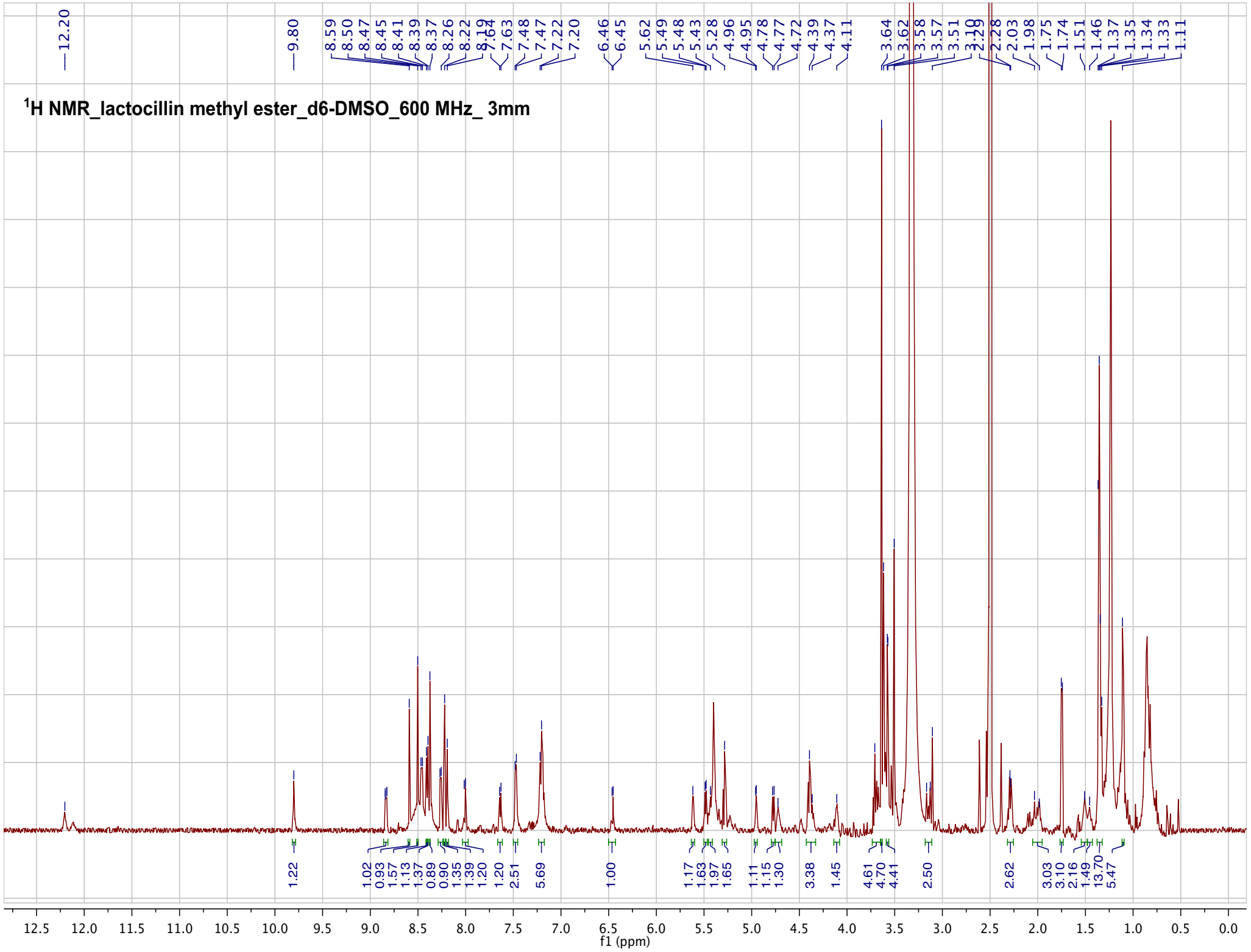
12.20
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8.39
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8.22
8.19
8.14
7.63
7.48
7.47
7.22
7.20
6.46
6.45
5.62
5.49
5.48
5.43
5.28
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4.95
4.78
4.77
4.72
4.39
4.37
4.11
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3.58
3.57
3.51
3.10
2.29
2.28
2.03
1.98
1.75
1.74
1.51
1.46
1.37
1.35
1.34
1.33
1.11
1H NMR_lactocillin methyl ester_d6-DMSO_600 MHz_ 3mm
1.22
1.02
0.93
1.57
1.13
1.37
0.89
0.90
1.35
1.39
1.20
1.20
2.51
5.69
1.00
1.17
1.63
1.97
1.65
1.11
1.15
1.30
3.38
1.45
4.61
4.70
4.41
2.50
2.62
3.03
3.10
2.16
1.49
13.70
5.47
12.5
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11.5
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6.0
5.5
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4.5
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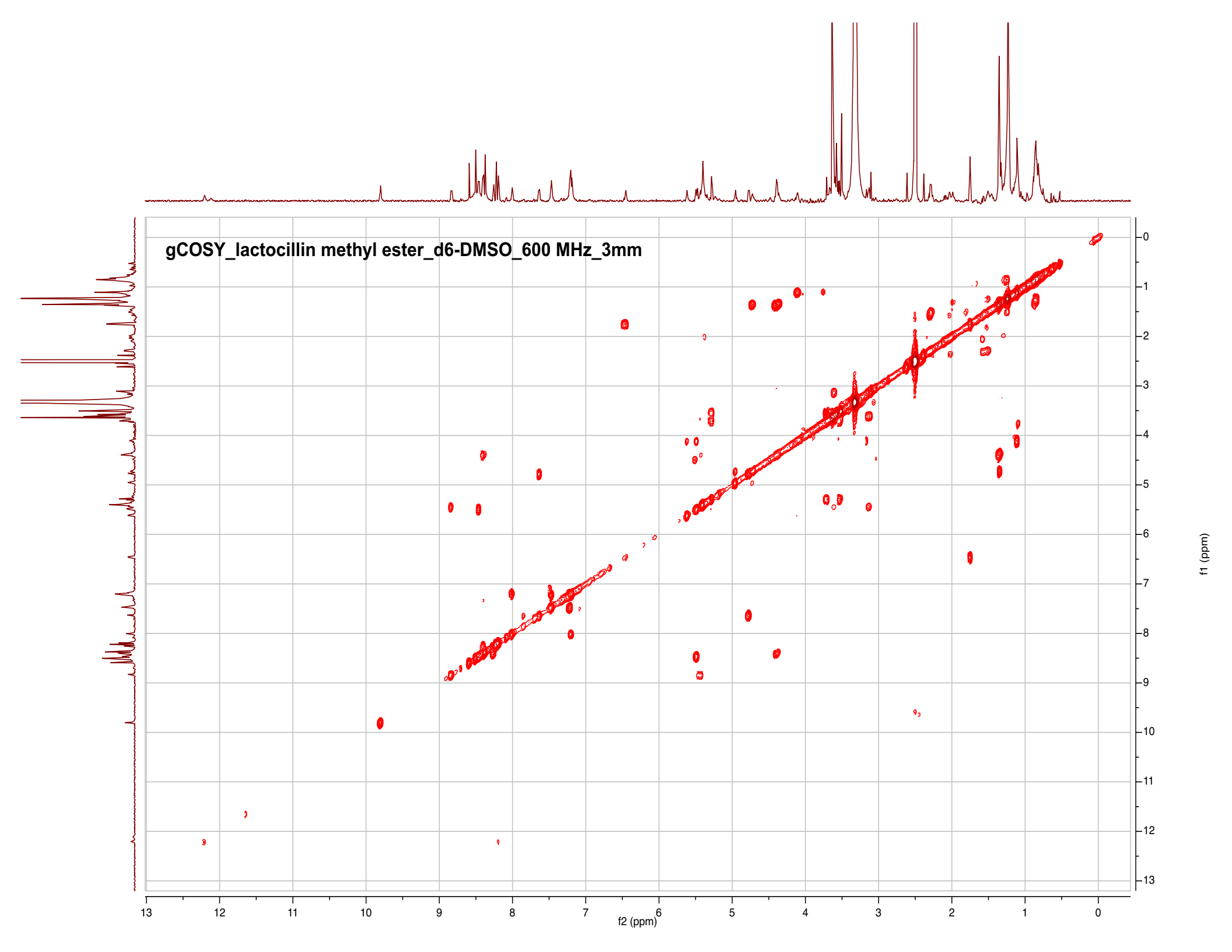
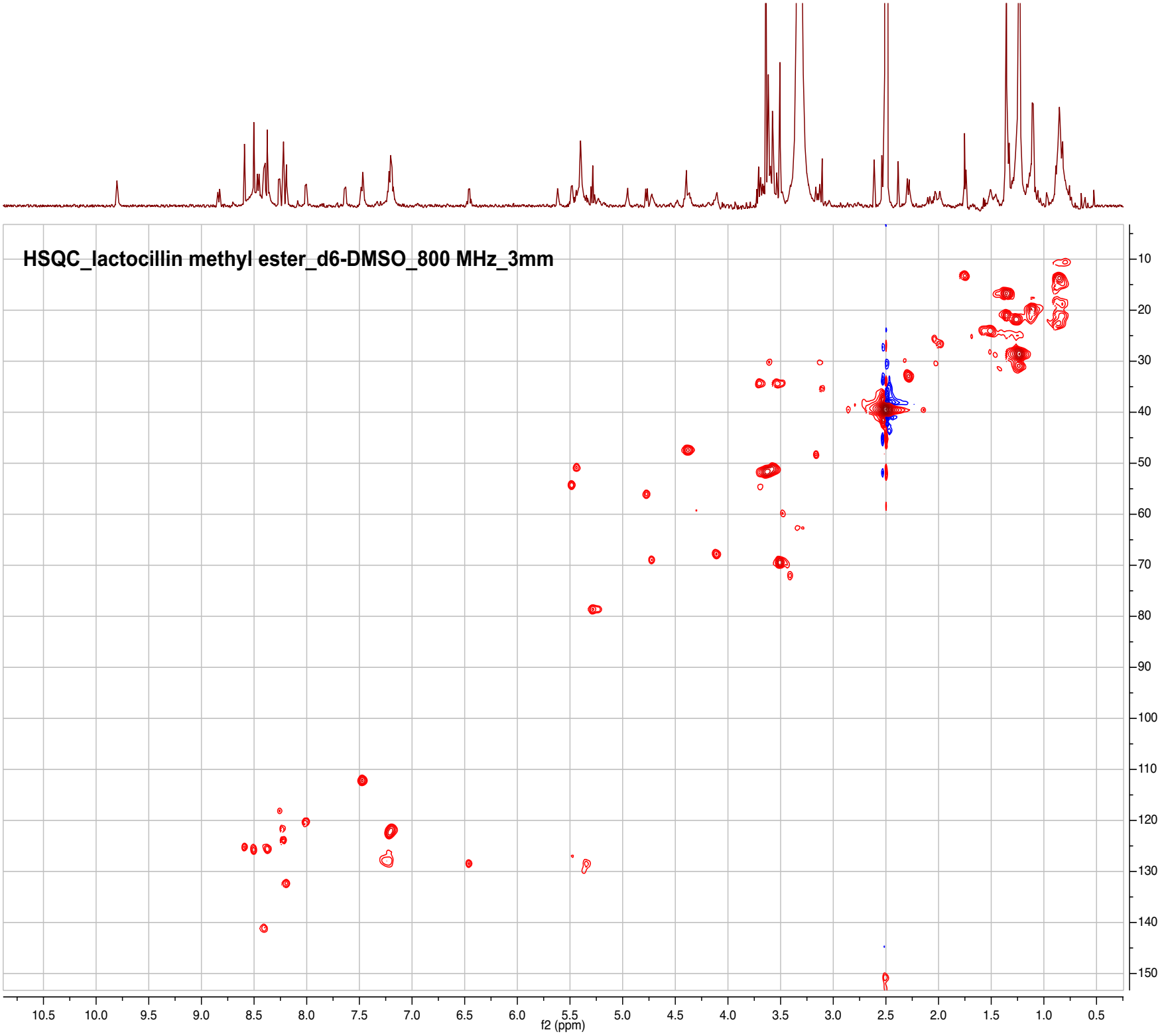
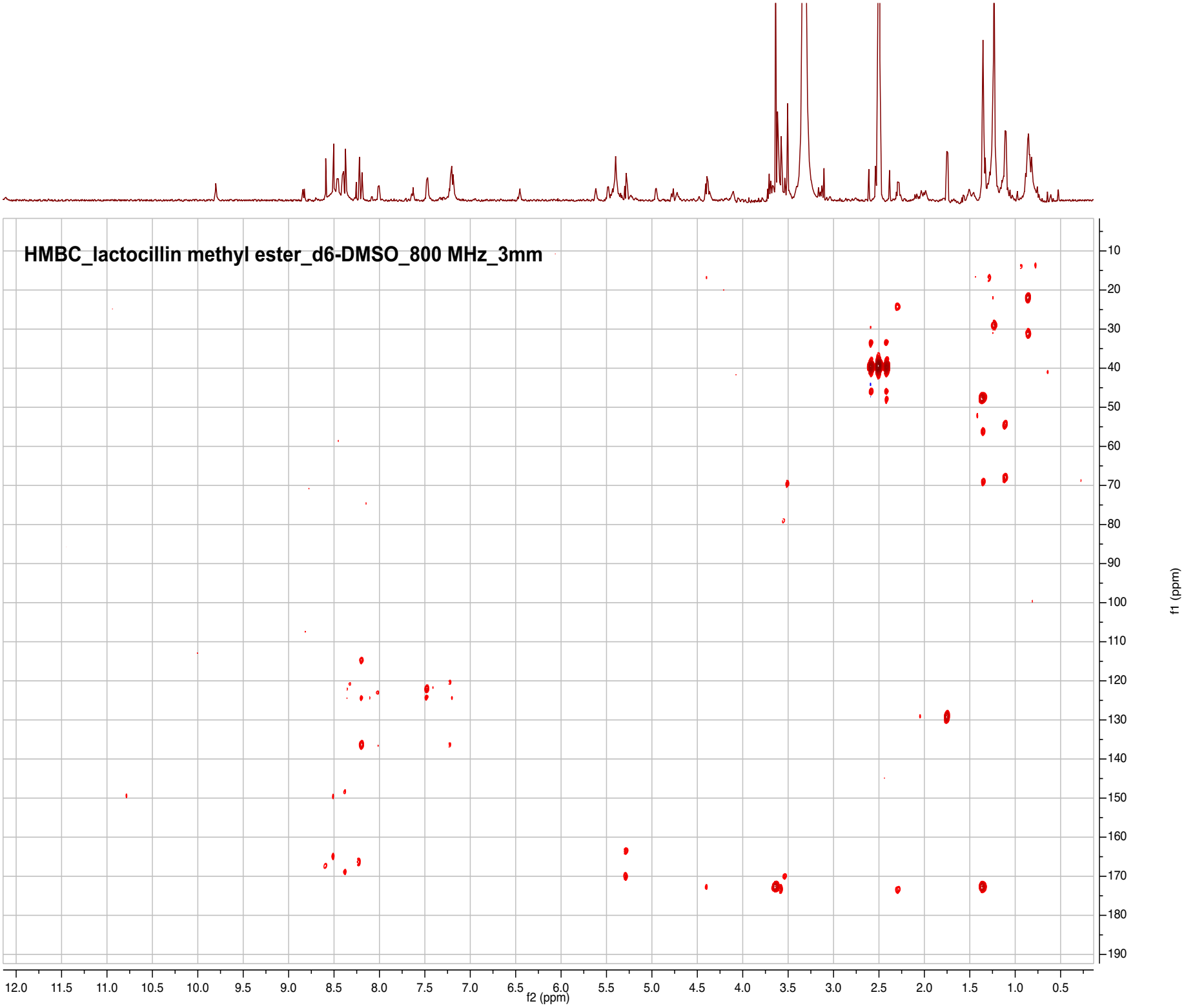
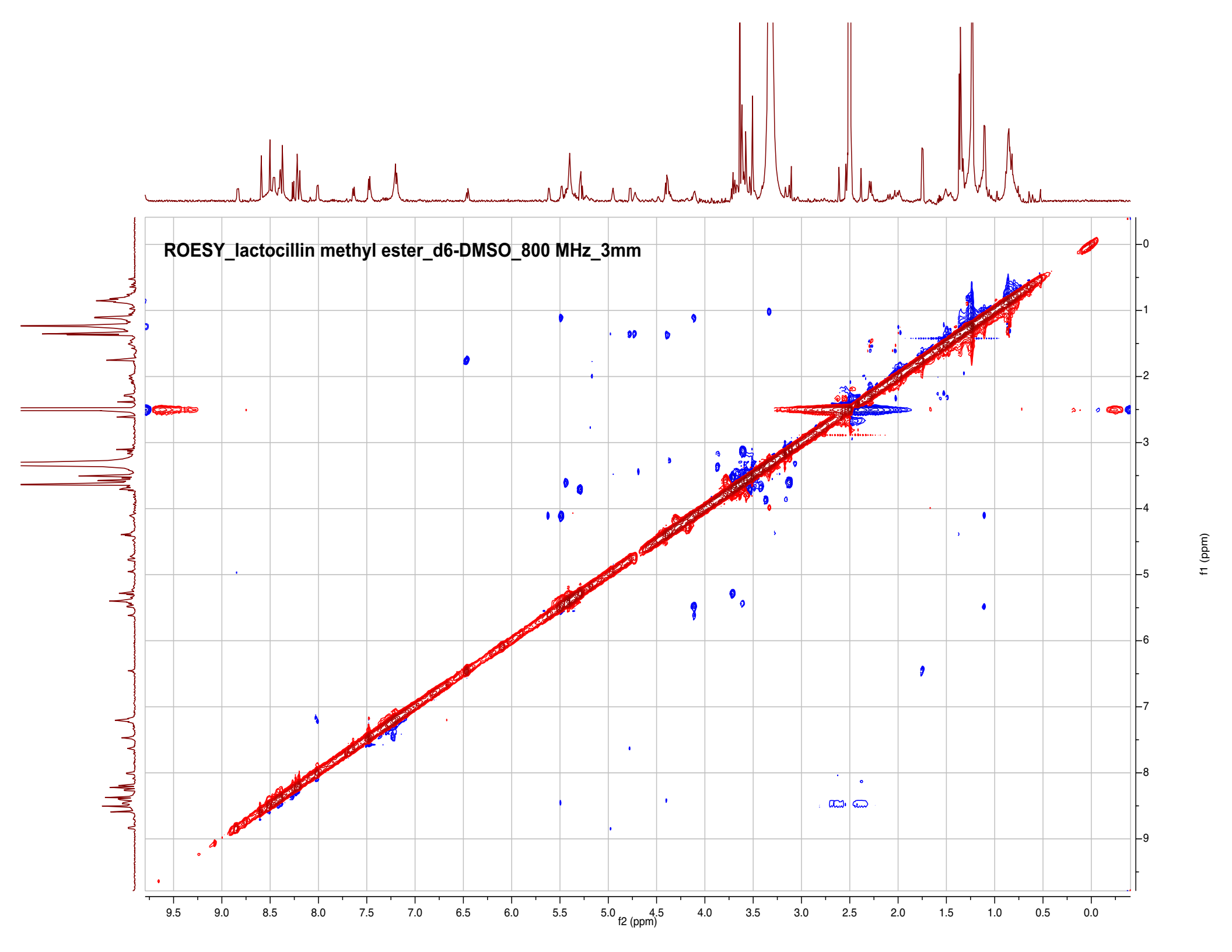
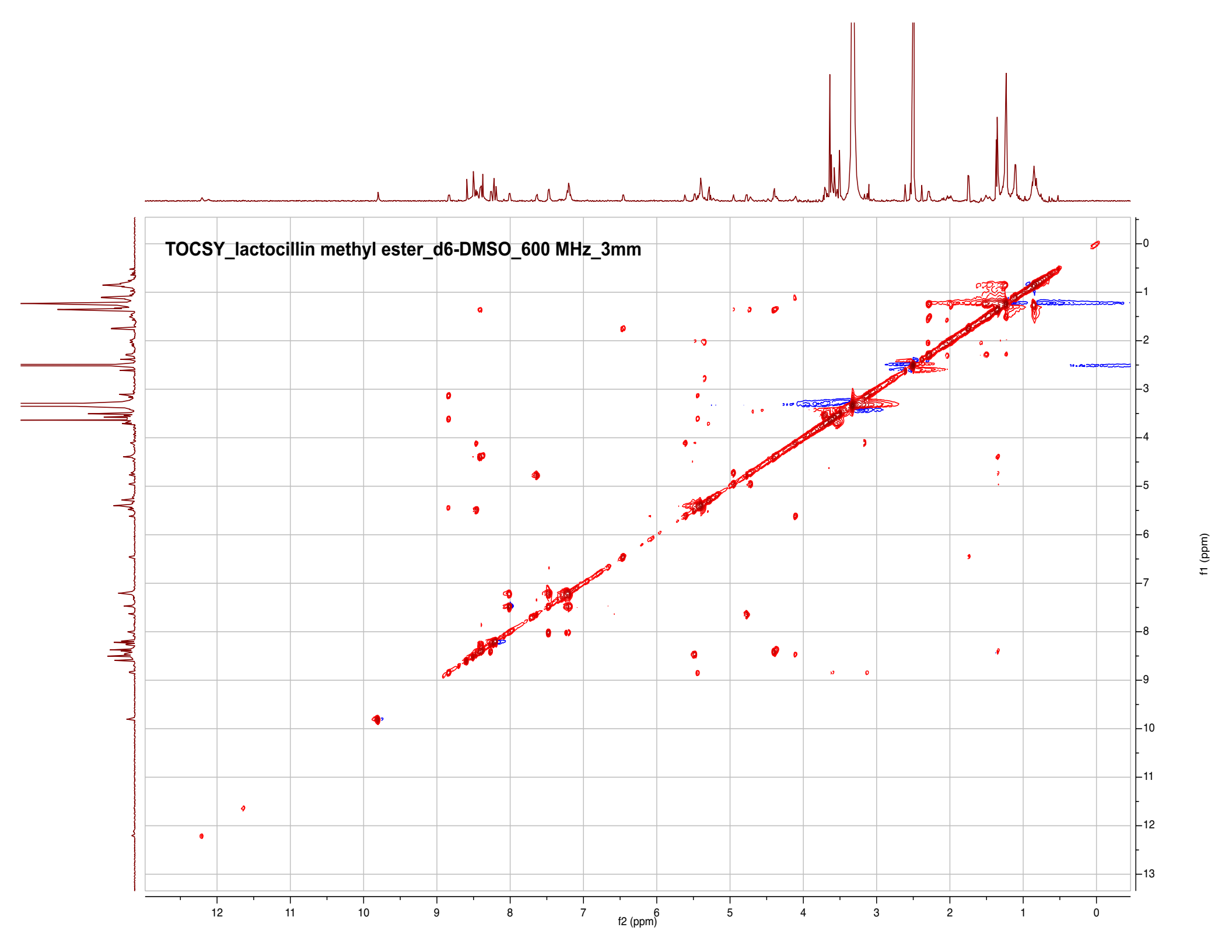
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

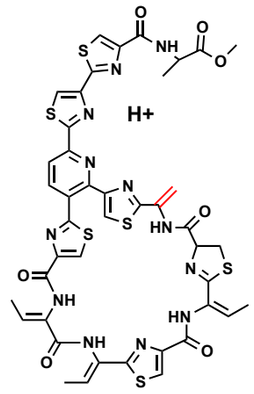

gCOSY_lactocillin methyl ester_d6-DMSO_600 MHz_3mm
f2 (ppm)
f1 (ppm)


HSQC_lactocillin methyl ester_d6-DMSO_800 MHz_3mm
f2 (ppm)
f1 (ppm)


HMBC_lactocillin methyl ester_d6-DMSO_800 MHz_3mm
f2 (ppm)
f1 (ppm)

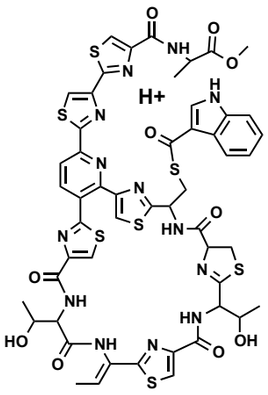

ROESY_lactocillin methyl ester_d6-DMSO_800 MHz_3mm
f2 (ppm)
f1 (ppm)


TOCSY_lactocillin methyl ester_d6-DMSO_600 MHz_3mm
f2 (ppm)
f1 (ppm)

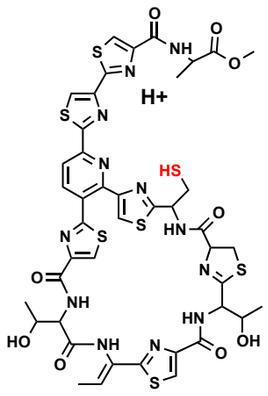


Chemical Formula: $C_{43}H_{37}N_{12}O_7S_6^+$
Calculated Exact Mass: 1025.12323
Observed Exact Mass: 1025.12187
01.3 ppm

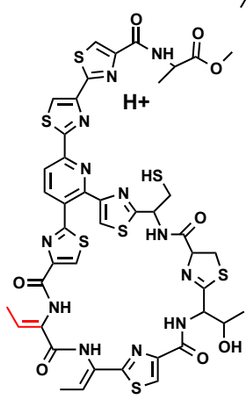
CID/35



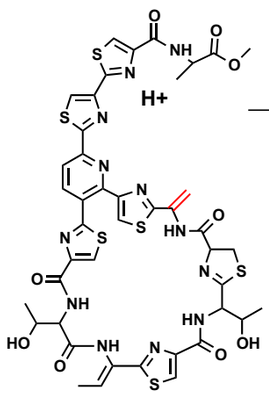
Chemical Formula: $C_{52}H_{48}N_{13}O_{10}S_7^+$
Calculated Exact Mass: 1238.16919
Observed Exact Mass: 1238.16916
-0.02 ppm



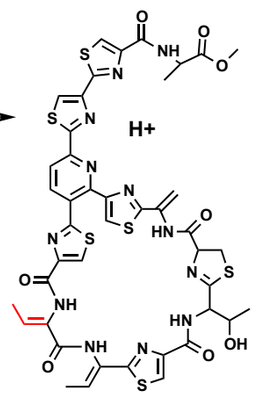
Chemical Formula: $C_{43}H_{43}N_{12}O_9S_7^+$
Calculated Exact Mass: 1095.13207
Observed Exact Mass: 1095.13268
0.5 ppm



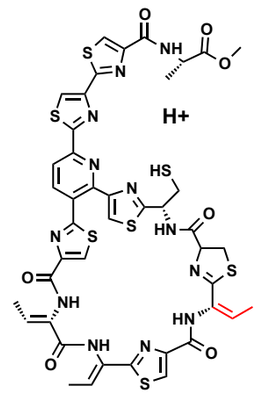
Chemical Formula: $C_{43}H_{41}N_{12}O_8S_7^+$
Calculated Exact Mass: 1077.12151
Observed Exact Mass: 1077.12203
0.5 ppm



Chemical Formula: $C_{43}H_{41}N_{12}O_9S_6^+$
Calculated Exact Mass: 1061.14435
Observed Exact Mass: 1061.14433
-0.02 ppm

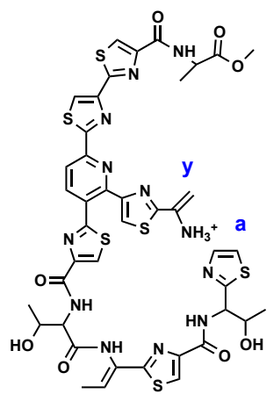


Chemical Formula: $C_{43}H_{39}N_{12}O_8S_6^+$
Calculated Exact Mass: 1043.13379
Observed Exact Mass: 1043.13345
-0.3 ppm

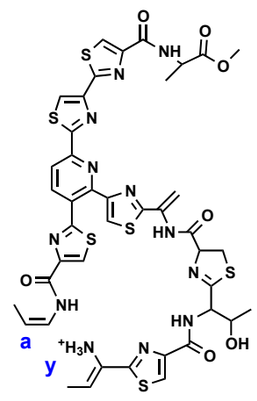


Chemical Formula: $C_{43}H_{39}N_{12}O_7S_7^+$
Calculated Exact Mass: 1059.11095
Observed Exact Mass: 1059.11080
-0.1 ppm

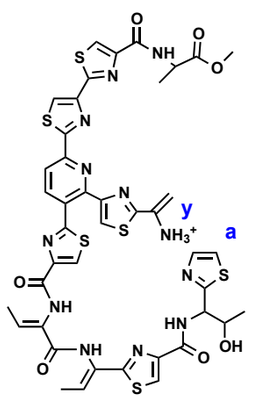
HCD/35



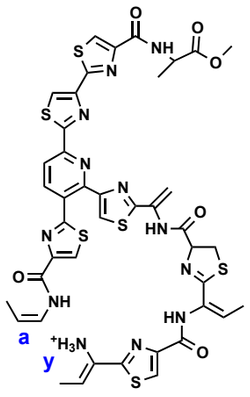
Chemical Formula: $C_{42}H_{41}N_{12}O_8S_6^+$
Calculated Exact Mass: 1033.14944
Observed Exact Mass: 1033.15260
3 ppm



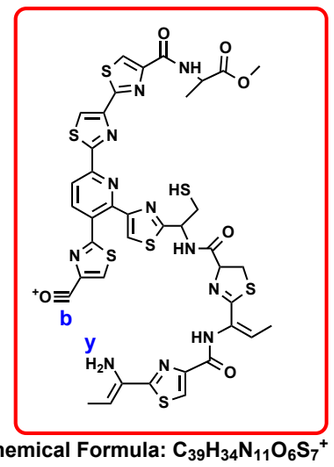
Chemical Formula: $C_{42}H_{41}N_{12}O_7S_6^+$
Calculated Exact Mass: 1017.15452
Observed Exact Mass: 1017.15650
2 ppm



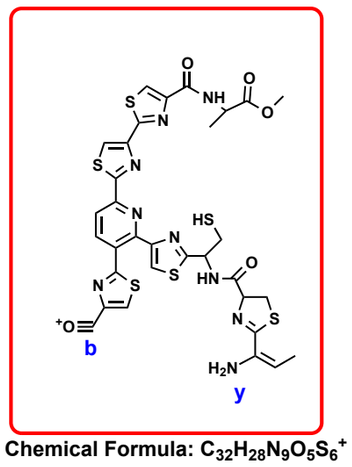
Chemical Formula: $C_{42}H_{39}N_{12}O_7S_6^+$
Calculated Exact Mass: 1015.13887
Observed Exact Mass: 1015.13887
0 ppm



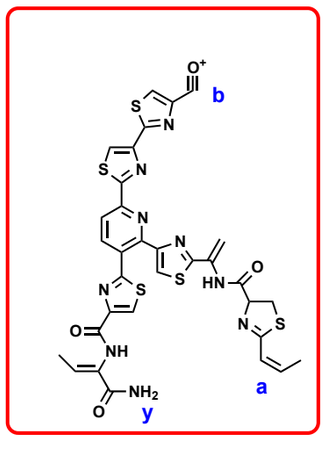
Chemical Formula: $C_{42}H_{39}N_{12}O_6S_6^+$
Calculated Exact Mass: 999.14396
Observed Exact Mass: 999.14389
-0.07 ppm



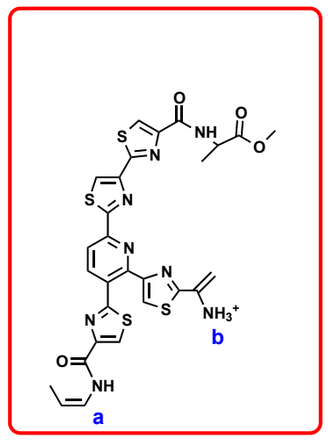
Chemical Formula: $C_{39}H_{34}N_{11}O_6S_7^+$
Calculated Exact Mass: 976.07384
Observed Exact Mass: 976.07460
-0.8 ppm



Chemical Formula: $C_{32}H_{28}N_9O_5S_6^+$
Calculated Exact Mass: 810.05375
Observed Exact Mass: 810.05343
-0.4 ppm



Chemical Formula: $C_{32}H_{24}N_9O_4S_5^+$
Calculated Exact Mass: 758.05547
Observed Exact Mass: 758.05552
0.06 ppm



Chemical Formula: $C_{28}H_{25}N_8O_4S_4^+$
Calculated Exact Mass: 665.08815
Observed Exact Mass: 665.08798
-0.3 ppm

Chemical shifts of lactocillin in DMSO-d_6 (600 MHz)

Position	δ H (ppm)	m	*J* (Hz)	δ C (ppm)[a]	Residue
1	3.64	s	-	51.8	Ala
2	-	-	-	172.5	Ala
3	4.39	m[b]		47.5	Ala
4	1.36	d	7.0	16.7	Ala
5	8.41	d	7.2	NH	Ala
6	-	-	-	169.8	Thiazole 1
7	-	-	-	n.o.	Thiazole 1
8	8.59	s	-	125.3	Thiazole 1
9	-	-	-	167.2	Thiazole 1
10	-	-	-	n.o.	Thiazole 2
11	8.50	s	-	125.7	Thiazole 2
12	-	-	-	164.8	Thiazole 2
13	-	-	-	n.o.	Pyridine
14	8.39	d	8.0	141.8	Pyridine
15	8.27	d	8.1	118.5	Pyridine
16	-	-	-	n.o.	Pyridine
17	-	-	-	n.o.	Pyridine
18	-	-	-	n.o.	Thiazole 3
19	8.37	s	-	125.6	Thiazole 3
20	-	-	-	168.7	Thiazole 3
21	5.44	m[b]		50.7	Cys
22	3.13	m[b]		30.3	Cys
	3.61	m[b]		30.3	Cys
23	-	-	-	n.o.	Indole
24	-	-	-	114.5	Indole
25	8.19	br s		132.4	Indole
26	12.2	br s		NH	Indole
27	-	-	-	136.2	Indole
28	7.47	d	7.3	112.2	Indole
29	7.22	m[b]		122.6	Indole
30	7.19	m[b]		121.8	Indole
31	8.01	d	8.2	120.2	Indole
32	-	-	-	124.2	Indole
33	8.84	d	9.7	NH	Cys
34	-	-	-	n.o.	Thiazoline
35	5.28	dd	9.4, 9.4	78.8	Thiazoline
36	3.53	dd	9.0, 11.3	34.4	Thiazoline
	3.70	dd	9.8, 11.0	34.4	Thiazoline
37	-	-	-	169.8	Thiazoline
38	5.48	dd	3.7, 9.7	54.3	Thr 1
39	4.1	br m[b]		68.0	Thr 1
40	1.11	d	6.2	19.8	Thr 1
41	5.61	br m[b]		OH	Thr 1
42	8.46	d	9.3	NH	Thr 1
43	-	-	-	n.o.	Thiazole 4
44	-	-	-	n.o.	Thiazole 4
45	8.23	s	-	121.6	Thiazole 4
46	-	-	-	166.1	Thiazole 4

47	-	-	-	n.o.	Dhb
48	6.46	q	7.1	128.5	Dhb
49	1.75	d	7.0	13.2	Dhb
50	9.80	s	-	NH	Dhb
51	-	-	-	n.o.	Thr 2
52	4.77	d	9.6	56.0	Thr 2
53	4.73	br m[b]		69.1	Thr 2
54	1.35	d	7.2	21.0	Thr 2
55	4.95	d	4.6	OH	Thr 2
56	7.64	d	8.4	NH	Thr 2
57	-	-	-	n.o.	Thiazole 5
58	-	-	-	n.o.	Thiazole 5
59	8.22	s	-	123.8	Thiazole 5
60	-	-	-	166.1	Thiazole 5

[a] Chemical shifts determined from gHSQC and gHMBC NMR data (800 MHz). [b] Muliplicities unresolved due to signal overlap or broadening. n.o.- Resonance not observed in two dimensional heteronuclear spectra. The relative positions of the five distinct thiazoles and the two distinct threonines cannot be differentiated based on the NMR data.