Supporting Information

Alkaloids and polyketides from the South China Sea sponge *Agelas* aff. *nemoechinata*

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Computational details

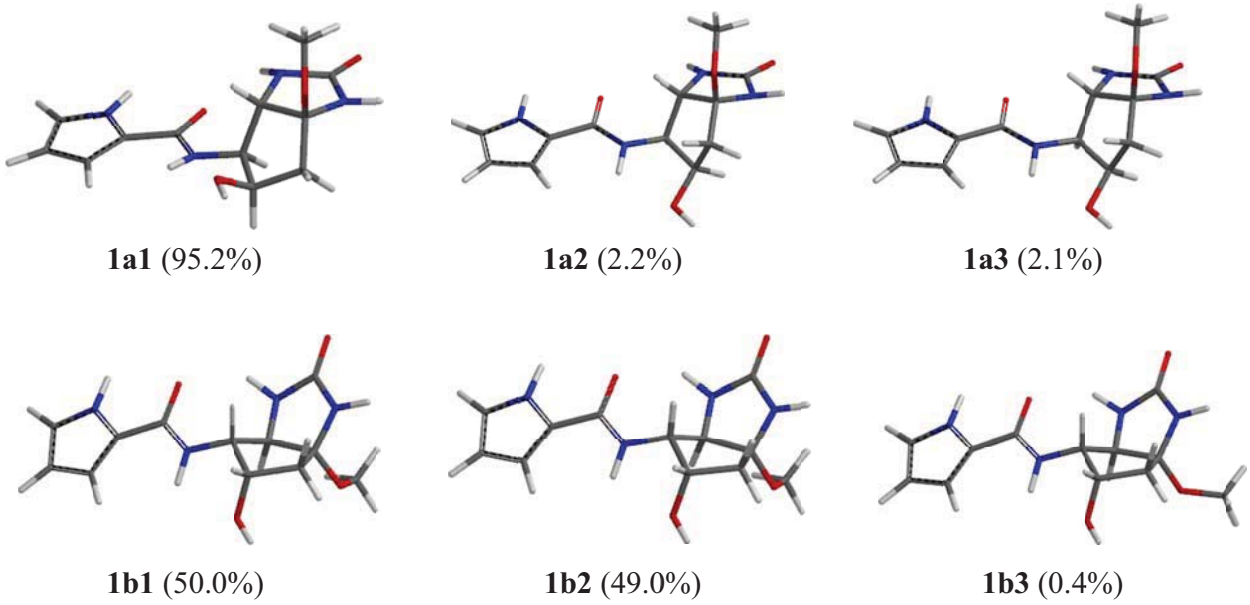


Figure S1. Stable conformers of compound **1** with 8*S*,9*R*,11*S*,15*S* (**1a**) and 8*R*,9*S*,11*R*,15*R* (**1b**) configurations, respectively.

Table S1. Important thermodynamic parameters (a.u.) of the optimized compound **1** at B3LYP/6-31G(d,p) level in the gas phase

conformations	E+ZPE	G	conformations	E+ZPE	G
1a1	-986.573227	-986.620643	**1b1**	-986.573227	-986.620644
1a2	-986.569661	-986.617074	**1b2**	-986.573222	-986.620626
1a3	-986.573222	-986.620626	**1b3**	-986.568791	-986.616183

Table S2. Optimized Z-Matrixes of compound **1** in the Gas Phase (Å) at B3LYP/6-31G(d,p) level.

1a1				**1a2**				**1a3**			
C	-3.325098	0.113642	0.003295	C	3.295978	-0.25099	0.003588	C	3.295977	-0.250933	0.003471
C	-4.087481	-1.033023	0.196773	C	4.036824	0.824308	0.480485	C	4.036949	0.824379	0.48014
C	-5.396861	-0.616918	0.536073	C	5.369274	0.37706	0.649473	C	5.369312	0.376975	0.649386
C	-5.401486	0.769759	0.538723	C	5.407789	-0.95681	0.27321	C	5.407713	-0.956929	0.27324
N	-4.148298	1.193251	0.217755	N	4.15308	-1.31913	-0.11205	N	4.152965	-1.319211	-0.111888
C	-1.928347	0.391032	-0.351494	C	1.894425	-0.46889	-0.37558	C	1.894417	-0.46881	-0.37566
N	-1.102512	-0.683342	-0.493671	N	1.049047	0.600823	-0.28773	N	1.049038	0.600902	-0.287772
C	0.302358	-0.530301	-0.814678	C	-0.29329	0.483455	-0.83189	C	-0.293325	0.483575	-0.831885

O	-1.541956	1.558428	-0.521373	O	1.501306	-1.5862	-0.74049	O	1.501252	-1.586119	-0.740515
C	0.958536	-1.891917	-1.092812	C	-1.00114	1.864379	-0.7965	C	-1.001172	1.864469	-0.796259
C	2.463633	-1.594913	-1.024012	C	-1.76259	1.886512	0.534924	C	-1.762513	1.886413	0.535222
C	1.187101	0.087324	0.30181	C	-1.18371	-0.45722	0.042494	C	-1.183685	-0.457231	0.042437
N	1.329636	1.528975	0.272208	N	-1.9545	-1.4359	-0.68831	N	-1.9545	-1.435851	-0.688431
C	2.518884	1.906079	-0.336857	C	-3.25464	-1.02763	-0.91425	C	-3.25462	-1.027503	-0.914362
C	2.632535	-0.449741	0.010111	C	-2.29241	0.45676	0.67769	C	-2.292359	0.456661	0.677784
N	3.259991	0.738517	-0.512127	N	-3.40891	0.167848	-0.20302	N	-3.408875	0.167857	-0.202944
O	2.862959	3.027836	-0.659199	O	-4.10192	-1.57864	-1.59194	O	-4.101877	-1.578362	-1.592204
O	0.518192	-2.754433	-0.040044	O	-0.03241	2.897353	-0.94584	O	-0.032501	2.897473	-0.945578
H	0.393416	0.102307	-1.705147	H	-0.24312	0.087294	-1.85267	H	-0.243162	0.087561	-1.852718
H	0.837757	-0.27542	1.273462	H	-0.57006	-0.91889	0.817526	H	-0.569973	-0.918976	0.817375
O	3.302874	-1.014049	1.12479	O	-2.56785	0.241086	2.047028	O	-2.567802	0.240803	2.047096
C	3.515343	-0.147033	2.233404	C	-3.00547	-1.06406	2.41197	C	-3.005465	-1.064379	2.411823
H	-3.746042	-2.053995	0.093836	H	3.661308	1.815807	0.693523	H	3.661594	1.816009	0.692855
H	-6.24386	-1.252434	0.751523	H	6.207754	0.957659	1.00675	H	6.20784	0.957532	1.006618
H	-6.197778	1.469836	0.743186	H	6.228068	-1.65882	0.254012	H	6.227934	-1.659009	0.254152
H	-3.809477	2.139684	0.119031	H	3.828965	-2.21794	-0.43948	H	3.828685	-2.218064	-0.439046
H	-1.379274	-1.585249	-0.130221	H	1.4272	1.537877	-0.23944	H	1.427166	1.537955	-0.239291
H	0.657855	-2.299061	-2.06843	H	-1.71932	1.892897	-1.62567	H	-1.719454	1.893038	-1.625346
H	2.819483	-1.259886	-2.002438	H	-2.56515	2.629858	0.56909	H	-2.565019	2.629816	0.569594
H	3.044635	-2.47321	-0.729478	H	-1.06673	2.085276	1.356155	H	-1.066608	2.085019	1.356455
H	0.499788	2.080361	0.080649	H	-1.52081	-2.12047	-1.28893	H	-1.52085	-2.120268	-1.289264
H	4.236993	0.792727	-0.755499	H	-4.34541	0.47769	0.013506	H	-4.34538	0.477787	0.013454
H	0.999605	-3.588825	-0.104097	H	-0.4849	3.74887	-0.90095	H	-0.484933	3.748982	-0.89994
H	2.572057	0.213567	2.662513	H	-2.24769	-1.82756	2.197359	H	-2.247691	-1.827874	2.197165
H	4.128585	0.720513	1.96296	H	-3.93675	-1.343	1.904672	H	-3.936735	-1.343208	1.904441
H	4.043311	-0.738906	2.983591	H	-3.18369	-1.0322	3.488478	H	-3.183762	-1.032656	3.488325
1b1				**1b2**				**1b3**			
C	3.325122	0.113575	0.003343	C	3.325051	0.113943	0.003438	C	3.39185	0.039199	0.018622
C	4.087439	-1.03308	0.197155	C	4.087638	-1.03258	0.196957	C	4.112943	-1.14197	0.15402
C	5.396858	-0.61695	0.536277	C	5.397067	-0.61624	0.535807	C	5.44287	-0.78884	0.484848
C	5.401563	0.769729	0.538523	C	5.401509	0.770436	0.538131	C	5.500488	0.595547	0.540619
N	4.148394	1.1932	0.217472	N	4.148174	1.193691	0.217375	N	4.259274	1.077876	0.258894
C	1.928383	0.390956	-0.35148	C	1.928201	0.391004	-0.35128	C	2.001394	0.383977	-0.30035
N	1.102492	-0.68339	-0.49353	N	1.102595	-0.68352	-0.4933	N	1.130635	-0.65086	-0.46761
C	-0.30234	-0.53026	-0.81467	C	-0.30231	-0.53107	-0.8145	C	-0.27094	-0.42892	-0.76027
O	1.542027	1.558335	-0.52155	O	1.541559	1.558327	-0.52119	O	1.659767	1.571098	-0.42107
C	-0.95859	-1.8918	-1.09299	C	-0.95818	-1.89306	-1.09164	C	-0.98253	-1.74968	-1.09671
C	-2.46366	-1.59465	-1.02432	C	-2.46338	-1.59648	-1.02278	C	-2.47993	-1.40905	-0.98349

C	-1.18712	0.087304	0.301813	C	-1.18715	0.087079	0.301549	C	-1.11855	0.165195	0.394564
N	-1.32959	1.528985	0.272347	N	-1.32985	1.528702	0.271305	N	-1.19741	1.611759	0.439513
C	-2.51887	1.906209	-0.3366	C	-2.51903	1.905666	-0.33769	C	-2.36504	2.070668	-0.14624
C	-2.63256	-0.44967	0.010022	C	-2.63248	-0.45001	0.009887	C	-2.58007	-0.28426	0.093734
N	-3.26002	0.738697	-0.512	N	-3.25944	0.737725	-0.51447	N	-3.15039	0.942473	-0.39501
O	-2.8629	3.028022	-0.6588	O	-2.86371	3.027521	-0.6591	O	-2.66572	3.218511	-0.41476
O	-0.51843	-2.75443	-0.04022	O	-0.51743	-2.75491	-0.03842	O	-0.55502	-2.68482	-0.1027
H	-0.39325	0.10246	-1.70507	H	-0.39358	0.100852	-1.70544	H	-0.34724	0.248954	-1.61825
H	-0.83781	-0.27552	1.273446	H	-0.8378	-0.27513	1.2734	H	-0.80178	-0.26387	1.348805
O	-3.30291	-1.01419	1.124589	O	-3.30371	-1.01265	1.124906	O	-3.14023	-0.7555	1.316158
C	-3.51527	-0.1474	2.233402	C	-3.51536	-0.14465	2.232871	C	-4.54268	-0.94647	1.315959
H	3.745939	-2.05407	0.094599	H	3.746313	-2.05364	0.094545	H	3.730852	-2.14454	0.018621
H	6.243822	-1.25246	0.751898	H	6.244176	-1.25162	0.751231	H	6.268462	-1.46357	0.660478
H	6.197895	1.46982	0.742781	H	6.197706	1.470702	0.742314	H	6.326172	1.256812	0.757326
H	3.809644	2.139622	0.11841	H	3.809426	2.140098	0.118217	H	3.954809	2.03941	0.203425
H	1.37924	-1.58535	-0.1302	H	1.379869	-1.5856	-0.13066	H	1.37419	-1.57576	-0.13995
H	-0.65785	-2.29891	-2.0686	H	-0.65756	-2.30076	-2.06704	H	-0.71482	-2.11283	-2.09879
H	-3.04485	-2.47294	-0.73012	H	-3.04394	-2.47463	-0.72697	H	-3.06372	-2.29325	-0.71094
H	-2.81929	-1.25931	-2.00272	H	-2.81965	-1.26274	-2.00148	H	-2.84826	-1.04315	-1.94639
H	-0.49975	2.08037	0.080759	H	-0.49994	2.080338	0.080832	H	-0.34435	2.136433	0.280808
H	-4.23706	0.79298	-0.7552	H	-4.23754	0.79225	-0.75351	H	-4.10769	1.060162	-0.68503
H	-1.00002	-3.58871	-0.1043	H	-0.99743	-3.59007	-0.10307	H	-1.0099	-3.52307	-0.25232
H	-2.57194	0.213081	2.662513	H	-4.12644	0.724155	1.961518	H	-4.87265	-1.65466	0.540079
H	-4.04319	-0.73942	2.98351	H	-2.57171	0.21403	2.662798	H	-5.08817	-0.00204	1.185677
H	-4.12851	0.720218	1.9632	H	-4.0454	-0.73498	2.982818	H	-4.79999	-1.36049	2.292939

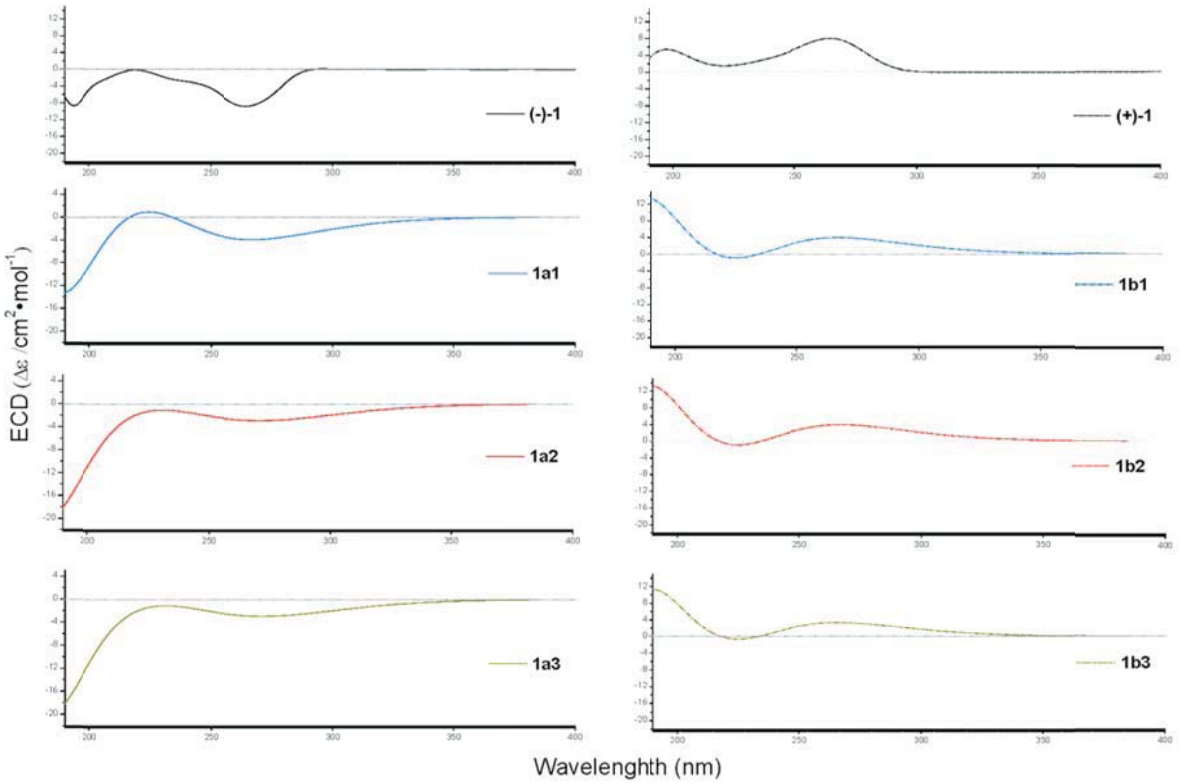
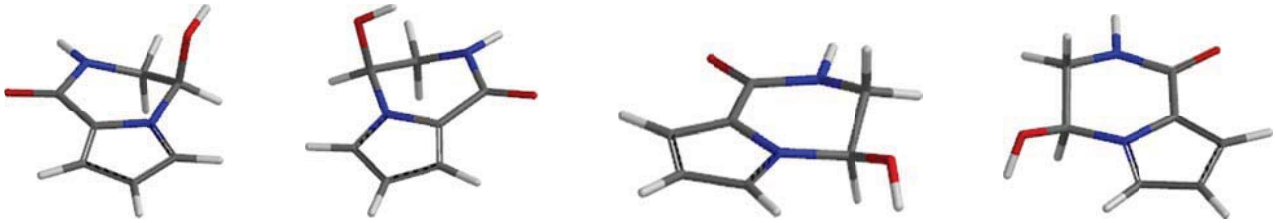


Figure S2. The corresponding calculated ECD spectra (redshifted by 15 nm) of structural candidates with respective 8*S*,9*R*,11*S*,15*S* (**1a**) and 8*R*,9*S*,11*R*,15*R* (**1b**) configurations.



2a1 (9*R*) (97.8%) **2a2 (9*S*)** (99.0%) **2b1 (9*R*)** (1%) **2b2 (9*S*)** (1%)

Figure S3. Stable conformers of (+)- and (-)-nemoechine B (**2**) with respective quasiaxial (**2a**) and quasiequatorial (**2b**) OH-9 conformations.

Table S3. Important thermodynamic parameters (a.u.) of the optimized compound **2** at B3LYP/6-31G(d,p) level in the gas phase

conformations	E+ZPE	G	conformations	E+ZPE	G
2a1	-531.375108	-531.408758	**2b1**	-531.370499	-531.404438
2a2	-531.375109	-531.408760	**2b2**	-531.370498	-531.404435

Table S4. Optimized Z-Matrixes of compound **2** in the Gas Phase (Å) at B3LYP/6-31G(d,p) level.

2a1				**2a2**			
C	-2.70067	-0.01677	-0.04461	C	2.70067	-0.01677	-0.04461
C	-1.87793	-1.11997	-0.19508	C	1.87793	-1.11997	-0.19508
N	-0.579	-0.69138	-0.20111	N	0.579	-0.69138	-0.20111
C	-0.55781	0.68816	-0.02724	C	0.55781	0.68816	-0.02724
C	-1.86903	1.1236	0.0638	C	1.86903	1.1236	0.0638
C	0.63362	-1.5042	-0.20376	C	-0.63362	-1.5042	-0.20376
C	1.74489	-0.64807	-0.82086	C	-1.74489	-0.64807	-0.82086
N	1.83488	0.60859	-0.0798	N	-1.83488	0.60859	-0.0798
C	0.70771	1.41954	0.06792	C	-0.70771	1.41954	0.06792
O	0.79653	2.61653	0.30759	O	-0.79653	2.61653	0.30759
O	0.97092	-1.97691	1.07589	O	-0.97092	-1.97691	1.07589
H	-3.78094	-0.03631	-0.02334	H	3.78094	-0.03631	-0.02334
H	-2.1152	-2.16879	-0.30083	H	2.1152	-2.16879	-0.30083
H	-2.16871	2.15337	0.19122	H	2.16871	2.15337	0.19122
H	0.45015	-2.3906	-0.81601	H	-0.45015	-2.3906	-0.81601
H	1.53613	-0.49181	-1.88956	H	-1.53613	-0.49181	-1.88956
H	2.69044	-1.18675	-0.72842	H	-2.69044	-1.18675	-0.72842
H	2.69158	1.14205	-0.16195	H	-2.69158	1.14205	-0.16195
H	1.28103	-1.2124	1.58639	H	-1.28103	-1.2124	1.58639
2b1				**2b2**			
C	-0.69769	0.632234	0.000381	C	0.697649	0.632158	0.000439
C	-0.91473	1.996118	-0.1026	C	0.914788	1.995987	-0.102826
N	0.351551	2.626615	-0.07621	N	-0.351427	2.62661	-0.076208
C	1.309972	1.633971	0.048065	C	-1.309902	1.634071	0.048288
C	0.671887	0.425043	0.079452	C	-0.671963	0.425076	0.07978
C	1.250928	-0.89329	0.352039	C	-1.251042	-0.89327	0.352024
C	0.352906	-1.93812	-0.308	C	-0.352875	-1.938033	-0.307994
N	-1.03156	-1.73631	0.094826	N	1.031539	-1.73638	0.095246
C	-1.64078	-0.49026	0.037235	C	1.640759	-0.490294	0.037237
O	-2.85892	-0.359	0.053559	O	2.858888	-0.358989	0.053352
O	2.537955	-1.01366	-0.19632	O	-2.537922	-1.01372	-0.196667
H	-1.88614	2.458757	-0.19624	H	1.886253	2.458478	-0.196679
H	0.552069	3.685599	-0.15619	H	-0.551919	3.685595	-0.156246
H	2.387201	1.697182	0.076983	H	-2.387114	1.697586	0.077535
H	1.267822	-1.0516	1.440167	H	-1.26815	-1.051771	1.440127
H	0.500967	-1.86147	-1.39569	H	-0.500657	-1.861146	-1.395712
H	0.683671	-2.92976	0.009465	H	-0.68379	-2.929681	0.009232
H	-1.67851	-2.50454	-0.02534	H	1.678467	-2.504552	-0.025464
H	3.185399	-0.73759	0.463546	H	-3.185565	-0.737088	0.462787

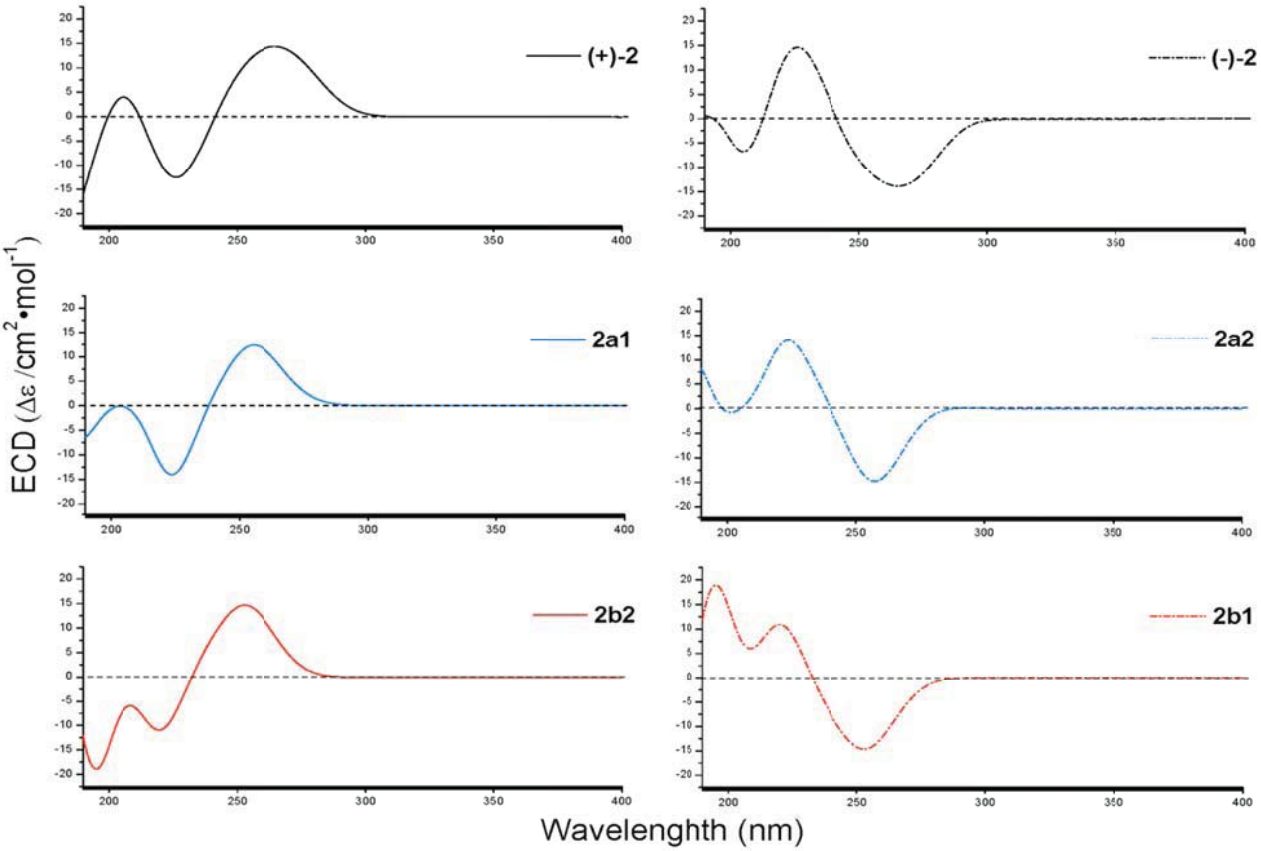
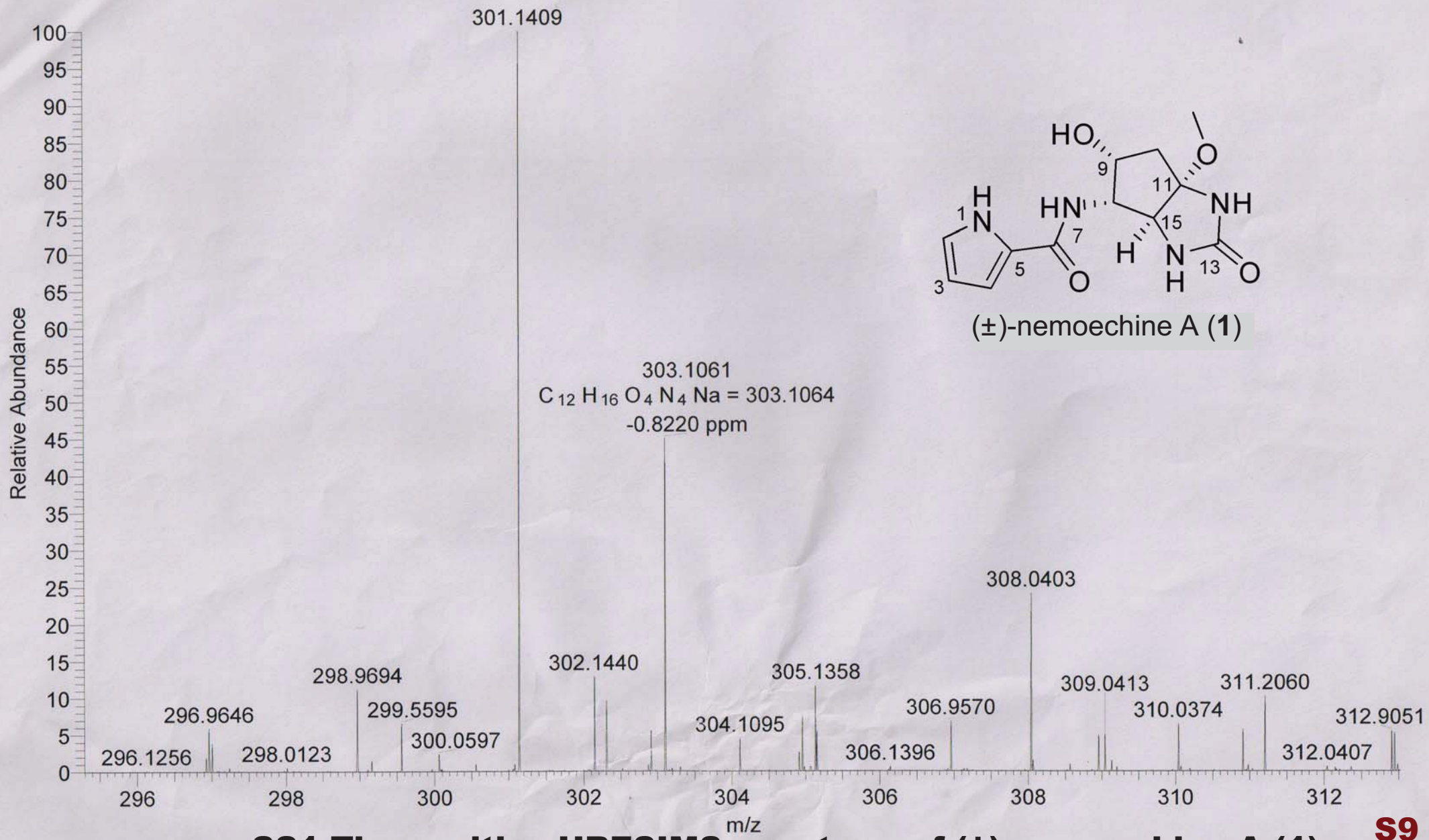


Figure S4. Experimental CD and calculated spectra (redshifted by 10 nm) of (+)- and (-)-nemoechine B (**2**) for the candidate stereostructures with respective quasiaxial (**2a**) and quasiequatorial (**2b**) OH-9 conformation.

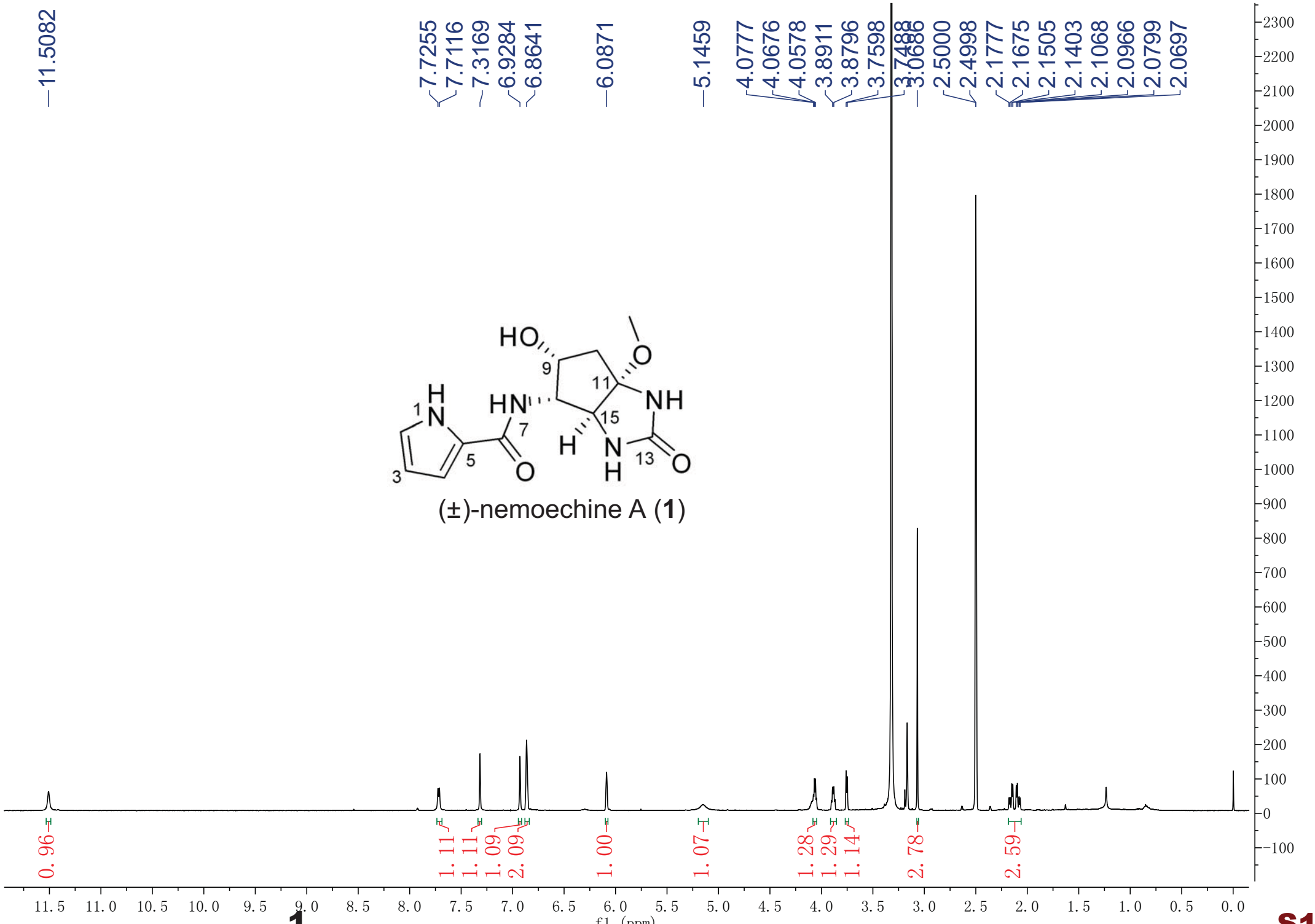
D:\MS-DATA\20131031-S62316_131031094958 10/31/2013 9:49:58 AM S62316

20131031-S62316_131031094958 #47-56 RT: 1.16-1.38 AV: 10 NL: 4.75E5
T: FTMS + p ESI Full ms [100.00-1000.00]



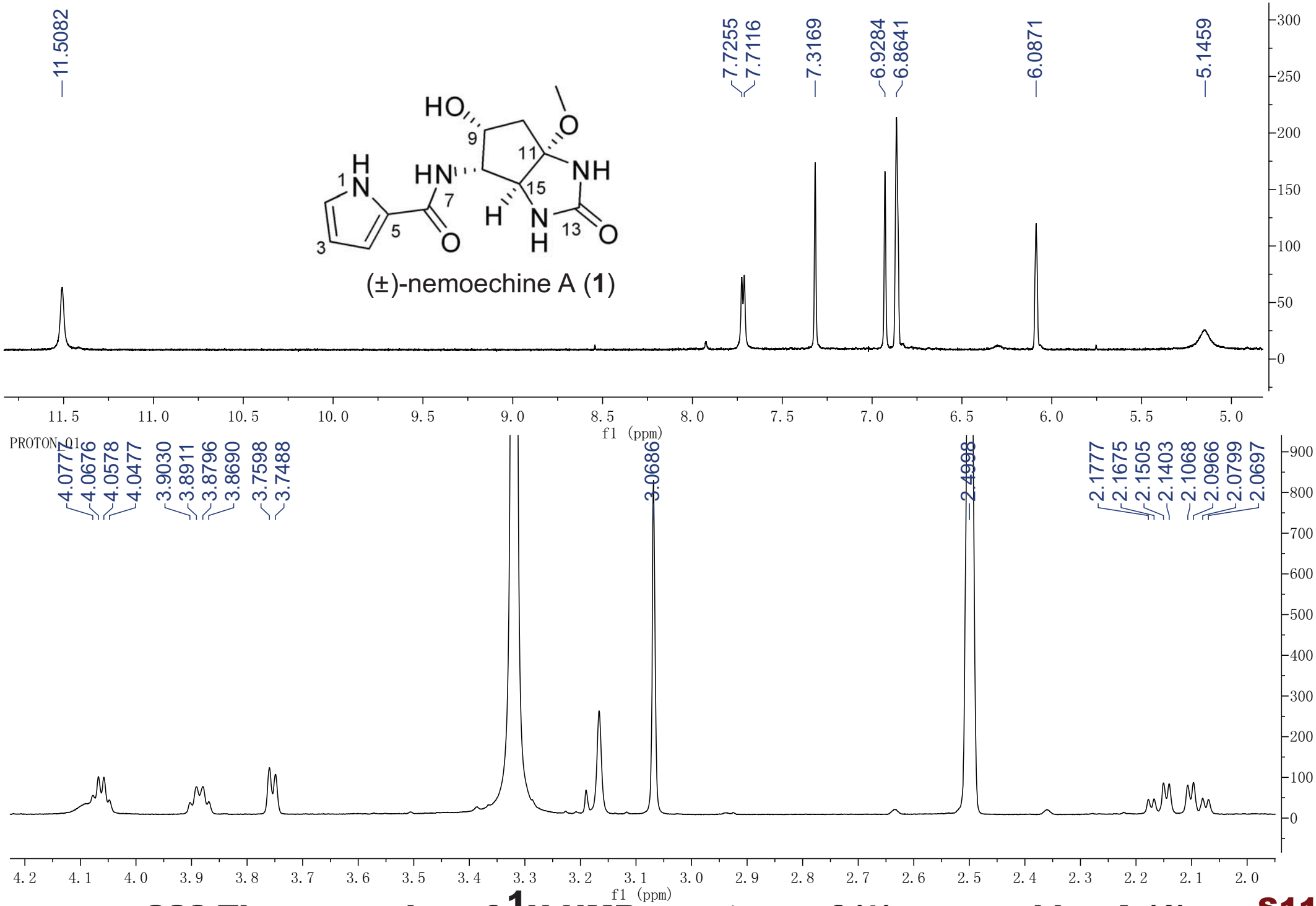
(±)-nemoechine A (**1**)

SS1 The positive HRESIMS spectrum of (±)-nemoechine A (1)

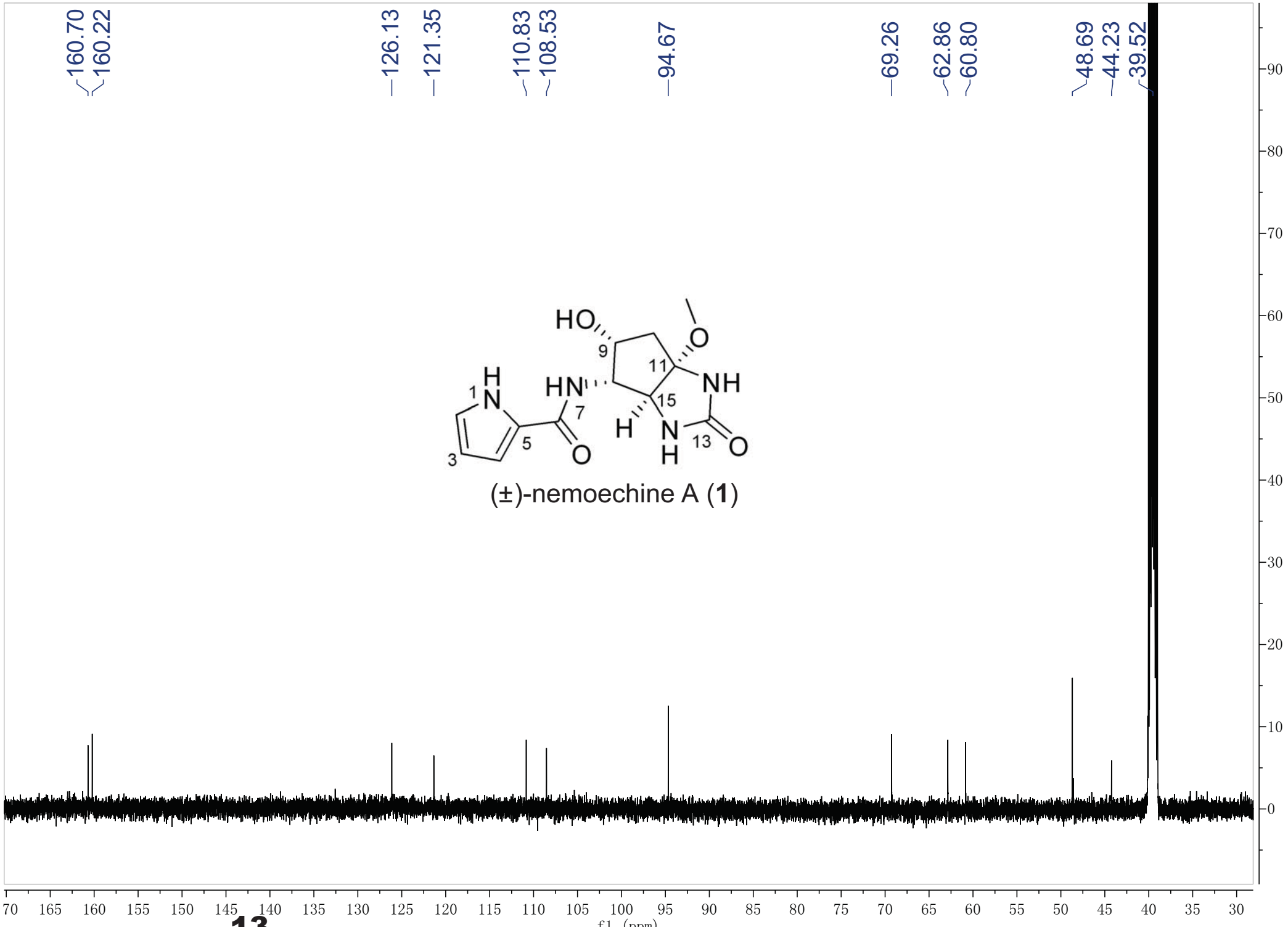


(±)-nemoechine A (**1**)

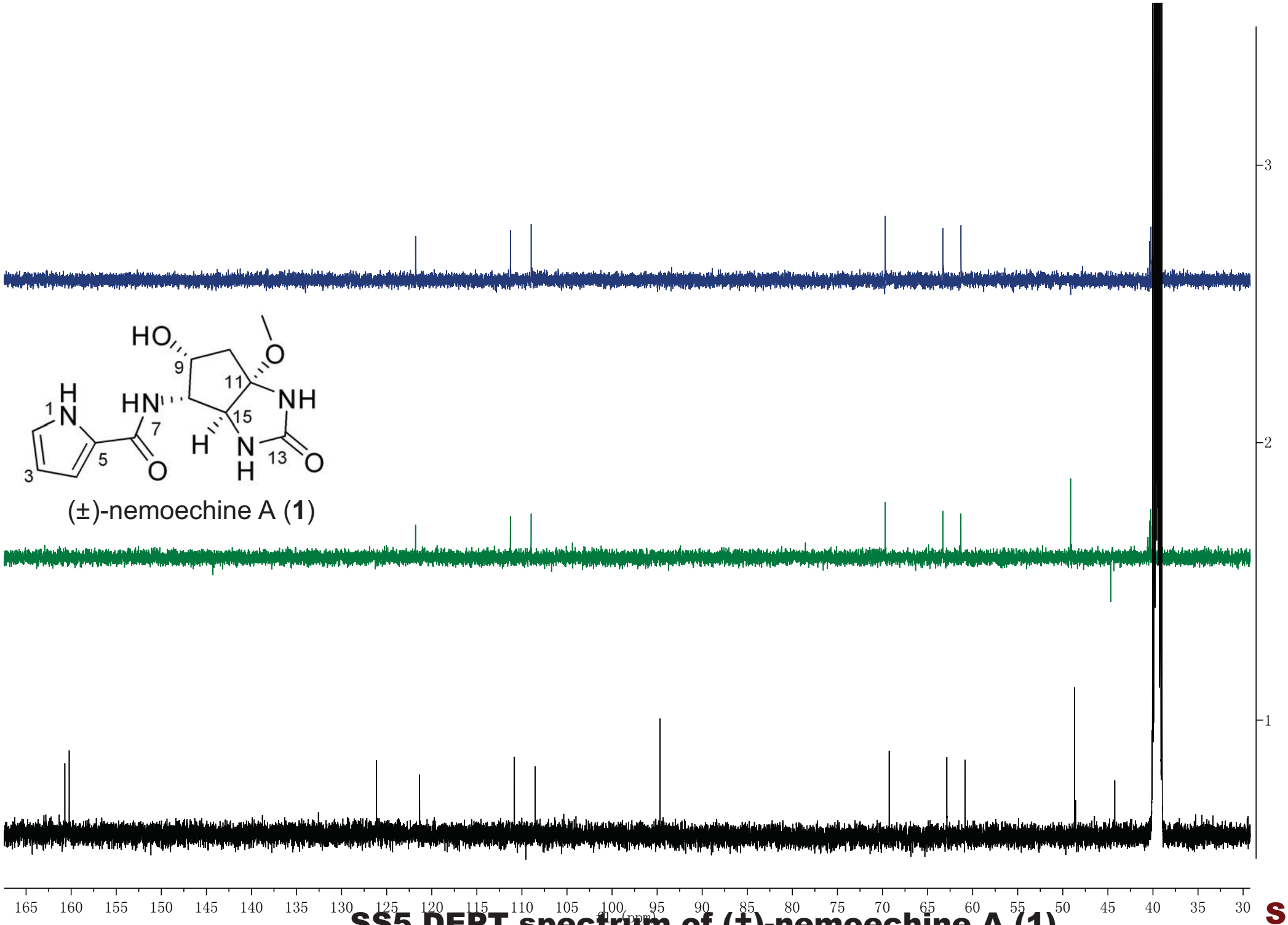
SS2 ^{1}H NMR (500 MHz, DMSO) spectrum of (±)-nemoechine A (1)



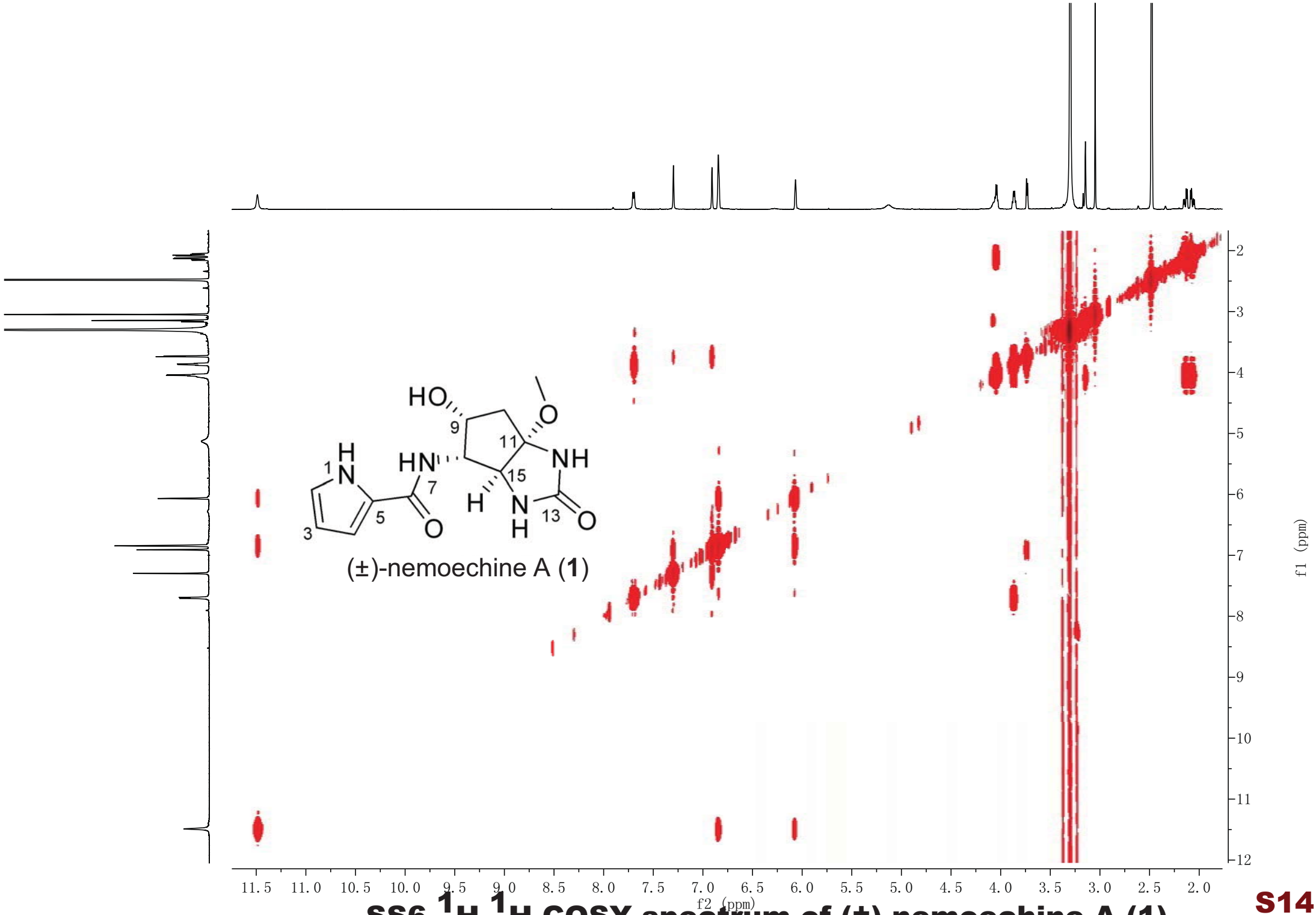
SS3 The expansion of ^{1}H NMR spectrum of (±)-nemoechine A (1)



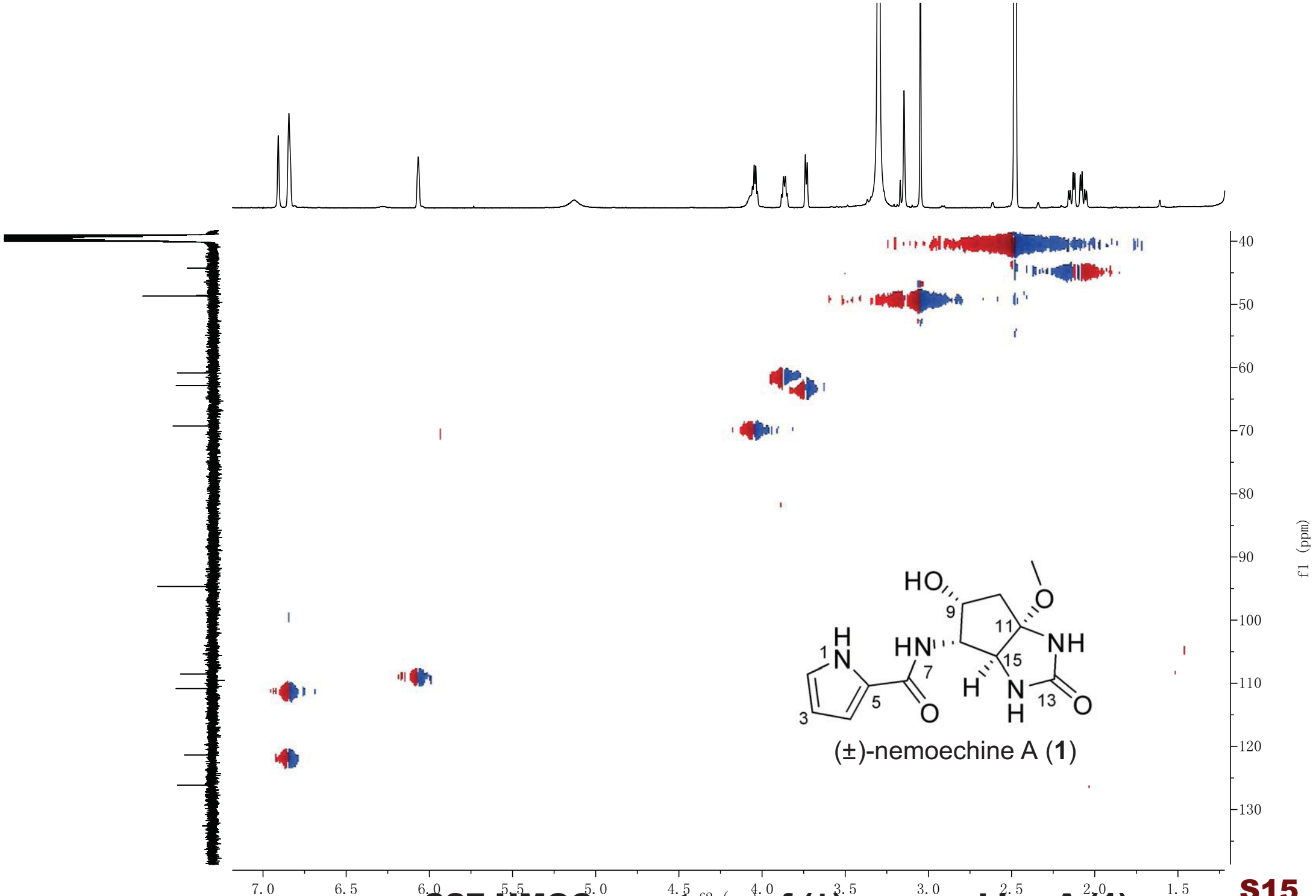
SS4 ^{13}C NMR (125 MHz, DMSO) spectrum of (±)-nemoechine A (1)



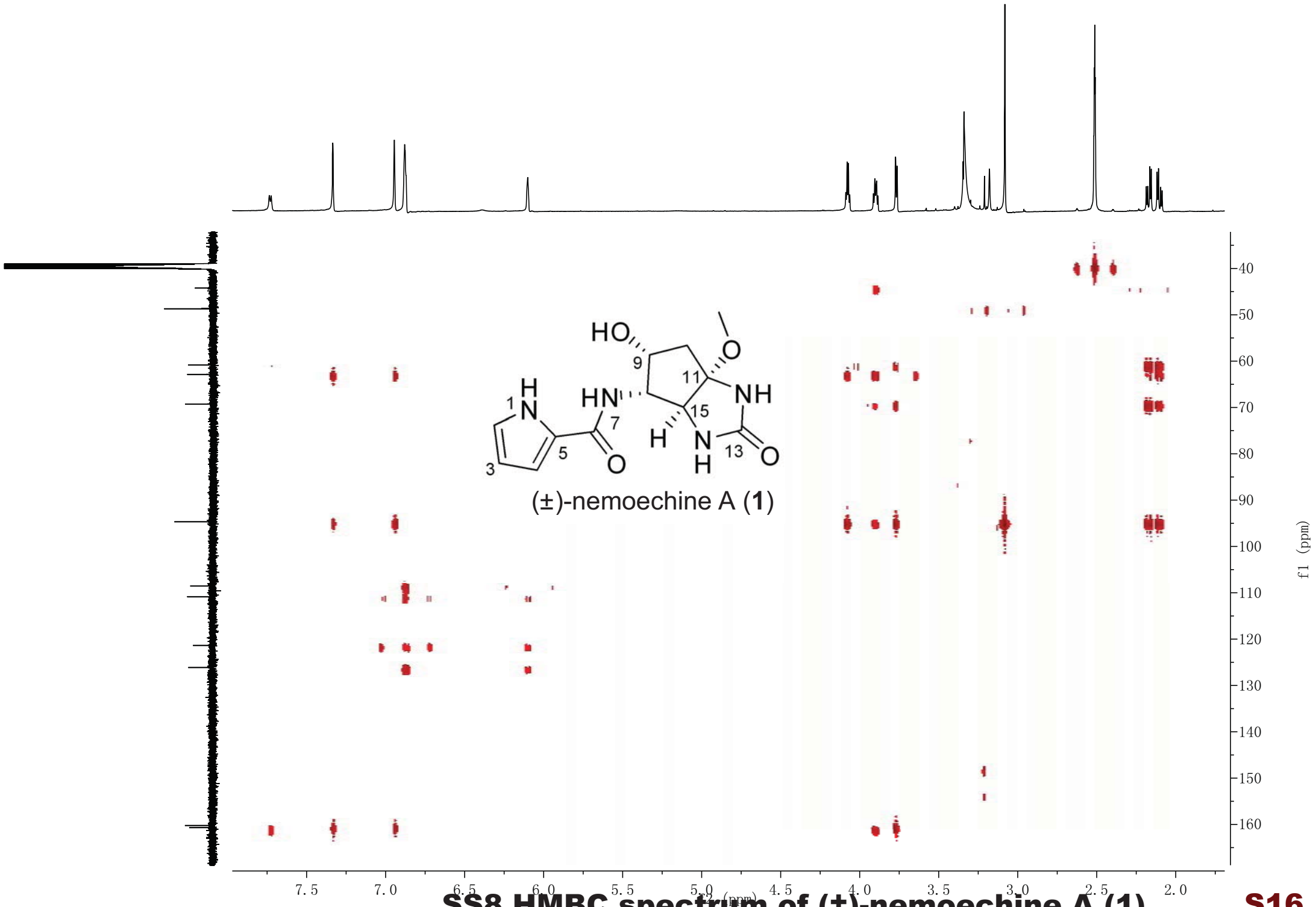
SS5 DEPT spectrum of (±)-nemoechine A (1)



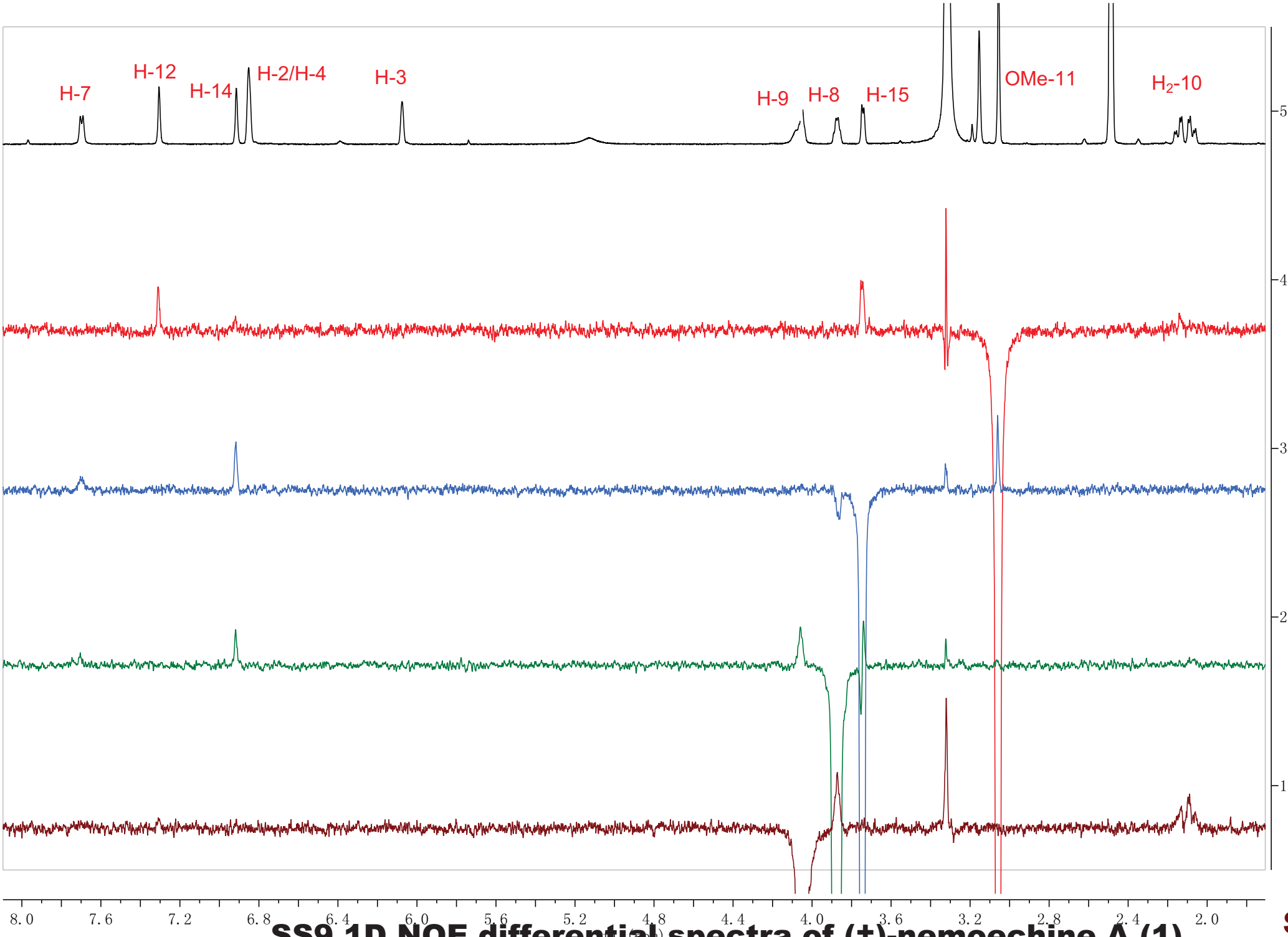
SS6 ^{1}H-^{1}H COSY spectrum of (±)-nemoechine A (1)



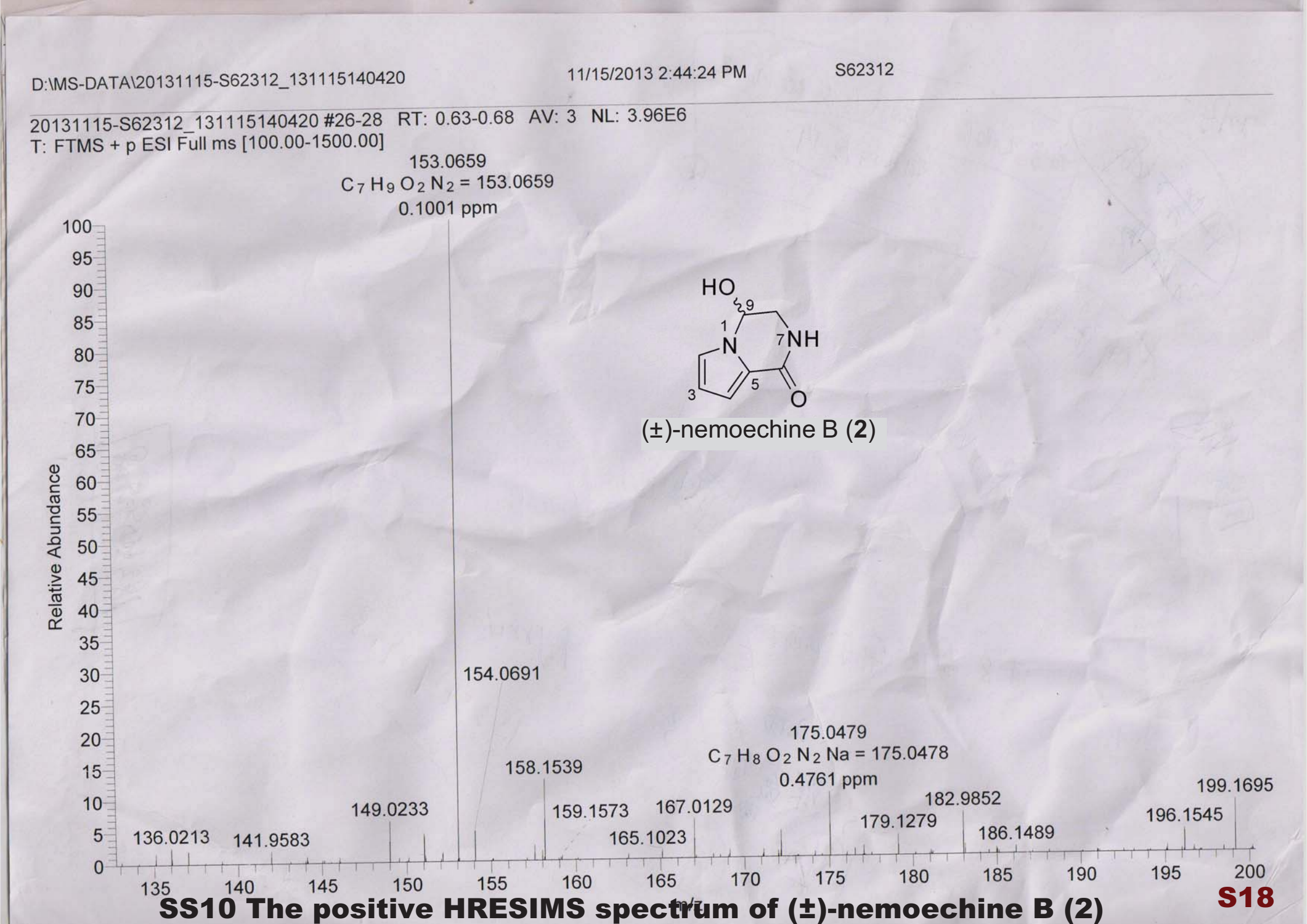
SS7 HMQC spectrum of (±)-nemoechine A (1)



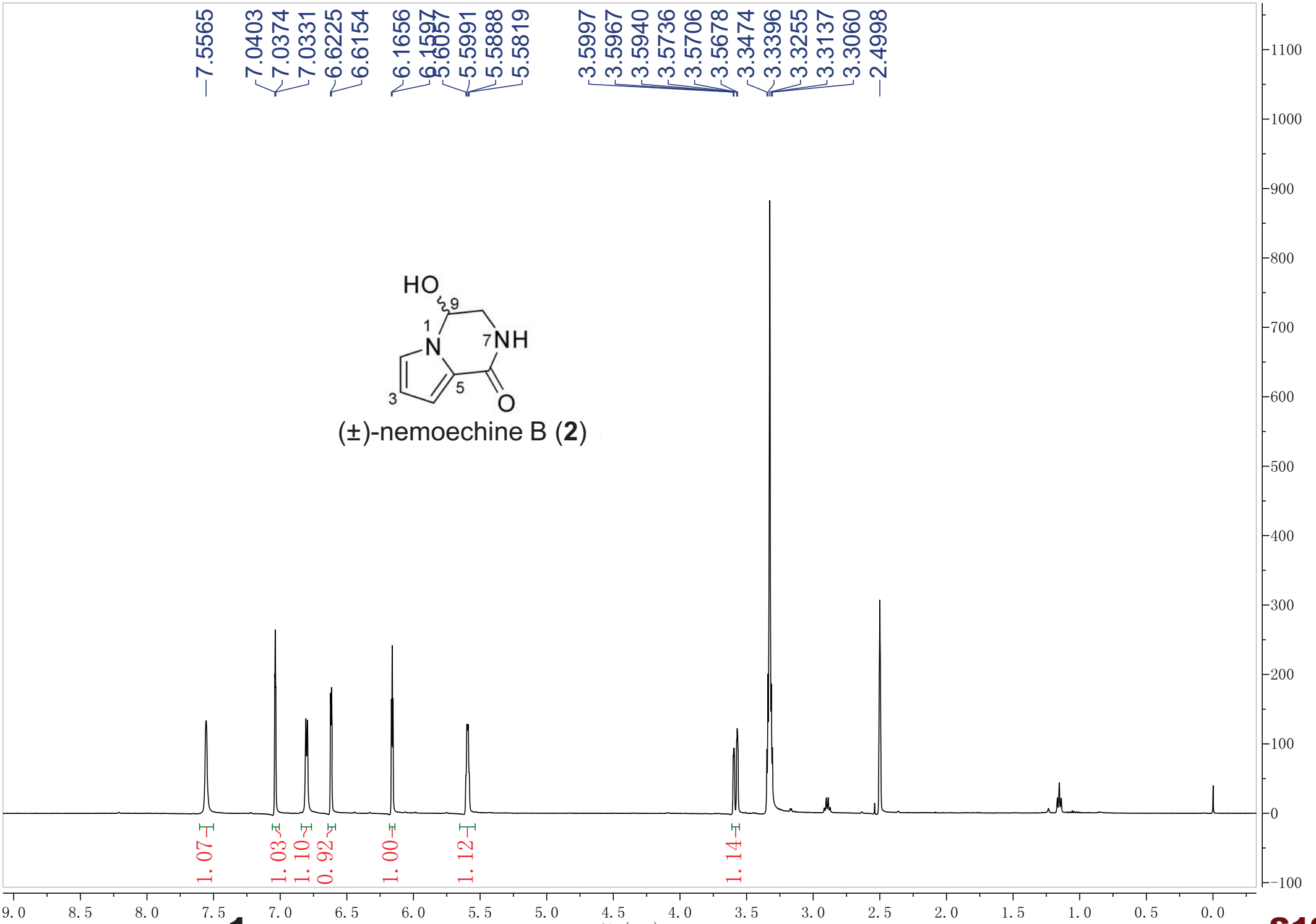
SS8 HMBC spectrum of (±)-nemoechine A (1)



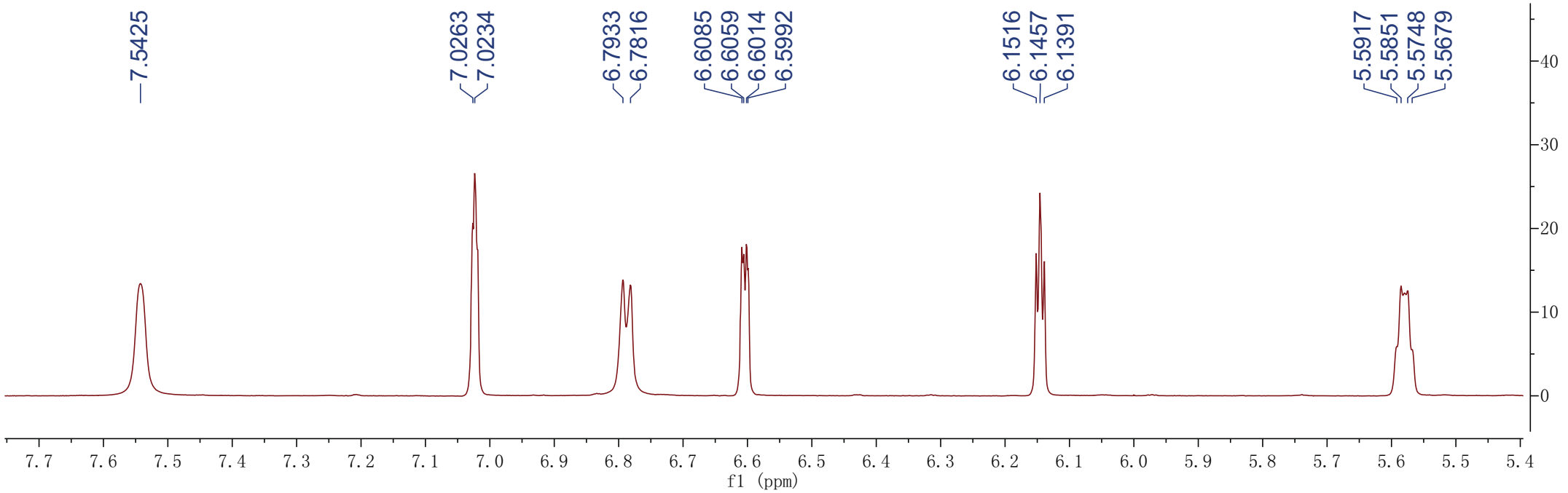
SS9 1D NOE differential spectra of (±)-nemoechine A (1)

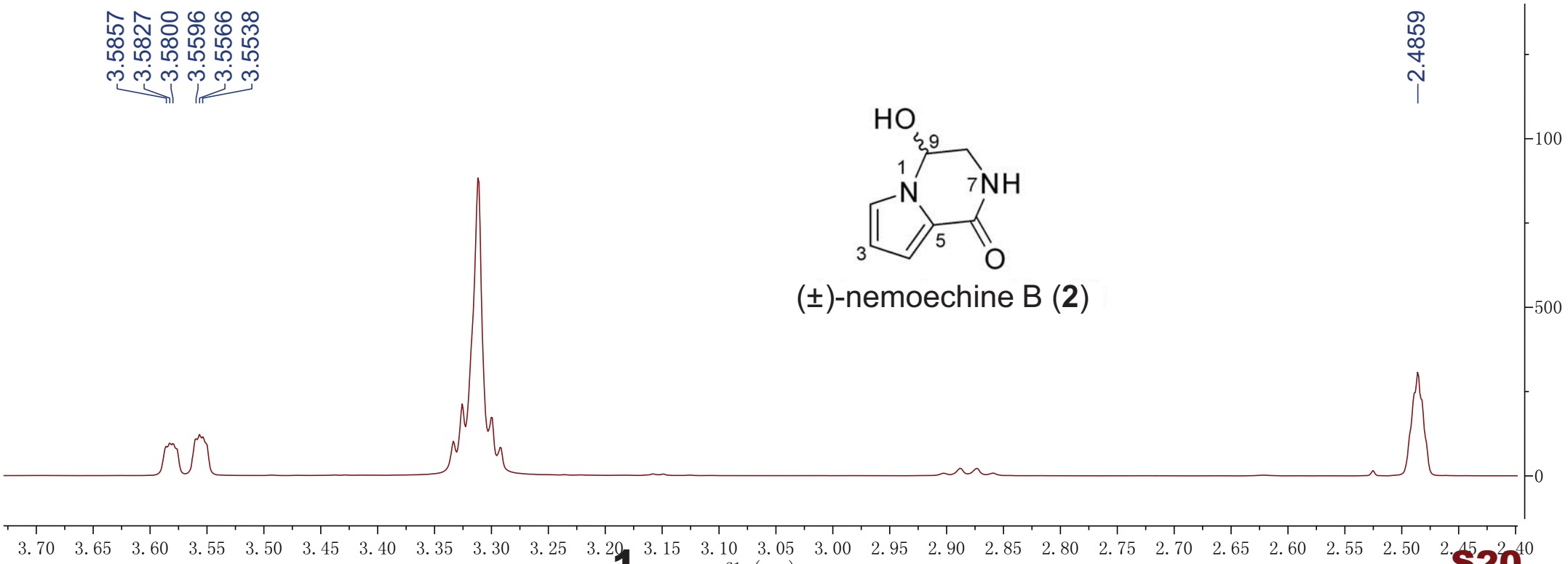


SS10 The positive HRESIMS spectrum of (±)-nemoechine B (2)



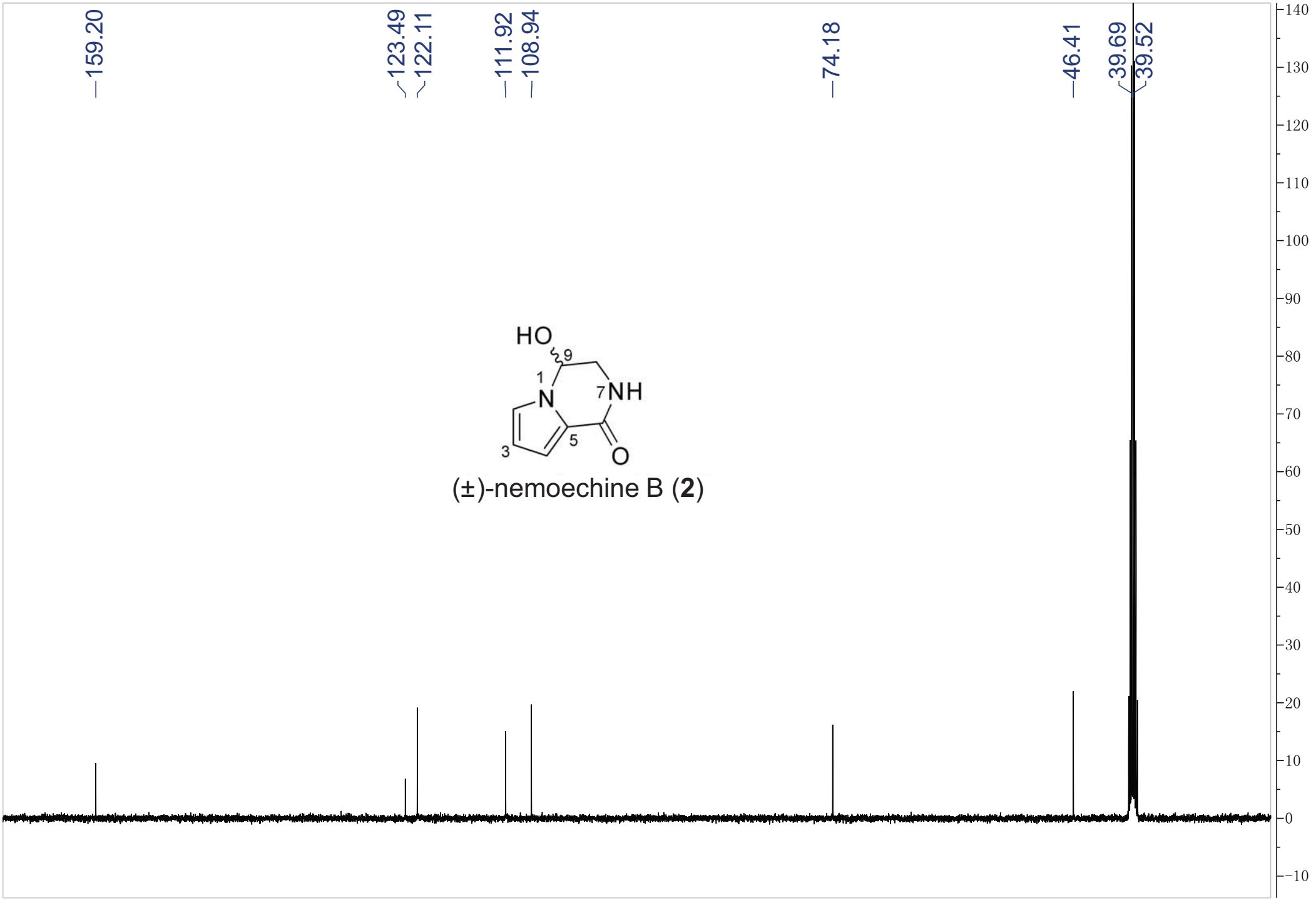
SS11 ^{1}H NMR (500 MHz, DMSO) spectrum of (±)-nemoechine B (2)



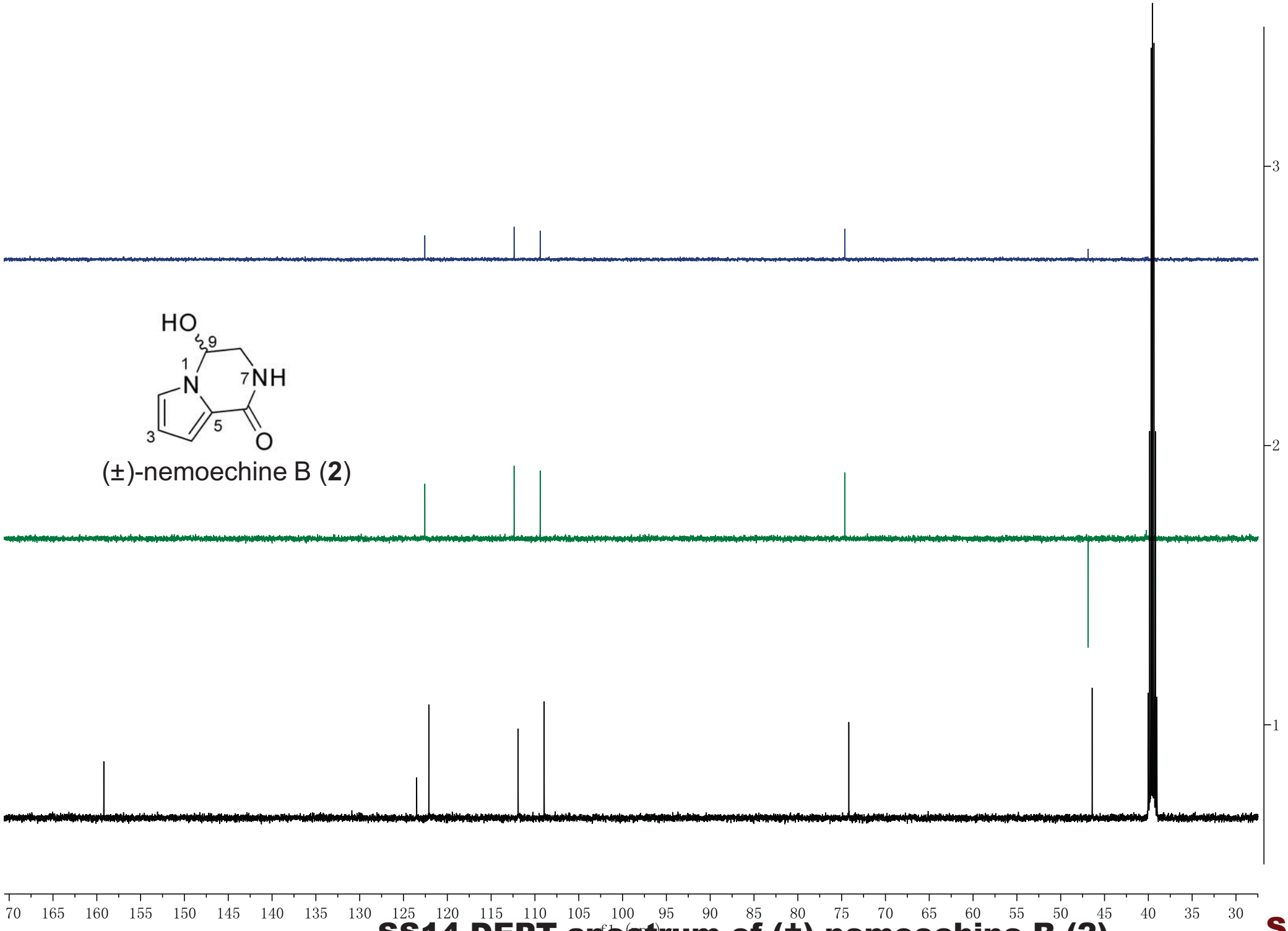


(±)-nemoechine B (**2**)

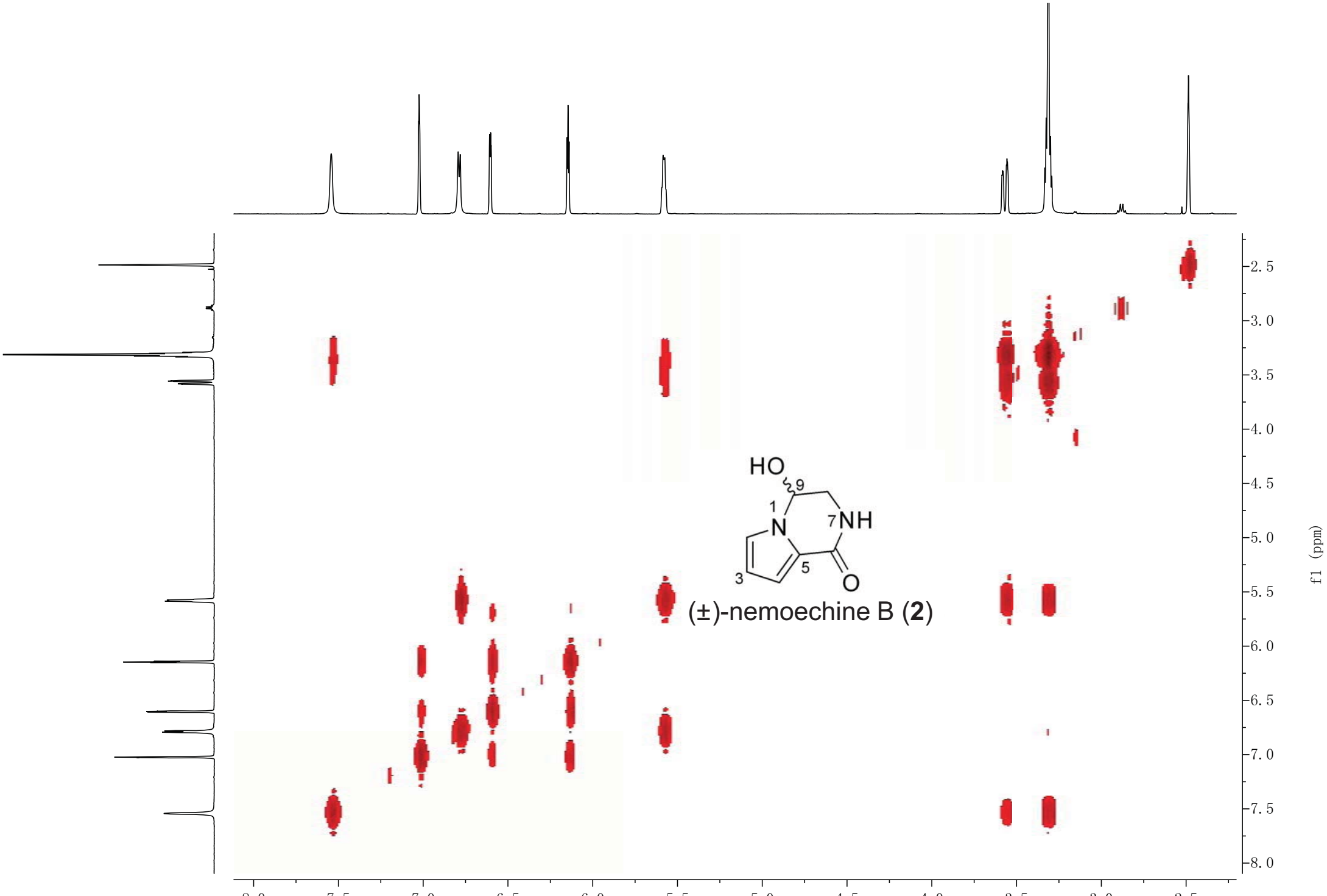
SS12 The expansion of ^{1}H NMR spectrum of (±)-nemoechine B (2)



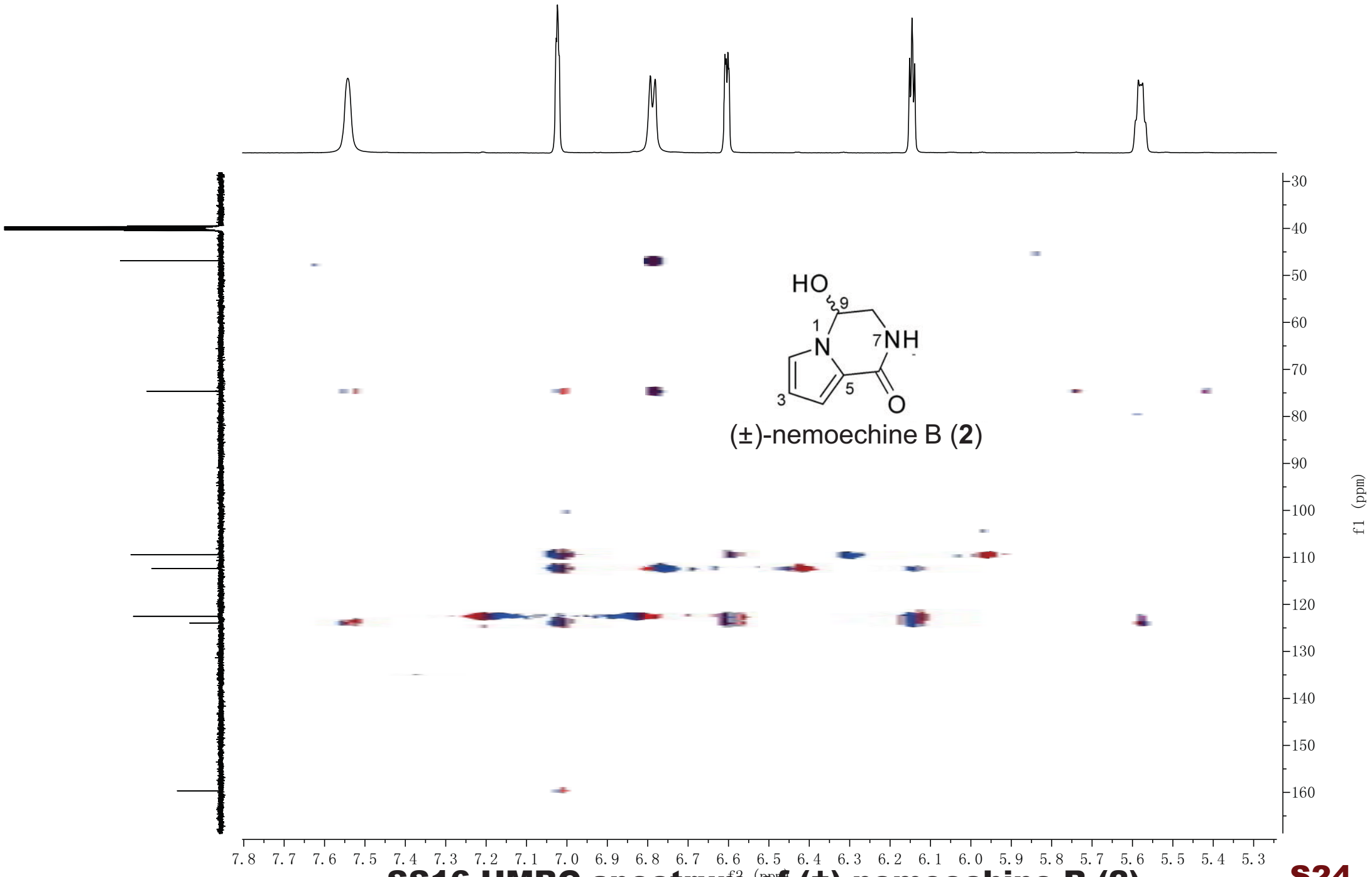
SS13 ^{13}C NMR (125 MHz, DMSO) spectrum of (±)-nemoechine B (2)



SS14 DEPT spectrum of (±)-nemoechine B (2)



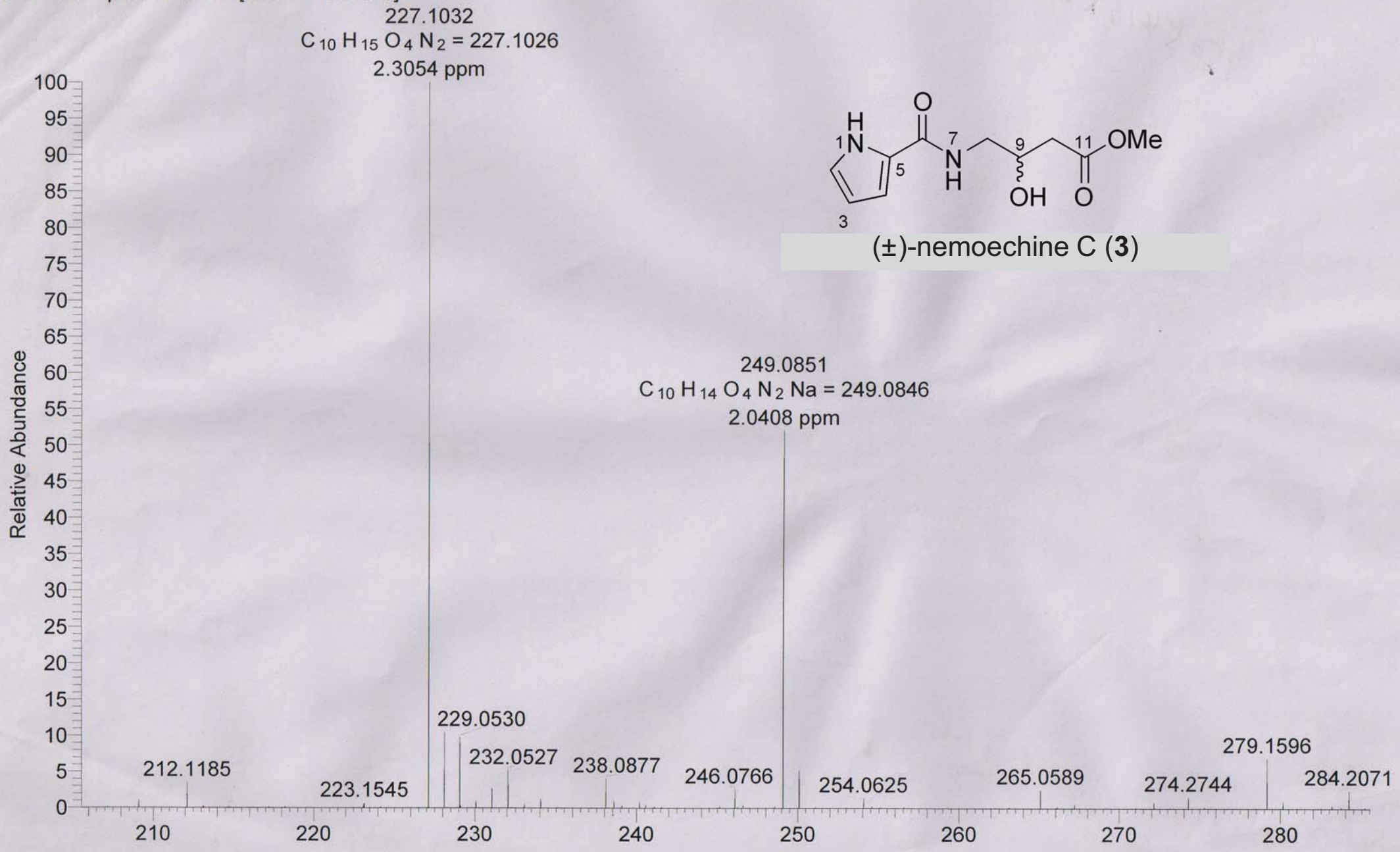
SS15 ^{1}H-^{1}H COSY spectrum of (±)-nemoechine B (2)



SS16 HMBC spectrum of (±)-nemoechine B (2)

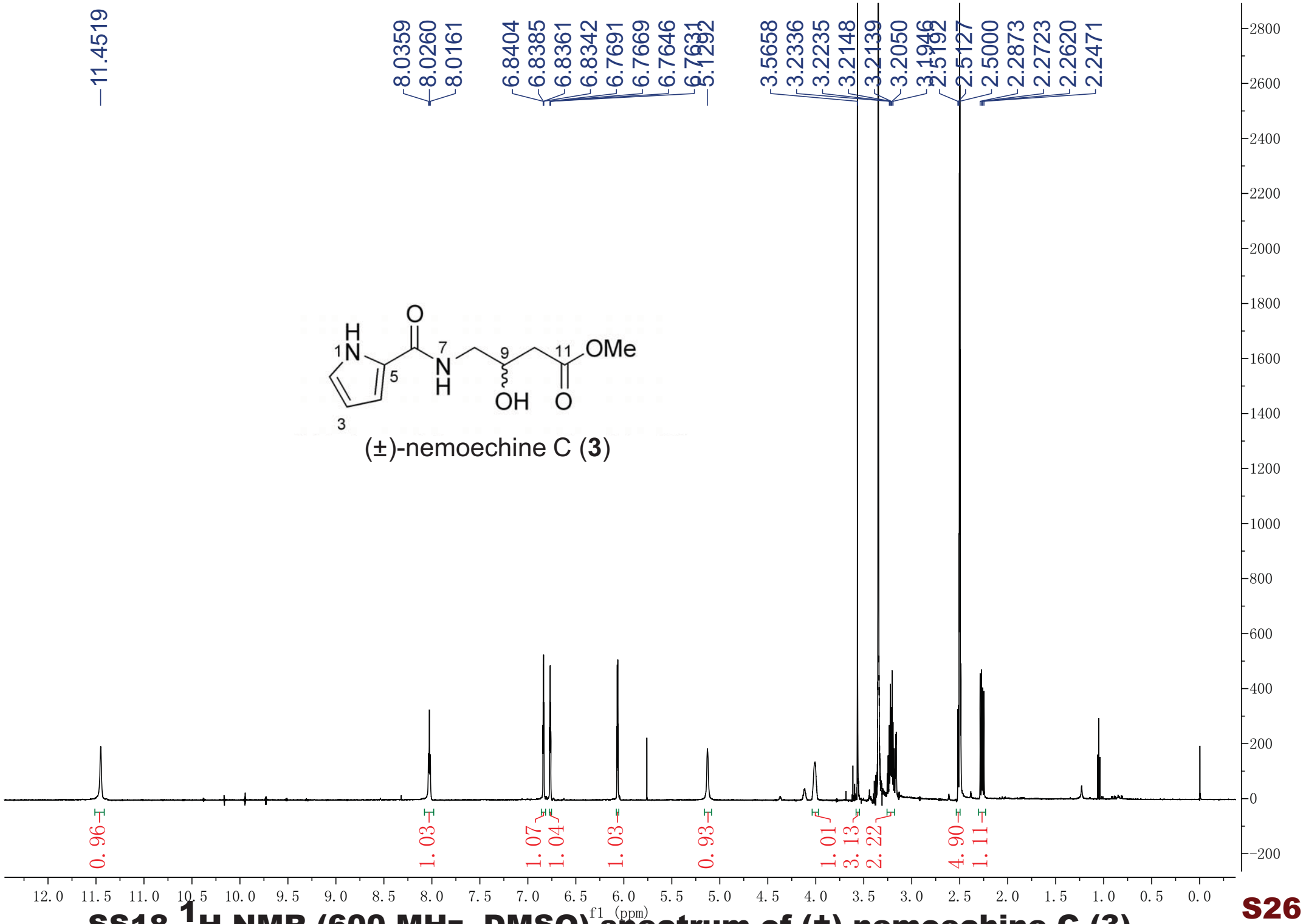
D:\MS-DATA\20131115-S5322_131115140420 11/15/2013 2:41:29 PM S5322

20131115-S5322_131115140420 #28-30 RT: 0.68-0.73 AV: 3 NL: 3.07E7
T: FTMS + p ESI Full ms [100.00-1500.00]



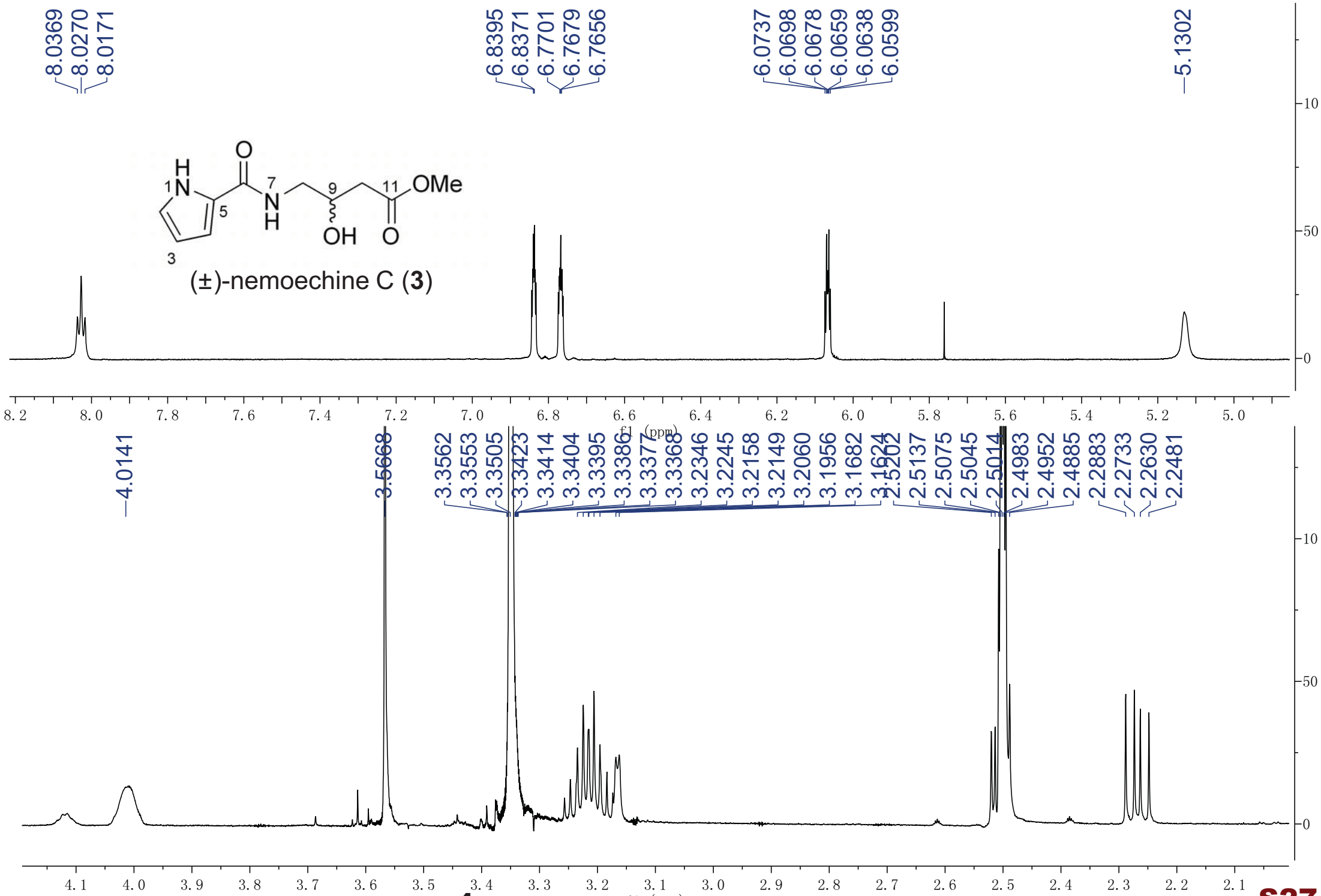
(±)-nemoechine C (**3**)

SS17 The positive HRESIMS spectrum of (±)-nemoechine C (3)

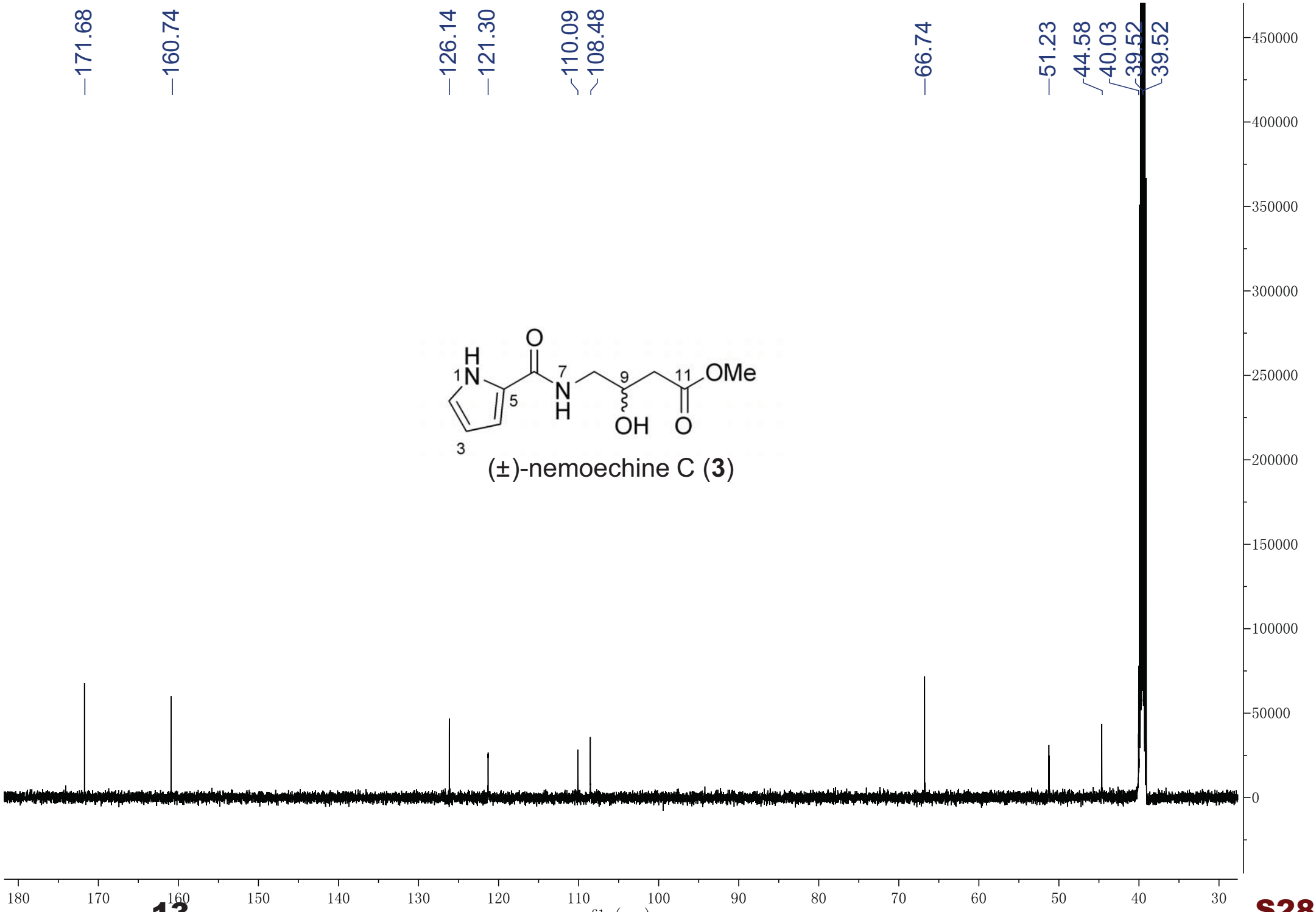


(±)-nemoechine C (**3**)

SS18 ^{1}H NMR (600 MHz, DMSO) spectrum of (±)-nemoechine C (3)

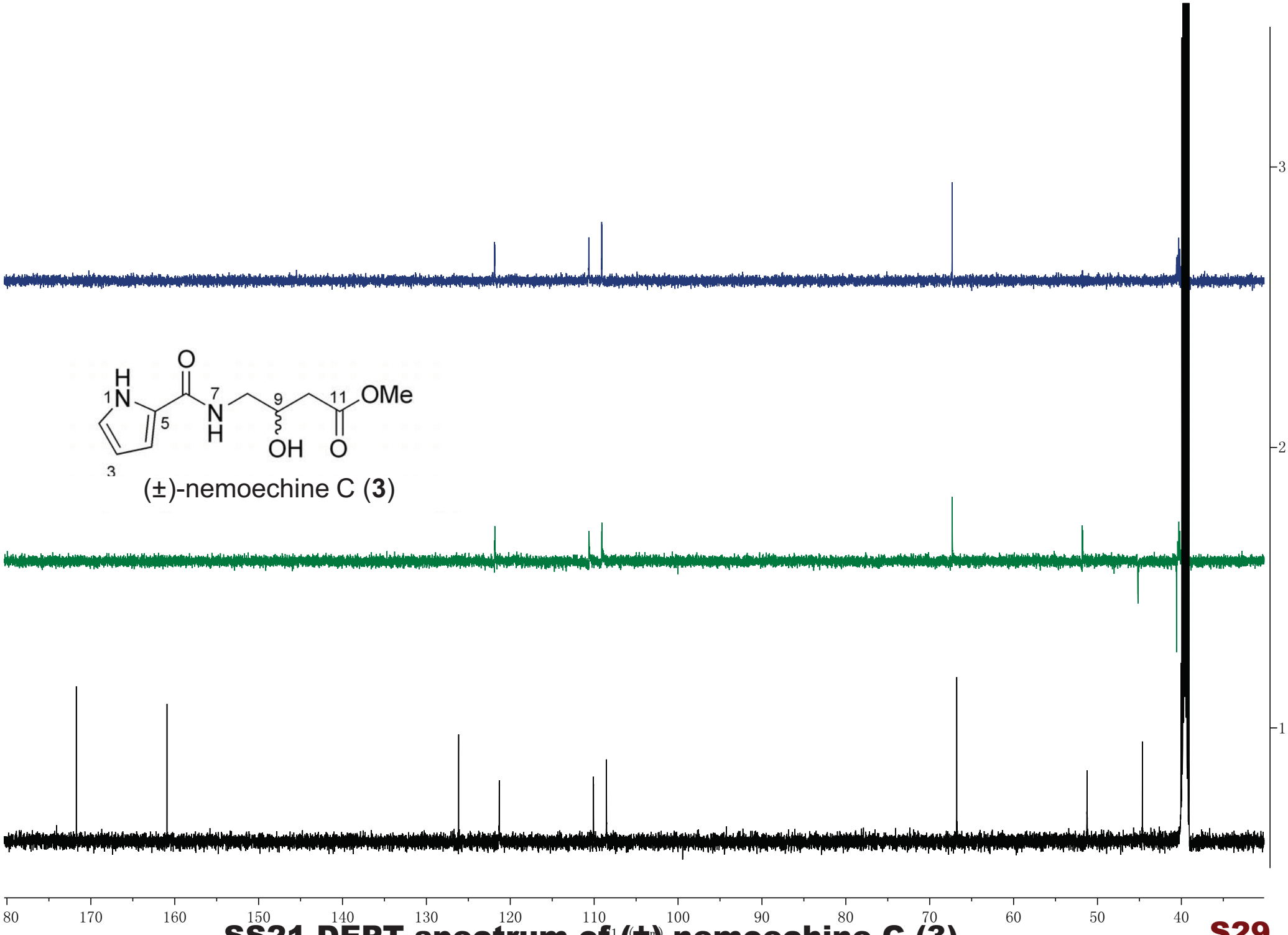


SS19 The expansion of ^{1}H NMR spectrum of (±)-nemoechine C (3)

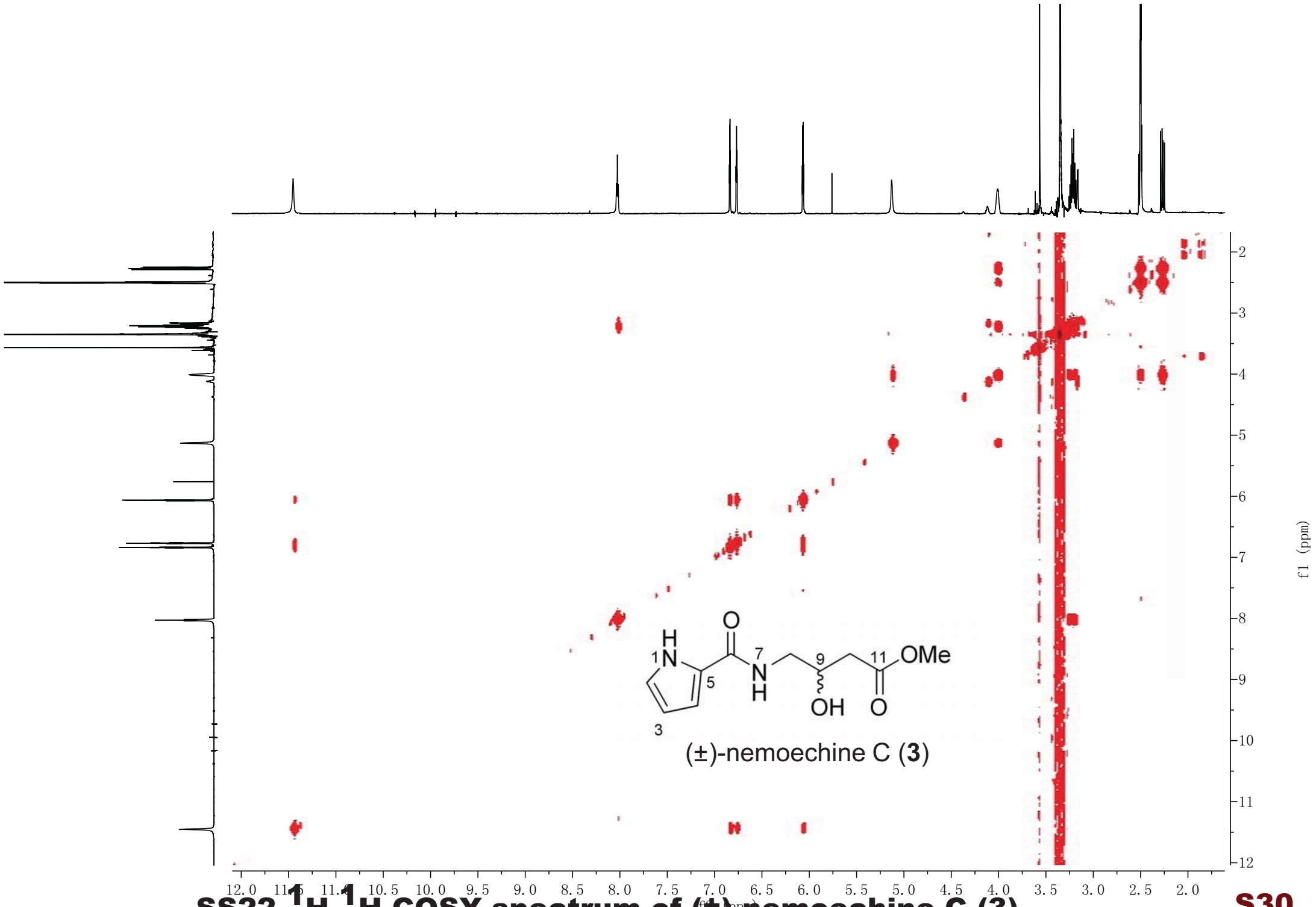


(±)-nemoechine C (**3**)

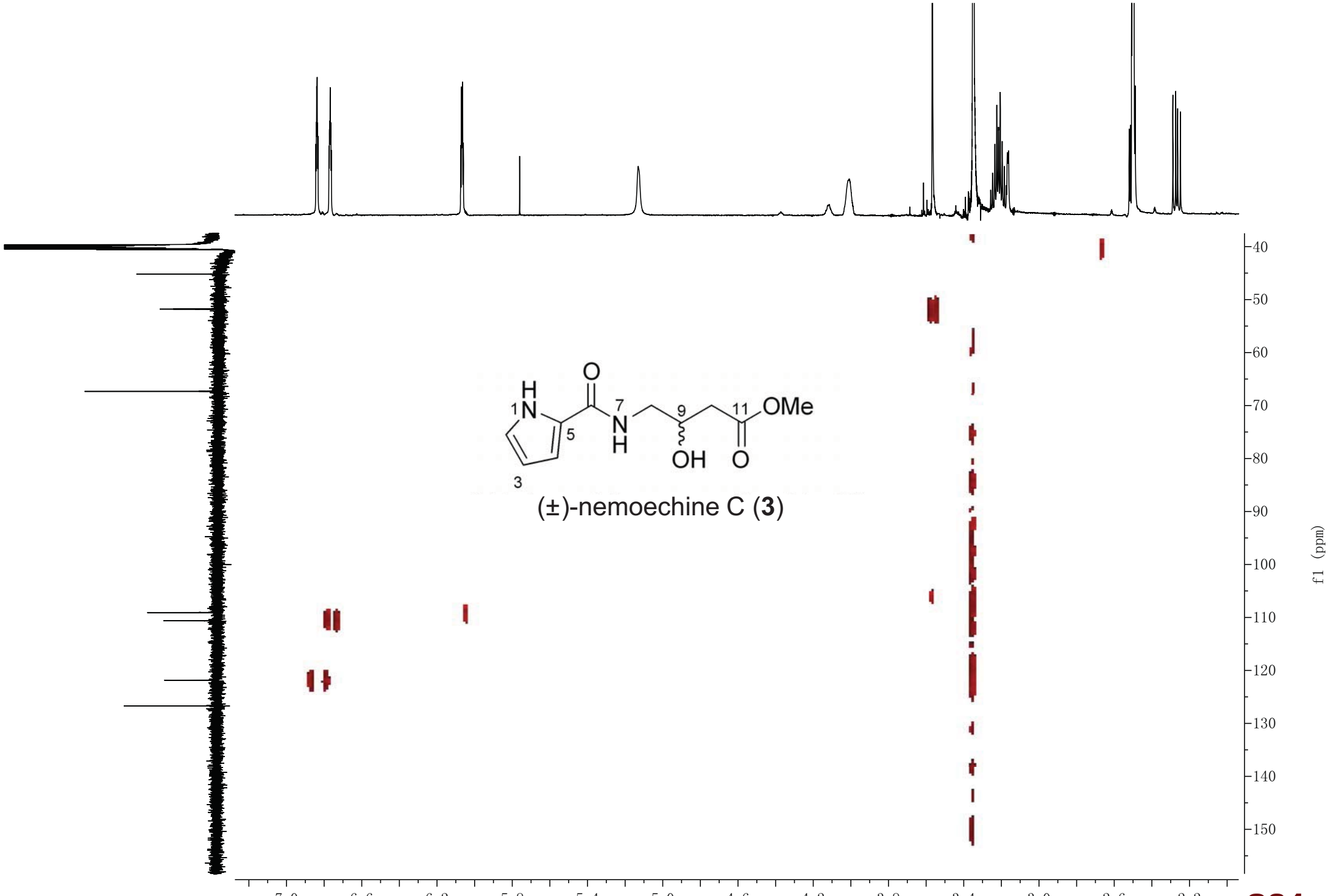
SS20 ^{13}C NMR (150 MHz, DMSO) spectrum of (±)-nemoechine C (3)



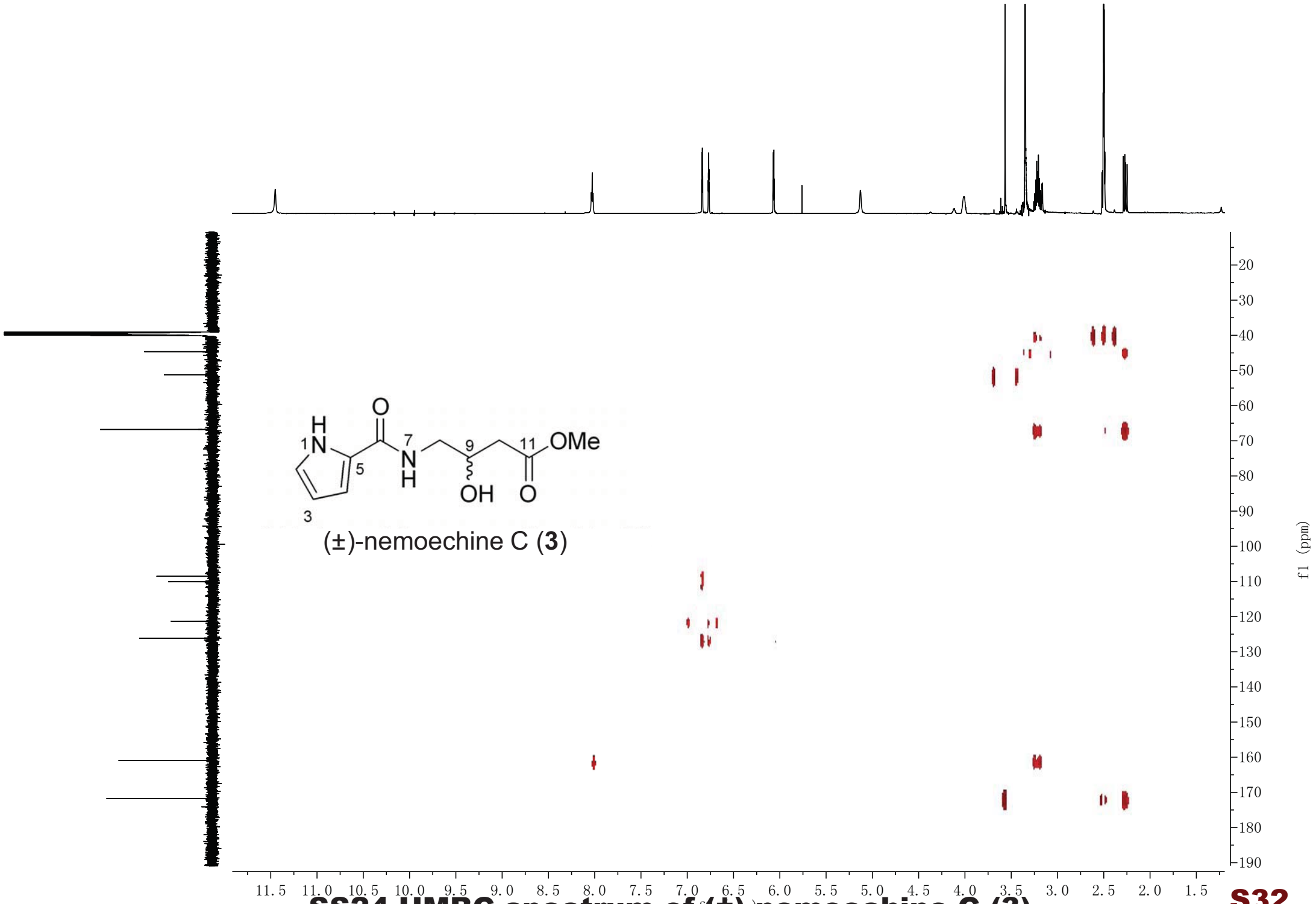
SS21 DEPT spectrum of (±)-nemoechine C (3)



SS22 ^{1}H-^{1}H COSY spectrum of (±)-nemoechine C (3)



SS23 HMQC spectrum of (±)-nemoechine C (3)

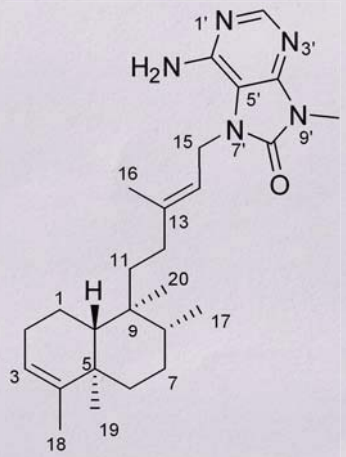


SS24 HMBC spectrum of (±)-nemoechine C (3)

D:\MS-DATA\20131115-S51322_131115140420 11/15/2013 2:10:40 PM S51322

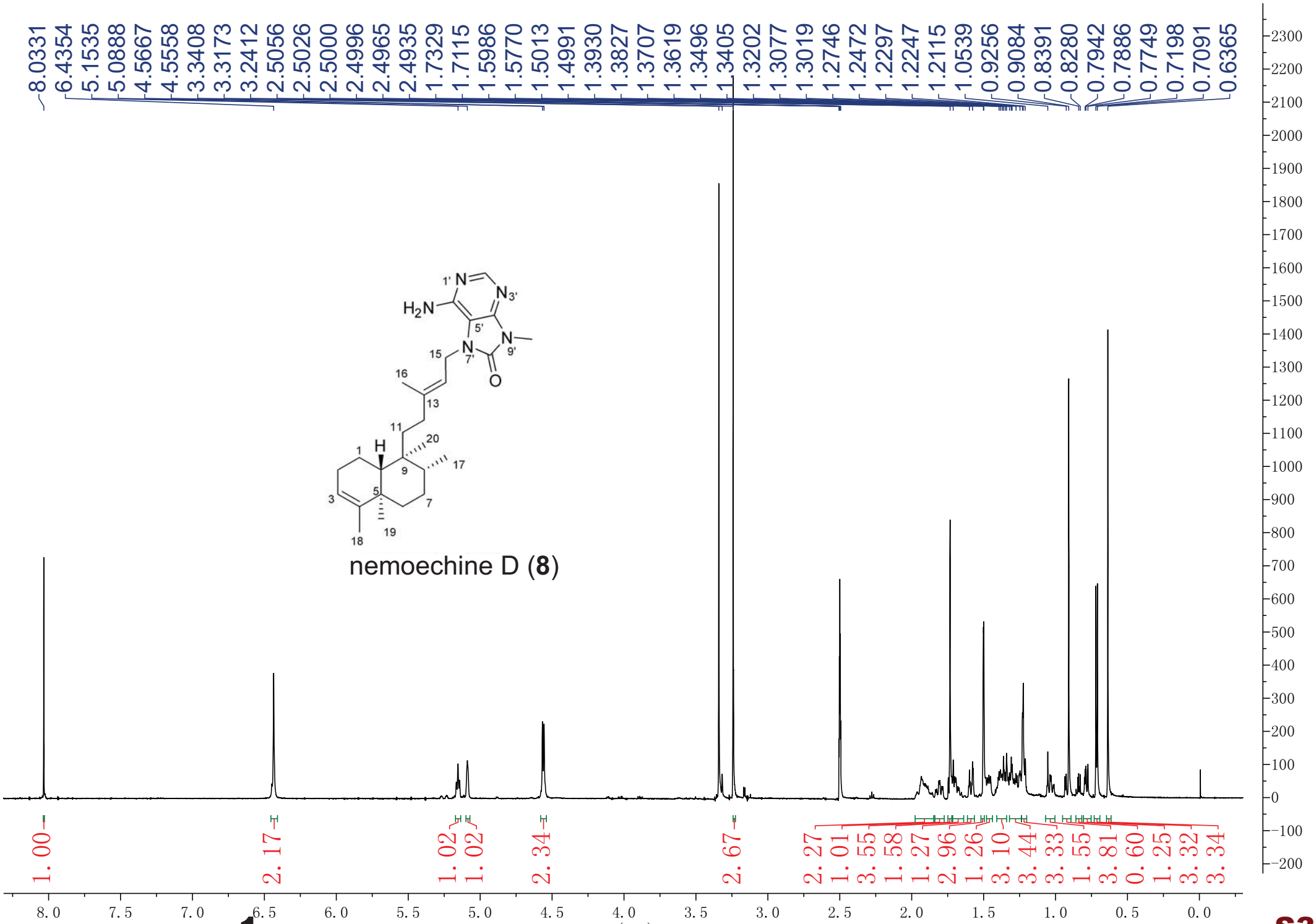
20131115-S51322_131115140420 #32-33 RT: 0.78-0.81 AV: 2 NL: 5.05E7
T: FTMS + p ESI Full ms [100.00-1500.00]

438.3239
$C_{26}H_{40}ON_5$ = 438.3227
2.6379 ppm

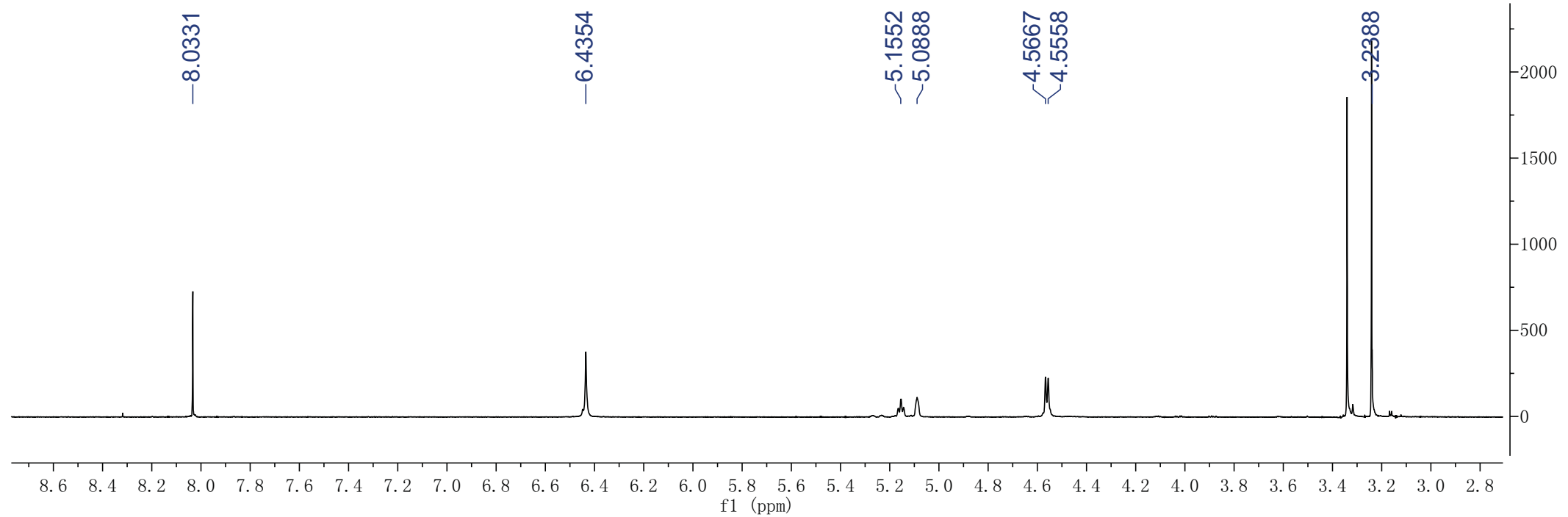


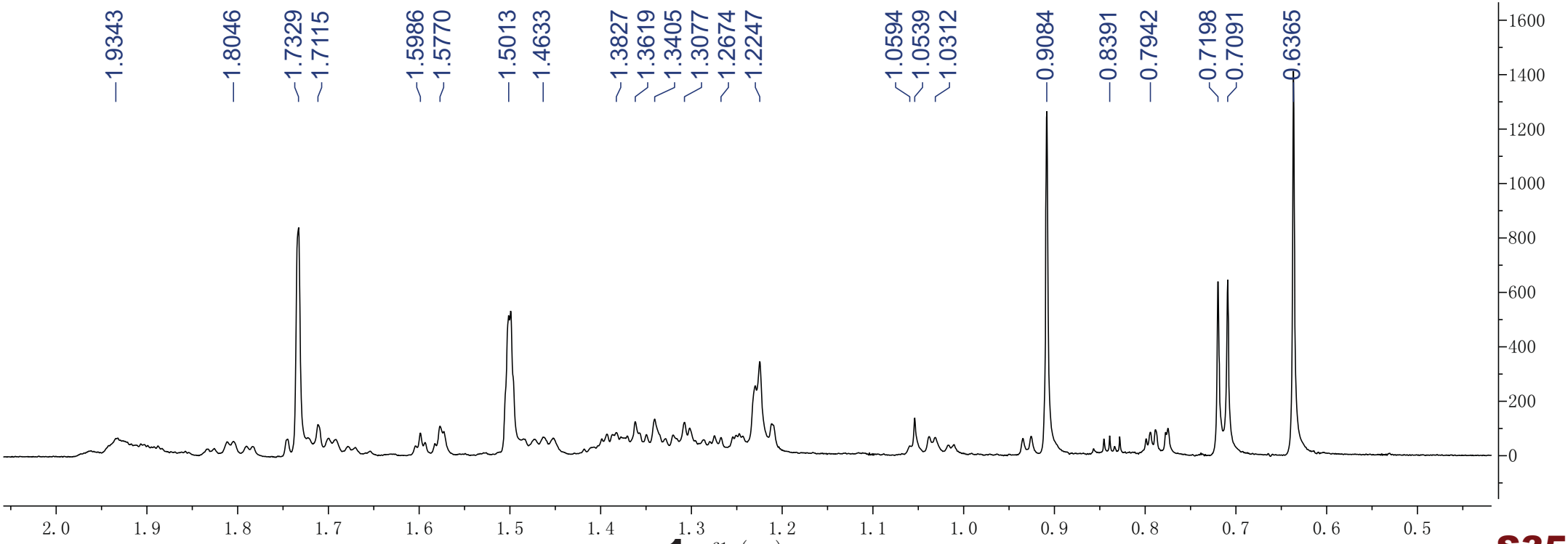
nemoechine D (**8**)

SS25 The positive HRESIMS spectrum of nemoechine D (8)

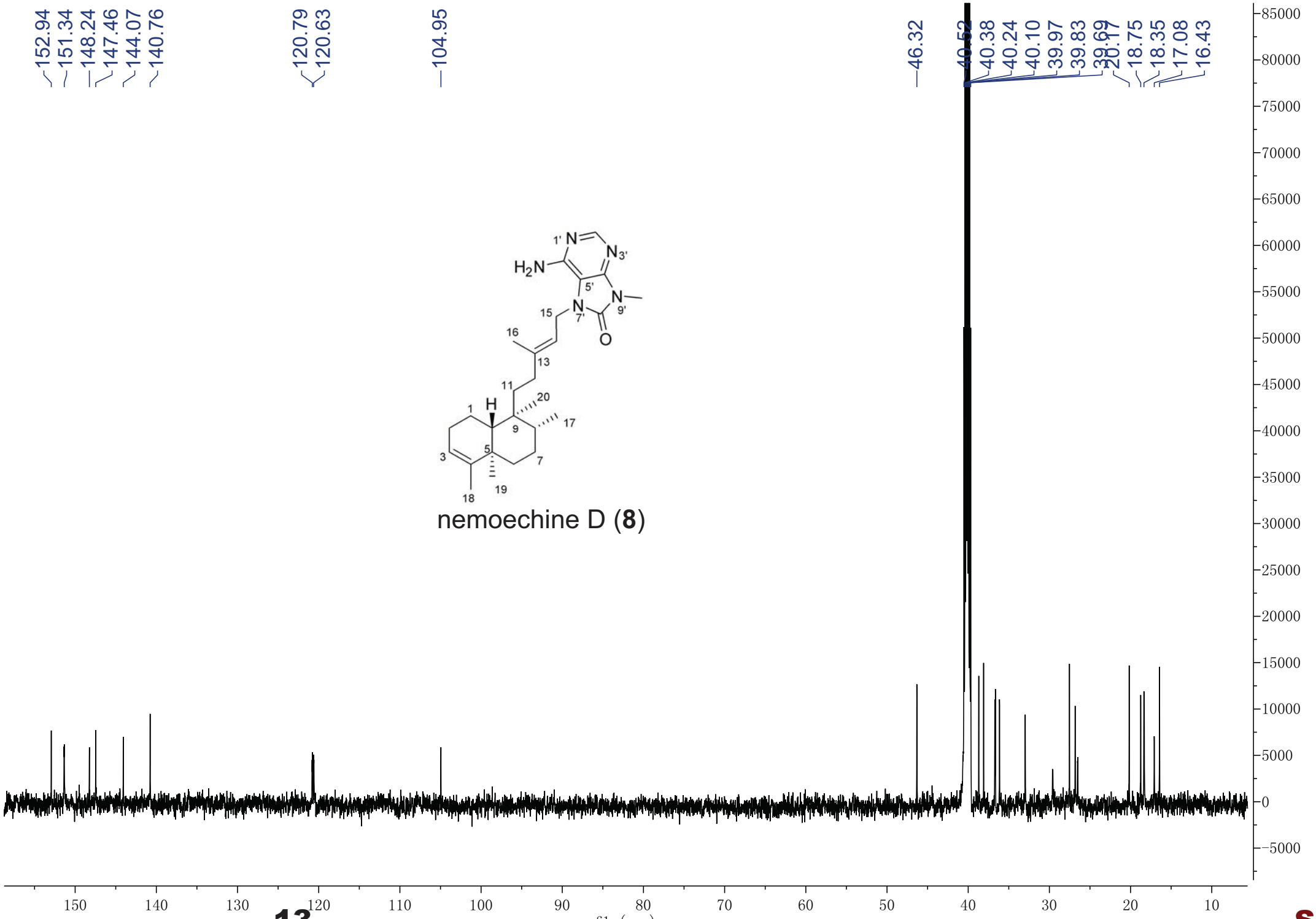


SS26 ^{1}H NMR (600 MHz, DMSO) spectrum of nemoechine D (8)

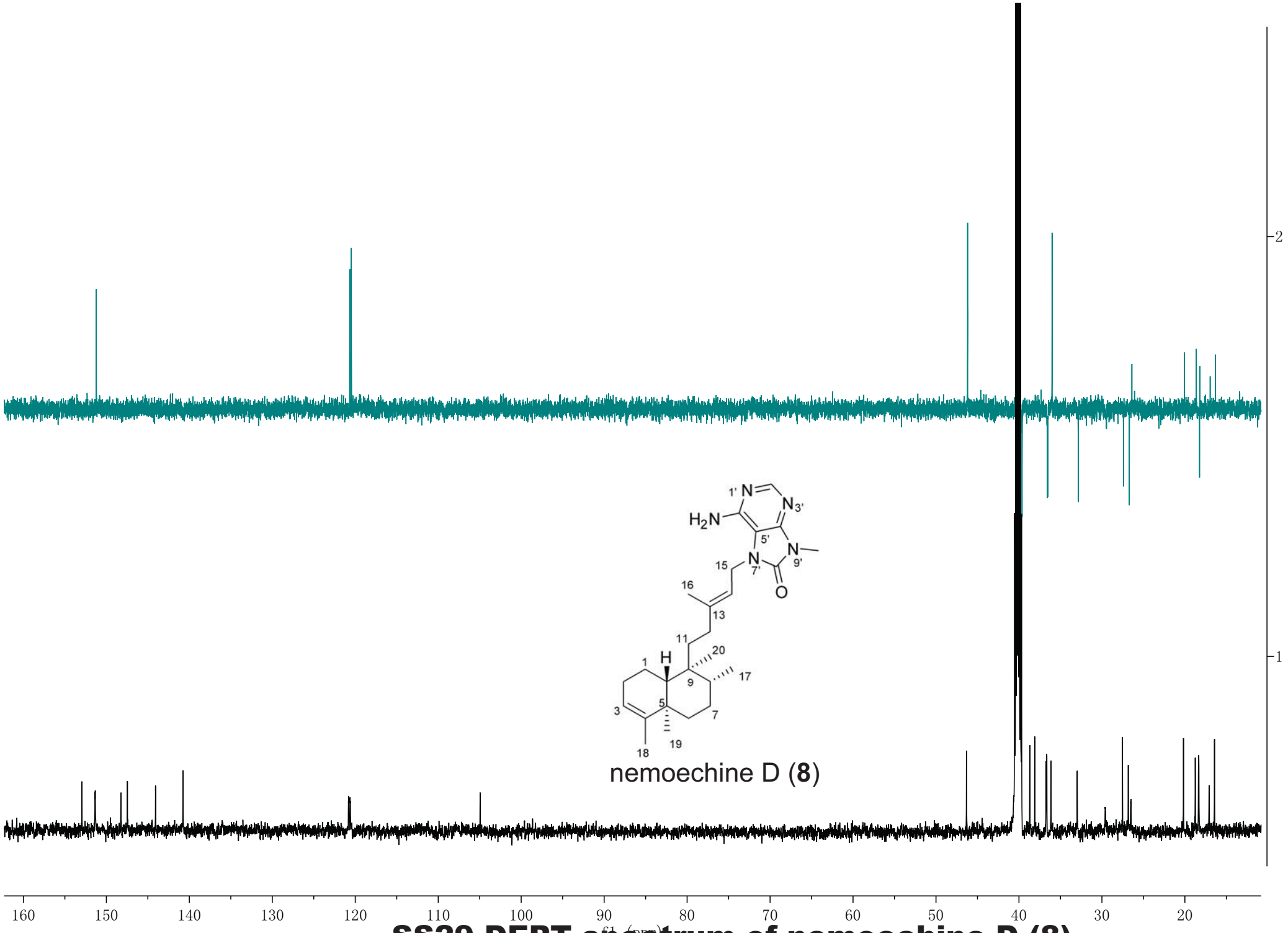




SS27 The expansion of ^{1}H NMR spectrum of nemoechine D (8)

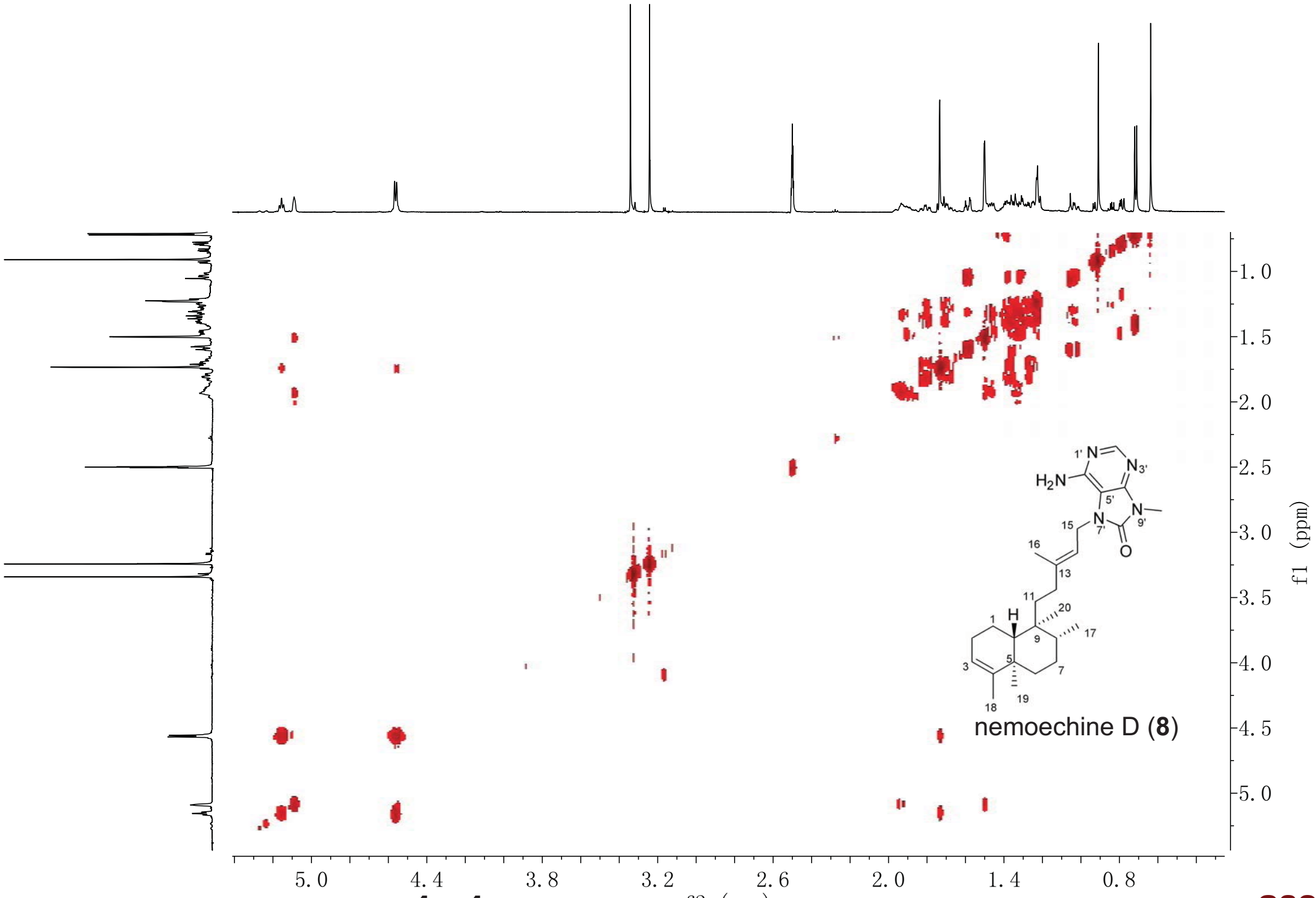


SS28 ^{13}C NMR (150 MHz, DMSO) spectrum of nemoechine D (8)

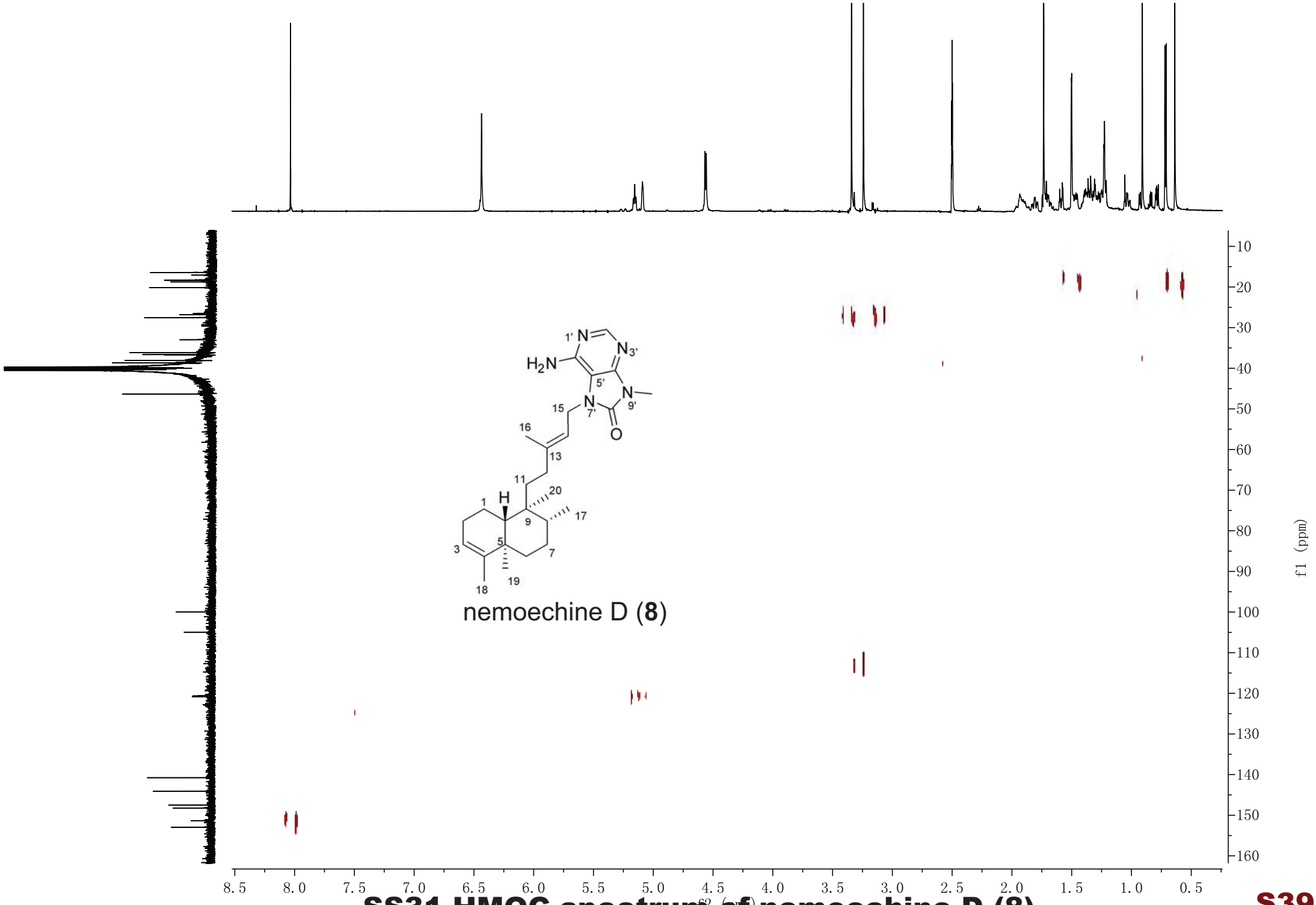


nemoechine D (**8**)

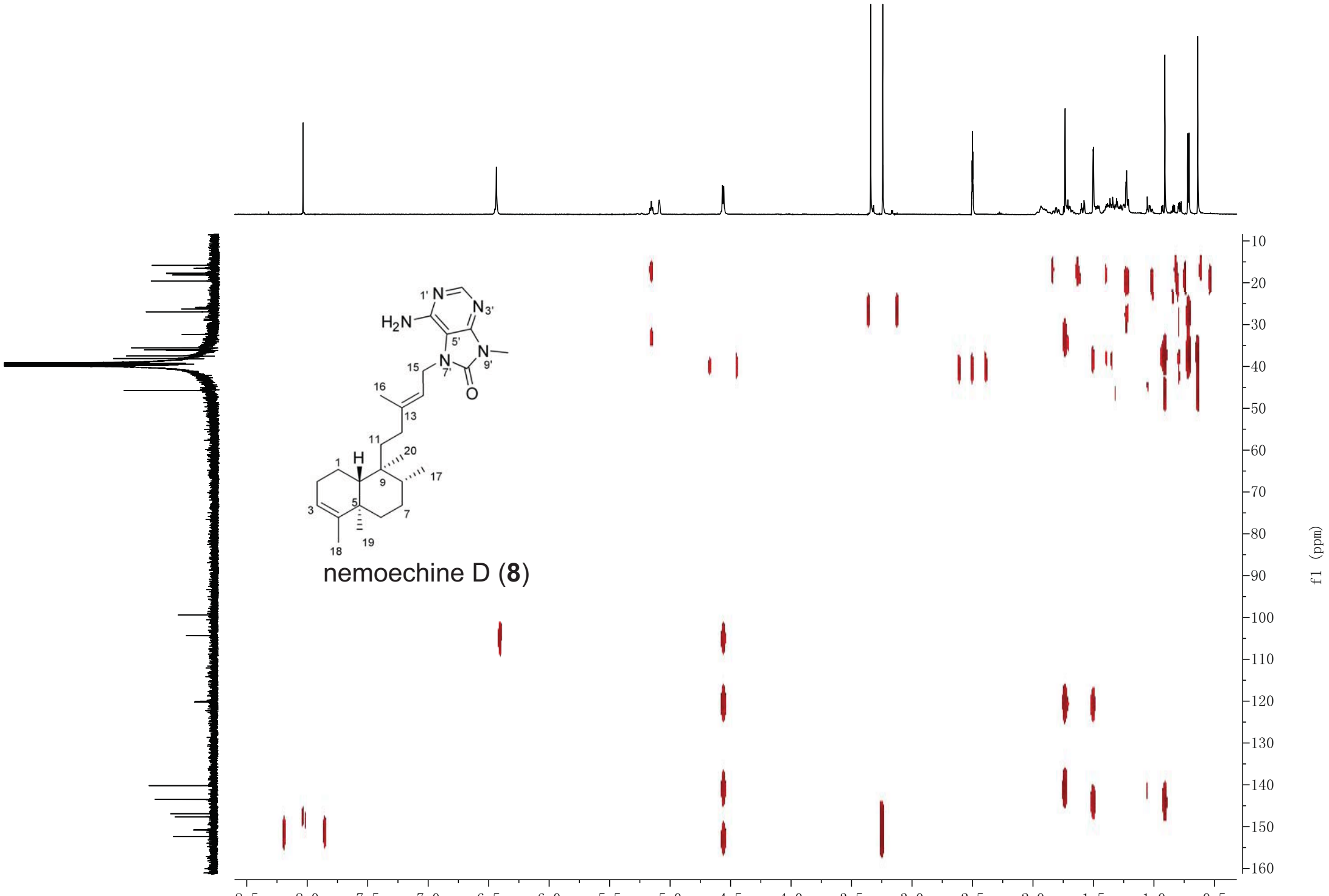
SS29 DEPT spectrum of nemoechine D (8)



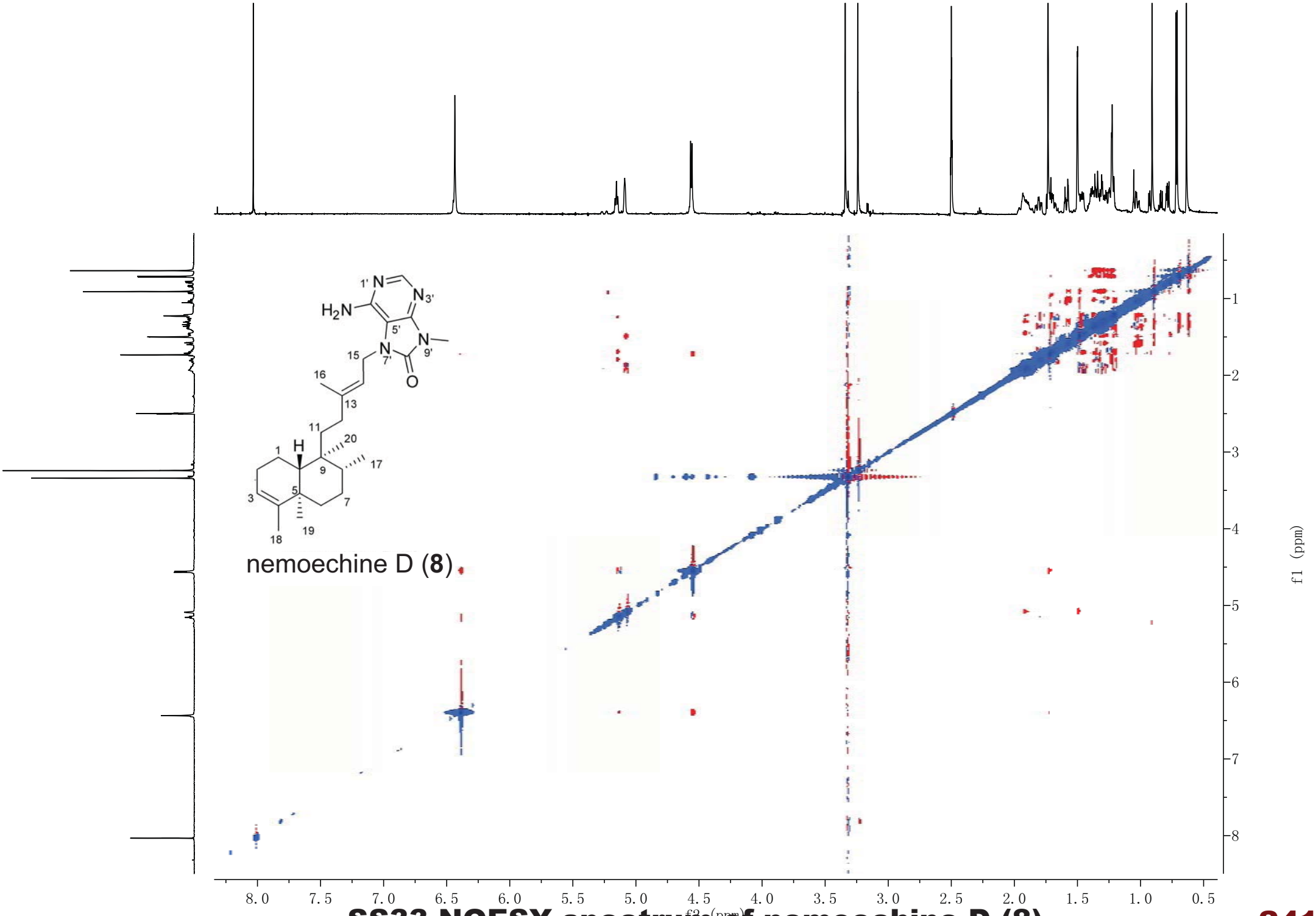
SS30 ^{1}H-^{1}H COSY spectrum of nemoechine D (8)



SS31 HMQC spectrum of nemoechine D (8)



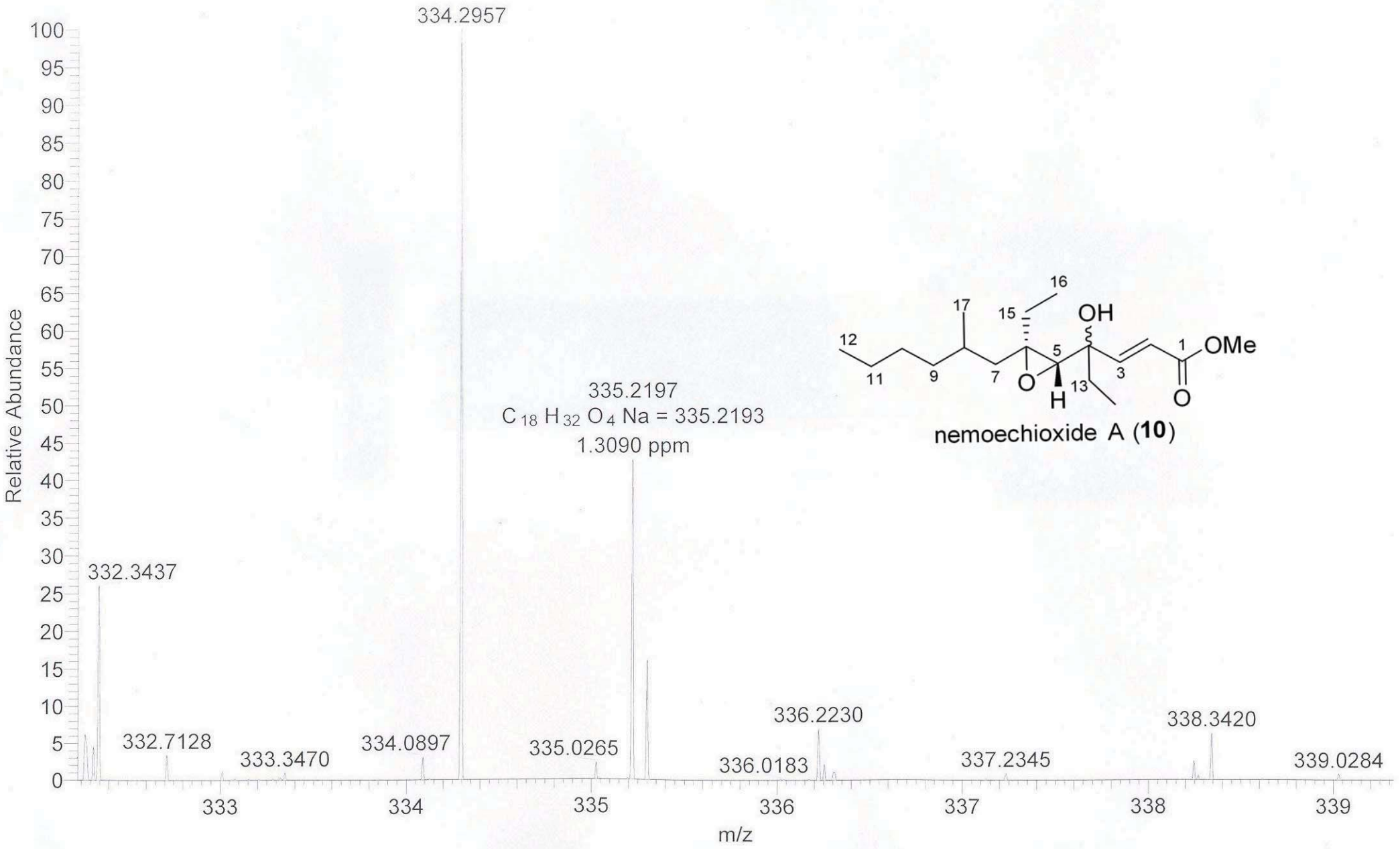
SS32 HMBC spectrum of nemoechine D (8)



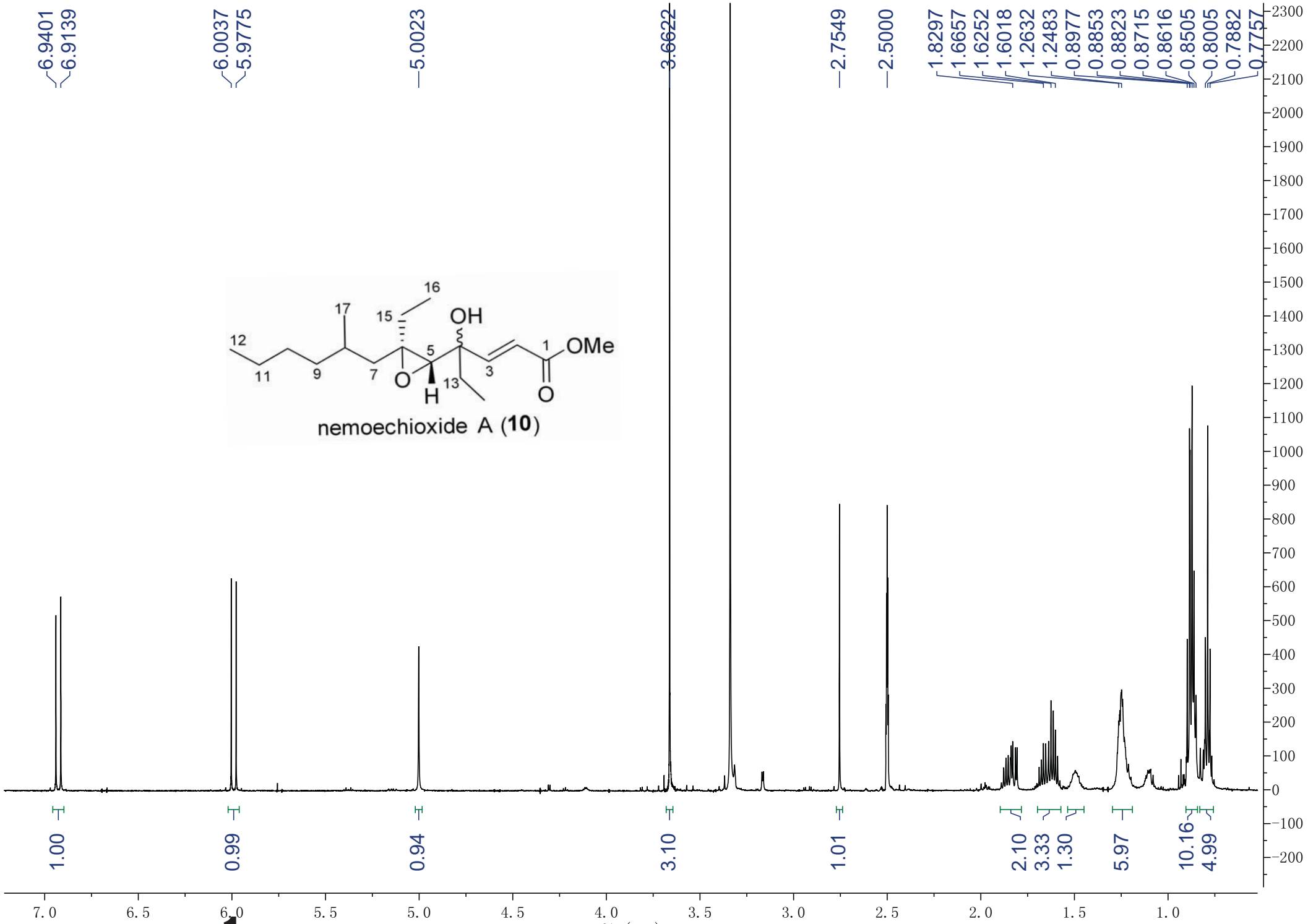
SS33 NOESY spectrum of nemoechine D (8)

20140526-S2-2-1-2-1_140520145817 5/26/2014 3:06:32 PM S2-2-1-2-1

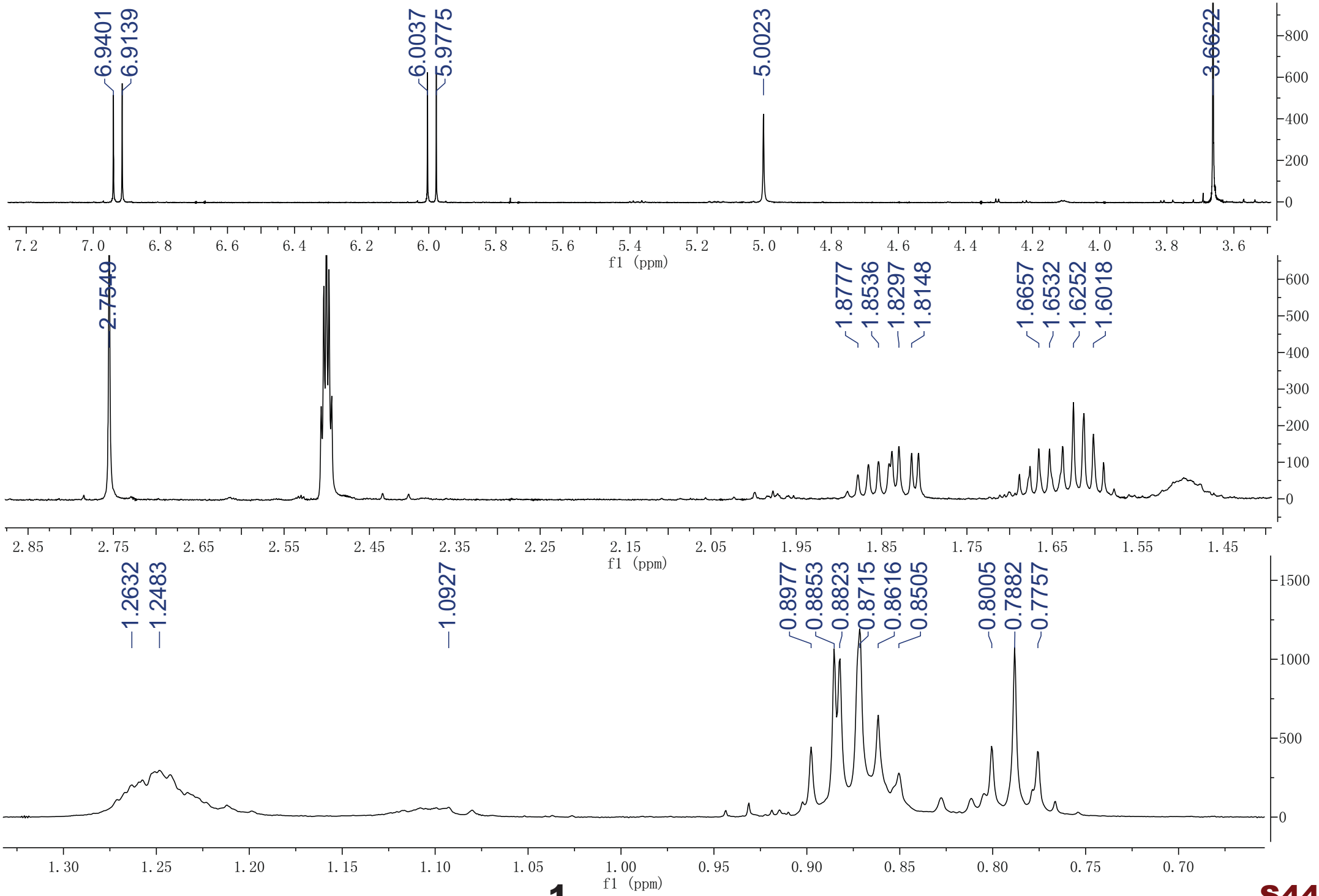
20140526-S2-2-1-2-1_140520145817 #31-40 RT: 0.73-0.95 AV: 10 NL: 6.42E5
T: FTMS + p ESI Full ms [150.00-2000.00]



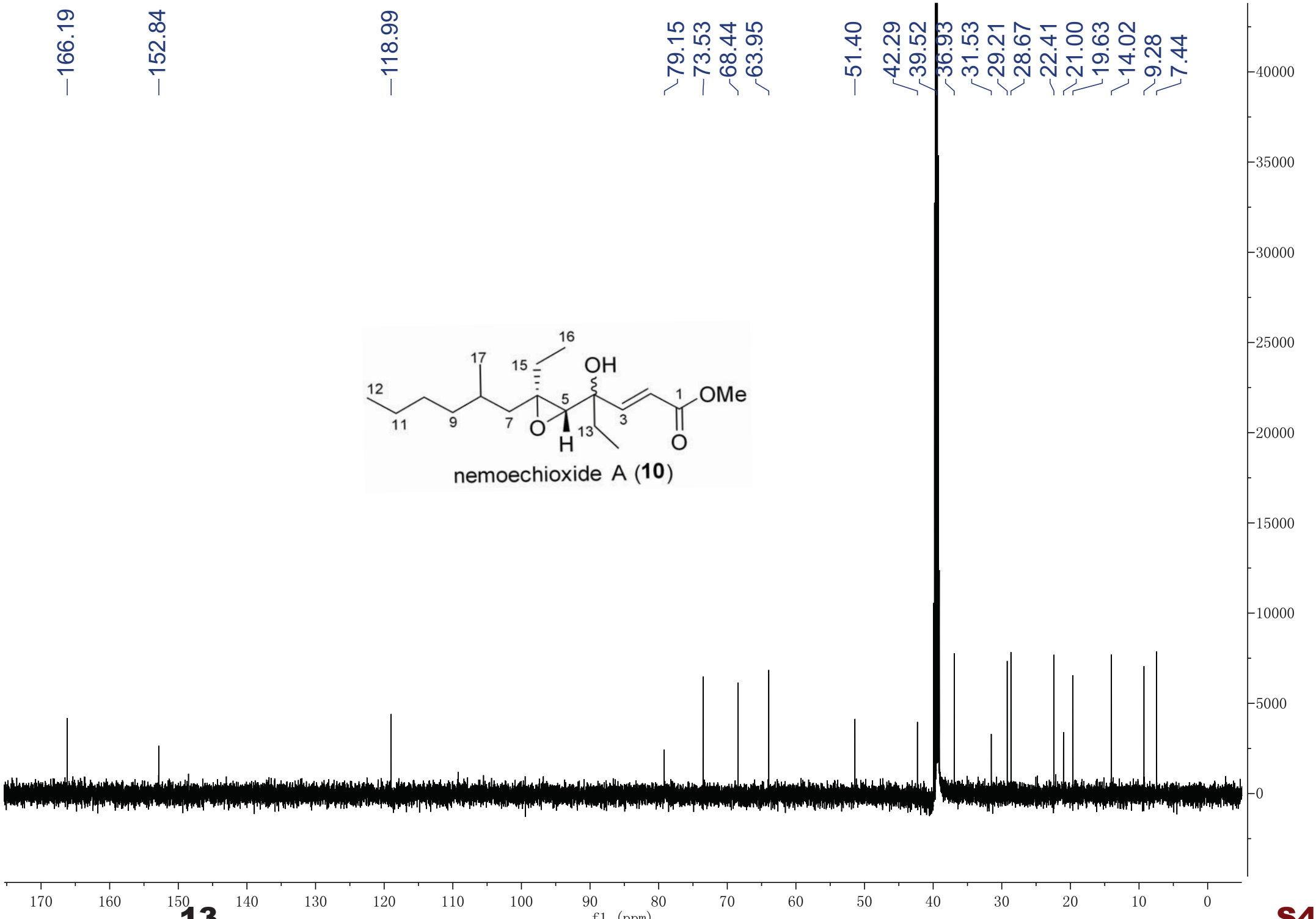
SS34 The positive HRESIMS spectrum of nemoechioxide A (10)



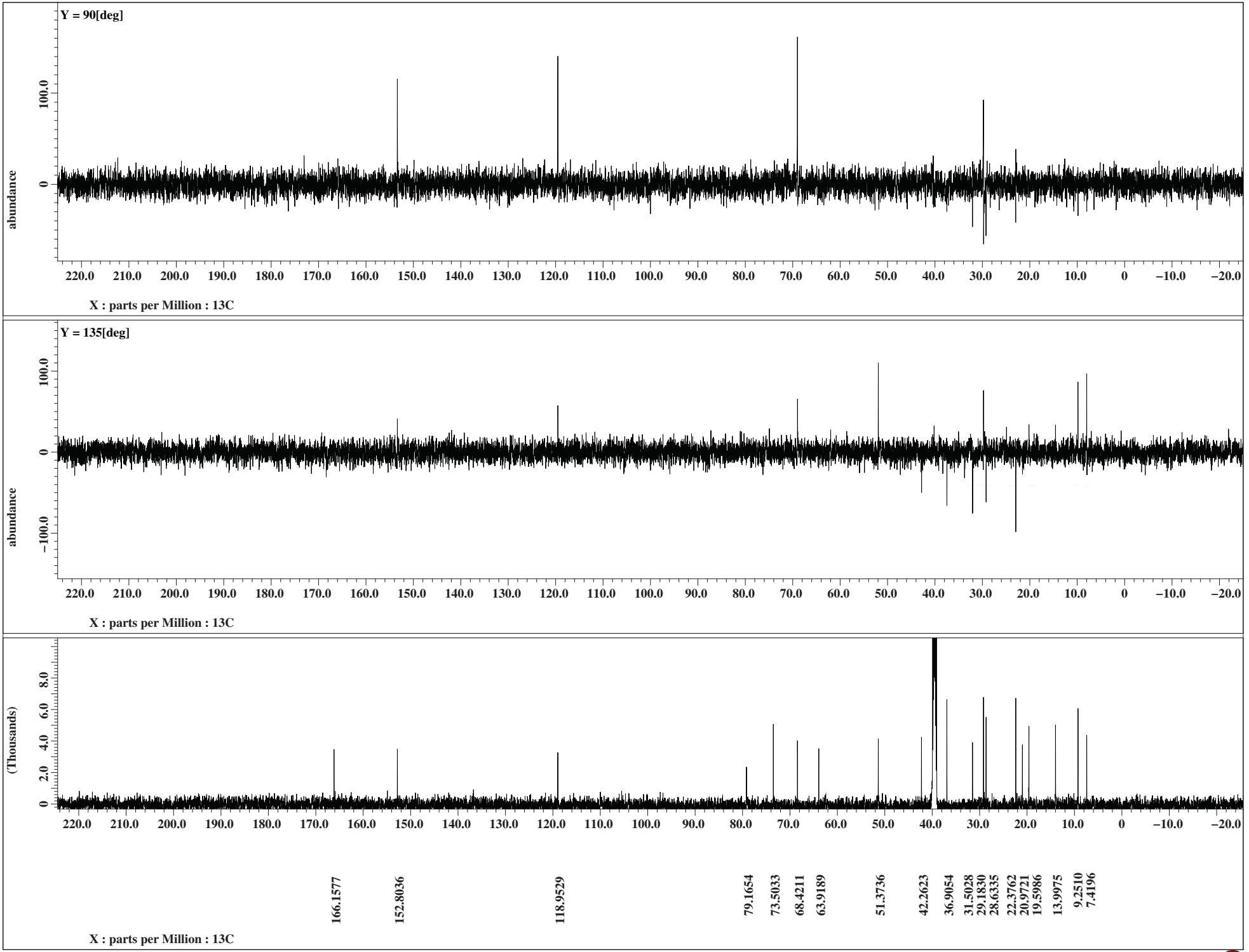
SS35 ^{1}H NMR (600 MHz, DMSO) spectrum of nemoechioxide A (10)



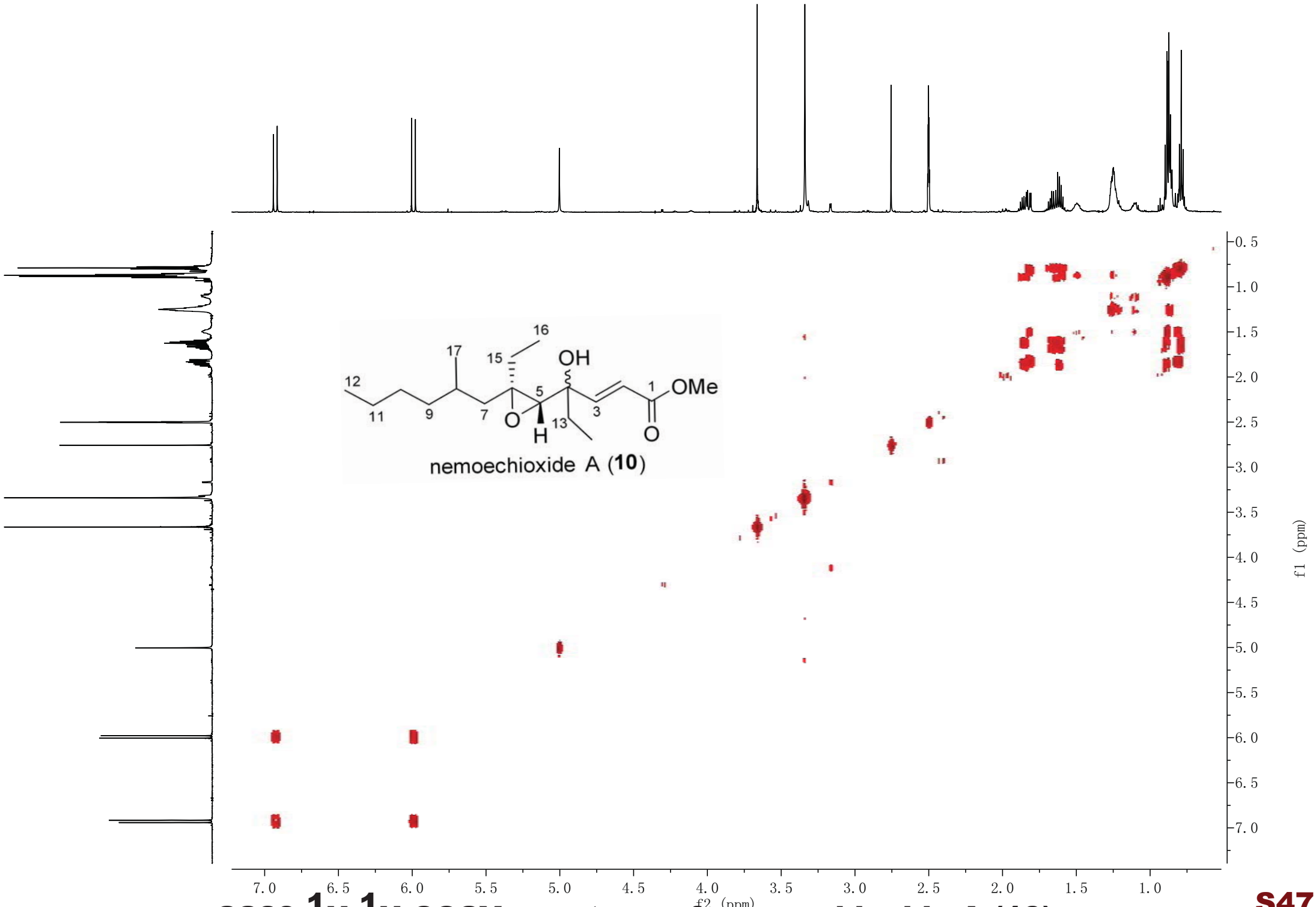
SS36 The expansion of ^{1}H NMR spectrum of nemoechioxide A (10)



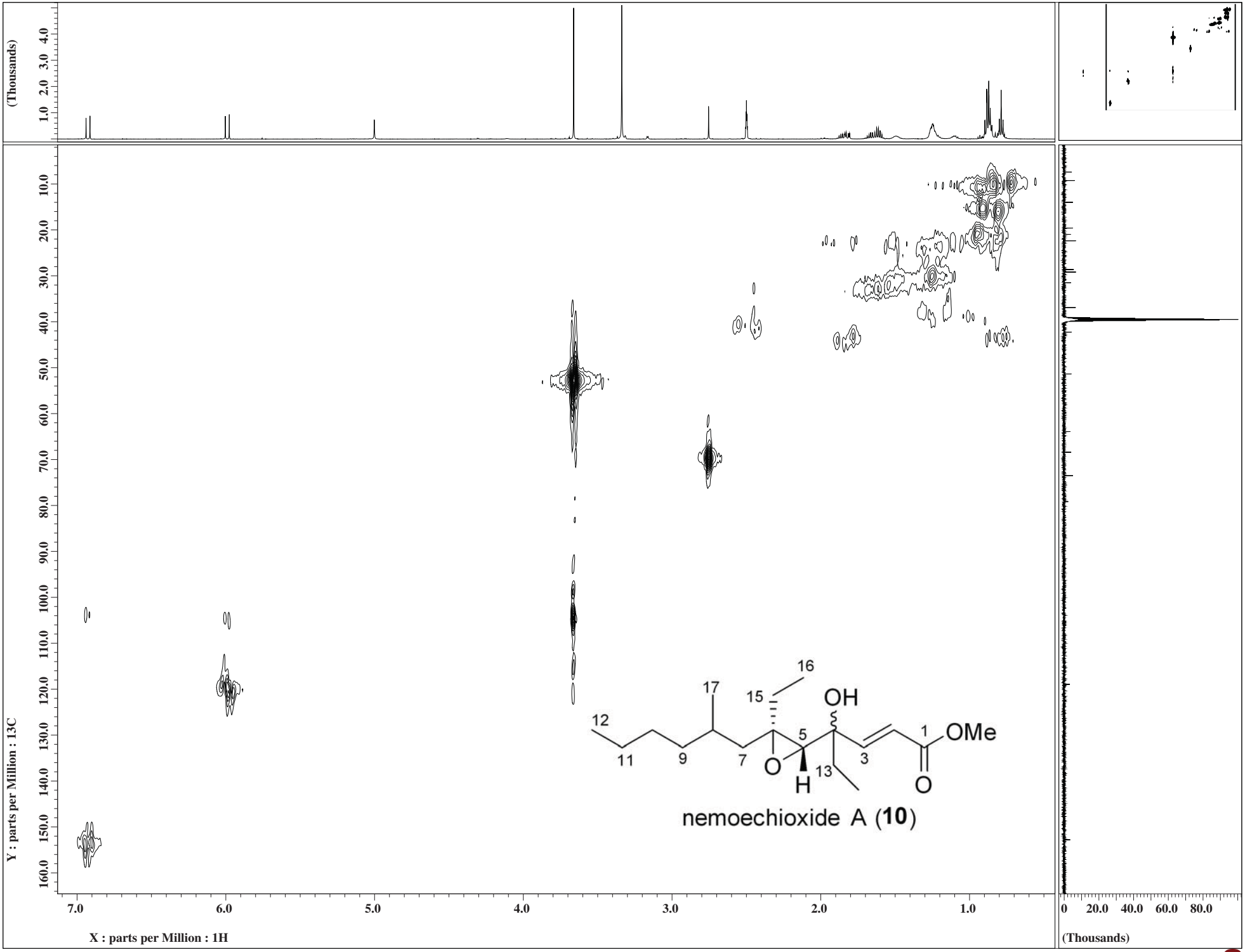
SS37 ^{13}C NMR (150 MHz, DMSO) spectrum of nemoechioxide A (10)



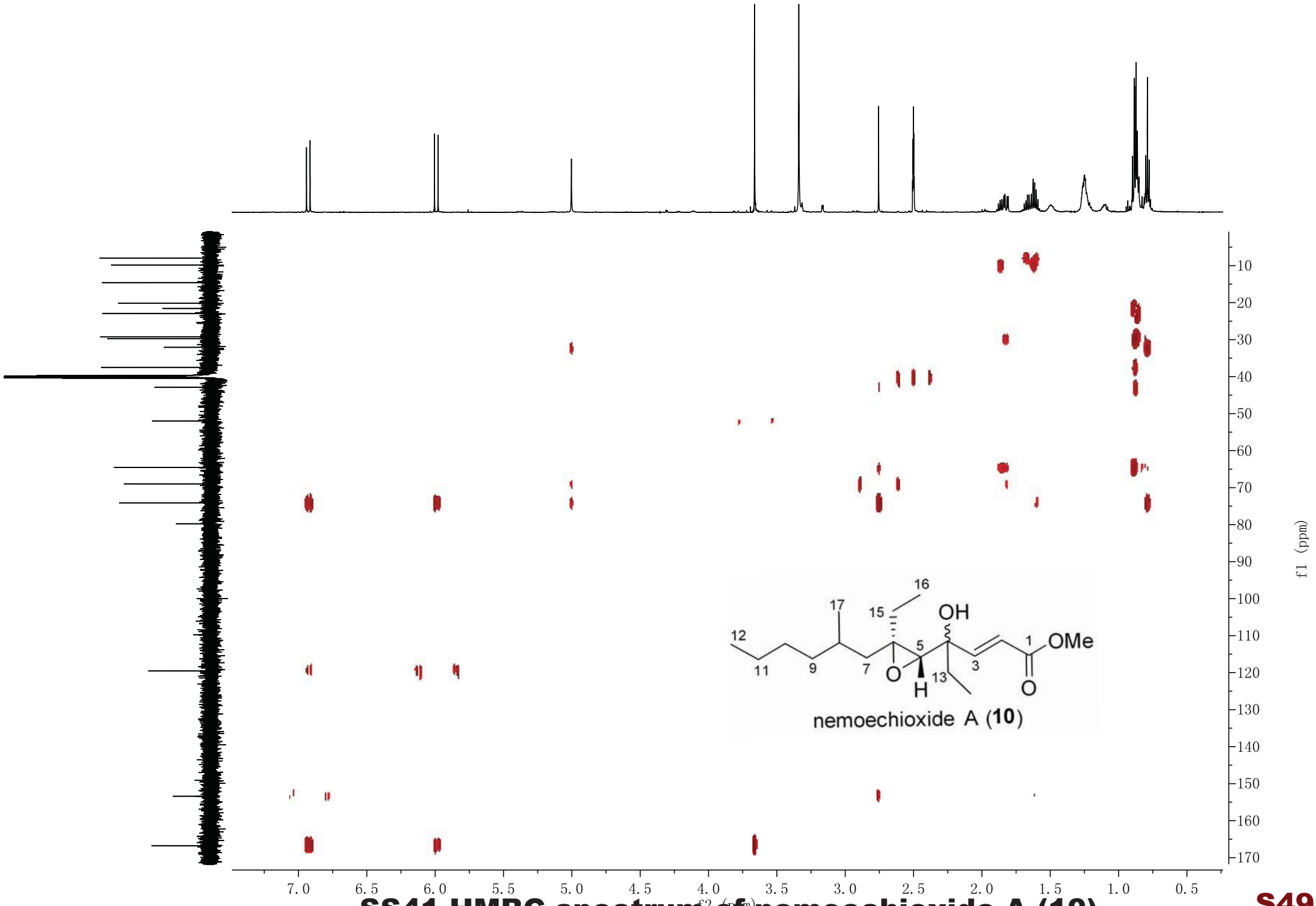
SS38 DEPT spectrum of nemoechioxide A (10)



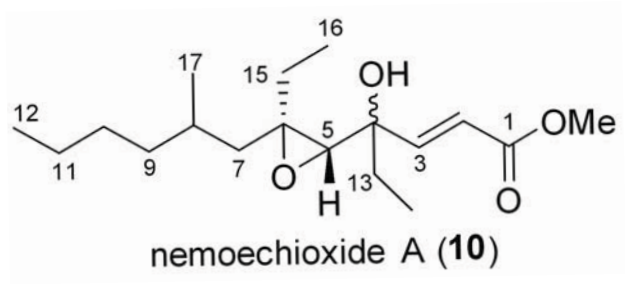
SS39 ^{1}H-^{1}H COSY spectrum of nemoechioxide A (10)



SS40 HMQC spectrum of nemoechioxide A (10)



SS41 HMBC spectrum of nemoechioxide A (10)



nemoechioxide A (**10**)

H-3
H-2
4-OH
H-5
Ha-15
Hb-15,
H_2-13
H_3-12,
H_3-16,
H_3-17,
H_3-14

7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5

f1 (ppm)

SS42 1D NOE differential spectrum of nemoechioxide A (10)