Supplementary Material

In-Depth Study of Alkaloids from *Strychnos longicaudata* Trunk Barks to Discover Original Antiplasmodial Compounds

Olivier Bonnet[a,*], Jessica Delrée[a], Mehdi A. Beniddir[b], Pierre Champy[b], Séverine Derbré[c], Charline Leroy[a], Allison Ledoux[a], Alembert Tiabou Tchinda[a,d], Luc Angenot[a], Michel Frédérich[a]

[a]Laboratory of Pharmacognosy, Center of Interdisciplinary Research on Medicines (CIRM), University of Liège, B36, 4000 Liège, Belgium.
[b]Equipe "Chimie des Substances Naturelles" BioCIS, CNRS, Université Paris-Saclay, 17 Avenue des sciences, 91400 Orsay, France.
[c]Department of Pharmacy, Faculty of Health Sciences, University of Angers, SONAS, SFR QUASAV, Angers, France.
[d]Institute of Medical Research and Medicinal Plants Studies (IMPM), PO Box 13033, Yaoundé, Cameroon.

Correspondence

Olivier Bonnet, University of Liège, B36, 4000 Liège, Belgium.

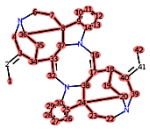
E-mail: Olivier.Bonnet@uliege.be

Table of contents

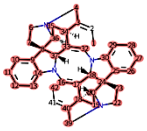
Table S1: List of identifications suggested by MixONat during the study of the alkaloidic crude extract from *S. longicaudata* trunk barks.

LTS numbers	Identifications
LTS0001938 LTS0021871 LTS0250825 LTS0006531	Bisnordihydrotoxiferine
LTS0178133 LTS0044492	Geissoschizol
LTS0234046 LTS0219283	Tubotaiwinal
LTS0227956	Normavacurine
LTS0163909	Yohimb-19-ene
LTS0025694	Normacusine B
LTS0072875	Caracurine V
LTS0119464 LTS0116794	Leucocinine C
LTS0205745 LTS0015052	Retuline ou isoretuline
LTS0157335 LTS0086061 LTS0097468	N-Desactylretuline ou N-Desactylisoretuline
LTS0126423	4',17-Dihydro-17α-tchibangensine ou 4',17-Dihydro-17β-tchibangensine
LTS0176270	Antirhine
LTS0012467	Antirhine lactone
LTS0100776	Dihydroantirhine (20R) ou Dihydroantirhine (20S)
LTS0040629	Longicaudatine
LTS0251284 LTS0191415	Longicaudatine Y
LTS0111579	Longicaudatine F
LTS0265114	Scholaricine
LTS0053790	11-Demethoxymyrtoidine
LTS0029735	5',6'-Dihydrousambarensine
LTS0210122	Tubifolidine
LTS0159100	4-tert-butyl-2-oxazolidinol
LTS0261346 LTS0005882	(Z)-Akuammidine
LTS0114913	(16R)-Isositsirkine ou (16S)-Isositsirkine

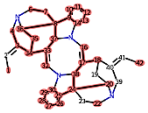
LTS0243393	1-[(18e)-18-ethylidene-6-hydroxy-8,14-diazapentacyclo[9.5.2.0^{1,9}.0^{2,7}.0^{14,17}]octadeca-2,4,6-trien-8-yl]propan-1-one
LTS0009899	Caracurine V
LTS0170796	3-Acetyl-indole
LTS0217769	10-methoxy-nor-C-fluorocurarine
LTS0180652	1-[(18e)-18-ethylidene-6-hydroxy-8,14-diazapentacyclo[9.5.2.0^{1,9}.0^{2,7}.0^{14,17}]octadeca-2,4,6-trien-8-yl]ethanone
LTS0259901	Methyl (1R,3'R,11R,12R,17S)-3'-methylspiro[8,14-diazapentacyclo[9.5.2.01,9.02,7.014,17]octadeca-2,4,6,9-tetraene-12,2'-oxirane]-10-carboxylate



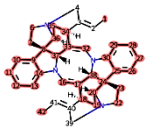
Rank: 1 MW: 552.75
LTS0001938
Score: 0.95 (36/38 C)
Deviation : 9.28 ppm



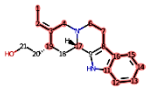
Rank: 2 MW: 552.75
LTS0021871
Score: 0.95 (36/38 C)
Deviation : 9.28 ppm



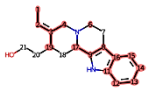
Rank: 3 MW: 552.75
LTS0250825
Score: 0.84 (32/38 C)
Deviation : 7.32 ppm



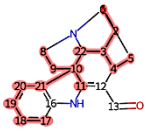
Rank: 4 MW: 552.75
LTS0006531
Score: 0.84 (32/38 C)
Deviation : 8.08 ppm



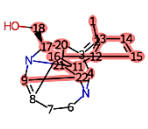
Rank: 5 MW: 296.41
LTS0178133
Score: 0.79 (15/19 C)
Deviation : 5.36 ppm



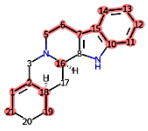
Rank: 6 MW: 296.41
LTS0044492
Score: 0.79 (15/19 C)
Deviation : 5.4 ppm



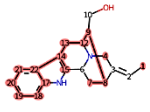
Rank: 7 MW: 294.39
LTS0234046
Score: 0.79 (15/19 C)
Deviation : 7.07 ppm



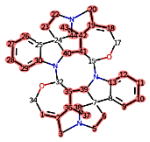
Rank: 8 MW: 294.39
LTS0227956
Score: 0.79 (15/19 C)
Deviation : 7.93 ppm



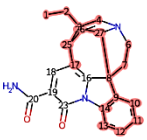
Rank: 9 MW: 278.39
LTS0163909
Score: 0.79 (15/19 C)
Deviation : 8.15 ppm



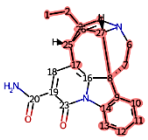
Rank: 10 MW: 294.39
LTS0025694
Score: 0.79 (15/19 C)
Deviation : 10.42 ppm



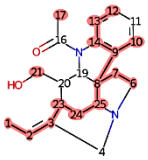
Rank: 11 MW: 584.75
LTS0072875
Score: 0.79 (30/38 C)
Deviation : 16.24 ppm



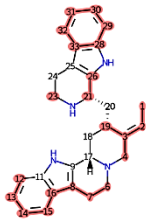
Rank: 12 MW: 359.42
LTS0119464
Score: 0.77 (17/22 C)
Deviation : 4.7 ppm



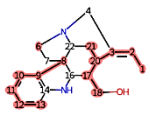
Rank: 13 MW: 359.42
LTS0116794
Score: 0.77 (17/22 C)
Deviation : 6.77 ppm



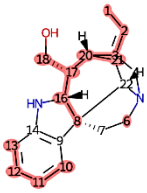
Rank: 14 MW: 338.44
LTS0205745
Score: 0.76 (16/21 C)
Deviation : 7.94 ppm



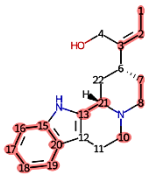
Rank: 15 MW: 436.59
LTS0126423
Score: 0.76 (22/29 C)
Deviation : 11.19 ppm



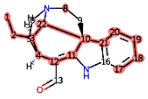
Rank: 16 MW: 296.41
LTS0157335
Score: 0.74 (14/19 C)
Deviation : 5.04 ppm



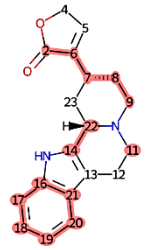
Rank: 17 MW: 296.41
LTS0086061
Score: 0.74 (14/19 C)
Deviation : 6.31 ppm



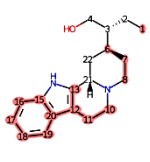
Rank: 18 MW: 296.41
LTS0176270
Score: 0.74 (14/19 C)
Deviation : 6.32 ppm



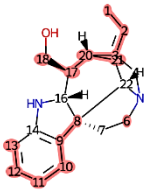
Rank: 19 MW: 294.39
LTS0219283
Score: 0.74 (14/19 C)
Deviation : 6.32 ppm



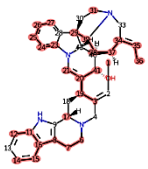
Rank: 20 MW: 308.37
LTS0012467
Score: 0.74 (14/19 C)
Deviation : 6.48 ppm



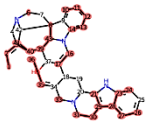
Rank: 21 MW: 298.42
LTS0100776
Score: 0.74 (14/19 C)
Deviation : 6.71 ppm



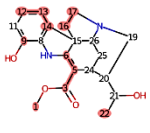
Rank: 22 MW: 296.41
LTS0097468
Score: 0.74 (14/19 C)
Deviation : 7.65 ppm



Rank: 23 MW: 570.77
LTS0251284
Score: 0.74 (28/38 C)
Deviation : 11.33 ppm



Rank: 24 MW: 570.77
LTS0191415
Score: 0.74 (28/38 C)
Deviation : 11.69 ppm



Rank: 25 MW: 356.42
LTS0265114
Score: 0.73 (11/15 C)
Deviation : 5.34 ppm

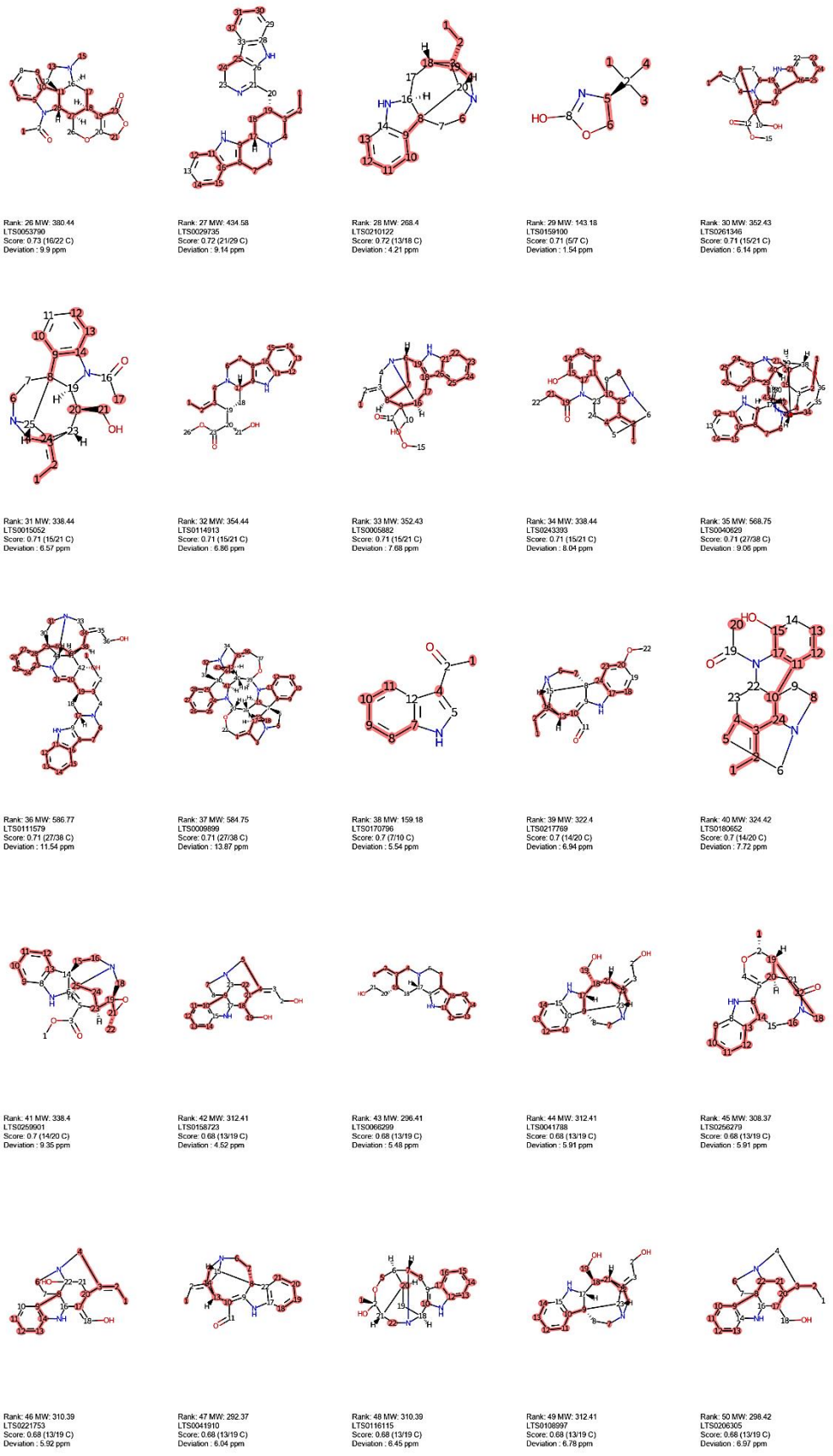


Figure S1: Identifications suggested by MixONat during the study of the alkaloidic crude extract from *S. longicaudata* trunk barks.

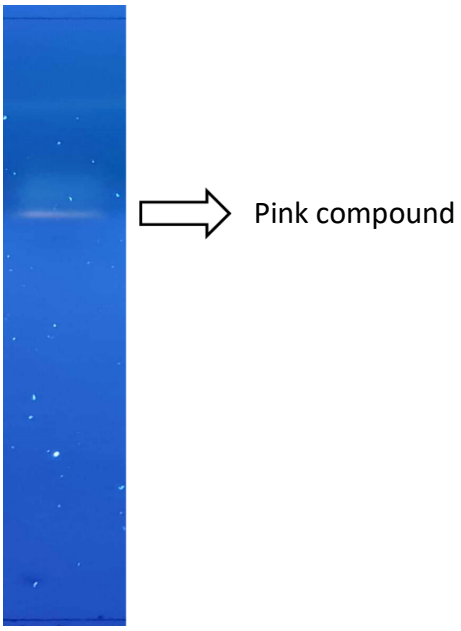


Figure S2: An example of TLC of the pink compound from the fraction 21 under UV at 366 nm.

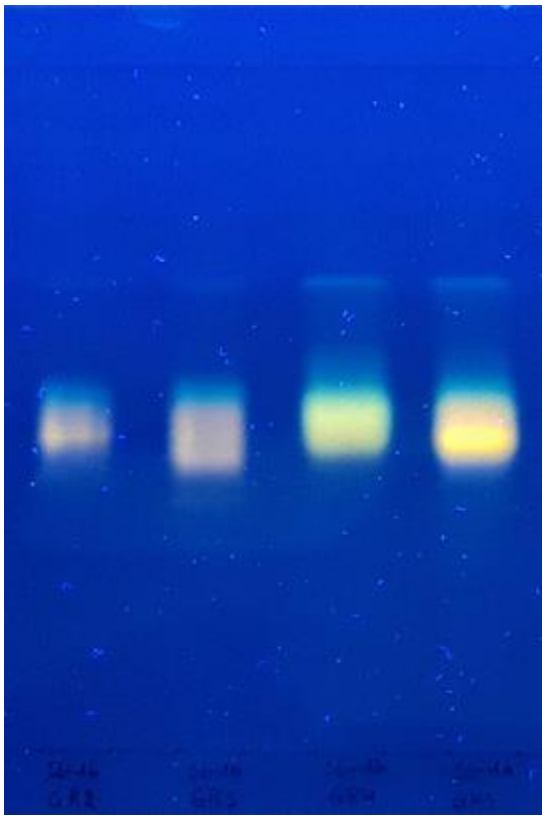


Figure S3: An example of TLC of the yellow-orange compounds from the fraction 16 under UV at 366 nm.

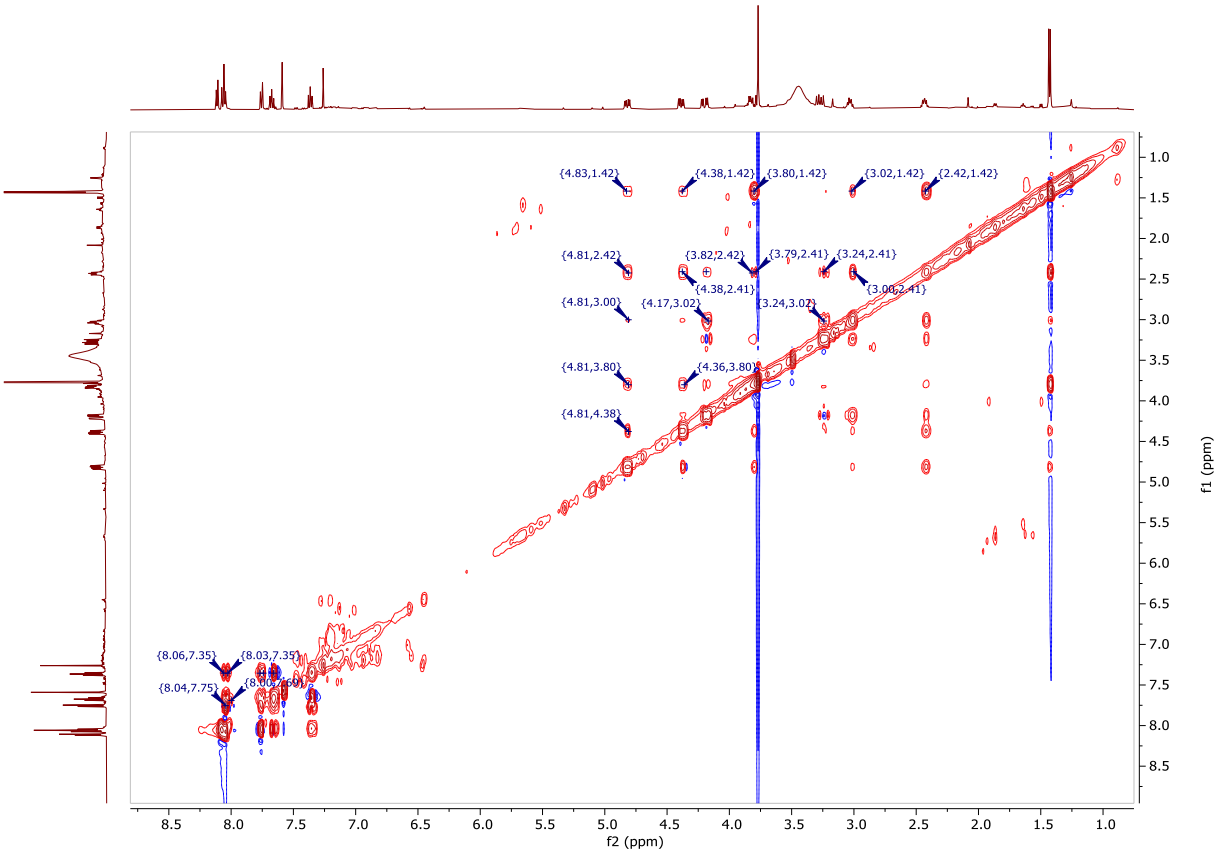
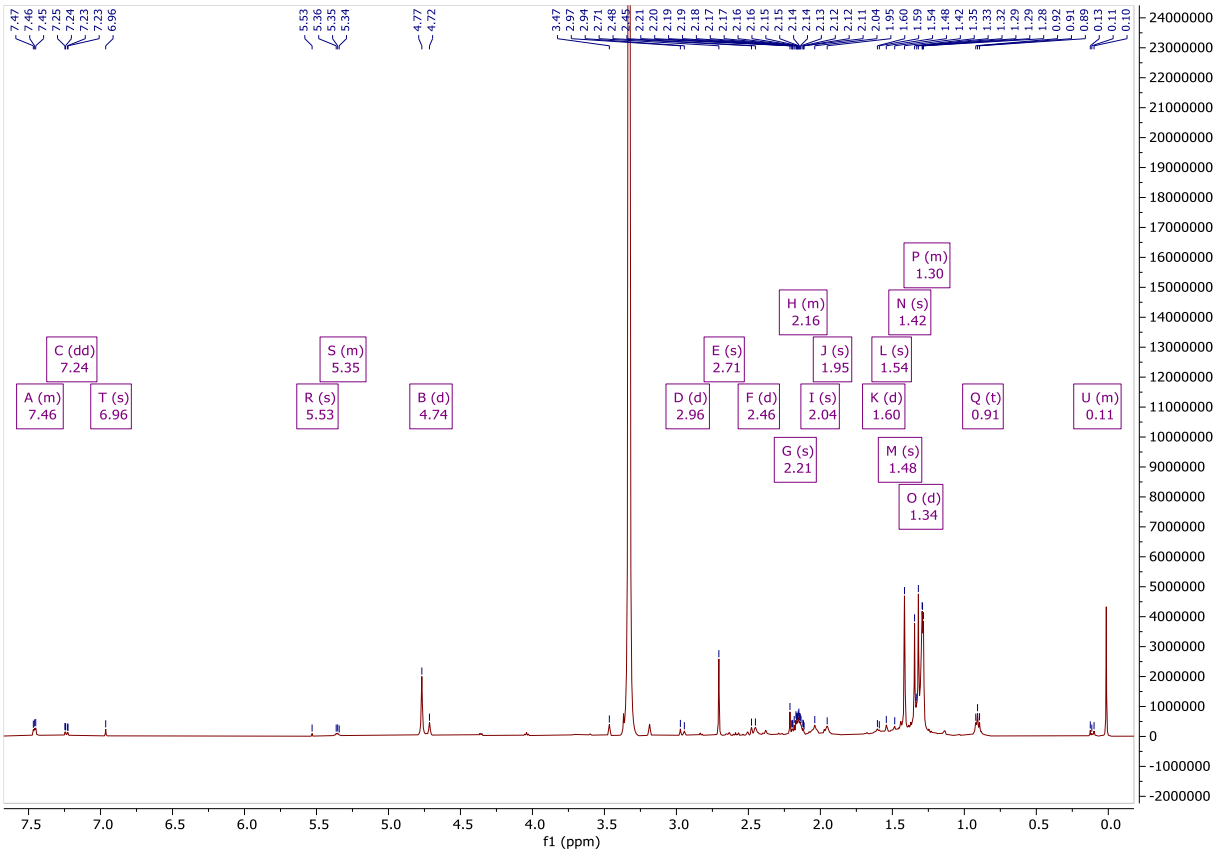
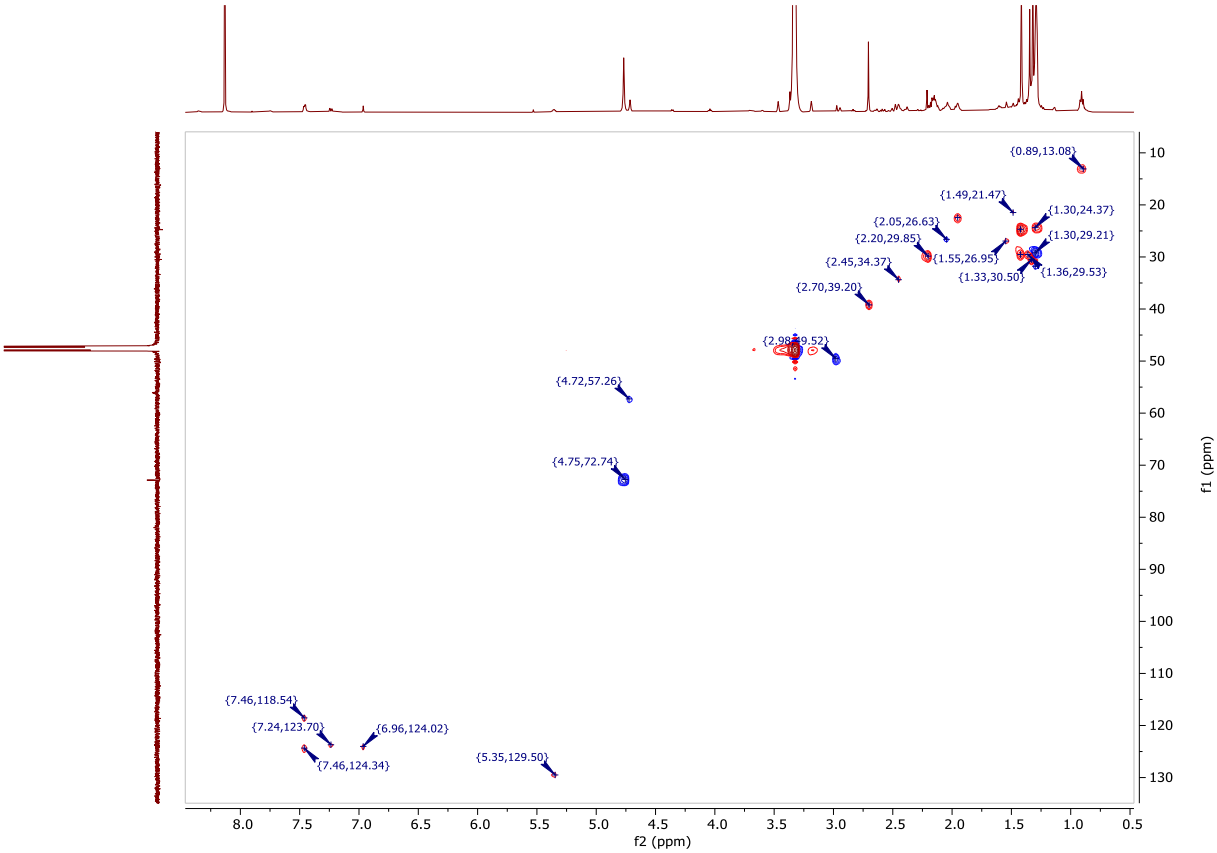


Figure S4: TOCSY spectrum of the fraction 14.


A (m) 7.46
C (dd) 7.24
T (s) 6.96
R (s) 5.53
S (m) 5.35
B (d) 4.74
D (d) 2.96
E (s) 2.71
F (d) 2.46
G (s) 2.21
H (m) 2.16
I (s) 2.04
J (s) 1.95
K (d) 1.60
L (s) 1.54
M (s) 1.48
N (s) 1.42
O (d) 1.34
P (m) 1.30
Q (t) 0.91
U (m) 0.11
f1 (ppm)


{0.89,13.08}
{1.49,21.47}
{1.30,24.37}
{2.05,26.63}
{2.20,29.85}
{1.30,29.21}
{1.55,26.95}
{2.45,34.37}
{1.33,30.50}
{1.36,29.53}
{2.70,39.20}
{2.98,39.52}
{4.72,57.26}
{4.75,72.74}
{7.46,118.54}
{7.24,123.70}
{6.96,124.02}
{7.46,124.34}
{5.35,129.50}
f2 (ppm)
f1 (ppm)

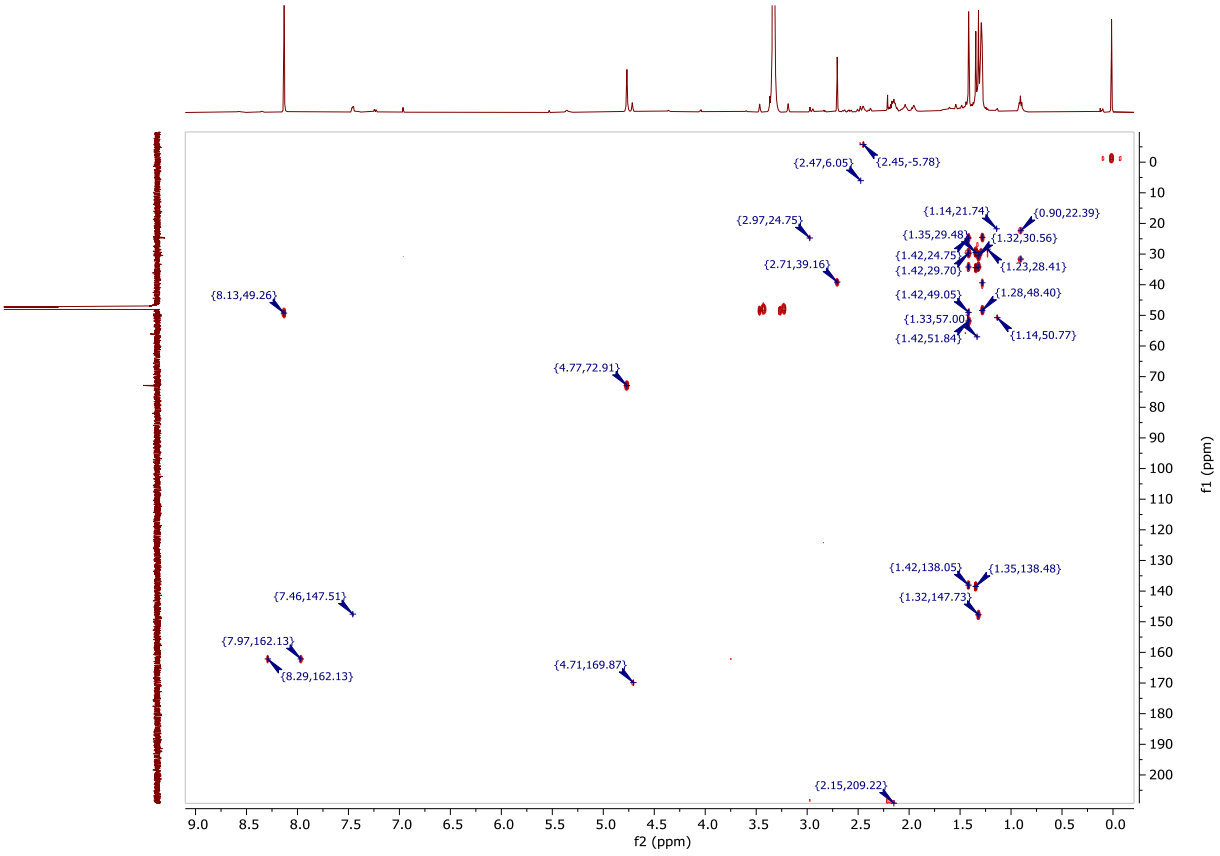


Figure S5: ^{1}H, HSQC, and HMBC spectra of the subfraction SL16 GR2+3.

Mass observed: 563.2820 *m/z*

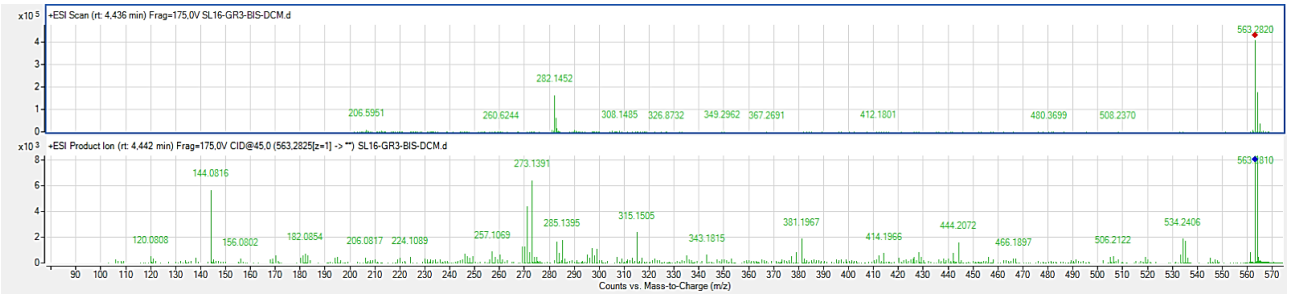


Figure S6: MS and MS/MS spectra of the subfraction SL16 GR2+3.

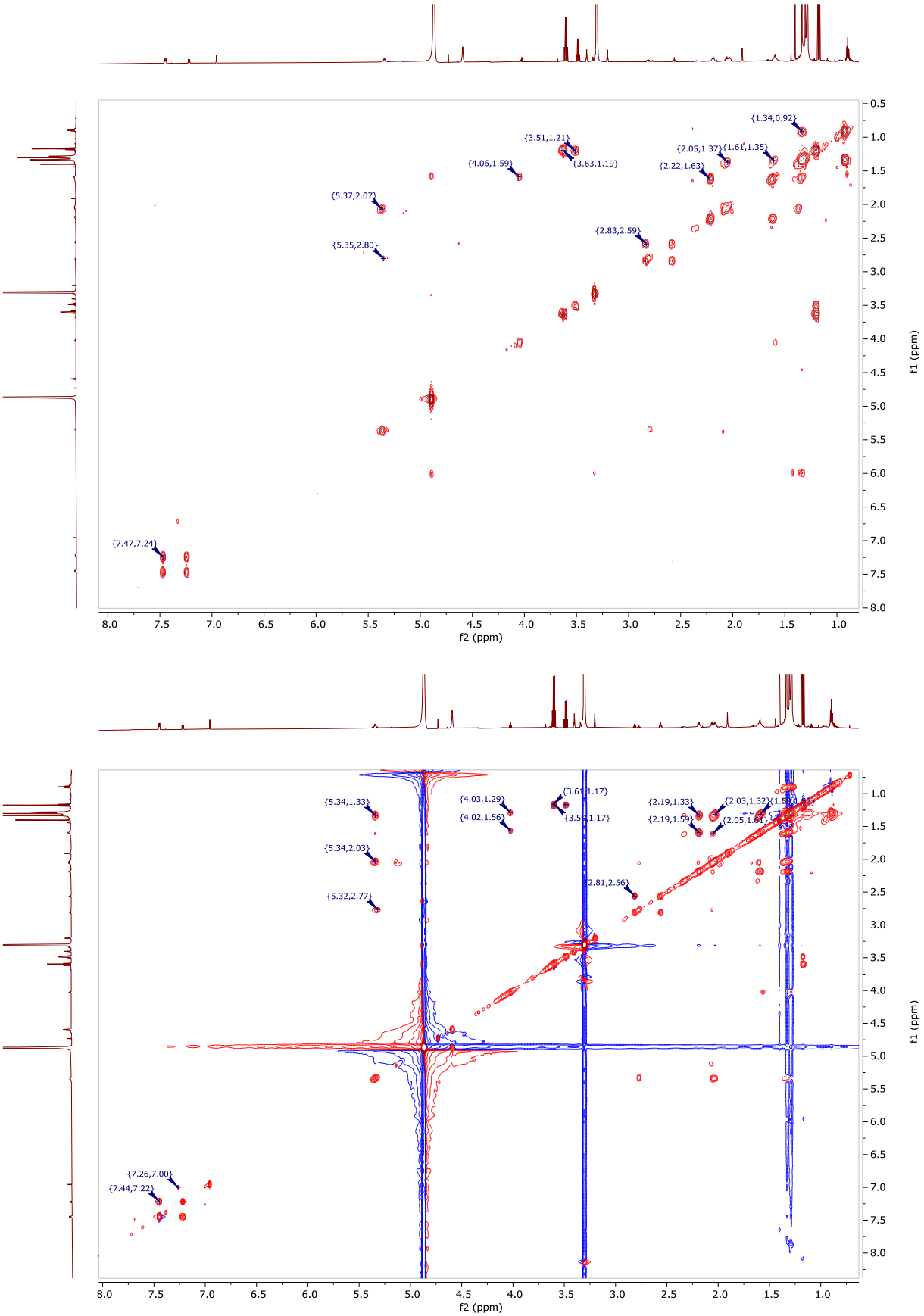
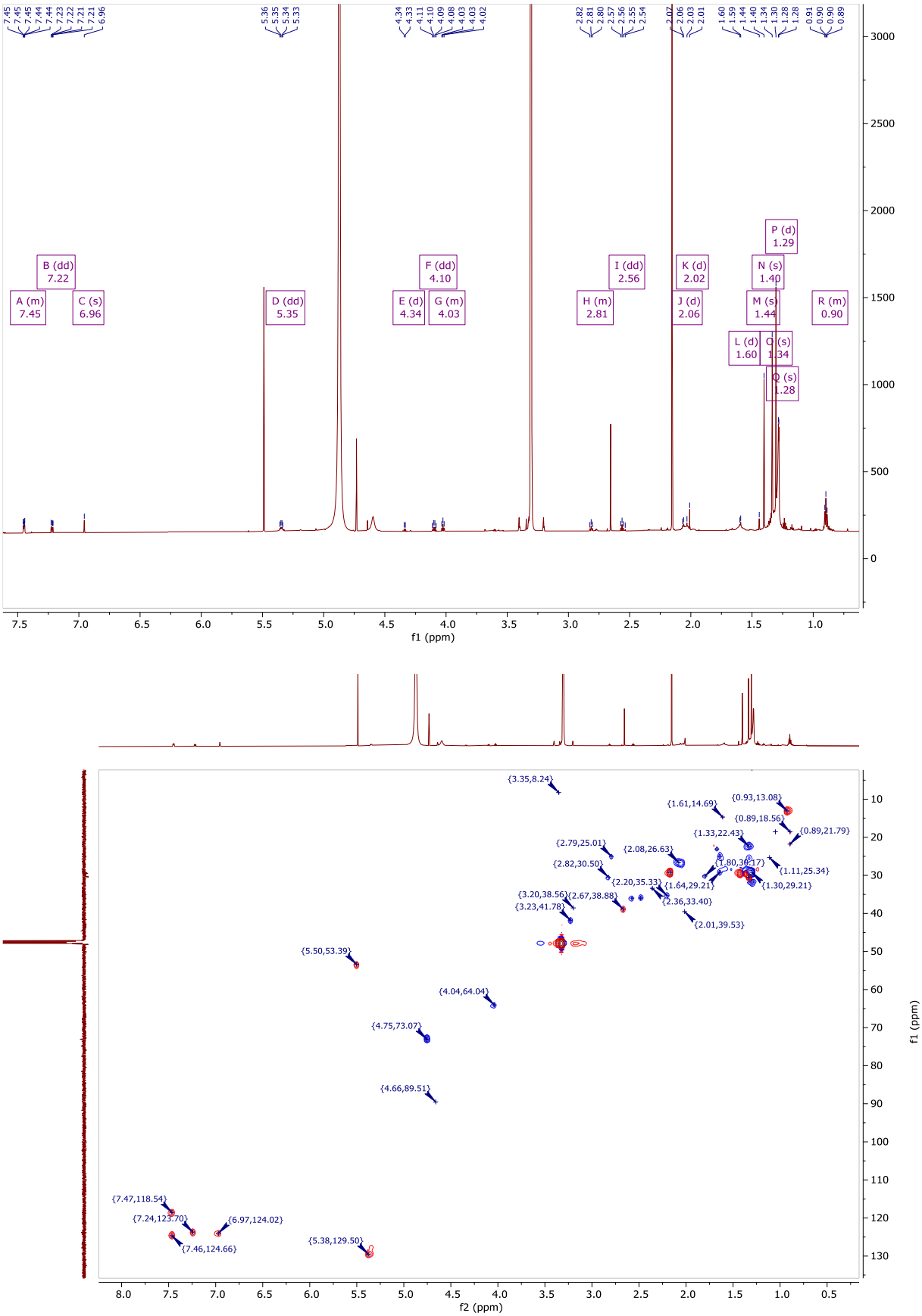


Figure S7: COSY and TOCSY spectra of the subfraction SL16 GR5.5.


A (m) 7.45
B (dd) 7.22
C (s) 6.96
D (dd) 5.35
E (d) 4.34
F (dd) 4.10
G (m) 4.03
H (m) 2.81
I (dd) 2.56
J (d) 2.06
K (d) 2.02
L (d) 1.60
M (s) 1.44
N (s) 1.40
O (s) 1.34
P (d) 1.29
Q (s) 1.28
R (m) 0.90
f1 (ppm)
{3.35,8.24}
{1.61,14.69}
{0.93,13.08}
{0.89,18.56}
{0.89,21.79}
{1.33,22.43}
{2.79,25.01}
{2.08,26.63}
{2.82,30.50}
{1.80,30.17}
{1.11,25.34}
{2.20,35.33}
{1.64,29.21}
{1.30,29.21}
{3.20,38.56}
{2.67,38.88}
{3.23,41.78}
{2.36,33.40}
{2.01,39.53}
{5.50,53.39}
{4.04,64.04}
{4.75,73.07}
{4.66,89.51}
{7.47,118.54}
{7.24,123.70}
{6.97,124.02}
{7.46,124.66}
{5.38,129.50}
f2 (ppm)
f1 (ppm)

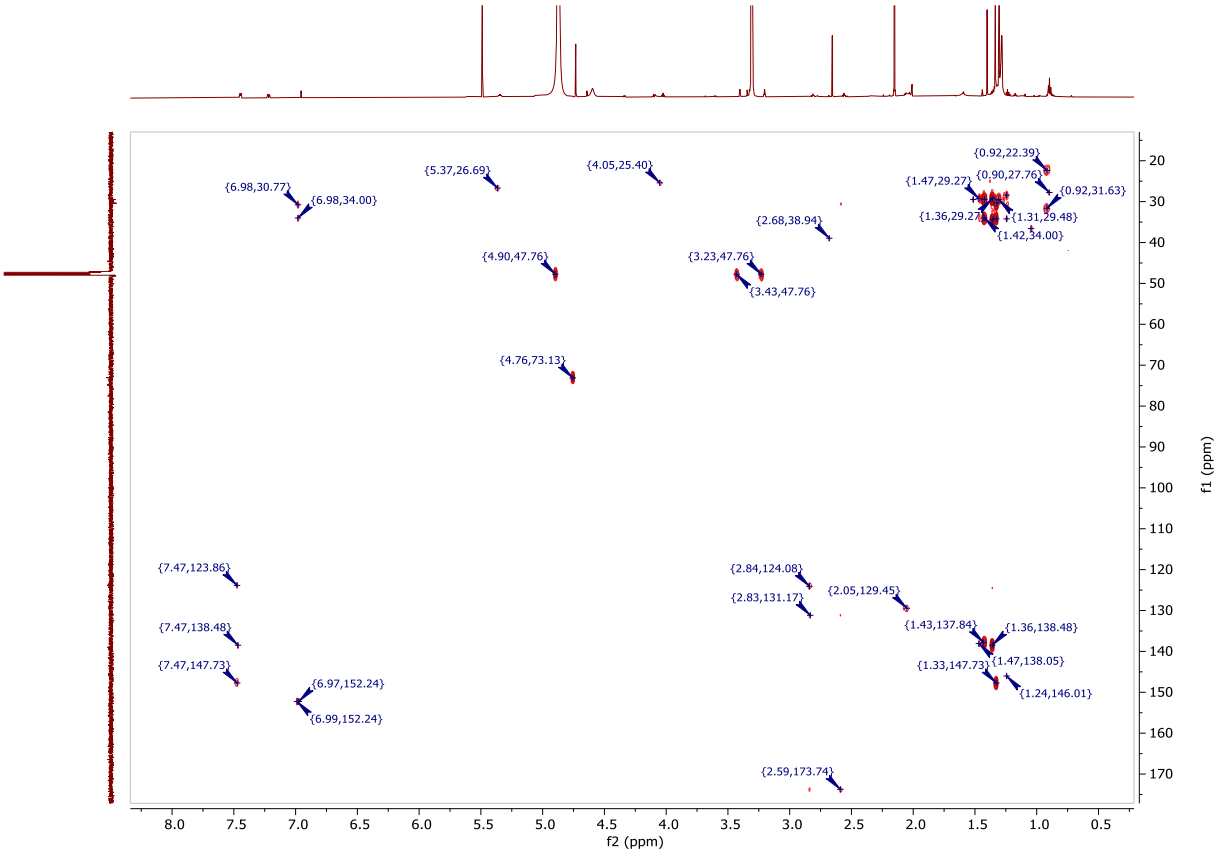
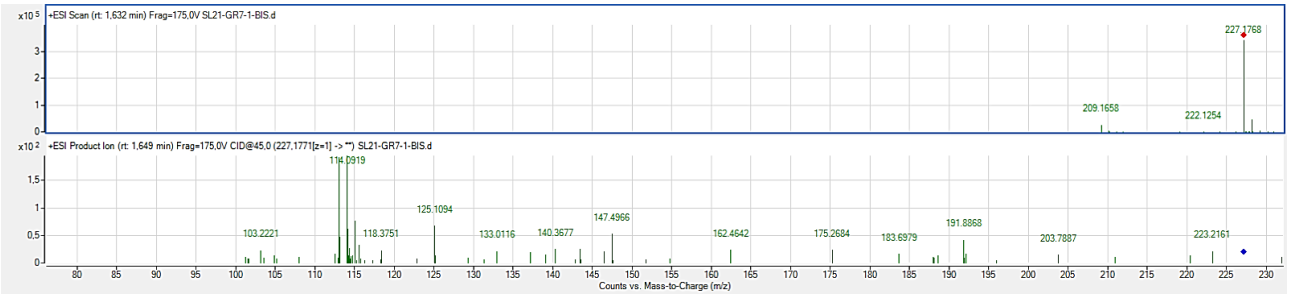
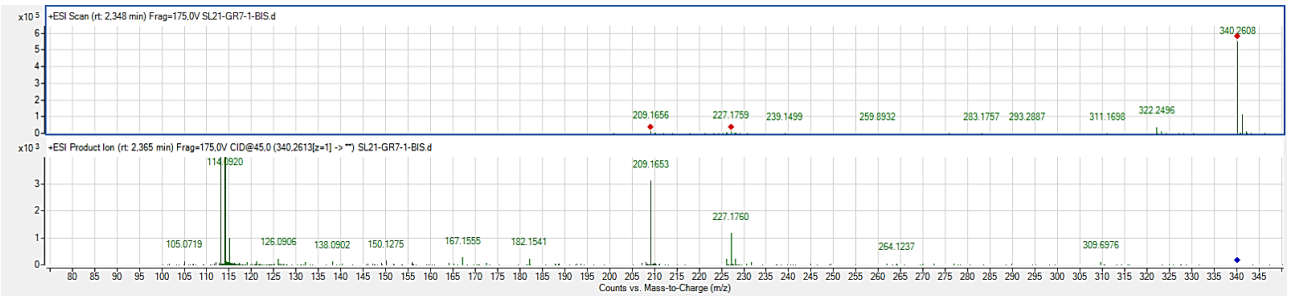


Figure S8: ^{1}H, HSQC, and HMBC spectra of the subfraction SL21 GR7.1.

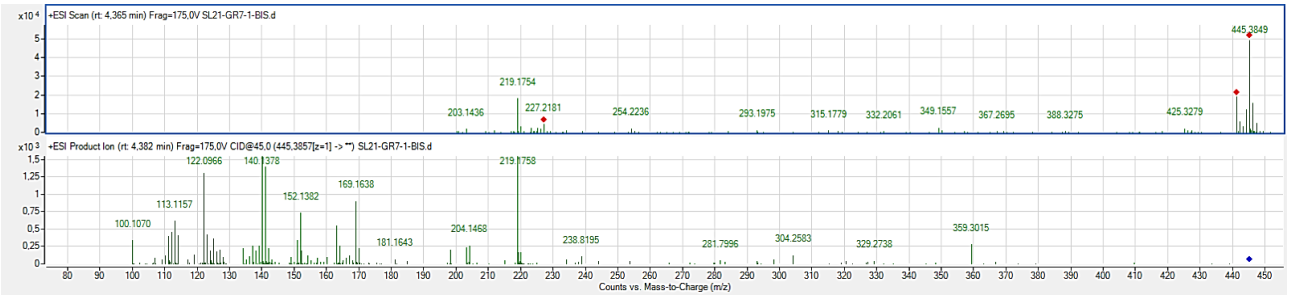
Mass observed: 227.1768 *m/z*



Mass observed: 340.2068 *m/z*



Mass observed: 445.3848 *m/z*



Mass observed: 453.3449 *m/z*

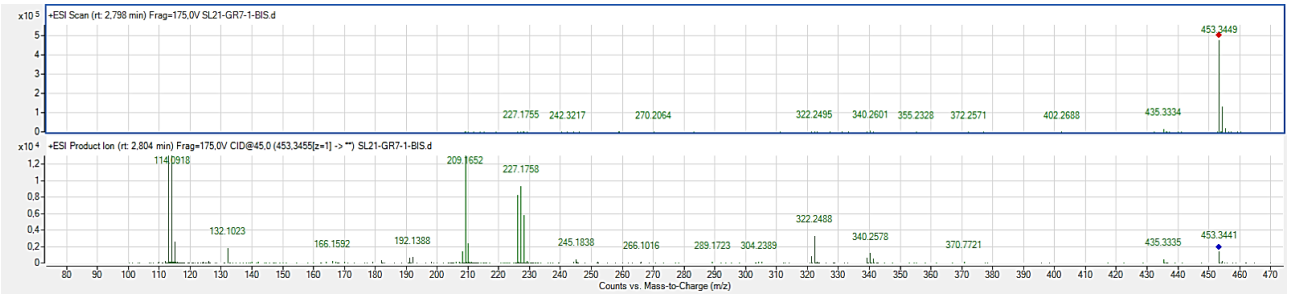
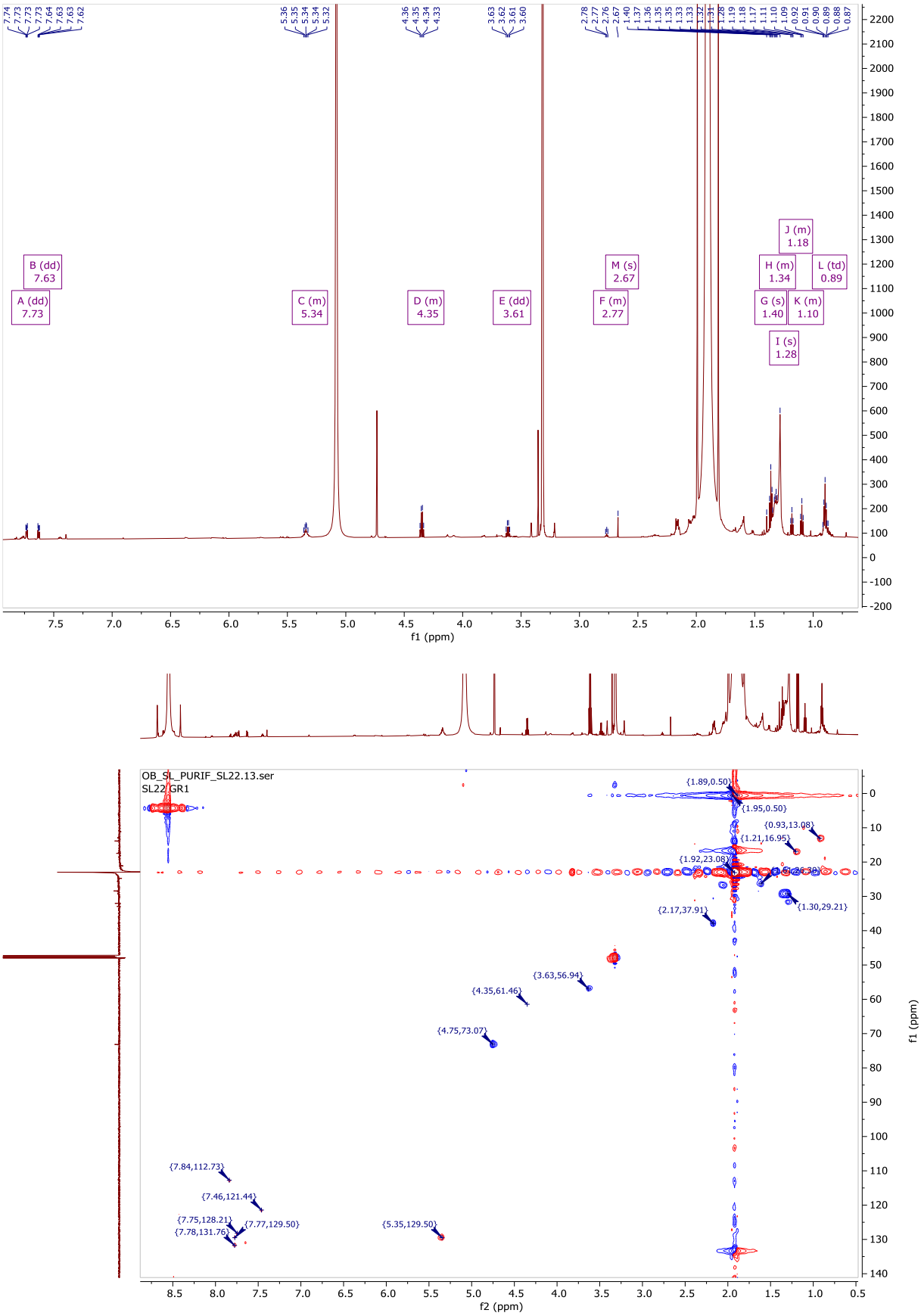


Figure S9: MS and MS/MS spectra of the subfraction SL21 GR7.1.


B (dd) 7.63
A (dd) 7.73
C (m) 5.34
D (m) 4.35
E (dd) 3.61
M (s) 2.67
F (m) 2.77
J (m) 1.18
H (m) 1.34
L (td) 0.89
G (s) 1.40
K (m) 1.10
I (s) 1.28
f1 (ppm)
OB_SL_PURIF_SL22.13.ser
SL22_GR1
{1.89,0.50}
{1.95,0.50}
{0.93,13.08}
{1.21,16.95}
{1.92,23.08}
{1.30,29.21}
{2.17,37.91}
{3.63,56.94}
{4.35,61.46}
{4.75,73.07}
{7.84,112.73}
{7.46,121.44}
{7.75,128.21}
{7.78,131.76}
{7.77,129.50}
{5.35,129.50}
f2 (ppm)
f1 (ppm)

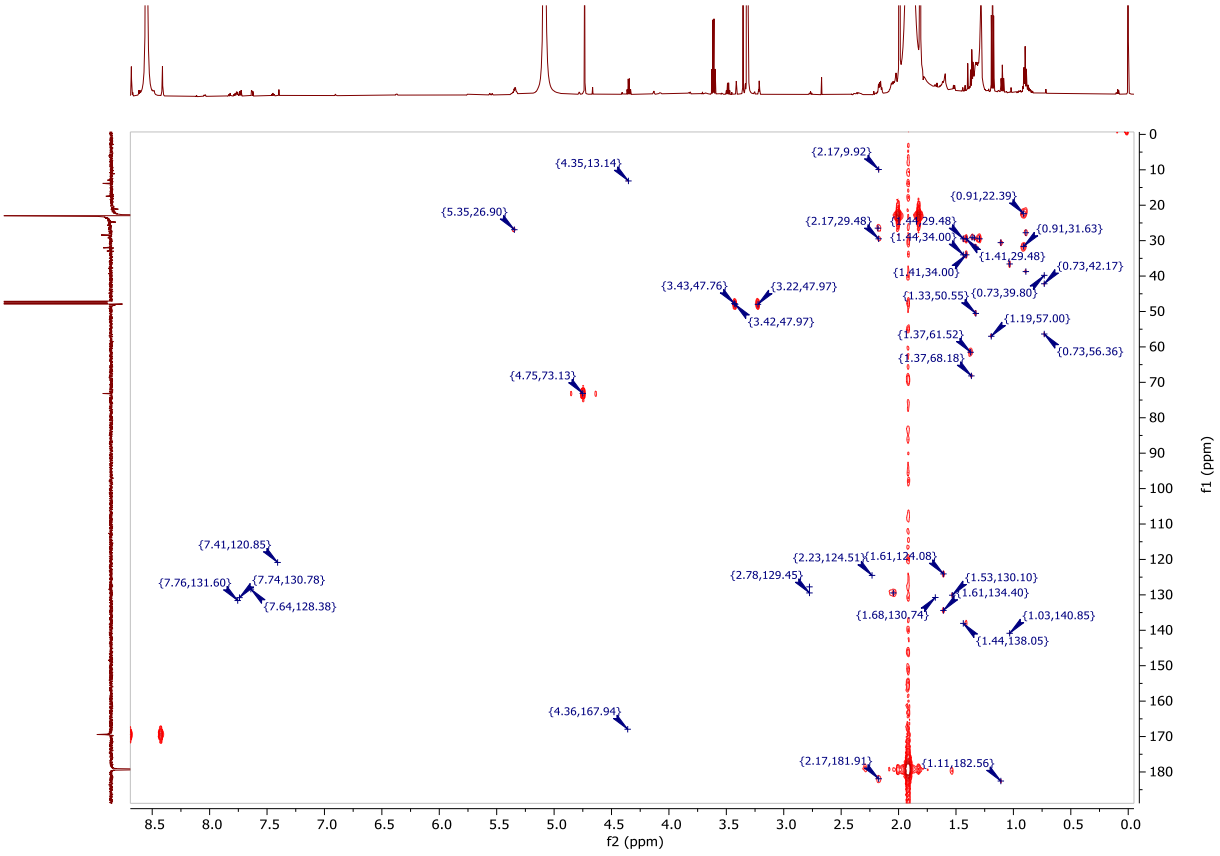
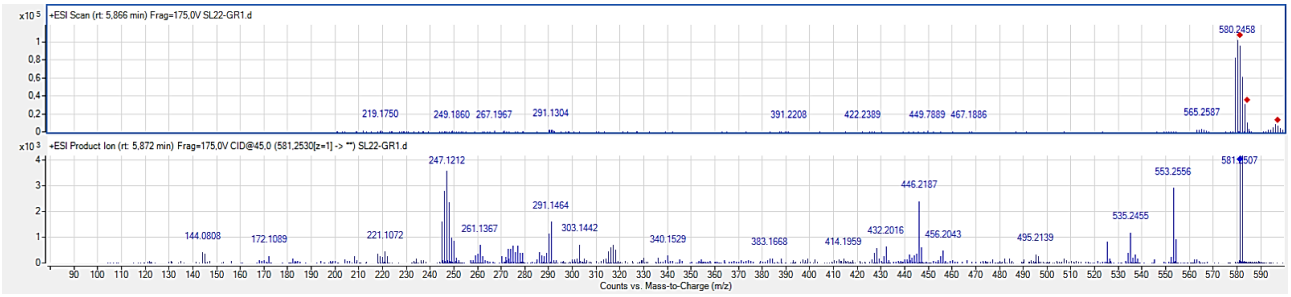


Figure S10: ^{1}H, HSQC, and HMBC spectra of the subfraction SL22 GR1.

Mass observed: 580.2458 *m/z*



Mass observed: 582.2616 *m/z*

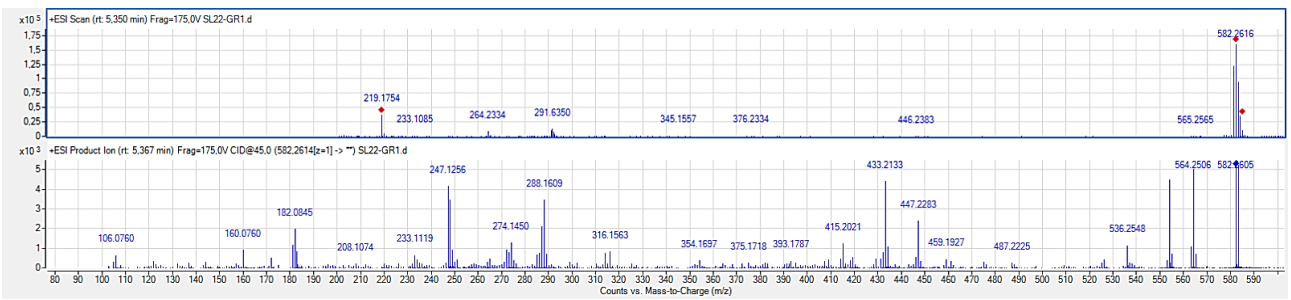
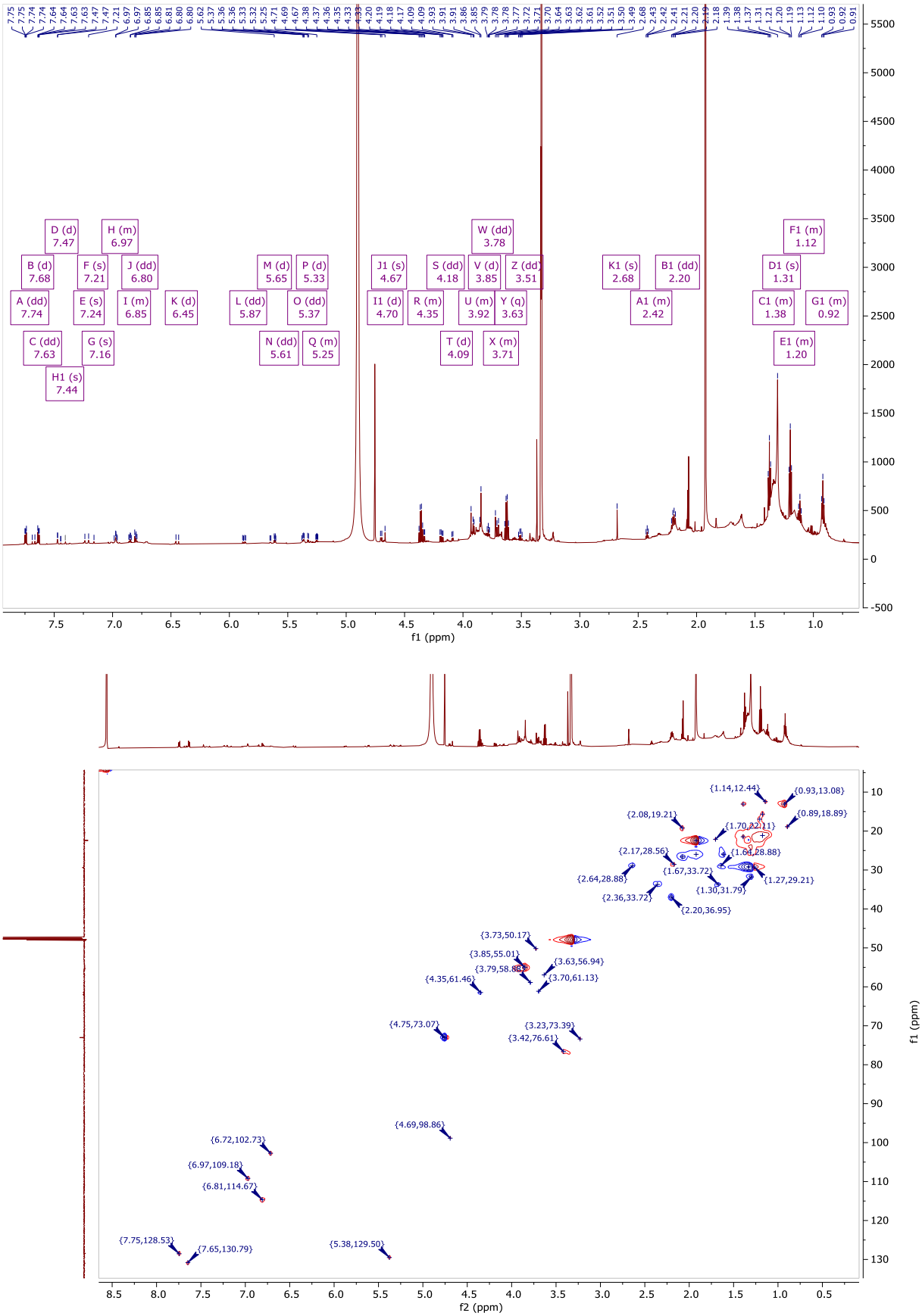


Figure S11: MS and MS/MS spectra of the subfraction SL22 GR1.


D (d) 7.47
H (m) 6.97
B (d) 7.68
F (s) 7.21
J (dd) 6.80
A (dd) 7.74
E (s) 7.24
I (m) 6.85
K (d) 6.45
C (dd) 7.63
G (s) 7.16
H1 (s) 7.44
M (d) 5.65
P (d) 5.33
L (dd) 5.87
O (dd) 5.37
N (dd) 5.61
Q (m) 5.25
J1 (s) 4.67
I1 (d) 4.70
S (dd) 4.18
R (m) 4.35
T (d) 4.09
W (dd) 3.78
V (d) 3.85
Z (dd) 3.51
U (m) 3.92
Y (q) 3.63
X (m) 3.71
K1 (s) 2.68
B1 (dd) 2.20
A1 (m) 2.42
F1 (m) 1.12
D1 (s) 1.31
C1 (m) 1.38
G1 (m) 0.92
E1 (m) 1.20
f1 (ppm)
{1.14,12.44}
{0.93,13.08}
{2.08,19.21}
{0.89,18.89}
{1.70,22.11}
{2.17,28.56}
{1.64,28.88}
{1.67,33.72}
{2.64,28.88}
{1.27,29.21}
{1.30,31.79}
{2.36,33.72}
{2.20,36.95}
{3.73,50.17}
{3.85,55.01}
{3.63,56.94}
{3.79,58.88}
{3.70,61.13}
{4.35,61.46}
{4.75,73.07}
{3.23,73.39}
{3.42,76.61}
{4.69,98.86}
{6.72,102.73}
{6.97,109.18}
{6.81,114.67}
{7.75,128.53}
{7.65,130.79}
{5.38,129.50}
f2 (ppm)
f1 (ppm)

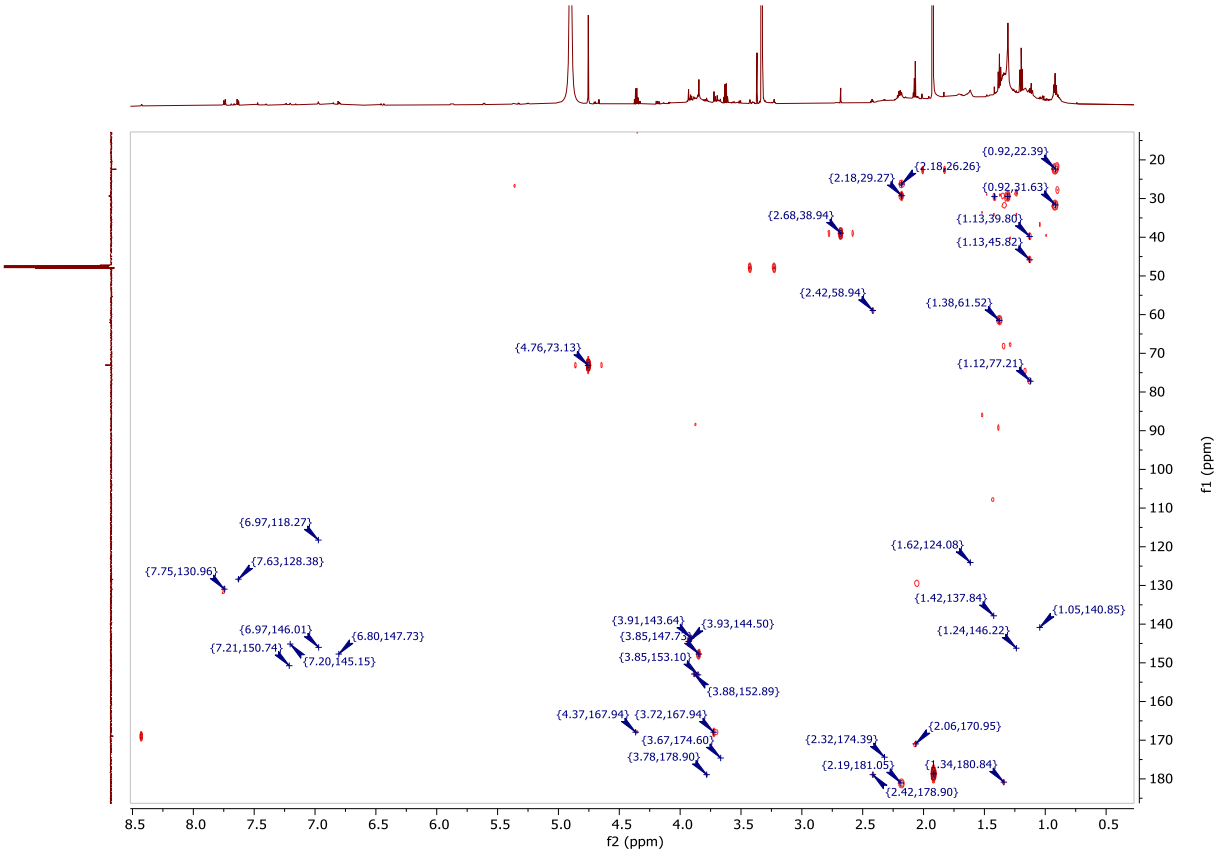


Figure S12: ^{1}H, HSQC, and HMBC spectra of the subfraction SL22 GR12.

Mass observed: 442.3397 *m/z*

Figure S13: MS and MS/MS spectra of the subfraction SL22 GR12.

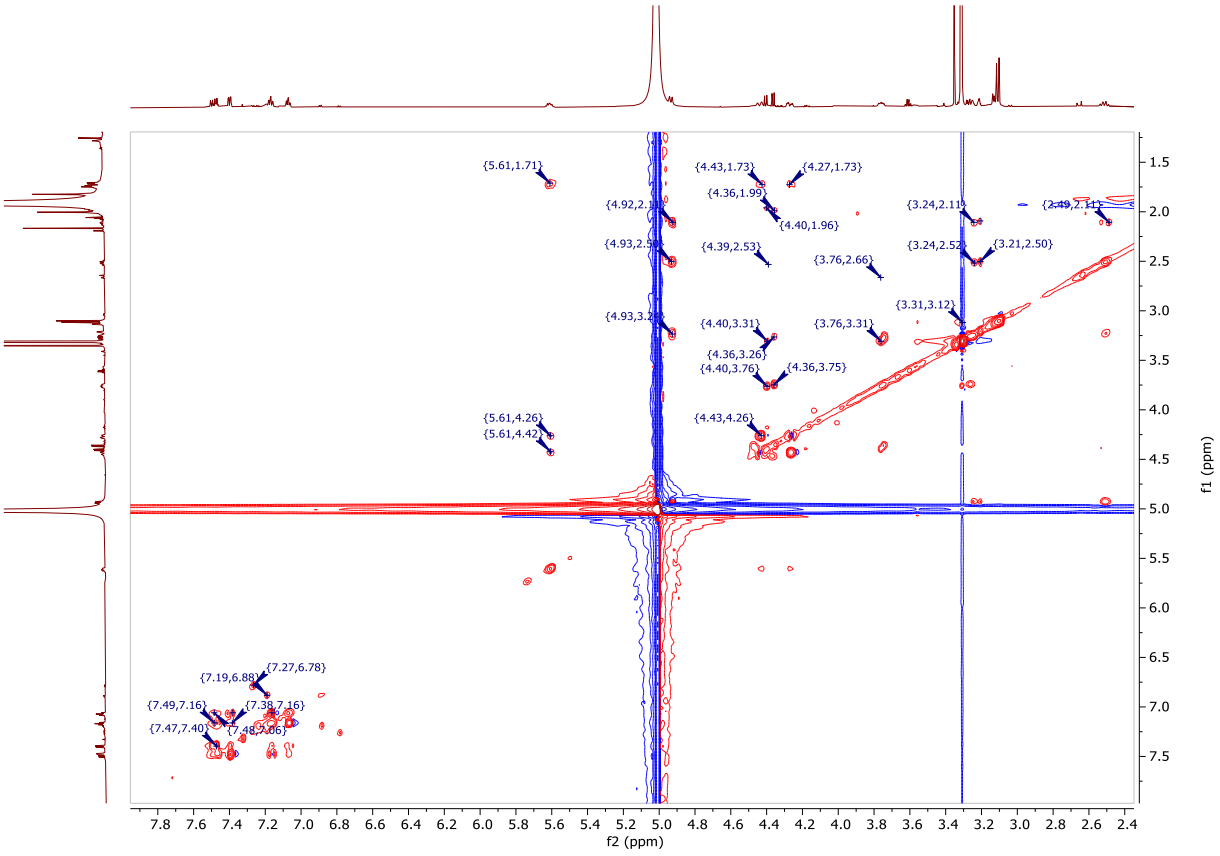
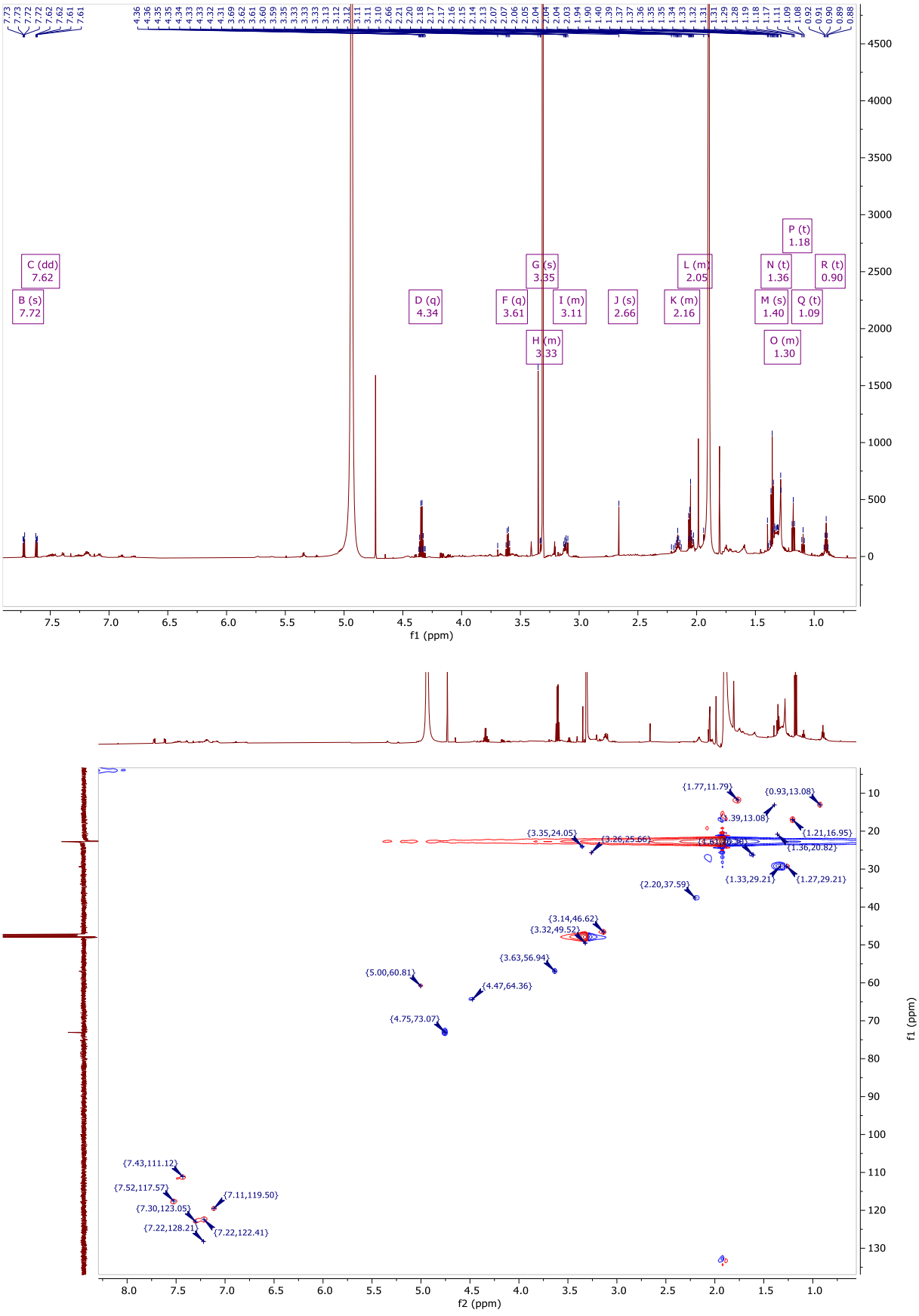


Figure S14: TOCSY spectrum of the subfraction SL23 GR3.


C (dd) 7.62
B (s) 7.72
D (q) 4.34
F (q) 3.61
G (s) 3.35
H (m) 3.33
I (m) 3.11
J (s) 2.66
K (m) 2.16
L (m) 2.05
M (s) 1.40
N (t) 1.36
O (m) 1.30
P (t) 1.18
Q (t) 1.09
R (t) 0.90
f1 (ppm)
f2 (ppm)
f1 (ppm)
{1.77,11.79}
{0.93,13.08}
{1.39,13.08}
{1.21,16.95}
{3.35,24.05}
{3.26,25.66}
{1.36,20.82}
{1.33,29.21}
{1.27,29.21}
{2.20,37.59}
{3.14,46.62}
{3.32,49.52}
{3.63,56.94}
{5.00,60.81}
{4.47,64.36}
{4.75,73.07}
{7.43,111.12}
{7.52,117.57}
{7.11,119.50}
{7.30,123.05}
{7.22,128.21}
{7.22,122.41}

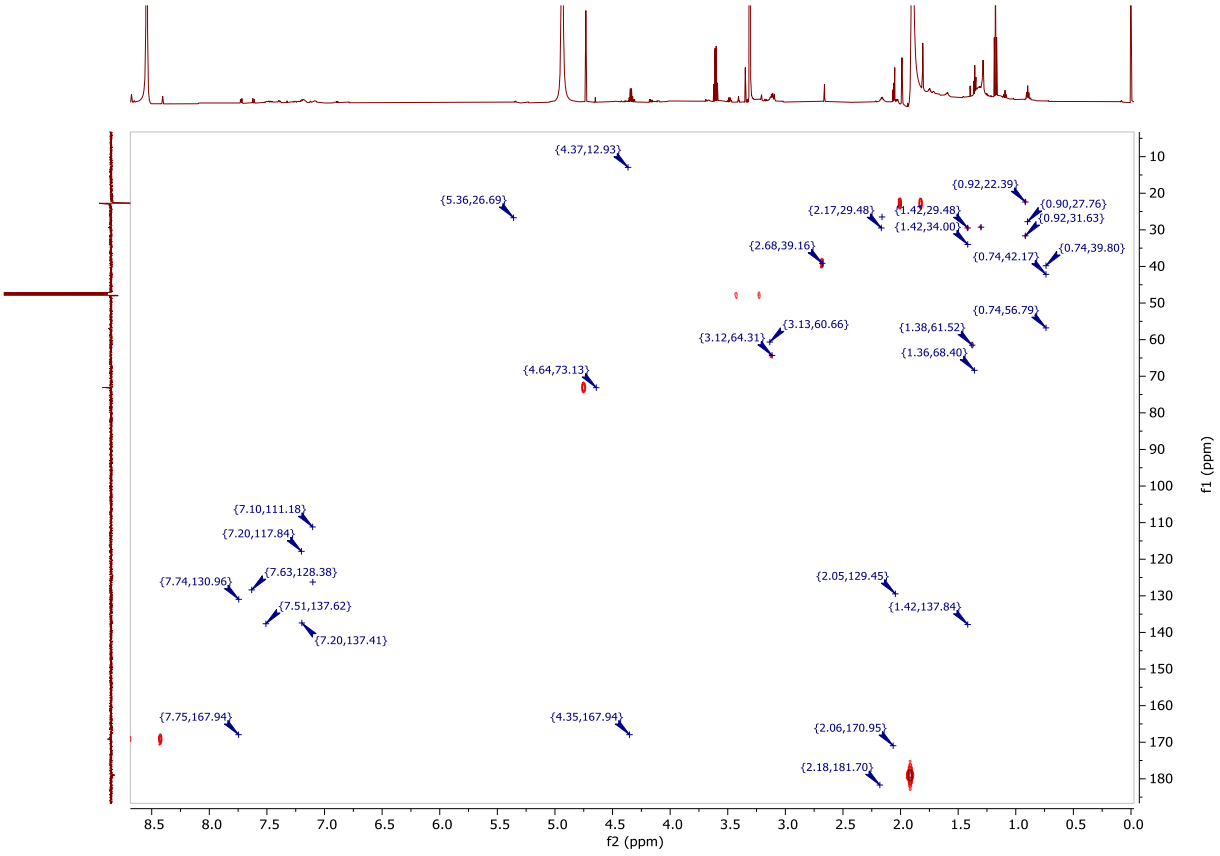
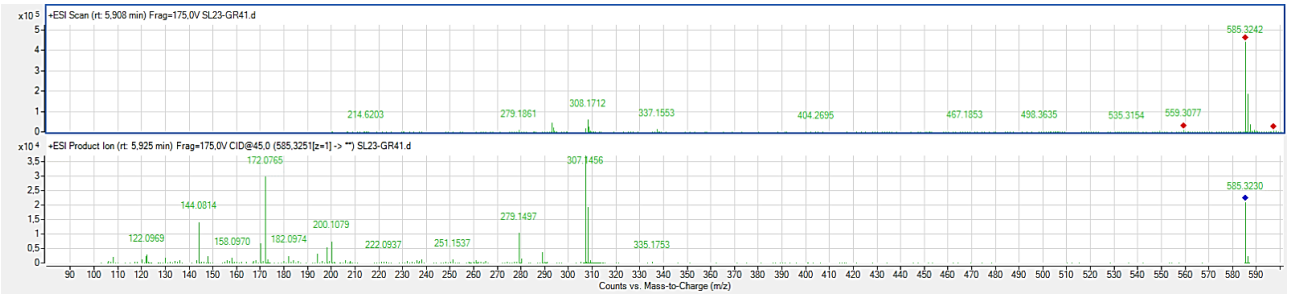


Figure S15: ^{1}H, HSQC, and HMBC spectra of the subfraction SL23 GR4.

Mass observed: 585.3242 *m/z*



Mass observed: 615.3348 *m/z*

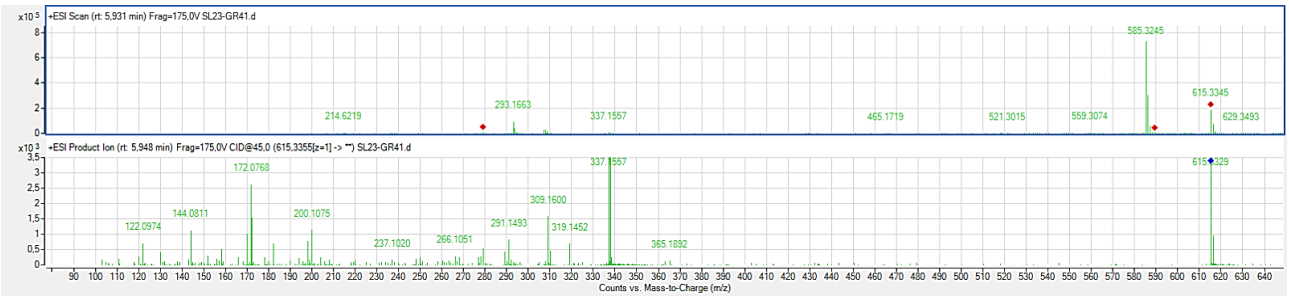


Figure S16: MS and MS/MS spectra of the subfraction SL23 GR4.