Solid-Phase Extraction Embedded Dialysis (SPEED) an Innovative procedure for the Investigation of Microbial Specialized Metabolites

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Supporting Information

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Table S1. Table of hit compounds dereplicated by GNPS database.

	Compound name	Score	Biological source
912.6279	Surugamide A	0.78	Marine-derived *Streptomyces* sp[1]
623.3375	Desferrioxamine E	0.89	*Streptomyces* species[2]
614.2724	Ferrioxamine B	0.76	Marine bacterium[3]
601.3555	Desferrioxamine E	0.84	*Streptomyces* species[2]
587.3401	Desmethylenylnocardamine	0.83	*Streptomyces* species[4]
585.3606	Dehydroxynocardamine	0.83	*Streptomyces* species[5]
561.3606	Desferrioxamine	0.92	*Streptomyces pilosus* ATCC 19797 [6]
549.2809	Antimycin A1	0.81	*Streptomyces* sp[7]
547.3451	N-[5-[[4-[4-[acetyl(hydroxy)amino]butylamino]-4-oxobutanoyl]-hydroxyamino]pentyl]-N'-(5-aminopentyl)-N'-hydroxybutanediamide	0.87	-
531.4093	Didodecyl 3,3'-thiodipropionate oxide	0.71	
535.2652	Antimycin A2	0.83	*Streptomyces* sp[7]
521.2498	Antimycin A3	0.83	*Streptomyces* sp[7]
507.2338	Antimycin A4	0.75	*Streptomyces* sp[7]
461.2607	4-[5-[[4-[5-[acetyl(hydroxy)amino]pentylamino]-4-oxobutanoyl]-hydroxyamino]pentylamino]-4-oxobutanoic acid	0.85	-
443.2500	4-[5-[[4-[5-[acetyl(hydroxy)amino]pentylamino]-4-oxobutanoyl]-hydroxyamino]pentylamino]-4-oxobutanoic acid	0.74	-
425.1919	Citreoviridin	0.72	*Penicillum citreoviride*[8]
369.1252	Tricresylphosphate	0.86	-
367.1501	1-beta-D-Glucopyranosyl-L-tryptophan	0.85	-
314.09	5'-Deoxy-5'-(methylsulfinyl)adenosine	0.86	-
261.1234	Cyclo(L-Tyr-L-Pro)	0.83	*Streptomyces* sp[9]
245.1286	L-prolyl-L-phenylalanine	0.80	-
188.0706	L-Tryptophan	0.91	-
174.0551	Quinoline-4-carboxylic acid	0.77	-
169.0756	Norharman	0.95	Plant and fungi metabolite[10]

Table S2 The *hit list* from the Dictionary of Natural Products® of 125 hit compounds of the molecular formula $C_{18}H_{22}O_6$ and their biological source

No.	compound name	biological source
1	aigialomycin D	*Aigialus parvus* BCC 5311 [11], *Fusarium* sp. LN-10 and *Paecilomyces* sp. SC0924
2	aigialomycin E	*Aigialus parvus* BCC 5311 [11]
3	2,2′,4,4′,5,5′-hexamethoxybiphenyl	-
4	2,2′,4,4′,6,6′-hexamethoxybiphenyl	-
5	1,2-Bis(4-hydroxy-3-methoxyphenyl)-1,3-propanediol;(1R,2R)-form, 1-Me ether	*Phyllanthus glaucus* [12]
6	1,2-Bis(4-hydroxy-3-methoxyphenyl)-1,3-propanediol;(1R,2S)-form, 1-Me ether	*Phyllanthus glaucus* [12]
7	1,2-Bis(4-hydroxy-3-methoxyphenyl)-1,3-propanediol;(1RS,2SR)-form, 1-Me ether	*Phyllanthus glaucus* [12]
8	1,2-Bis(4-hydroxy-3-methoxyphenyl)-1,3-propanediol;(1S,2R)-form, 1-Me ether	*Phyllanthus glaucus* [12]
9	1,2-Bis(4-hydroxy-3-methoxyphenyl)-1,3-propanediol;(1S,2S)-form, 1-Me ether	*Phyllanthus glaucus* [12]
10	1,2-Bis(3,4,5-trihydroxyphenyl)ethane; 3,3',4,4'-Tetra-Me ether	*Dendrobium cumulatum [13]*
11	dihydrobyssochlamic acid	*Byssochlamys fulva* [14]
12	chaetoaurin	*Chaetomium aureum* [15]
13	chermesinone C	*Penicillium chermesinum* ZH4-E2 [16]
14	combretastatin	*Combretum caffrum* [17]
15	cyclopaldic acid, 5-*O*-(3-methyl-2-butenyl), 3-Et ether	*Aspergillus duricaulis* [18]
16	3,7'-cyclo-1,2,3,4-tetrahydro-1,8'-lign-8-ene-2,3,3',4,4',5-hexol	-
17	3,7'-Cyclo-1,2,3,4-tetrahydro-1,8'-lign-8-ene-2,3,3',4,4',5-hexol; (1*R**,3*S**,4*R**,7'*R**,8'*S**)-form	-
18	3,7'-Cyclo-1,2,3,4-tetrahydro-1,8'-lign-8-ene-2,3,3',4,4',5-hexol; (1*R**,3S*,4*S**,7'*R**,8'*S**)-form	-
19	3,7'-Cyclo-1,2,3,4-tetrahydro-1,8'-lign-8-ene-2,3,3',4,4',5-hexol; (1*S*,2*S*,3*R*,4*S*,7'*S*,8'*R*)-form	-
20	cytosporone H	*Paraphaeosphaeria quadriseptata* [19]
21	cytosporone G	*Paraphaeosphaeria quadriseptata* [19]
22	cytosporone I	*Paraphaeosphaeria quadriseptata* [19]
23	Neocosmosin B	*Neocosmospora* sp. (UM-031509) [20]
24	Monocillin V	*Monocillium nordinii* [21]
25	9R-Hydroxymonocillin IV	*Paecilomyces sp. SC0924* [22]
26	3,5-Dihydroxy-4(15),10(14),11(13)-guaiatrien-12,8-olide; (1α,3α,5α,8α)-form, 10α, 146epoxide, 3-propanoyl	*Arctotis grandis* and *Venidium hirsutum*
27	3,5-Dihydroxy-4(15),10(14),11(13)-guaiatrien-12,8-olide; (1α,3β,5α,8α)-form, 10α, 146epoxide, 3-propanoyl	*Arctotis arctotoides*
28	1,8-Dihydroxy-2-oxo-3,7(11)-eudesmadien-12,8-olide; (1β,8βOH)-form, 8-Me ether, 1-Ac	*Salvia plebeia*
29	7-hydroxygerin	*Saussurea cauloptera* [23]

30	carayensin A	*Carya cathayensis* [24]
31	2-(3,4-Dihydroxyphenyl)-1-(3,4,5-trihydroxyphenyl)ethanol; *(R)*-form, *α*,3,3′,5-Tetra-Me ether (loddigesiinols C)	*Dendrobium loddigesii* [25]
32	nobilin B	*Dendrobium nobile* [26]
33	pithecellobiumol A	*Pithecellobium clypearia* [27]
34	combretol C	*Combretum yunnanense* [28]
35	3,8-dimethyl-2-naphthol; *O*-β-D-glucopyranoside	*Hibicus cannabinus* [29]
36	8,10-epoxy-*p*-mentha-1,3,5-triene-2,5,9-triol; 2-Me ether, 5-tigloyl, 9-Ac	*Mikania species* [30]
37	4,7'-epoxy-3,4,5,6-tetrahydro-3,8'-lign-8-ene-3,3',4,4',6-pentol	-
38	4,7'-epoxy-3,4,5,6-tetrahydro-3,8'-lign-8-ene-3,3',4,4',6-pentol; (3*R**,4*R**,7′S*,8′*S**)-form	-
39	4,7'-epoxy-3,4,5,6-tetrahydro-3,8'-lign-8-ene-3,3',4,4',6-pentol; (3*R**,4*R**,7′S*,8′*R**)-form	-
40	4,7'-epoxy-3,4,5,6-tetrahydro-3,8'-lign-8-ene-3,3',4,4',6-pentol; (3*S*,4*R*,6S,7′*S*,8′*R*)-form	-
41	6'-hydroxypestalotiopsone C	*Acremonium strictum* [31]
42	dihydroepiheveadride	Unidentified fungus IFM 52672 [32]
43	4'-O-Acetylsinapyl angelate	*Solidago decurrens*
44	Nervolan A	*Inula nervosa* [33]
45	15-hydroxy-1(10),4,11(13)-germacratrien-12,6-olid-14-oic acid; (1(10,*E*,4*Z*,6*α*)-form, Me ester, Ac	*Oyedaea verbesinoides* [34]
46	2',3'-Isopropylideneobtusinin	*Pterocaulon alopecuroides* [35]
47	5-(Hydroxymethyl)-7-methyl-6-(2,4,5-trimethoxyphenyl)-8-oxabicyclo[3.2.1]oct-3-en-2-one	-
48	Acorusin C	*Acorus tatarinowii* [36]
49	Acortatarone A	*Acorus tatarinowii* [36]
50	5-(Hydroxymethyl)-7-methyl-6-(2,4,5-trimethoxyphenyl)-8-oxabicyclo[3.2.1]oct-3-en-2-one; (1*S*,5*S*,6*R*,7*S*)-form	-
51	3-Hydroxyviscidone	*Gerbera saxatilis* [37]
52	Ilexisochroman	*Ilex pubescens* [38]
53	2,7'-Lignan-3,3',4,4',5,5'-hexol	-
54	2,7'-Lignan-3,3',4,4',5,5'-hexol, *(R)*-form	-
55	3,8'-Lignan-3',4,4',5,9,9'-hexol	-
56	3,8'-Lignan-3',4,4',5,9,9'-hexol, *(R)*-form	-
57	3,8'-Lignan-3',4,4',5,9,9'-hexol, *(S)*-form	-
58	3,8'-Lignan-3',4,4',5,9,9'-hexol, *(ξ)*-form	-
59	8,8'-Lignan-2,2',4,4',5,5'-hexol	-
60	8,8'-Lignan-2,2',4,4',5,5'-hexol;(8*R**,8'*S**)-form	-
61	8,8'-Lignan-2,2',4,4',5,5'-hexol;(8*RS*,8'*SR*)-form	-
62	8,8'-Lignan-2,3',4,4',5,7'-hexol	-
63	8,8'-Lignan-2,3',4,4',5,7'-hexol;(7'*S*,8*S*,8'*R*)-form	-
64	8,8'-Lignan-2,3',4,4',5,7'-hexol;(8ξ,8'ξ)-form	-
65	8,8'-Lignan-3,3',4,4',5,5'-hexol	-
66	8,8'-Lignan-3,3',4,4',5,5'-hexol;(8*R*,8'*R*)-form	-
67	8,8'-Lignan-3,3',4,4',5,5'-hexol;(8*RS*,8'*SR*)-form	-
68	8,8'-Lignan-3,3',4,4',5,5'-hexol;(8ξ,8'ξ)-form	-
69	8,8'-Lignan-3,3',4,4',5,7-hexol	-
70	8,8'-Lignan-3,3',4,4',5,7-hexol;(7ξ,8ξ,8'ξ)-form	-

71	8,8'-Lignan-3,3',4,4',5,9'-hexol	-
72	8,8'-Lignan-3,3',4,4',5,9-hexol	-
73	8,8'-Lignan-3,3',4,4',5,9-hexol;(8*S*,8'*R*)-form	-
74	8,8'-Lignan-3,3',4,4',5,9′-hexol;(8*S*,8'*R*)-form	-
75	8,8'-Lignan-3,3',4,4',7,7'-hexol	-
76	8,8'-Lignan-3,3',4,4',7,7'-hexol;(7*RS*,7'*RS*,8*SR*,8'*SR*)-form	-
77	8,8'-Lignan-3,3',4,4',7,7'-hexol;(7*RS*,7'*SR*,8*RS*,8'*RS*)-form	-
78	8,8'-Lignan-3,3',4,4',7,7'-hexol;(7*S*,7'*S*,8*S*,8'*S*)-form	-
79	8,8'-Lignan-3,3',4,4',9,9'-hexol	-
80	8,8'-Lignan-3,3',4,4',9,9'-hexol;(8*R**,8'*R**)-form	-
81	8,8'-Lignan-3,3',4,4',9,9'-hexol;(8*R*,8'*R*)-form	-
82	8,8'-Lignan-3,3',4,4',9,9'-hexol;(8*R**,8'*S**)-form	-
83	8,8'-Lignan-3,3',4,4',9,9'-hexol;(8*RS*,8'*RS*)-form	-
84	8,8'-Lignan-3,3',4,4',9,9'-hexol;(8*RS*,8'*SR*)-form	-
85	8,8'-Lignan-3,3',4,4',9,9'-hexol;(8S,8'*S*)-form	-
86	8,8'-Lignan-3,3',4,4',9,9'-hexol;(8ξ,8'ξ)-form	-
87	8,8'-Lignan-3,3',5,5',7,7'-hexol	-
88	8,8'-Lignan-3,3',5,5',7,7'-hexol;(7*R**,7'*R**,8*R**,8'*S**)-form	-
89	2β-Hydroxynagilactone L	*Podocarpus nagi* [39]
90	3β-Hydroxynagilactone L	*Podocarpus nagi* [39]
91	15-Hydroxynagilactone L	*Podocarpus nagi* [39]
92	Laxiflorin U	*Isodon eriocalyx* var. *laxiflora* [40]
93	Andrographidoid D	*Andrographis paniculata* [41]
94	Octandrenolone;3,4-Dihydro, 3α,4β-dihydroxy	*Melicope erromangensis* [42]
95	Octandrenolone;9,10-Dihydro, 9α,10β-dihydroxy	*Melicope erromangensis* [42]
96	Oncocalyxone D;11-Me ether(11β-)	*Cordia oncocalyx* [43]
97	Oxirapentyne B	*Isaria felina* (DC.) Fr [44]
98	Oxirapentyne C	*Isaria felina* (DC.) Fr [44]
99	4,8'-Oxylignan-3,3',4',7',9-pentol	-
100	4,8'-Oxylignan-3,3',4',7',9-pentol;(7'*R*,8'*R*)-form	-
101	4,8'-Oxylignan-3,3',4',7',9-pentol;(7'*R**,8'*R**)-form	-
102	4,8'-Oxylignan-3,3',4',7',9-pentol;(7'*R*,8'S)-form	-
103	4,8'-Oxylignan-3,3',4',7',9-pentol;(7'*R*,8'S)-form	-
104	4,8'-Oxylignan-3,3',4',7',9-pentol;(7'*S*,8'S)-form	-
105	4,8'-Oxylignan-3,3',4',9,9'-pentol	-
106	4,8'-Oxylignan-3,3',4',9,9'-pentol;(*R*)-form	-
107	4,8'-Oxylignan-3,3',4',9,9'-pentol;(*S*)-form	-
108	4,8'-Oxylignan-3,4',7',9,9'-pentol	-
109	4,8'-Oxylignan-3,4',7',9,9'-pentol;(7′*RS*,8'*RS*)-form	-
110	4,8'-Oxylignan-3,4',7',9,9'-pentol;(7′*RS*,8'*SR*)-form	-
111	Streblusligнanol H	*Streblus asper* [45]
112	Streblusol D	*Streblus asper* [46]
113	tetrodecamycin	*Streptomyces nashvillensis* MJ885-mF8 [47]
114	1,6,10-trihydroxy-7(11),8-eremophiladien-12,8-olide;(1β,6β,10α)-form,1-Ketone, 6-propanoyl	*Senecio nemorensis*
115	8-Acryloylhydroxyisonobilin	*Anthemis nobilis* [48]
116	Combretastatin B1	*Combretum caffrum* [49] and *Combretum kraussi*

117	Bussealin B	*Bussea sakalava* [50]
118	11,12-Epoxyzearalenone	*Fusarium graminearum* [51]
119	4R-Hydroxyzearalenone	*Fusarium* sp. PSU-ES123 [52]
120	5R-Hydroxyzearalenone	*Gibberella zeae, Fusarium graminearium* and the marine-derived *Fusarium* sp. 05ABR26 [53]
121	5S-Hydroxyzearalenone	*Gibberella zeae* and *Fusarium graminearium* [51]
122	6R-Hydroxyzearalenone	*Fusarium* sp. PSU-ES123 [52]
123	8R-Hydroxyzearalenone	*Fusarium* sp. PSU-ES73 [54]
124	8S-Hydroxyzearalenone	*Fusarium* sp. PSU-ES123 [52]
125	10-Hydroxyzearalenone	*Fusarium graminearum* [51]

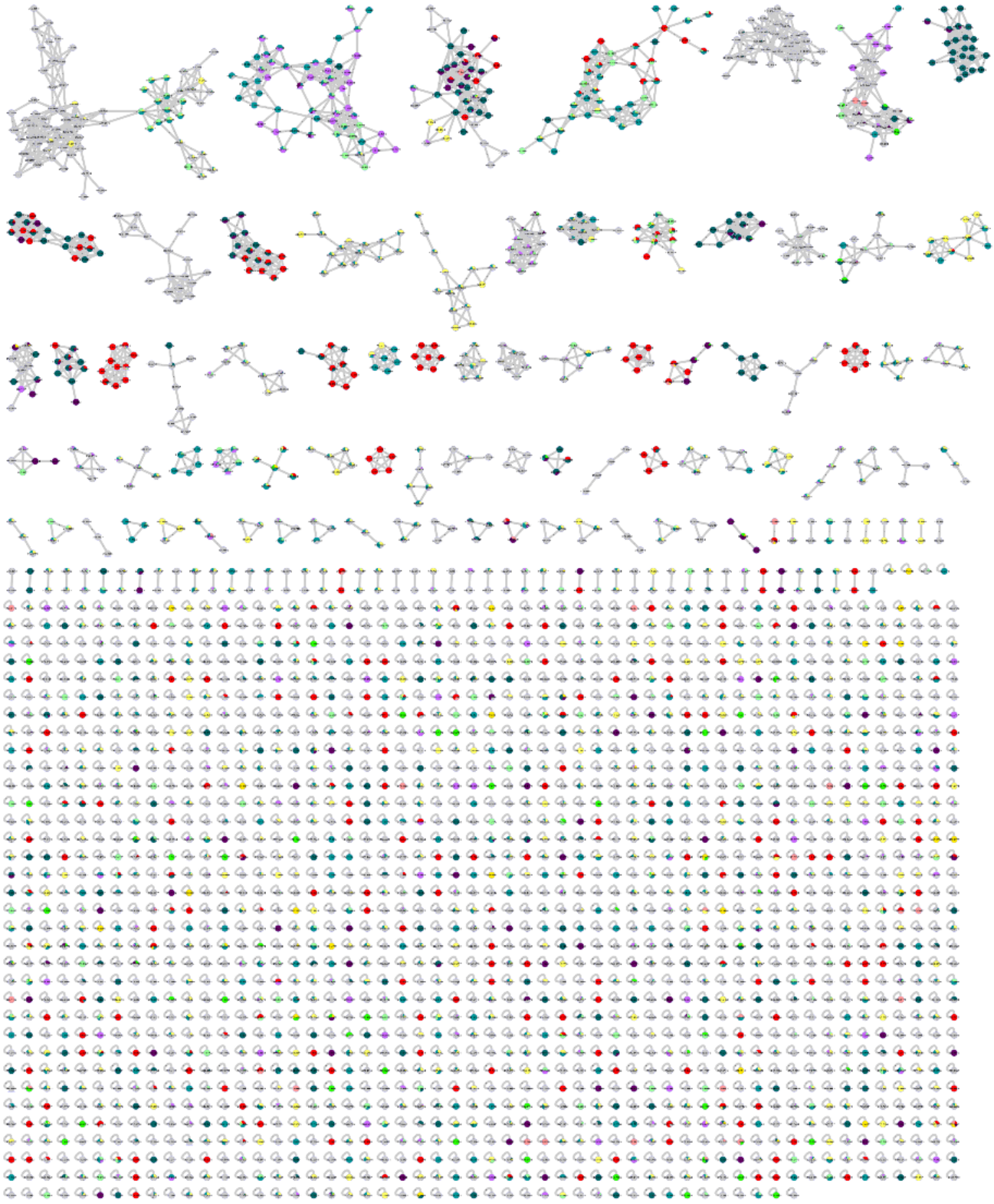

Figure S1. The molecular networking of the strain extracts from different condition cultures and the control extracts. Different culture condition is represented by different color code.

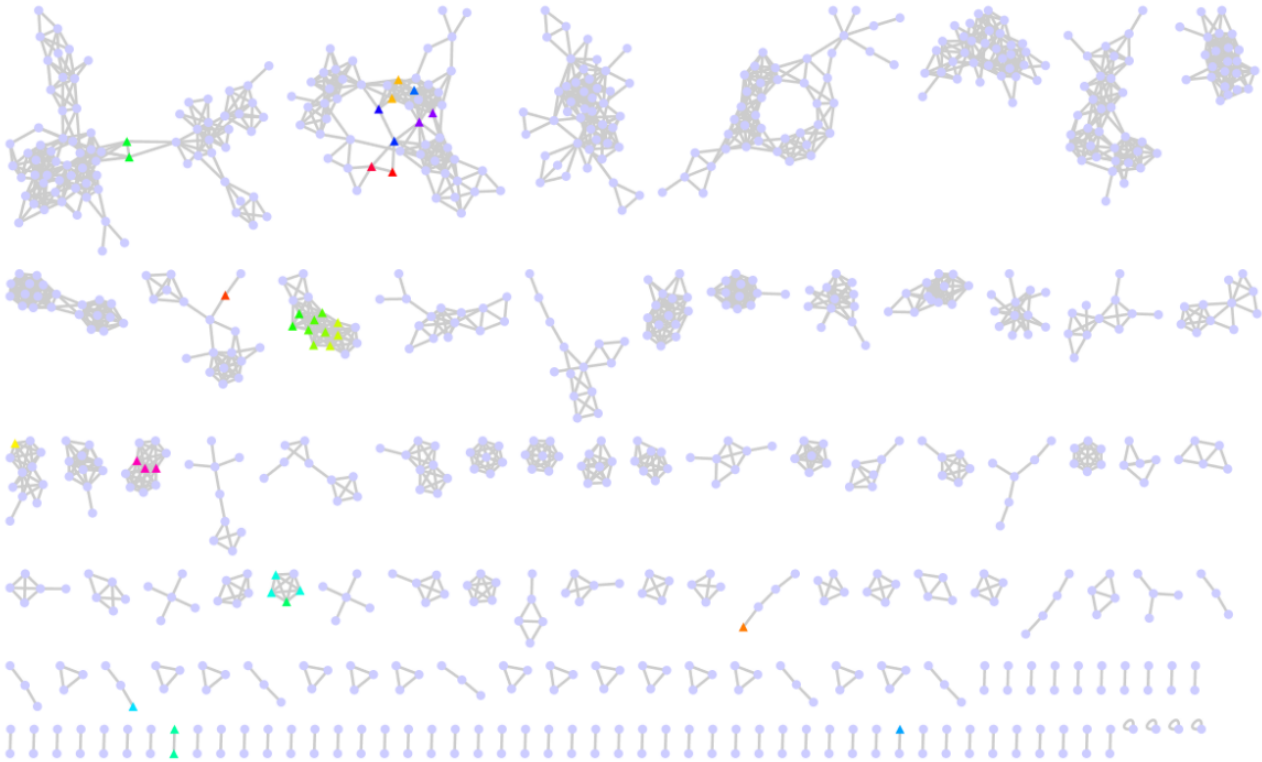

Figure S2. The molecular networking with dereplicated nodes that are mapped by rainbow color codes while others stayed purple.

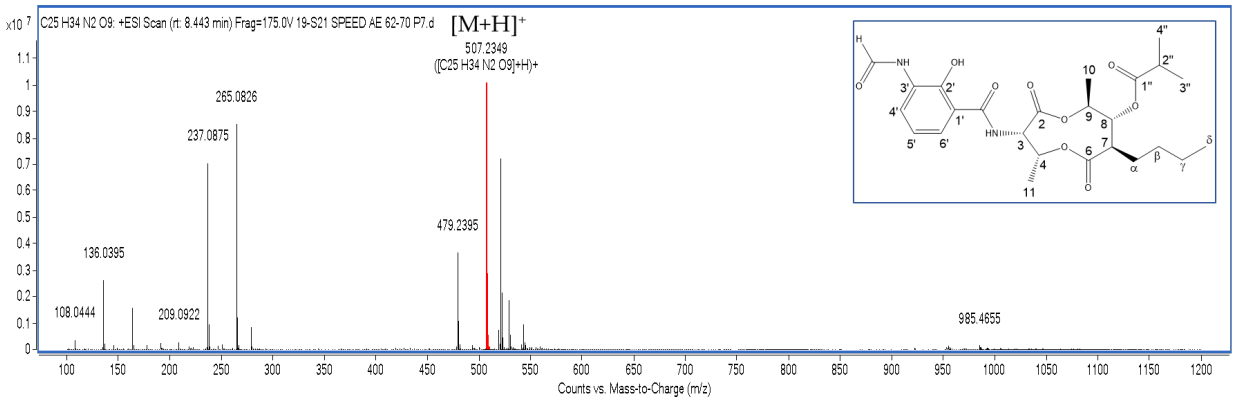

Figure S3. The HRESIMS spectrum of Antimycin A4a

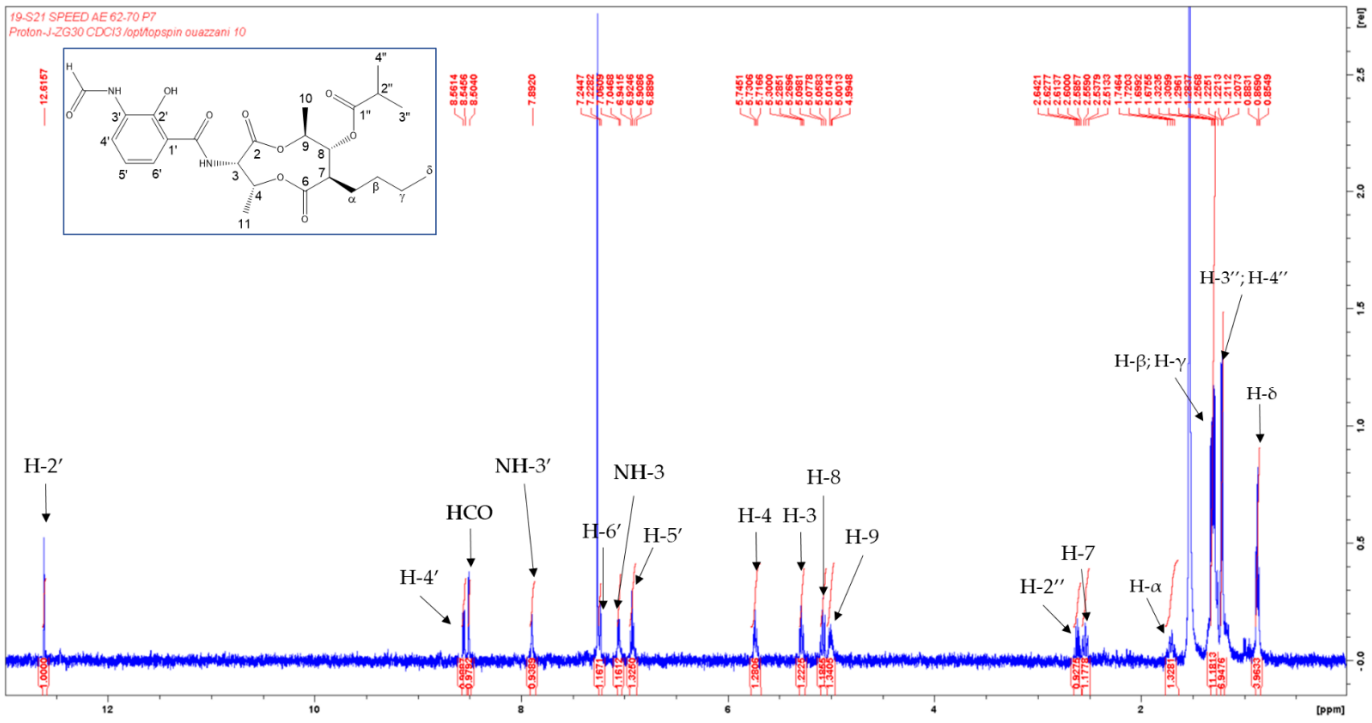

Figure S4. ^{1}H NMR spectrum of Antimycin A4a in $CDCl_3$ (500 MHz)

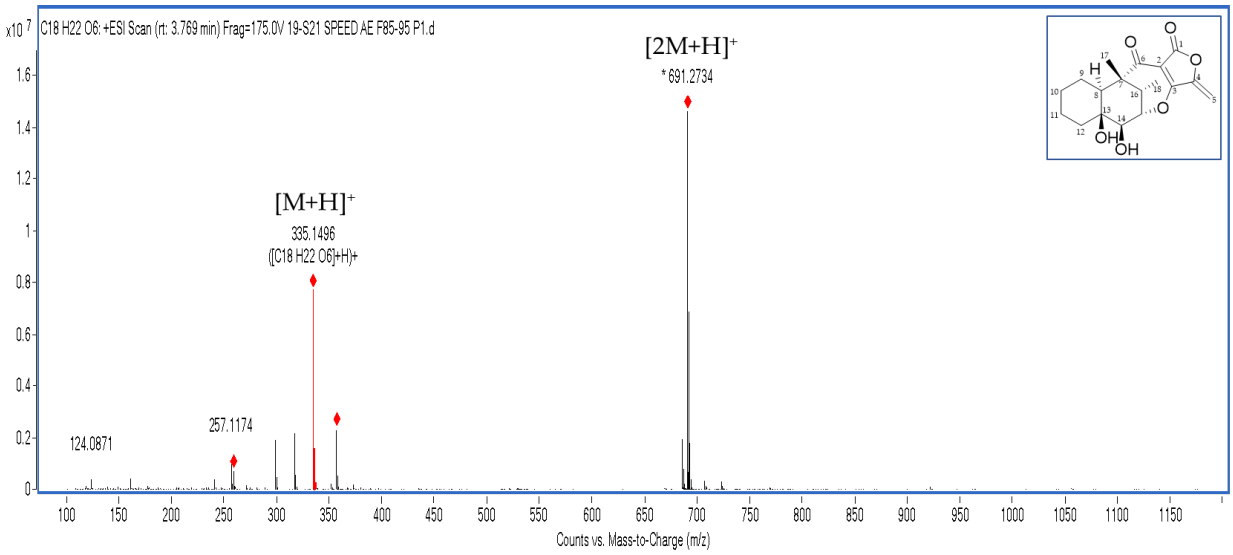

Figure S5. The HRESIMS spectrum of tetrodecamycin

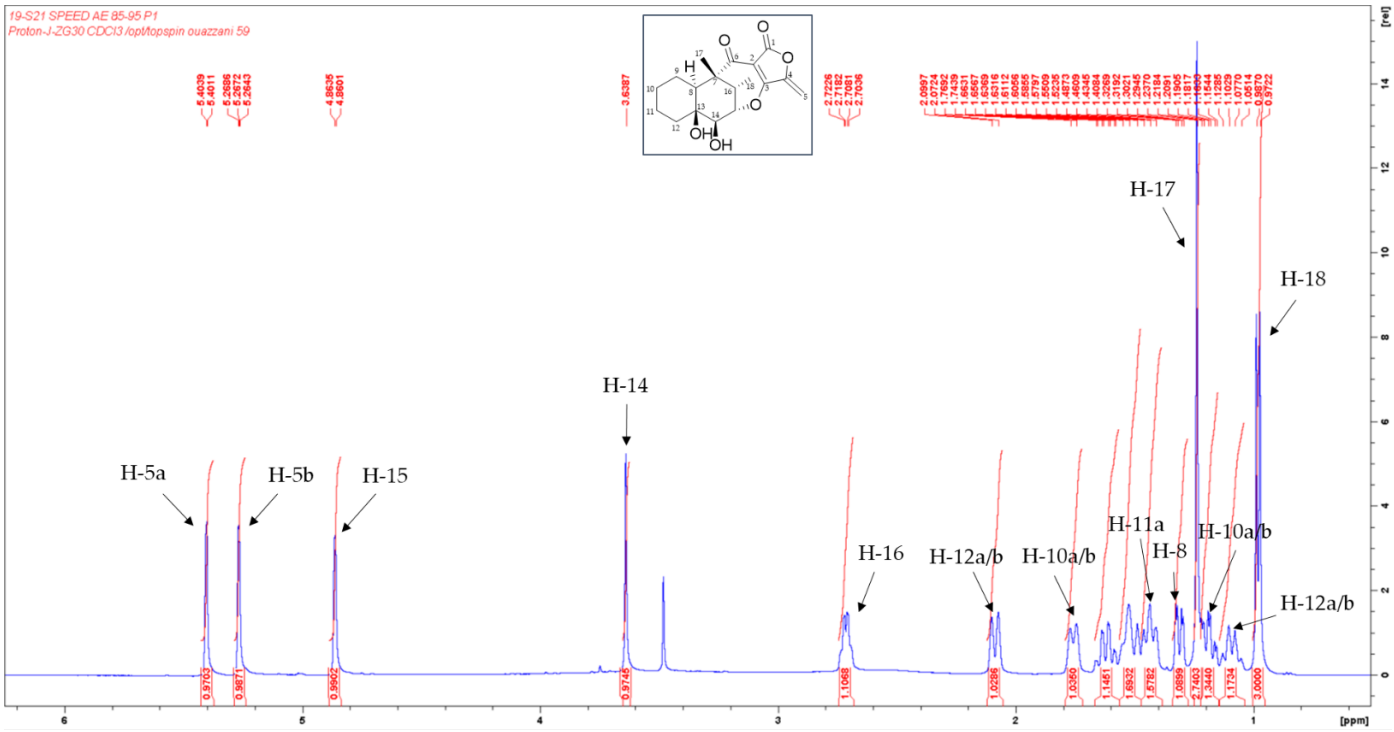

Figure S6. ^{1}H NMR spectrum of tetrodecamycin in $CDCl_3$ (500 MHz)

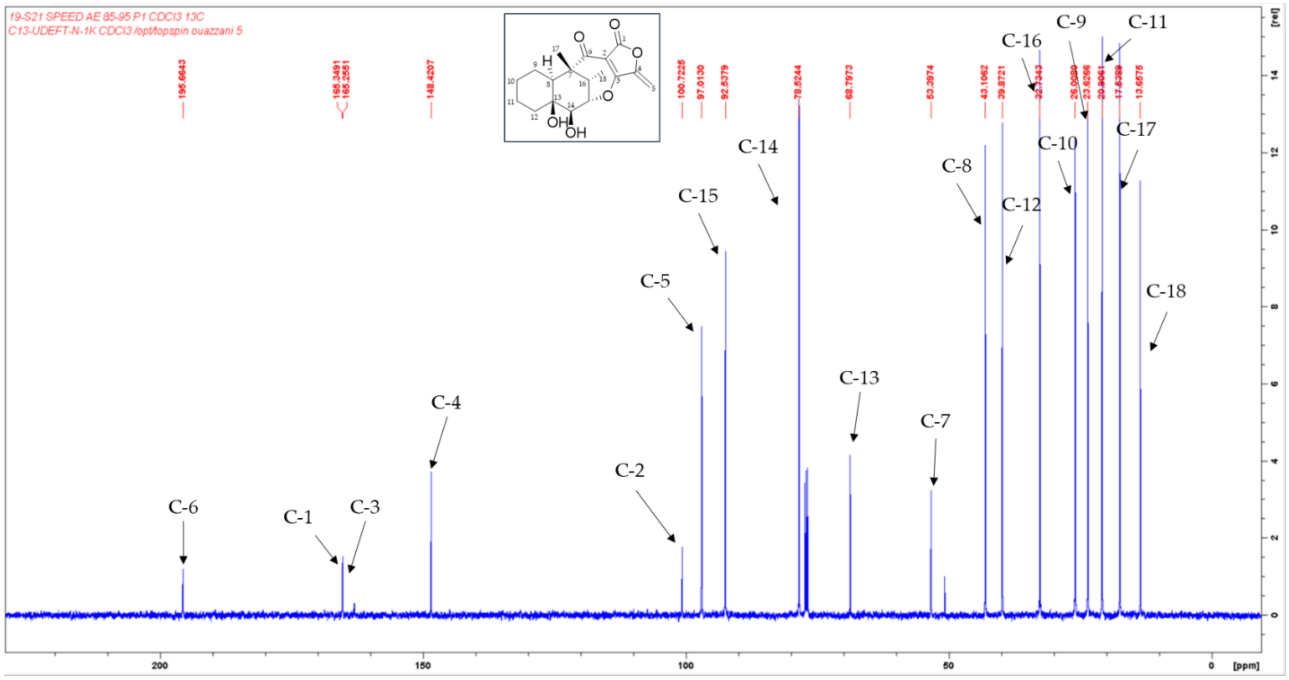

Figure S7. ^{13}C NMR spectrum of tetrodecamycin in $CDCl_3$ (125 MHz)

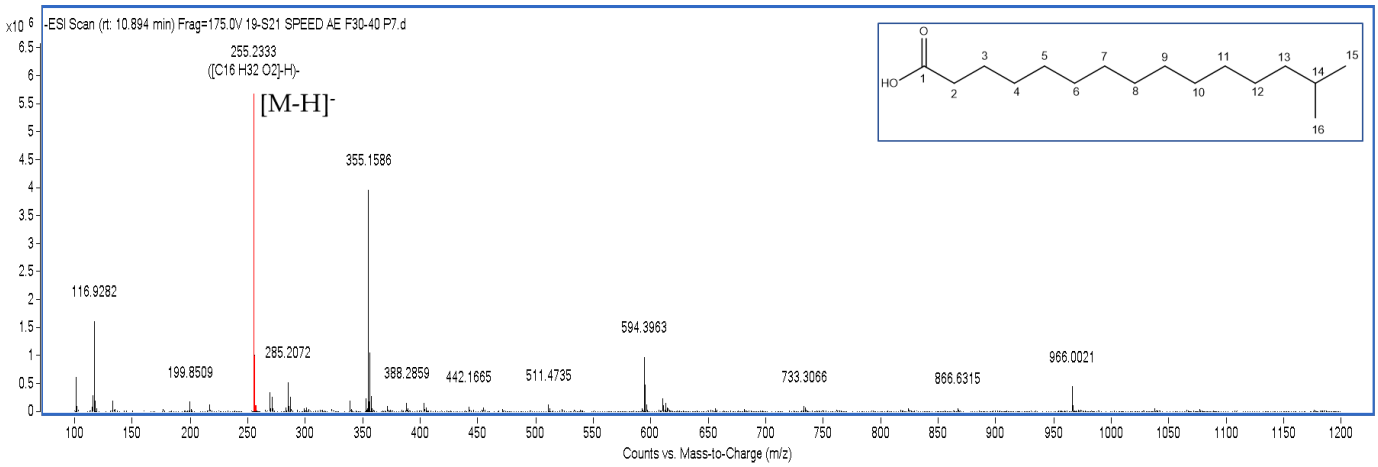

Figure S8. The HRESIMS spectrum of 14-methylpentadecanoic acid

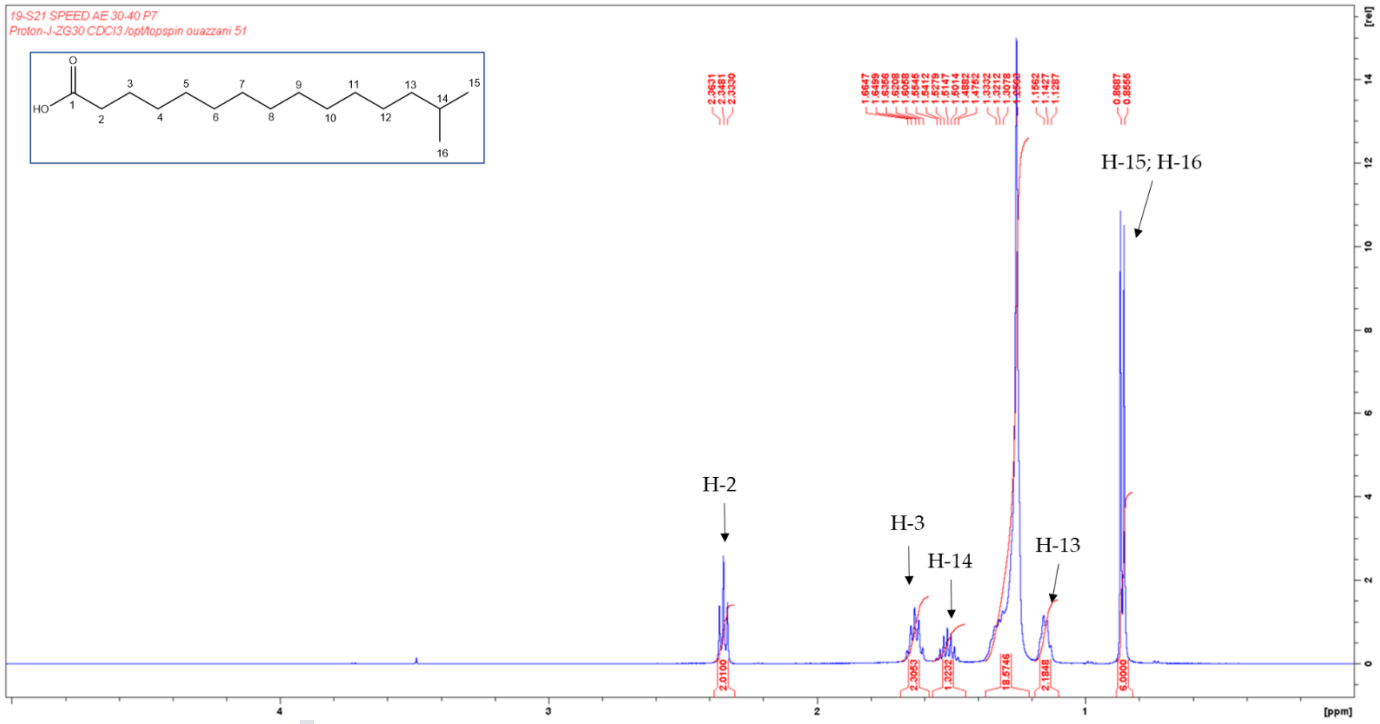

Figure S9. ^{1}H NMR spectrum of 14-methylpentadecanoic acid in $CDCl_3$ (500 MHz)

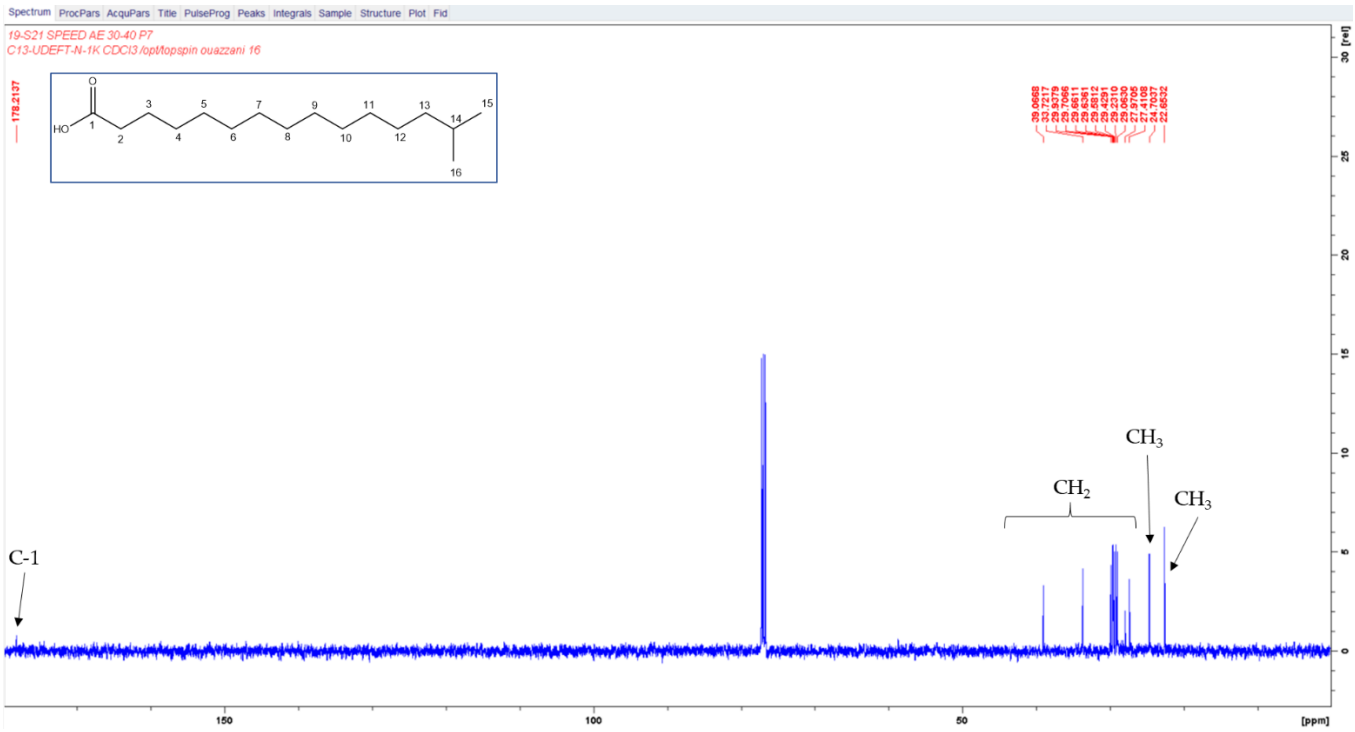

Figure S10. ^{13}C NMR spectrum of 14-methylpentadecanoic acid in $CDCl_3$ (125 MHz)

Figure S11. Further SPEED pictures

References

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