methoxyphenols	MWOOGOJBH1ARPG-UHFFFAOYSA-N	O=CC1=CC=C(O)C(OC)=C1
1384	4. 234	381. 1911	Histamine-trifluoromethyltoluide	[M+H] ⁻	381. 19077	C19H25F3N4O	Trifluoromethylbenzenes	PMKJGBBYNEYP-UHFFFAOYNA-N	O=C(NC1=CC=C(C=C1)C(F)(F)F)C(CCC(NC2C=CN=CN2)C
1385	4. 236	182. 08073	Tyrosine	[M+H] ⁺	182. 08099	C9H11NO3	Tyrosine and derivatives	OUYCCASQSFEME-UHFFFAOYSA-N	O=C(O)C(N)CC1=CC=C(O)C=C1
1386	4. 253	433. 1106	Vitexin	[M+H] ⁺	433. 11292	C21H20O10	Flavonoid 8-C-glycosides	SGEWCQFVRRZDC-YPRICQMDSA-N	OC[C-H]1O[C-H]1([C-H](O)[C-H](O)[C-H]1O)C1=C(O)C=C(O)C2=C1OC(=CC2=O)C1=CC=C(O)C=C1
1387	4. 255	320. 2059	Tributyrin	[M+H] ⁺	320. 207	C15H26O6	Triacylglycerols	UYXTWCETRIEDR-UHFFFAOYSA-N	O=C(OC)C(OC(=O)CCC)COC(=O)CCC
1388	4. 258	211. 14357	Cyclo(Leu-Pro)	[M+H] ⁺	211. 1441	C11H18N2O2	Alpha amino acids and derivatives	SZJNCZMRZAUNQT-UHFFFAOYNA-N	O=C1N2CCCC2C(O)=NC1CC(C)C
1389	4. 259	189. 07564	Hydroxysuberic acid	[M+H] ⁻	189. 0766	C8H14O5	Organic acids	ARJZZFXSNJKGR-UHFFFAOYNA-N	O=C(O)CCCC(O)CC(=O)O
1390	4. 261	357. 09692	5-Hydroxy-2',4',7,8-Tetramethoxyflavone	[M+H] ⁻	357. 09796	C19H18O7	8-O-methylated flavonoids	AHUAGKIYEMQITH-UHFFFAOYSA-N	O=C1C=C(OC2=C(OC)C(OC)=CC(O)=C12)C=C3CC(OC)=CC3OC
1391	4. 264	380. 94601	PFSA-H	[M+H] ⁻	380. 94601	C6H2F12O3S	PFSA	DOWJLTPWFGXFD-UHFFFAOYSA-N	O=S(=O)(O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F
1392	4. 265	369. 09677	Acacetin Diacetate	[M+H] ⁺	369. 09686	C20H16O7	4'-O-methylated flavonoids	VYHHSBHXZYSILO-UHFFFAOYSA-N	O=C(OC=C1C=C(OC(=O)C)C=C2(C(=O)C2C1)C=C3CC(OC)=CC3)C
1393	4. 266	347. 11563	Toraseamide	[M+H] ⁻	347. 11835	C16H20N4O3S	Pyridinesulfonamides	NGBFQHCQMULJNZ-UHFFFAOYSA-N	CC(C)N=C(NS(C1=CN=C=CC1=NC2=CC=CC(C)=C2)(=O)=O)=O
1394	4. 276	179. 15379	6,7-Dihydroxycoumarin;esculetin	[M+H] ⁺	179. 14999	C9H6O4	6,7-dihydroxycoumarins	ILEDWLMCKZNDJK-UHFFFAOYSA-N	O=C1OC=2C=C(O)C(O)=CC2=C1
1395	4. 282	510. 25674	[3,4,5-trihydroxy-6-[[[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxymethyl]oxan-2-yl]-2,6,6-trimethylcyclohexene-1-carboxylate	[M+H] ⁺	510. 25449	C22H36O12	0-glycosyl compounds	URTXFXGQVQACIC-UHFFFAOYSA-N	O=C(OC1OC(COC2OC(CO)C(O)C(CO)C2O)C(O)C1O)C3OC(C)CCC(C3)C
1396	4. 288	253. 10754	Phomalone	[M+H] ⁻	253. 10814	C13H18O5	Alkyl-phenylketones	PTDQWUHUOMDVS-UHFFFAOYSA-N	O=C(C1=C(O)C(=C(C(=O)C=C1OC)CCO)CCC
1397	4. 288	496. 24182	Silodosin (Rapaflo)	[M+H] ⁺	496. 242	C25H32F3N3O4	Indolecarboxamides and derivatives	CNCPYILMDWPEY-QGZVFWFLSA-N	O=C(N)C1=CC(=CC2=C1N(CCC2)CCO)CC(NCOC=3C=CC=3OCC(F)(F)F)C
1398	4. 289	470. 29544	(E)-5-hydroxy-N-[3-[5-[3-[(E)-5-hydroxy-3-methylpent-2-enoyl]aminol]propyl]-3,6-dioxopiperazin-2-yl]propyl]-3-methylpent-2-enamide	[M+H] ⁺	470. 2973	C22H36N4O6	Alpha amino acids and derivatives	CNQCBOHTKBVCFM-WXUJJIITCSA-N	OC(=NCCC1N=C(O)(N=C1O)CCCN=C(O)C(C)C(CO)C=C(C)CCO
1399	4. 299	508. 27811	Epothilone B	[M+H] ⁺	508. 27301	C27H41NO6S	Epothilones and analogues	QXRSDHAAWVKZLJ-FBAHCSNKS-N	O=C1OC(C(=CC=2N(C(SC2)C)CC3OC(C)CCCC(C)C(C(=O)C(C(=O)C1)C
1400	4. 303	203. 04448	THYMOQUINONE	[M+H] ⁺	203. 04689	C10H12O2	P-benzoquinones	KEQHJBSNCLWCAE-UHFFFAOYSA-N	O=C1C=C(C(=O)C=C1)C(C)C
1401	4. 304	343. 12796	2,6-dihydroxy-7-methoxy-1,1,4a-trimethyl-3,4,10,10a-tetrahydro-2H-phenanthren-9-one	[M+H] ⁺	343. 13062	C18H24O4	Diterpenoids	JKTSLDANJEZMK-UHFFFAOYSA-N	O=C1C2=CC(OC)=C(O)C=C2C3(C)CCC(O)C(C)C(C3)C1
1402	4. 306	538. 27393	taurohyocholic acid	[M+H] ⁺	538. 28003	C26H45NO7S	Trihydroxy bile acids, alcohols and derivatives	XSOLDPYUICRHJX-DSNLCWFJSA-N	O=S(=O)(O)CCN=C(O)CCC(C)C1CCC2C3C(O)C(O)C4CC(O)CCC4(C)C3CCC12C
1403	4. 307	409. 11041	(1s)-1,5-anhydro-1-[2,4,6-trihydroxy-3-(4-hydroxybenzoyl)phenyl]-d-glucitol	[M+H] ⁺	409. 11292	C19H20O10	Phenolic glycosides	BZYKNVLTWVYEFA-ZJJKXBQSA-N	O=C(C1=CC=C(C=C1)C2=C(O)C=C(O)C(=C2O)C3OC(CO)C(O)C(O)C3O
1404	4. 311	269. 03339	kavain	[M+H] ⁺	269. 02936	C14H14O3	Kavalactones	XEAQIWGXBCYFX-GUOLPTJISA-N	O=C1OC(C=CC=2C=CC=CC2)CC(OC)=C1
1405	4. 311	329. 21667	Peramivir Trihydrate	[M+H] ⁺	329. 21799	C15H34N4O7	Gamma amino acids and derivatives	RFUCJKFZFXN1GB-ZBHRWQZSA-N	O=C(O)C1CC(NC(=N)N)C(C1O)C(NC(=O)C)C(C)CC.O.O.O
1406	4. 312	607. 16565	Flavonol base + 3O, 1MeO, 0-diflex-diflex	[M+H] ⁻	607. 16571	C28H32O15	Flavonol 0-glycosides	DGFGSUQDQJHFL-UHFFFAOYNA-N	O=C3C(OC2OC(C)C(OC1OC(C)C(O)C(O)C1(O)C(C2)O))=C(OC4(C(C(OC)CC(O)C4O)C4O)=C5C=CC(CO)C=C5)C
1407	4. 314	543. 23834	Symplocosin	[M+H] ⁺	543. 23749	C26H32O11	Lignan glycosides	QLJNETOQQXTLI-UHFFFAOYSA-N	OC1=CC=C(C=C1OC)C2OC3C(OC23)C4=CC=C(C(OC5O)C(O)C(O)C5O)C(OC)=C4
1408	4. 322	116. 07043	L-(-)-Proline	[M+H] ⁺	116. 0706	C5H9NO2	Proline and derivatives	ONIBWKKTOPOVIA-BYPYZUCNSA-N	OC(=O)[C@H]1CCCN1
1409	4. 331	284. 14798	Metolachlor	[M+H] ⁺	284. 14117	C15H22ClN2O2	Anilides	WYQBLGZPHOPPO-UHFFFAOYNA-N	CCC1=CC=CC(C)=C1N(C(C)OCC)C(=O)CC1
1410	4. 333	385. 11234	Sinapoylhexoside (isomer of 955)	[M+H] ⁻	385. 1131	C17H22O10	Sinapinic acid and derivatives	XRXBRPFTFKHEF-UHFFFAOYNA-N	O=C(OC1OC(CO)C(O)C(O)C1O)C(=O)C=CC=2C=C(OC)C(O)=C(OC)C=2
1411	4. 336	341. 13715	Flavanone base + 3O, 1Prenyl	[M+H] ⁺	341. 13721	C20H20O5	Prenylated flavanones	LPEFZZAVJPLNZ-UHFFFAOYNA-N	O=C2C=C(O)C=CC(O)=C(C=3(OC(C1=CC=C(O)C=C1)C2)CC=C(C)C(C
1412	4. 337	405. 15057	Desoxyrhaponticin	[M+H] ⁺	405. 14999	C21H24O8	Stilbene glycosides	MFMQRDLLSRLLJY-DXKBKAGUSA-N	OC=1C=C(OC2OC(CO)C(O)C(C2O)C=C(C=CC3=CC=C(OC)C=C3)C1
1413	4. 339	149. 0959	ANETHOLE	[M+H] ⁺	149. 09608	C10H12O	Anisoles	RUV1NXPYWBROJD-ARJAWSKDSA-N	O(C1=CC=C(C=C1)C=CC)C
1414	4. 354	309. 09512	D-(-)-salicin	[M+H] ⁺	309. 09448	C13H18O7	Phenolic glycosides	NGFM1CBJZRJ1BI-UHFFFAOYSA-N	OC=C1C=CC=CC1OC2OC(CO)C(O)C2O
1415	4. 355	560. 15576	(2S)-6-[(2S)-5,7-dihydroxy-2-(4-hydroxyphenyl)-4-oxo-2,3-dihydrochromen-8-yl]-5,7-dihydroxy-2-(4-hydroxyphenyl)-2,3-dihydrochromen-4-one	[M+H] ⁺	560. 15509	C30H22O10	Biflavonoids and nolyflavonoids	YBD1ZQWDBOOFB-GOTSBHOMSA-N	O=C1C=2C(O)=CC(O)C(C2OC(C3=CC=C(O)C=C3)C1)C=4C(O)=CC=5OC(C6=CC=C(O)C=C6)CC(=O)C5C4O
1416	4. 356	227. 01837	Trinitrotoluene	[M+H] ⁻	227. 01839	C7H5N3O6	Nitrobenzenes	SPSSLHKKWKEEL-UHFFFAOYSA-N	CC1=C(C=C(C=C1N(=O)=O)N(=O)=O)N(=O)=O
1417	4. 364	237. 03891	SINAPIC ACID METHYL ETHER	[M+H] ⁻	237. 04083	C12H14O5	Coumaric acids and derivatives	YTFVRYKXDAIBI-SNAWJCMRSA-N	O=C(O)C=CC1=CC(OC)=C(OC)C(OC)=C1

1418	4. 37	154. 15851	d-LIMONENE	[M+H] ⁺	154. 15901	C10H16	Menthane monoterpenoids	XMGQYMWDOXHJM-JTQLQTEISA-N	C=C(C)C1CC=C(C)CC1
1419	4. 375	326. 13467	Boldine	[M-H] ⁻	326. 13977	C19H21N04	Alkaloids	LZJRNLRASBVRXR-UHFFFAOYNA-N	CC1=CC2=C(C(CCN(C)CCC4=CC(O)=C(O)C)C2=C34)C=C10
1420	4. 375	387. 19943	Sinapoylhexoside	[M+H] ⁺	387. 20081	C17H22010	Sinapinic acid and derivatives	XRKBRPFTFKHEF-ONEGZZKNNA-N	O=C(OC1OC(CO)C(O)C(C)C1O))C=CC=CC(C)C(C)=C(OC)C=C2
1421	4. 377	490. 31979	Oxysporidinone_130003	[M+H] ⁺	490. 31699	C28H43N06	Terpene glycosides	CYNJYDGSURTLL-CPNJWEJPSA-N	O=C1C(=C(O)C(=CN1C)C2(O)CCC(=O)CC2O)C3OC(C(=CC(C)CC(C)C)C(C)C)C3
1422	4. 388	647. 16846	4-(3-oxobutyl)phenyl 6-O-[(2E)-3-(4-hydroxyphenyl)prop-2-enoyl]-2-O-(3,4,5-trihydroxybenzoyl)-beta-D-glucopyranoside	[M+H] ⁺	647. 16998	C32H32013	Phenolic glycosides	Q1EOAENKXYTH-IQDFXJLSA-N	O=C(OC1OC(OC2=C(C(=C2)CCC(=O)C)C(OC(=O)C3=CC(O)=C(CO)C(O)=C3)(CO)C1O)C=C4C=CC=C(O)C=C4
1423	4. 39	314. 11316	5-[(E)-3-hydroxybut-1-enyl]-4-[4-[(E)-3-oxobut-1-enyl]anilino]oxolan-2-one	[M-H] ⁻	314. 11084	C18H21N04	Cinnamic acids and derivatives	HGCMCLAKARHJW-OBXOXFIQSA-N	O=C1OC(C=CC(O)C)C(CN2=CC=C(C=CC(=O)C)C=C2)C1
1424	4. 392	413. 14447	3-oxo-3-[[[(2R,3S,4S,5R,6S)-3,4,5-trihydroxy-6-(4-hydroxy-5-methyl-2-propan-2-ylphenoxy)oxan-2-yl]methoxy]propanoic acid	[M-H] ⁻	413. 14532	C19H26010	Terpene glycosides	VJVG7GQETNCOEX-LQDZTQBFSA-N	O=C(O)CC(=O)CC1OC(OC2=CC(=C(O)C=C2C(C)C)C(C)C(O)C(C)O)C1O
1425	4. 395	304. 1167	N-(6-methoxypyridin-3-yl)-1-methyl-1H-indole-6-carboxamide	[M+H] ⁺	304. 10999	C16H15N302	Indolecarboxamides and derivatives	IEYPTSQYHVVDAC-UHFFFAOYSA-N	O=C(NC1=CN=C(OC)C=C1)C=CC=CC=CC(C)C(C)C
1426	4. 395	454. 16919	Phlorhizin	[M+H] ⁺	454. 17078	C21H24010	Flavonoid O-glycosides	IOUVKUPGOMBWBT-QNDFHXLGSA-N	O=C(C=C1C(O)=CC(O)=CC1OC2OC(CO)C(O)C(O)C2O)CCC3=CC=C(O)C=C3
1427	4. 398	178. 01389	S-CARBOXYMETHYL-L-CYSTEINE	[M-H] ⁻	178. 017	C5H9N04S	L-cysteine-S-conjugates	GBFLZEXEOZUWRN-VKHMYEASA-N	O=C(O)CSC(N)C(=O)O
1428	4. 399	250. 10684	Goniothalenol	[M+H] ⁺	250. 10738	C13H1204	Furoprans	ZK1RVBNLJG1EM-UHFFFAOYSA-N	O=C1OC2C(OC(C=3C=CC=CC3)C2O)C=C1
1429	4. 409	385. 21753	(4aR)-5-hydroxy-6-methoxy-1,1-dimethyl-7-propan-2-yl-2,3,4,9,10,10a-hexahydrophenanthrene-4a-carboxylic acid	[M+H] ⁺	385. 21786	C21H3004	Diterpenoids	QQNSARJGBPMQ1-MZVUKIXXSA-N	O=C(O)C1C2=CC(O)=C(OC)C(C=CC3CC1C(C)C(C)CC2)C(C)C
1430	4. 415	347. 10925	Demethyleneberberine	[M+H] ⁺	347. 10999	C19H18N04+	Protoberberine alkaloids and derivatives	HVTCCKMWZDWOY-UHFFFAOYSA-O	OC=1C=CC2=CC=C4C=CC(OC)=C(OC)C4=C1N+3CCC2=CC1O
1431	4. 415	327. 11804	Dendrophanol	[M+H] ⁺	327. 12	C17H2005	Stilbenes	YTRAVU1KLRAOQ-UHFFFAOYSA-N	OC1=CC=C(C=C1OC)CCC2=CC(OC)=C(O)C(C)C(=C2
1432	4. 417	288. 18002	(4-oxido-2,3,5,6,7,8-hexahydro-1H-pyrrolizin-4-ium-1-yl)methyl 2,3-dihydroxy-3-methylpentanoate	[M+H] ⁺	288. 18054	C14H25N05	Pyrrolizidines	QRYNXLBAFAPSKQ-UHFFFAOYSA-N	O=C(OC1CCN2(=O)CCCC12)C(O)C(O)C(C)CC
1433	4. 428	367. 18542	Tobramycin 1-N- or 3-N-carbamoyl, ion source fragment	[M+H] ⁺	367. 18301	C14H30N407	Aminocyclitol glycosides	IUFQFQNF1GWHJ-FZEEZGWEXSA-N	OC1OC(OC2C(O)C(OCN(C)C(C)C2N)C(O)C(C)N)C1O
1434	4. 434	267. 16922	Panaxynol	[M+H] ⁺	267. 17001	C17H240	Long-chain fatty alcohols	UGJAEDFOKNAQD-ZHACJMWSA-N	OC(C)CCCCC=CCCCCCCCC)C=C
1435	4. 44	285. 15955	Tropisetron	[M+H] ⁺	285. 15976	C17H20N202	Indolecarboxylic acids and derivatives	ZNRGQMMCGHDTET-UHFFFAOYNA-N	O=C(OC1C2N(C)C(C)C2)C1C3=CC=C(C=CC=CC3
1436	4. 445	273. 14383	Sempervirine	[M+H] ⁺	273. 13861	C19H16N2	Beta carbolines	UQVUEULZDJRMJR-UHFFFAOYSA-N	C1CCC2=CC3=C4N=C5C=CC=C5=C4C=CC3=C2C1
1437	4. 448	271. 16354	19-Norandrosta-4,9-dien-3,17-dione	[M+H] ⁺	271. 16299	C18H2202	Oxosteroids	BHTWZQKERRCPZ-RYRKJORJSA-N	O=C1C=C2C(=C3CCC4(C(=O)CC4C3CC2)C)CC1
1438	4. 465	313. 13956	6-(1,1-DIMETHYLLALLYL)-2-(1-HYDROXY-1-METHYLETHYL)-2,3-DIHYDRO-7H-FURO[3,2-G]CHROMEN-7-ONE	[M-H] ⁻	313. 14453	C19H2204	Psoralens	JCDLLLYA1CSQV-INIZCTEOSA-N	O=C1OC=CC=CC3C(C3=CC2=C1C(C=C)C(C)C(C)C)C1O
1439	4. 467	299. 13745	3-Hydroxy-3',4'-Dimethoxyflavone	[M+H] ⁺	299. 13629	C17H1405	Flavonols	BXLAVJWSFYZDPF-UHFFFAOYSA-N	O=C1C(O)C(=C(C=CC=CC21)C=3C=CC(OC)C(=O)C)C3
1440	4. 471	327. 1333	8,8-dimethyl-2-phenylpyrano[2,3-f]chromen-4-one	[M+H] ⁺	327. 13269	C20H1603	Pyranoflavonoids	RBKXJAHRWPNPM-UHFFFAOYSA-N	O=C1C=C(C=CC2C1=CC=C3OC(=CC32)C(C)C=4C=CC=CC4
1441	4. 484	305. 15897	1-(3aS,6Z,10Z,11aR)-6-(hydroxymethyl)-3-methylindene-2-oxo-3a,4,5,8,9,11a-hexahydrocyclohexa[h]furan-10-yl)methyl acetate	[M-H] ⁻	305. 15668	C17H2205	Germacranolides and derivatives	XGODCDTVQAHYAH-DZPPMGJRSA-N	O=C1OC2C=C(COC(=O)C)CCC=C(CO)CCC2C1=C
1442	4. 486	463. 12106	(1S,3R,6R,7S,8S,9R,10S,13S,16S,17R)-8-tert-butyl-6,9,12,17-tetrahydroxy-16-methyl-2,4,14,19-	[M+H] ⁺	463. 12106	C20H24011	Ginkgolides and bilobalides	AMOGMTLMADEGQ-PDZSGAKNSA-N	O=C1OC2OC34C(=O)CC5C(O)C(C(C)C)C2(C1O)C54C(O)C6OC(=O)C(C)C63O
1443	4. 486	325. 10226	Licarin A	[M-H] ⁻	325. 10001	C20H2204	2-arylbenzofuran flavonoids	ITDFOWJEDZPCF-AATRIKPKSA-N	OC1=CC=C(C=C1OC)C2OC=3C(OC)=CC(C=CC)=CC3C2C
1444	4. 488	351. 1058	1-(4-hydroxyphenyl)-3-[(2R,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxypropan-1-one	[M+H] ⁺	351. 10504	C15H2008	Fatty acyl glycosides of mono- and disaccharides	NPAQLFPPEOMKAL-VXXRCYHCSA-N	O=C(C1=CC=C(O)C=C1)CCOC2OC(CO)C(O)C(C)C2O
1445	4. 49	411. 18939	Picaline	[M+H] ⁺	411. 19101	C23H26N205	Corynanthan-type alkaloids	DXTJMQCRVFNWBD-FTHUSJGSA-N	O=C(OC(C1(=O)C(=O)C2C(=CC)CN34OC5(NC=6C=CC=C6C51C4)C3=C2)C
1446	4. 494	165. 05476	3-Phenyllactic acid	[M-H] ⁻	165. 05573	C9H1003	Phenylpropanoic acids	VOXXWSYKYCBWHO-UHFFFAOYNA-N	O=C(O)C(C)CC=1C=CC=CC1
1447	4. 528	281. 06595	Feruloyl Lactate	[M-H] ⁻	281. 06479	C13H1407	Ferulic acid and derivatives	ZWAYKTOAUP1GML-HWKANZRONA-N	CC1=CC=C(C=C1C=C(C(=O)O)C(C)C(=O)O)C=C1O
1448	4. 531	109. 02869	CATECHOL	[M-H] ⁻	109. 029	C6H602	Catechols	YCTMNLNLNPGFHC-UHFFFAOYSA-N	OC=1C=CC=CC1O
1449	4. 535	316. 2113	[5-hydroxy-3-(hydroxymethyl)-2-oxo-6-propan-2-ylcyclohex-3-en-1-yl] 3-methylpentanoate	[M+H] ⁺	316. 21182	C16H2605	Menthane monoterpenoids	BUOADWXPJXXRM-UHFFFAOYSA-N	O=C(OC1C(=O)C(=CC(O)C1C(C)C)CO)CC(C)CC
1450	4. 541	188. 03438	4-HYDROXY-2-QUINOLINECARBOXYLIC ACID	[M-H] ⁻	188. 035	C10H7N03	Quinoline carboxylic acids	HCZHIE1FKROPDY-UHFFFAOYSA-N	O=C(O)C1C(=C(C=O)C=CC=CC2N1
1451	4. 542	167. 03738	3,4-Dihydroxyphenylacetic acid	[M-H] ⁻	167. 03499	C8H804	Catechols	CFPZDZCDUFSOFZ-UHFFFAOYSA-N	O=C(O)CC1=CC=C(O)C(C)=C1
1452	4. 543	120. 08041	Indoline	[M+H] ⁺	120. 08077	C8H9N	Indolines	LPAGFVYQRIESJQ-UHFFFAOYSA-N	C1=CC=C2C(=C1)CCN2
1453	4. 543	208. 09602	N-Acetylphenylalanine	[M+H] ⁺	208. 09682	C11H13N03	Phenylalanine and derivatives	CPQJSKFNMDLON-UHFFFAOYNA-N	O=C(O)C(C(N=C(O)C)CC=1C=CC=CC1
1454	4. 544	275. 01813	6-Phospho-D-gluconic acid	[M-H] ⁻	275. 01736	C6H13010P	Monosaccharide phosphates	BTBSGZKFKXLSJQ-SQOUCZDYSA-N	O[C@H](COP(O)(O)=O)[C@H](O)[C@H](O)[C@H](O)C(O)=O
1455	4. 545	429. 20035	elegantissine	[M+H] ⁺	429. 20001	C23H28N206	Indolizidines	TIWZEO1NXXJHCY-DWROLHPLSA-N	O=C(OC)C1=CC(C)C2CN3CC4(C(=O)NC5=C(OC)C(OC)=CC=C54)C3CC12
1456	4. 549	367. 20892	3-[2-(6,7-dihydroxy-1,2,4a-trimethylspiro[3,4,6,7,8,8a-hexahydro-2H-naphthalene-5,2'-oxirane]-1-yl)ethyl]-2-hydroxy-2H-furan-5-one	[M+H] ⁺	367. 21152	C20H3006	Butenolides	QMWJAHMURTIJMQ-UHFFFAOYSA-N	O=C1OC(C)C(=C1)CCC2(C)C(C)CC3(C)C2OC(C)C(C)C43OC4
1457	4. 549	534. 34595	9-hydroxy-5b,8,11a-trimethyl-1-prop-1-en-2-yl-1,2,3,4,5,6,7,7a,9,10,11,11b,12,13,13a,13b-	[M+H] ⁺	534. 34253	C30H4407	Triterpenoids	FTKGHGVFGGOMW-UHFFFAOYSA-N	O=C(O)C12CCC(C(=C(C)C)C2C3CC4C5(C)CCC(O)C(C(=O)O)C(C)C5C(C4)C)C3(C(=O)O)C1
1458	4. 552	233. 00833	FT-sulfone	[M-H] ⁻	233. 01009	C6H9F304S	PFSA	FTHRJQNFESLACH-UHFFFAOYSA-N	O=C(O)CCS(=O)(=O)CCC(F)F
1459	4. 562	562. 25378	(S)-2-(((S)-7-acetamido-1,2,3-trimethoxy-9-oxo-5,6,7,9-tetrahydrobenzofalantalen-10-yl)amino)-N-(4-methoxyphenyl)propanamide	[M+H] ⁺	562. 26001	C31H35N307	Alpha amino acid amides	RVLHHzKCFQNH1I-XDHUDOTRSA-N	O=C1C=C2C(=CC(C1NC(=O)NC3=CC=C(OC)C=C3)C)C4=C(OC)C(CO)C(=O)C(=O)C=C4CC(C)C2NC(=O)C
1460	4. 563	322. 09183	Metazachlor ESA	[M-H] ⁻	322. 0867	C14H17N304S	Anilides	IPVCEPCEVHQOV-UHFFFAOYSA-N	CC1=CC=CC(C)=C1N(CN1C=CC=N1)C(=O)CS(O)(=O)=O

1461	4.564	255.12265	DL-Liquiritigenin	[M-H] ⁻	255.12166	C15H12O4	Flavanones	FURUXTVLHOCNA-UHFFFAOYSA-N	O=C1C2=CC(=O)C=C2OC(C3=CC(=O)C=C3)C1
1462	4.568	217.09651	4-Formyl-antipyrine	[M-H] ⁺	217.09715	C12H12N2O2	Phenylpyrazoles	QFYZYDOEJZMDX-UHFFFAOYSA-N	CN1N(C(=O)C(C=O)=C1)C1=CC=CC=C1
1463	4.573	357.17981	Arnicolide C	[M-H] ⁺	357.17001	C19H26O5	Sesquiterpene lactones	WKUOPGZYLRFCHJ-APDQSUKSA-N	O=C(OC1C2C(OC(=O)C2)CC(C)C3CC(=O)C13)C(C)C
1464	4.582	308.11105	Tolnaftate	[M-H] ⁺	308.10999	C19H17NO5	Naphthalenes	FUSMLNFJXSJDI-UHFFFAOYSA-N	S=C(OC(=O)C-CO-2C-CC(=C2C1)N(C3=CO-CC(=C3)C)C
1465	4.588	301.11749	Pesticide9_Desmedipham_C16H16N2O4_3-[(Ethoxycarbonyl)amino]phenyl phenylcarbamate	[M-H] ⁺	301.11801	C16H16N2O4	Phenylcarbamic acid esters	WJZJMKBKWXKTQ-UHFFFAOYSA-N	OC(=NC(=O)CC(=O)C)=2C=CC(=N(C(=O)O)CC)C2
1466	4.591	171.06548	1,4-Cyclohexanedicarboxylic acid	[M-H] ⁻	171.06628	C8H12O4	Dicarboxylic acids and derivatives	PGZQGDETEZPERC-UHFFFAOYSA-N	O=C(O)C1CCC(C(=O)O)CC1
1467	4.594	254.06645	methyl 2-[(2,3-dihydroxybenzoyl)amino]-3-hydroxypropanoate	[M-H] ⁻	254.067	C11H13NO6	Hippuric acids and derivatives	NQIZIOLKJAGJU-UHFFFAOYSA-N	O=C(OC)C(N(=O)C=C1C=CC(=O)C1)CO
1468	4.596	481.12912	Lusitanicoside	[M-H] ⁺	481.13086	C21H30O10	Phenolic glycosides	DAELTIGCCPYTP-ZLQZEYEIS-N	OC1C(O)C(OC2OC(OC3=CC(=O)C(CO)CC(C)C(O)C2)OC(C1)C
1469	4.603	299.10245	Scutellarein 4'-methyl ether	[M-H] ⁻	299.10306	C16H12O6	4'-O-methylated flavonoids	XVMEYCPXYZLAI-UHFFFAOYSA-N	O=C1C=C(OC2=CC(O)=C(C)C(O)=C12)C=3C=CC(OC)=CC3
1470	4.604	339.11752	Licodione base + 30, 2Prenyl	[M-H] ⁻	339.12079	C20H20O5	Prenylated licodiones	I3XMKVKYGAGJGJ-UHFFFAOYSA-N	O=C(C(=O)C1=CC=C(C)C=C1)C=2C=C(C(=O)=CC=2(O))CC=C(C)C
1471	4.615	153.01921	2,3-Dihydroxybenzoic acid	[M-H] ⁻	153.01933	C7H6O4	Salicylic acids	GLDQAMCGOIJDV-UHFFFAOYSA-N	O=C(O)C(=O)C=C(C(=O)C)O
1472	4.617	204.02948	XANTHURENIC ACID	[M-H] ⁻	204.03	C10H7NO4	Quinoline carboxylic acids	FBZXONHGGBHHY-UHFFFAOYSA-N	O=C(O)C1=CC(=O)C=C2C=CC(=O)C2CN1
1473	4.618	207.0112	2-Naphthalenesulfonic acid	[M-H] ⁻	207.01213	C10H8O3S	2-naphthalene sulfonates	KVBGVZZKJNLNJU-UHFFFAOYSA-N	OS(=O)(=O)C1=CC2=CC=CC=C2C=C1
1474	4.62	317.11447	Rhodocladonic Acid	[M-H] ⁻	317.11322	C15H10O8	Naphthofurans	XKWWCTISHMFJB-UHFFFAOYSA-N	O=C1C(=O)C=2C(O)=C3C(O)=(OC3=CC2(=O)=C1OC)C(=O)C
1475	4.623	217.10738	Hydroxysebacic acid	[M-H] ⁻	217.10789	C10H18O5	Organic acids	OQYZCKCJQHIE-UHFFFAOYNA-N	O=C(O)CCCCCCC(O)CC(=O)O
1476	4.629	269.11374	Galangin	[M-H] ⁻	269.11237	C15H10O5	Flavonols	VCCRNZQBSJXYJD-UHFFFAOYSA-N	O=C1C(O)=C(OC=2C(C)C(C(=O)C12)C=3C=CC=CC3
1477	4.635	301.09186	2-(3-hydroxy-5-methoxyphenoxy)-6-(hydroxymethyl)oxane-3,4,5-triol	[M-H] ⁻	301.0929	C13H18O8	Phenolic glycosides	SJBWDSQMCPAGHA-UHFFFAOYSA-N	OC=1C=C(OC)C(C(OC2OC(CO)C(C)C(O)C2)O)C1
1478	4.648	363.23743	2-[(2E)-3,7-dimethylocta-2,6-dienyl]-3-methoxy-5-(2-phenylethyl)phenol	[M-H] ⁻	363.23294	C25H32O2	Stilbenes	ZDSBUUDXDQSCSK-DIEDYNTISA-N	OC=1C=C(C(=O)OC)C1CC=C(C)CCC=C(C)C)CCC=2C=CC=CC2
1479	4.651	587.29132	[(2R,3S,4S,5R,6S)-6-[3,5-dihydroxy-4-{3-(4-hydroxyphenyl)orphanovyl}phenoxy]-3,4,5-trihydroxyoxan-2-yl)methyl 3,4,5-	[M-H] ⁻	587.29706	C28H28O14	Flavonoid O-glycosides	YPFUHFNAEWDRD-ZKPBI.SLZSA-N	O=C(OC1OC(OC2=CC(O)=C(C)C(=O)C2)C(C)OC1C3=CC=C(C)C(C3)C
1480	4.653	370.07071	Pesticide6_Diniconazole_C15H17Cl2N3O_(1E)-1-(2,4-Dichlorophenyl)-4,4-dimethyl-2-((1E-1,2,4-triazol-1-yl)pent-1-en-3-yl)	[M-H] ⁻	370.073	C15H17Cl2N3O	Cinnamyl alcohols	FBOUTAKEJMZPGG-WNNJVPZSA-N	C1C1=CC=C(C=C(N2N=CN=C2)C(O)C(C)C(C)C(C1)=C1
1481	4.658	224.12704	4-Hydroxybenzoylecholine	[M-H] ⁺	224.12756	C12H18NO3	Benzoic acid esters	BAPAICNRGTBJT-UHFFFAOYSA-O	C[N+](C)(C)CCCC(O)=C1C=CC(=O)C=C1
1482	4.658	315.11966	Pinoqueretin	[M-H] ⁻	315.11609	C16H12O7	Flavonols	DTFXGVGIKNSQQ-UHFFFAOYSA-N	O=C1C(O)=C(OC2=CC(O)=C(C)=C12)C=C3C=CC(O)=C(O)C3
1483	4.66	503.24872	4-[(E)-3-[(2R,3R,4S,5S,6R)-3-{[(2S,3R,4R)-3,4-dihydroxy-4-(hydroxymethyl)oxolan-2-yl]oxy}-5,6-dihydroxy-6-(hydroxymethyl)oxan-2-yl]-3aS,8R,8aR)-8-hydroxy-6,8-dimethyl-3-methylidene-2-oxo-3a,4,5,8a-	[M-H] ⁺	503.24869	C24H38O11	Fatty acyl glycosides of mono- and disaccharides	IDPRQTHASGHSD-BTOUMF1XSA-N	O=C1C=C(C)C(C=CC(OC2OC(CO)C(C)C(OC2)OC(CO)C(CO)C(CO)C1)C(C
1484	4.667	279.14386	tetrahydrocyclohepta[b]furan-7-yl]propanoic acid	[M-H] ⁻	279.14893	C15H20O5	Terpene lactones	PPUVIGSWLRHCY-PSPSQSSA-N	O=C1OC2C(C1=C)CCC(=C(CCC(=O)O)C2(O)C)C
1485	4.668	457.19702	2,7,7,11,15,17-hexamethyl-18-methylidene-5,13,16-trioxo-6,14-dioxatetracyclo[9.8.0.02,9.022,22]nonadec-3-en-10-yl acetate	[M-H] ⁻	457.19882	C26H34O7	Naphthopyrans	JFYFYCQXZYIOBKU-UHFFFAOYSA-N	O=C1OC(C)(C)C2CC(OC(=O)C)C3(C)C4C(=O)OC(C(=O)C4(C)=C(C)C3C2(C1)C)C
1486	4.669	220.0966	Aniracetam	[M-H] ⁺	220.097	C12H13NO3	Benzoic acids and derivatives	ZXNRKTGTJPIJK-UHFFFAOYSA-N	O=C(C1=CC=C(OC)C=C1)N2C(=O)CCC2
1487	4.67	230.14677	N-cyano-N'-(1,1-dimethylpropyl)-N'-3-pyridinyl-guanidine	[M-H] ⁻	230.14111	C12H17N5	Pyridines and derivatives	HKZNDVXGKQDL-UHFFFAOYSA-N	N#N=C(NC(=O)C=NC(=O)C1)NC(C)(C)CC
1488	4.672	481.19406	[3-(13-methyltetradecyl)-5-sulfoxyphenyl] hydrogen sulfate	[M-H] ⁺	481.19241	C21H36O8S2	Phenylsulfates	NGWLEVPXPLCINC-UHFFFAOYSA-N	O=S(=O)(O)OC1=CC(=O)S(=O)(=O)C(=O)C1)CCCCCCCCCCCC(C)C
1489	4.678	271.18942	(E)-2-decylpent-2-enedioic acid	[M-H] ⁺	271.19037	C15H26O4	Long-chain fatty acids	BWSQDEWQMUVIG-ACCUITESSA-N	O=C(O)C(=CCC(=O)O)CCCCCCCCC
1490	4.681	572.34351	Veratrosine	[M-H] ⁺	572.34998	C33H49NO7	Fluorenes	WXQHBVNTJNGJJR-UHFFFAOYSA-N	OC1OC(OC2OC3=CC4C5=CC=C(C(=C5OC4C3(C)C2)C(C)C)C6CC(C)C6)C(C)C(C)C1O
1491	4.685	467.28165	10-hydroxyusambarine	[M+2H] ²⁺	467.28	C30H34N4O	Harmala alkaloids	QYONROBKPAESK-YBTNASEISA-N	OC=1C=CC=2NC3=C(C2C1)CC4C(C=C)C(OC5=6NC=7OC=CC7C6CCN5)CC34
1492	4.687	589.30579	12-O-[deca-2Z,4E,6E-trienoyl]-13-isobutyroyloxy-4-deoxyphorbol	[M-H] ⁺	589.31	C34H46O7	Trigiane and ingenane diterpenoids	WHPZSYIEWQPEHY-OMZKPLISA-N	O=C(OC1C(C)C2(O)C3C=C(C(=O)C3C(=CC2)C4C1(OC(=O)C)C(C)C4(C)C(C)C(C)C=C(C

1504	4. 736	250. 10771	Dimethachlor OXA	[M-H] ⁻	250. 10847	C13H17N04	Alpha amino acids and derivatives	MHGMSAFFNAKIRZ-UHFFFAOYSA-N	COCCN(C(=O)C(=O)=O)C1=C(C)C=CC=C1C
1505	4. 741	308. 11472	CP_M308a	[M+H] ⁺	308. 11603	C15H18ClN3O2	Chlorobenzenes	IVFRBVSPOAYOOK-UHFFFAOYNA-N	C1C1C1(CO)C(CN2C=NC=N2)(C3=CC=C(C(=C3)C1)O
1506	4. 741	326. 12619	Monocrotaline	[M+H] ⁺	326. 12665	C16H23N06	Pyrrolizines	QVCMHGNNRFMAD-XFGHUUIASA-N	O=C1OC2CNC3CC=C(COC(=O)C(=O)C(=O)C1C)C32
1507	4. 741	182. 08051	Tyr	[M+H] ⁺	182. 08118	C9H11N03	Tyrosine and derivatives	OUYCCASQSFEME-QMMGPOBSA-N	N[C=H](CC1=CC=C(C(=O)C=C1)C(=O)=O
1508	4. 744	199. 086	Harmol Hydrochloride	[M+H] ⁺	199. 08658	C12H10N02	Harmala alkaloids	LBBJNGFCXDQYMQ-UHFFFAOYSA-N	O=C1C=CC=2C(=C1)NC=3C2C=CN3C
1509	4. 775	176. 03455	FORMYL-L-METHIONYL PEPTIDE	[M-H] ⁻	176. 03799	C6H11N03S	Methionine and derivatives	PYUSHNNKPOHWEZ-UHFFFAOYSA-N	=O-CNC(C(=O)O)CCSC
1510	4. 784	369. 09335	psulowin	[M-H] ⁻	369. 09796	C20H1807	Furanoid lignans	CAQZFLPHBKTRT-WMISUXOKSA-N	OC12COC(C3=CC=C4OCOC4=C3)C2COC1C5=CC=C6OCOC6=C5
1511	4. 787	291. 12567	curvularin	[M-H] ⁻	291. 12378	C16H2005	Macrolides and analogues	VDUTGYAPXSXCJFC-UHFFFAOYSA-N	O=C1OC(C)CCCCC(=O)C=2C(=O)=CC(O)=CC2C1
1512	4. 792	308. 11157	altenuin	[M+H] ⁺	308. 11285	C15H1406	Biphenyls and derivatives	ADPBTBPP11KLEH-UHFFFAOYSA-N	O=C(O)C1=C(C(=O)C=C(O)C=C1C=2C=C(C(=O)C(=O)=CC2C
1513	4. 794	437. 16907	Picropodophyllin	[M+H] ⁺	437. 16586	C22H2208	Podophyllotoxins	YJGVMLPVUAXIQN-HAEOHJBNSA-N	O=C1OC2C(=O)C3=CC=4OCOC4=C3C(C5=CC(OC)=C(C(=O)C(OC)=C5)C12
1514	4. 804	326. 09903	Tumonoic acid E	[M+H] ⁺	326. 10001	C18H31N04	Proline and derivatives	UUFOMZNGYHUJH-XTVPCCRVSA-N	O=C(O)C1N(C(=O)C(C(=O)C(=O)C(CCC(C)CCC(C)CCC1
1515	4. 835	305. 09125	Oxypeucedanin hydrate	[M+H] ⁺	305. 10001	C16H1606	Psoralens	PEFPWDOPJISUOK-CYBMJFWSA-N	O=C1OC=2C=C3OC=CC3=C(OC(C)C(=O)C(C)C)C2C=C1
1516	4. 844	208. 13234	Benzoylcholine	[M+H] ⁺	208. 13266	C12H18N02	Benzoic acid esters	HOPVGFKDVOOCHD-UHFFFAOYSA-N	C[N+](C)(C)CCOC(=O)C1=CC=CC=C1
1517	4. 847	281. 09552	culpin	[M+2H] ²⁺	281. 09384	C16H1802	Prenylated hydroquinones	QMWWKFPZKRYCUMA-UHFFFAOYSA-N	OC1=CC(=C(C(=O)C=C1C#CC(=C(C)C)CC=C(C)C
1518	4. 848	283. 12842	biochanin A	[M-H] ⁻	283. 13037	C16H1205	4'-O-methylisoflavones	WUADCCVRTIWANL-UHFFFAOYSA-N	O=C1C(=COC=2C=C(C(=O)C(C(=O)C12)C=3C=CC(OC)=CC3
1519	4. 852	621. 18243	5-[4,5-dihydroxy-6-(hydroxymethyl)-3-(3,4,5-trihydroxyoxan-2-yl)oxyoxan-2-yl]oxy-7,8-dimethoxy-3-(4-methoxyphenoxy)chromen-4-one	[M-H] ⁻	621. 1825	C29H34015	Isoflavonoid O-glycosides	NGUSMSQYMPBGF-UHFFFAOYSA-N	O=C1C(=COC=2C(OC)=C(C)C=C(C(OC3OC(CO)C(=O)C3OC4OC(C(=O)C4O)C12)C=5C=CC(=O)C=C5
1520	4. 853	539. 22491	methyl (1S,2R,4R,8R,9S,10R,13R,15R)-2-(acetoxyl)-13-(furan-3-yl)-9-(2-methoxy-2-oxoethyl)-4,8,10,12-tetramethyl-7-oxo-16-methoxy-2-oxoethyl)-3,4,5-tri	[M-H] ⁻	539. 22864	C30H3609	Limonoids	NHOIBRJQOAYQJTR-WILUJPLZSA-N	O=C(OC1C2OC3C(=C(C)C(C4=OC=C4)C3)C2(C)C(CC(=O)OC)C5(C(=O)C6C7C(C(=O)C7)C6)C1C15)C1C
1521	4. 854	543. 21814	methyl 3-(1-(2-(1H-indol-3-yl)ethyl)-2-hydroxy-6-methyl-4-oxo-1,4-dihydroxyridin-3-yl)-3-(3,4,5-trimethoxyphenoxy)propanoate	[M+H] ⁺	543. 21002	C29H32N207	3-alkylindoles	OUBFEEIFMSTDPQ-UHFFFAOYSA-N	O=C1C=C(C(N(C(=O)=C1C(C2=CC(OC)=C(C(=O)C(OC)=C2)CC(=O)OC)CC(C3=CC=C4C=C(C=C4)C3
1522	4. 854	664. 09021	NICOTINAMIDE HYPOXANTHINE DINUCLEOTIDE	[M-H] ⁻	664. 09302	C21H26N6O15P2	(5'->5')-dinucleotides	DGVSIBCYUVRNA-UHFFFAOYSA-N	O=C1N=CN2C=C1N=CN2C3OC(COP(=O)(O)OP(=O)([10-])OC4OC(C[N+]=5C=C(C=C5)C(=O)N(C(=O)C4O)C(=O)C3O
1523	4. 858	186. 11198	3-(2-amino-2-oxoethyl)-5-methyl-hexanoic acid	[M-H] ⁻	186. 11099	C9H17N03	Medium-chain fatty acids	NPDKTSLVWGFPQG-UHFFFAOYSA-N	O=C(O)CC(CC(=N)O)CC(C)C
1524	4. 864	280. 09427	9-Methoxy-2,2-dimethyl-2,6-dihydro-pyran[3,2-c]quinolin-5-one	[M+2H] ²⁺	280. 09439	C15H15N03	Pyraquinolines	IXRKGKGFPFCIR-UHFFFAOYSA-N	OC1=NC=2C=CC(OC)=CC2C=3OC(C=CC13)C(C)C
1525	4. 867	178. 04965	Alliin	[M+H] ⁺	178. 05	C6H11N03S	L-alpha-amino acids	XUHLIQGRKURPH-JDLXGLENSA-N	O=C(O)C(N)CS(=O)CC=C
1526	4. 869	300. 19412	(5S)-5-hydroxy-1,7-diphenylheptan-3-one	[M+H] ⁺	300. 1958	C19H2202	Linear diarylheptanoids	CCKNTMMNRPJQHV-SFHVURJKSA-N	O=C(CCC(=C=CC=CC1)CC(O)CCC=2C=OC=CC2
1527	4. 871	362. 18076	2-[1-hydroxy-1-(4-methoxyphenyl)propan-2-yl]oxy-6-(hydroxymethyl)oxane-3,4,5-triol	[M+H] ⁺	362. 18094	C16H2408	O-glycosyl compounds	JYWSARFDLXXOHT-UHFFFAOYSA-N	OCOC1OC(C(C)C(=O)C2=CC=C(OC)C=C2)C(C(=O)C(=O)C1O
1528	4. 873	285. 13025	3-Hexen-1-ol O-b-D-glucopyranoside	[M+H] ⁺	285. 13	C12H2206	Fatty acyl glycosides of mono- and disaccharides	OZ1PFYKAOOVJEJ-ODUUMNUISA-N	OCOC1OC(CCCC=CC)C(C)C(O)C1O
1529	4. 875	479. 18799	4-(2-Nitroethyl)phenyl 6-O-?-D-xylopyranosyl-?-D-glucopyranoside	[M+H] ⁺	479. 18713	C19H27N012	Phenolic glycosides	ZHVLKFAODFQST-BMWMOQNNSA-N	O=N(=O)CCC1=CC=C(C(OC2OC(COC3OC(C(=O)C3O)C(=O)C(=O)C2O)C=C1
1530	4. 894	423. 12613	2-[[1-(2R,3S)-2-(3,4-dihydroxyphenyl)-3,5-dihydroxy-3,4-dihydro-2H-chromen-7-yl]oxy]oxane-3,4,5-triol	[M+H] ⁺	423. 1264	C20H22010	Flavonoid-7-O-glycosides	UQKKDJWFQZJLPT-PTYVBHFSNA-N	OC1=CC=C(C=C1O)C2OC3=CC(OC4OC(CO)C(=O)C4O)=CC(O)=C3CC2O
1531	4. 905	430. 30078	PF-1052_130138	[M+H] ⁺	430. 29599	C26H39N04	N-alkylpyrrolidines	NPWKEUKXVOMELT-LXVKXUELSA-N	O=C1OC(C(=O)C(N1C)C(C)C(C)=O)C2C(C=CC3OC(C)CC(C)C32)C4(OC4)C
1532	4. 912	383. 13275	Ochrephilon	[M+H] ⁺	383. 13297	C23H2605	Cyclohexenones	GAIVGINVGXHEIA-ZAAJWPAISA-N	O=C1OC2(C(=O)C=C3C=C(OC=C3C2C1C(=O)C)C=C(=CC(C)CC)C
1533	4. 917	428. 21677	Pesticide2_Benfuracarb_C20H30N2O5S_Oncol	[M+H] ⁺	428. 22198	C20H30N2O5S	Coumarans	FYZBOYWSHKHDMT-UHFFFAOYSA-N	O=C(OC1=CC=CC2=C1OC(C)C2)N(SN(CCC(=O)OCC)C(C)C)C
1534	4. 926	197. 11649	Lolilide	[M+H] ⁺	197. 117	C11H1603	Benzofurans	XEVQXKKKAVVSMW-UHFFFAOYSA-N	O=C1OC2(C(=C1)C(C)C)CC(O)C2)C
1535	4. 928	193. 04929	Monoethyl phthalate	[M-H] ⁻	193. 05063	C10H1004	Benzoic acid esters	YVWHKOHZJFMIE-UHFFFAOYSA-N	CCOC(C1=CC=CC=C1C(=O)O)=O
1536	4. 932	631. 17334	4-(3-Oxobutyl)phenyl 6-O-[(2E)-3-phenyl-2-propenoyl]-2-O-(3,4,5-trihydroxybenzoyl)-beta-D-glucopyranoside	[M+H] ⁺	631. 17999	C32H32012	Phenolic glycosides	AHLBWJHZDLMJQJ-SIJHJTGPPSA-N	O=C(OCOC1OC(C2=CC=C(C=C2)CCC(=O)C)C(OC(=O)C(C3=CC(O)=C(O)C(=O)C3)C(C)C1O)C(=O)C(C1O)C(=O)C(=O)C(=O)C(C4
1537	4. 94	331. 1752	(3R,4S,5S,6R)-2-(6-hydroxy-2,6-dimethylocta-2,7-dienoxy)-6-(hydroxymethyl)oxane-3,4,5-triol	[M-H] ⁻	331. 17621	C16H2807	Fatty acyl glycosides of mono- and disaccharides	WEHZNHJZBEGME-SPGNZJCFSA-N	OCOC1OC(CCCC(=O)C(C(=O)C)C(C(=O)C)C1O
1538	4. 943	451. 22998	[4,8-dihydroxy-3-(3-methoxy-3-oxoprop-1-en-2-yl)-8a-methyl-5-oxo-1,2,3,4,4a,6,7,8-octahydronaphthalen-2-yl]-3,4-dihydroxy-2-(4aS,6aR,6bR,10S,12aR)-1,2,6b,9,9,12a-hexamethyl-10-[(2R,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy-	[M+H] ⁺	451. 2262	C20H2809	Beta hydroxy acids and derivatives	NOGWMYITAXOCY-UHFFFAOYSA-N	O=C(OC(C(=O)C1C(C(=O)C2C(C(=O)C2)C(C1OC(=O)C(=O)C(=O)C(=O)C(=O)C12C(=CC3C4(C)CCC(OC5OC(C(=O)C(=O)C5O)C(C)C(C)C4CCC3(C)C6C(C)C(C)C7C6(C=C(=O)O)CC2
1539	4. 944	666. 42291	(4aS,6aR,6bR,10S,12aR)-1,2,6b,9,9,12a-hexamethyl-10-[(2R,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy-	[M+H] ⁺	666. 42114	C36H56010	Triterpene saponins	AXNXSFBKZQIMPF-RIBCLQTCSA-N	O=C(OC)CC1C(C(=O)C(=O)CC2OC34C(=O)C(CCC4(C)C(OC(=O)C3)C5=O)C=C5)C21C
1540	4. 945	471. 24402	3Alpha-Hydroxy-3-Deoxyangolensic Acid Methyl Ester	[M-H] ⁻	471. 24536	C27H3607	Delta valerolactones	QFRZVNPYNYLAN-UOICJKMOSAN	O=C(O)CCC(NC(=O)C1=CC=C(C=C1)C(C#CC)CC=2N=C3C(=N)C=N(C(=O)C1)C(=O)O
1541	4. 945	478. 18442	Pralatrexate (Folotyln)	[M+H] ⁺	478. 18301	C23H23N705	Glutamic acid and derivatives	QFSBUKJUDHAQEA-WMCAAGNNSA-N	O=C(OC)C1=C(NC(=C(C(=O)OC)C1C=2C=CC=CC2N(=O)=O)C)C
1542	4. 946	347. 12262	Nifedipine	[M+H] ⁺	347. 12375	C17H18N206	Dihydropyridinecarboxylic acids and derivatives	HYTMSNHJQBLINT-UHFFFAOYSA-N	O=C(OC)C1=C(NC(=C(C(=O)OC)C1C=2C=CC=CC2N(=O)=O)C)C
1543	4. 952	148. 03983	4-Hydroxymandelonitrile	[M-H] ⁻	148. 04041	C8H7N02	1-hydroxy-2-unsubstituted benzeneids	HOOPXDSCKBLFG-UHFFFAOYNA-N	N#CC(O)C1=CC=C(C)C=C1
1544	4. 97	231. 1232	Melatonin	[M-H] ⁻	231. 12207	C13H16N202	3-alkylindoles	DRLFMBDRBRZALE-UHFFFAOYSA-N	OC(=NCCC1=CNC=2C=CC(OC)=CC21)C
1545	4. 974	601. 3418	Desferrioxamine E	[M+H] ⁺	601. 34198	C27H48N609	Macrolactams	NHKCCADZLTPPO-UHFFFAOYSA-N	O=C1N(O)CCCCN=C(C)CCC(=O)N(O)CCCCCN=C(C)CCC(=O)N(O)CC(CCCN=C(O)CC1
1546	4. 98	327. 04868	Acid Orange 7 (free acid)	[M-H] ⁻	327. 04449	C16H12N204S	Naphthols and derivatives	RDUJRVXKAIYTDH-UHFFFAOYSA-N	C1=CC=C2C(=C1)C=CC(=C2N3CC=C(C(=C3)S(O)(=O)=O

1547	4. 98	361. 1012	Demethoxycurcumin	[M+H] ⁺	361. 10001	C20H18O5	Curcuminoids	HJTJVQHVGMGKONQ-LUZRFALSA-N	O=C(C=CC1=CC=C(C)C)CC(=O)C=CC2=CC=C(C)C(OC)=C2
1548	4. 985	262. 09906	(E)-3-(3-chlorobut-2-en-1-yl)-2, 8-dimethylquinolin-4-ol	[M+H] ⁺	262. 10001	C15H16ClN0	Hydroquinolones	YRXDKQKQWMHRSY-JXMRQGBWSA-N	C1C(=CCC1=C(C)C=2C=CC=C(C2N=C1C)C)C
1549	4. 993	268. 16434	Azacyclonol	[M+H] ⁺	268. 17001	C18H21N0	Diphenylmethanes	ZMISODWVFHHNR-UHFFFAOYSA-N	OC(=C1C=CC=CC1)C(=C2C=CC=C2)C3CNC3
1550	4. 994	440. 20276	Protostemonine	[M+H] ⁺	440. 20001	C23H31N06	Stemamide-type alkaloids	JDGNFRYDHRXNL-ROHJGGRPSA-N	O=C1OC(C(OC)=C1C)=C2OC3CCN4C(CCC4C3C2)C5OC(=O)C(C)C5
1551	4. 999	150. 09082	2'-Methylacetanilide	[M+H] ⁺	150. 09134	C9H11N0	Acetanilides	BPEXTIMJLDWTL-UHFFFAOYSA-N	CC1=CC=CC=C1N=C(C)O
1552	5. 003	423. 29526	licoricidin	[M-H] ⁻	423. 2905	C26H32O5	5-O-methylated isoflavonoids	GBRZTJUCDFSHM-KRWQZBQSA-N	OC1=CC=C(C(OC)=C1OC=C(C)C)C2OC3=CC(=O)C(C(OC)=C3C2)CC=C(C)C
1553	5. 015	357. 16394	Hycanthone	[M+H] ⁺	357. 16312	C20H24N2O2S	Thiochromenes	MFZWMTSUNWVBU-UHFFFAOYSA-N	CCN(CC)CCN1=C2C(=O)C3=CC=CC=C3SC2=C(C)C=C1
1554	5. 017	146. 05962	Indole-3-carboxyaldehyde	[M+H] ⁺	146. 06004	C9H7N0	Indoles	OLNJUISKUQNTW-UHFFFAOYSA-N	O=CC1=CC2=CC=CC=C12
1555	5. 017	524. 26886	sodium (2R)-2'-((2R, 5S, 6R)-6'-((3E, 5E)-6-((3aR, 4S, 7aS)-4-(1H-pyrrole-2-carbonyl)-2, 3, 3a, 4, 5, 7a-hexahydro-1H-inden-5-yl)hexa-3, 5-dien-3-yl)-5-	[M+H] ⁺	524. 27002	C30H40NNaO4	Aryl alkyl ketones	BPSPGNVGAIGAXI-AREVZEEPSA-M	[Na ⁺]. O=C([O-]
1556	5. 018	361. 20032	Cortisone	[M+H] ⁺	361. 20093	C21H28O5	21-hydroxysteroids	MFYSYFVPBJMBGN-ZPOLXVRWSA-N	1)C(C)C1OC(C(=CC=CC2=CC3CCC3C2)C(=O)C4=CC(=C4)C)C(C
1557	5. 021	407. 20593	[6, 10a-dihydroxy-4-(hydroxymethyl)-4, 7, 11b-trimethyl-9-oxo-1, 2, 3, 4a, 5, 6, 6a, 7, 11, 11a-decahydronaphtho[2, 1-f][1]benzofuran-5-yl]	[M-H] ⁻	407. 20752	C22H32O7	Naphthofurans	GWEGFCVAPNYPY-UHFFFAOYSA-N	O=C1OC2(O)C=C1)C(C)C3C(O)C(OC(=O)C)C4C(C)(CO)CCCC4(C)C3C2
1558	5. 021	379. 14713	Glyasperin C	[M+H] ⁺	379. 14999	C21H24O5	5-O-methylated isoflavonoids	RCZMWKVBFOCEE-UHFFFAOYSA-N	OC1=CC=C(C(OC)=C1)C2COC3=CC(=O)C(C(OC)=C3C2)CC=C(C)C
1559	5. 023	609. 33606	Reserpine	[M+H] ⁺	609. 33337	C33H40N2O9	Yohimbin alkaloids	QEVHRUUCGRFIF-MDEJGZSSA-N	O=C(OC1CC2CN3CC=CC=CC(OC)=C5NC4C3CC2C(C(=O)OC)C1O
1560	5. 028	361. 13901	Nitrendipine	[M+H] ⁺	361. 13901	C18H20N2O6	Dihydropyridinecarboxylic acids and derivatives	PVHUJELLJLJGLN-UHFFFAOYSA-N	C)C6=CC(OC)=C(OC)C(OC)=C6
1561	5. 03	144. 04489	4-Hydroxyquinoline	[M-H] ⁻	144. 04549	C9H7N0	Hydroquinolones	PMZDQRJGMBQBF-UHFFFAOYSA-N	O=C(OC)C1=C(NC(=C(C(=O)OC)C1C=2C=CC=C2)[N+](=O)[O-])C(C
1562	5. 031	206. 11729	Dehydrosalsolidine	[M+H] ⁺	206. 11755	C12H15N02	Others	VASUQTGAZAPKFK-UHFFFAOYSA-N	O=C1C=CC2=CC=CC=C12
1563	5. 036	269. 12769	(3aS, 5aS, 9bR)-5a, 9-dimethyl-3-methylidene-3a, 4, 6, 7, 8, 9b-hexahydrobenzo[<i>c</i>][1]benzofuran-2, 5-dione	[M+H] ⁺	269. 12912	C15H18O3	Eudesmanolides, seudesmanolides, and Cinnamic acids and derivatives	CPHFAWJXZHHPEN-PSOPSSQASA-N	OC1=OC2=C(C(=C1OC)C(C)=O)CC2C1=C)C
1564	5. 036	221. 08017	Dihydrodiplartine	[M+H] ⁺	221. 078	C17H21N05	Fatty acyl glycosides of mono- and disaccharides	HPXUNEGPCPBQBF-BQYQJAHWSA-N	O=C(C=C(C1=CC(OC)=C(OC)C(OC)=C1)N2C(=O)CCCC2
1565	5. 04	427. 16019	(2R, 3S, 4S, 5R, 6R)-2-[1-(2R, 3S, 4S, 5R)-3, 4-dihydroxy-5-(hydroxymethyl)oxolan-2-yl]oxymethyl]-6-[<i>E</i>]-[3-phenyliron-2-enox]oxane-3, 4, 5-triol	[M-H] ⁻	427. 16095	C20H28O10		IEBPEMIXHIISM-RJSCAXEBSA-N	OC1OC(OC2OC(OC=CC=CC=CC3C(C)C(C)C2O)C(C)C1O
1566	5. 055	195. 06493	trans-4-Hydroxy-3-methoxycinnamate	[M+H] ⁺	195. 06519	C10H10O4	Hydroxycinnamic acids	KSEBMQBYZTHIS-HWKANZROSA-N	OC(=C(C)C)C=CC(\C=C(C)C)=O)=C1
1567	5. 062	305. 18475	Piperanine	[M+H] ⁺	305. 18594	C17H21N03	Benzodioxoles	QHWOPMXDKFORMO-XVNBXDJSA-N	O=C(C=CCCC1=CC=C2OCOC2=C1)N3CCCC3
1568	5. 068	276. 08633	ACTIPHENOL	[M+H] ⁺	276. 08603	C15H17N04	Alkyl-phenylketones	YTLMIHBTPTWTEV-UHFFFAOYSA-N	O=C1N=C(C)CC(C1)CC(=O)C=2C=C(C=C(C2O)C)C
1569	5. 075	218. 21074	Triacetin	[M+H] ⁺	218. 21001	C9H14O6	Triacylglycerols	URAYPUMNDPQOKB-UHFFFAOYSA-N	O=C(OC(C(=O)C)COC(=O)C)C
1570	5. 084	415. 19446	Hexose + C13H19O (isomer of 1062)	[M-H] ⁻	415. 19489	C19H30O7	Terpene glycosides	SZOPSAFLRCYJXC-UHFFFAOYNA-N	O=C2C=C(C)C(C(=CC(OC1OC(CO)C(C)C(C)C1)C(C)C(C)C)C(C)C2
1571	5. 092	470. 2735	Hypocanine	[M+H] ⁺	470. 27399	C24H39N08	Aconitane-type diterpenoid alkaloids	BQTYHFZQSAKNQU-UHFFFAOYSA-N	OC1C(OC)C2(O)CC3C(C2O)C1(O)C4C(OC)C5C6(COC)CN(C)C4C3SC(OC)C6
1572	5. 094	197. 16608	(1R, 3r, 8S, 9r)-1, 8-dimethyl-3, 6-diazatricyclo[4. 3. 1. 1 (3, 8)]undecan-9-ol	[M+H] ⁺	197. 164	C11H20N2O	1, 4-diazepanes	JNARJHDJLSPXGM-UHFFFAOYSA-N	OC1C2(C)CN3CCN(C2)CC1(C)C3
1573	5. 121	179. 06984	Coniferylaldehyde	[M+H] ⁺	179. 07027	C10H10O3	Methoxyphenols	DKZBBWMURDFHNE-UHFFFAOYSA-N	O=CC=CC1=CC=C(C)C(OC)=C1
1574	5. 136	345. 14279	Tyr-Tyr	[M+H] ⁺	345. 1445	C18H20N2O5	Dipeptides	JAQGKXUEKGKTKX-UHFFFAOYNA-N	O=C(C)C(N=C(C)C(N)CC1=CC=C(C)C1)CC2=CC=C(C)C=C2
1575	5. 143	164. 10643	N-acetyl-2-phenylethylamine	[M+H] ⁺	164. 10698	C10H13N0	N-acetyl-2-arylethylamines	MOCKMIXGCKTLE-UHFFFAOYSA-N	OC(=NCCC=CC=CC1)C
1576	5. 143	443. 20349	Perlatolic acid	[M-H] ⁻	443. 20001	C25H32O7	Depsides and depsidones	UTAQXQVSEK1WBB-UHFFFAOYSA-N	O=C(C)C1=C(C)C=C(OC(=O)C2=C(C)C(OC)C=C2CCCC)C=C1CCC(C
1577	5. 15	381. 20328	1-Myristoyl-2-hydroxy-sn-glycero-3-phosphate	[M-H] ⁻	381. 20477	C17H35O7P	1-acylglycerol-3-phosphates	FAZBDRGXCKPJJU-MRXNPFEDSA-N	CCCCCCCCCCCC(=O)OC([C@H](O)COP(O)(O)=O
1578	5. 151	509. 30313	18b-glycyrrhetic acid	[M-2H] ²⁺	509. 30276	C30H46O4	Triterpenoids	MPDGHEJMBKOTSU-AWOGJAJBSA-N	O=C(C)C1(C)CCC2(C)CCC3(C(=CC(=O)C4C5(C)CCC(O)C(C)C)C5(C)C4C)C2(C)C
1579	5. 152	369. 22314	5-(3-methoxyphenyl)-N-((octahydro-1H-quinolinizin-1-yl)methyl)-1H-pyrazole-3-carboxamide	[M+H] ⁺	369. 23001	C21H28N4O2	Phenylpyrazoles	ZZFSKJIAK1BPSR-UHFFFAOYSA-N	O=C(NCC1CCN2CCCCC21)C3=NNC(=C3)C=CC=C(C(OC)C4
1580	5. 152	382. 14096	Capecitabine (Xeloda)	[M+H] ⁺	382. 138	C15H22FN3O6	5'-deoxyribonucleosides	GAGWJHPBLXJQN-GMTLJSCSSA-N	O=C(OC(CCC)NC1=CC(=O)N(C=C1F)C2OC(C)C(C)C2O
1581	5. 152	353. 16904	meso-dihydroguaiaietic acid	[M+H] ⁺	353. 17001	C20H26O4	Dibenzylbutane lignans	ADPOLUXMYCTRR-ZIAGYMGSSA-N	OC1=CC=C(C=C1OC)CC(C)C(C)CC2=CC=C(C)C(OC)=C2
1582	5. 153	193. 1331	Isoproteron-monodemethyl	[M+H] ⁺	193. 13354	C11H16N2O	N-phenylureas	DOULWSSZVEPIN-UHFFFAOYSA-N	ON=C(C)NC1=CC=C(C=C1)C(C)C
1583	5. 157	282. 13272	4, 7, 8-trimethoxy-3, 5-dimethylchromen-2-one	[M+H] ⁺	282. 13361	C14H16O5	Coumarins and derivatives	PKKTAMCHLIVDS-UHFFFAOYSA-N	O=C1OC2=C(C)C(C(OC)=CC(=C2OC)=C1C)C
1584	5. 159	383. 19971	Venocristine	[M-H] ⁻	383. 19763	C22H28N2O4	Alkaloids	OYMQKBZKMFJMH-UHFFFAOYNA-N	COC(=O)C1CC2CC(C(C)C)C1N(C3)CCC1=C2NC2=CC=C(C(OC)C=C12
1585	5. 174	174. 18509	MENTHOL(-)	[M+H] ⁺	174. 18523	C10H20O	Menthane monoterpeneoids	NOOLISFMXDJSKH-UHFFFAOYSA-N	OC1CC(C)CCC1C(C)C
1586	5. 175	401. 1597	aschantin	[M+H] ⁺	401. 15948	C22H24O7	Furanoid lignans	ONDWGDNAPRACN-VIEDXXQZSA-N	O(C=C1C=C(C(OC)C1OC)C2OC3C(OC2C3)C4=CC=C5OC(C=C4)C
1587	5. 176	327. 08426	Isosaxalin	[M+H] ⁺	327. 08401	C16H16O6	Psoralens	FOINLJRVEBYARJ-UHFFFAOYSA-N	O=C1OC=2C(C=C1)=CC=3C=CC3C2OCC(O)C(O)C(C)C
1588	5. 179	209. 07835	Sinapyl alcohol	[M-H] ⁻	209. 08194	C11H14O4	Methoxyphenols	LZPOPEXOUVTGJS-UHFFFAOYSA-N	OC=1C(OC)=CC(C=CCO)=CC1OC
1589	5. 184	309. 11179	Warfarin	[M+H] ⁺	309. 11212	C19H16O4	4-hydroxycoumarins	PJYWKTKQMONHTI-UHFFFAOYNA-N	CC(CC(C1=CC=CC=C1)C2=C(C3=CC=CC=C3OC2=O)O)=O

1590	5.186	427.15753	9,11,12a-trihydroxy-2,3-dimethoxy-8-(3-methylbut-2-enyl)-6,6a-dihydrochromeno[3,4-b]chromen-12-one	[M-H]-	427.16016	C23H24O8	Rotenones	LAUXTJGTOIBBOB-UHFFFAOYSA-N	O=C1C2=C(O)C(C=O)C(C=C2)OC(=O)C(=O)C(C=C1)C(=O)C
1591	5.186	187.09703	Azelaic acid (Not validated)	[M-H]-	187.0974	C9H16O4	Organic acids	BDJRBEYXGNGYIS-UHFFFAOYSA-N	O=C(O)CCCCCCC(=O)O
1592	5.189	276.99207	FT-PFCA	[M-H]-	276.99167	C6H3F9O2	PFSA	PMVMXTIBUIRJHZ-UHFFFAOYSA-N	O=C(O)CC(F)(F)C(F)(F)C(F)(F)C(F)(F)F
1593	5.191	317.065	methyl 2-(2,6-dihydroxy-4-methylbenzoyl)-3,5-dihydroxybenzoate	[M-H]-	317.06668	C16H14O7	Benzophenones	G1JDACRMFMBET-UHFFFAOYSA-N	O=C(OC)C=C(C=O)C(C=O)C1C(=O)C2=C(O)C=C(C=C2)C
1594	5.191	466.23239	Norgenaime D_130072	[M+H]+	466.233	C26H31N3O5	Pyrrroloindoles	DM1IGSHOPYKWKW-RRGUOAIQSA-N	O=C1N2CCCC2(O)C(=O)N3C1CC4(O)C5=CC=C6OC(C=C6)=C5N34C(=C)C(C)C
1595	5.195	651.35663	Lopinavir (ABT-378)	[M+H]+	651.35199	C37H48N4O5	Valine and derivatives	KJHKTHMKYKJE-SUGCFRTWSA-N	O=C1NCCN1C(C(=O)NC(C=CC(=O)C2)CC(O)C(NC(=O)COC=3C(=CC(=C3)C)CC=4C(=O)C741C1C
1596	5.197	493.13254	Anthocyanidin base + 40, 2MeO, 0-Hex	[M+H]+	493.13281	C23H25O12	Anthocyanidin O-glycosides	PUXQTDZNOHRLW1-UHFFFAOYNA-O	O=C2C=C(O)C=3C=C(OC1OC(C)C(O)C1(O)C)C(=[O+]=C3(C=C2))C=C4C(OC)C(O)=C(OC)C=4
1597	5.197	293.1012	Benzyl glucopyranoside	[M+H]+	293.10001	C13H18O6	O-glycosyl compounds	GKHCBYBLTXYEY-UJPOAA1JSA-N	OC1OC(OC=C2C=CC2)C(O)C(O)C1O
1598	5.197	310.20081	Metadone	[M+H]+	310.20099	C21H27NO	Diphenylmethanes	USSIQVCVUKGNF-UHFFFAOYSA-N	O=C(CC)C(C=C1CC=CC1)(C=CC=CC2)CC(N(C)C)C
1599	5.199	288.25189	Emodin	[M+H]+	288.25159	C15H10O5	Hydroxyanthraquinones	RHMXJGYXNZAPX-UHFFFAOYSA-N	O=C1C=2C(C(O)C=C(O)C2)C(O)C3=C(O)C=C(C=C13)C
1600	5.201	189.11185	Azelaic acid	[M+H]+	189.11211	C9H16O4	Medium-chain fatty acids	BDJRBEYXGNGYIS-UHFFFAOYSA-N	O=C(O)CCCCCCC(=O)O
1601	5.205	295.06955	alpha-Naphthoflavone	[M+H]+	295.07001	C19H12O2	Flavones	VFMMPHCGEFGIP-UHFFFAOYSA-N	O=C1C=C(OC2=C1C=CC=CC2)C=C(C=C1)C
1602	5.242	367.16376	4-(4-(2,3-dihydrobenzo[b][1,4]dioxin-6-yl)-3-methyl-1H-pyrazol-5-yl)-6-propylbenzene-1,3-diol	[M+H]+	367.164	C21H22N2O4	Phenylpyrazoles	FOUM01ACEBZPT-UHFFFAOYSA-N	OC=1C=C(O)C(C=CC1C=2N=C(C2C3=CC=C4OCOC4=C3)C)CCC
1603	5.251	365.14929	1-hydroxy-4-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxynaphthalene-2-carboxylic acid	[M-H]-	365.15024	C17H18O9	Phenolic glycosides	STXNGSCHXKQJX-OQAPJJDNSA-N	O=C(O)C1=C(C(OC2OC(CO)C(O)C2O)C2O)C3=C=CC=CC3C1O
1604	5.251	235.16858	Curcumenol	[M+H]+	235.16925	C15H22O2	Guianes	ISPMXVMWEWJGJ-UHFFFAOYSA-N	OC12OC(C1C(C)C)C(C)C(C(=C2)C)CCC3C
1605	5.251	316.03421	Efavirenz	[M+H]+	316.03467	C14H9ClF3NO2	Benzoazazines	XPOQHMRABVBWR-UHFFFAOYNA-N	C1CC1C=CC2(C=3C=C(C=CC3=N(C)O2)C1)C(F)F
1606	5.253	351.11884	Isoflavone base + 20 + 1MeO + 1Prenyl	[M-H]-	351.1218	C21H20O5	Prenylated isoflavones	JQNSUD1G1GIOL-UHFFFAOYSA-N	O=C1C=COC(=C2C=C(O)C(=C(O)C1)C2)CC(C)C3=C=CC(=O)C=C3
1607	5.255	377.12982	Griseofulvic Acid	[M+H]+	377.12964	C16H15ClO6	Benzofurans	KUTVEHZNKAAAO-UHFFFAOYSA-N	O=C1C=C(O)C2(OC=3C1)C(=O)C=C(O)C(OC3C2=O)C(C)C1
1608	5.265	515.18005	Cilnidipine	[M+H]+	515.17902	C27H28N2O7	Dihydropyridinecarboxylic acids and derivatives	KJEBULYHNRNJT-EHJHZJOJSA-N	O=C(OC=CC(=O)C=CC1)C2=C(NC(=C(C(=O)O)C2)C=CC=C(C3)N4=C(O)C=CC3)C
1609	5.268	435.16284	4-[(2R,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxypentan-2-yl (E)-3-(4-hydroxyphenyl)propanoate	[M+H]+	435.16254	C20H28O9	Fatty acyl glycosides of mono- and disaccharides	RMFDCHYDYYNFA-AKVWERCLSA-N	O=C(OC(C)CC(OC1OC(CO)C(O)C(O)C1O)C)C=C2C=CC=C(O)C=C2
1610	5.282	355.14804	Isoxanthohumol	[M+H]+	355.14999	C21H22O5	8-prenylated flavanones	YKGCBLLMDSAV-SHVURJKSA-N	O=C1C=2C(OC)=CC(O)C(C2OC(C3=CC=C(O)C=C3)C1)CC=C(C)C
1611	5.287	643.38629	Cimigenol-3-O-alpha-L-arabinoside	[M+2H]2+	643.38202	C35H56O9	Cucurbitacin glycosides	BTPYUWOBZFGKA1-BKJHYQRZSA-N	OC1OC(OC2CC34CC4COC(C)C7C(C)CC8OC(OC8(O)(C)C)C(O)C1)C(C)C5CC3C2(C)C(C)C1O
1612	5.302	206.08046	Methoxyindoleacetic acid	[M+H]+	206.08118	C11H11NO3	Indole-3-acetic acid derivatives	COCNDHOP1DHTH-UHFFFAOYSA-N	CCO1=CC2(C=O)CC3(C)C2(O)CC4C=CC(=O)C(=CC=C4)C6C8C(C(C=C7)C(C8)C(C)C)C(C)C7
1613	5.303	570.35529	Secopentitrem D_120253	[M+2H]2+	570.35699	C37H47NO4	Naphthopyrans	YZRQMJFFPMHJA-Y-DTOWOETISA-N	OC1C=C2C(OC1(C)C)CC3(C)C2(O)CC4C=CC(=O)C(=CC=C4)C6C8C(C(C=C7)C(C8)C(C)C)C(C)C7
1614	5.328	225.1481							

1633	5. 469	497. 19168	Strictosamide	[M-H] ⁻	497. 19171	C26H30N2O8	Carbolines	LBRPLJCNRXLSL-UHFFFAOYNA-N	O=C5C2=COC(OC1OC(CO)C(O)C(C1)C(C)=C)C2OC6C=4NC=3C=CC=C3C=4CNC56
1634	5. 47	265. 11737	conocarpan	[M-H] ⁻	265. 12051	C18H18O2	2-arylbenzofuran flavonoids	GXJSAXNLJFDPQ-CGBXWHS-CSA-N	OC1=CC=C(C=C1)C2OC3=CC=C(C=CC)C=C3C2C
1635	5. 471	403. 16257	(Z)-3-(4-hydroxyphenyl)-N-[4-[[[(E)-3-(4-hydroxyphenyl)prop-2-en-1-yl]amino]butyl]amino-2-aminidene	[M+H] ⁺	403. 16281	C22H24N2O4	Coumaric acids and derivatives	PYVBFDXJDSMM-MFUUIURDSA-N	OC(=NCCCCN(C)O)C=C1=CC=C(O)C=C1C=C2=CC=C(O)C=C2
1636	5. 474	417. 13855	7-hydroxy-2-[4-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyphenyl]-2,3-dihydrochromen-4-one	[M-H] ⁻	417. 13687	C21H22O9	Flavonoid O-glycosides	DEMKZLAVYISIA-UZQFATADSA-N	O=C1C2=CC=C(C)C=C2OC(C3=CC=C(C(OC4OC(CO)C(O)C(O)C4O)C=C3)OC1
1637	5. 475	449. 14609	Isosakuranin	[M+H] ⁺	449. 14499	C22H24O10	Flavonoid-7-O-glycosides	KEEWIHTDSNESJZ-JZHVRRPSA-N	O=C1C2=C(C)C=C(C(OC3OC(CO)C(O)C(O)C3O)C=C2OC(C4=C(C)C(OC)C=C4)C1
1638	5. 495	430. 27469	Mifepristone	[M+H] ⁺	430. 27405	C29H35NO2	Oxosteroids	VKHAHZOOSURJNA-UHFFFAOYNA-N	O=C1C=C2C(=C3C(=CC(=CC(=C3)C(OC5(C)C(OC5(C)C(OC)C3C2)C1
1639	5. 498	183. 07932	Triethylphosphate	[M+H] ⁺	183. 07808	C6H15O4P	Trialkyl phosphates	DQWPFSLDJDLRL-UHFFFAOYSA-N	CCOP(=O)(OC)OC
1640	5. 504	619. 36914	Desferrioxamine G1	[M+2H] ²⁺	619. 37	C27H50ON6O10	N-acyl amines	MIVGUYBAQIHKPJ-UHFFFAOYSA-N	O=C(O)CCC(=O)N(O)CCCCCNC(=O)CCC(=O)N(O)CCCCCNC(=O)CCC(=O)N(O)CCCCCNC
1641	5. 511	335. 1221	5-hydroxy-2,2-dimethyl-10-(2-methylbut-3-en-2-yl)pyrano[3,2-g]chromen-8-one	[M+H] ⁺	335. 12537	C19H20O4	Linear pyranocoumarins	WYMMGQSPNWCIK-UHFFFAOYSA-N	O=C1OC2=C(C=C1)C(O)=C3C=CC(OC3=C2C(C=C)C(C)C)C(C)
1642	5. 512	617. 36523	Cimicidanol-3-O-alpha-L-arabinoside	[M+H] ⁺	617. 37	C35H52O9	Cycloartanols and derivatives	PYBFXJMIKJNNAJ-UHFFFAOYSA-N	O=C(C(C)C)C1C(=O)CC2(C3=CC4C(C)C(C)C(OC5OC(C)C(O)C5O)C(C)C4)CC6(C)C(C)C(C)C2C1
1643	5. 515	325. 14825	4-amino-2-hydroxy-5-[[1-hydroxy-1-(5-oxo-6-bicyclo[4.1.0]hept-3-en-2-yl)propan-2-yl]amino]-5-oxopentanoic acid	[M-H] ⁻	325. 14774	C15H22N2O6	Glutamic acid and derivatives	SYGQXRLXOXXDRP-UHFFFAOYSA-N	O=C(O)C(C)CC(N(C)O)=NC(C)C(O)C1C2(=O)C=C-CC2C1
1644	5. 52	284. 12744	Coumaroyl tyramine	[M+H] ⁺	284. 12851	C17H17NO3	Coumaric acid and derivatives	RXGUTQKRCXHALN-UHFFFAOYSA-N	O=C(C=CC1=CC=C(C)C=C1)NCCC2=CC=C(O)C=C2
1645	5. 523	389. 25284	Ilicicolin A	[M-H] ⁻	389. 2518	C23H31ClO3	Sequiterpenoids	MHWOMRMBQSGSTFS-JTCWOHRSA-N	O=CC1=C(O)C(=C(C)C)C(C)=C1OC=CC(C)CCC=C(C)CCC=C(C)C
1646	5. 537	213. 07297	N,N-Dimethyl-N'-p-tolylsulphamide	[M-H] ⁻	213. 07033	C9H14N2O2S	Sulfanilides	UPCDOJQOXWCCSD-UHFFFAOYSA-N	CN(C)S(=O)(=O)NC1=CC=C(C)C=C1
1647	5. 551	257. 12698	6-ethyl-2,3,5-trimethyl-7H-furo[3,2-g]chromen-7-one	[M+H] ⁺	257. 12	C16H16O3	Psoralens	USSZROTZVDHBM-UHFFFAOYSA-N	O=C1OC=2C=C3OC(=C(C3=CC2=C1CC)C)C(C)
1648	5. 568	650. 4295	(1S,2R,4aS,6aR,6bR,10S,12aR,14bS)-1,2,6b,9,9,12a-hexamethyl-10-[1-(2R,3R,4S,5S,6R)-3,4,5-trihydroxy-6-methylhexan-2-yl]oxy-5-[(8aS)-2,5,5,8a-tetramethyl-3-oxo-4a,6,7,8-tetrahydro-4H-naphthalen-1-yl]-3-methylpentanoic acid	[M+H] ⁺	650. 42621	C36H56O9	Triterpene saponins	PUOQHFWBKXTHST-MPLMRMBSA-N	O=C(O)C1C2(=CCC3C4(C)CC(OC5OC(C)C(O)C5O)C(C)C4)CC3(C)C(C)C(C)C2C1
1649	5. 573	321. 24225	5-[(8aS)-2,5,5,8a-tetramethyl-3-oxo-4a,6,7,8-tetrahydro-4H-naphthalen-1-yl]-3-methylpentanoic acid	[M+H] ⁺	321. 2424	C20H32O3	Diterpenoids	BARZJLALPXZLMN-RJGDCVCESA-N	O=C(O)CC(C)CCC=C(C(=O)CC2C1(C)CCC2(C)C)C1
1650	5. 582	322. 12711	HERALENOL	[M+H] ⁺	322. 12851	C16H16O6	Psoralens	FOINLJRVEBYARJ-UHFFFAOYSA-N	O=C1OC=2C(C=C1)=CC=3C=CC3C2OCC(O)C(O)C(C)
1651	5. 588	179. 03394	4-Hydroxyphenylpyruvic acid	[M-H] ⁻	179. 03499	C9H8O4	Phenylpyruvic acid derivatives	KKADPXVIOXHKN-UHFFFAOYSA-N	O=C(O)C(=O)CC1=CC=C(C)C=C1
1652	5. 588	259. 09692	6-methoxy-7-(3-methylbut-2-enoxy)chromen-2-one	[M-H] ⁻	259. 09756	C15H16O4	Coumarins and derivatives	ZLPLFUBVEZYDX-UHFFFAOYSA-N	O=C1OC=2C=C(OC=C(C)C)C(OC)=CC2=C1
1653	5. 596	433. 17191	osmanthuside H	[M+H] ⁺	433. 17044	C19H28O11	O-glycosyl compounds	IVRQZYXJBVMHCW-OTCFHACESA-N	OC1=CC=C(C=C1)COC2OC(COC3OC(C)C(CO)C3O)C(C)C2O
1654	5. 598	263. 12848	Abscisic acid	[M-H] ⁻	263. 12888	C15H20O4	Abscisic acids and derivatives	JLIDBQLQVAYINE-UHFFFAOYNA-N	O=C(O)C(=C(C=CC1(C)C(=CC(=O)CC1(C)C)C)C
1655	5. 601	137. 02368	4-Hydroxybenzoic acid	[M-H] ⁻	137. 02441	C7H6O3	Hydroxybenzoic acid derivatives	FJKROLJGYXJWQN-UHFFFAOYSA-N	OC(=O)C1=CC=C(C)C=C1
1656	5. 602	843. 35504	(8R,10R,11S,11aS,13S)-9-ethyl-8,13-dihydroxy-7-(2-(((10S,13R)-14-hydroxy-10,13-dimethyl-17-(5-oxo-2,5-dihydrofuran-3-yl)hexadecahydro-1H-	[M+H] ⁺	843. 34998	C45H61BrN2O7	Cardenolides and derivatives	JPBBOIVVPLQMCQ-VYWZAZLPAS-M	[Br-] 1,10,11,17-tetrahydro-2H-pyran-2-yl)-5-oxo-2,5-dihydrofuran-3-yl]hexadecahydro-1H-
1657	5. 604	507. 15305	Scutellarioside II	[M-H] ⁻	507. 15079	C24H28O12	Coumaric acid esters	MVTLFXPHKDVATC-LAQGVYQA-SN	O=C(OC12OC2(C)C3C(=CC(OC4OC(CO)C(O)C(O)C4O)C31)C=CC5=CC=C(O)C=C5
1658	5. 604	352. 16827	Usaramine	[M+H] ⁺	352. 17001	C18H25NO6	Macrolides and analogues	BCJMNZRGJAVLD-VMOBWIEOSA-N	O=C1OC2C8NCC=C(COC(=O)C(O)C(C)C(C)C1=CC)C32
1659	5. 608	265. 1431	(9E)-11a-hydroxy-3,6,10-trimethyl-6,7,8,11-tetrahydro-4H-cyclodeca[h]furan-2,5-dione	[M+H] ⁺	265. 14343	C15H20O4	Germacranolides and derivatives	SCOXKWLFRILEY-WEVYVXLNSA-N	O=C1OC2(C)C(=C(C)CC(=O)C(C)CCC=C(C)C2
1660	5. 608	273. 13394	afzelechin	[M-H] ⁻	273. 13797	C15H14O5	Flavan-3-ols	RSYUFYQTACJFML-DZGQCQFKSA-N	OC1=CC=C(C=C1)C2OC=3C=C(C)C=C(O)C3CC2O
1661	5. 612	255. 11237	Nepafenac	[M+H] ⁺	255. 11301	C15H14N2O2	Benzophenones	QEFAQIPZVLVERP-UHFFFAOYSA-N	O=C(N)CC=C1C=CC=C(C(=O)C=2C=CC=CC2)C1N
1662	5. 614	448. 27548	Jervine	[M+H] ⁺	448. 28	C27H39NO3	Jerveratrum-type alkaloids	CLEXFLHGFJONT-UHFFFAOYSA-N	O=C1C2=C(C)C3(OC4CC(C)CNC4C3)CCC2C5CC=O6CC(O)CC6(C)C15
1663	5. 619	274. 08472	Pomalidomide	[M+H] ⁺	274. 082	C13H11N3O4	Phthalimides	UYSMNLNDYGZFPF-UHFFFAOYSA-N	O=C1C=2C=CC(=O)N(C2C(=O)N1C3C(=O)NC(=O)C3
1664	5. 63	479. 15591	Isolindleyin	[M+H] ⁺	479. 155	C23H26O11	Phenolic glycosides	KHUVRRVIZOSFTI-UHFFFAOYSA-N	O=C(OC1C(OC2=CC=C(C=2)CCC(=O)C(OC(CO)C(O)C1O)C3=CC(=O)C(OC(CO)C=C3
1665	5. 664	457. 2757	Mundulone	[M+H] ⁺	457. 2749	C26H26O6	6-prenylated isoflavones	KJTDAZHLWHEULN-UHFFFAOYSA-N	O=C1C(=CC=2C=C3OC(C)C(C)C(OC3=C21)=4C=CC=5OC(C=CC5=COC)C(C
1666	5. 668	218. 1898	Prolintane	[M+H] ⁺	218. 19032	C15H23N	Amphetamines and derivatives	OJQPSBCUMRIPEL-UHFFFAOYNA-N	CCCC(C(C)=CC=C(C)C)N1CCCC1
1667	5. 67	331. 12057	sulochrin	[M-H] ⁻	331. 11725	C17H16O7	Benzophenones	YJRLSCDYLRBITZ-UHFFFAOYSA-N	O=C(OC)C=C1C=C(O)C=C(OC)C1(=O)C2=C(O)C=C(C=C2O)C
1668	5. 672	255. 11191	Obtusaquinone	[M+H] ⁺	255. 11137	C16H14O3	P-quinomethanes	LUZUAYAKZLCOCQ-BHHNPLQBSA-N	O=C1C=C(C(OC)C(=CC=CC=CC2=CC=CC2)C=C1O
1669	5. 674	465. 18945	2-[[[4-(2,4-dihydroxy-3,5,6-trimethylbenzoyl)oxy-2-hydroxy-6-methylbenzoyl]amino]-3-hydroxybutanoic acid	[M+H] ⁺	465. 18674	C22H25NO9	Depside and depsidones	NJVCQZYVEIAGLE-UHFFFAOYSA-N	O=C(O)C(N=C(C)O)C1=C(C)C(OC(=O)C=C2(C)C(=O)C(C2)C(C)=C1(C)C(O)C
1670	5. 676	319. 20114	Chaulmoogric Acid	[M+H] ⁺	319. 20337	C18H32O2	Long-chain fatty acids	XMQQWNRDPAAUJB-UHFFFAOYSA-N	O=C(O)CCCCCCCCCCCCC1C=CCC1
1671	5. 677	238. 14311	N,N-Diethyl-3,4-dimethoxybenzamide	[M+H] ⁺	238. 14377	C13H19NO3	Dimethoxybenzenes	ZXTJMIZZI CSORJ-UHFFFAOYSA-N	CN(C)CC(C(=O)C1=CC(OC)=C(OC)C=C1O)C=C1
1672	5. 678	463. 28424	Methyl-mappain	[M+H] ⁺	463. 28201	C30H38O4	Stilbenes	MRXGJOCASBBDTM-FVFOHYRDSA-N	OC=1C=C(C=CC=2C(OC)C(C)=C(C2)CC=C(C)CCC=C(C)C(C)C(=O)C1C=C(C)C
1673	5. 68	208. 13298	Pesticide3_Fenobucarb_C12H17N02_Bassa	[M+H] ⁺	208. 133	C12H17NO2	Phenyl methylcarbamates	D1RFUJHNVNOMY-UHFFFAOYSA-N	OC(=NC)OC=1C=CC=CC1C(C)CC
1674	5. 681	479. 15488	calceolarioside A	[M+H] ⁺	479. 15479	C23H26O11	Coumaric acids and derivatives	UHGZLYCYRQESL-VJWFJHQPSA-N	O=C(OC1C(OC)C(O)C(OC)C2=CC=C(O)C(O)C2)OC1OC(C=CC3=CC=C(C)C3)C(C)C
1675	5. 684	281. 19653	Aspidofractinine	[M+H] ⁺	281. 20099	C19H24N2	Aspidofractine alkaloids	BITBZWCWSCFPBB-MRCYZYCBSA-N	C=C1C=C2C(C(C1)NC34CC5(CCCN6CCC23C65)CC4

1676	5.684	267.11902	Ponatinib (AP24534)	[M+H] ⁺	267.11801	C29H27F3N6O	Benzanilides	PHXJVRSECI GDHY-UHFFFAOYSA-N	O=C(NC(=C(C=C(C=C1)C(F)(F)F)N2C3C(C(C2)C3=CC=C(C(C(=C4)C=CN=C5C=C(C(=N4)S)=C3)C
1677	5.686	229.10693	2-(6-hydroxyhexyl)-3-methylidenebutanedioic acid	[M-H] ⁻	229.10814	C11H18O5	Medium-chain hydroxy acids and derivatives	DHYXMTJVCPCBB-UHFFFAOYSA-N	O=C(O)(C=C(C=C(C(=O)O)CCCCO
1678	5.687	504.23227	N-(1-(2-amino-2-oxoethyl)piperidin-4-yl)-3-(4-(hydroxy-6-methyl-2-oxo-2H-pyran-3-yl))-3-(2,3,4-trimethoxyphenyl)propanamide	[M+H] ⁺	504.23001	C25H33N3O8	Alpha amino acid amides	YE1WCPFXBQSECZ-UHFFFAOYSA-N	O=C1OC(=C(O)=C1C(C2=CC=C(C(=O)C(C(=C2O)CC(=O)N3C3C(C(C(=O)N)C3)C
1679	5.693	349.13013	[(10Z)-6,10-bis(hydroxymethyl)-3-methylidene-2-oxo-3a,4,5,6,7,8,9,11a-octahydrocyclodecabifuran-4-yl]-2-methylpropan-2-enoate	[M-H] ⁻	349.13354	C19H26O6	Germaconanilides and derivatives	RJHSXEZOOJQAF-ZSO1EALJSA-N	O=C(OC1CC(CO)CCCC(=CC2OC(=O)C(C2)CO)C(=C)C
1680	5.702	279.1813	cyclopeptide	[M-H] ⁻	279.17978	C17H16N2O2	1,4-benzodiazepines	KSQNKZMAGACTL-UHFFFAOYSA-N	O=C1C=2C=CC=CC2N=C(O)C(N1C)CC=3C=CC=CC3
1681	5.72	488.97534	Pesticide1 Temephos_C16H20O6P2S3, O, O', O'-Tetramethyl O, O'-(sulfanedialdi-4,1-nphenylene) bis(phosphorothioate)	[M+H] ⁺	488.979	C16H20O6P2S3	Phenyl thiophosphates	WJZJWCUNJNYAI-UHFFFAOYSA-N	S=P(OC1=CC=C(CSC2=CC=C(COP(=S)(OC)OC)=C2)C=C1)(OC)OC
1682	5.723	483.30066	TRIDESACETOXYKHIVORIN	[M+H] ⁺	483.30237	C26H36O7	Limonoids	MQOMSFBIYXTTE-F1YJXLSPSA-N	O=C1OC(C2=CC=C(C2)C3(C)CC4C5(C)C(O)CC(O)C(C)C(C)C5CC(O)C4(C)C6OC7C16
1683	5.725	477.15842	Benzyl alcohol + Hex-Hex	[M-H] ⁻	477.15961	C19H28O11	Alkyl benzyl hexosides	WXKRKUZTXJFY-UHFFFAOYNA-N	OC3OC(OC1=CC=CC=C1)C(OC2OC(C)C(O)C(O)C2(O)C(O)C3(O)C
1684	5.727	370.21509	(1S,8R,16S,17R)-11,12-dimethoxy-5,15-diazahexacyclo[13.4.2.0,02.02.02.02.02.02.02]henicosic-2,9,11,13-tetraen-	[M+H] ⁺	370.21249	C21H24N2O3	Aminoguanolines and derivatives	BOPPHZK1KFBHB-GEOUA10SA-N	O=C1N2C3=CC(OC)=C(OC)C=C3C4C5NCC5=CC6(C1)CCC4C256
1685	5.727	537.16302	[(1aS,1bS,2S,5aR,6aS)-1a-(hydroxymethyl)-2-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy-2,5a,6,6a-tetrahydro-1bH-	[M-H] ⁻	537.16138	C25H30O13	Comaric acids and derivatives	LRHHPZILMP1MIY-GGKSNITSA-N	O=C(OC1C2OC(CO)C3C(OC=C1C3)OC4OC(CO)C(CO)C2(O)C4O)C=CC=C(CO)C(CO)=C5
1686	5.727	161.0594	4-Methylcoumarin	[M+H] ⁺	161.05971	C10H8O2	Coumarins and derivatives	PSGQCSGKJLRL-UHFFFAOYSA-N	CC1=CC(=O)OC2=CC=CC=C12
1687	5.727	295.04913	Butin	[M+H] ⁺	295.04999	C15H12O5	Flavanones	MJBPQUQJNAPAZ-AWEZNCPLSA-N	O=C1C2=CC=C(CO)C=C2OC(C3=CC=C(CO)C(CO)=C3)C1
1688	5.727	439.18497	Diferuloyl putrescine	[M-H] ⁻	439.18689	C24H28N2O6	Ferulic acid and derivatives	CHEZHJQHCYLF1-UHFFFAOYSA-N	OC(=NCCCC(CO)C(=O)CC=1C=CC(O)=C(OC)C=C1)C=CC2=CC(OC)=C(C(=O)C2
1689	5.727	336.07516	Gossypetin	[M+H] ⁺	336.07138	C15H10O8	Flavonols	YRRAGUMVDQZ1Y-UHFFFAOYSA-N	O=C1C(O)=C(OC=2C(O)=C(O)C=C(CO)C12)C=3C=CC(O)=C(O)C3
1690	5.727	341.05438	lecanoric acid	[M+H] ⁺	341.06	C16H14O7	Depsides and depsidones	HEMSJKZDNNSEW-UHFFFAOYSA-N	O=C(O)C1=C(O)C(C(OC(=O)C=2C(O)=CC(O)=CC2)C=C1
1691	5.727	339.08389	methyl 2-(9-hydroxy-1-methyl-5,10-dioxo-3,4-dihydro-1H-benzogliso chromen-3-yl)acetate	[M+H] ⁺	339.08389	C17H16O6	Benzoisochromanequinones	FMEUW1KCS1JB-UHFFFAOYSA-N	O=C(OC)CC1OC(C=2C(O)=C3C(O)=CC=CC3(=O)C2C1)C
1692	5.729	881.39075	3-[(3S,10S,13R)-14-hydroxy-3-[4-methoxy-6-methyl-5-[3,4,5-trihydroxy-6-[[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy)methyl]oxan-2-yl]oxyoxan-	[M+H] ⁺	881.39313	C42H66O17	Cardenolide glycosides and derivatives	1TKDSJDYFJAVTJ-BMRHGRNRS-N	O=C1OCC(=C1)C2CC3(CO)C4CC5C5C(=O)OC(CO)C(OC7OC(COC8OC(CO)C(CO)C8O)C(CO)C(CO)C7O)C(CO)C3(CO)C(CO)C2(CO)C1C
1693	5.73	289.08957	(2S,3S)-2-(3,4-dihydroxyphenyl)-3,7-dihydroxy-2,3-dihydrochromen-4-one	[M+2H] ²⁺	289.08755	C15H12O6	Flavanonols	FNUPYFWXZM1E-CABCYRRESA-N	O=C1C2=CC=C(CO)C=C2OC(C3=CC=C(CO)C(CO)=C3)C1O
1694	5.732	290.08984	(2R,3R,4S,5R)-2-(6-amino-9H-purin-9-yl)-5-(hydroxymethyl)tetrahydrofuran-3,4-diol	[M+2H] ²⁺	290.09	C10H13N5O4	Purine nucleosides	O1RDTQYTFABQOQ-KQYNXCUSA-N	OC1OC(N2C=NC=NC(=NC(N3C2)N)C(CO)C1O
1695	5.732	879.37732	[(2R,3R,4R,5R,6S)-6-[(6E)-3,7-dimethyl-8-oxo-8-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxoacetal-1,6-dien-3-yl]oxy-5-hydroxy-	[M+H] ⁺	879.3775	C42H64O17	Saccharolipids	O1MSOLEDHKDCY-WJHJMGTLA-N	O=C(OC1OC(CO)C(O)C(O)C1O)C(=CCCC(OC2OC(CO)C(OC(=O)C(=C(CCC(OC(CO)C8O)C(CO)C(CO)C8)C(CO)C(CO)C7O)C(CO)C(CO)C7O)C(CO)C1C
1696	5.732	325.9588	Bifenox free acid	[M-H] ⁻	325.96286	C13H7Cl2NO5	Diphenylethers	IUSYSZLVZMUVD-UHFFFAOYSA-N	C1=CC(=C(C=C1C1)C1)OC=

1719	5.897	238.10706	Bupropion	[M-H]-	238.10042	C13H18ClNO	Alkyl-phenylketones	SNNPWTUOZRMVNY-UHHFFAONYA-N	O=C(C(=C=CC=C(C1)C)(NC(C)(C)C)C
1720	5.899	542.33514	(3E,7E,11E,15E)-5,9,13,17,18-pentahydroxy-4,6,8,10-tetramethyl-2-[(E)-2-methylbut-2-enyl]nonadeca-3,7,11,15-tetraenedioic acid	[M-H]+	542.33234	C28H44O9	Very long-chain fatty acids	YKAENKKQWMYF-SLELSECNSA-N	O=C(O)C(O)C(O)C(OC)=CC(C)C(O)C(=CC(C)C)C(O)C(=CC(C(=O)OC)=CC(C)C)C
1721	5.939	296.10309	1-Methylguanosine	[M-H]-	296.10004	C11H15N5O5	Purine nucleosides	UTAITYHAJNQDW-UHHFFAONYA-N	O=C1C=2N=C(C2NC(N)N1C)C3OC(CO)C(O)C3O
1722	5.941	213.0648	3-(2-hydroxyethyl)quinazolin-4(3H)-one	[M-H]+	213.06	C10H10N2O2	Quinazolines	OCFLUNGSKQZSJ-UHHFFAONYA-N	O=C1C=2C=CC=CC2N=CN1COO
1723	5.941	284.05457	Cladribine	[M-H]-	284.0556	C10H12ClN5O3	Purine 2'-deoxynucleosides	PTOARAEWMLNO-UHHFFAONYA-N	C1C=1N=C(N)C=2N=C(C2N1)C3OC(CO)C(O)C3
1724	5.943	285.03915	3',4',5,7-tetrahydroflavone	[M-H]-	285.04047	C15H10O6	Flavones	JPNAAANSBPFGQ-UHHFFAONYA-N	O=C1C=C(OC=2C(C)C)C(C)C12=C=3C=CC(O)=C(O)C3
1725	5.947	562.35303	(6aR,8aS)-10-(4-(N-acetylacetamido)-3-methylbutyl)-6a,8a,9-trimethyl-3,4,5,6,6a,6b,7,8,8a,8b,11a,12,12a,12b-tetradecahydro-1H-	[M-H]+	562.34998	C33H49NO6	Furostanes and derivatives	WURLGASLEZVNHV-PLECQWPSA-N	O=C(O)CC1CC2=CC3C(CCC4(C)C5C(=C(OC5CC34))CCC(C)CN(C)=O)C1C=C1C(C)C(C)C2(C)C(C)C1C
1726	5.954	425.20551	Benazepril hydrochloride	[M-H]+	425.207	C24H29ClN2O5	Dipeptides	VPSRQEHTIMQM-FKLPMAJSA-N	C1.O=C(O)CN1C(=O)C(NC(=O)OC)CCC=2C=CC=CC2.CCC=3C=CC=CC3
1727	5.954	268.11746	Citrinin	[M-H]+	268.11795	C13H14O5	Benzopyrans	CQUIUKYOEOPUDV-IYSWYEDSA-N	O=C(O)C(=C(=O)C)=C2C(=C(C)C(C)C2)C1O)C
1728	5.979	393.16168	Corynanthin	[M-H]+	393.1575	C21H26N2O3	Yohimbine alkaloids	BLGFXZZNTWLAY-UHHFFAONYA-N	O=C(O)C(C)C1C(O)CC2CN3CCC=4C=SC=CC5N4C3CC12
1729	5.979	415.31894	diosgenin	[M-H]+	415.32001	C27H42O3	Triterpenoids	WQLVFSAGJTQC-KVROHFGNSA-N	OC1CC2=CC3C(CCC4(C)C3CC5OC6(OC(C)OC6(C)C54)C2(C)CC1
1730	5.982	577.36346	Polyphyllin A	[M-H]+	577.37	C33H52O8	Steroidal saponins	WXMARHXAKWRND-GAMIEDRGS-N	OC1OC10C2CC3=CC4C(CCC5(C)C4CC6OC7(OC(C)C(C)C(C)C65)C3(C)C2)C(C)C(C)C1O
1731	5.988	317.06497	3-O-methylquercetin	[M-H]+	317.065	C16H12O7	3-O-methylated flavonoids	WEPPBGSIAWZTEJR-UHHFFAONYA-N	O=C1C(OC)=C(CC=2C(C)C)C(C)C12=C=3C=CC(O)=C(O)C3
1732	6.001	464.09738	Delphinidin-3-glucoside	[M-H]-	464.09549	C21H21O12	Anthocyanidin-3-O-glycosides	XENHPQLDPAYIJ-UHHFFAONYA-O	OC=1C=C(C)C=2C=C(OC3OC(C)C(O)C(C)C3O)C(=[O+])C2(C)C=4C=C(C)C(O)=C(O)C4
1733	6.004	251.16333	2-[(1S,2S,4aR,8aS)-1-hydroxy-1a-methyl-8-methylenedioxy-1,2,3,4,5,6,7,8a-octahydronaphthalen-2-yl]irono-2-enoic acid	[M-H]+	251.16417	C15H22O3	Eudesmane, Isoeudesmane or cycloisoeudesmane	QTSGCVLTMMKDP-SFDCRBFBSA-N	O=C(O)C(C=C)CCCC(C)CCCC(=O)C2C1O
1734	6.005	270.11206	(2Z)-2-benzylidene-6-methoxy-1-benzofuran-3(2H)-one	[M-H]+	270.11246	C16H12O3	Aurene flavonoids	LKWJJGLULNRBP-DHDCSXOGS-N	O=C1C(OC2=CC(OC)=CC2C1)=CC=3C=CC=CC3
1735	6.005	297.06497	(5E)-4-methoxy-5-[methoxy{1(2R,3S)-3-phenyloxiran-2-yl)methylenedioxy}furan-2-one	[M-H]+	297.06296	C15H14O5	Butenolides	RTNGMUTUMJOABT-ONKYJICLSA-N	O=C1OC(C(OC)=C1)C(OC)C2OC2=3C=CC=CC2
1736	6.007	301.06006	Carbazochrome sulfonate	[M-H]+	301.06012	C10H12NaO5S	Indole and derivatives	OZCACMPSTYSQM-UHHFFAONYA-N	CN1C(CC2=CC(NNC(O)=N)C(C)=O)C(C)S12(O)=O
1737	6.008	537.15936	(1S,4aS,7r,8aS)-7-hydroxy-7-[[1(E)-3-(4-hydroxyphenyl)prop-2-enoyl]oxymethyl]-1-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-	[M-H]+	537.16028	C25H28O13	Iridoid O-glycosides	WIJPBKJNJIZGY-QZOILURDPSA-N	O=C(O)C1=CC(OC2OC(C)C(O)C(C)C2O)C3C1C=CC3(O)CC(=O)C=C(C)C=C(C)C(C)C4
1738	6.008	283.26233	Oleic acid	[M-H]+	283.26401	C18H34O2	Long-chain fatty acids	ZGPPMHWFCSIRJ-MDZMXPLPSA-N	O=C(O)CCCCCCCC=CCCCCCCCCC
1739	6.018	201.1127	Sebacic acid	[M-H]-	201.11324	C10H18O4	Medium-chain fatty acids	CXMXPHRMRROMY-UHHFFAONYA-N	OC(=O)CCCCCCCC(=O)=O
1740	6.019	301.03595	Ellagic Acid	[M-H]-	301.03583	C14H6O8	Hydrolysable tannins	AFSDNFLWKVMVB-UHHFFAONYA-N	O=C1OC2=C(O)C(O)=CC=3C(=O)C(=O)C(=O)C=C1C4C23
1741	6.021	581.14795	Flavanone base + 40, O-Hex, C-Pen	[M-H]-	581.15021	C26H30O15	Flavanone C,O-glycosides	QETQGQBDBULWC-UHHFFAONYA-N	OC1OC(OC2=CC(O)=C(C3OC(C)C(O)C(C)C3O)C3=C2C(=O)CC(C)C2)=CC(O)=C(O)C(C)C(C)C1O
1742	6.024	579.35144	(1S,2S,5R,7R,10S,11S,14R,16R,19S,20S,23R,25R)-5,14-diethyl-2,11,20,23-tetramethyl-4,13,22,28,29,30-	[M-H]-	579.35382	C32H52O9	Macrolides and analogues	MXXZIBZNZOHER-VHWZAHMSA-N	O=C1OC(C)CC2OC(C2)C(C)=O(C(C)C(C)C3OC(C)C(C)=O)OC(C(C)CC4OC(C4)C)C1C
1743	6.024	527.26678	3Beta-Acetoxydeoxydihydrogedunin	[M-H]-	527.26721	C30H40O8	Limonoids	LCTHUKJMKQYDV-ZYIGBFLPSA-N	O=C(OC1CC2(C)C(C)C(C)C2O)C3OC(=O)C5OC54C3(C)C(OC(=O)C)CC2(C)C(C)C6=OOC(C6)C
1744	6.03	375.10605	2-(3,4-dimethoxyphenyl)-5,7-dihydroxy-3,6-dimethoxy-4H-chromen-4-one	[M-H]+	375.10699	C19H18O8	6-O-methylated flavonoids	SDTFURCSWUESP-UHHFFAONYA-N	O=C1C(OC)=C(OC2=CC(O)=C(CO)C(OC)=C12)C=3C=CC(OC)=C(OC)C3
1745	6.03	487.25217	Alpha-Dihydrogedunol	[M-H]+	487.25009	C28H38O7	Limonoids	JVHWYVNBMTROCV-AJIGNVKSA-N	O=C(OC1CC2C(C)C(C)C(O)CC2(C)C3CC4(C)C(C)OC(=O)C5OC54C13(C)C6=OOC(C6)C
1746	6.033	491.29947	caudatin	[M-H]+	491.29999	C28H42O7	Gluco/mineralocorticoids , progestogens and	VVLXIXALPNYWFH-UVJZLUHSA-N	O=C(OC1CC2C(O)CC=C3C(O)CC3CC2)C4(O)CCC(O)C(C(=O)C)C14
1747	6.034	272.12668	3-(alpha, alpha-dimethylallyl)psoralen	[M-H]+	272.12811	C16H14O3	Psoralens	FVCCUUNGXGKNJV-UHHFFAONYA-N	O=C1OC=2C=C3OC=C3C=CC2=C1C(C=C)C(C)C
1748	6.034	524.3335	Phosphatidylcholine lyso 16	[M-H]-	524.33575	C24H48NO7P	2-acyl-sn-glycerol-3-phosphocholines	GMEZONVWDGOWJ-XXVXOECA-N	CCCCCCCCCCCCC=C/C(OC(=O)OC(CO)OP([O-])([O-])OP([O-])N1C)C(C)C1
1749	6.054	453.19968	5-[(2R,3S)-6-hydroxy-2-(4-hydroxyphenyl)-4-[(E)-2-(4-hydroxyphenyl)ethenyl]-2,3-dihydro-1-benzofuran-3-yl]benzene-1,3-diol	[M-H]-	453.20023	C28H22O6	2-arylbenzofuran flavonoids	FQWLMRXWZGLFI-PAKEJIOWSA-N	OC1=CC=C(C=C1)C=C(C=2C(C)C=C3OC(=O)C4=CC=C(C)C=C4)C(=SC=C(O)C(C)C(C)C5)C32
1750	6.057	285.08676	(2R,3R)-3,7-dihydroxy-6-methoxy-2-phenyl-2,3-dihydrochromen-4-one	[M-H]-	285.0853	C16H14O5	6-O-methylated flavonoids	GLMPFOLJOLXCLA-JKSUJKBHSA-N	O=C1C2=CC(OC)=C(C)C=C2OC(C=3C=CC=CC3)C1O
1751	6.071	174.08405	Citrulline	[M-H]-	174.08841	C6H13N3O3	L-alpha-amino acids	RHGKRLQHDJDR-UHHFFAONYA-N	O=C(O)C(N)CCNC(=O)O
1752	6.085	765.43829	2-[2-[19-acetamido-6-(3,4-dicarboxybutanoyloxy)-16,18-dihydroxy-5,9-dimethylcosan-7-yl]oxy-2-oxoethyl]butanedioic aci	[M-H]+	765.43793	C36H61NO15	Fumonisin	GGCJWFDPDAKUS-UHHFFAONYA-N	O=C(O)CC(C(=O)C)CC(=O)OC(C)C(C)CCCC(C)CC(C)N(C)C(=O)C(C)C(=O)OC(C(=O)C)C(C

1762	6. 168	357. 09528	Byakangelicin	[M+H] ⁺	357. 095	C17H1807	5-methoxypsoralens	PKRPFNXROFUNDE-LLYKDONJSA-N	O=C1OC=2C (OCC (O) C (O) C) C=C3OC=CC3=C (OC) C2C=C1
1763	6. 169	309. 14288	Biflorin	[M+H] ⁺	309. 14301	C20H2003	Naphthoquinones	DSVUBIQQVPVZST-UHFFFAOYSA-N	O=C1C (=O) C (=C2OC=C (C=3C=CC (=C1C23) C) CCC=C (C) C) C
1764	6. 171	343. 21268	ERGONOINE MALEATE	[M+H] ⁺	343. 21283	C19H23N302	Lysergamides	WVYSZNPYNCNODU-XTQGRXLLSA-N	OC (=NC (O) C) C1C=C2C=3C=CC=4NC=C (C43) CC2N (C) C1
1765	6. 172	495. 28561	2-[[[6,7-dimethoxy-1,2,3,4-tetrahydroisoquinolin-1-yl)methyl]-3-ethyl-9,10-dimethoxy-5-oxido-2,3,4,6,7,11h-hexahydro-1H-benzofalaminolizin-5-ium	[M-H] ⁻	495. 28644	C29H40N205	Emetine alkaloids	SSQAAXSNCRMBPJ-UHFFFAOYSA-N	O=N12CCC3=CC (OC) =C (OC) C=C3C2CC (CC4NCC5=C (OC) C=C (OC) C=C5) C1C (OC) C1
1766	6. 172	547. 2948	Cymarine	[M-H] ⁻	547. 29126	C30H4409	Cardenolide glycosides and derivatives	XQCGNURMLWFJR-ZNDDOCHDSA-N	O=C1C2CCC (OC3OC) C (O) C (OC) C3) CC2 (O) CCC4C1CC5 (C) C (C6=C=CC (=O) OC6) CC450
1767	6. 187	168. 02977	N-(2-Furoyl)glycine	[M-H] ⁻	168. 03023	C7H7N04	N-acyl-alpha amino acids	KSPQDMRTZZYQLM-UHFFFAOYSA-N	O=C (O) CNC (=O) C=1OC=CC1
1768	6. 189	349. 21048	Roxatidine acetate HCl	[M+H] ⁺	349. 21201	C19H29C1N204	N-benzylpiperidines	FEWCTJHCXOHWNL-UHFFFAOYSA-N	C1. O=C (OCC (=O) NCCCOC1=CC=CC (=C1) CN2CCCCC2) C
1769	6. 19	305. 10461	15,17-dihydroxy-9-methyl-4,10-dioxatricyclo[[11.4.0.0?;7]heptadec-1(17),13,15-triene-2,11-dione	[M-H] ⁻	305. 10306	C16H1806	Aryl alkyl ketones	BVDHPBILFRQGE-UHFFFAOYSA-N	O=C1OC (C) CCCC2OC2 (C) C=3C (O) =CC (O) =CC3C1
1770	6. 217	897. 38678	3-[(3S,5R,10S,13R,14S,17S)-14-hydroxy-3-[(2R,3S,4S,5S,6S)-3-hydroxy-4-methoxy-6-methyl-5-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-3-hydroxy-5,5,8a-trimethyl-3,4,4a,6,7,8-hexahydronaphthalene-2-carboxylic acid	[M+H] ⁺	897. 38806	C42H66018	Cardenolide glycosides and derivatives	GZVMBXDQJRICT-OZPZHNRSA-N	O=C1OCC (=C1) C2CC3 (O) C4CC5CC (OC6OC) C (C) OC7OC (OC8OC (C) C (O) C) C8O) C (O) C (O) C7O) C (OC1OC6) CCC5 (C) C4OCC23C
1771	6. 225	256. 19073	3-hydroxy-5,5,8a-trimethyl-3,4,4a,6,7,8-hexahydronaphthalene-2-carboxylic acid	[M+H] ⁺	256. 1907	C14H2203	Beta hydroxy acids and derivatives	LQZAHKUYJVAAR-UHFFFAOYSA-N	O=C (O) C1=C2C (O) CCCC (C) C2CC1O
1772	6. 23	257. 17358	alpha-dihydrolysergol	[M+H] ⁺	257. 17001	C16H20N20	Clavines and derivatives	UFKTZIXVYHGAES-XEGUGMAKSA-N	OC1CN (C) C2CC3=CN=C4=CC=CC (=C43) C2C1
1773	6. 235	584. 2735	Tricoumaroyl spermidine (isomer of 2952)	[M+H] ⁺	584. 27441	C34H37N306	Coumaric acid and derivatives	PFDWJJCSDYDRMZ-UHFFFAOYSA-N	O=C (C=CC1=CC=C (O) C=C1) NCCCN (C (=O) C=C2C=CC=C (O) C=C2) CCC (CNC (=O) C=C3=CC=CC (O) C=C3)
1774	6. 248	483. 29504	(2R,3S,4S,5S,6R)-2-[[[7-hydroxy-4-[(2)-5-hydroxy-3-methylpent-3-enyl]-4a,8,8-trimethyl-3-methylidene-2,4,5,6,7,8a-hexahydro-1H-naphthalen-2-3-[5-hydroxy-7-methoxy-2,3-dimethyl-6-(3-methylbut-2-enyl)-4-oxo-2,3-dihydrochromen-8-yl]hexanoic acid	[M-H] ⁻	483. 29633	C26H4408	Diterpene glycosides	JECOCDCQZSANS-RFKAOMIISA-N	OC=C (C) CCC1C (=C) C (OC2OC) C (O) C (O) C2O) CC3C (C) C (C) C (O) CC13C
1775	6. 254	403. 14877	3-[5-hydroxy-7-methoxy-2,3-dimethyl-6-(3-methylbut-2-enyl)-4-oxo-2,3-dihydrochromen-8-yl]hexanoic acid	[M-H] ⁻	403. 14771	C23H3206	Chromones	UDNTMMLZUXNQM-UHFFFAOYSA-N	O=C (O) CC (C1=C (OC) C (=C) C2=C1OC (C) C (C2=O) C) CC=C (C) C) CC=C
1776	6. 274	339. 17966	coronardine	[M+H] ⁺	339. 17966	C21H26N202	Ibogan-type alkaloids	NVVDQMVGALBDGE-UHFFFAOYSA-N	O=C (OC) C12C=3NC=4CC=CC4C3CCN5CC (CC (CC) C51) C2
1777	6. 275	345. 18036	Formoterol	[M+H] ⁺	345. 18088	C19H24N204	Amphetamines and derivatives	BPZSYCZ1ITTYBL-UHFFFAOYNA-N	OC=NC1=CC=C (CC=C1O) C (O) CNC (C) CC2=CC=C (OC) C=C2
1778	6. 296	188. 03595	Acetylisatin	[M-H] ⁻	188. 03532	C10H7N03	Indoles and derivatives	LPGEHBASRKTDG-UHFFFAOYSA-N	O=C1C (=O) N (C (=O) C) C=2C=CC=CC12
1779	6. 296	271. 10748	naringenin	[M-H] ⁻	271. 10629	C15H1205	Flavanones	FTWIRXFLQLPI-UHFFFAOYSA-N	O=C1C=2C (O) =CC (O) =CC2OC (C3=CC=C (O) C=C3) C1
1780	6. 312	512. 20221	(R,E)-6-acetyl-7,9-dihydroxy-2-((3-(3-(2-methoxyethyl)-1,2,4-oxadiazol-5-yl)propyl)amino)ethylidene)-8,9b-dimethylidenezofb,difuran-1,3(2H,9H)-4a,8,8-trimethyl-3-methylidene-2,4,5,6,7,8a-hexahydro-1H-naphthalen-2-8-[(2R,3S)-5,7-dihydroxy-2-(4-hydroxyphenyl)-4-oxo-2,3-dihydrochromen-3-yl]-5,7-dihydroxy-2-(4-hydroxyphenyl)chromen-4-one	[M+H] ⁺	512. 20001	C26H29N308	Acetophenones	GCKXCHKHNLGAF-WGKDYUESA-N	O=C1C=C2OC3=C (C (=O) C) C=C (O) =C3C2 (C (=O) C1=C (NCCC4=NC (C4O) CCCC4) C) C=C
1781	6. 312	539. 16595	8-[(2R,3S)-5,7-dihydroxy-2-(4-hydroxyphenyl)-4-oxo-2,3-dihydrochromen-3-yl]-5,7-dihydroxy-2-(4-hydroxyphenyl)chromen-4-one	[M-H] ⁻	539. 16309	C30H20010	Biflavonoids and polyflavonoids	YOGANETYUQWTM-PXJZQJOASA-N	O=C1C=C (OC=2C1=C (O) C=C (O) C) C2C3C (=O) C=C4 (O) =CC (O) =CC4OC3=C5=CC=C (O) C=C5) C=6C=CC (O) =CC6
1782	6. 316	250. 0712	Phenylacetylaspartic acid	[M-H] ⁻	250. 0713	C12H13N05	Amino acids	SVFKZPQPMZHLZ-UHFFFAOYNA-N	O=C (O) CC (NC (=O) CC1=CC=CC=C1) C (=O) O
1783	6. 325	877. 35803	4-[[[7R,11S,14S,16R)-14-[[[4-methoxy-6-methyl-5-[[[2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-[[[2R,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-(7S,9E,11S,12R,13S,14S,15S,16R,17S,18S,19E,21Z)-13-(acetyloxy)-26-(dimethylamino)-15,17-dihydroxy-11-methoxy-3,7,12,14,16,18,22-hexamethyl-	[M+H] ⁺	877. 36182	C42H62017	O-glycosyl compounds	DVFXYUYOYUOTA-DYCWBJYSA-N	O=C1OCC (=C1) C2=C=CC34OC54OC6OC (OC7OC) C (OC8OC (COC9OC (C) C) C (O) C9O) C (O) C (O) C8O) C (OC) C7) CCCC6 (C) C5OCC723C
1784	6. 326	879. 3772	(7S,9E,11S,12R,13S,14S,15S,16R,17S,18S,19E,21Z)-13-(acetyloxy)-26-(dimethylamino)-15,17-dihydroxy-11-methoxy-3,7,12,14,16,18,22-hexamethyl-	[M+H] ⁺	879. 37	C47H56N2013	Macrolactams	CRQDRGLGJNQTJ-ZXWRESOLSA-N	O=C (OC=1C=2C (=O) C=3NC (=O) C (=CC=CC (O) C) C (O) C (O) C (C) C (OC (=O) C) C (C) C (OC) C=C=CC4 (OC=C (C4=O) C2C (=O) C3N (C) C1) C1
1785	6. 326	202. 0515	Indole-3-pyruvic acid	[M-H] ⁻	202. 05096	C11H9N03	Indolyl carboxylic acids and derivatives	RSTKLPEZGYGAPY-UHFFFAOYSA-N	O=C (O) C (O) C1=C=CC=2C=C=CC21
1786	6. 328	649. 27307	(S)-2-(((S)-7-acetamido-1,2,3-trimethoxy-9-oxo-5,6,7,9-tetrahydrobenzo[f]hentalen-10-yl)amino)-4-(methylthio)-N-(2-(2-	[M+H] ⁺	649. 27002	C32H42N407S	Methionine and derivatives	PMKXQVXLVOSJT-ZCQVQJMSA-N	O=C1C=C2C (=CC=C1NC (C (=O) NCCN3C (=O) CCC3) CCSC) C4=C (OC) C (OC) =C (OC) C=C4OCC2NC (=O) C
1787	6. 337	211. 13293	(+)-Jasmonic acid	[M+H] ⁺	211. 13287	C12H1803	Jasmonic acids	ZNJFBWYDHLGLCU-HWKKXFMVSA-N	CC)C=C/C=C[H]1[C=H]1C=H] (CC (O) =O) OCC1=O
1788	6. 346	389. 00107	PFAP-FT diPAP	[M-H] ⁻	389. 00061	C8H9F1004P	PFSA	ZPRPFGDLJHJEV-UHFFFAOYSA-N	O=P (O) (OCCC (F) (F) F) OCCC (F) (F) C (F) (F) C (F) F
1789	6. 357	515. 30316	Ganoderic acid LM2	[M+H] ⁺	515. 29999	C30H4207	Triterpenoids	YVIVANDTNNUXHR-UGRWEMWSA-N	O=C (O) C (=CC (O) CC (C) C1CC (=O) C2 (C3=C (C (=O) CC12C) C4 (C) CCC (=O) C (C) C) C4CC30) C) C
1790	6. 358	307. 12851	Caffeoyl lysine	[M-H] ⁻	307. 12729	C15H20N205	Caffeic acid and derivatives	WVFMZTORJFNZPK-UHFFFAOYNA-N	NC (CCCCNC (=O) C=C1=CC (O) =C (O) C=C1) C (O) =O
1791	6. 36	249. 10913	2-hydroxylantolactone	[M+H] ⁺	249. 10852	C15H2003	Eudesmanolides, secoeudesmanolides, and	FZSKLHDEGWSLTB-ATYMOLOSSA-N	O=C1OC2CC3 (C (=CC2C1=C) C (C) CC (O) C3) C
1792	6. 36	229. 03857	3-methyl-3,4-dihydro-1H-1,4-benzodiazepine-2,5-dione	[M+H] ⁺	229. 03738	C10H10N202	1,4-benzodiazepines	LJONJQLKOKMKBR-UHFFFAOYSA-N	OC1=NC (C (O) =NC=2C=CC=CC12) C
1793	6. 361	326. 09048	Midazolam	[M+H] ⁺	326. 086	C18H13C1FN3	Imidazo[1,5-a][1,4]benzodiazepines	DDLJGOFVUZHBH-UHFFFAOYSA-N	FC=1C=CC=CC1C2=NCC3=CN=C (N3C=4C=CC (C1) C=CC24) C
1794	6. 366	369. 18057	8-hydroxy-6-methoxy-7-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxychromen-2-one	[M-H] ⁻	369. 17978	C16H18010	Coumarin glycosides	RVWWDDKQXKCJ-ZOLYHUHESA-N	O=C1OC=2C (O) =C (OC3OC) C (O) C (O) C3O) C (OC) =CC2C=C1
1795	6. 383	302. 19473	heliocurassavicine n-oxide	[M+H] ⁺	302. 194	C15H27N05	Pyrrolizidines	DLNWZIVYKXLTN-YOPIWALVSA-N	O=C (OCC1CC[N+](=I) ([O-]) OCC12) C (O) (C) C (O) C (C) C
1796	6. 384	431. 314	Hecogenin	[M+H] ⁺	431. 31558	C27H4204	Triterpenoids	QOLRLFLJMLZLQJ-LORDNJQFSA-N	O=C1CC2C (CCC3CC (O) CCC3C) C4CC5OC6 (OCC (C) CC6) C (C) C5C14C
1797	6. 395	601. 37	Timosaponin A1	[M+H] ⁺	601. 37	C33H5408	Steroidal saponins	ZNEI1ZXNGXIAL-UHFFFAOYSA-N	OC1OC (OCC2CC3 (C) C (CCC4C3CC5 (C) C4C6OC7 (OCC (C) CC7) C (C) C65) C2) C (O) C (O) C1O
1798	6. 411	429. 11752	Formononetin-7-O-glucoside	[M-H] ⁻	429. 11911	C22H2209	Isoflavone O-glycosides	MGJLSBDCWOSMHL-UHFFFAOYNA-N	OC1=C=CC=C (C=C1) C1=COC2=CC (OC3OC) C (O) C (O) C3O) =CC=C2C1=O
1799	6. 415	300. 18002	Tegaserod	[M-H] ⁻	300. 18298	C16H23N50	Indoles and derivatives	JXDXRFUJZDKKGDV-UHFFFAOYSA-N	N=C (NNC=C1C=NC=2C=CC=CC1) NCCCC
1800	6. 436	375. 27365	(E)-5-[(1S,4aR,8aR)-2-formyl-5,5,8a-trimethyl-1,4,4a,6,7,8-hexahydronaphthalen-1-yl]-3-(acetylloxymethyl)pent-2-enoic acid	[M-H] ⁻	375. 27643	C22H3205	Diterpenoids	KLGPVOFYVYHEGO-VBJQW1QDSA-N	O=CC1=CCC2C (C) (CCC2C) C1CCC (=CC (=O) O) OOC (=O) C
1801	6. 436	545. 27655	7-Deacetylkhivorin	[M+H] ⁺	545. 27448	C30H4009	Limonoids	MRMHZVITOFZZID-WXWNNQMSA-N	O=C (OC1CC (=O) C) C2 (C) C (CC (O) C3 (C) C2CC4 (C) C (OC (=O) C5 (OC43) C6=C6) C4) C1C
1802	6. 445	777. 2204	methyl (1S,4aS,7aS)-5'-oxo-1-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy-4'-[(1S)-1-[(R)-3-[4-[(2S,3R,4S,5S,6R)-3,4,5-	[M-H] ⁻	777. 22473	C36H42019	Iridoid O-glycosides	AFY1WKNGSYXQC-WLJLAZQSA-N	O=C (OC (C1=CC2 (OC1=O) C=CC3=C=CC (OC4OC) C (O) C (O) C4O) C=32) C (O) OC1) C1=C=C5=C=C=C (OC6OC) C (O) C (O) C6O) C=C5
1803	6. 447	481. 34943	brassinolide	[M+H] ⁺	481. 35001	C28H4806	Brassinolides and derivatives	IXVMHGQKLDRKH-KNBKMWSGSA-N	O=C1OCC2C3CCC (C (C) C (O) C (O) C (C) C) C3 (C) CC2C4 (C) CC (O) 1C (O) CC14
1804	6. 452	303. 25253	2-Myristoylglycerol	[M+H] ⁺	303. 25299	C17H3404	2-monooacylglycerols	TYVMZSOXQNHWO-UHFFFAOYSA-N	O=C (OC (CO) CO) CCCCCCCCCCCC

[illegible]

[illegible]

[illegible]

[illegible]

1977	7.623	304.26459	Fenpropimorph	[M+H] ⁺	304.26349	C20H33NO	Phenylpropanes	RYAUSQKQZMAI-UHFFFAOYNA-N	CC(C1C=CC=C(C=C1)C(C)C(C)C)CN2CC(C)OC(C)C2
1978	7.624	390.28265	Roquefortine C	[M+H] ⁺	390.27811	C22H23N5O2	Pyrrololindoles	SPWSUFUPTSJWNG-LHMLNZRCSA-N	O=C1C(N=C(O)C2N1C3NC=4C(=CC=C4C3)C2)C(C=C)C(C)C)-CC5=CN=C5
1979	7.65	284.29617	1-desoxymethylsphinganine	[M+H] ⁺	284.29401	C17H37NO	1,2-aminoalcohols	UGVBHUWZNNKIR-QGZVFWFLSA-N	OC(CN)CCCCCCCCCCCC
1980	7.662	172.16907	Chrysanthemyl Alcohol	[M+H] ⁺	172.16959	C10H18O	Monocyclic monoterpeneoids	HIPIENKVKJCMAP-DTWKNJWSA-N	0CC1C(C=C(C)C)C1(C)C
1981	7.664	599.17377	4-[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy-9-(3,4,5-trimethoxyphenyl)-5a,6,8a,9-tetrahydro-5H-[2]benzofuro[6,5-	[M+H] ⁺	599.17352	C28H32O13	Lignan glycosides	PAIASCUMTHMGHU-UHFFFAOYSA-N	O=C1OCC2C3C=C(OC4OC(CO)C(CO)C4O)C=5OCC5C=C3C(C6=CC(OC)=C(OC)C(OC)=C6)C12
1982	7.668	199.12221	Tacrine	[M+H] ⁺	199.12297	C13H14N2	Acridines	YLJREFDVOIBQDA-UHFFFAOYSA-N	N=C1C=2C=CC=CC2NC3=C1CCCC3
1983	7.669	254.17445	MPL-dm	[M+H] ⁺	254.17506	C14H23NO3	Tyrosols and derivatives	CUKXSBOATJILRY-UHFFFAOYNA-N	CC(C)NCC(COC)=CC=C(C=C1)CCO1O
1984	7.679	292.18994	(4aS)-6,7-dihydroxy-1,1,4a-trimethyl-3,4,10,10a-tetrahydro-2H-phenanthren-9-one	[M+H] ⁺	292.1907	C17H22O3	Diterpenoids	JMBKXUYCBKSSY-OMOCHNIRSA-N	O=C1C2=C(CO)=C(CO)C=C2C3(C)CCCC(C)C3C1
1985	7.684	449.22769	Irigenin, 7-Benzyl Ether	[M+H] ⁺	449.22553	C25H22O8	3'-hydroxy,4'-methoxyisoflavonoids	WSKWDWDFVUKY-UHFFFAOYSA-N	O=C1C(=COC=2C=C(OC=3C=CC=C3)C(OC)=C(CO)C12)C=C4C=C(CO)C(OC)=C(OC)C4
1986	7.684	957.50177	Soyasaponin Ba	[M+H] ⁺	957.50647	C48H78O19	Triterpene saponins	WFRQIKSNAYUJZ-UHFFFAOYNA-N	CC1(C)CC(O)C2(C)CC(C)C=C(OC4C5(C)CCC(OC6OC(C)C(CO)C6)C6OC6OC(C)C(CO)C6OC6OC(C)C(CO)C6)C(C)C
1987	7.69	433.09933	Reynoutrin	[M+H] ⁺	433.10001	C20H18O11	Flavonoid-3-O-glycosides	PZZRDJXEMZMDF-QDQGBAFUSA-N	O=C1C(OC2OCC(CO)C2O)=C(OC=3C=C(CO)C(CO)C13)C=4C=CC(C)=C(CO)C4
1988	7.695	389.20721	3-[3-[(2E)-3,7-dimethylocta-2,6-dienyl]-4-hydroxyphenyl]-7-hydroxychromen-4-one	[M+H] ⁺	389.20807	C25H26O4	Isoflavones	ZBHUUXLHDOUMKM-REZTVBANSAN	O=C1C(=COC2=CC(O)=CC(C12)=3C=CC(O)=C(C3)CC=C(C)CCC=C(C)C1C
1989	7.706	281.14209	4-(2,6-dihydroxy-6-methylheptan-2-yl)-3-hydroxybenzoic acid	[M+H] ⁺	281.13943	C15H22O5	Sesquiterpenoids	YCUWMGYPKGLQKF-UHFFFAOYSA-N	O=C(O)C1=CC=C(C(O)=C1)C(O)C(C)CCC(O)C(C)C
1990	7.707	326.14691	6-(2-aminopyrimidin-4-yl)-4-butyl-7-hydroxy-8-methyl-2H-chromen-2-one	[M+H] ⁺	326.14999	C18H19N3O3	7-hydroxycoumarins	KMPN1YIOWJCPY-UHFFFAOYSA-N	O=C1OC2=C(C=C(C=3N=C(N=CC3)N)C(O)=C2O)C(=C1)CCCC
1991	7.707	274.27383	ISOPALMITIC ACID	[M+H] ⁺	274.27405	C16H32O2	Long-chain fatty acids	ZONJATNKKGVSV-UHFFFAOYSA-N	O=C(O)CCCCCCCCCCCCC(C)C
1992	7.71	455.13159	(2R,3S,4S,5R,6R)-5-[(2S,3R,4R)-3,4-dihydroxy-4-(hydroxymethyl)oxolan-2-yl]oxy-2-(hydroxymethyl)-6-(2-phenylethoxy)oxane-3,4-diol	[M+H] ⁺	455.13141	C19H28O10	O-glycosyl compounds	UWKRNCNWJCHGZ-DERWJZPFA-N	OC1OC(OC=2C=CC=CC2)C(OC3OCC(O)(CO)C3O)C(O)C1O
1993	7.719	192.13783	DEET	[M+H] ⁺	192.13829	C12H17NO	N,N-dialkyl-m-toluidides	MMOXZBCLQITDF-UHFFFAOYSA-N	CCN(CC)C(C1=CC=CC(C)=C1)=O
1994	7.733	357.26324	5-[6-[3-(hydroxy-4-methoxyphenyl)-1,3,3a,4,6,6a-hexahydrofuro[3,4-c]furan-3-yl]-2-methoxyphenyl]	[M+H] ⁺	357.2594	C20H22O6	Furanoid lignans	VRIHVMFGDGRFLP-UHFFFAOYSA-N	OC1=CC(=CC(C1OC)C2OC3C(OC23)C4=CC=C(OC)C(O)=C4
1995	7.733	325.20099	FA 18:3+30	[M+H] ⁺	325.20071	C18H30O5	Oxidized fatty acids	PLJHEKVESBJRJC-UHFFFAOYNA-N	O=C(O)CCCCCCCC(=O)C=CC(O)C(CO)CC=CCC
1996	7.752	617.36725	(2S,3R,4S,5R)-2-[(2-hydroxy-22-(2-hydroxypropan-2-yl)-3,8,8,17,19-pentamethyl-23,24-	[M+H] ⁺	617.36951	C35H54O9	Cycloartanols and derivatives	LTVCFOSN1VOVBK-RSGHPYSYSA-N	OC1OCC(OC2OCC34CC54C(=CCC3C2(C)C)C6(C)C(O)C78OC(C)C(C)C78(C)C)C5(C)C4(C)C(C)C1O
1997	7.771	663.37299	Medicagenic acid base + O-Hex	[M+H] ⁺	663.37347	C36H56O11	Triterpene saponins	XCHARI1ZLLEBL-UHFFFAOYNA-N	O=C(O)C6(C)C(C(OC1OC(CO)C(CO)C1O)C(CO)C5(C)C(C6(C)C(C)C(C5(C)C=C24CC(C)C)C4)C(C=O)C(OC23(C)1)1)1)1
1998	7.773	391.23688	Perilogenin	[M+H] ⁺	391.23999	C23H34O5	Cardenolides and derivatives	QJPCKAJTLHONCS-FBAXFMHRSAN	O=C1OCC(=C1)C2OCC(CO)C4CC(CO)C(CO)C(C5(C)C4OCC23C
1999	7.774	221.0811	Monoisobutyl phthalate	[M+H] ⁺	221.08194	C12H14O4	Benzoic acid esters	RZJSUWQGFCHNFS-UHFFFAOYSA-N	CC(C)COC(C1=CC=CC=C1C(=O)O)=O
2000	7.775	317.07245	(3aR,4R,6E,10Z,11aR)-4-h						

2020	7. 974	250. 17645	N, O-Didesmethylvenlafaxine	[M+H] ⁺	250. 18016	C15H23N02	Cyclohexanols	MMSWXJSQCAEDLK-UHFFFAOYNA-N	CNOC(C1=CC=C(O)C=C1)C1(O)CCCC1
2021	7. 979	449. 0849	astilbin	[M-H] ⁻	449. 07956	C21H22O11	Flavonoid-3-O-glycosides	ZROGCCBNZBKLE-MPHRSVQHS-A-N	O=C1C=2C(O)=CC(O)=CC2OC(C3=CC=C(O)C(O)=C3)C1OC4OC(C)C(C(=O)O)C4O
2022	7. 984	595. 36383	(2R,6R)-6-[(3R,10S,12S,13R,17R)-3-(2-carboxyacetyl)oxy-12-hydroxy-4,4,10,13,14-pentamethyl-2,3,5,6,7,11,12,15,16,17-decahydro-1H-	[M+H] ⁺	595. 36047	C34H52O7	Triterpenoids	HMOGSPWDYKCAH-CBLCVTABSA-N	O=C(O)CC(=O)CC1OC2C(C3=C(CCC2C1)C)C4(C)CCC(C(C)CCC(=O)C(C(=O)O)C)C4(C)C(C)C(C)C
2023	7. 997	270. 07587	Dimethenamid OXA	[M-H] ⁻	270. 08057	C12H17N04S	Alpha amino acids and derivatives	HOYCASTVMCEOTP-UHFFFAOYNA-N	COCC(C)N(C(=O)(O)=O)C1=C(C)SC=C1C
2024	8. 008	407. 17255	Secoisolariciresinol	[M-H] ⁻	407. 17114	C20H26O6	Lignols	PUEUDUXMCLALY-UHFFFAOYNA-N	COC1=CC(CC(O)C(O)C)CC2=CC=C(C(O)C(OC)=C2)=CC=C1O
2025	8. 009	272. 09085	(E)-8-(1-(hydroxyimino)ethyl)-4,9-dimethyl-2H-furo[2,3-h]chromen-2-one	[M+H] ⁺	272. 09	C15H13N04	Angular furanocoumarins	VEUCARGUJVDOP-CXUHZMBSA-N	O=C1OC2=C(C=CC=OC(C(=NO)C)=C(C2)C)C(C(=C1)C
2026	8. 009	601. 26843	_130131	[M+H] ⁺	601. 263	C30H42O11	Terpene lactones	LB RJFDBQNUVAGM-VGCGLKNISA-N	O=C(O)C1=C=CC2C(C(=O)OC1)C(O)(COC(=O)C3=CC4C(C(=O)OC3)C(C(O)CCC4C(C)C)CC2C(C)C
2027	8. 022	252. 23137	(2E,4E)-N-(2-methylpropyl)dodeca-2,4-dienamide	[M+H] ⁺	252. 23218	C16H29NO	N-acyl amines	BBRMJCAPNGJKEK-AQASXUMVSA-N	OC(=NCC(C)C)C=CC=CCCCCCC
2028	8. 023	533. 27032	9-hydroxy-9-[[[(E)-2-(hydroxymethyl)-3-[3-(hydroxymethyl)-6-propan-2-yl]cyclohex-2-en-1-yl]nonan-2-oxo]loxymethyl]-1-oxo-6-nonan-2-yl]-	[M-H] ⁻	533. 27557	C29H42O9	Terpene lactones	R0OCBDNPGVEDL-KEBDBYFISA-N	O=C(O)C1=CC2C(C(=O)OC1)C(O)(COC(=O)C(=CC3C=C(O)CCC3(C)C)C(O)CC2C(C)C
2029	8. 036	495. 12662	[(4E)-7-acetyloxy-6-hydroxy-2-methyl-10-oxo-2,3,6,7,8,9-hexahydrooxecin-3-yl](F)-but-2-enoate	[M+H] ⁺	495. 12616	C24H24O10	Hydroxycinnamic acid glycosides	IAVJHQVGTGRSIOM-UVMZMRP TSA-N	O=C(OC1OC(OC(=O)C=CC2=CC=C(C)C(O)C(O)C)C=CC3=C(C(=O)C)C=C3
2030	8. 052	213. 14804	Dihydrojasmonic Acid	[M+H] ⁺	213. 14851	C12H20O3	Jasmonic acids	PQEYTAGBXNEUQL-UHFFFAOYSA-N	O=C(O)CC1CCC(=O)C1CCCC
2031	8. 055	598. 30341	5-[[[4-[5-[[[4-[5-[acetyl(hydroxy)amino]pentylamino]-4-oxobutanoyl]-hydroxyamino]pentylamino]-4-oxobutanoyl]-hydroxyamino]pentanoic acid	[M+H] ⁺	598. 30585	C25H45N5O10	N-acyl amines	ZMCWALAGRPU LMT-UHFFFAOYSA-N	O=C(O)CCCC(C)C(=O)CCC(O)=NCCCCC(O)C(=O)CCC(O)=NCCCCC(N)(O)C(=O)C
2032	8. 055	167. 14282	Dihydrojasnone	[M+H] ⁺	167. 14304	C11H18O	Cyclic ketones	YCI XWYOBMYNTGB-UHFFFAOYSA-N	CCCCC1=C(C)CCC1=O
2033	8. 057	103. 03149	Ethylenethiourea	[M+H] ⁺	103. 03245	C3H6N2S	Imidazolidines	PDQAZBWRQCBEV-UHFFFAOYSA-N	C1CNC(=N1)S
2034	8. 058	279. 09235	Triphenylphosphine oxide	[M+H] ⁺	279. 09332	C18H15OP	Phenylphosphines and derivatives	FIQMIBFVRAXMOP-UHFFFAOYSA-N	C1=CC=C(C=C1)P(C2=CC=CC=C2)(C3=CC=CC=C3)=O
2035	8. 063	360. 21573	9-phenyl-1-(2,4,6-trihydroxyphenyl)nonan-1-one	[M+H] ⁺	360. 21692	C21H26O4	Alkyl-phenylketones	OOGZXWIAHJUYAH-UHFFFAOYSA-N	O=C(C(=C(O)C)=CC(O)=CC1O)CCCCCCCCC2C=CC=CC2
2036	8. 066	260. 20001	Vesamicol	[M+H] ⁺	260. 2009	C17H25NO	Phenylpiperidines	YSSBJODGTYRAMI-UHFFFAOYNA-N	OC1CCCCC1N2CC(C=CC=CC=C3)CC2
2037	8. 075	316. 1167	Pipltartine	[M-H] ⁻	316. 11905	C17H19NO5	Cinnamic acids and derivatives	VABYUUNZAVNPG-BQYQJAHWSA-N	O=C(C=CC1=CC(OC)=C(OC)C(OC)=C1)N2C(=O)C=CCC2
2038	8. 078	236. 1111	1-(4-methoxyphenyl)isoquinoline	[M+2H] ²⁺	236. 11	C16H13NO	Phenylpyridines	VRGXPRJRDJGSKC-UHFFFAOYSA-N	N=C1CC=CC=CC=C2C1C=3C=CC(OC)=CC3
2039	8. 083	367. 20914	Pesticide4_Boscalid_C18H12Cl2N2O_3-Pyridinecarboxamide, 2-chloro-N-(4'-chloro[1,1'-biphenyl]-2-yl)-	[M-H] ⁻	367. 203	C18H12Cl2N2O	Aromatic anilides	WYEMLYFITZORAB-UHFFFAOYSA-N	C1C=1CC(=CC1)C=2C=CC=CC2N=C(O)C3=CC=CC=C3C1
2040	8. 087	286. 1058	arborinine	[M+H] ⁺	286. 10599	C16H15N04	Acridones	ATBZZQPALSPNMF-UHFFFAOYSA-N	O=C1CC2CC3=C(CN4=C3C(OC)=C(OC)C(O)=C13)C
2041	8. 091	223. 16907	KOBUSONE	[M+H] ⁺	223. 16925	C14H22O2	Ketones	UETZJEZFKASPR-UZTWUQPSA-N	O=C1CC2CC2(C)CCC3C1CC3(C)C
2042	8. 093	234. 11253	Euparin	[M+H] ⁺	234. 11246	C13H12O3	Benzofurans	OPUFUNZTKHPZHM-UHFFFAOYSA-N	O=C(C1=CC=CC=C2C(=CC2=C1O)C(=C)C)C
2043	8. 097	397. 21783	Mitragynine	[M-H] ⁻	397. 21329	C23H30N2O4	Alkaloids	LELBFTMXC1IKXX-UHFFFAOYNA-N	CCC1CN2CCC3=C(NC4=C3C(OC)=CC4)C2CC1C(=O)CC(C(=O)C
2044	8. 098	743. 19354	jaceidin	[M+H] ⁺	743. 18933	C18H16O8	6-O-methylated flavonoids	XUWTZJRCPPNJR-UHFFFAOYSA-N	O=C1C(OC)=CC(OC2=CC(O)=C(OC)C(O)=C12)C=CC=CC(O)=C(OC)C3
2045	8. 1	497. 28586	Epoxgedunin	[M-H] ⁻	497. 28519	C28H34O8	Limonoids	AZGNIKZHFJEPJ-FJONONFLSA-N	O=C(OC1CC2C(C(=O)C3OC3C2(C)C4CC5(C)C(OC(=O)C6OC65C14C)C7=CC=C7)C)C1C
2046	8. 104	193. 08611	Butylparaben	[M-H] ⁻	193. 08702	C11H14O3	p-Hydroxybenzoic acid alkyl esters	QFOHBWFCXYLES-UHFFFAOYSA-N	CCCCOC(C1=CC=C(C=C1)O)=O
2047	8. 107	617. 40112	Phorbol-12-Myristate-13-Acetate	[M+H] ⁺	617. 40002	C36H56O8	Phorbol esters	PHEDXBVP1ONIQT-RGYGYFBSA-N	O=C(OC12C(OC(=O)CCCCCCCCC)C(C)C3(O)C(C(=O)CC4(O)C(=O)C(=CC43)C)C1C2(C)C)C
2048	8. 123	419. 32953	(3S,10R,13R,14R,17R)-17-((2R,E)-5,6-dimethylhept-3-en-2-yl)-10,13-dimethyl-2,3,4,9,10,11,12,13,14,15,16,17-dodecahydro-1H-	[M+H] ⁺	419. 32999	C28H44O	Ergosterols and derivatives	DNVPQKSNVMLRS-QRFHLYGJSA-N	OC1CC2C=CC3(CCC4(C)C3CCC4C(C=CC(C)C(C)C)C2(C)CC1
2049	8. 129	308. 22067	Dihydrocapsaicin	[M+H] ⁺	308. 22101	C18H29NO3	Methoxyphenols	XJQPQKLURWNAAH-UHFFFAOYSA-N	OC1=CC=C(C=C1OC)CN=C(O)CCCCC(C)C
2050	8. 142	340. 22595	Propoxyphene	[M+H] ⁺	340. 22711	C22H29NO2	Stilbenes	XLMALTXPSGGQBX-UHFFFAOYNA-N	O=C(OC(C=1C=CC=C1)C(=CC=CC=CC2)C(C)CN(C)C)CC
2051	8. 144	403. 13757	Hexamethylquercetagenin	[M+H] ⁺	403. 138	C21H22O8	7-O-methylated flavonoids	CHXSDBWSFDZEU-UHFFFAOYSA-N	O=C1C(OC)=CC(OC=2C=C(OC)C(OC)=C(OC)C12)C=CC=CC(OC)=C(OC)C3
2052	8. 16	387. 14737	Cetirizine	[M-H] ⁻	387. 1481	C21H25ClN2O3	Diphenylmethanes	ZKLPARSLTMPFCP-UHFFFAOYNA-N	OC(=O)COCN1CN(CCC1)C(C1=CC=CC=C1)C1=CC=C(C1)C=C1
2053	8. 163	322. 20074	Jasmonyl isoleucine	[M-H] ⁻	322. 203	C22H32O8	Trichothecenes	PNKLMTPXERFKEN-UHFFFAOYSA-N	O=C(OC12CC(OC(=O)CC(C)C)C(=CC2OC3C(O)C(O)C1(C)C43OC4)C
2054	8. 164	375. 10617	Casticin	[M+H] ⁺	375. 10745	C19H18O8	7-O-methylated flavonoids	PJQLSMYMKWUJG-UHFFFAOYSA-N	COCC1=C(O)C=C(C=C1)C1=C(OC)C2=C(O)C(OC)=C(OC)C=C2O
2055	8. 167	417. 23776	N-(3-(dimethylamino)propyl)-2-((3,4,8,8-tetramethyl-2-oxo-2,8,9,10-tetrahydroxyranol[2,3-f]chromen-5-yl)oxy)acetamide	[M+H] ⁺	417. 23801	C23H32N2O5	Angular pyranocoumarins	SYJCVRCHBPLGHM-UHFFFAOYSA-N	O=C1OC2=C(C(OC(=O)N)NCCCN(C)C)=CC=3OC(C(C)CCC2C)C(=C1C)C
2056	8. 18	385. 20999	Corynoxine	[M+H] ⁺	385. 20999	C22H28N2O4	Indolizidines	DAXYLDFNWXHGB-RCFOJTTRSA-N	O=C(OC)C(=COC)C1CC2N(CCC2C(=O)NC=4C=CC=CC4)CC1CC
2057	8. 181	286. 20013	Viridiflorine	[M+H] ⁺	286. 20129	C15H27NO4	Pyrrrolizidines	WQSRLRZOVFVJH-ABHRYQDASA-N	CC(C)[C-](O)([C=H])C(O)C(=O)OC[C@H]1CN2NCCC[C@H]12
2058	8. 182	400. 23981	Karacoline	[M+H] ⁺	400. 23999	C22H35NO4	Aconitane-type diterpenoid alkaloids	HKQZUYOVMYOFT-JEJCSOMWSA-N	OC1CC2(C)CN(CCC)C3C4CC2C1C=CC5C6C(O)C5C4(O)CC6OC
2059	8. 192	376. 03693	Pesticide4_Prochloraz_C15H16Cl3N3O2	[M+H] ⁺	376. 03799	C15H16Cl3N3O2	Phenol ethers	TVLSRXXTLMFWEO-UHFFFAOYSA-N	O=C(N1C=NC=C1)N(CCOC=2C(C1)=CC(C1)=CC2C1)CCC
2060	8. 204	589. 16992	genipin 1-gentiobioside	[M+H] ⁺	589. 16925	C23H34O15	Iridoid O-glycosides	FYZXYLPBWLGI-AUOPOVQUSA-N	O=C(OC)C1=CC(OC2OC(COC3OC(CO)C(O)C(O)C3O)C(O)C(O)C2O)C4C(=CC4)CO
2061	8. 213	827. 25452	2-[[[4-[4,6-dihydroxy-3-(3-methylbut-2-enyl)-2-[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyphenyl]-3-hydroxy-2-(4-hydroxyphenyl)-5-	[M+H] ⁺	827. 25208	C39H48O18	Flavonoid-7-O-glycosides	GQOCHOCFYNMUJ-UHFFFAOYSA-N	OC1=CC=C(C=C1)C2OC=CC(OC4OC(CO)C(O)C4O)C=C(OC)C3(C(=C5C)C=CC(O)=C(C5OC6OC(CO)C(O)C6O)C=C(C)C)C2O
2062	8. 227	505. 27747	Tonantzitlolone B	[M+H] ⁺	505. 28101	C28H42O9	Fatty acid esters	BKJAMMLKHPQMJI-SMKITLBYSA-N	O=C(OC1C(OC2OC1(O)C(O)C3(OC(C3)C(=CC(=O)C)C(C)C)C(=C(C)C)C(OC(=O)C)C

2063	8.245	281.09052	4-hydroxy-1'-methylspiro[benzo[e][1,3]oxazine-2,3'-indolin]-2'-one	[M+H] ⁺	281.09	C16H12N2O3	Benzoxazines	OZPNYAHEDUKMPF-UHFFFAOYSA-N	O=C1N(C(=2C=CC=C2C31N=C(O)C(=4C=CC=CC4O3)C
2064	8.256	384.15884	Meropenem	[M+H] ⁺	384.159	C17H25N3O5S	Thienamycins	DMJNNHOUXLYBY-UHFFFAOYSA-N	O=C(O)C1=C(SC2CNC(C(=O)N(C)C)C2)C(C)C31C(=O)C3C(O)C
2065	8.258	578.31488	(2S,3R)-2-(1-((S)-2-(tert-butoxycarbonyl)-1,2,3,4-tetrahydroisoquinoline-3-carbonyl)-4-phenylpiperidine-3-carboxamido)-3-methylpentanoic acid	[M+H] ⁺	578.32001	C33H43N3O6	Hybrid peptides	NBWLCAFFGQXOGJ-ILRLXPBVS-N	O=C(OC(C)(C)O)N1C=2C=CC=C2C1C(=O)N3CCC(C(=O)NC(C(=O)O)(C)C)C(C(=4C=CC=CC4)C)C
2066	8.258	306.27872	[(1R,5R,9S,13S)-5,9,13-trimethyltetraacyclo[11.2.1.0 ^{9,2} .0 ^{2,9}]hexadec-14-en-5-yl]methanol	[M+H] ⁺	306.27911	C20H32O	Diterpenoids	C1GQQQTZIDQQR-SGWMQEPOSA-N	OC(C1)CCCC(C)C3CCC4(C=C/C3)C(CCC12)C4)C
2067	8.258	583.2702	4-((11aS)-1,3-dioxo-5-(p-tolyl)-11,11a-dihydro-1H-imidazo[1',5':1,6]pyrido[3,4-b]indol-2(3H,5H,6H)-yl)-N-(4-phenylbutan-2-	[M+H] ⁺	583.27002	C37H34N4O3	Beta carbolines	VIMCLONZOXFDPI-QPQITGAISA-N	O=C(NC(C)CCC=1C=CC=C1)C2=CC=C(C=C2)N3C(=O)N4C(C5=CC=C(C(=5)C)C=C6NC=7C=CC=C7C6)C4C3O
2068	8.258	306.16904	Anisodamine	[M+H] ⁺	306.17001	C17H23NO4	Tropane alkaloids	WTQYWNWRJXNDEG-UHFFFAOYSA-N	O=C(OC1CC2N(C)C(C1)C(O)C2)C(C=3C=CC=C3)CO
2069	8.26	323.18753	calopocarpin	[M-H] ⁻	323.19284	C20H20O4	Pterocarpan	CYXCYFWIZXENQ-JXKFEZNVSA-N	OC1=CC=C2C(OC3C4=CC(=O)C=C4CC23)CC=C(C)C=C1
2070	8.267	461.24326	7-(3,4-dihydroxyphenyl)-1-(4-hydroxyphenyl)-5-[(2S,3R,4S,5R)-3,4,5-trihydroxyoxan-2-yl]oxhexan-3-one	[M-H] ⁻	461.2435	C24H30O9	Linear diarylheptanoids	KQLSXWIDDTWR-WUOZLOAJSA-N	O=C(CCC1=CC=C(O)C=C1)CC(OC2CCC(O)C(O)C2)CCC3=CC=C(O)C(O)=C3
2071	8.276	267.14206	3,6-diphenylcyclohexane-1,2-diol	[M-H] ⁻	267.13904	C18H20O2	Cyclohexanols	KIDYUEHQXIEBKG-UHFFFAOYSA-N	OC1C(O)C(C=2C=CC=CC2)CCC1C=3C=CC=CC3
2072	8.284	527.45996	N-lignoceroyl-5-hydroxytryptamide	[M+H] ⁺	527.45801	C34H58N2O2	Long-chain N-acylserotonins	QLZQXTNKCAWVES-UHFFFAOYSA-N	O=C(NCCC1=CNC=2C=CC(O)=CC21)CCCCCCCCCCCCCCCCCCCC
2073	8.284	635.4093	O-glucopyranosylepideragenin, 28-	[M+H] ⁺	635.40997	C36H58O9	Triterpene saponins	WJMBWVSQAPLFO-DLQTVUGOSA-N	O=C(OC1OC(C)C(O)C(O)C1O)C23OC(C)(C)C3C4=CC5CC(C)CC(C)C(O)C(O)C6OC7C(C)C4(C)C72
2074	8.284	165.09103	Phenethylacetate	[M+H] ⁺	165.091	C10H12O2	Benzene and substituted derivatives	MDHYEMXUFSJLGV-UHFFFAOYSA-N	O=C(OC(=1C=CC=CC1)C
2075	8.303	485.2753	MGMG 16:3	[M-H] ⁻	485.27411	C25H42O9	Lipids	LJJVATEJUGJSPWF-UHFFFAOYNA-N	O=C(OC(CO)COC1OC(CO)C(O)C1(O))C3CCCC=CC=CCO=CCO
2076	8.326	511.15887	(2R,3S,4S,5R,6S)-2-[[[(2R,3R,4R)-3,4,4-dihydroxy-4-(hydroxymethyl)oxolan-2-yl]oxymethyl]-6-[4-hydroxy-3-(3-methylbut-2-en-1-yl)phenoxyl]oxane-3,4,5-triol	[M+H] ⁺	511.15762	C22H32O11	Phenolic glycosides	UEAATLPMPTZOFF-PYEGHPNJS-A-N	OC1=CC=C(OC2OC(CO3CCC(O)(CO)C3O)C(O)C2O)CC1C=CC=C(C)C
2077	8.331	243.15901	(5E)-3,4,9-trihydroxy-2-propyl-2,3,4,7,8,9-hexahydrooxecin-10-one	[M-H] ⁻	243.15417	C12H20O5	Oxocins	KQJGPGHQDZVJH-ZZXKWFJSA-N	O=C1OC(CCC(C)C(O)C(O)C=CCCC1O
2078	8.332	529.31622	(2S,3R,5S,9R)-2,3-dihydroxy-14-(hydroxymethyl)-5,9-dimethyl-14-[[[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-	[M-H] ⁻	529.31628	C26H42O11	Diterpene glycosides	QUCCBQWLVOVBR-BBJJSLPGSA-N	O=C(O)C1(C)CCCC2(C)C3OC4OC3(CO4)OC5OC(C)(O)C(O)C5O)CO(CO)C(O)C12
2079	8.333	313.1467	Clomipramine	[M-H] ⁻	313.14771	C19H23ClN2	Dibenzazepines	GDL1GK1OYRNDHA-UHFFFAOYSA-N	C1C1=CC=C2C(=C1)N(C=3C=CC=CC3CC2)CCCN(C)C
2080	8.35	582.25183	Tricoumaroyl spermidine	[M-H] ⁻	582.25781	C34H37N3O6	Coumaric acid and derivatives	PFDFWJCSQYDMZ-UHFFFAOYSA-N	O=C(C=C(C1=CC=C(O)C=C1)NCCC(N(C)=O)C=CC2=CC(O)C=C2)CCC(NC(=O)C=C3C=CC=C(O)C=C3
2081	8.352	343.08032	Coptisine	[M+H] ⁺	343.07999	C19H14NO4+	Protoberberine alkaloids and derivatives	XYHOBMEDLZIMP-UHFFFAOYSA-N	O1C=2C=CC3=CC=4C5=CC=6OCOC6=C5CC[N+](=4)C=C3CC2O1
2082	8.354	304.15405	Cetraxate	[M-H] ⁻	304.15543	C17H23NO4	Phenylpropanoic acids	FHRSHSOEWXUORL-UHFFFAOYSA-N	O=C(O)CCC1=C=C(OC(=O)C2CCC(CN)CC2)C=C1
2083	8.358	310.27383	Bentyl	[M+H] ⁺	310.27399	C19H35NO2	Carboxylic acid esters	CURUTKGFNZGFE-UHFFFAOYSA-N	O=C(OC(CN)CC(CO)C1(OC(=O)C1)C2CCCCC2
2084	8.366	356.27881	Aphidicolin	[M+H] ⁺	356.27951	C20H34O4	Aphidicolane and steroidane diterpenoids	NOFOAYPPHUXJR-APNQZ1XSA-N	OC(C1)CC2CC3C1CC3CCC4(C)(CO)C(O)CC42C
2085	8.393	230.24718	N,N-Dimethyldecylamine N-oxide	[M+H] ⁺	230.24785	C14H31NO	Long-chain alkyl amine oxides	SYELZBGXA1XKHU-UHFFFAOYSA-N	CCCCCCCCCCCC(C)(C)=O
2086									

2106	8.688	425.37234	17 (21)-Hopen-6-one	[M+H] ⁺	425.37201	C30H480	Hopanoids	OZFAGHUNGAZEMO-VKNUIDEPSA-N	O=C1CC2(C)C(CCC3C4(C(=C(C(C4)C(C)C)CC3C2(C)C5(C)CCCC(C)1)C(C15
2107	8.709	298.09604	5'-Methylthiadenosine	[M+H] ⁺	298.09683	C11H15N5O3S	5'-deoxy-5'-thionucleosides	WUUGPSXJNOTRMR-UHFFFAOYNA-N	OC1C(O)C(OC1N2C=NC=3C(=NC=NC32)N)CSC
2108	8.72	252.13965	(E)-3-phenyl-N-(2-phenylethyl)prop-2-enamide	[M+H] ⁺	252.13829	C17H17N0	Cinnamic acid amides	BOSUEWCNVFBGV-VAWYSNFS-A-N	OC(=NCCC=1C=CC=CC1)C=C=CC=CC=CC2
2109	8.733	343.08133	5,7-dihydroxy-3,6-dimethoxy-2-(4-methoxyphenyl)-4H-chromen-4-one	[M-H] ⁻	343.08099	C18H16O7	6-O-methylated flavonoids	DWZAJFEYZI1HFO-UHFFFAOYSA-N	O=C1C(OC)=C(OC2=CC(O)=C(C(OC)C(O)=C12)C=3C=CC(OC)=CC3
2110	8.733	285.12445	Brazilin	[M-H] ⁻	285.11926	C16H14O5	l-benzopyrans	UWHUTZOC7ZJUK-JKSUJKBHSA-N	OC1=CC=C2C(OC3(C)CC4=CC(O)=C(O)C=C4C3)C=C1
2111	8.768	187.13326	10-Hydroxydecanoic acid	[M-H] ⁻	187.13397	C10H20O3	Medium-chain hydroxy acids and derivatives	YJCJVMMDTBEITC-UHFFFAOYSA-N	O=C(O)CCCCCCCCO
2112	8.771	282.15103	N-normuifeirine	[M+H] ⁺	282.14999	C18H19NO2	Aporphines	QKQAHDMMPQAC-UHFFFAOYSA-N	O(C=1C=C2C3=C(C1OC)C4=C=CC=C4CC3NCC2)C
2113	8.783	633.40021	Echinocystic acid-3-O-glucoside	[M-H] ⁻	633.40082	C36H58O9	Triterpene saponins	WYDPEADEZMKNM-UHFFFAOYNA-N	CC1(C)CC2(C)CC3(C)C(=CCC4C5(C)CC(C6OC(C)C(O)C(C)C6O)C(C)C(C5CCC34C)C2C1)C(O)=O
2114	8.784	559.30896	MGMG 18:3	[M-H] ⁻	559.31073	C27H46O9	Lipids	HUS1SCNTLUEZCN-UHFFFAOYNA-N	O=C(OC(C)COC1OC(CO)C(O)C(C)O)CCCCCCCC=CC=CCC=CCC
2115	8.786	346.3306	icos-19-ene-1,2,4-triol	[M+H] ⁺	346.33154	C20H40O3	Long-chain fatty alcohols	QVLYXPULBQ7JW-UHFFFAOYSA-N	CCC(O)CC(O)CCCCCCCCCCCCC=C
2116	8.791	561.32367	(2S,3R,4S,5S,6R)-2-[4-[[[(3S,4R,5S)-3-hydroxy-5-(4-hydroxy-3-methoxyphenyl)-4-(hydroxymethyl)oxolan-3-yl]methyl]-2-methoxyphenoxy]-6-	[M+H] ⁺	561.32379	C26H34O12	Lignan glycosides	SGXSYHDLSPXCM-CTQXEDXS-A-N	OC1=CC=C(C=CC1OC)C2OC(C)C(C3=C(C=C(C4OC4O)C(C)C(O)C4O)1)C(O)=C3C2O
2117	8.795	287.18497	2-decyl-3-hydroxypentanedioic acid	[M-H] ⁻	287.1864	C15H28O5	Long-chain fatty acids	KOLGVIQEZBW1Q-UHFFFAOYSA-N	O=C(O)CC(O)C(C)C(=O)O)CCCCCCCC
2118	8.825	765.44208	Cauloside C (3-Glu(1-2)Ara Hederagenin) (NMR)	[M-H] ⁻	765.44305	C41H66O13	Triterpenoids	BRQGRHRLVQSG-UUWFFIQNSA-N	CC1(C)CC[C@]2(CC[C@]3(C)C(=CC[C@H]4[C@]5[C@]C(C)[C@H](O)C=C4)C(C)[C@H](O)C=C1)C(C)[C@H](O)C=C1
2119	8.825	438.34378	tomatidine	[M+H] ⁺	438.34	C27H45NO2	Spirostanes and derivatives	XYNPHXGMVJBLV-JYAGXCGRSA-N	OC1CCC2(C)C(CCC3C2CC4(C)C3CC5OC6(NOC(C)C6)C(C)C5)C1(C)C
2120	8.835	302.17462	Dobutamine	[M+H] ⁺	302.17508	C18H23NO3	Catecholamines and derivatives	JRWZLRBJNMZMF-UHFFFAOYNA-N	CC(CCC1=CC=C(O)C=C1)NCC1=CC(O)=C(O)C=C1
2121	8.859	179.10637	(4-methylcyclohex-3-ene-1,1-diyl)dimethanol	[M+H] ⁺	179.10001	C9H16O2	Primary alcohols	JTRLVUONADOHI-UHFFFAOYSA-N	OC(C)C(OC)CC(C)CC1
2122	8.859	359.11212	5-hydroxy-3,6,7-trimethoxy-2-(4-methoxyphenyl)-4H-chromen-4-one	[M+H] ⁺	359.112	C19H18O7	7-O-methylated flavonoids	ADNCMDZHONBR-UHFFFAOYSA-N	O=C1C(OC)=C(OC2=CC(OC)C(OC)=C(O)C12)C=3C=CC(OC)=CC3
2123	8.866	453.34576	Boldenone Undecylenate	[M+H] ⁺	453.33633	C30H44O3	Steroid esters	ADMSNQOPMLSX-KEZAGTACSA-N	CC12CC[C@H]3C(CCC4=C(C)C=CC43)[C@H]1CC[C@H]2OC(=O)CCCCCCC=
2124	8.904	297.1116	[(2E)-2-hexa-2,4-diynylidene-1,6-dioxaspiro[4.4]nona-3,7-dien-9-yl] 3-methylbut-2-enoate	[M+H] ⁺	297.11212	C18H16O4	Fatty acid esters	VJOI1YQDMELSH-OVCL1PMQSA-N	O=C(OC1C=CC21OC(=CC=CC=C2)C=C2)C(C)C
2125	8.957	519.2373	neoandrographolide	[M+H] ⁺	519.23547	C26H40O8	Diterpene glycosides	YGCYRQKJYQXHG-RNQFMQVSA-N	O=C1OCC=C1CC2C(=C)CCC3C(C)C(C4OC(CO)C(C)C4O)CCCC2O
2126	8.958	547.34485	N-[5-[[4-[4-(acetyl(hydroxy)amino)butylamino]-4-oxobutanoyl]-hydroxylaminomethyl]-N''-(5-aminononyl)-N'-hydroxybutanediamide	[M+H] ⁺	547.34497	C24H46N6O8	N-acyl amines	GUZJCKBQAGXGH-UHFFFAOYSA-N	O=C(N(O)CCCCN(C)O)CCC(=O)N(O)CCCCN=C(O)CCC(=O)N(O)CCC(CO)C
2127	8.968	373.12799	Isoisinenetin	[M+H] ⁺	373.12799	C20H20O7	8-O-methylated flavonoids	UYCWETUOAG7IL-UHFFFAOYSA-N	O=C1C=C(OC=2C(OC)=C(OC)C(OC)C12)C=3C=CC(OC)=C(OC)C3
2128	8.974	343.08334	Eupatilin	[M-H] ⁻	343.08234	C18H16O7	6-O-methylated flavonoids	DRRWBCNQKKOL-UHFFFAOYSA-N	COCl=CC=C(C=C1OC)C1=CC(=O)C2=C(O)C(OC)=C(O)C=C2O1
2129	8.974	353.23441	Prostaglandin E1	[M-H] ⁻	353.23334	C20H34O5	Prostaglandins and related compounds	GMVPFGQO1O1MI-UHFFFAOYNA-N	O=C(O)CCCCCCC1C(=O)CC(O)C1C=CC(OC)CCCC
2130	8.984	301.21802	dehydroabietic acid	[M+H] ⁺	301.21701	C20H28O2			

[illegible]

[illegible]

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[illegible]

[illegible]

[illegible]

2407	12.593	427.38852	3-Epilupeol	[M+H] ⁺	427.39343	C30H500	Triterpenoids	MQXYUHLBZPQQO-1SZJTHHZA-S-N	OC1CCC(C)(C)CCC3(C)C2CC4C5C(C(=C)C)CC5(C)CCC43C(C1(C)=O)
2408	12.613	409.23532	beta-TOXICAROL	[M-H] ⁻	409.23636	C23H2207	Rotenones	MTTUVGLGBORBP1-UHFFFAOYSA-N	O=C1C=C(C)OC3CC4=CC(OC)=C(O)C(=C)C13C=C5OC(C=C5=C2O)(C)C
2409	12.622	249.14821	2-[(2S,4aR,8aS)-2-hydroxy-4a-methyl-8-methylidene-3,4,5,6,7,8a-hexahydro-1H-naphthalen-2-yl]non-2-enoic acid	[M-H] ⁻	249.14961	C15H2203	Eudesmane, isoeudesmane or cycloeudesmane	WQMBGCHXXVLQTE-CFVMTHKISA-N	O=C(O)C(=O)C1(O)CC2(C)CCCC(=O)C2C1
2410	12.637	277.14157	3,7-Epoxyxycaryophyllan-6-ol	[M+2H] ²⁺	277.14157	C15H2602	Oxepanes	KSMZUKWIDPCGBS-UHFFFAOYSA-N	OC1CCC2(OC1(C)CCC3C2CC3(C)C)C
2411	12.648	499.25668	Lucidenic acid C	[M+H] ⁺	499.26001	C27H4007	Triterpenoids	X1MQDJNNEMWDH-VHPIRQCPISA-N	O=C(O)CCC(C)C1CC(=O)C2(C3=C(C(=O)C(O)C12C)C4(C)CCC(O)C(C)C4C30)C
2412	12.653	247.64191	Imatinib Mesylate	[M+2H] ²⁺	247.63699	C30H35N7O4S	Benzanilides	YLMAHNUQAMNNX-UHFFFAOYSA-N	O=C(NC1=CC=C(C(=C1)NC=2N=CC=C(N2)C3=CN=CC(=C3)C4=CC=C(C=C4)CN5C(N)C(C5)=S(=O)=O)C
2413	12.655	462.09622	7-Methylthioheptyl glucosinolate	[M-H] ⁻	462.09317	C15H29N09S3	Alkylglucosinolates	SHJVBSHKTUXLG-MFRQQAQSA-N	CSCCCCCVC(C(S(C[H])10(C[H])(CO)1(C[H])(O)1(C[H])10)=N(S(=O)(=O)2O)4)C
2414	12.662	517.22748	Angeloylgomisins H	[M+H] ⁺	517.22394	C28H3608	Hydrolyzable tannins	ZSAUXCVJDVCLRS-XSRHQFTISA-N	O=C(OC1=C(OC)C(OC)=C2(C3=C(C(OC)C(OC)=C(OC)C=C3C(OC)C(C)C2)C(=O)C
2415	12.68	134.04462	L-Aspartic acid	[M+H] ⁺	134.04478	C4H7N04	Aspartic acid and derivatives	CKLJMWJ2IHZCS-REOHLBHS-A-N	C(C(=H)C(=O)O)N(C(=O)O)
2416	12.69	277.1413	3-hydroxy-1a,5-bis(hydroxymethyl)-5,6b-dimethyl-1,3,3a,4,6,6a-hexahydrocyclopropan[c]inden-2-one	[M+2H] ²⁺	277.14102	C14H2204	Cyclic alcohols and derivatives	CUAPOUHDJKWLB-UHFFFAOYSA-N	O=C1C(O)C2CC(C)(CO)CC2C3(C)CC13CO
2417	12.696	347.22128	2-[4a-methyl-8-methylidene-4-(3-methylpentanoyloxy)-1,2,3,4,5,6,7,8a-octahydronaphthalen-2-yl]non-2-enoic acid	[M-H] ⁻	347.22278	C21H3204	Eudesmane, isoeudesmane or cycloeudesmane	QVSFEQJQPOHP-UHFFFAOYSA-N	O=C(O)C(=O)C(=O)C1CC(OC(=O)CC(C)C)C2(C)CCCC(=O)C2C1
2418	12.698	519.32819	(2E,4E)-1-[(1R,3S,8R,10S,14S)-12-[(2E,4E)-hexa-2,4-dienoyl]-1,6,8,13-tetrahydroxy-3,7,10,14-tetramethyl-2,9-	[M+H] ⁺	519.32812	C28H3208	Oxepanes	VATYWO1GRKMMCM-QHSDNFTQSA-N	O=C(C(=O)CC)C1C(=O)C2(C3C(C(=O)C=CC(=O)C(=O)C4(C)C1C5(C)C4(C)C3)C(C5)O)C
2419	12.699	499.25378	(3E,5S,7R,8R,11E,13S,15R,16R)-3,5,7,11,13,15-hexamethyl-8,16-bis(1,3-oxazol-5-ylmethyl)-1,9-dioxacyclohexadeca-3,11-diene-2,10-dione	[M+H] ⁺	499.25061	C28H38N2O6	Macrolides and analogues	LAJRJVLDAKYLGO-FQSDNCTISA-N	O=C1OC(C=C2OC=NC2)C(C)CC(C(=O)C(=O)C(=O)C(=O)C(=O)C(C)CC(C(=O)C)C(C)C
2420	12.7	443.26395	Strophanthidin	[M+2H] ²⁺	443.25845	C23H3206	Cardenolides and derivatives	ODJLBQGV1NUJMM-HXZDTFASAA-N	O=CC12CCC(O)CC2(O)CCC3C1CCC4(C)C(C5=CC(=O)OC5)CCC34O
2421	12.701	451.26227	Repaglinide	[M-H] ⁻	451.26022	C27H36N2O4	Phenylpiperidines	FAEKWTJYAMJFK-UHFFFAOYNA-N	O=C(O)C1=CC=C(C(=C1)CC)CC(O)C(C(=O)C2C(=O)C(=O)C(=O)C2)CC(C)C
2422	12.708	458.97763	Pesticide3_Hexaflumuron_C16H8C12F6N2O3	[M-H] ⁻	458.97501	C16H8C12F6N2O3	N-benzoyl-N'-phenylureas	RGNPBRKPHBKXN-UHFFFAOYSA-N	O=C(NC(=O)C(=O)C(F)=CC(=O)F)N2=CC(C1)=C(OC(F)F)C(F)F(C)C1)=O
2423	12.719	499.33569	Poricoic acid A	[M+H] ⁺	499.34	C31H4605	Triterpenoids	KYAQLXUMUEKGR-SMFZJLCSA-N	O=C(O)CCC1(C2=CC3(C)C(C)C(C)C3(C2=CCC1C(=O)C)C(C)C(=O)C(=O)CCC(=O)C(C)C
2424	12.721	471.22241	(2R,3S,4S,5R,6R)-2-[[[2(R,3R,4R,5S)-3,4-dihydroxy-5-(hydroxymethyl)oxolan-2-yl]oxymethyl]-6-[(2E)-3,7-dimethylocta-2,6-dienoxyloxa-3,4,5-triol	[M+H] ⁺	471.22006	C21H36010	Terpene glycosides	AWDKYYAAQLEFP-XRSPUIAFSA-N	OC11OC(OC2OC(OC=C(C)CCC=C(C)C)C(O)C(O)C2O)C(O)C1O
2425	12.721	258.12772	Telmisartan (Micardis)	[M+H] ⁺	258.12601	C33H30N4O2	Biphenyls and derivatives	RMMXLNWKUUMAY-UHFFFAOYSA-N	O=C(O)C(=O)C(=O)C(=O)C1=CC(=O)C2(C3C4=CC(=O)C(=O)C4=CC(=O)C3)C(C)C1C
2426	12.748	621.43817	Ginsenoside compound K	[M-H] ⁻	621.43719	C36H6208	Triterpenoids	FVJZARNDLYOMSU-UHFFFAOYNA-N	CC(C)=CCCC(C)(OC1OC(CO)C(O)C1O)C1OC2(C)C1C(O)CC1C3(C)C(CCC(O)C(C)C3)C2C1C
2427	12.752	333.27866	(1R,2R,4aS,8aS)-1-((S)-3-hydroxy-3-methylpentyl)-2,5,5,8a-tetramethyl-8,9-dihydro-1H-naphthalen-2-ol	[M+H] ⁺	333.28	C20H3802	Diterpenes	VWPNQCLIQCRGC-HHUQCJWSA-N	OC(C)(CC)CCC1(O)C(OC)C2(C)(C)CCCC12C
2428	12.771	515.31677	2-hydroxy-3-[(1R,3S,4S,5R,6R)-2-hydroxy-5-(hydroxymethyl)oxolan-						

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2493	13.815	438.05661	(2R)-2-Hydroxy-2-phenethylglucosinolate	[M-H]-	438.05341	C15H21NO10S2	Glucosinolates	GAPDDBFHNHZIS-UHFFFAOYNA-N	OC[C@]1(SO(C(C(CO)C2=C(CO)C=C2)=NOS(O)(=O)=O)(C(O)C(O)C1O
2494	13.823	335.14978	Pyrenophorol	[M-H]+	335.14999	C16H24O6	Macrolides and analogues	RBQNDQKFC1JGL-UTBFYLPBSA-N	O=C1OC(C)CCC(O)C=CC(=O)OC(C)CCC(O)C=C1
2495	13.825	471.2706	Ingenol-5,20-acetonide-3-O-angetate	[M-H]+	471.26999	C28H38O6	Fatty acid esters	STFFIQUHWFISBB-RKHHLFRASA-N	O=C(OC1C(=C(C2C3(=O)C(C=C(C4OC(OC412O)(C)C)C5C(C3C3)C5(C)C)C)C(=C(CO)C
2496	13.831	403.26736	ascochlorin	[M-H]-	403.26532	C23H29C104	Hydroxybenzaldehydes	SETVRSKZJJWOPA-FLDGXSQCSA-N	O=C1C(=O)C(C(=C(O)C(C1)=C1)C)CO=C(C(=CC2(C)C(=O)CCC2)C)C
2497	13.839	277.21613	a-Linolenic acid (NMR)	[M-H]-	277.21732	C18H30O2	Linoleic acids and derivatives	DTSISQBPPRVQHS-PBXOOCHISA-N	CC\C=C/C\C=C/C\C=C/C\CCCCCCCC(O)=O
2498	13.853	751.46173	alpha-Hederin	[M-H]+	751.46271	C41H66O12	Triterpenoids	KEOITPILCOILGM-UHFFFAOYNA-N	CC1OC(OC2(C)(O)C)OC2OC2CC3(C)C(OC4(C)C3OC=C3C5OC(C)(C)CCC5(CCC43C)C(O)=O)C2(C)OC(C)(O)C(C)C1O
2499	13.871	381.29797	2,3-dihydroxypropyl stearate	[M-H]+	381.29999	C21H42O4	l-monoacylglycerols	VBICXKHEKHSIBG-FQEVSJTJZA-N	O=C(OCC(O)(O)O)CCCCCCCCCCCCCCCCCC
2500	13.884	280.16101	Schinifoline	[M-H]+	280.16	C17H23NO	Hydroquinonoles	HCUSLQJBQAQC-BUHFFFAOYSA-N	O=C1C=C(N(C=2C=CC=C12))CCCCCCC
2501	13.896	507.27579	(2E,4E)-1-[(2R,6S,14S,22S,25R)-25-(3,3-dimethyloxiran-2-yl)-15-methyl-1,3,13,15-	[M-H]-	507.27655	C32H36NaO2	Alpha carbolines	XZF5MUXYAYCHO-QREHLEPSA-N	O=C(C(=CC=C)N1CCCC23C4OC(=CC4N5NC6=CC=CC7=C6S3CCN(C7C7R8OC)C(C1)2)C
2502	13.905	417.29654	6-[[[5-(hydroxymethyl)-2,5,8a-trimethyl-1,4,4a,6,7,8-hexahydronaphthalen-1-yl]methyl]-3-methylidene-7-oxabicyclo[4.1.0]heptane-2,4,5-triol	[M-H]+	417.29257	C22H34O5	Oxepanes	GYERARYFYBXXO-UHFFFAOYSA-N	OC[C@](C)(CCCC(C)C)C(C(=C(CC12)C)C3C4OC4(O)C(=C)C(O)C3O
2503	13.92	581.30774	Isocucurbitacin B	[M-H]+	581.30902	C32H46O8	Cucurbitacins	WTBZNVRBNJWSFP-OUKQBFQZSA-N	O=C(O)C(=C(O)C(O)C(C)C1C(O)C2(C)C3OC=C4C(C(=O)C(O)C(C)C4(C)C)C3(C)C(=O)C12C)C(C)C(C)C
2504	13.93	542.16547	Doxorubicin	[M-H]-	542.16681	C27H29NO11	Anthracyclines	AOJJ5UZOXBQZNB-DIHIFYAZSA-N	O=C1C=2C=C=C(CO)C2C(=O)C=3C(O)=C4C(=C(O)C13)CC(O)C(C(=O)C)CC4OC5OC(C)C(O)(N)C5
2505	13.937	691.43793	MONENSIN SODIUM (monensin A is shown)	[M-H]+	691.43915	C37H63NaO10	Ketals	GYPNBQSUNTBSD-DUDHYVAZSA-M	[Na+].[O-]C([O-])C(C)C(OC)C(C)C1OC2(OC(C)C2)C3OC(C)C(C)C3C4OC(C4C)C
2506	13.94	278.14941	cyclo(tyrosyl-propyl)	[M+2H]2+	278.1499	C14H16N2O3	Alpha amino acids and derivatives	LSGOTAXPMUCUK-UHFFFAOYSA-N	O=C1N2CCCC2(O)=NC1C3C=CC(O)C(O)=C3
2507	13.943	250.02029	Clothianidin	[M-H]+	250.01601	C6H8ClN5O2S	2,5-disubstituted thiazoles	PGOOBECOWQEB-UHFFFAOYSA-N	CN=C(NC1=CN(C)C1S)NN(=O)=O
2508	13.949	281.24762	Trans-Vaccenic acid	[M-H]-	281.2486	C18H34O2	Long-chain fatty acids	UWHZ1QPFPDPJM-BQVQJAHWSA-N	CCCCC/C=C\CCCCCCCC(O)=O
2509	13.954	511.21042	Flemphilippinin A	[M-H]+	511.20999	C30H32O6	6-prenylated isoflavanonones	VBTMMYSEYFPKP-UHFFFAOYSA-N	O=C1C(=COC=2C1=C(O)C=3C=C(C(OC3C2OC=C(C)C)C(C)C(=C(C)C)C)C(=C(C)C)C(=C(C)C)C
2510	13.957	577.44592	Daucosterol;Sitogluside	[M-H]+	577.44702	C35H60O6	Stigmastanes and derivatives	NPJCTIMALKLTFW-OFUAXYQCSA-N	OC1CC(OC2OC3=CC4C(CCC5(C)C(CCC45)C(C)CCC(C)C(C)C)C3(C)C2)C(C)C(O)C1O
2511	13.959	529.34937	Gymnemenin	[M-H]+	529.34998	C30H50O6	Triterpenoids	VKJLHZPVYLJKG-ABHXHSUSA-N	OC[C@](C)C(OC)C2(C)C3OC=C4C5OC(C)C(C)C(O)C(C)C5(CO)C(O)C(C4)C3(C)C(C)C12
2512	13.96	269.14359	4-benzyl-7-hydroxy-1-hydroxymethyl-3,5,6,7-tetrahydro-8h-pyrrolizinium	[M-H]+	269.14001	C15H20NO2+	Alkaloids and derivatives	MPDVGSUYGBLA-ARHFVFGLSA-N	OC[C@]1CN1J2(CC=3C=CC=C3)CCC(O)C12
2513	13.97	439.30093	(2E,4E,6E,8E,10E,12E,14E,16E)-2,6,11,15-tetramethyl-17-(2,6,6,6-trimethyl-1-cyclohexen-1-yl)-2,4,6,8,10,12,14,16-octadecaacetanilal	[M-H]+	439.29999	C30H40O	Triterpenoids	DFWMFLMMAQZH-DOKBYWTLISA-N	O=CC(=CC(CO)C(=CC(CO)C(C(=CC(CO)C(C(=CC(CO)C(C)C)C
2514	13.971	338.27582	5-(1,2,4a,5-tetramethyl-7-oxo-3,4,8,8a-tetrahydro-2H-naphthalen-1-yl)-3-methylnonanonic acid	[M-H]+	338.26895	C20H32O3	Colansene and clerodane diterpenoids	RNWJUFUZQBBLK-UHFFFAOYSA-N	O=C(O)C(C)CC(C)C(C)C(C)CC2(C(=CC(O)C)CC2)C
2515	13.972	231.02675	D-(-)-quinic acid	[M-H]+	231.02655	C7H12O6	Quinic acids and derivatives	AAWZDTNLSGCEK-LNVDRNJUSA-N	O=C(O)C1(C)CC(O)C(O)C(O)C1
2516	14.043	497.35797	Soyasapogenol A	[M-H]+	497.35999	C30H50O4	Triterpenoids	CDWRAYFUPQLRZ-UHFFFAOYSA-N	OC[C@](C)C(OC)CC2(C)C1CC3(C)C2CC=C4C5OC(C)C(O)C(C)C5(C)CC43C
2517	14.067	595.25153	6-(furan-3-yl)-12,16,21-trihydroxy-7,15-dimethyl-9-oxo-3,17,19-trioxahentacyclo[9.9.3.0]2,9.						

2536	14.413	421.27527	3-[(7S,8S)-5-hydroxy-2,2,1,8-tetramethyl-6-oxo-7,8-dihydroprano[3,2-b]chromen-10-yl]-3,4-dihydrobenzoic acid	[M-H] ⁻	421.27563	C25H2606	Pyranochromenes	CEJSHVIZUAMEQY-CBVZESEGA-N	O=C(O)CC(C=C(C=CC1)C=C(C2=C(C3=C(C4=C(C5=C(C6=C(C7=C(C8=C(C9=C(C10=C(C11=C(C12=C(C13=C(C14=C(C15=C(C16=C(C17=C(C18=C(C19=C(C20=C(C21=C(C22=C(C23=C(C24=C(C25=C(C26=C(C27=C(C28=C(C29=C(C30=C(C31=C(C32=C(C33=C(C34=C(C35=C(C36=C(C37=C(C38=C(C39=C(C40=C(C41=C(C42=C(C43=C(C44=C(C45=C(C46=C(C47=C(C48=C(C49=C(C50=C(C51=C(C52=C(C53=C(C54=C(C55=C(C56=C(C57=C(C58=C(C59=C(C60=C(C61=C(C62=C(C63=C(C64=C(C65=C(C66=C(C67=C(C68=C(C69=C(C70=C(C71=C(C72=C(C73=C(C74=C(C75=C(C76=C(C77=C(C78=C(C79=C(C80=C(C81=C(C82=C(C83=C(C84=C(C85=C(C86=C(C87=C(C88=C(C89=C(C90=C(C91=C(C92=C(C93=C(C94=C(C95=C(C96=C(C97=C(C98=C(C99=C(C100=C(C101=C(C102=C(C103=C(C104=C(C105=C(C106=C(C107=C(C108=C(C109=C(C110=C(C111=C(C112=C(C113=C(C114=C(C115=C(C116=C(C117=C(C118=C(C119=C(C120=C(C121=C(C122=C(C123=C(C124=C(C125=C(C126=C(C127=C(C128=C(C129=C(C130=C(C131=C(C132=C(C133=C(C134=C(C135=C(C136=C(C137=C(C138=C(C139=C(C140=C(C141=C(C142=C(C143=C(C144=C(C145=C(C146=C(C147=C(C148=C(C149=C(C150=C(C151=C(C152=C(C153=C(C154=C(C155=C(C156=C(C157=C(C158=C(C159=C(C160=C(C161=C(C162=C(C163=C(C164=C(C165=C(C166=C(C167=C(C168=C(C169=C(C170=C(C171=C(C172=C(C173=C(C174=C(C175=C(C176=C(C177=C(C178=C(C179=C(C180=C(C181=C(C182=C(C183=C(C184=C(C185=C(C186=C(C187=C(C188=C(C189=C(C190=C(C191=C(C192=C(C193=C(C194=C(C195=C(C196=C(C197=C(C198=C(C199=C(C200=C(C201=C(C202=C(C203=C(C204=C(C205=C(C206=C(C207=C(C208=C(C209=C(C210=C(C211=C(C212=C(C213=C(C214=C(C215=C(C216=C(C217=C(C218=C(C219=C(C220=C(C221=C(C222=C(C223=C(C224=C(C225=C(C226=C(C227=C(C228=C(C229=C(C230=C(C231=C(C232=C(C233=C(C234=C(C235=C(C236=C(C237=C(C238=C(C239=C(C240=C(C241=C(C242=C(C243=C(C244=C(C245=C(C246=C(C247=C(C248=C(C249=C(C250=C(C251=C(C252=C(C253=C(C254=C(C255=C(C256=C(C257=C(C258=C(C259=C(C260=C(C261=C(C262=C(C263=C(C264=C(C265=C(C266=C(C267=C(C268=C(C269=C(C270=C(C271=C(C272=C(C273=C(C274=C(C275=C(C276=C(C277=C(C278=C(C279=C(C280=C(C281=C(C282=C(C283=C(C284=C(C285=C(C286=C(C287=C(C288=C(C289=C(C290=C(C291=C(C292=C(C293=C(C294=C(C295=C(C296=C(C297=C(C298=C(C299=C(C300=C(C301=C(C302=C(C303=C(C304=C(C305=C(C306=C(C307=C(C308=C(C309=C(C310=C(C311=C(C312=C(C313=C(C314=C(C315=C(C316=C(C317=C(C318=C(C319=C(C320=C(C321=C(C322=C(C323=C(C324=C(C325=C(C326=C(C327=C(C328=C(C329=C(C330=C(C331=C(C332=C(C333=C(C334=C(C335=C(C336=C(C337=C(C338=C(C339=C(C340=C(C341=C(C342=C(C343=C(C344=C(C345=C(C346=C(C347=C(C348=C(C349=C(C350=C(C351=C(C352=C(C353=C(C354=C(C355=C(C356=C(C357=C(C358=C(C359=C(C360=C(C361=C(C362=C(C363=C(C364=C(C365=C(C366=C(C367=C(C368=C(C369=C(C370=C(C371=C(C372=C(C373=C(C374=C(C375=C(C376=C(C377=C(C378=C(C379=C(C380=C(C381=C(C382=C(C383=C(C384=C(C385=C(C386=C(C387=C(C388=C(C389=C(C390=C(C391=C(C392=C(C393=C(C394=C(C395=C(C396=C(C397=C(C398=C(C399=C(C400=C(C401=C(C402=C(C403=C(C404=C(C405=C(C406=C(C407=C(C408=C(C409=C(C410=C(C411=C(C412=C(C413=C(C414=C(C415=C(C416=C(C417=C(C418=C(C419=C(C420=C(C421=C(C422=C(C423=C(C424=C(C425=C(C426=C(C427=C(C428=C(C429=C(C430=C(C431=C(C432=C(C433=C(C434=C(C435=C(C436=C(C437=C(C438=C(C439=C(C440=C(C441=C(C442=C(C443=C(C444=C(C445=C(C446=C(C447=C(C448=C(C449=C(C450=C(C451=C(C452=C(C453=C(C454=C(C455=C(C456=C(C457=C(C458=C(C459=C(C460=C(C461=C(C462=C(C463=C(C464=C(C465=C(C466=C(C467=C(C468=C(C469=C(C470=C(C471=C(C472=C(C473=C(C474=C(C475=C(C476=C(C477=C(C478=C(C479=C(C480=C(C481=C(C482=C(C483=C(C484=C(C485=C(C486=C(C487=C(C488=C(C489=C(C490=C(C491=C(C492=C(C493=C(C494=C(C495=C(C496=C(C497=C(C498=C(C499=C(C500=C(C501=C(C502=C(C503=C(C504=C(C505=C(C506=C(C507=C(C508=C(C509=C(C510=C(C511=C(C512=C(C513=C(C514=C(C515=C(C516=C(C517=C(C518=C(C519=C(C520=C(C521=C(C522=C(C523=C(C524=C(C525=C(C526=C(C527=C(C528=C(C529=C(C530=C(C531=C(C532=C(C533=C(C534=C(C535=C(C536=C(C537=C(C538=C(C539=C(C540=C(C541=C(C542=C(C543=C(C544=C(C545=C(C546=C(C547=C(C548=C(C549=C(C550=C(C551=C(C552=C(C553=C(C554=C(C555=C(C556=C(C557=C(C558=C(C559=C(C560=C(C561=C(C562=C(C563=C(C564=C(C565=C(C566=C(C567=C(C568=C(C569=C(C570=C(C571=C(C572=C(C573=C(C574=C(C575=C(C576=C(C577=C(C578=C(C579=C(C580=C(C581=C(C582=C(C583=C(C584=C(C585=C(C586=C(C587=C(C588=C(C589=C(C590=C(C591=C(C592=C(C593=C(C594=C(C595=C(C596=C(C597=C(C598=C(C599=C(C600=C(C601=C(C602=C(C603=C(C604=C(C605=C(C606=C(C607=C(C608=C(C609=C(C610=C(C611=C(C612=C(C613=C(C614=C(C615=C(C616=C(C617=C(C618=C(C619=C(C620=C(C621=C(C622=C(C623=C(C624=C(C625=C(C626=C(C627=C(C628=C(C629=C(C630=C(C631=C(C632=C(C633=C(C634=C(C635=C(C636=C(C637=C(C638=C(C639=C(C640=C(C641=C(C642=C(C643=C(C644=C(C645=C(C646=C(C647=C(C648=C(C649=C(C650=C(C651=C(C652=C(C653=C(C654=C(C655=C(C656=C(C657=C(C658=C(C659=C(C660=C(C661=C(C662=C(C663=C(C664=C(C665=C(C666=C(C667=C(C668=C(C669=C(C670=C(C671=C(C672=C(C673=C(C674=C(C675=C(C676=C(C677=C(C678=C(C679=C(C680=C(C681=C(C682=C(C683=C(C684=C(C685=C(C686=C(C687=C(C688=C(C689=C(C690=C(C691=C(C692=C(C693=C(C694=C(C695=C(C696=C(C697=C(C698=C(C699=C(C700=C(C701=C(C702=C(C703=C(C704=C(C705=C(C706=C(C707=C(C708=C(C709=C(C710=C(C711=C(C712=C(C713=C(C714=C(C715=C(C716=C(C717=C(C718=C(C719=C(C720=C(C721=C(C722=C(C723=C(C724=C(C725=C(C726=C(C727=C(C728=C(C729=C(C730=C(C731=C(C732=C(C733=C(C734=C(C735=C(C736=C(C737=C(C738=C(C739=C(C740=C(C741=C(C742=C(C743=C(C744=C(C745=C(C746=C(C747=C(C748=C(C749=C(C750=C(C751=C(C752=C(C753=C(C754=C(C755=C(C756=C(C757=C(C758=C(C759=C(C760=C(C761=C(C762=C(C763=C(C764=C(C765=C(C766=C(C767=C(C768=C(C769=C(C770=C(C771=C(C772=C(C773=C(C774=C(C775=C(C776=C(C777=C(C778=C(C779=C(C780=C(C781=C(C782=C(C783=C(C784=C(C785=C(C786=C(C787=C(C788=C(C789=C(C790=C(C791=C(C792=C(C793=C(C794=C(C795=C(C796=C(C797=C(C798=C(C799=C(C800=C(C801=C(C802=C(C80
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[illegible]

			(3S)-5-[(1R,2R,8aS)-2-hydroxy-2,5,8a-tetramethyl-3,4,4a,6,7,8-hexahydro-1H-naphthalen-1-yl]-3-methylnicotanoic acid	[M-H] ⁺	325.27371	C20H36O3	Diterpenoids	KHCOSRVJDOANA-ZOSGAXDSSA-N	O=C(O)CC(C)CCC1C(C)(C)CCCC12C
2623	15.329	802.52032	Scytophycin B	[M-H] ⁻	802.51599	C45H73NO12	Diterpene lactones	LGYQYCWQMRLJJ-DAAXTDNESA-N	O-CN(CC(=O)C(C)OC(C)=O)CCC(C)(C)C(C)C1OC(=O)C-C=CC(C)C(C)CC2OC(C=CC2)C(C)C(C)C(C)C(C)C(C)C(C)C(C)
2624	15.386	372.28827	Buxtamine	[M-H] ⁺	372.29001	C24H37NO2	Triterpenoids	KTASKRCJBGXHM-WMYNZDBHS-A	O=C(C)C1C(C)CC(C)C3CCOC4=C(C)(NC)OCC54C3SCCO12C
2625	15.407	378.33545	Ursocholic Acid	[M-H] ⁺	378.33664	C24H40O2	Bile acids, alcohols and derivatives	RPKLZQLYOUPWTW-LVVAJZHISA-N	O=C(O)CCC(C)C1CCC2C3CCC4CCCC4(C)C3CCC12C
2626	15.418	363.28772	2-methoxy-4-pentadecylbenzoic acid	[M-H] ⁺	363.289	C23H38O3	0-methoxybenzoic acids and derivatives	HGXGHYZLPCLUJI-UHHFFAOYSA-N	O=C(O)C1=CC=C(C=C1)CCCCCCCCCC
2627	15.423	397.34457	Ergosterol	[M-H] ⁺	397.3465	C28H44O	Ergosterols and derivatives	DNPYPKGSXYMLRS-UHHFFAOYNA-N	OC1CC2=CC=C3C(CCC4(C)C3CCC4=C(C)C(C)C(C)C2(C)CC1
2628	15.447	432.35431	korseveriline	[M-H] ⁺	432.35001	C27H45NO3	Cerveratrum-type alkaloids	NGVOUYEGZOZEN-CADWWJYS-A	OC1CCC2(C)C(C)C(C)OC3AC2C4C5CNBCC(C)CCC6(C)C5CCC43O
2629	15.449	437.37778	(3beta)-stigmast-5-en-3-ol	[M-H] ⁺	437.38	C29H50O	Stigmasteranes and derivatives	KZJWDPNJALLNS-VJSFXLFPS-A	OC1CC2=CCC3C(CCC4(C)C(C)CCC4)C(C)CCC(C)(C)C(C)C2(C)C
2630	15.45	607.25134	3-(2-((3-{(2-carboxyethyl)-4-methyl-5-oxo-4-vinyl-1H-pyrrol-2(5H)-ylidene)methyl}-1H-pyrrol-2-yl)methyl)-4-methyl-5-(4)-(4-	[M-H] ⁺	607.25	C33H36N4O6	Billirubins	BPYKITZIUTYGOLF-IDASCNNAS-N	O=C(O)CC1=C(NC(C=C2NC(=O)C(C=C2)C)C(C)OC(=O)3NC(C=N C(=O))C(C)=C4C=C(C3CCTC(=O)O))C
2631	15.491	398.34741	Solanidine (not validated)	[M-H] ⁺	398.34091	C27H43NO	Steroidal saponins	JVKYIZPBMZFJNJ-UHHFFAOYNA-N	OC6OC5=CC4C(CCC3(C)(C4(C2N1C(C)CC1C(C)C23)))C5(C)C O6
2632	15.502	285.21609	Acacetin	[M-H] ⁺	285.21265	C16H12O5	4'-O-methylated flavonoids	DANYIYRPLHOXC-UHHFFAOYSA-N	O=C1C=C(OC=2C=C(O)C=C(O)C12)C=3C=CC(OC)=CC3
2633	15.541	917.53845	Notoginsenoside Ftl	[M-H] ⁺	917.53998	C47H80O17	Triterpenoids	LXLVPXTOKTYXHUGLCNCSA-N	OC1OOC(OC2OCC3(C)C(CCC4(C)C3OC(C)C5(CCC54)C(C)OC CC=C(C)C)C2(C)C(C)OC6OC(C)(C)OC7OC7OC(C)(C)C7O)C(C)C
2634	15.575	698.48297	10-[3-acetamido-4,5-dihydroxy-6-(hydroxymethyl)oxan-2-ylo]oxy-5-hydroxy-2,2,6a,6b,9,9,12a-hexamethyl-1,3,4,5,6,6a,7,8,8a,10,11,12,13,14b-	[M-H] ⁺	698.48602	C38H61NO9	Triterpene saponins	ZCVZUHMTUSANI-UHHFFAOYSA-N	O=C(C)C12CCC(C)(C)OC2C3=CC4C5(C)CC(C)OC6OC(C)(C)C7O(C)CBN=C(C)C(C)C(C)C5CC4(C)C3(C)C1O
2635	15.576	383.32977	Cholest-4,6-Dien-3-One	[M-H] ⁺	383.33081	C27H42O	Cholesterols and derivatives	XJWMKRKFYSISJ-GVMKIIDSA-N	O=C1C=C2C=CC3C(CCC4(C)C3CCC4(C)CCCC(C)C)C2(C)C(C)C1
2636	15.58	321.21909	Bis(2-ethylhexyl)phosphate	[M-H] ⁻	321.22003	C16H35O4P	Dialkyl phosphates	SEGLCEGVDFDPX-UHHFFAOYNA-N	CCCC(C)COP(O)(=O)OCC(C)CCCC
2637	15.588	591.25671	3-[[{3R,5S,10R,13R,14S,17R)-5,14-dihydroxy-10,13-dimethyl-3-[(2R,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yloxy-(3Z)-3-[[[1,6-dimethyl-2-(1E,3E)-penta-1,3-dienyl]-4a,5,6,7,8,8a-hexahydro-2H-naphthalen-1-yl]]-hydroxymethylidenel-5-(1-	[M-H] ⁺	591.25659	C29H44O10	Gardenolid glycosides and derivatives	PFCZYMDHYKVIA-MHLHJPMSA-N	O=C1OCC(=O)C2OCC3(C)OC4(C5(C)OC(C)OC6OC(C)(O)C(C)O)C6O OC75(C)C4OCC23C
2638	15.589	398.23196	{3Z)-3-[[[1,6-dimethyl-2-(1E,3E)-penta-1,3-dienyl]-4a,5,6,7,8,8a-hexahydro-2H-naphthalen-1-yl]]-hydroxymethylidenel-5-(1-	[M-H] ⁻	398.23367	C24H33NO4	Pyrrolines	AIFXSMDWBXFPT-SNXGECCISA-N	O=C1C(C)O=NC1O(C)=C(O)C2(C)C(C=C(C)C)=CC3CC(C)CCC3 2
2639	15.595	357.33517	conessone	[M-H] ⁺	357.32999	C24H40N2	Conanine-type alkaloids	GPLGAQQNMWMM-CVFNKAMPSA-N	C1=C2C(N(C)C)CCC2(C)C3CCC45CN(C)C(C)C5CCCC4C3C1
2640	15.635	654.18976	7-chloro-6'-hydroxy-4,6-dimethoxy-'1,3',8''-trimethyl-5'-(3,4,5-trimethoxyphenyl)-8'',9''-dihydro-1'H-spiro[benzofuran-2,7'-pyrimidinol-4,5'	[M-H]	654.19	C32H32ClN3O10	Phenylquinolines	BEALVDNRJVATFR-UHHFFAOYSA-N	O=C1C2=C(N=C3C=C(O)C4(C)OC=5C(C1)=C(OC)C(C)OC54=C(O)C(C)C3C2C=C(C)C(=O)C(C)C(C)=C6)N(C(C)O)N1(C)C
2641	15.637	653.17877	[2-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yloxy]phenyl]methyl 6-hydroxy-2-methoxy-3-[3,4,5-trihydroxy-6-	[M-H] ⁺	653.18365	C27H34O16	Phenolic glycosides	WQJLTIVDGZXMHF-XAYMNBSA-N	O=C(OC)C=C(C)C(C)C1OC2OC(C)(C)OC2O=C3C(O)=CC=C(OC4(C)OC(C)(O)C4O)C3OC
2642	15.645	463.27945	Pristimerin derivative	[M-H] ⁺	463.27701	C30H38O4	Methyl esters	LQBQRDRDYGCBI-RKHSHXAASA-N	O=C1C=C2C(=CC=C3C4(C)CC(C5(C)CCC(C)=O)OC)CC4C3(C)CC2(C5=C(C)OC(C)C(C)C1)C(C)C
2643	15.646	479.25531	6-oxopristimerol derivative	[M-H] ⁺	479.25	C30H38O5	3-hydroxysteroids	LOTZFUXLMRODN-IUOWYMDSA-N	O=C1C=C2C=C(C)C4(C)CCC(C(C)=O)OC)CC4C3(C)CC

[illegible]

[illegible]

[illegible]

[illegible]

2837	19.834	225.06013	1,8,9-Anthracenetriol	[M-H] ⁻	225.05573	C14H10O3	Anthracenes	YUTJCNFTO1OGT-UHFFFAOYSA-N	OC1=CC=CC2=CC3=CC=CC(O)=C3C(O)=C12
2838	19.835	370.72946	2-(hydroxymethyl)-6-[[[(1R,4S)-2,4,4-trimethyl-3-oxabicyclo[2.2.2]octan-5-yl]oxloxane-3,4,5-triol]	[M-H] ⁺	370.72919	C16H28O7	O-glycosyl compounds	NWYZT2HMCWGOF-HLJZFUEWSA-N	OC(C1OC(OC2CC3CC2(OC3(C)C)C)C(O)C(O)C)C1O
2839	19.836	742.53802	Phosphatidylethanolamine 18	[M-H] ⁻	742.53925	C41H78NO8P	Phosphatidylethanolamines	CJVLVBK1FVTUPS-JSCMWKRNA-N	CCCCCCCCCCCCCCCC(=O)OC(COP(O)(=O)OCN)OC(=O)CC(C)/C=C/C(=C)CCCC
2840	19.836	161.02267	Salicylic acid	[M+H] ⁺	161.02	C7H6O3	Salicylic acids	YGSDEFSMJLEOE-UHFFFAOYSA-N	O=C(O)C=CC=CC1O
2841	19.836	167.01692	URATE	[M-H] ⁻	167.021	C5H4N4O3	Xanthines	LEHOTFFKMJEONL-UHFFFAOYSA-N	O=C1NC(=O)C=2NC(=O)NC2N1
2842	19.837	177.0397	D-GULONIC ACID GAMA-LACTONE	[M-H] ⁻	177.03999	C6H12O7	Medium-chain hydroxy acids and derivatives	RGHJNZXEOKURBD-QTBDOELSSA-N	O=C(O)C(O)C(O)C(O)C(O)CO
2843	19.837	267.07068	Norberto Lopes	[M-H] ⁻	267.07001	C16H12O4	4'-O-methylisoflavones	HKYGTGCTOTHOMP-UHFFFAOYSA-N	O=C1C(=COC2=CC(O)=CC=C21)C=3C=CC(OC)=CC3
2844	19.837	117.0185	Succinic acid (not validated)	[M-H] ⁻	117.0182	C4H6O4	Organic acids	KDYFGRWQYBRFD-UHFFFAOYSA-N	O=C(O)CCC(=O)O
2845	19.841	134.03107	Thiazolidine-4-carboxylic acid	[M+H] ⁺	134.02702	C4H7NO2S	L-alpha-amino acids	DZLNHFMRPBULJ-UHFFFAOYNA-N	O=C(O)C1NCSC1
2846	19.842	264.08609	2,3',4,6-Tetrahydroxybenzophenone	[M+H] ⁺	264.08664	C13H10O5	Benzophenones	QWRYPHZJTQLFX-UHFFFAOYSA-N	O=C(C1C=CC=C(O)C1)C=2C(O)=CC(O)=CC2O
2847	19.845	223.01393	(7R,8R)-7,8-dihydroxy-3,5,7-trimethyl-8H-isochromen-6-one	[M+H] ⁺	223.01343	C12H14O4	Azaphilones	JVUYBLROBJEJN-NEPJUHUUSA-N	O=C1C(=C2C=C(OC=C2(O)C1(O)C)C)C
2848	19.845	184.01772	Pesticide1_Acephate_C4H10NO3PS_O,S-Dimethyl acetylphosphoramidothioate	[M+H] ⁺	184.019	C4H10NO3PS	Organothiophosphorus compounds	YASYMFAVPKPKE-UHFFFAOYSA-N	O=P(N=C(O)C)OC)SC
2849	19.846	327.25266	1,2-dihydroxyheptadec-16-yn-4-yl acetate	[M+H] ⁺	327.25296	C19H34O4	Long-chain fatty alcohols	FHGZOCZNYHWAL-UHFFFAOYSA-N	O=C(OC(CCCCCCCCCCCC)CC(O)CO)C
2850	19.848	101.02376	2-Oxobutyric acid	[M-H] ⁻	101.02441	C4H6O3	Short-chain keto acids and derivatives	TYEYBOSBBHJIV-UHFFFAOYSA-N	CCC(=O)C(O)=O
2851	19.848	193.03444	D-(+)-Galacturonic acid	[M-H] ⁻	193.03537	C6H10O7	Glucuronic acid derivatives	AEMOLEFTQBMNLQ-YMDCURPLSA-N	OC1O[C@H]([C@H](O)[C@H](O)[C@H]1O)C(O)=O
2852	19.848	163.03859	Umbelliferone	[M+H] ⁺	163.03897	C9H6O3	7-hydroxycoumarins	ORHBXUUXSCNDEV-UHFFFAOYSA-N	OC1=CC2=C(C=C1)C=CC(=O)O2
2853	19.851	160.04372	Brompheniramine	[M+H] ⁺	160.04401	C20H23BrN2O4	Pheniramines	SRGKFVASLQWBO-BTJKTKAUSA-N	O=C(O)C=C(=O)O.BrC1=CC=C(C=C1)C(C2=NC=CC=C2)CCN(C)C
2854	19.854	158.11694	Homostachydrine	[M+H] ⁺	158.11757	C8H15NO2	Alpha amino acids	XULZWQRXYTVUTE-ZETCQVMHSA-N	C[N+](C)CCCC(=C[H]1C(=O)[O-])
2855	19.855	165.07521	1,5-Anhydrosorbitol	[M+H] ⁺	165.07574	C6H12O5	Monosaccharides	MPCAJMNYNOGPB-UHFFFAOYNA-N	OC1OC(C)C(O)C1O
2856	19.859	100.11179	Cyclohexylamine	[M+H] ⁺	100.11208	C6H13N	Cyclohexylamines	PAFZNILMFXTIMY-UHFFFAOYSA-N	C1CCC(CC1)N
2857	19.861	478.29318	Phosphatidylethanolamine lyso 18	[M-H] ⁻	478.29391	C23H46NO7P	2-acyl-sn-glycero-3-phosphoethanolamines	FEVAUEZKXSRQS-PFONDGANA-N	CCCCCCCCCCCCC/C=C/C(=O)OC(CO)COP(O)(=O)OCN
2858	19.861	183.08594	Sorbitol	[M+H] ⁺	183.08627	C6H14O6	Sugar alcohols	FDPFZTCFMRRESA-JGWLTMVSA-N	CCC(O)C(O)C(O)C(O)CO
2859	19.862	274.27481	Palmitic Acid	[M+H] ⁺	274.27411	C16H32O2	Long-chain fatty acids	IPCSVSSVZVIGE-UHFFFAOYSA-N	O=C(O)CCCCCCCCCCCCC
2860	19.862	301.23651	Roccellic Acid	[M+H] ⁺	301.23734	C17H32O4	Long-chain fatty acids	CADNMISJDLVPCK-LSOHHALUSA-N	O=C(O)C(C)C(C(=O)O)CCCCCCCCCCCC
2861	19.864	199.01796	MCPA	[M-H] ⁻	199.01674	C9H9ClO3	Chlorophenoxyacetates	WHKUVPPKQRBVB-UHFFFAOYSA-N	CC1=CC(=CC=C1OCC(=O)O)C1
2862	19.869	284.91183	Homoptercarpin	[M+H] ⁺	284.91422	C17H16O4	1-benzopyrans	GIWAJLOUBQKKA-UHFFFAOYSA-N	O(C1C=CC2(OC3OC4=CC(OC)=CC=C4C23)=C1)C
2863	19.873	189.03371	4-nitroquinoline 1-oxide	[M-H] ⁻	189.03056	C9H6N2O3	4-nitroquinoline N-oxides	YHQDZJICGQWFKH-UHFFFAOYSA-N	O=N(=O)C1=CC=N(=O)C=2C=CC=CC12
2864	19.892	167.99811	2-Mercaptobenzothiazole	[M+H] ⁺	167.99362	C7H5NS2	Benzothiazoles	YX1WHUQKZSMYRE-UHFFFAOYSA-N	C1=CC=C2C(=C1)N=C(S)S2
2865	19.898	83.0601	3-Methylpyrazole	[M+H] ⁺	83.06037	C4H6N2	Pyrazoles	XKVUYEYANWF1JX-UHFFFAOYSA-N	CC=C1C=CN1
2866	19.898	351.16913	hirsutanone	[M+H] ⁺	351.16895	C19H20O5	Linear diarylheptanoids	VWHYFMQJYFLCC-DUXPYHPUSA-N	O=C(C=CCCC1=CC=C(O)C(O)=C1)CCC2=CC=C(O)C(O)=C2
2867	19.904	265.09631	D-Tryptophan	[M+H] ⁺	265.09698	C11H12N2O2	Indolyl carboxylic acids and derivatives	Q1VBCCIJJIAJPQS-SECBINFHSA-N	O=C(O)C(N)CC1=CNC=2C=CC=CC21
2868	19.904	449.26535	Mappain	[M+H] ⁺	449.26901	C29H36O4	Stilbenes	GJZKDVGLDGLPMB-ZVBRSEKESA-N	OC=1C=C(C=CC2=CC(O)=C(C)=C2)CC=C(C)C=C(C1O)CC=C(C)C(=C(C)C
2869	19.91	130.04935	Pyroglutamic acid	[M+H] ⁺	130.04987	C5H7NO3	Alpha amino acids and derivatives	ODHCTXKNWHXJC-UHFFFAOYNA-N	O=C(O)C1N=C(O)CC1
2870	19.92	87.04472	Isobutyric acid	[M-H] ⁻	87.04515	C4H8O2	Carboxylic acids	KQNPFPQTMSNSAP-UHFFFAOYSA-N	O=C(O)C(C)C
2871	19.925	357.12521	Pioglitazone	[M+H] ⁺	357.12674	C19H20N2O3S	Phenol ethers	HYAFETHFCAUJAY-UHFFFAOYNA-N	CCC=1C=CC(COC2=CC=C(C=C2)CC3C(=NC(=O)S3)O)=NC1
2872	19.927	224.04832	1-Hydroxyanthraquinone	[M-H] ⁻	224.0479	C14H8O3	Anthraquinones	BTLXPCBPYBNQR-UHFFFAOYSA-N	C1=CC=C2C(=C1)C(C=3C=CC=C(C3C2=O)O)=O
2873	19.928	199.02962	Herniarin	[M+H] ⁺	199.03	C10H8O3	Coumarins and derivatives	L1IALPBMIOVAHH-UHFFFAOYSA-N	O=C1OC=2C=C(OC)C=CC2C=C1
2874	19.929	237.02075	6,7,8-trimethoxycoumarin	[M+H] ⁺	237.02609	C12H12O5	Coumarins and derivatives	RAVQKHLZHPYEJ-UHFFFAOYSA-N	O=C1OC=2C(OC)=C(OC)C(OC)=CC2C=C1
2875	19.932	134.05969	INDOXYL SULFATE	[M+H] ⁺	134.06	C8H7NO4S	Arylsulfates	BXFFHSIDQOFMLE-UHFFFAOYSA-N	O=S(=O)(O)OC1=CNC=2C=CC=CC12
2876	19.933	316.25439	Decanoyl-L-carnitine	[M+H] ⁺	316.24823	C17H33NO4	Acyl carnitines	LZOSYCMHQXPBU-UHFFFAOYSA-N	O=C(1(O)CC(OC(=O)CCCCCCCC)[N+](C)(C)C
2877	19.936	221.99419	HISTAMINE DIHYDROCHLORIDE	[M+H] ⁺	221.99615	C5H11ClN3	2-arylethylamines	PPZMYIBUHIPZOS-UHFFFAOYSA-N	C1.C1.N1=CNC(=C1)CCN
2878	19.939	207.1373	Ibuprofen	[M+H] ⁺	207.13699	C13H18O2	Phenylpropanoic acids	HEPNNSXXWATRW-UHFFFAOYSA-N	O=C(O)C(C1=CC=C(C=C1)CC(C)C)C
2879	19.944	116.07018	Proline	[M+H] ⁺	116.07	C5H9NO2	Proline and derivatives	ONIBWKTPOPIA-BYPYZUCNSA-N	O=C(O)C1NCCC1

2880	19.946	178.04254	Isoxanthopterin	[M-H] ⁻	178.03705	C6H5N5O2	Pterins and derivatives	GLKCOBII ZKYKFN-UHFFFAOYSA-N	N=C1N=C(O)C=2N=CC(O)=NC2N1
2881	19.951	169.12199	Geranic acid	[M+H] ⁺	169.1223	C10H16O2	Acyclic monoterpenoids	ZHYZqXUYZJNEHD-UHFFFAOYSA-N	O=C(O)C=C(C)CC=C(C)C
2882	19.952	207.06438	7,8-dimethoxy-2H-chromen-2-one	[M+H] ⁺	207.064	C11H10O4	Coumarins and derivatives	CHBBSMUTOCUYDW-UHFFFAOYSA-N	O=C1OC=2C(OC)=C(OC)C=C2C=C1
2883	19.965	254.10156	10-Azabenz[a]pyrene	[M+H] ⁺	254.09642	C19H11N	Pyrenes	BYF1UFNRSNKODH-UHFFFAOYSA-N	C1=CC=2C=CC3=CC=4C=CC=NC4C=5C(=C1)C2C35
2884	19.969	148.06073	L-Glutamic acid	[M+H] ⁺	148.06044	C5H9NO4	Glutamic acid and derivatives	WHUUTDBJXJRKMK-VKHYHEASA-N	C(CC(=O)O)[C@H](C(=O)O)N
2885	19.97	200.1277	Methylecgonine	[M+H] ⁺	200.12801	C10H17NO3	Tropane alkaloids	Q1QNNBXHAYSQRY-UHFFFAOYSA-N	O=C(OC)C1C(O)CC2N(C)C1CC2
2886	19.971	253.05798	rubiadin	[M-H] ⁻	253.0596	C15H10O4	Hydroxyanthraquinones	IRZTUXPRITUZXP-UHFFFAOYSA-N	O=C1C=2C=CC=CC2C(=O)C3=C(O)C(=C(O)C(=C13)C
2887	19.972	149.04596	Arabinose	[M-H] ⁻	149.04555	C5H10O5	Pentoses	PYMYPHUHKUWMLA-UHFFFAOYNA-N	O=CC(O)C(O)C(O)CO
2888	19.972	193.03604	D-sorbose	[M-H] ⁻	193.03539	C6H10O7	Sugar acids and derivatives	VBUYCZFBWCYFD-FLRLBIABSA-N	O=C(O)C(=O)C(O)C(O)CO
2889	19.972	135.0304	Threonine	[M-H] ⁻	135.02989	C4H8O5	Sugar acids and derivatives	JP1JQSOTBSSVTP-UHFFFAOYNA-N	O=C(O)C(O)C(O)CO
2890	19.975	185.02164	m-Xylene-4-sulfonic acid	[M-H] ⁻	185.02779	C8H10O3S	p-Methylbenzenesulfonates	CHZLVSBMXZSPNN-UHFFFAOYSA-N	CC(=O)C(=O)C(=O)S(O)(=O)=O
2891	19.985	177.04108	Gluconic acid-γ-lactone	[M-H] ⁻	177.04047	C6H10O6	Glucolactones	PHQVHQSTUBQK-UHFFFAOYNA-N	O=C1OC(CO)C(O)C(O)C1O
2892	19.989	145.04993	3-METHYLGUTARIC ACID	[M-H] ⁻	145.05	C6H10O4	Methyl-branched fatty acids	XJMMNTG1MDZPMU-UHFFFAOYSA-N	O=C(O)CC(C)CC(=O)O
2893	19.989	117.01871	SUCCINATE	[M-H] ⁻	117.019	C4H6O4	Dicarboxylic acids and derivatives	KDYFGRWQYBRFD-UHFFFAOYSA-N	O=C(O)CCC(=O)O
2894	19.991	197.06747	Harmol	[M-H] ⁻	197.07204	C12H10N2O	Alkaloids	SATMZMMKDDTOSQ-UHFFFAOYSA-N	CC1=C2NC3=C(C=CC(O)=C3)C2=CC=NC1
2895	19.993	130.05026	Pyroglutamic acid (not validated, isomer of 89)	[M+H] ⁺	130.0504	C5H7NO3	Amino acids	ODHCTXNWHXJC-UHFFFAOYNA-N	O=C(O)C1NC(=O)CC1
2896	19.998	146.02515	1H-Isoidole-1,3(2H)-dione	[M-H] ⁻	146.02475	C8H5NO2	Phthalimides	XKJCHHZQLQNZHY-UHFFFAOYSA-N	C1=CC=C2C(=C1)C(=NC2=O)O
2897	19.998	217.03114	4,4'-Thiodiphenol	[M-H] ⁻	217.03287	C12H10O2S	Diaryliethers	VWGKEVFBQIAND-UHFFFAOYSA-N	C=C1C=C(C=CC1O)SC2=CC=C(C=C2)O
2898	19.998	138.02016	4-Nitrophenol	[M-H] ⁻	138.01967	C6H5NO3	Nitrophenols	BTJ1UGIUPKRLHP-UHFFFAOYSA-N	O=N(O)C1=CC=C(O)C=C1
2899	19.999	129.01863	Itaconic acid (Not validated)	[M-H] ⁻	129.0188	C5H6O4	Organic acids	LVBHZNLOWSRM-UHFFFAOYSA-N	O=C(O)C(=C)CC(=O)O
2900	20	159.06561	3-Methyladipic acid	[M-H] ⁻	159.06628	C7H12O4	Medium-chain fatty acids	SYEOWNSTUDRG-UHFFFAOYNA-N	O=C(O)CCC(C)CC(=O)O
2901	20.004	156.06519	Indole-3-acetonitrile	[M+H] ⁺	156.06821	C10H8N2	3-alkylindoles	DMCFQDLJMLSNC-UHFFFAOYSA-N	N#CCCC1=CC=C(C=C1)C#N
2902	20.014	337.20325	Bavachinin A	[M-H] ⁻	337.20111	C21H22O4	6-prenylated flavanones	HOVCSQHKPZS1KB-FQEVSTJZSA-N	O=C1C2=CC(=C(OC)C=C2OC(C3=CC=C(O)C=C3)C1)CC=C(C)C
2903	20.017	261.0162	isofraxidin	[M+H] ⁺	261.01599	C11H10O5	7-hydroxycoumarins	HOEVRIHMDJKUMZ-UHFFFAOYSA-N	O=C1OC=2C(OC)=C(O)C(OC)=CC2C=C1
2904	20.019	296.1842	Esmolol	[M+H] ⁺	296.18564	C16H25NO4	Phenol ethers	AGNDDEOPVVGCPG-UHFFFAOYNA-N	O=C(OC)CCC1=CC=C(OC(O)CNC(C)C)C=C1
2905	20.02	297.11691	Enterolactone	[M-H] ⁻	297.11322	C18H18O4	Lignols	HVDGDHABMCBLR-UHFFFAOYNA-N	OC1=CC(C2CCOC(=O)C2CC2=CC(O)=CC=C2)=CC=C1
2906	20.024	249.99564	2-[(4,6-diamino-1,3,5-triazin-2-yl)thio]-Ethanesulfonic acid	[M-H] ⁻	250.00101	C5H9N5O3S2	1,3,5-triazine-2,4-diamines	VQJSEYJDXBICY-UHFFFAOYSA-N	O=S(=O)(O)CCSC1=NC(=N)NC(=N)N1
2907	20.024	164.06999	Clozapine (Clozaril)	[M+H] ⁺	164.073	C18H19ClN4	Dibenzodiazepines	QZUDENBUXUHMW-UHFFFAOYSA-N	C1C1=CC=C2NC=3C=CC=C3C(=NC2=C1)N4CCN(C)CC4
2908	20.03	306.97766	(2E)-2-[hydroxy(phenyl)methylidene]-6-methoxy-1-benzofuran-3-one	[M+H] ⁺	306.97165	C16H12O4	Aurone flavonoids	TXVHAPNXGBCXJ-JQ1JEIRASA-N	O=C1C(OC2=CC(OC)=CC=C21)=C(O)C=3C=CC=C3
2909	20.031	228.98563	Hymecromone Methyl Ether	[M+H] ⁺	228.98586	C11H10O3	Coumarins and derivatives	UDFPKNSWSYB1HO-UHFFFAOYSA-N	O=C1OC=2C=C(OC)C=CC2C(=C1)C
2910	20.037	169.08588	FA 9:2+10	[M-H] ⁻	169.08591	C9H14O3	Oxidized fatty acids	QHVBPAALYZNWPK-UHFFFAOYSA-N	O=C(O)C=CC(=O)CCCC
2911	20.041	193.03444	D-GLUCURONIC ACID	[M-H] ⁻	193.035	C6H10O7	Glucuronic acid derivatives	AEMOLEFTQBMLQ-UHFFFAOYSA-N	O=C(O)C1OC(C(O)C(O)C1O
2912	20.042	179.05533	Psicose	[M-H] ⁻	179.05611	C6H12O6	Monosaccharides	BJH1KHVHCXPLS-UHFFFAOYNA-N	O=C(CO)C(O)C(O)CO
2913	20.043	133.04961	Dihydroxy-Valerate	[M-H] ⁻	133.0497	C5H10O4	Fatty acids	JTEYKUFKXGDTU-UHFFFAOYNA-N	O=C(O)C(O)C(O)C(C)C
2914	20.044	122.09614	2,4,6-Trimethylpyridine	[M+H] ⁺	122.09643	C8H11N	Methylpyridines	BWZVCCNYMEVEX-UHFFFAOYSA-N	CC1=CC(C)=NC(C)=C1
2915	20.044	96.04408	3-Hydroxypyridine	[M+H] ⁺	96.04439	C5H5NO	Hydroxypyridines	GRFNBEZ1AWKCO-UHFFFAOYSA-N	c1cc(cnc1)O
2916	20.045	177.0397	D-GLUCONATE	[M-H] ⁻	177.03999	C6H12O7	Medium-chain hydroxy acids and derivatives	RGLNJXEOKUBD-UHFFFAOYSA-N	O=C(O)C(O)C(O)C(O)CO
2917	20.047	211.00325	Pesticide5_Acibenzolar-S-methyl_C8H6N2OS2_Actigard	[M+H] ⁺	210.99899	C8H6N2OS2	Benzothiadiazoles	UEL1TFHSLAHKR-UHFFFAOYSA-N	O=C(SC)C1=CC=CC(=C1)N=C1C
2918	20.051	163.039	2-Coumaric acid	[M-H] ⁻	163.04007	C9H8O3	Hydroxycinnamic acids	PMOWT1HVNWYF1-AATRIKPKSA-N	OC(=O)C=Cc1cc(C)=CC=C1O
2919	20.052	125.02366	Benzene-1,2,4-triol	[M-H] ⁻	125.02441	C6H6O3	Hydroxyquinols and derivatives	GGQRNBQZJCCN-UHFFFAOYSA-N	OC1=CC=C(C(=O)O)C=C1
2920	20.055	167.03416	Homogenetic acid	[M-H] ⁻	167.03499	C8H8O4	2(hydroxyphenyl)acetic acids	IGMNYECUMZDDF-UHFFFAOYSA-N	OC(=O)CC1=CC(O)=CC=C1O
2921	20.056	161.04457	Hydroxymethylglutaric acid	[M-H] ⁻	161.0451	C6H10O5	Organic acids	NPOAOTPXNNWTSU-UHFFFAOYSA-N	O=C(O)CC(O)(C)CC(=O)O
2922	20.061	101.07047	Gyromitrin	[M+H] ⁺	101.07094	C4H8N2O	N-alkylated hydrazones	IMAGWKUTFZRWBS-HWKANZROSA-N	O=CN(N=CC)C

2923	20.062	224.09085	Pesticide3_Dioxacarb_C11H13N04_Phenol, 2-(1,3-dioxolan-2-yl)-, methylcarbamate	[M+H] ⁺	224.091	C11H13N04	Phenoxy compounds	SDKQRNRDYGKY-UHFFFAOYSA-N	OC(=NC)OC=1C=CC=CC1C20CCO2
2924	20.063	195.05006	Xanthone	[M-H] ⁻	195.0452	C13H8O2	Xanthenes	JNELGWHKGNBSMD-UHFFFAOYSA-N	O=C1C=2C=CC=CC2OC=3C=CC=CC31
2925	20.069	146.05243	3-Formylindole	[M+H] ⁺	146.06004	C9H7NO	Indoles	OLNJUISUQQNIM-UHFFFAOYSA-N	O=CC1=CN2C=CC=CC=C12
2926	20.07	206.08853	1-phenylisoquinoline	[M+H] ⁺	206.09	C15H11N	Phenylpyridines	LPWDYWZ1WDTCV-UHFFFAOYSA-N	N=1C=CC=2C=CC=CC21C=3C=CC=CC3
2927	20.07	108.08051	2,6-Dimethylpyridine	[M+H] ⁺	108.08077	C7H9N	Methylpyridines	O1SVCGZHLKMSJ-UHFFFAOYSA-N	CC=1C=CC=C(C)N1
2928	20.071	183.101	Angelical anhydride	[M+H] ⁺	183.10001	C10H14O3	Dicarboxylic acids and derivatives	L1HLSLRANKCHLY-SFECWDFSA-N	O=C(OC(=O)C(=CC)C)C(=CC)C
2929	20.071	118.08569	Valine	[M+H] ⁺	118.086	C5H11NO2	Valine and derivatives	KZSNJWFQEVHDMF-UHFFFAOYSA-N	O=C(O)C(N)C(C)C
2930	20.076	269.08661	7,3',4'-Trihydroxyflavone	[M-H] ⁻	269.08456	C15H10O5	Flavones	PVFGJHYLIHMCQD-UHFFFAOYSA-N	O=C1C=C(OC2=CC(O)=CC=C12)C=3C=CC(O)=C(O)C3
2931	20.078	103.03949	3-HYDROXYBUTANOIC ACID	[M-H] ⁻	103.04	C4H8O3	Beta hydroxy acids and derivatives	WHBMMWSBFZVSSR-GSVUUGTDSA-N	O=C(O)CC(O)C
2932	20.079	196.09613	Glucosaminic Acid	[M+H] ⁺	196.09639	C6H13NO6	D-alpha-amino acids	UFYKDFXCZBTL00-TXICZTDVSA-N	O=C(O)C(N)C(O)C(O)C(O)CO
2933	20.083	72.08051	Pyrrolidine	[M+H] ⁺	72.08078	C4H9N	Pyrrolidines	RWRDLPDLKQPQOW-UHFFFAOYSA-N	C1CCNC1
2934	20.093	131.11752	N-Acetylputrescine	[M+H] ⁺	131.11789	C6H14N2O	Carboximide acids	KLZGKIDSEJWEDW-UHFFFAOYSA-N	CC(O)=NCCCN
2935	20.094	147.06473	Phenyltetrazole	[M+H] ⁺	147.06653	C7H6N4	Phenyltetrazoles and derivatives	MARUHZGHZWCQU-UHFFFAOYSA-N	C1=CC=C(C=C1)C2=NNN=N2
2936	20.1	267.07315	INOSINE	[M-H] ⁻	267.073	C10H12N4O5	Purine nucleosides	UQQMVRMYASKQ-UHFFFAOYSA-N	O=C1N=CN2C=C1N=CN2C3OC(CO)C(O)C3O
2937	20.118	180.10094	Phenacetin	[M+H] ⁺	180.10201	C10H13NO2	Acetanilides	CFJSUEIXXCENMM-UHFFFAOYSA-N	O=C(NC1=CC=C(C(OC)C=C1)C
2938	20.12	278.8667	3,5-dibromo-2-methoxyphenol	[M-H] ⁻	278.866	C7H6Br2O2	Methoxyphenols	YFCZJZFKAEGT-UHFFFAOYSA-N	BrC=1C=C(Br)C(OC)=C(O)C1
2939	20.122	156.06592	3-Methylcrotonylglycine	[M-H] ⁻	156.06662	C7H11NO3	N-acyl-alpha amino acids	PFWQSHXPNKRLIV-UHFFFAOYSA-N	O=C(O)CN=C(O)C=C(C)C
2940	20.123	74.05972	N,N-Dimethylformamide	[M+H] ⁺	74.06004	C3H7NO	Tertiary carboxylic acid amides	ZMXDDKWL CZAD1W-UHFFFAOYSA-N	O=CN(C)C
2941	20.124	90.0547	Alanine	[M+H] ⁺	90.05495	C3H7NO2	Alanine and derivatives	QNAYEMKLOCPYVGJ-UHFFFAOYNA-N	O=C(O)C(N)C
2942	20.127	167.03412	Vanillic acid	[M-H] ⁻	167.03499	C8H8O4	M-methoxybenzoic acids and derivatives	WKOLLVMJNQ1ZCI-UHFFFAOYSA-N	COC1=CC(=CC=C1O)C(O)=O
2943	20.129	187.05923	Rhamnose	[M+H] ⁺	187.05769	C6H12O5	Hexoses	PNNNSAQSRJYSB-BXKXVDMCESA-N	C[C@H](O)[C@H](O)[C@H](O)[C@H](O)C=O
2944	20.133	246.12245	4-Acetamidoantipyrine	[M+H] ⁺	246.1237	C13H15N3O2	Phenylpyrazoles	O1AGWXKSCXPNNZ-UHFFFAOYSA-N	CN1N(C(=O)C(N=C(C)O)=C1)C1=CC=CC=C1
2945	20.137	297.15091	ostruthin	[M-H] ⁻	297.1496	C19H22O3	Terpene lactones	INBMTJJPUABOQJ-VGOFMYFVSA-N	O=C1OC=2C=C(O)C(=CC2=C1)CC=C(C)CCC=C(C)C
2946	20.14	122.05975	Benzamide	[M+H] ⁺	122.06004	C7H7NO	Benzamides	KDAEFPNCMNJSK-UHFFFAOYSA-N	C1=CC=C(C=C1)C(=N)O
2947	20.141	170.08087	Pyridoxine	[M+H] ⁺	170.08099	C8H11NO3	Pyridoxines	LXNHXLTXMVPWM-UHFFFAOYSA-N	OC=1C(=NC=C(C1CO)CO)C
2948	20.152	169.08575	2-(3-oxobutyl)cyclopentane-1,3-dione	[M+H] ⁺	169.09	C9H12O3	Beta-diketones	XRLGHWYZNGYZOW-UHFFFAOYSA-N	O=C(C)CCC1C(=O)CCC1=O
2949	20.152	397.07581	Propoxycarbazon	[M-H] ⁻	397.08234	C15H18N4O7S	Benzoic acid esters	JTHMVBQQLD1Y-UHFFFAOYSA-N	CCCC1=NN(C(C(=NS(C2=CC=CC=C2O)OC(=O)=O)O)C(N1C)=O
2950	20.158	205.08662	1-[4-hydroxy-3-(3-methylbut-2-enyl)phenyl]ethanone	[M+H] ⁺	205.08617	C13H16O2	Alkyl-phenylketones	QJAPFSSVKIZTMR-UHFFFAOYSA-N	O=C(C1=CC=C(O)C(=C1)CC=C(C)C)C
2951	20.167	182.08046	2-(4-aminotetrahydro-2H-pyran-4-yl)acetic acid	[M+H] ⁺	182.08	C7H13NO3	Pyranoid amino acids and derivatives	QRIAWCUEIMQLGG-UHFFFAOYSA-N	O=C(O)CC1(N)CCOCC1
2952	20.169	241.07086	lusianthridin	[M-H] ⁻	241.0719	C15H14O3	Hydrophenanthrenes	RDKD1PDDUFMMMT-UHFFFAOYSA-N	OC=1C=CC2=C(C1)CCC3=CC(OC)=CC(O)=C23
2953	20.173	132.10143	Leucine	[M+H] ⁺	132.1019	C6H13NO2	Leucine and derivatives	ROHPNLRQFUHQCH-UHFFFAOYNA-N	O=C(O)C(N)CC(C)C
2954	20.177	169.04903	2,6-Dimethoxyquinone	[M+H] ⁺	169.04953	C8H8O4	P-benzoquinones	OLBNOBQQZRLMP-UHFFFAOYSA-N	O=C1C=C(OC)C(=O)C(OC)=C1
2955	20.179	76.039	Acetohydroxamic acid	[M+H] ⁺	76.03931	C2H5NO2	Acetohydroxamic acids	RRUDCFGSUDOHG-UHFFFAOYSA-N	ON=C(O)C
2956	20.181	166.04961	Phthalamic acid	[M+H] ⁺	166.04987	C8H7NO3	Benzoic acids	CYMRPDYINXWJFU-UHFFFAOYSA-N	C1=CC=C(C(=C1)C(=N)O)C(=O)O
2957	20.189	182.11749	Homoveratrylamine	[M+H] ⁺	182.11755	C10H15NO2	Dimethoxybenzenes	ANOUKFYBOAKOIR-UHFFFAOYSA-N	O(C1=CC=C(C(=C1O)CCN)C
2958	20.19	103.04034	2-Hydroxyisobutyric acid	[M-H] ⁻	103.04007	C4H8O3	Alpha hydroxy acids and derivatives	BWLBGMLXKSTLSX-UHFFFAOYSA-N	O=C(O)C(O)C(C)C
2959	20.191	202.09972	(1S,2S)-2-(methylamino)-1-phenylpropan-1-ol hydrochloride	[M+H] ⁺	202.10001	C10H16ClNO	Phenylpropanes	BALXUFOVQVENTIU-KXNXZCPBSA-N	C1.CC(C=C1C=CC(C1)C(N)C
2960	20.194	511.46915	Gallamine	[M+H] ⁺	511.46909	C30H60N3O3	Phenol ethers	OZLPUNFCJDMJD-UHFFFAOYSA-N	CC[N+](CC)(CC)CCOC1=CC=CC(OC([N+](O)C)(CC)C)=C1OCC([N+](CC)(CC)C
2961	20.194	89.0237	GLYCERALDEHYDE	[M-H] ⁻	89.0239	C3H6O3	Monosaccharides	MNQXJOMYWMBOU-UHFFFAOYSA-N	O=CC(O)CO
2962	20.201	253.1801	ilicic acid	[M+H] ⁺	253.17999	C15H24O3	Eudesmane, isoeudesmane or cycloeudesmane	FXKCGBBUBCRPUS-QHSBEEBCSA-N	O=C(O)C(=C)C1CCC2(C)CCCC(O)C(C)C2C1
2963	20.204	99.04379	alpha-Methylene-gamma-butyrolactone	[M+H] ⁺	99.04405	C5H6O2	Gamma butyrolactones	GSLDEZOOSBFGP-UHFFFAOYSA-N	O=C1OCCC1=C
2964	20.204	207.06506	Citroten	[M+H] ⁺	207.065	C11H10O4	Coumarins and derivatives	NXJCRELRQHZBQA-UHFFFAOYSA-N	O=C1OC2=CC(OC)=CC(OC)=C2C=C1
2965	20.21	217.07001	Caffeine	[M+H] ⁺	217.07001	C8H10N4O2	Xanthines	RYVYLZVUV1JVGH-UHFFFAOYSA-N	O=C1C2=C(N=CN2C)N(C(=O)N1C)C

[illegible]

3009	20.79	164.99457	maltol	[M+H] ⁺	164.99486	C6H6O3	Pyranones and derivatives	XPCTZQVDEJYUGT-UHFFFAOYSA-N	O=C1C=COC(=C1O)C
3010	20.816	194.98166	Orotic Acid	[M+H] ⁺	194.98027	C5H4N2O4	Pyrimidinecarboxylic acids	PXQPEWDEAKTCGB-UHFFFAOYSA-N	O=C(O)C=1N=C(O)N=C(O)C1
3011	20.832	379.08411	Justicidin G	[M+H] ⁺	379.08124	C21H14O7	Lignols	VINGQMKGDIELG-UHFFFAOYSA-N	COC1=C2OCOC2=CC2=C(C3=C(C=C12)C(=O)OC3)C1=CC2=C(OC2)C=C1
3012	20.835	269.2471	methyl palmitoleate	[M+H] ⁺	269.2475	C17H32O2	Fatty acid methyl esters	IZFGRAGOVZCUFB-HJWRWDRZSA-N	O=C(OC)CCCCCCCC=CCCCCCC
3013	20.838	148.03912	Isatin	[M+H] ⁺	148.03931	C8H5NO2	Indolines	JXDYKVIHCLTXOP-UHFFFAOYSA-N	O=C1NC2=CC=CC=C2C1=O
3014	20.877	162.11195	L-Carnitine	[M+H] ⁺	162.11247	C7H15NO3	Carnitines	PHIQHXFUZVPYII-ZCFTWIBFSA-N	C[N+](C)(C)C[C=H](CC(=O)[O-])O
3015	20.885	123.05493	Nicotinamide	[M+H] ⁺	123.05529	C6H6N2O	Nicotinamides	DFPAKSUCGFDDF-UHFFFAOYSA-N	N=C(O)C=1C=NC=CC1
3016	20.89	261.18573	falcarindiol	[M+H] ⁺	261.18491	C17H24O2	Long-chain fatty alcohols	QW'CNQXNAFCBLLV-RCQSYPMMSA-N	OC(C#CC#CC(O)C=CCCCCCC)C=C
3017	20.894	236.01015	Pesticidel_Omethoate_C5H12N04PS_	[M+H] ⁺	236.011	C5H12N04PS	Secondary carboxylic acid amides	PZXOQEXFMJCDPG-UHFFFAOYSA-N	O=C(NC)CSP(=O)(OC)OC
3018	20.914	130.0658	Indole-3-carbinol	[M+H] ⁺	130.06512	C9H9NO	3-alkylindoles	IVYPNXXAYMYVSP-UHFFFAOYSA-N	OCC1=CNC2=CC=CC=C12
3019	20.951	251.99133	Pesticidel_Dimethoate_C5H12N03PS2_Phosphorodithioic acid, O,O-dimethyl S-[2-(methylamino)-2-oxoethyl] ester	[M+H] ⁺	251.989	C5H12N03PS2	Dithiophosphate O-esters	MCW'XGJITAZMZEV-UHFFFAOYSA-N	S=P(OC)(OC)SCC(O)=NC

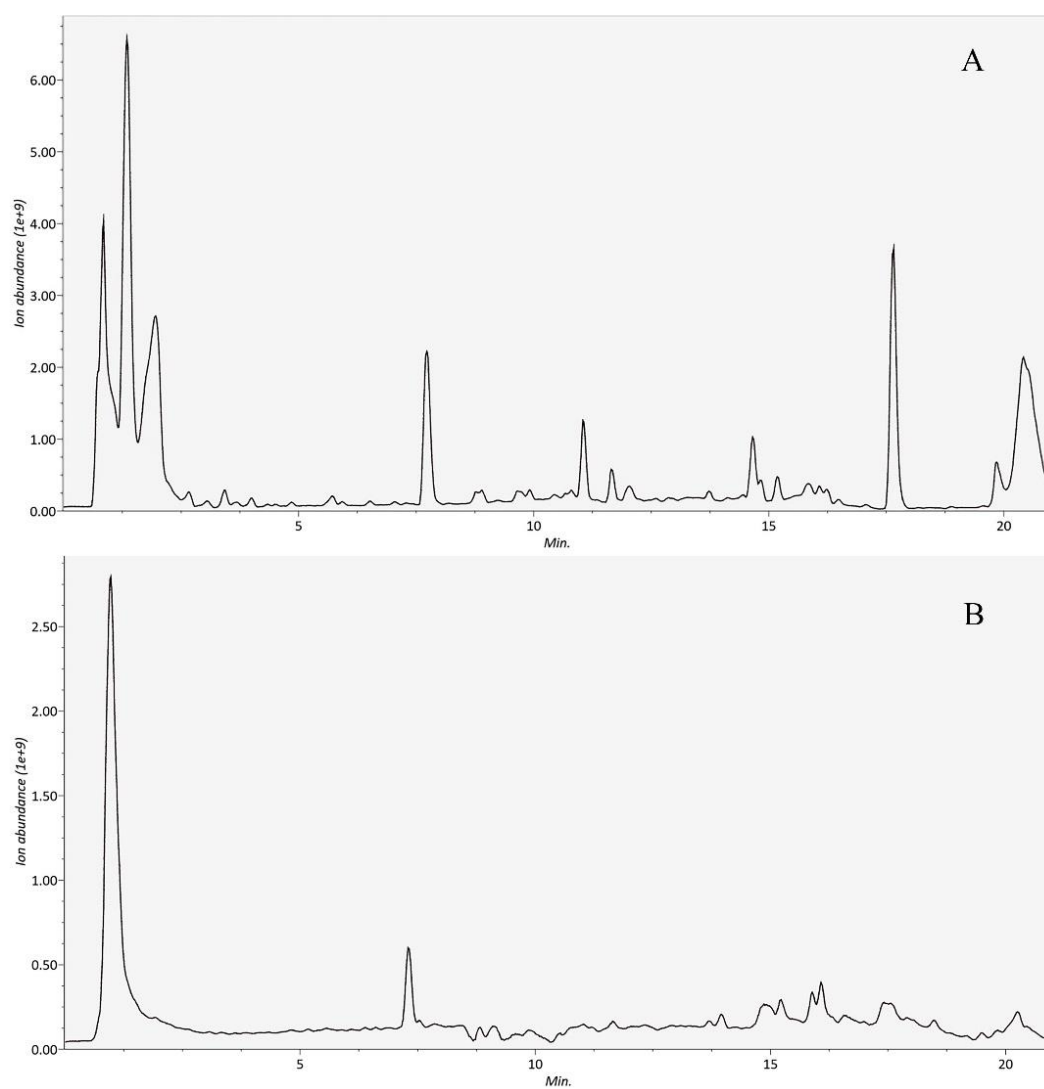


Figure S1. Total ion flow diagram in positive ion mode (**A**) and negative ion mode (**B**) of LC-MS/MS.