Nitrogen enriched solid-state cultivation for the overproduction of azaphilone red pigments by *Penicillium sclerotiorum* SNB-CN111

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Table S1: Cluster A features annotated by MS/MS database query. In-house database was built upon annotations from Hebra et al.[1]

ClusterA									
$[M+H]^+$	**Error (ppm)**	**Formula**	**Name**	**Database**	**Cosine score**	**Annotation**	**Ref**	**$\varepsilon(\lambda_{nm})$**	**Minimal condition**
357.1706	-2.7	$C_{21}H_{24}O_5$		In-house	0.97	Level 2	[1,2]		CZK
359.1863	-2.8	$C_{21}H_{26}O_5$		In-house	0.72	Level 3	[1]		PD
363.1349	-2.4	$C_{20}H_{23}ClO_4$		In-house	0.88	Level 2	[1]		CZK
371.1859	-1.6	$C_{22}H_{26}O_5$		In-house	0.85	Level 2	[1]		PD
385.2013	-0.9	$C_{23}H_{28}O_5$		In-house	0.86	Level 3	[1]		PD
391.1315	-2.1	$C_{21}H_{23}ClO_5$	Sclerotiorin	MS-Dial	0.84	Level 1	[3,4]	12000(445)	CZK
395.1633	-3.4	$C_{21}H_{27}ClO_5$	Isochromophilone IV	MS-Dial	0.66	Level 2	[5]	39400(390)	CZK
399.2177	-2.8	$C_{24}H_{30}O_5$		In-house	0.9	Level 3	[1]		PD
405.1473	-2.4	$C_{22}H_{25}ClO_5$	Sclerketide B	In-house	0.95	Level 2	[6]	17(332)	PD
407.1261	-1.3	$C_{21}H_{23}ClO_6$		In-house	0.73	Level 3	[1]		PD
419.163	-2.4	$C_{23}H_{27}ClO_5$		In-house	0.93	Level 3	[1]		PD
433.1785	-2.0	$C_{24}H_{29}ClO_5$		In-house	0.7	Level 3	[1]		PD
435.1578	-2.1	$C_{23}H_{27}ClO_6$		In-house	0.63	Level 3	[1]		PD

Level 0 corresponds annotations from isolated pure compounds; level 1 to annotations by comparison with standards; level 2 to putative annotations (e.g., MS/MS library comparison or tentative structure); level 3 to a chemical class assignment

Figure S1: Spectral comparison with databases of cluster A annotated molecules with their theoretical protonated *m/z*.

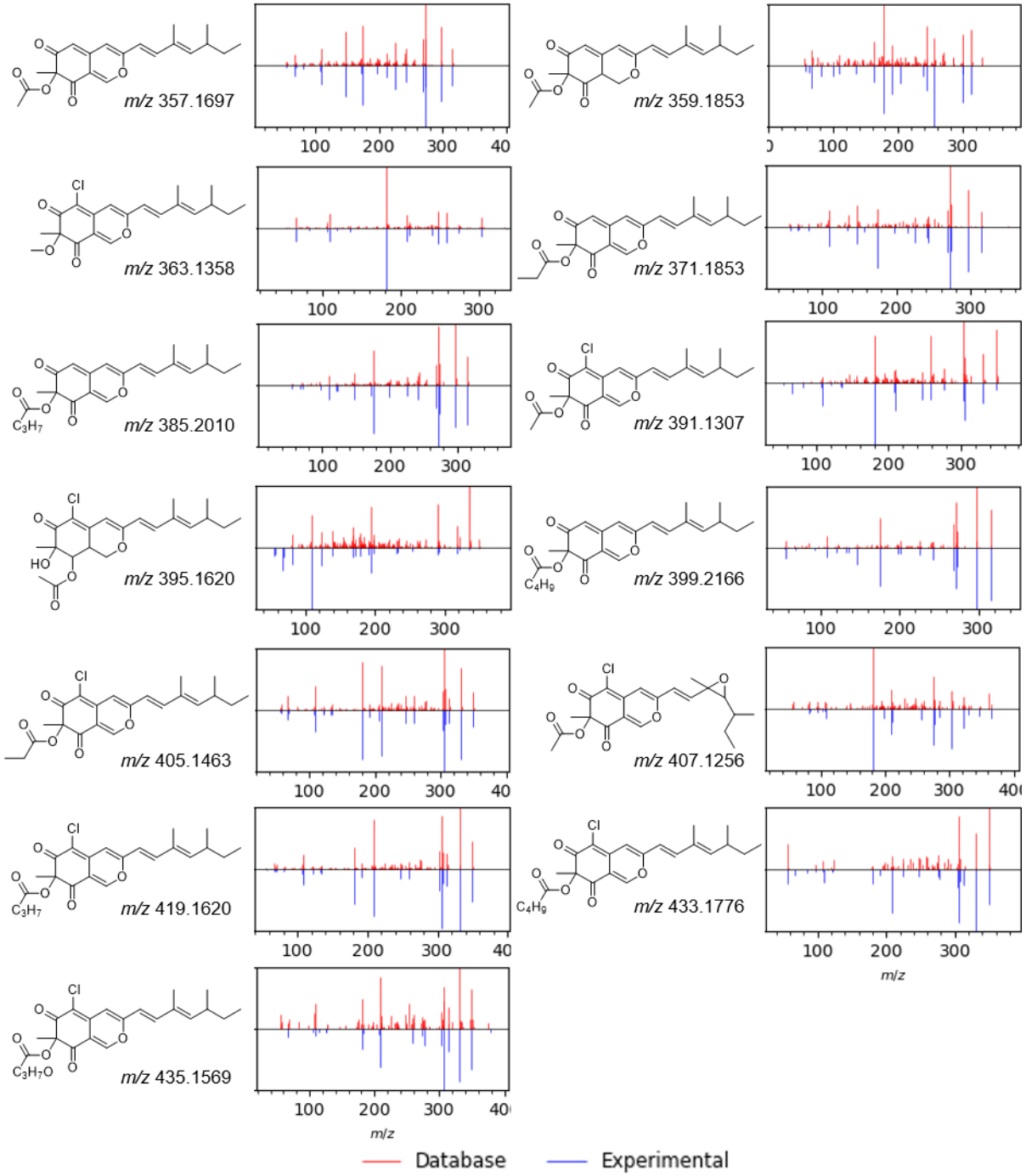

Table S2: Cluster B features annotated by MS/MS database query. In-house database was built upon annotations from Hebra et al.[1]

ClusterB									
$[M+H]^+$	**Error (ppm)**	**Formula**	**Name**	**Database**	**Cosine score**	**Annotation**	**Ref**	**$\varepsilon(\lambda_{nm})$**	**Minimal condition**
383.1865	-3.1	$C_{23}H_{26}O_5$	Ochrephilone	MS-Dial	0.8	Level 2	[7]	22000(415)	CZK
399.1805	-0.7	$C_{23}H_{26}O_6$		In-house	0.9	Level 3	[1]		CZK
417.1471	-1.9	$C_{23}H_{25}ClO_5$	Isochromophilone I	GNPS	0.71	Level 2	[8]	15700(412)	CZK

Level 0 corresponds annotations from isolated pure compounds; level 1 to annotations by comparison with standards; level 2 to putative annotations (e.g., MS/MS library comparison or tentative structure); level 3 to a chemical class assignment

Figure S2: Spectral comparison with databases of cluster B annotated molecules with their theoretical protonated *m/z*.

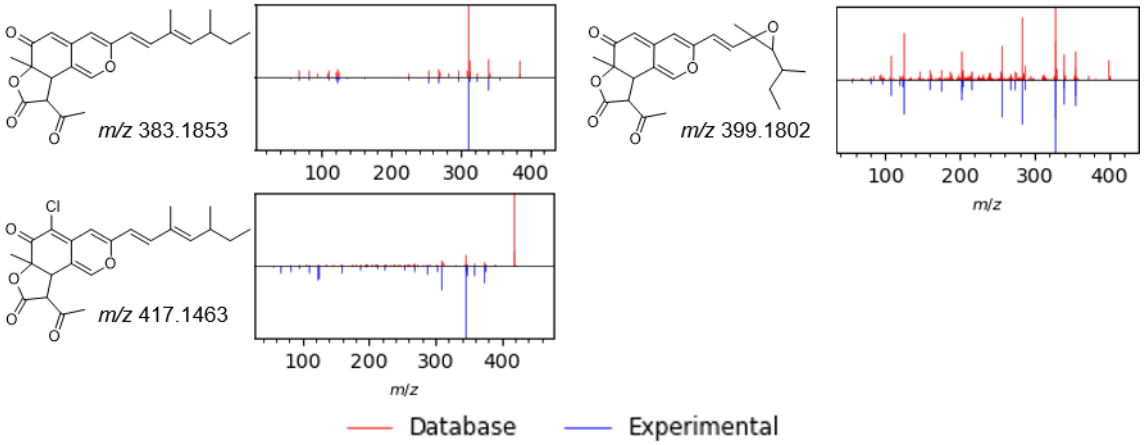

Table S3: Cluster C features annotated by MS/MS database query. In-house database was built upon annotations from Hebra et al.[1]

ClusterC									
$[M+H]^+$	Error (ppm)	Formula	Name	Database	Cosine score	Annotation	Ref	$\varepsilon(\lambda_{nm})$	Minimal condition
356.1859	-0.8	$C_{21}H_{25}NO_4$		In-house	0.94	Level 2	[1]		PD
362.1527	-2.6	$C_{20}H_{24}ClNO_3$		In-house	0.94	Level 2	[1]		YE
390.1469	-0.6	$C_{21}H_{24}ClNO_4$	Sclerotioramine	MONA	0.94	Level 1	[1,9]	20 000(331)	PD
404.1626	-0.7	$C_{22}H_{26}ClNO_4$		In-house	0.99	Level 2	[1]		PD
406.1420	-1.0	$C_{21}H_{24}ClNO_5$		In-house	0.95	Level 3	[1]		YE
418.1786	-1.5	$C_{23}H_{28}ClNO_4$		In-house	0.97	Level 3	[1]		YE
432.1946	-2.3	$C_{24}H_{30}ClNO_4$		In-house	0.93	Level 3	[1]		PD
434.1739	-2.4	$C_{23}H_{28}ClNO_5$		In-house	0.91	Level 3	[1]		PD

Level 0 corresponds annotations from isolated pure compounds; level 1 to annotations by comparison with standards; level 2 to putative annotations (e.g., MS/MS library comparison or tentative structure); level 3 to a chemical class assignment

Figure S3: Spectral comparison of cluster C molecules with databases with their theoretical protonated *m/z*.

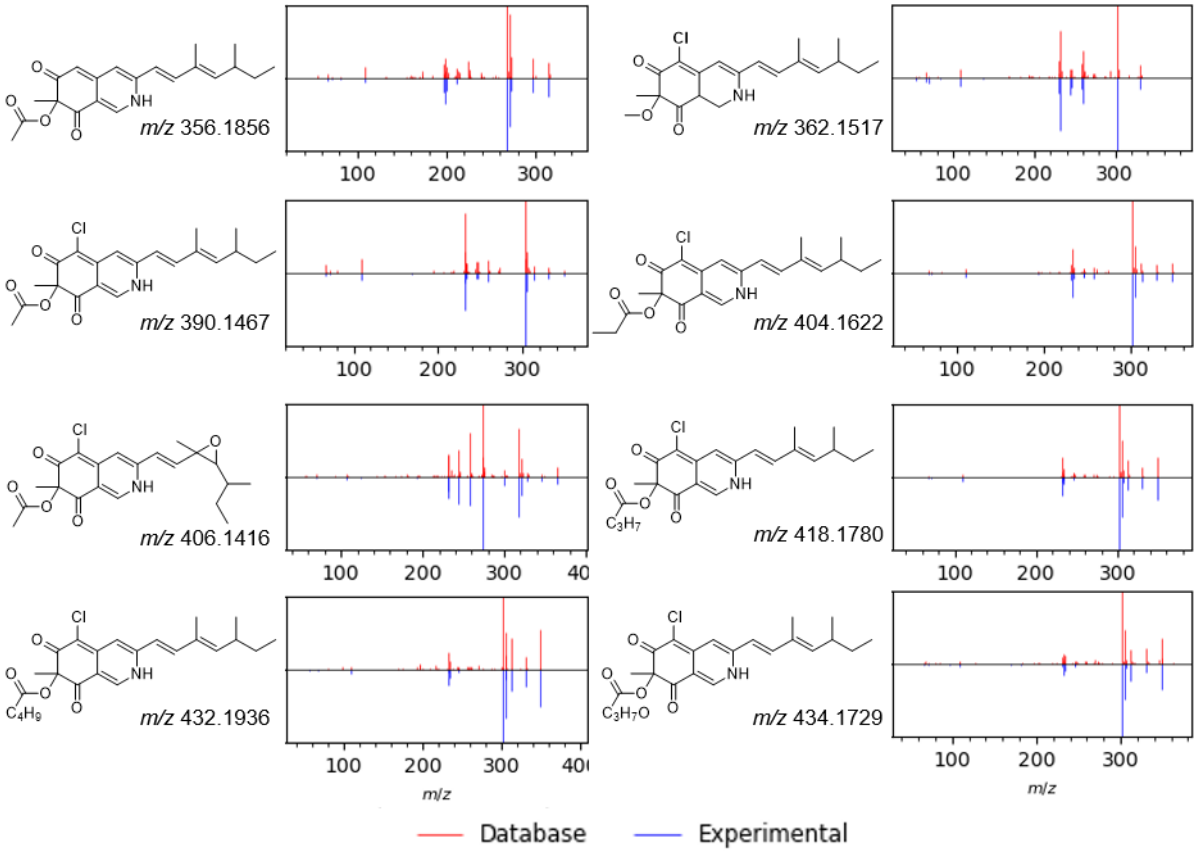

Table S4 : Cluster D features annotated by MS/MS database query. In-house database was built upon annotations from Hebra et al.[1]

ClusterD									
$[M+H]^+$	Error (ppm)	Formula	Name	Database	Cosine score	Annotation	Ref	$\varepsilon(\lambda_{nm})$	Minimal condition
400.2138	-4.9	$C_{23}H_{29}NO_5$		In-house	0.81	Level 2	[1]		PD
434.1732	-0.8	$C_{23}H_{28}ClNO_5$	Isochromophilone VI	MS-Dial	0.83	Level 1	[5]	23400(370)	CZK
448.1526	-1.0	$C_{23}H_{26}ClNO_6$		In-house	0.88	level 2	[1]		YE
448.1903	-4.0	$C_{24}H_{30}ClNO_5$		In-house	0.91	Level 2	[1]		YE
460.1530	-1.9	$C_{24}H_{26}ClNO_6$		In-house	0.87	Level 3	[1]		PD
476.1840	-1.2	$C_{25}H_{30}ClNO_6$	Isochromophilone IX	MONA	0.88	Level 2	[10]	No data	YE
478.1617	2.1	$C_{24}H_{28}ClNO_7$		In-house	0.9	Level 3	[1]		YE
490.1997	-1.2	$C_{26}H_{32}ClNO_6$		In-house	0.91	Level 3	[1]		YE
505.1737	-0.2	$C_{25}H_{29}ClN_2O_7$		In-house	0.93	Level 3	[1]		PD
519.1902	-1.8	$C_{26}H_{31}ClN_2O_7$		In-house	0.94	Level 3	[1]		YE
520.1735	-0.5	$C_{26}H_{30}ClNO_8$		In house	0.83	Level 3	[1]		PD

Level 0 corresponds annotations from isolated pure compounds; level 1 to annotations by comparison with standards; level 2 to putative annotations (e.g., MS/MS library comparison or tentative structure); level 3 to a chemical class assignment

Figure S4: Spectral comparison of cluster D molecules with databases and their theoretical protonated *m/z*.

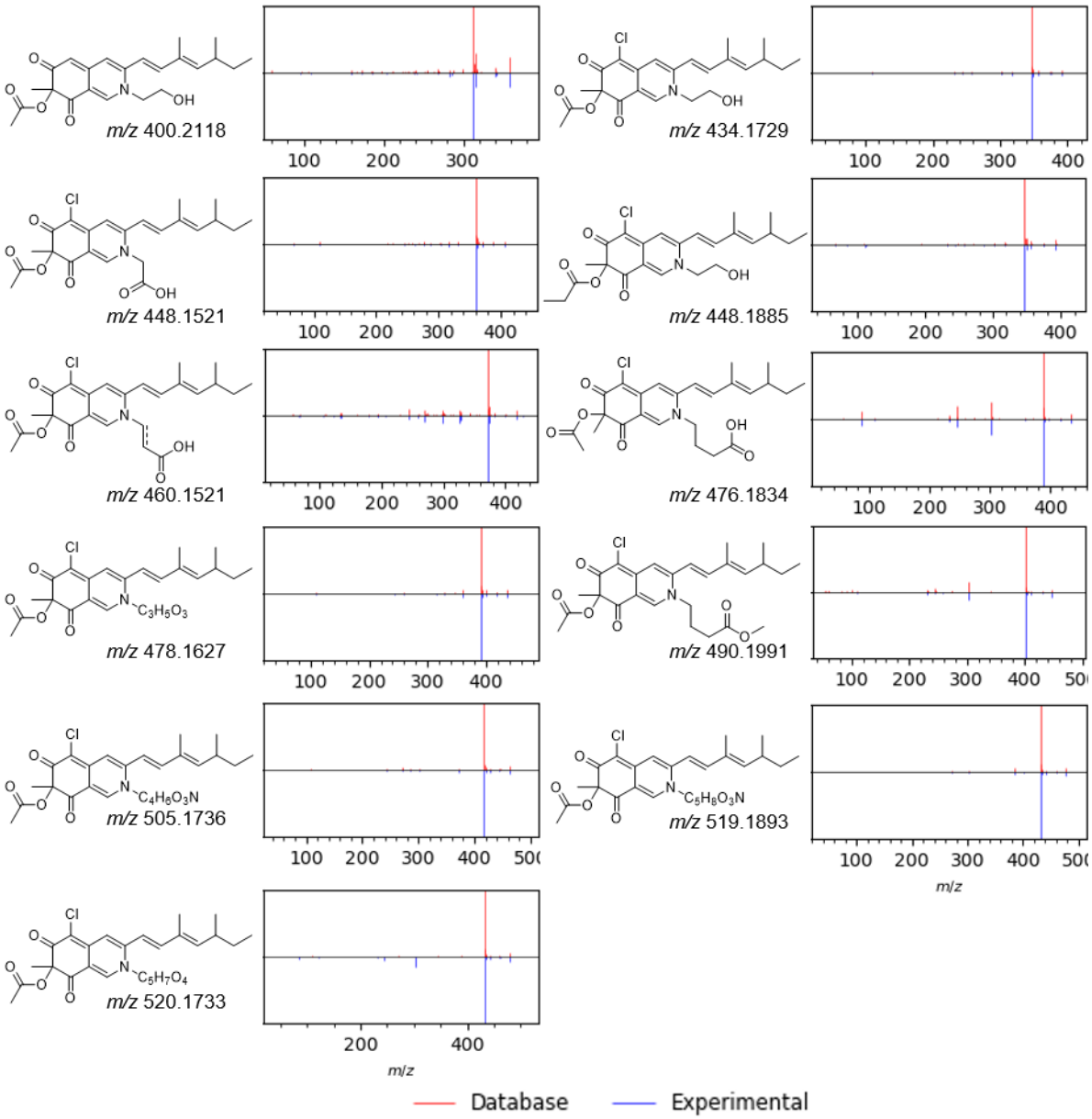

Table S5: Cluster E features annotated by MS/MS database query. In-house database was built upon annotations from Hebra et al.[1]

ClusterE									
$[M+H]^+$	Error (ppm)	Formula	Name	Database	Cosine score	Annotation	Ref	$\varepsilon(\lambda_{nm})$	Minimal condition
380.1860	-1.0	$C_{23}H_{25}NO_4$	Peniazaphilone E	In house	0.93	Level 1	[1]	9100(548)	PD
381.1705	-2.2	$C_{23}H_{24}O_5$		In-house	0.79	Level 2	[1]		PD
392.1618	1.3	$C_{21}H_{26}ClNO_4$	Deacetyl-isochromophilone VI	In-house	0.91	Level 1	[1]		YE
424.2119	-0.1	$C_{25}H_{29}NO_5$	Peniazaphilone A	In-house	0.93	Level 1	[1,11]	10900(541)	CZK

Level 0 corresponds annotations from isolated pure compounds; level 1 to annotations by comparison with standards; level 2 to putative annotations (e.g., MS/MS library comparison or tentative structure); level 3 to a chemical class assignment

Figure S5: Spectral comparison of cluster E molecules with databases and their theoretical protonated *m/z*.

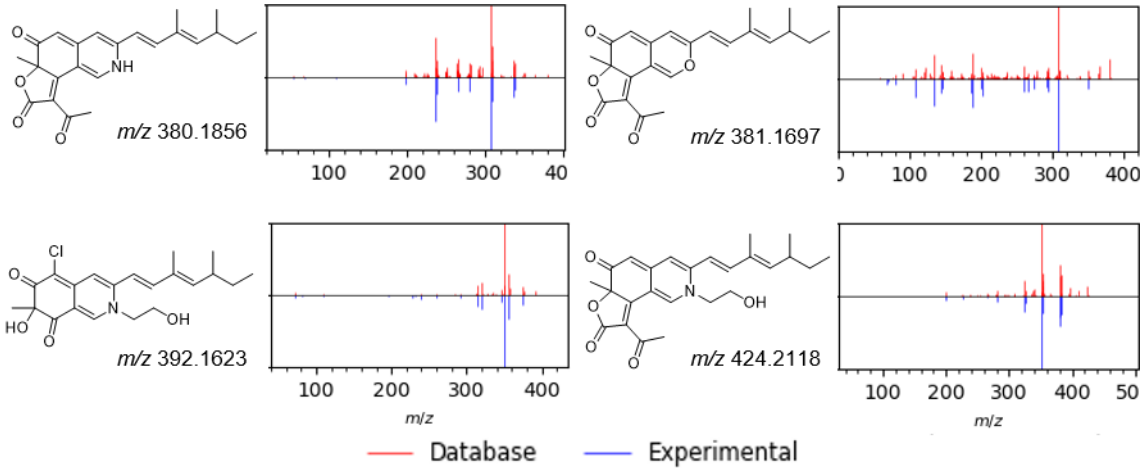

Table S6: Annotation of azaphilones from cluster D-I with proposed chain structure from molecular network data and KEGG compound database.[12]

Cluster D-I							
ID	**[M+H]$^+$**	**Error (ppm)**	**Chain Formula**	**Kegg_ID**	**Chain**	**Acylation**	**Supplementary information**
4	434.1732	-0.8	C_2H_7NO	C00189	Ethanolamine	Acetyl	
6	400.2138	-4.9	C_2H_7NO	C00189	Ethanolamine	Acetyl	No Cl on azaphilone scaffold
7	404.1635	-3.0	CH_5N	C00218	Methylamine	Acetyl	
8	446.1734	-1.2	C_3H_7NO	C01888 C05665	Aminoacetone 3-Aminopropanal	Acetyl	
9	446.1746	-3.9	C_3H_7NO	C01888 C05665	Aminoacetone 3-Aminopropanal	Acetyl	
10	448.1526	-1.0	$C_2H_5NO_2$	C00037	Glycine	Acetyl	
11	448.1901	-3.5	C_2H_7NO	C00189	Ethanolamine	Propionyl	
12	460.1530	-1.9	$C_3H_5NO_2$	C02218 C20253	Dehydroalanine Aminoacrylate	Acetyl	
13	460.1901	-3.4	C_3H_7NO	C01888 C05665	Aminoacetone 3-Aminopropanal	Propionyl	
14	460.1901	-3.4	C_4H_9NO	C00555	4-Aminobutanal	Acetyl	
15	460.2261	-2.6	$C_5H_{13}N$	C02640	Isoamylamine	Acetyl	
16	462.1690	-2.6	$C_3H_7NO_2$	C00041	Alanine	Acetyl	
17	474.2052	-2.2	$C_5H_{11}NO$	C01842 C12455	Pentanamide 5-Aminopentanal	Acetyl	
18	474.2054	-2.6	$C_5H_{11}NO$	C01842 C10974	Pentanamide 4-Methylaminobutanal	Acetyl	
19	476.1834	-0.1	$C_4H_9NO_2$		Methoxyacetamide	Acetyl	
20	476.1840	-1.2	$C_4H_9NO_2$	C00334	4-Aminobutanoate	Acetyl	
21	478.1617	2.1	$C_3H_7NO_3$	C00065	Serine	Acetyl	
22	490.1997	-1.2	$C_5H_{11}NO_2$	C00183	Valine	Acetyl	
23	501.2175	-4.9	$C_6H_{12}N_2O$	C19809	Piperidine-2-carboxamide	Acetyl	
24	504.2157	-1.9	$C_6H_{13}NO_2$	C00123 C00407	Leucine Isoleucine	Acetyl	
25	505.1740	-0.8	$C_4H_8N_2O_3$	C00152	Asparagine	Acetyl	
26	518.2314	-2.0	$C_6H_{13}NO_2$	C00123 C00407	Leucine Isoleucine	Propionyl	
27	519.1902	-1.8	$C_5H_{10}N_2O_3$	C00064	Glutamine	Acetyl	
28	519.2266	-1.9	$C_6H_{14}N_2O_2$	C00047	Lysine	Acetyl	
29	520.1735	-0.4	$C_5H_9NO_4$	C00025	Glutamate	Acetyl	
30	536.2054	-1.6	$C_6H_{13}NO_4$	C22301	Dihydroxyisoleucine	Acetyl	
31	538.2001	-1.9	$C_9H_{11}NO_2$	C00079	Phenylalanine	Acetyl	
32	547.2212	-1.2	$C_7H_{14}N_2O_3$	C00437	N-Acetylornithine	Acetyl	
33	550.2214	-2.2	$C_6H_{13}NO_4$	C22301	Dihydroxyisoleucine	Propionyl	
34	552.2173	4.6	$C_9H_{11}NO_2$	C00079	Phenylalanine	Propionyl	
35	554.1929	2.0	$C_9H_{11}NO_3$	C00082	Tyrosine	Acetyl	

Table S7: Annotation of azaphilones from cluster D-II with proposed chain structure from molecular network data and KEGG compound database.[12]

Cluster DII							
ID	**$[M+H]^+$**	**Error (ppm)**	**Chain Formula**	**Kegg_ID**	**Chain**	**Acylation**	**Supplementary information**
36	460.2493	-2.3	$C_8H_{11}N$	C02455	Phenylethylamine	Acetyl	No Cl on azaphilone scaffold
37	476.2427	1.0	$C_8H_{11}NO$	C00483 C01183	Tyramine Phenylethanolamine	Acetyl	No Cl on azaphilone scaffold
38	484.2012	2.6	$C_5H_9N_3$	C00388	Histamine	Acetyl	
39	494.2105	-2.5	$C_8H_{11}N$	C02455	Phenylethylamine	Acetyl	
40	503.2301	1.3	$C_6H_{14}N_2O$	C02714	N-Acetylputrescine	Acetyl	
41	508.2254	-1.0	$C_8H_{11}N$	C02455	Phenylethylamine	Propionyl	
42	510.2046	-0.8	$C_8H_{11}NO$	C00483 C01183	Tyramine Phenylethanolamine	Acetyl	
43	510.2055	-2.6	$C_8H_{11}NO$	C00483 C01183	Tyramine Phenylethanolamine	Acetyl	
44	522.1721	-1.8	$C_5H_{11}NO_2S$	C00073	Methionine	Acetyl	
45	522.2418	-2.4	$C_8H_{11}N$	C02455	Phenylethylamine	Butyl	
46	524.2208	-1.9	$C_8H_{11}NO$	C00483 C01183	Tyramine Phenylethanolamine	Propionyl	
47	526.1997	-1.2	$C_8H_{11}NO_2$	C03758 C04227	Dopamine Octopamine	Acetyl	
48	540.2140	1.4	$C_8H_{11}NO_2$	C03758 C04227	Dopamine Octopamine	Propionyl	

Table S8: Annotation of azaphilones from cluster D-III with proposed chain structure from molecular network data and KEGG compound database.[12]

Cluster DIII							
ID	**$[M+H]^+$**	**Error (ppm)**	**Chain Formula**	**Kegg_ID**	**Chain**	**Acylation**	**Supplementary information**
49	541.2108	-1.5	$C_8H_{12}N_2O_2$	C00534	Pyridoxamine	Acetyl	
50	577.2112	-2.1	$C_{11}H_{12}N_2O_2$	C00078	Tryptophane	Acetyl	

Figure S6: Subdivision of Cluster D based on annotated features

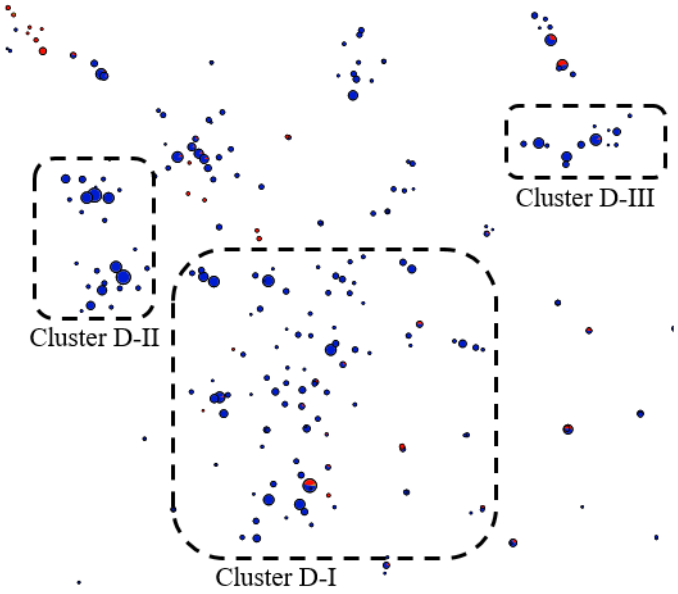

Table S9: Annotation of azaphilones from cluster E with proposed chain structure from molecular network data and KEGG compound database.[12]

Cluster E						
ID	**$[M+H]^+$**	**Error (ppm)**	**Chain Formula**	**Kegg_ID**	**Chain**	**Supplementary information**
5	380.186	-1.0	NH_3	C00014	Ammonium	
51	396.1809	-0.9	NH_3	C00014	Ammonium	Epoxy-azaphilone
52	424.2119	-0.1	C_2H_7NO	C00189	Ethanolamine	
53	436.212	-0.4	C_3H_7NO	C01888 C05665	Aminoacetone 3-Aminopropanal	
54	450.2646	-1.6	$C_5H_{13}N$	C02640	Isoamylamine	
55	484.2491	-1.8	$C_8H_{11}N$	C02455	Phenylethylamine	
56	494.2551	-2.8	$C_6H_{13}NO_2$	C00123 C00407	Leucine/Isoleucine	
57	500.2439	-1.5	$C_8H_{11}N$	C02455	Tyramine Phenylethanolamine	Epoxy-azaphilone
58	500.2445	-2.7	$C_8H_{11}NO$	C00483 C01183	Tyramine Phenylethanolamine	
59	516.2394	-2.6	$C_8H_{11}NO$	C00483 C01183	Tyramine Phenylethanolamine	Epoxy-azaphilone
60	528.2386	-1.0	$C_9H_{11}NO_2$	C00079	Phenylalanine	
61	534.2005	7.0	$C_8H_{11}NO$	C00483 C01183	Tyramine Phenylethanolamine	Chlorination
62	567.2502	-2.2	$C_{11}H_{12}N_2O_2$	C00078	Tryptophane	

Figure S7: Annotation of cluster E with hypothetical chain structures integrated to the azaphilone scaffold, proposed from molecular network data and KEGG compound database.[12] epoxy means The 3,5-dimethyl-1,3-heptadienyl unit bear an epoxide on position 3. Cl means azaphilone is chlorinated

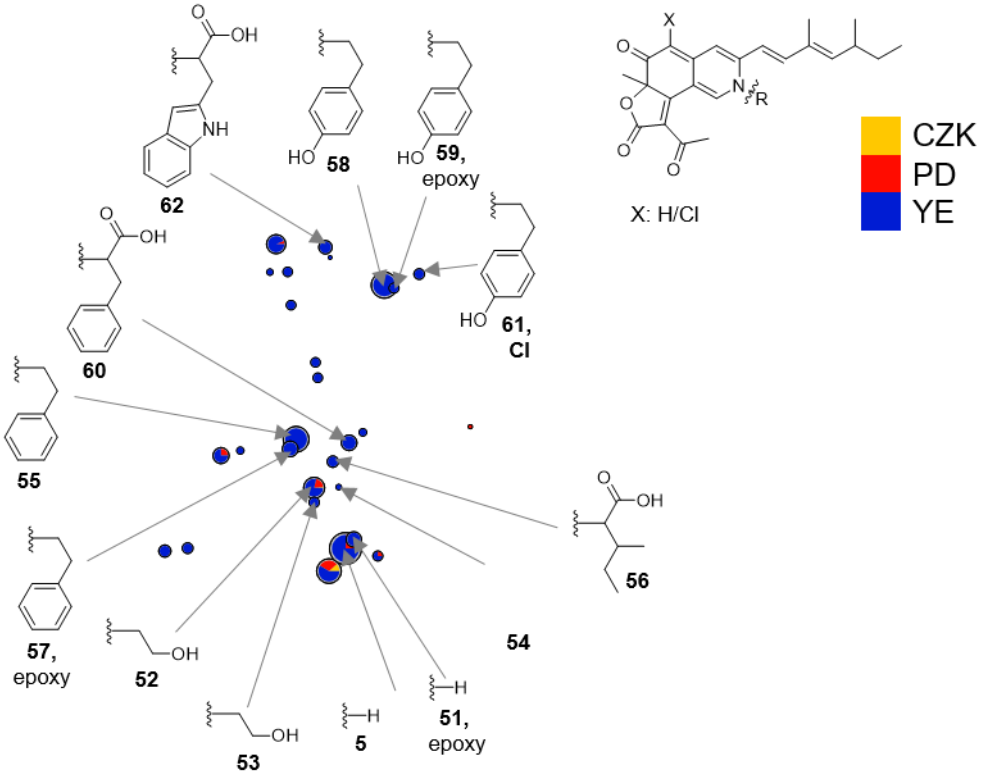

Figure S8: HRMS spectrum for compound **24'**

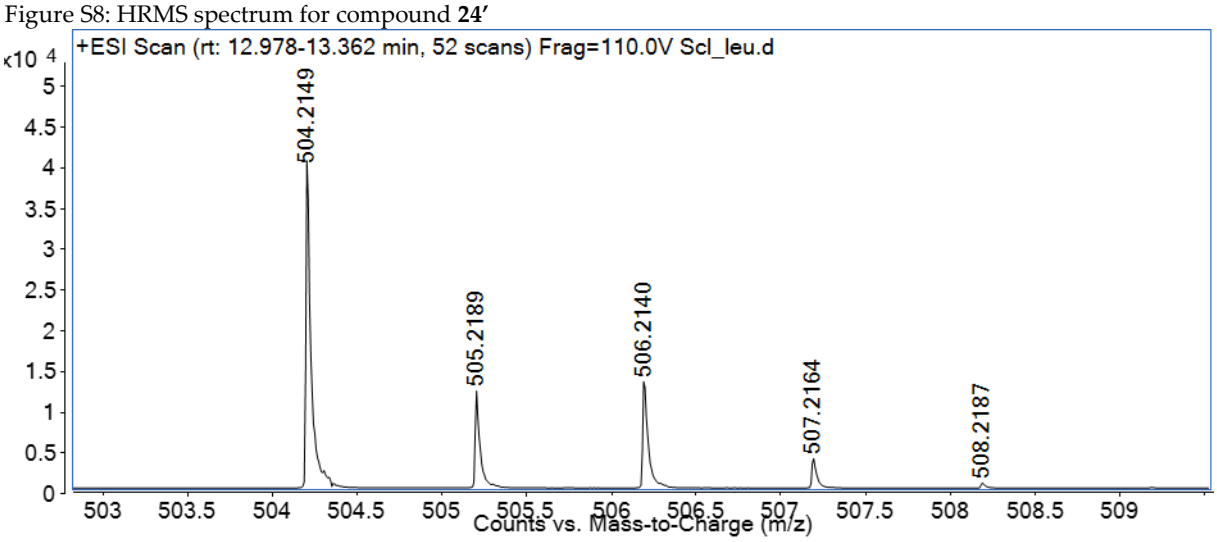

Figure S9: ^{1}H NMR spectrum (500 MHz, CD_3CN) of compound **24'**

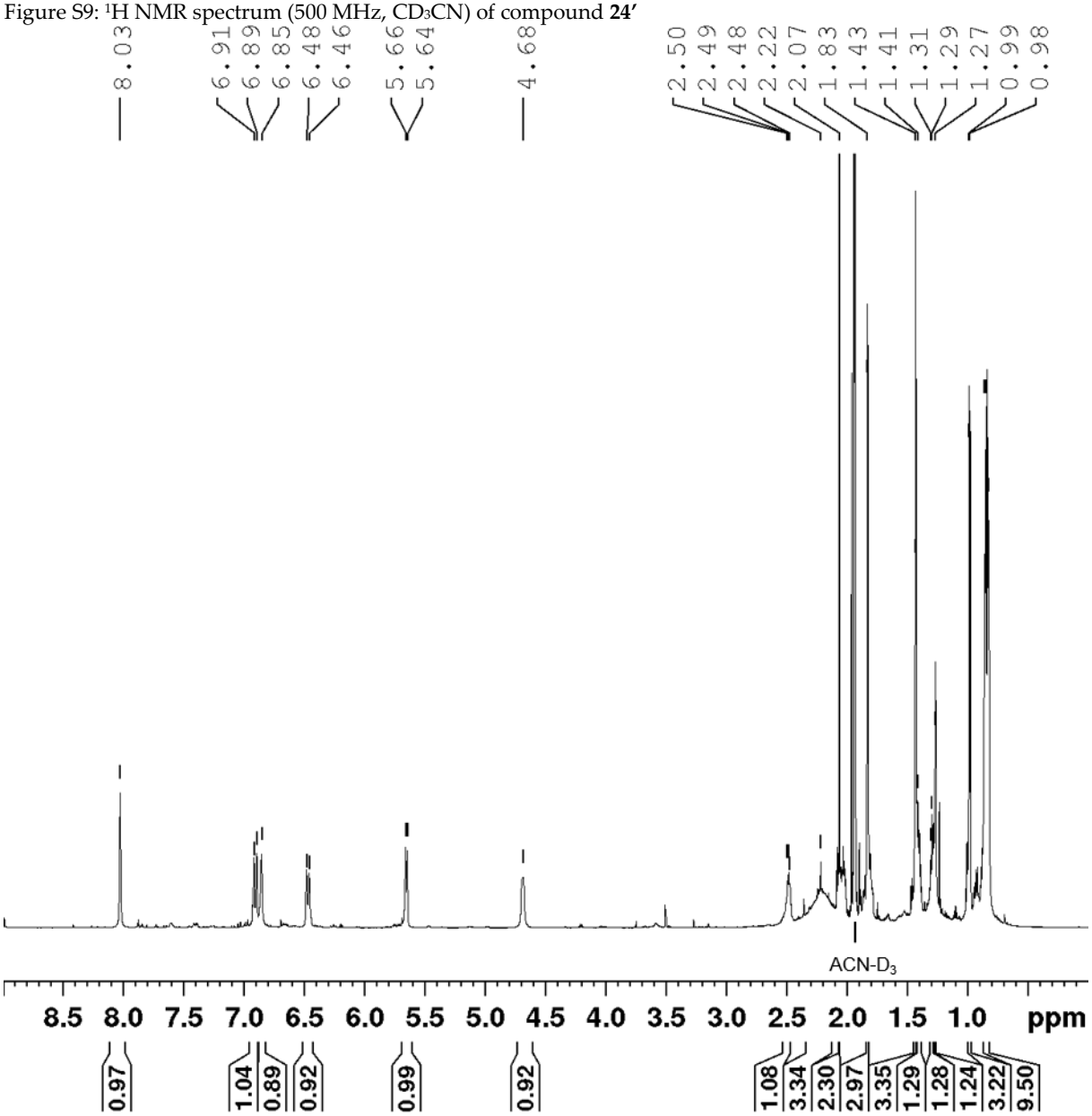

Figure S10: ^{13}C NMR spectrum (700 MHz, CD_3CN) of compound **24'**

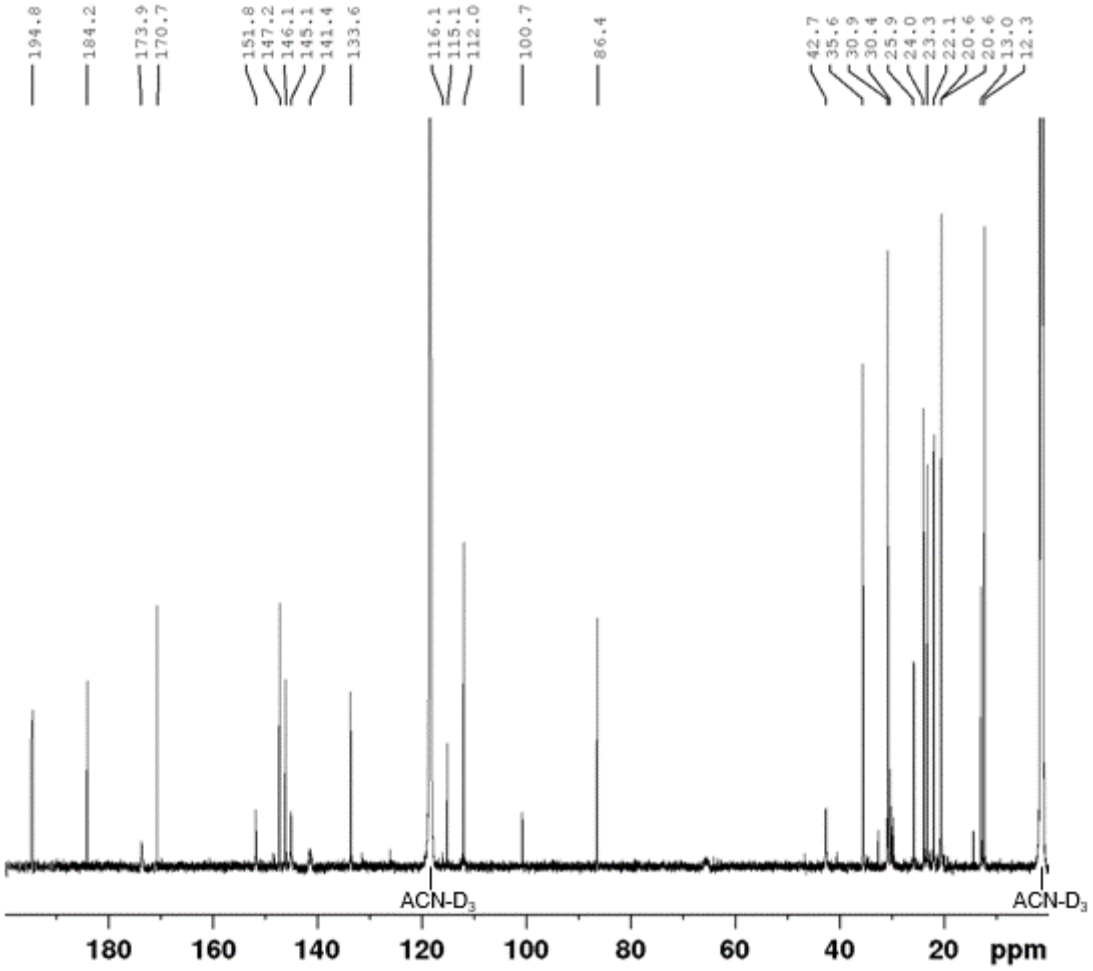

Figure S 11: HRMS spectrum for compound **39′**

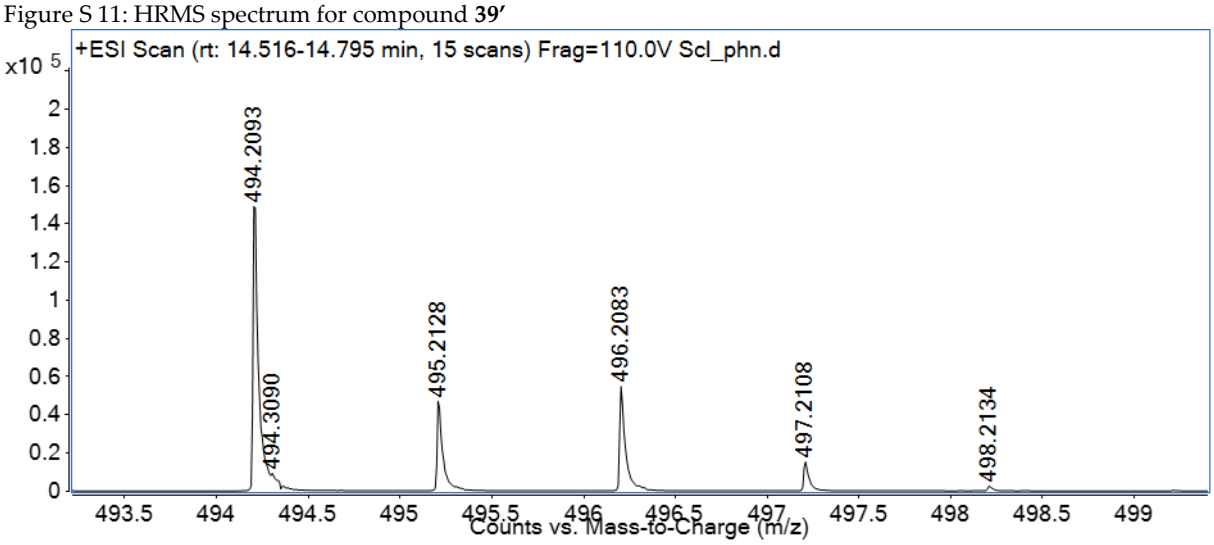

Figure S12: ^{1}H NMR spectrum (500 MHz, $CDCl_3$) of compound **39′**

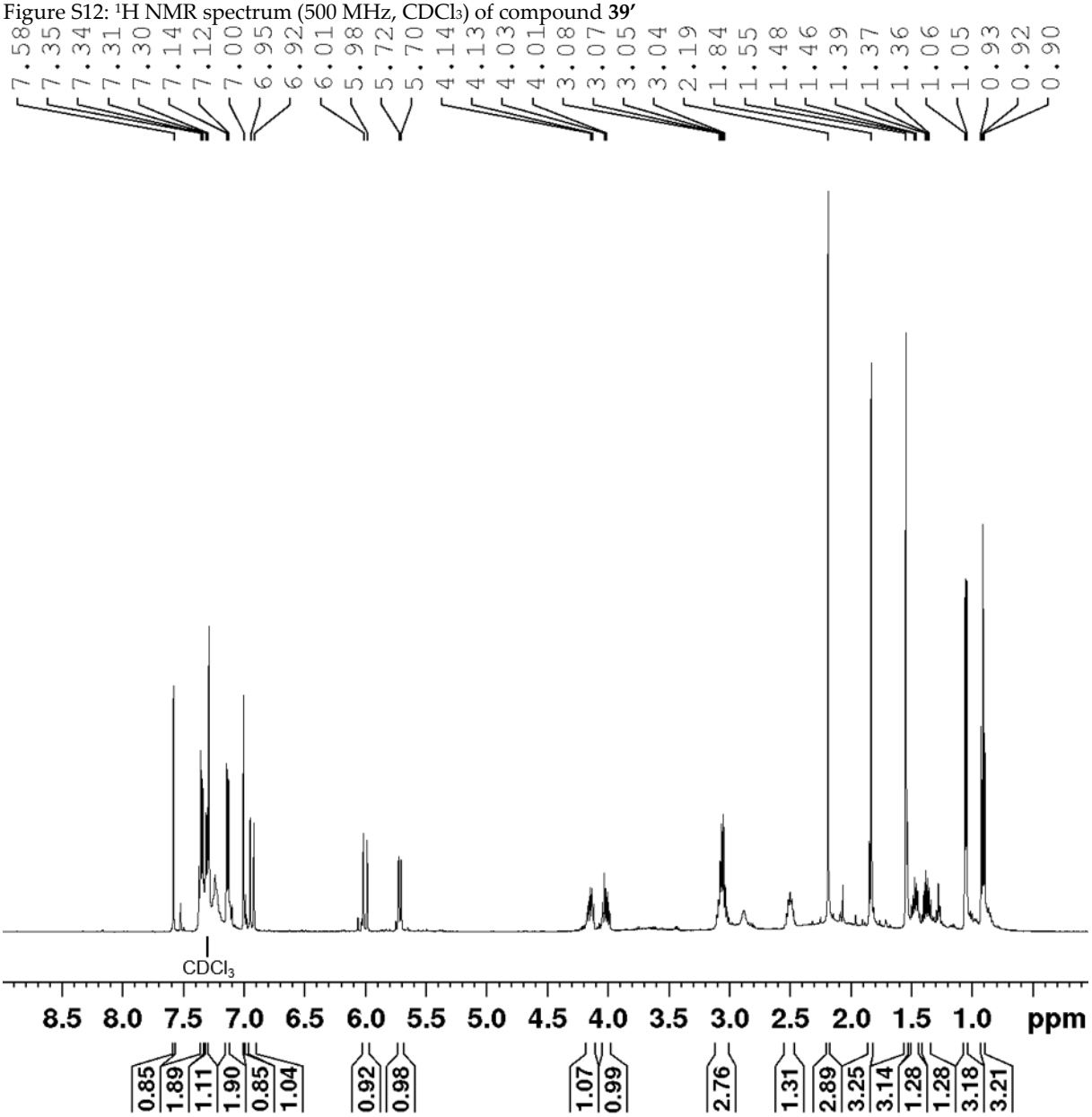

Figure S13: ^{13}C NMR spectrum (500 MHz, $CDCl_3$) of compound **39′**

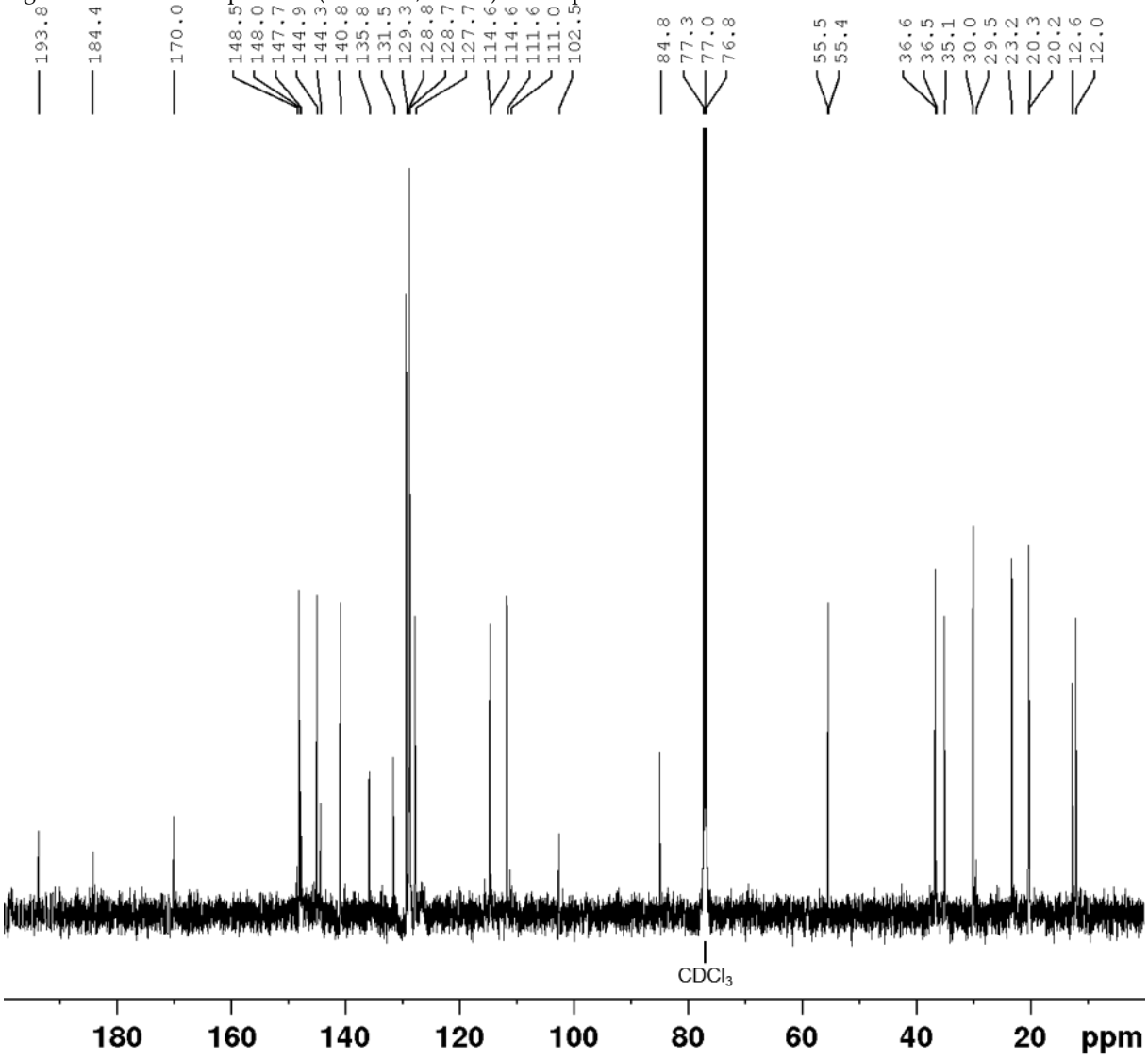

Figure S14: HRMS spectrum for compound **50′**

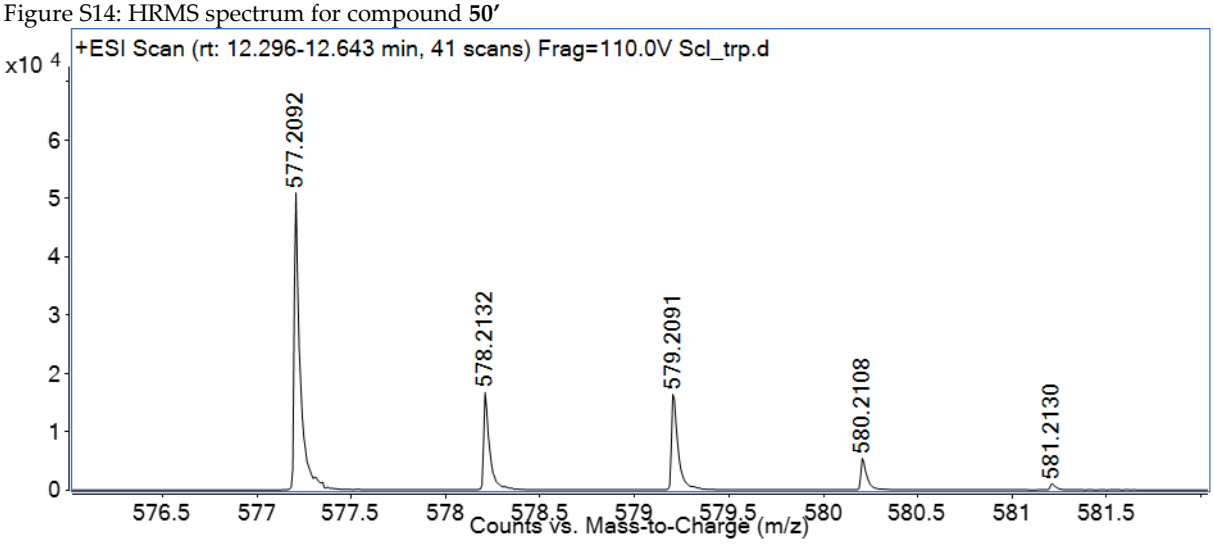

Figure S15: ^{1}H NMR spectrum (500 MHz, MeOD) of compound **50′**

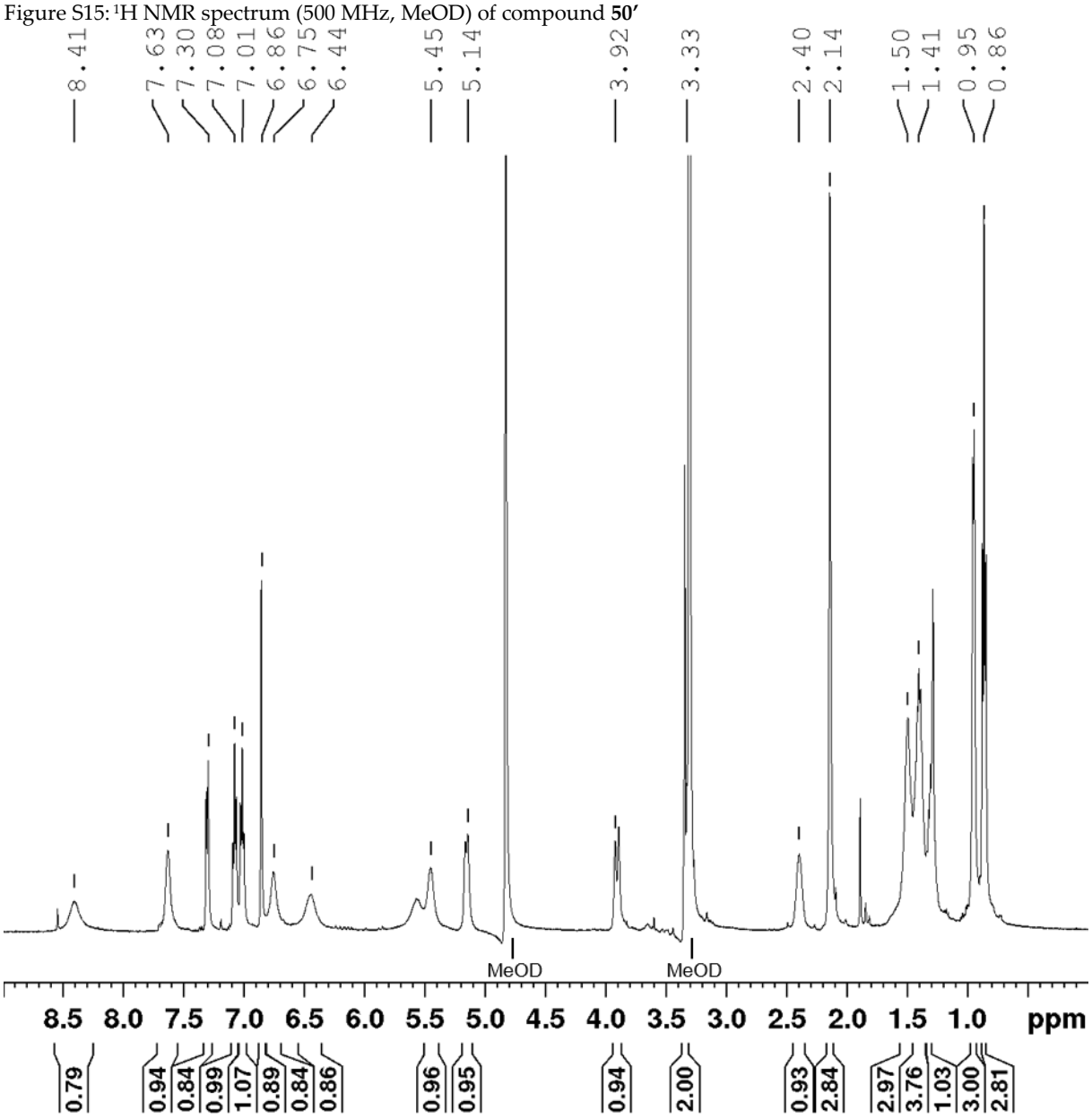

Figure S16: ^{13}C NMR spectrum (500, MHz, MeOD) of compound **50'**

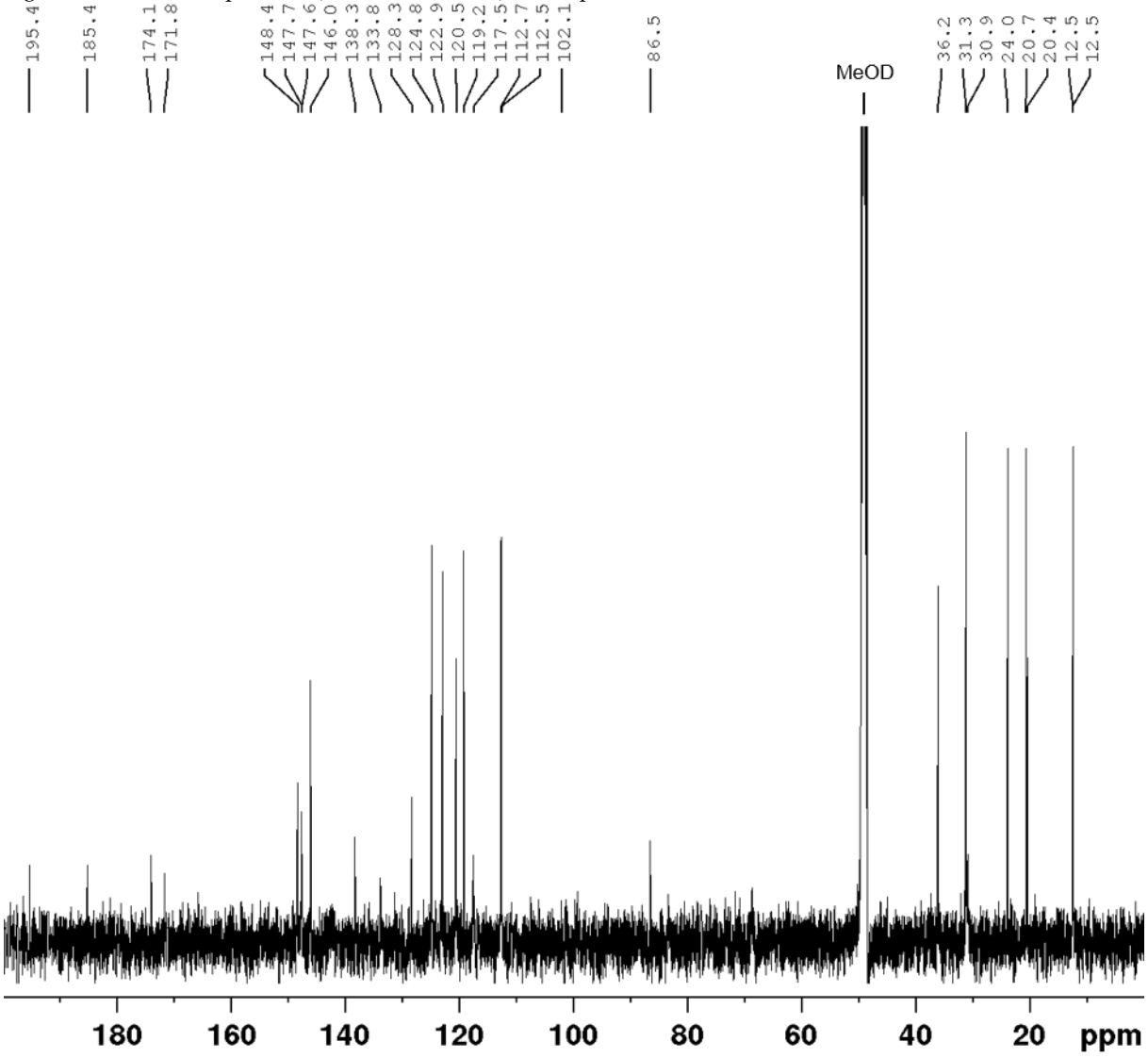

Figure S17: Comparison of fragmentation spectra and retention time from hemisynthetized standards with metabolites **24**, **39** and **50** produced by *P. sclerotiorum* SNB-CN111.

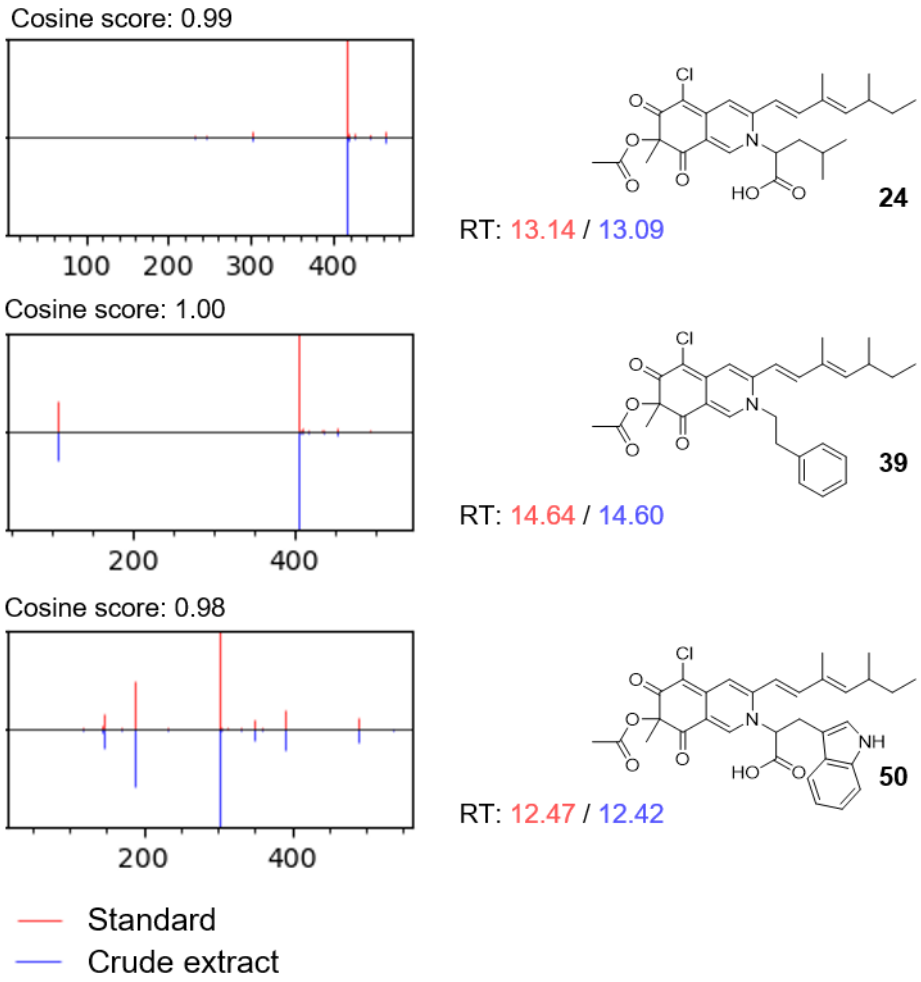

Table S10: Absorbance at 500, 460 and 400 nm of *P. sclerotiorum* SNB-CN111 crude extracts from fermentation on solid CZK, PD and YE. Values are given in $AU.g^{-1}$ of culture medium.

$AU_{nm}.g^{-1}$	CZK	PD	YE
OD_{500}	0.4	6.0	59.6
OD_{460}	1.0	10.4	64.9
OD_{400}	4.9	47.5	213.2

Table S11: Absorbance at 500, 460 and 400 nm of *P. sclerotiorum* SNB-CN111 crude extracts from fermentation on solid CZK supplemented with ammonium acetate or ethanolamine at 0, 0.1, 0.5 and 2 $g.L^{-1}$. Values are given in $AU.g^{-1}$ of culture medium.

	CZK + ammonium acetate ($g.L^{-1}$)				CZK + ethanolamine ($g.L^{-1}$)			
$AU_{nm}.g^{-1}$	0	0.1	0.5	2	0	0.1	0.5	2
OD_{500}	0.4	0.5	0.4	0.2	0.4	0.5	0.5	0.4
OD_{460}	1.0	1.1	0.8	0.6	1.0	1.1	1.1	0.7
OD_{400}	4.9	4.2	2.8	2.7	4.9	4.0	4.4	2.4

Figure S18: Extracted chromatogram for molecules **1** ([M+H]$^+$, *m/z* 391.1307), **3** ([M+H]$^+$, *m/z* 390.1467) and **4** ([M+H]$^+$, *m/z* 434.1729) as a function of the concentration of ammonium acetate or ethanolamine added to solid CZK medium.

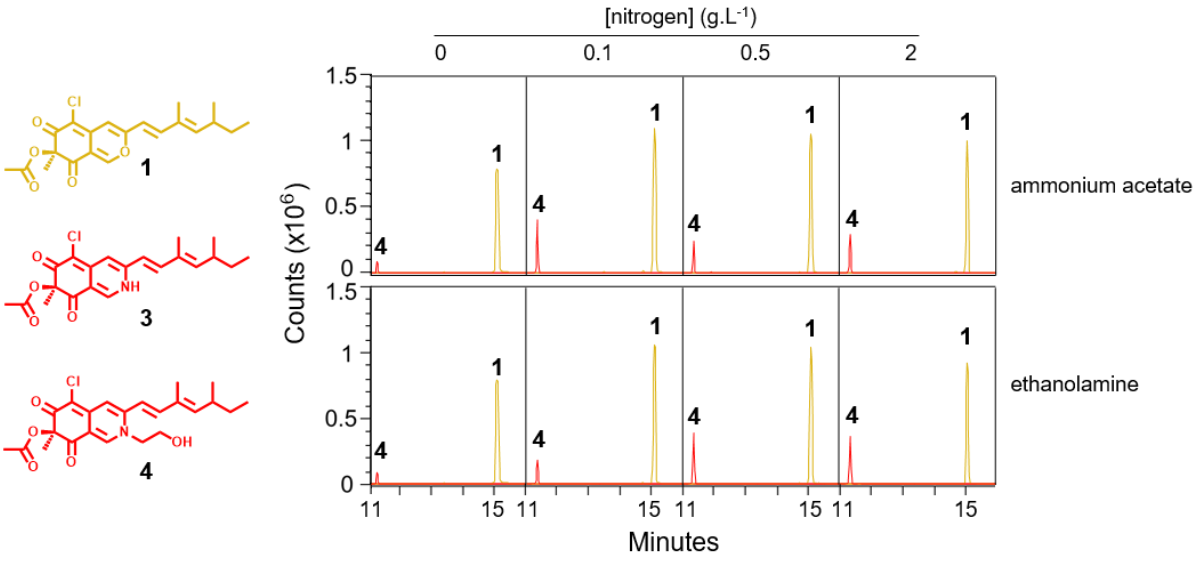

Table S12: Absorbance at 500, 460 and 400 nm of *P. sclerotiorum* SNB-CN111 crude extracts from two step fermentation process on porous cellophane membrane on solid CZK supplemented with ammonium acetate or ethanolamine at 0, 0.1, 0.5 and 2 g.L^{-1}. Values are given in AU.g^{-1} of culture medium.

	Two step fermentation CZK + ammonium acetate (g.L^{-1})				Two step fermentation CZK + ethanolamine (g.L^{-1})			
$AU_{nm}.g^{-1}$	0	0.1	0.5	2	0	0.1	0.5	2
OD_{500}	0.4	0.9	1.6	4.5	0.4	1.8	2.2	4.6
OD_{460}	1.0	2.1	3.2	10.3	1.0	4.2	5.1	8.9
OD_{400}	4.9	10.3	11.8	37.1	4.9	16.1	21.2	40.0

Table S13: Absorbance at 500, 460, and 400 nm of *P. sclerotiorum* SNB-CN111 crude extracts from two step fermentation process on porous cellophane membrane on solid CZK supplemented with propargilamine at 0, 0.1, 0.5 and 2 g.L^{-1}. Values are given in AU.g^{-1} of culture medium.

	Two step fermentation CZK + propargilamine (g.L^{-1})			
$AU_{nm}.g^{-1}$	0	0.1	0.5	2
OD_{500}	0.4	22.5	68.0	49.9
OD_{460}	1.0	38.3	91.7	68.2
OD_{400}	4.9	155.1	335.4	258.6

Figure S19: Metabolic profile of from *P. sclerotiorum* SNB-CN111 fermentation on solid CZK crude extract and two step fermentation process on porous cellophane membrane on solid CZK supplemented with propargilamine 0.5 $g.L^{-1}$.

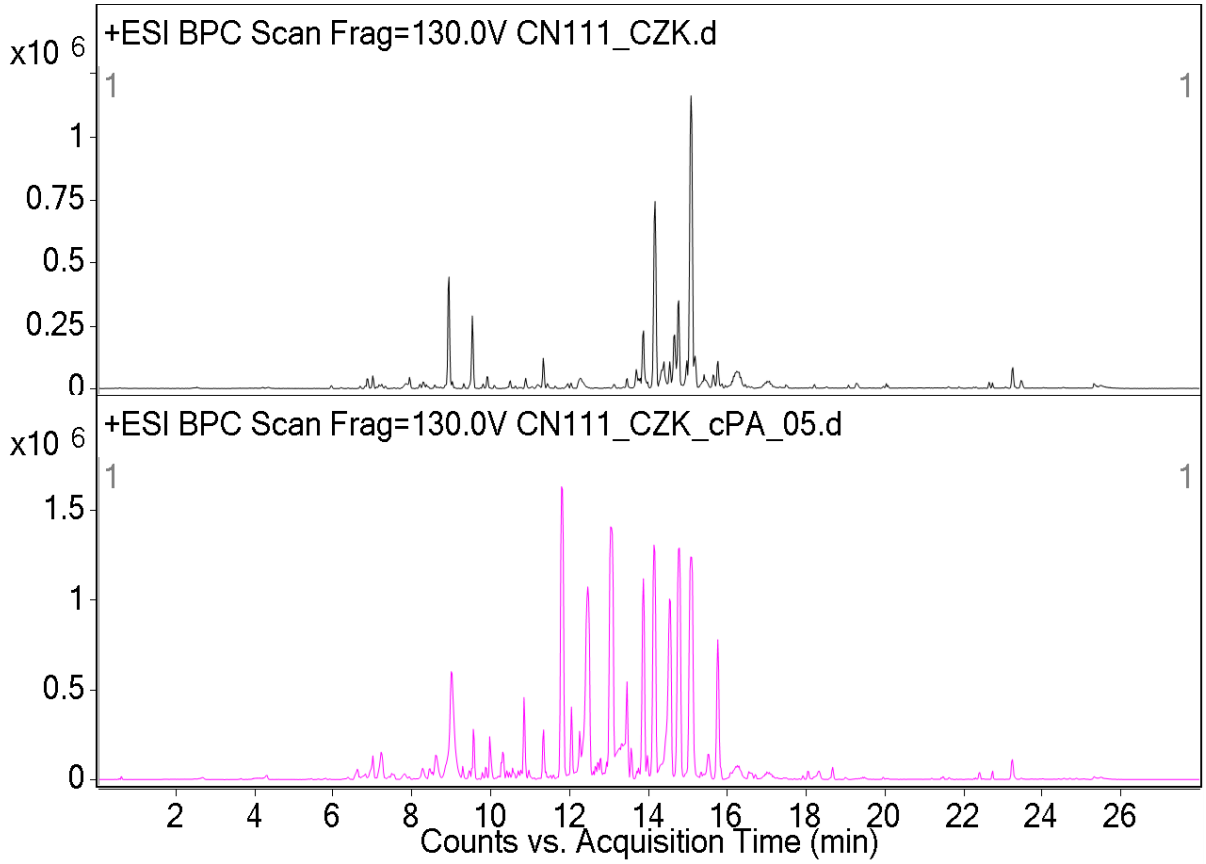

Figure S20: Base pic chromatogram of fraction F1 from flash chromatography of pulled two step fermentation process on porous cellophane membrane on solid CZK supplemented with propargilamine crude extracts.

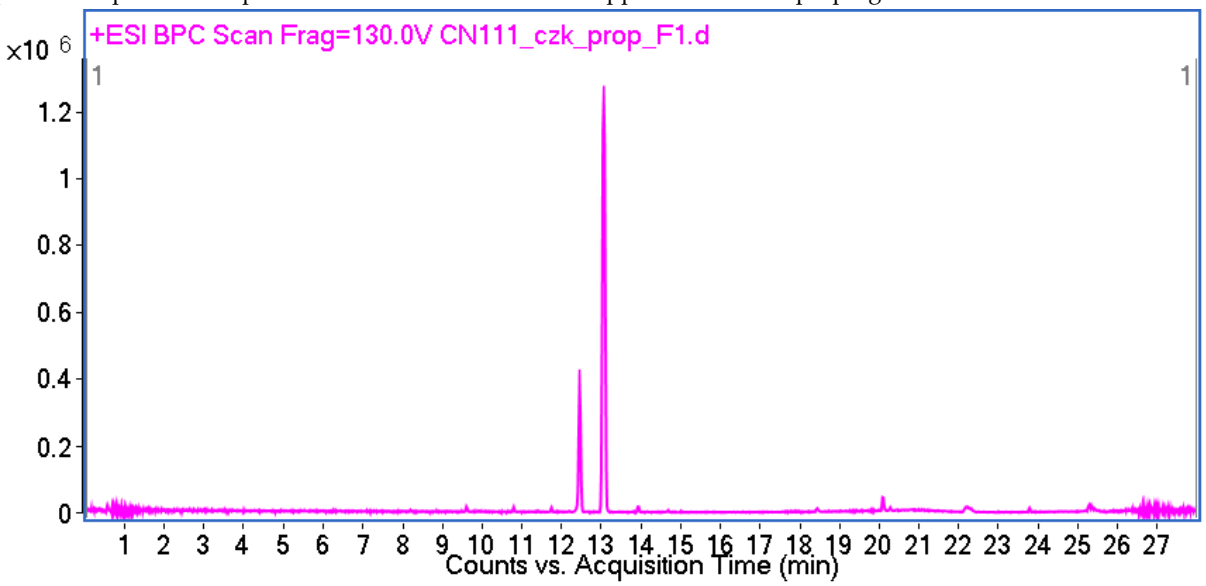

Figure S21 HRMS of compound **63**.

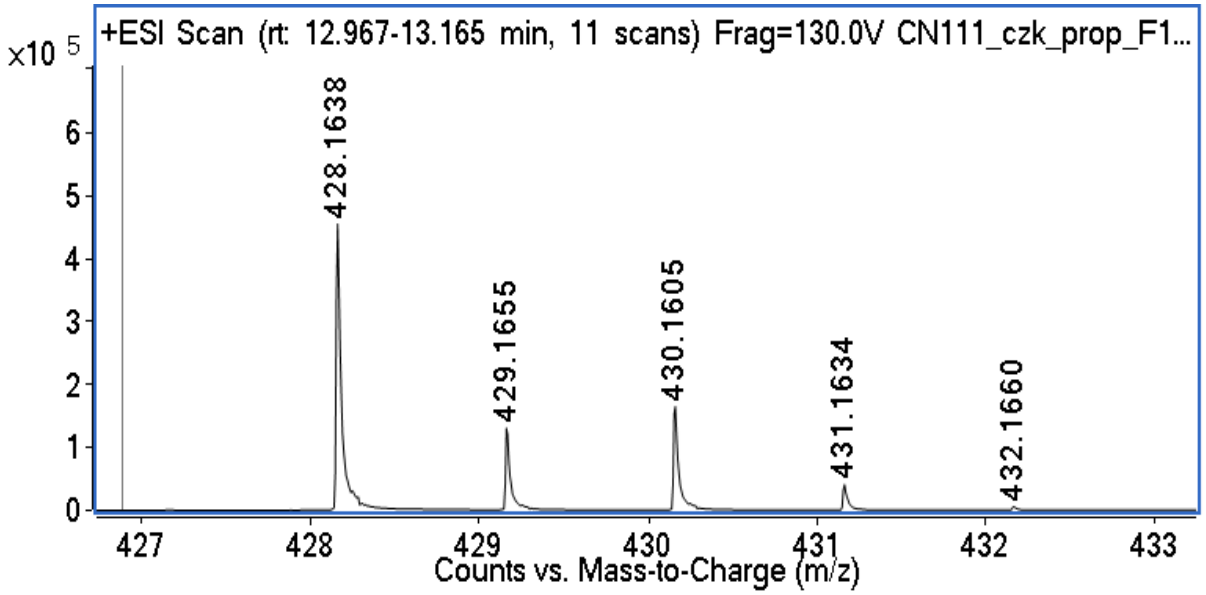

Figure S22: ^{1}H NMR spectrum (500 MHz, $CDCl_3$) of compound **63**.

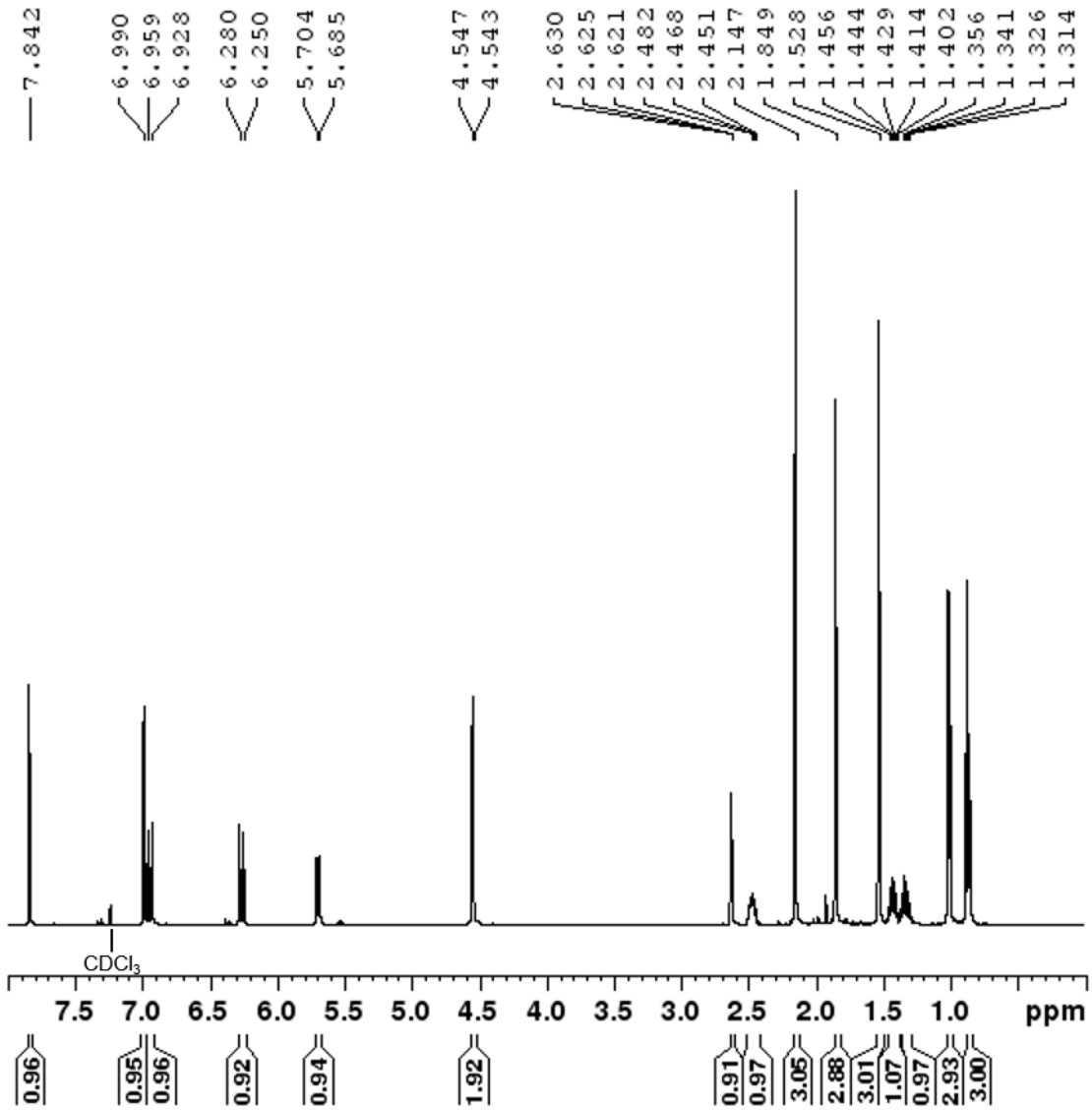

Figure S23: ^{13}C NMR spectrum (500 MHz, $CDCl_3$) of compound **63**.

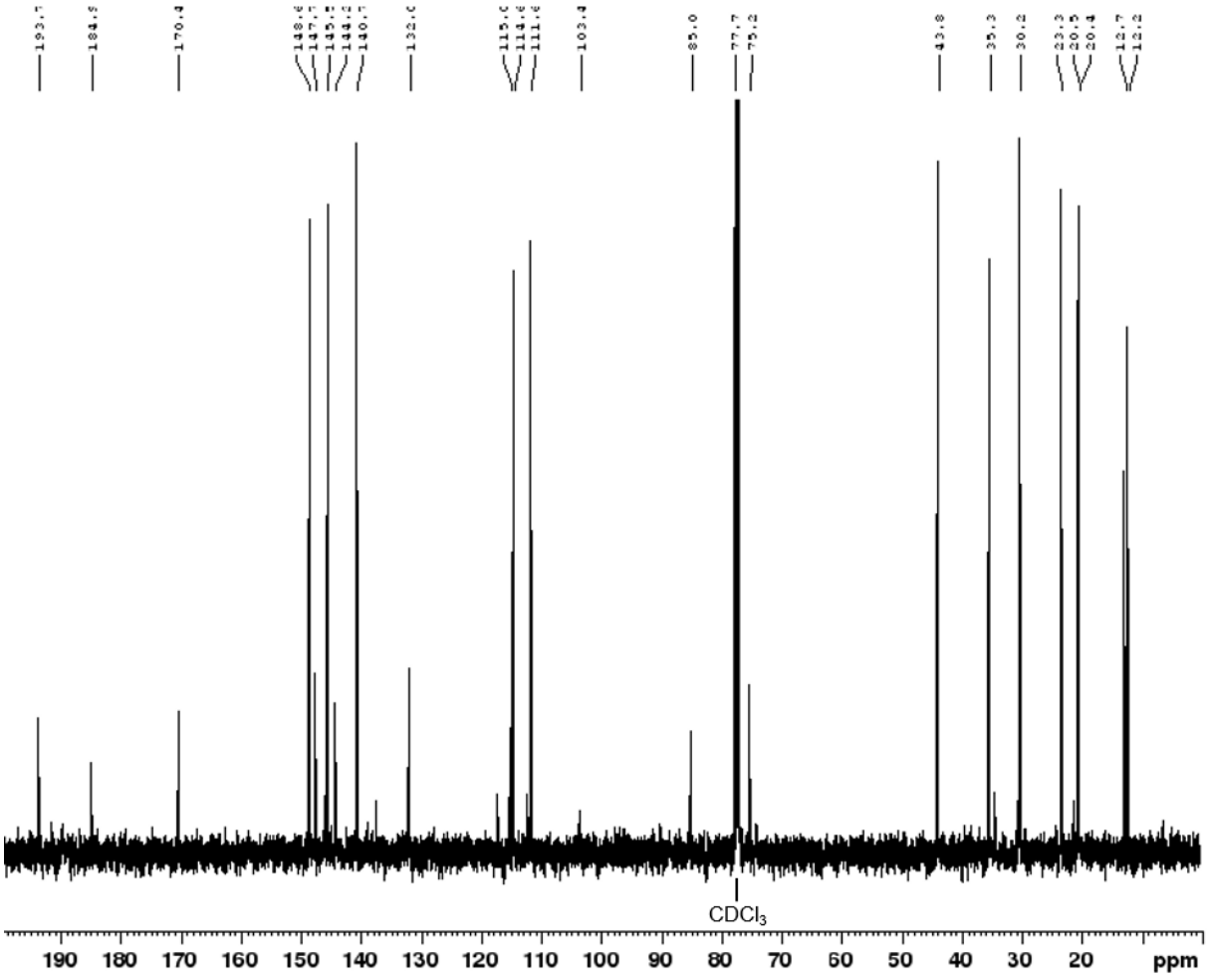

Figure S 24: COSY NMR spectrum (500 MHz, $CDCl_3$) of compound **63**.

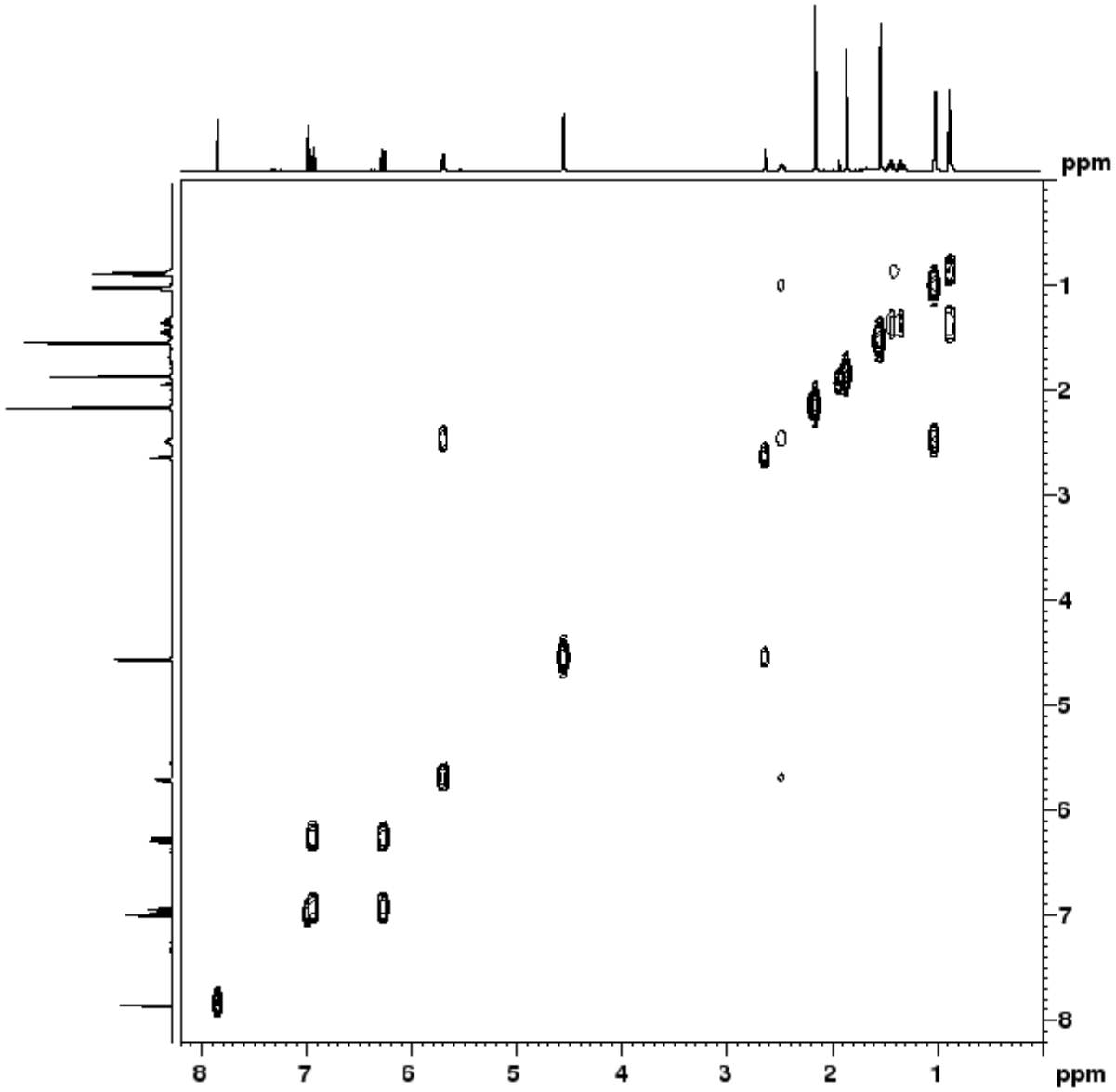

Figure S 25: HSQC NMR spectrum (500 MHz, $CDCl_3$) of compound **63**.

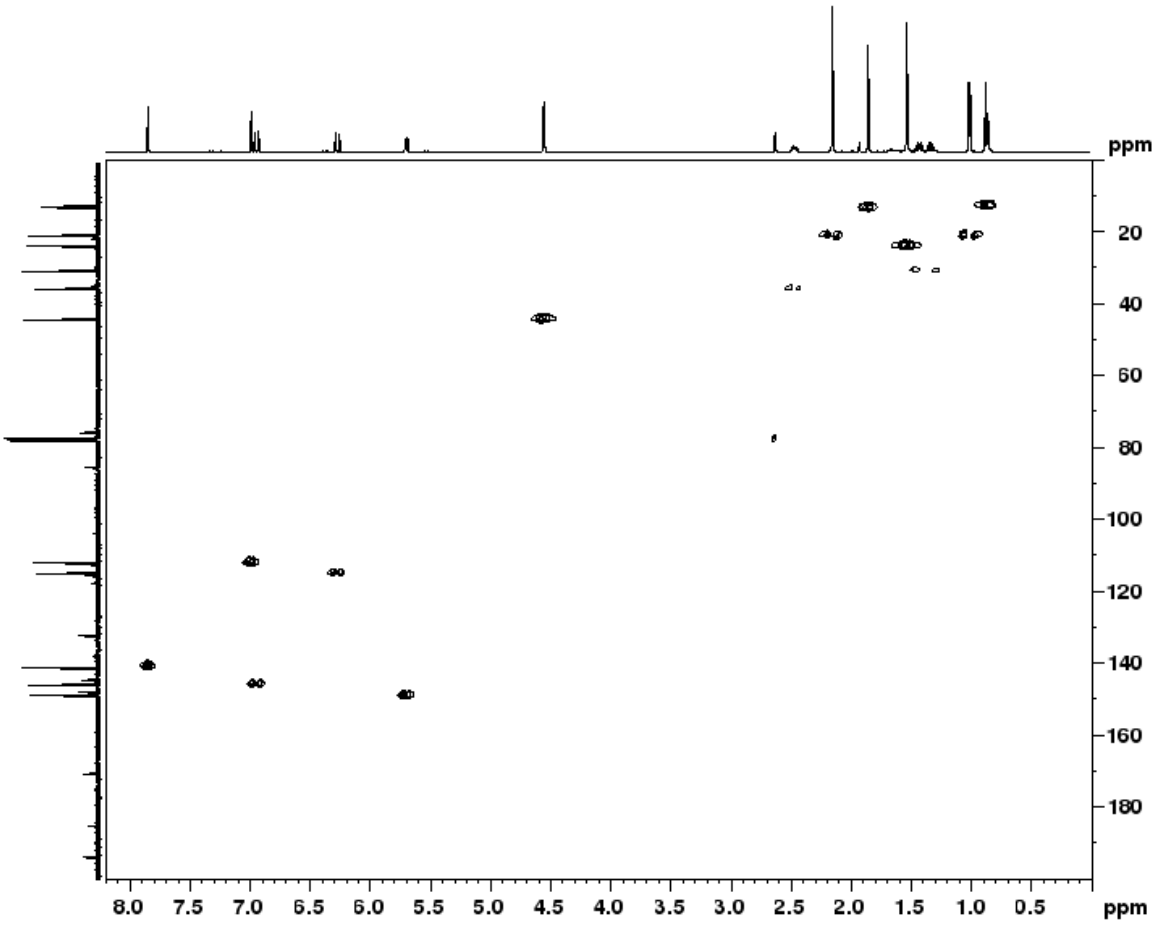

Figure S 26 HMBC NMR spectrum (500, MHz, $CDCl_3$) of compound **63**.

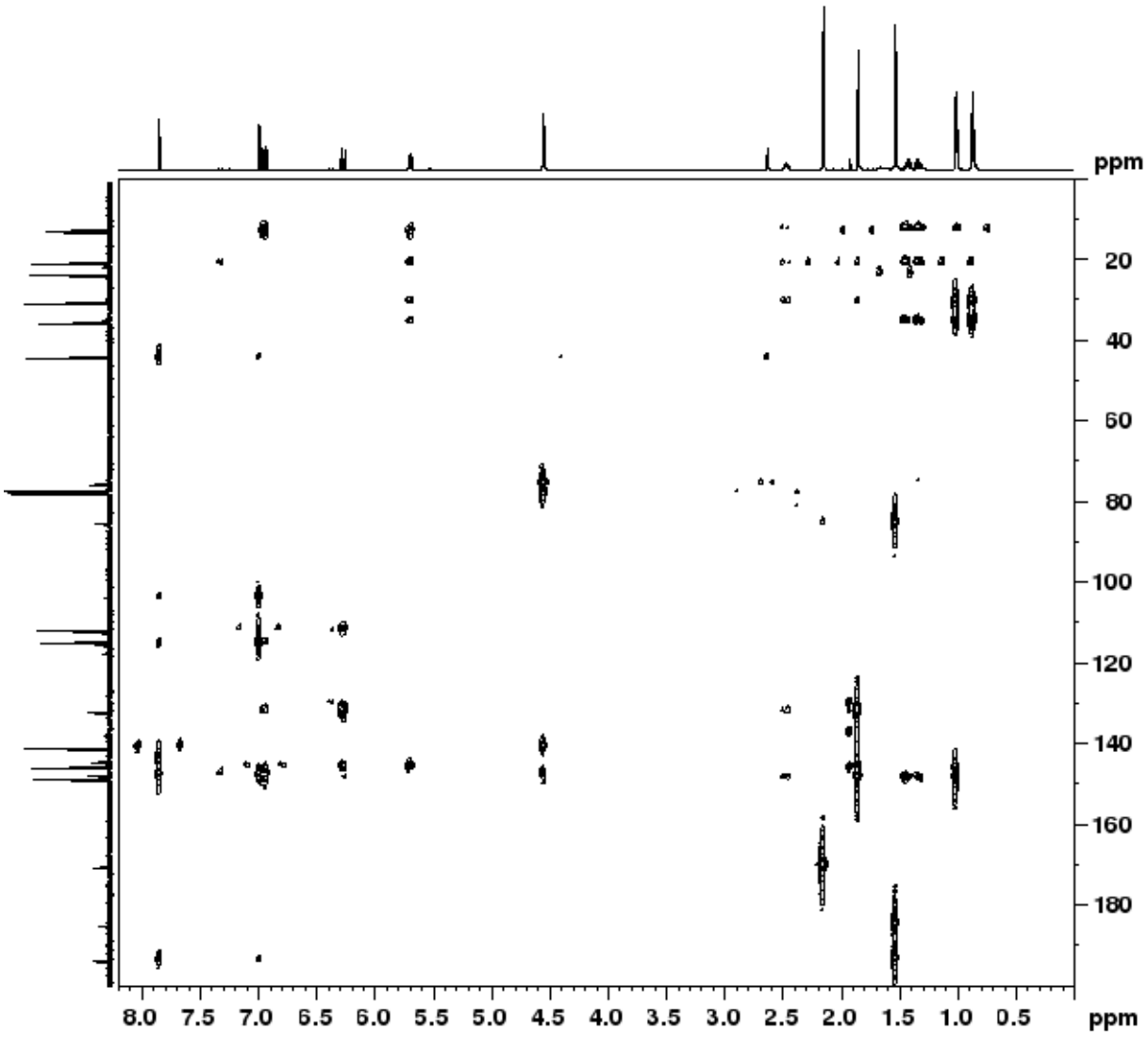

Figure S27: Key $^{1}H–^{1}H$ COSY (bold bonds) and $^{1}H–^{13}C$ (plain arrow) correlations of compound **63.**

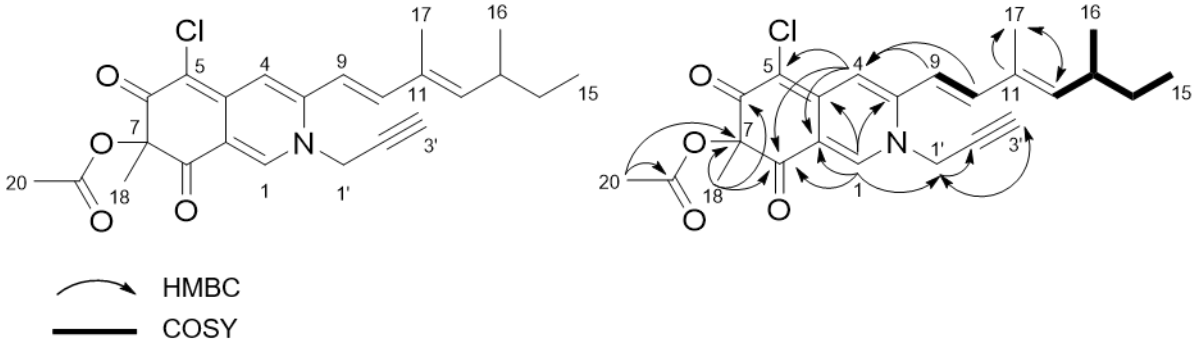

Table S14: ^{1}H NMR spectroscopic data for compounds **3**, **4**, **39′** and **63** recorded at 500 MHz on $CDCl_3$, **24′** recorded at 500 MHz on CD_3CN and **50′** recorded at 500 MHz on MeOD. Compounds **3** and **4** were described on a previous study.[1]

Position	δH (*J* in Hz)					
	3	**4**	**24′**	**39′**	**50′**	**63**
1	7.93, s	7.83, s	8.03, s	7.58, s	8.4, s	7.84, s
4	6.86, s	6.99, s	6.85, s	7, s	6.85, s	6.99, s
9	6.13, d(16.1)	6.23, d(15.9)	6.47, d(15.6)	6, d(15.3)	6.46, d(15.4)	6.26, d(15.2)
10	7.04, d(16.7)	6.91, d(15.6)	6.9, d(15.3)	6.94, d(15.4)	6.75, d(15.2)	6.94, d(15.6)
12	5.69, d(9.9)	5.68, d(9.9)	5.65, d(9.1)	5.71, d(10.0)	5.45, d(8.2)	5.70, d(9.7)
13	2.47, m	2.47, m	2.49, m	2.52, m	2.40, m	2.47, m
14	1.40/1.30, m	1.42/1.32, m	1.41/1.29, m	1.47/1.37	1.40/1.30, m	1.43/1.33, m
15	0.84, t(7.5)	0.86, t(7.5)	0.84, m	0.91, t(7.4)	0.87, t(7.3)	0.87, t(7.4)
16	0.99, d(6.6)	1.00, d(6.7)	0.99, d(6.7)	1.05, d(6.9)	0.95, d(6.3)	1.00, d(6.9)
17	1.83, s	1.82, s	1.83, s	1.84, s	1.50, s	1.84, s
18	1.57, s	1.52, s	1.43, s	1.55, s	1.41, s	1.53, s
20	2.16, s	2.13, s	2.2, s	2.19, s	2.14, s	2.14, s
1'		3.99, m	4.69, m	4.17/4.01, s	3.91, m	4.55, d(2.3)
2'		3.91, m		3.07, m		
3'			2.06, m		3.30, m	2.63, t(2.3)
4′			1.27, m	7.34, d(7.2)		
5′			0.84, m	7.13, d(7.4),	5.15, m	
6′			0.84, m	7.30, d(7.2)		
7′				7.13, d(7.4),		
8′				7.34, d(7.2)	7.31, d(7.8)	
9′					7.01, t(7.7)	
10′					7.08, t(7.1)	
11′					7.63, d(7.8)	

Table S15: ^{13}C NMR spectroscopic data for compounds **3**, **4**, **39′** and **63** recorded at 500 MHz on $CDCl_3$, **24′** recorded at 700 MHz on CD_3CN and **50′** recorded at 500 MHz on MeOD. Compounds **3** and **4** were described on a previous study.[1]

Position	δC, type					
	3	**4**	**24′**	**39′**	**50′**	**63**
1	138.4, CH	142.0, CH	141.4, CH	141, CH	138.3, CH	140.7, CH
3	146.3, C	144.8, C	151.8, C	144.5, C	147.7, C	144.2, C
4	110.3, CH	111.8, CH	112, CH	111.8, CH	124.9, CH	111.7, CH
4a	147.1, C	148.5, C	145.1, C	147.9, C	148.4, C	147.7, C
5	101.5, C	102.2, C	100.7, C	102.7, C	102.1, C	103.5, C
6	183.7, C	184.4, C	184.2, C	184.6, C	185.4, C	184.9, C
7	85.4, C	84.9, C	86.4, C	85.0, C	86.5, C	85.0, C
8	193.3, C	194.0, C	194.8, C	194, C	195.4, C	193.7, C
8a	114.2, C	114.6, C	116.1, C	114.8, C	117.5, C	115.0, C
9	116.4, CH	115.1, CH	115.1, CH	114.8, CH	112.7, CH	114.6, CH
10	142.9, CH	145.1, CH	146.1, CH	145.1, CH	146.0, CH	145.6, CH
11	132.0, C	131.7, C	133.6, C	131.7, C	133.8, C	132.0, C
12	148.7, CH	148.0, CH	147.2, CH	148.2, CH	147.7, CH	148.6, CH
13	35.1, CH	35.0, CH	35.5, CH	35.2, CH	36.2, CH	35.3, CH
14	30.6, CH_2	30.0, CH_2	30.9, CH_2	30.2, CH_2	31.3, CH_2	30.2, CH_2
15	12.0, CH_3	12.0, CH_3	12.3, CH_3	12.2, CH_3	12.5, CH_3	12.2, CH_3
16	20.1, CH_3	20.2, CH_3	20.6, CH_3	20.5, CH_3	20.7, CH_3	20.4, CH_3
17	12.4, CH_3	12.6, CH_3	13.0, CH_3	12.8, CH_3	12.5, CH_3	12.7, CH_3
18	23.6, CH_3	23.3, CH_3	24.0, CH_3	23.4, CH_3	24.0, CH_3	23.3, CH_3
19	170.9, C	170.2, C	170.7, C	170.2, C	171.7, C	170.4, C
20	20.6, CH_3	20.3, CH_3	20.6, CH_3	20.5, CH_3	20.4, CH_3	20.5, CH_3
1'		55.4, CH_2	42.7, CH	55.6, CH_2	56.6, CH	43.8, CH_2
2'		60.9, CH_2	173.9, C	36.8, CH	174.1, C	75.2, C
3'			30.4, CH_2	136, CH	28.6, CH_2	77.7, CH
4′			25.9, CH	128.8, CH	109.4, C	
5′			22.1, CH_3	129.5, CH	68.9, CH	
6′			23.3, CH_3	127.9, CH		
7′				129.5, CH	ND	
8′				128.8, CH	112.6, CH	
9′					120.6, CH	
10′					122.9, CH	
11′					119.2, CH	
12′					128.3, C	

ND : not determined

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