compounds

MDPI

Article

GC-MS Analysis and In Silico Approaches of *Indigofera heterantha* Root Oil Chemical Constituents

Muhammad Aurang Zeb [1,2,*], Taj Ur Rahman [3,*], Muhammad Sajid [2], Weilie Xiao [1,*], Syed Ghulam Musharraf [4], Shabana Bibi [5], Takashiro Akitsu [6] and Wajiha Liaqat [3]

1 Key Laboratory of Medicinal Chemistry for Natural Resource, Ministry of Education and Yunnan Province, School of Chemical Science and Technology, Yunnan University, Kunming 650091, China
2 Department of Biochemistry, Hazara University, Mansehra 21120, Pakistan; sajid931@hotmail.com
3 Department of Chemistry, Mohi-Ud-Din Islamic University, AJ&K 12080, Pakistan; gia_248@yahoo.com
4 H.E.J. Research Institute of Chemistry, ICCBS, University of Karachi, Karachi 75270, Pakistan; musharraf1977@yahoo.com
5 Yunnan Herbal Laboratory, School of Ecology and Environmental Sciences, Yunnan University, Kunming 650091, China; dazzling.grin@gmail.com
6 Department of Chemistry, Faculty of Science Division II, Tokyo University of Science, Tokyo 162-8601, Japan; akitsu2@rs.tus.ac.jp
* Correspondence: muhammad_aurangzeb@hotmail.com (M.A.Z.); taj_urrehman81@yahoo.co.uk (T.U.R.); xiaoweilie@ynu.edu.cn (W.X.); Tel.: +92-300-596-1093 (M.A.Z)

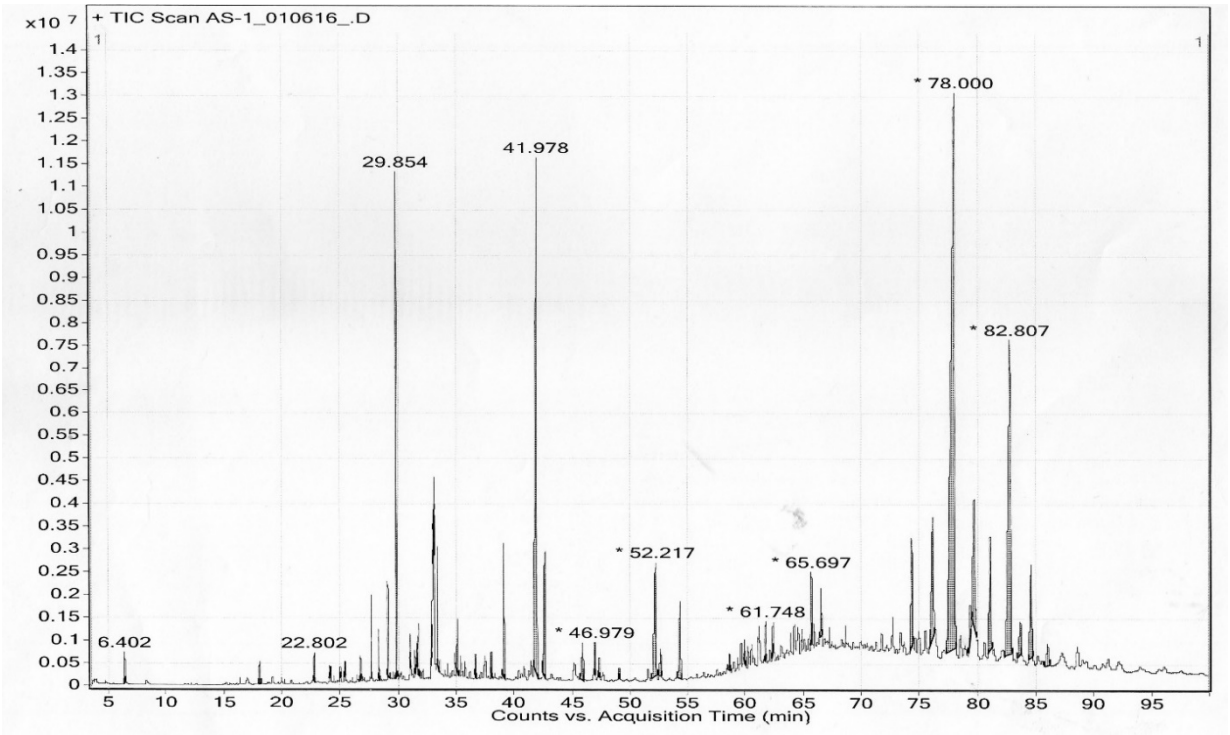

Figure S1. GC-MS chromatogram of IhA.

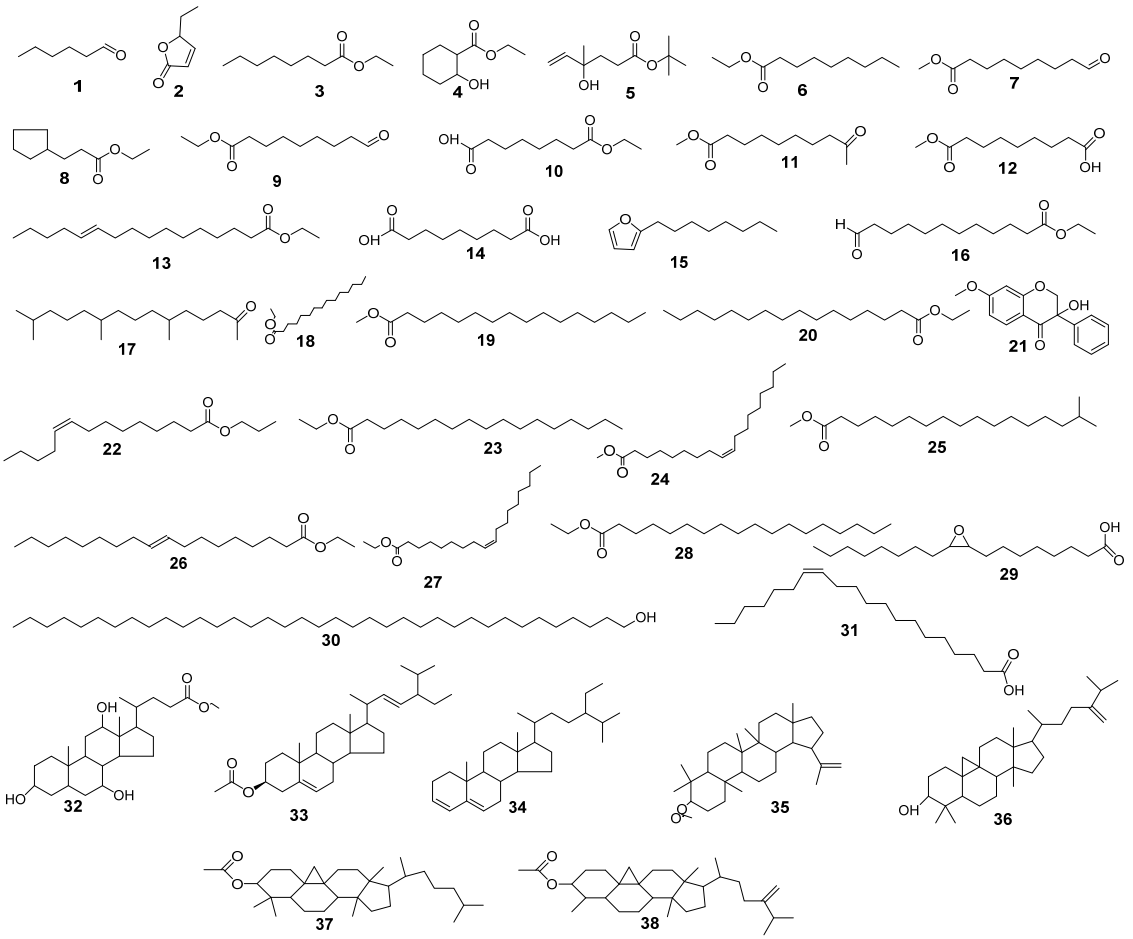

Figure S2. Structure of chemical constituent identified in sample IhA 1-38.

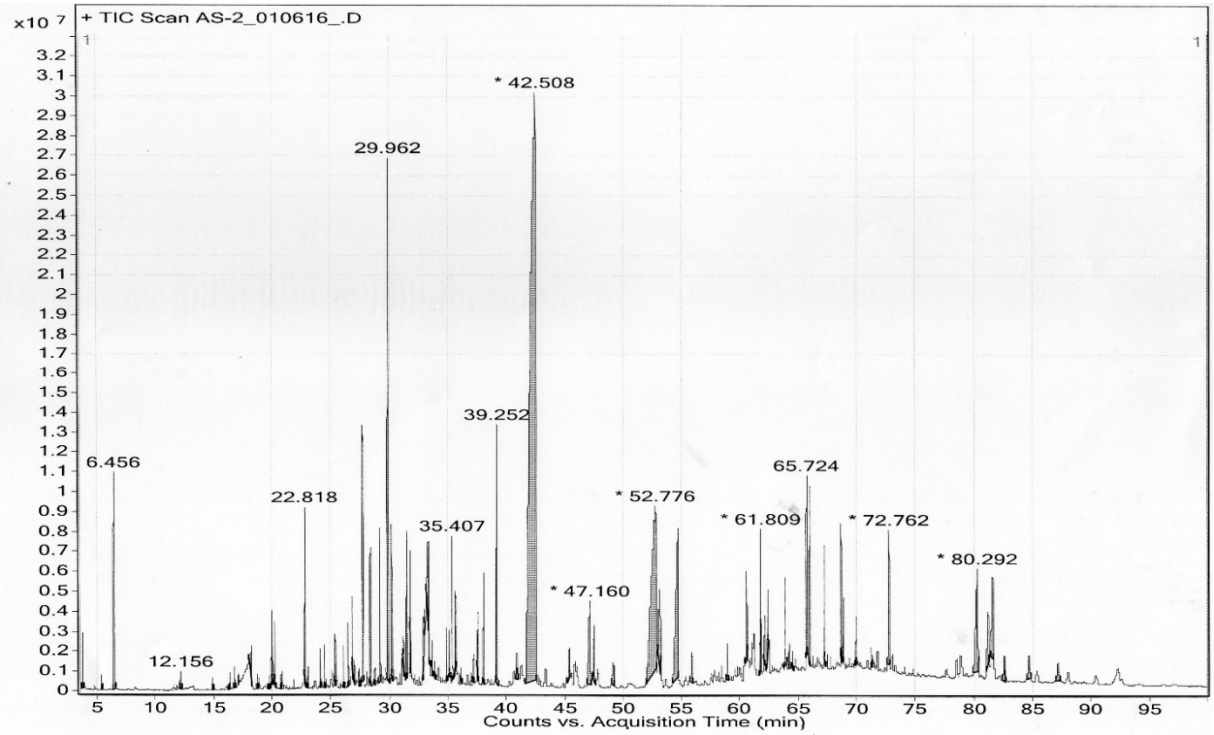

Figure S3. GC-MS chromatogram of IhB.

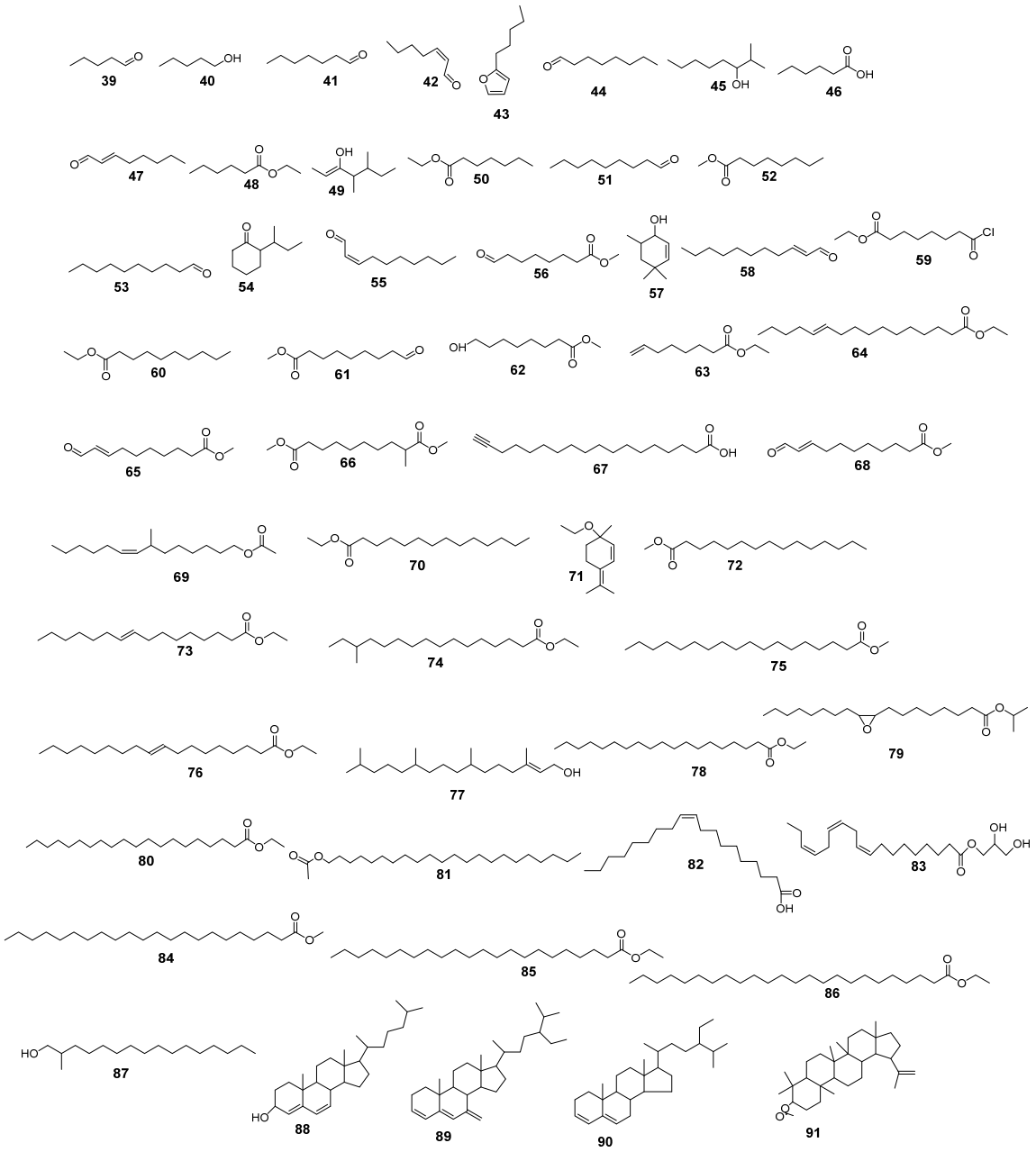

Figure S4. Structure of chemical constituent identified in IhB **39-91.**

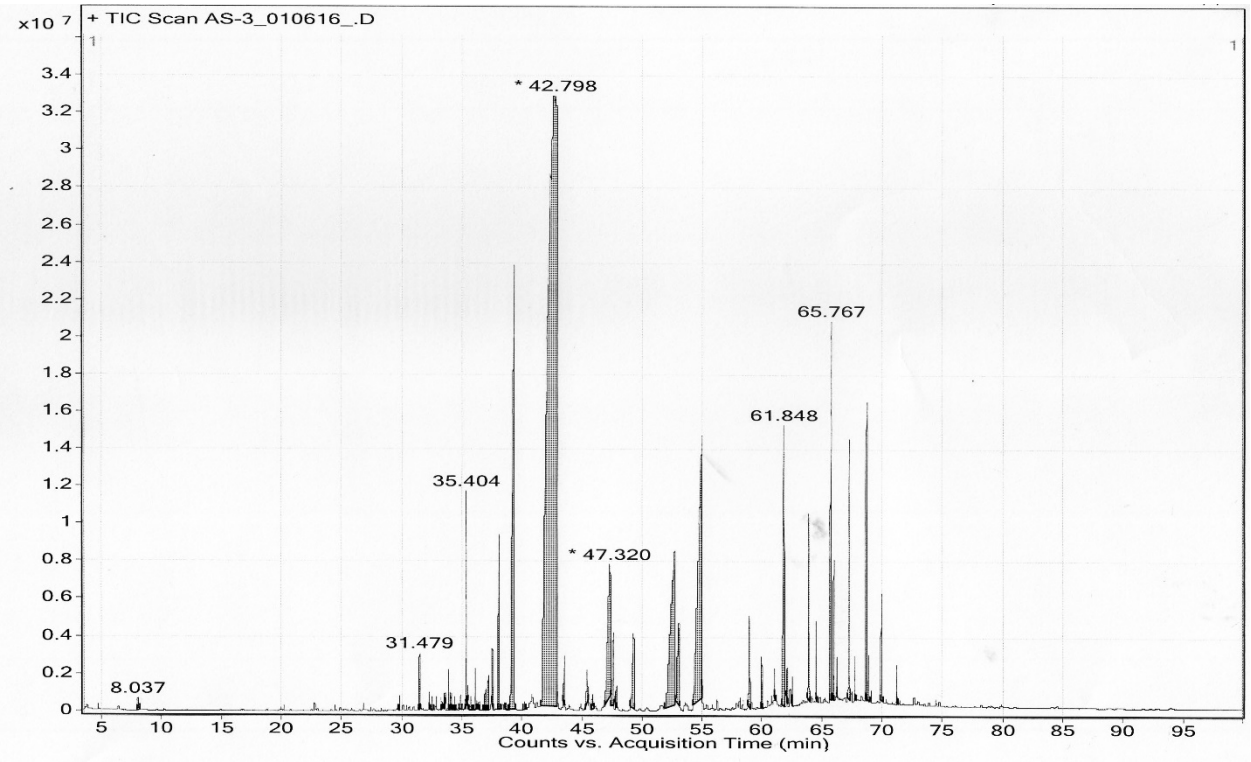

Figure S5. GC-MS chromatogram of IhC.

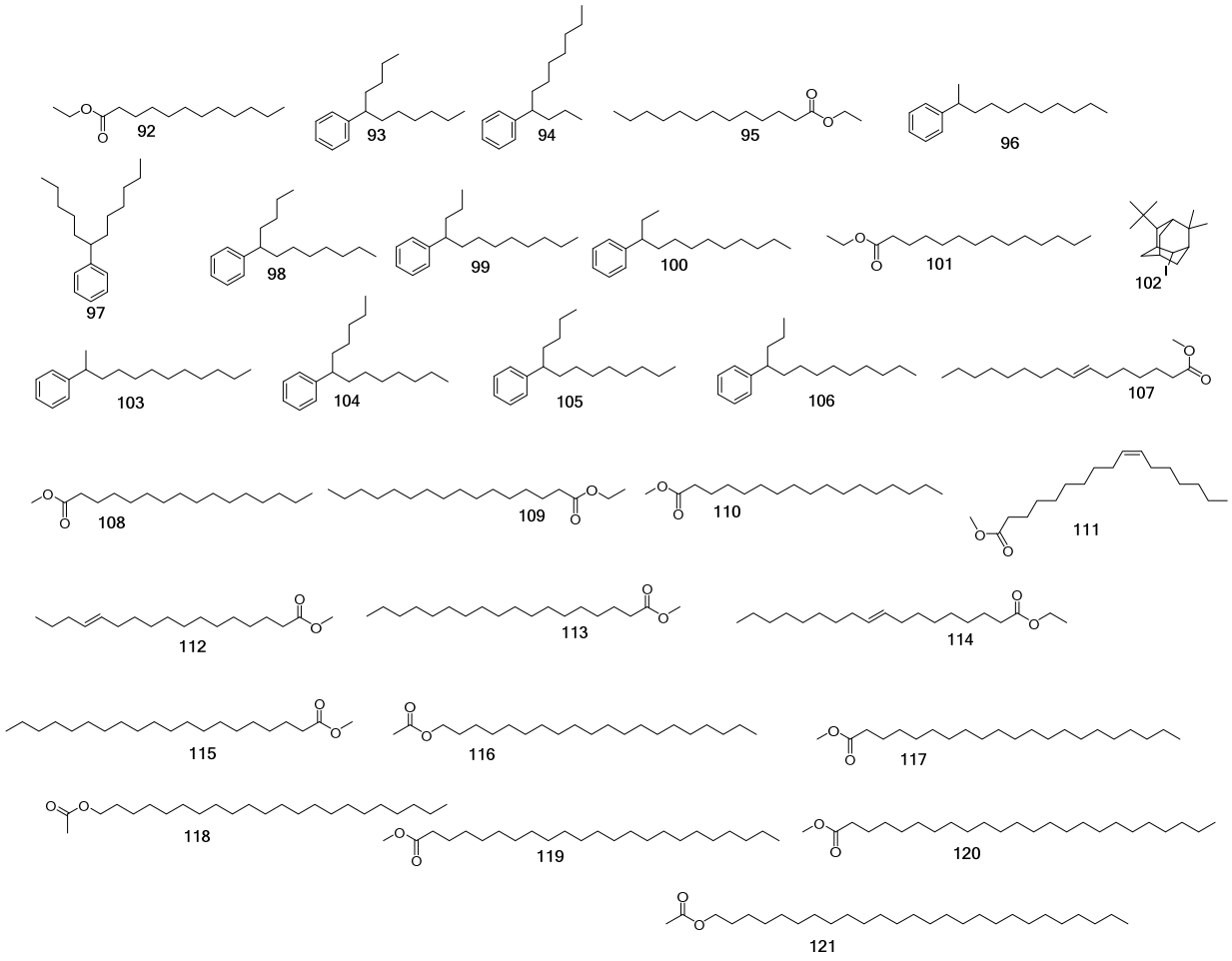

Figure S6. Structure of chemical constituent identified in IhC **92-121.**

Table S1. List of identified compounds in IhA.

S. No	Compound Name	Smile ID	MF	MW	CAS-NO	Docking Score against Alpha-Amylase	Docking Score against Alpha-Glucosidase
1	Hexanal	CCCCCC=O	$C_6H_{12}O$	100.09	66-25-1	−4.31266499	−4.99079609
2	2(5H)-Furanone, 5-ethyl-	O=C1OC(CC)C=C1	$C_6H_8O_2$	112.05	2407-43-4	−4.27905607	−4.9228735
3	Octanoic acid, ethyl ester	CCCCCCCC(OCC)=O	$C_{10}H_{20}O_2$	172.15	106-32-1	−5.485264	−6.54436159
4	Cyclohexanecarboxylic acid, 2-hydroxy-, ethyl ester	OC1CCCCC1C(OCC)=O	$C_9H_{16}O_3$	172.11	NA	−5.35771751	−6.12163973
5	4-Hydroxy-4-methylhex-5-enoic acid, tert.-butyl ester	C=CC(O)(C)CCC(OC(C)(C)C)=O	$C_{11}H_{20}O_3$	200.14	NA	−5.31870127	−6.61857176
6	Nonanoic acid, ethyl ester	CCOC(CCCCCCCC)=O	$C_{11}H_{22}O_2$	186.16	123-29-5	−5.48971462	−7.03561306
7	Nonanoic acid, 9-oxo-, methyl ester	COC(CCCCCCCC=O)=O	$C_{10}H_{18}O_3$	186.13	1931-63-1	−5.34788609	−6.91497087
8	3-Cyclopentylpropionic acid, ethyl ester	CCOC(CCC1CCCC1)=O	$C_{10}H_{18}O_2$	170.13	17931-64-5	−5.14433193	−6.46507025
9	Nonanoic acid, 9-oxo-, ethyl ester	CCOC(CCCCCCCC=O)=O	$C_{11}H_{22}O_3$	200.14	3433-16-7	−5.47711182	−7.22573948
10	Ethyl hydrogen suberate	OC(CCCCCCC(OCC)=O)=O	$C_{10}H_{18}O_4$	202.12	14113-01-0	−5.5131135	−6.88290501
11	Decanoic acid, 9-oxo-,methyl ester	COC(CCCCCCCC(C)=O)=O	$C_{11}H_{20}O_3$	200.14	2575-07-7	−5.56907511	−7.37059641
12	Nonanedioic acid, monomethyl ester	COC(CCCCCCCC(O)=O)=O	$C_{10}H_{18}O_4$	202.12	2104-19-0	−5.57761002	−7.15866947
13	(*E*)-11-Hexadecenoic acid, ethyl ester	CCCC/C=C/CCCCCCCCCC(OCC)=O	$C_{18}H_{34}O_2$	282.26	NA	−6.53635454	−8.24896908
14	Azelaic Acid	OC(CCCCCCCC(O)=O)=O	$C_9H_{16}O_4$	188.10	123-99-9	−5.33855867	−6.61465979
15	2-n-Octylfuran	CCCCCCCCC1=CC=CO1	$C_{12}H_{20}O$	180.15	4179-38-8	−5.1912365	−6.75099754
16	12-Oxododecanoic acid, ethyl ester	[H]C(CCCCCCCCCCC(OCC)=O)=O	$C_{14}H_{26}O_3$	242.19	NA	−5.92969322	−7.79101896
17	2-Pentadecanone, 6, 10, 14-trimethyl-	CC(C)CCCC(C)CCCC(C)CCCC(C)=O	$C_{18}H_{36}O$	268.29	502-69-2	−6.276546	−8.76418304
18	Pentadecanoic acid, ethyl ester	CCOC(CCCCCCCCCCCCCC)=O	$C_{17}H_{34}O_2$	270.45	41114-00-5	−6.46793652	−8.13654137
19	Hexadecanoic acid, methyl ester	COC(CCCCCCCCCCCCCCC)=O	$C_{17}H_{34}O_2$	270.26	112-39-0	−6.43439007	−7.87997484
20	Hexadecanoic acid, ethyl ester	CCCCCCCCCCCCCCCC(OCC)=O	$C_{18}H_{36}O_2$	284.27	628-97-7	−6.5955987	−8.75007629
21	3-Hydroxy-7-methoxy-3-phenyl-4-chromanone	COC1=CC=C(C(C(C2=CC=CC=C2)(O)CO3)=O)C3=C1	$C_{16}H_{14}O_4$	270.09	NA	−5.65472698	−7.05745459
22	n-Propyl 9-tetradecenoate	CCCC/C=C\CCCCCCCC(OCCC)=O	$C_{17}H_{32}O_2$	268.24	NA	−6.57248163	−7.82908297

S. No	Compound Name	Smile ID	MF	MW	CAS-NO	Docking Score against Alpha-Amylase	Docking Score against Alpha-Glucosidase
23	Heptadecanoic acid, ethyl ester	CCOC(CCCCCCCCCCCCCCCC)=O	$C_{19}H_{38}O_2$	298.29	14010-23-2	−6.77076817	−9.1118927
24	9- Octadecenoic acid(Z)-, methyl ester	COC(CCCCCCC/C=C\CCCCCCCC)=O	$C_{19}H_{36}O_2$	296.48	112-62-9	−6.59404707	−8.75259495
25	Heptadecanoic acid, 16-methyl-, methyl ester	COC(CCCCCCCCCCCCCCC(C)C)=O	$C_{19}H_{38}O_2$	298.28	5129-61-3	−6.80502367	−8.50299454
26	(E)-9-Octadecenoic acid ethyl ester	CCCCCCCC/C=C/CCCCCCCC(OCC)=O	$C_{20}H_{38}O_2$	310.29	6114-18-7	−7.15074158	−9.11989594
27	Ethyl Oleate	CCOC(CCCCCCC/C=C\CCCCCCCC)=O	$C_{20}H_{38}O_2$	310.51	111-62-6	−7.05047369	−8.97215843
28	Octadecanoic acid, ethyl ester	CCOC(CCCCCCCCCCCCCCCCCC)=O	$C_{20}H_{40}O_2$	312.30	111-61-5	−6.95561504	−8.56285477
29	Oxiraneoctanoic acid, 3-octyl-, cis-	CCCCCCCCC(O1)C1CCCCCCCC(O)=O	$C_{18}H_{34}O_3$	298.25	24560-98-3	−6.79044151	−8.45058346
30	1-Heptatriacotanol	CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCO	$C_{37}H_{76}O$	536.59	NA	Not Docked	Not Docked
31	cis-13-Eicosenoic acid	CCCCCC/C=C\CCCCCCCCCCCC(O)=O	$C_{20}H_{38}O_2$	310.29	17735-94-3	−6.93859339	−8.71145344
32	Ethyl iso-allocholate	CC(CCC(OCC)=O)C1CCC2C3C(O)CC4CC(O)CCC4(C)C3CC(O)C21C	$C_{26}H_{44}O_5$	436.32	NA	−6.57296314	−8.12089443
33	Stigmasta-5,22-dien-3-ol, acetate, 3β	CCC(/C=C/C(C(CCC1C(CC=C2C[C@H](C3)OC(C)=O)C(CC4)C23C)C14C)C)C(C)C	$C_{31}H_{50}O_2$	458.41	4651-48-3	−706750381	−4.1289
34	Stigmastan-3,5-diene	CC12C(C=CCC2)=CCC3C1CCC4(C)C3CCC4C(CCC(C(C)C)CC)C	$C_{29}H_{48}$	396.38	4970-37-0	−6.51642656	−7.713274
35	Lup-20(29)-en-3-ol, acetate, (3β)-	O=C(OC1CCC(C(CCC2C3(C)CCC4(C)C2C(C(C)=C)CC4)C3(C)CC5)(C)C5C1(C)C)C	$C_{32}H_{52}O_2$	468.40	1617-68-1	−6.550179	−5.50565338
36	9, 19-Cyclolanostan-3-ol, 24-methylene-, (3β)-	OC1CCC2(C3)C(CCC4C23CCC5(C)C4(C)CCC5C(CCC(C(C)C)=C)C)C1(C)C	$C_{31}H_{52}O$	440.40	1449-09-8	−6.87323761	−7.1842041
37	9, 19-Cyclolanostan-3-ol, acetate, (3β)-	CC(OC1C(C)(C)C(CCC2C3(C)C(C(C(CCCC(C)C)C)CC3)(C)CC4)C5(C24C5)CC1)=O	$C_{32}H_{54}O_2$	470.41	4575-74-0	−7.1042161	−7.37506437
38	9, 19- Cycloergost-24 (28)-en-3-ol, 4, 14-dimethyl-, acetate, (3β, 4α, 5α)-	CC(OC1C(C)C(CCC2C3(C)C(C(C(CCC(C(C)C)=C)C)CC3)(C)CC4)C5(C24C5)CC1)=O	$C_{32}H_{52}O_2$	468.40	10376-42-8	−7.17082357	−7.33567381

Table S2. List of identified compounds in IhB.

S. No	Compound Name	Smile ID	MF	MW	CAS-NO	Docking Score against Alpha-Amylase	Docking Score against Alpha-Glucosidase
39	Pentanal	CCCCC=O	$C_5H_{10}O$	86.07	110-62-3	−4.32325125	−4.93257999
40	1-Pentanol	CCCCCO	$C_5H_{12}O$	88.09	71-41-0	−3.87824464	−4.77271938
41	Heptanal	CCCCCCC=O	$C_7H_{14}O$	114.10	111-71-7	−4.03811502	−5.37939739
42	2-Heptenal, (Z)-	CCCC/C=C\C=O	$C_7H_{12}O$	112.09	57266-86-1	−4.48092222	−5.05973959
43	Furan, 2-pentyl-	CCCCCC1=CC=CO1	$C_9H_{14}O$	138.10	3777-69-3	−4.82865477	−5.86127758
44	Octanal	O=CCCCCCCC	$C_8H_{16}O$	128.12	124-13-0	−4.3046174	−5.86470699
45	3-Octanol, 2-methyl-	CCCCCC(C(C)C)O	$C_9H_{20}O$	144.15	26533-34-6	−4.78631783	−6.10976982
46	Hexanoic acid	CCCCCC(O)=O	$C_6H_{12}O_2$	116.08	142-62-1	−4.58951378	−5.33519888
47	2-Octenal, (E)-	O=C/C=C/CCCCC	$C_8H_{14}O$	126.10	2548-87-0	−4.2365818	−5.40431356
48	Hexanoic acid, ethyl ester	CCCCCC(OCC)=O	$C_8H_{16}O_2$	144.12	123-66-0	−4.6092453	−6.06598473
49	2-Hepten-3-ol, 4, 5-dimethyl-	C/C=C(C(C)C(C)CC)\O	$C_9H_{18}O$	142.14	55956-37-1	−4.5863843	−5.74066496
50	Heptanoic acid, ethyl ester	CCOC(CCCCCC)=O	$C_9H_{18}O_2$	158.13	106-30-9	−5.10614061	−5.75709963
51	Nonanal	CCCCCCCCC=O	$C_9H_{18}O$	142.14	124-19-6	−4.95700645	−5.70021248
52	Octanoic acid, methyl ester	COC(CCCCCCC)=O	$C_9H_{18}O_2$	158.13	111-11-5	−5.0524044	−5.58636475
53	Decanal	CCCCCCCCCC=O	$C_{10}H_{20}O$	156.15	112-31-2	−5.05645657	−6.73987961
54	2-Sec-Butylcyclohexanone	O=C1C(C(C)CC)CCCC1	$C_{10}H_{18}O$	154.14	14765-30-1	−5.03070116	−5.70856428
55	2-Decenal, (Z)-	O=C/C=C\CCCCCCC	$C_{10}H_{18}O$	154.14	2497-25-8	−4.95901442	−6.27999401
56	Methyl 8-oxooctanoate	O=CCCCCCCC(OC)=O	$C_9H_{16}O_3$	172.11	4316-48-7	−5.12607718	−6.21193838
57	4, 4, 6-Trimethyl-cyclohex-2-en-1-ol	CC1(C)CC(C)C(O)C=C1	$C_9H_{16}O$	140.12	NA	−4.52863503	−5.51741457
58	2-Undecenal	CCCCCCCC/C=C/C=O	$C_{11}H_{20}O$	168.15	2463-77-6	−4.93627262	−6.62668419
59	Octanoic acid, 8 – chloro -8- oxo-, ethyl ester	CCOC(CCCCCCC(Cl)=O)=O	$C_{10}H_{17}ClO_3$	220.09	14113-02-1	−5.67675924	−6.43358374
60	Decanoic acid, ethyl ester	CCOC(CCCCCCCCC)=O	$C_{12}H_{24}O_2$	200.18	110-38-3	−5.60674953	−7.02947712
61	Nonanoic acid, 9-oxo-, methyl ester	COC(CCCCCCCC=O)=O	$C_{10}H_{18}O_3$	186.13	1931-63-1	−5.29726171	−6.27741861
62	Methyl 8-hydroxyoctanoate	OCCCCCCCC(OC)=O	$C_9H_{18}O_3$	174.12	NA	−5.04441357	−6.31654358
63	7-Octenoic acid, ethyl ester	C=CCCCCCC(OCC)=O	$C_{10}H_{18}O_2$	170.13	35194-38-8	−5.21281576	−5.88366032
64	E-11-Hexadecenoic acid, ethyl ester	CCCC/C=C/CCCCCCCCCC(OCC)=O	$C_{18}H_{34}O_2$	282.26	NA	−6.50866795	−8.24960423
65	Methyl 10-oxo-8-decenoate	O=C/C=C/CCCCCCC(OC)=O	$C_{11}H_{18}O_3$	198.13	65114-83-2	−5.52289963	−6.80319262

S. No	Compound Name	Smile ID	MF	MW	CAS-NO	Docking Score against Alpha-Amylase	Docking Score against Alpha-Glucosidase
66	Dimethyl 2-methyldecane-1, 10-dioate	COC(CCCCCCCC(C)C(OC)=O)=O	$C_{13}H_{24}O_4$	244.17	NA	−6.10659981	−7.56790543
67	17-Octadecynoic acid	OC(CCCCCCCCCCCCCCCC#C)=O	$C_{18}H_{32}O_2$	280.24	34450-18-5	−6.43764019	−8.18279076
68	Methyl 11-oxo-9-undecenoate	O=C/C=C/CCCCCCCC(OC)=O	$C_{12}H_{20}O_3$	212.14	53613-55-1	−5.65583229	−6.90458632
69	7- Methyl - Z- tetradecen- 1- ol-acetate	CCCCC/C=C\C(C)CCCCCCOC(C)=O	$C_{17}H_{32}O_2$	268.24	NA	−6.44342041	−8.32530499
70	Tetradecanoic acid, ethyl ester	CCOC(CCCCCCCCCCCCC)=O	$C_{16}H_{32}O_2$	256.24	24-06-1	−6.22171164	−7.88299227
71	6-Octadiene, 3-ethoxy-3, 7-dimethyl-	C/C(C)=C1CCC(C)(OCC)C=C/1	$C_{12}H_{20}O$	180.15	NA	−5.12247133	−6.11779451
72	Pentadecanoic acid, methyl ester	COC(CCCCCCCCCCCCCC)=O	$C_{16}H_{32}O_2$	256.24	7132-64-1	−6.18482256	−8.04787731
73	Ethyl 9-hexadecenoate	CCCCCC/C=C/CCCCCCCC(OCC)=O	$C_{18}H_{34}O_2$	282.26	54546-22-4	−6.36167288	−8.08851337
74	Ethyl 14-methyl-hexadecanoate	CCC(C)CCCCCCCCCCCC(OCC)=O	$C_{19}H_{38}O_2$	298.29	NA	−6.75107527	−8.20447445
75	Octadecenoic acid, methyl ester	COC(CCCCCCCCCCCCCCCCC)=O	$C_{19}H_{38}O_2$	298.29	NA	−6.98113012	−8.40727997
76	(E) -9- Octadecenoic acid ethyl ester	CCCCCCCC/C=C/CCCCCCCC(OCC)=O	$C_{20}H_{38}O_2$	310.29	6114-18-7	−6.87963486	−8.37716389
77	3, 7, 11, 15- Tetramethyl -2-hexadecen-1 -ol	CC(C)CCCC(C)CCCC(C)CCC/C(C)=C/CO	$C_{20}H_{40}O$	296.31	102608-53-7	−7.20854521	−8.05761528
78	Nonadecanoic acid, ethyl ester	CCCCCCCCCCCCCCCCCCC(OCC)=O	$C_{21}H_{42}O_2$	326.32	18281-04-4	−7.19974422	−9.01764488
79	Octadecanoic acid,9 ,10-epoxy-, isopropyl ester	CCCCCCCCC1C(O1)CCCCCCCC(OC(C)C)=O	$C_{21}H_{40}O_3$	340.30	NA	−6.90465403	−9.27101898
80	Eicosanoic acid, ethyl ester	CCCCCCCCCCCCCCCCCCCC(OCC)=O	$C_{22}H_{44}O_2$	340.33	18281-05-5	−7.15885353	−8.50954723
81	1-Docosanol, acetate	O=C(C)OCCCCCCCCCCCCCCCCCCCCC	$C_{24}H_{48}O_2$	368.37	822-26-4	−7.39843893	−9.11747551
82	cis-10-Nonadecenoic acid	CCCCCCCC/C=C\CCCCCCCCC(O)=O	$C_{19}H_{36}O_2$	296.27	73033-09-7	−6.76501608	−8.4207592
83	9, 12, 15- Octadecatrienoic acid, 2, 3-dihydroxypropyl ester, (Z, Z, Z)-	CC/C=C\C/C=C\C/C=C\CCCCCCCC(OCC(O)CO)=O	$C_{21}H_{36}O_4$	352.26	NA	−6.97605228	−9.59869957
84	Docosanoic acid, methyl ester	CCCCCCCCCCCCCCCCCCCCCC(OC)=O	$C_{23}H_{46}O_2$	354.35	929-77-1	−7.36427069	−8.77867508
85	Docosanoic acid, ethyl ester	CCCCCCCCCCCCCCCCCCCCCC(OCC)=O	$C_{24}H_{48}O_2$	368.37	5908-87-2	−7.12757349	−9.34544277
86	Ethyl tetracosanoate	O=C(OCC)CCCCCCCCCCCCCCCCCCCCCC	$C_{26}H_{52}O_2$	396.40	24634-95-5	−8.25968075	−9.31482697
87	1-Hexadecanol, 2-methyl-	CCCCCCCCCCCCCCC(C)CO	$C_{17}H_{36}O$	256.28	2490-48-4	−6.16457653	−8.13131428

S. No	Compound Name	Smile ID	MF	MW	CAS-NO	Docking Score against Alpha-Amylase	Docking Score against Alpha-Glucosidase
88	Cholesta-4,6-dien-3-ol, (3β)-	OC1CCC2(C)C(C=CC3C2CCC4(C)C3CCC4C(CCCC(C)C)C)=C1	$C_{27}H_{44}O$	384.34	14214-69-8	−6.55595922	−6.86098099
89	Stigmasta-3,5-dien-7-one	CC12C(C=CCC1)=CC(C3C2CCC4(C)C3CCC4C(CCC(CC)C(C)C)C)=C	$C_{29}H_{46}O$	410.35	NA	−6.19042683	−7.28196764
90	Stigmastan-3,5-dien	CC12C(C=CCC2)=CCC3C1CCC4(C)C3CCC4C(C)CCC(C(C)C)CC	$C_{29}H_{48}$	396.38	NA	−6.40985394	−7.53033066
91	Lup- 20 (29)- en-3 -ol, acetate, (3β) -	O=C(OC1CCC(C(CCC2C3(C)CCC4(C)C2C(C(C)=C)CC4)C3(C)CC5)(C)C5C1(C)C)C	$C_{32}H_{52}O_2$	468.40	1617-68-1	−6.93653917	−5.68568516

Table S3. List of identified compounds in IhC.

S. No	Compound Name	Smile ID	MF	MW	CAS-NO	Docking Score against Alpha-Amylase	Docking Score against Alpha-glucosidase
92	Dodecanoic acid, ethyl ester	CCOC(CCCCCCCCCCC)=O	$C_{14}H_{28}O_2$	228.21	106-33-2	−5.71854591	−7.29325151
93	Benzene, (1-butylheptyl)-	CCCCC(C1=CC=CC=C1)CCCCCC	$C_{17}H_{28}$	232.22	4537-15-9	−5.47292233	−7.02896166
94	Benzene, (1-propyloctyl)-	CCCC(C1=CC=CC=C1)CCCCCCC	$C_{17}H_{28}$	232.22	4536-86-1	−5.93453646	−7.02986383
95	Ethyl tridecanoate	CCCCCCCCCCCCC(OCC)=O	$C_{15}H_{30}O_2$	242.22	28267-29-0	−6.41103649	−8.04990196
96	Benzene, (1-methyldecyl)-	CCCCCCCCCC(C)C1=CC=CC=C1	$C_{17}H_{28}$	232.22	4536-88-3	−5.64050913	−7.06706905
97	Benzene, (1-pentylheptyl)-	CCCCCC(CCCCCC)C1=CC=CC=C1	$C_{18}H_{30}$	246.23	2719-62-2	−5.75403023	−6.58053255
98	Benzene, (1-butyloctyl)-	CCCCC(CCCCCCC)C1=CC=CC=C1	$C_{18}H_{30}$	246.23	2719-63-3	−6.01381588	−7.09059381
99	Benzene, (1-propylnonyl)-	CCCC(CCCCCCCC)C1=CC=CC=C1	$C_{18}H_{30}$	246.23	2719-64-4	−5.88937235	−7.27823877
100	Benzene, (1-ethyldecyl)-	CCC(CCCCCCCCC)C1=CC=CC=C1	$C_{18}H_{30}$	246.23	2400-00-2	−5.80677986	−7.47779083
101	Tetra decanoic acid, ethyl ester	CCOC(CCCCCCCCCCCCC)=O	$C_{16}H_{32}O_2$	256.24	124-06-1	−6.42799234	−8.04944801
102	9-t-Butyl-4-iodo-2,2-dimethyladamantane	I[C@@H]1[C@H](C2)C(C)(C)[C@H]3[C@H](C(C)(C)C)[C@@H]1C[C@@H]2C3	$C_{16}H_{27}I$	346.12	NA	−5.0323143	−6.39810419
103	Benzene, (1-methylundecyl)-	CC(C1=CC=CC=C1)CCCCCCCCCC	$C_{18}H_{30}$	246.23	2719-61-1	−6.17118549	−7.12832546
104	Benzene, (1-pentyloctyl)-	CCCCCCCC(CCCCC)C1=CC=CC=C1	$C_{19}H_{32}$	260.25	4534-49-0	−5.96058226	−7.64328575
105	Benzene, (1-butylnonyl)-	CCCCC(CCCCCCCC)C1=CC=CC=C1	$C_{19}H_{32}$	260.25	4534-50-3	−5.8515029	−7.66689396
106	Benzene, (1-propyldecyl)-	CCCC(CCCCCCCCC)C1=CC=CC=C1	$C_{19}H_{32}$	260.25	4534-51-4	−6.13278246	−7.51954603
107	7-Hexadecenoic acid, methyl ester, (Z)-	CCCCCCCC/C=C/CCCCCC(OC)=O	$C_{17}H_{32}O_2$	268.24	56875-67-3	−6.34425068	−7.73232126

S. No	Compound Name	Smile ID	MF	MW	CAS-NO	Docking Score against Alpha-Amylase	Docking Score against Alpha-glucosidase
108	Hexadecenoic acid, methyl ester	COC(CCCCCCCCCCCCCCC)=O	$C_{17}H_{34}O_2$	270.26	NA	−6.58620548	−8.07269287
109	Hexadecenoic acid, ethyl ester	CCCCCCCCCCCCCCCC(OCC)=O	$C_{18}H_{36}O_2$	284.27	NA	−6.41025019	−8.1135788
110	Heptadecanoic acid, methyl ester	COC(CCCCCCCCCCCCCCCC)=O	$C_{18}H_{36}O_2$	284.27	1731-92-6	−6.44106197	−8.43236828
111	cis-10-Heptadecenoic acid, methyl ester	CCCCCC/C=C\CCCCCCCCC(OC)=O	$C_{18}H_{34}O_2$	282.26	NA	−6.84707069	−8.07504368
112	trans-13-Octadecenoic acid, methyl ester	CCC/C=C/CCCCCCCCCCCC(OC)=O	$C_{19}H_{36}O_2$	296.27	NA	−6.73890829	−8.29063797
113	Octadecanoic acid, methyl ester	CCCCCCCCCCCCCCCCCC(OC)=O	$C_{19}H_{38}O_2$	298.50	112-61-8	−6.91980696	−8.48671246
114	(E) -9- Octadecenoic acid, ethyl ester	CCCCCCCC/C=C/CCCCCCCC(OCC)=O	$C_{20}H_{38}O_2$	310.29	6114-18-7	−7.27659082	−8.62704754
115	Eicosanoic acid, methyl ester	COC(CCCCCCCCCCCCCCCCCCC)=O	$C_{21}H_{42}O_2$	326.32	1120-28-1	−7.16555834	−8.67712688
116	Eicosyl acetate	CC(OCCCCCCCCCCCCCCCCCCCC)=O	$C_{22}H_{44}O_2$	340.33	822-24-2	−6.92805481	−8.52007294
117	Heneicosanoic acid, methyl ester	COC(CCCCCCCCCCCCCCCCCCCC)=O	$C_{22}H_{44}O_2$	340.33	6064-90-0	−7.13835382	−8.73273849
118	Docosano, acetate	O=C(C)OCCCCCCCCCCCCCCCCCCCCC	$C_{24}H_{48}O_2$	368.37	NA	−7.71306992	−8.78453636
119	Tricosanoic acid, methyl ester	CCCCCCCCCCCCCCCCCCCCCC(OC)=O	$C_{24}H_{48}O_2$	368.37	2433-97-8	−7.57870722	−9.3228426
120	Tetracisanoic acid, methyl ester	COC(CCCCCCCCCCCCCCCCCCCCC)=O	$C_{25}H_{50}O_2$	382.38	NA	−7.7322011	−8.98537827
121	Hexacosyl acetate	CC(OCCCCCCCCCCCCCCCCCCCCCC)=O	$C_{28}H_{56}O_2$	424.43	822-32-2	−8.2944994	−9.73762512