Supplementary Information

New protein tyrosine phosphatase inhibitors from fungus *Aspergillus gorakhpurensis* F07ZB1707†

Yannan Ji [a], Qiqi Zhou [a], Guosheng Liu [a], Tianhui Zhu [a], Yufang Wang [a], Yan Fu [a], Yeying Li [b], Ruolan Li [b], Xuexia Zhang [b], Mei Dong [c], Françoise Sauriol [d], Yucheng Gu [e], Qingwen Shi *[, a, c], Xinhua Lu*[,b] and Zhiyu Ni*[, f]

[a]*School of Pharmaceutical Sciences, Hebei Medical University, Shijiazhuang 050017, China; jiyannan@yeah.net (Y.J.); chuxinzqq@163.com (Q.Z.); lgs199504@163.com (G.L.); tian_hui_zhu@126.com (T.Z.); wang-yu-fang@163.com (Y.W.); fuyan0228@hebmu.edu.cn (Y.F.)*

[b]*New Drug Research & Development Center of North China Pharmaceutical Group Corporation, National Microbial Medicine Engineering & Research Center, Hebei Industry Microbial Metabolic Engineering & Technology Research Center, Key Laboratory for New Drug Screening Technology of Shijiazhuang City, Shijiazhuang 050015, China; li_yeying@sohu.com (Y.L.); liruolan2013@163.com (R.L.); zhangxuexiazxx@163.com (X.Z.)*

[c]*Hebei Key Laboratory of Forensic Medicine, and Collaborative Innovation Center of Forensic Medical Molecular Identification, Hebei Medical University, Shijiazhuang 050017, China; meimeidong11@126.com*

[d]*Department of Chemistry, Queen's University, Kingston, K7L 3N6, Canada; francoise.sauriol@chem.queensu.ca*

[e]*Syngenta Jealott's Hill International Research Centre, Bracknell, Berkshire, RG42 6EY, UK; yucheng.gu@syngenta.com*

[f]*School of Basic Medical Science, Hebei University, Baoding 071002, China; nizhiyu@hbu.edu.cn*

**Correspondence: shiqingwen405@163.com (Q.S.); luxinhua89@yeah.net (X.L.); nizhiyu@hbu.edu.cn (Z.N.); Tel.: +86-311-8626-1270 (Q.S.); +86-311-8815-2439 (X.L.); +86-312-507-9625 (Z.N.)*

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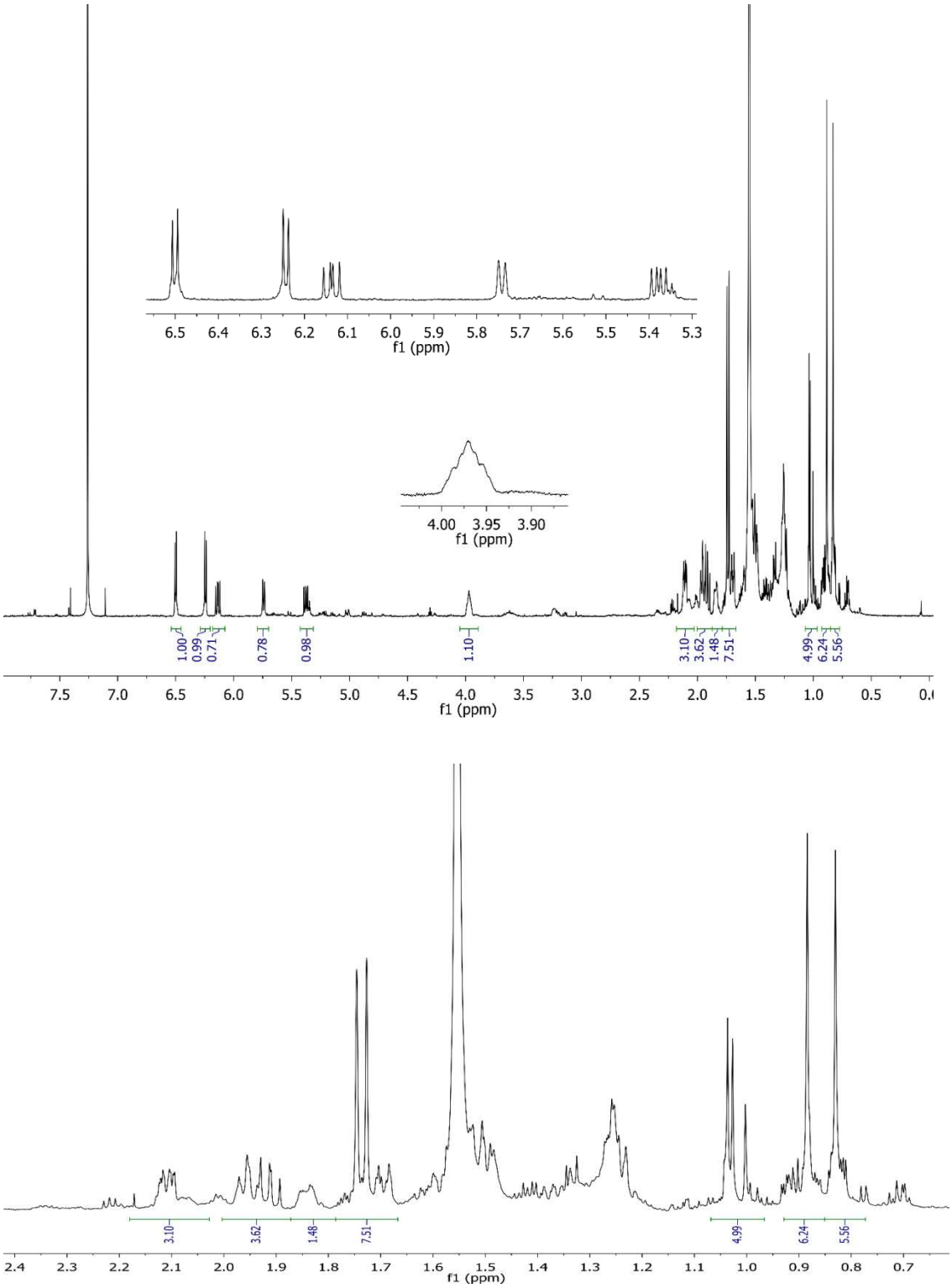
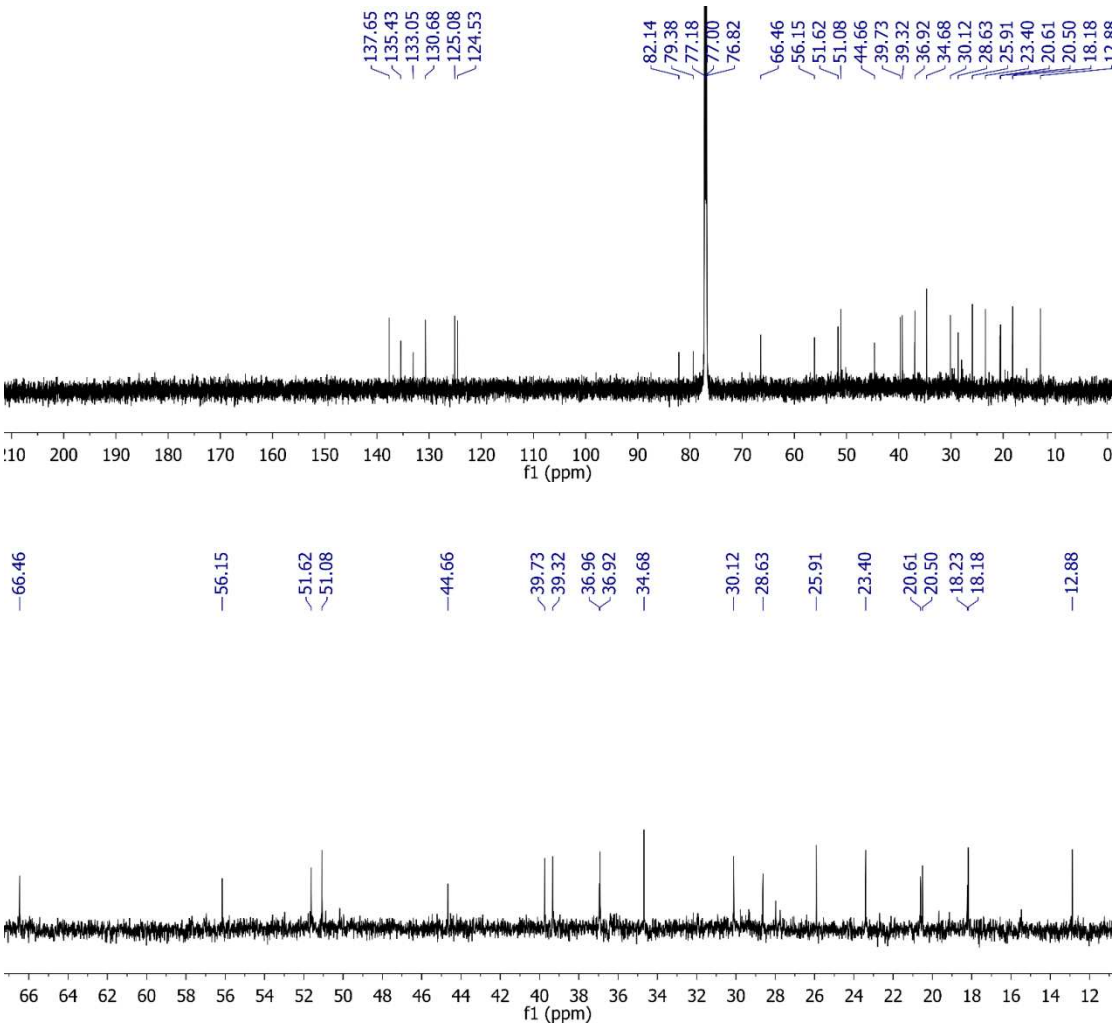
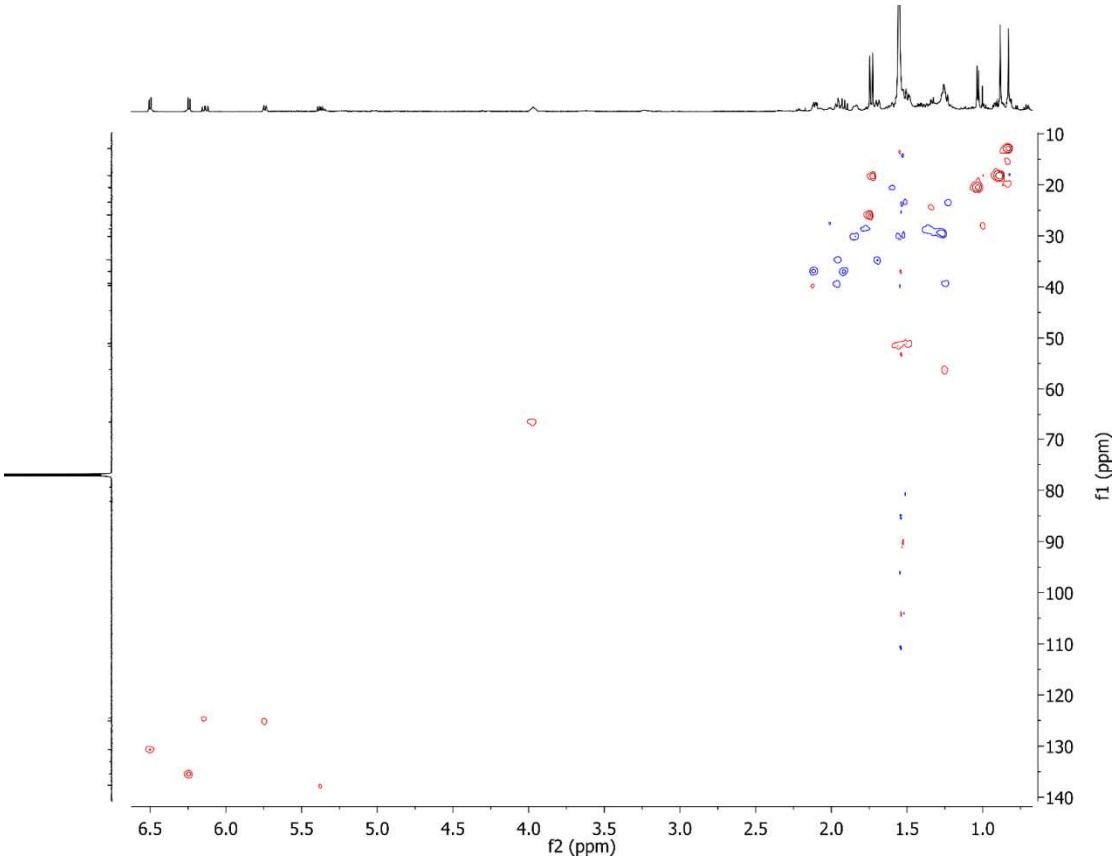
S1 ^{1}H NMR (700 MHz, $CDCl_3$) spectrum of aspergorakhins A (**1**).



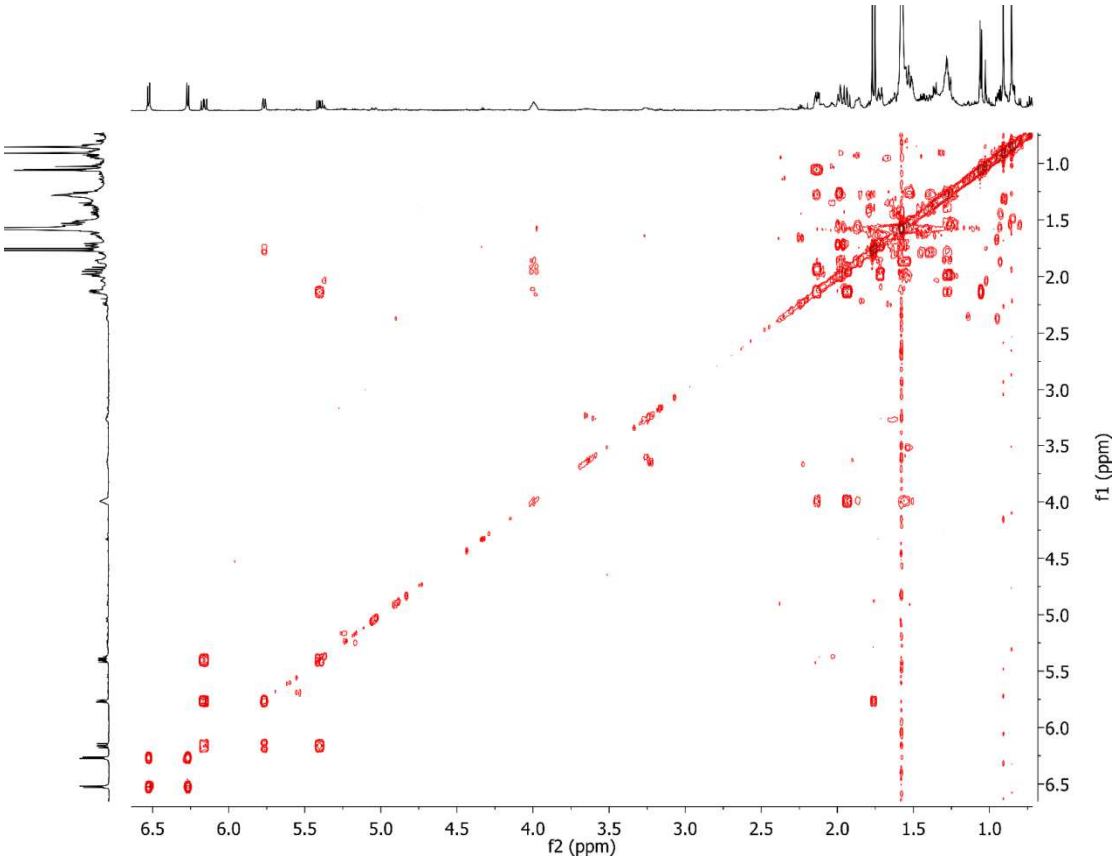
S2 ^{13}C NMR (175 MHz, $CDCl_3$) spectrum of aspergorakhins A (**1**).



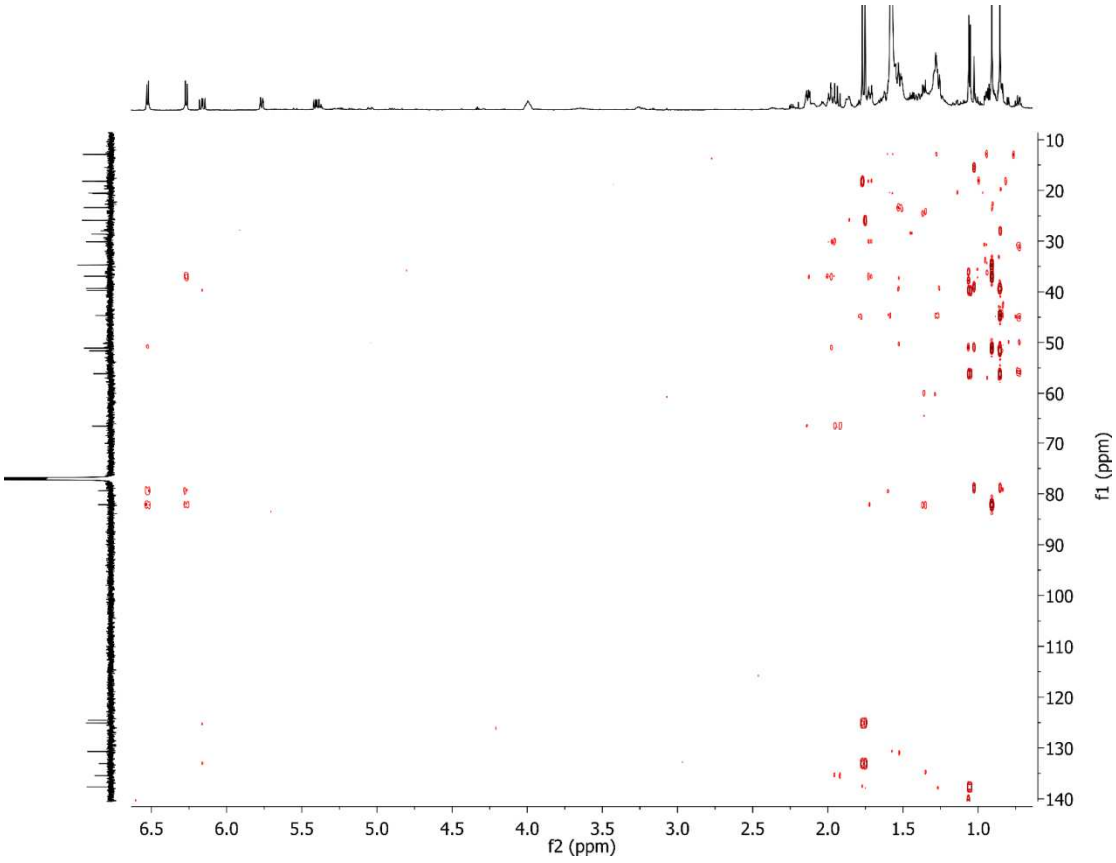
S3 HSQC spectrum of aspergorakhins A (**1**).



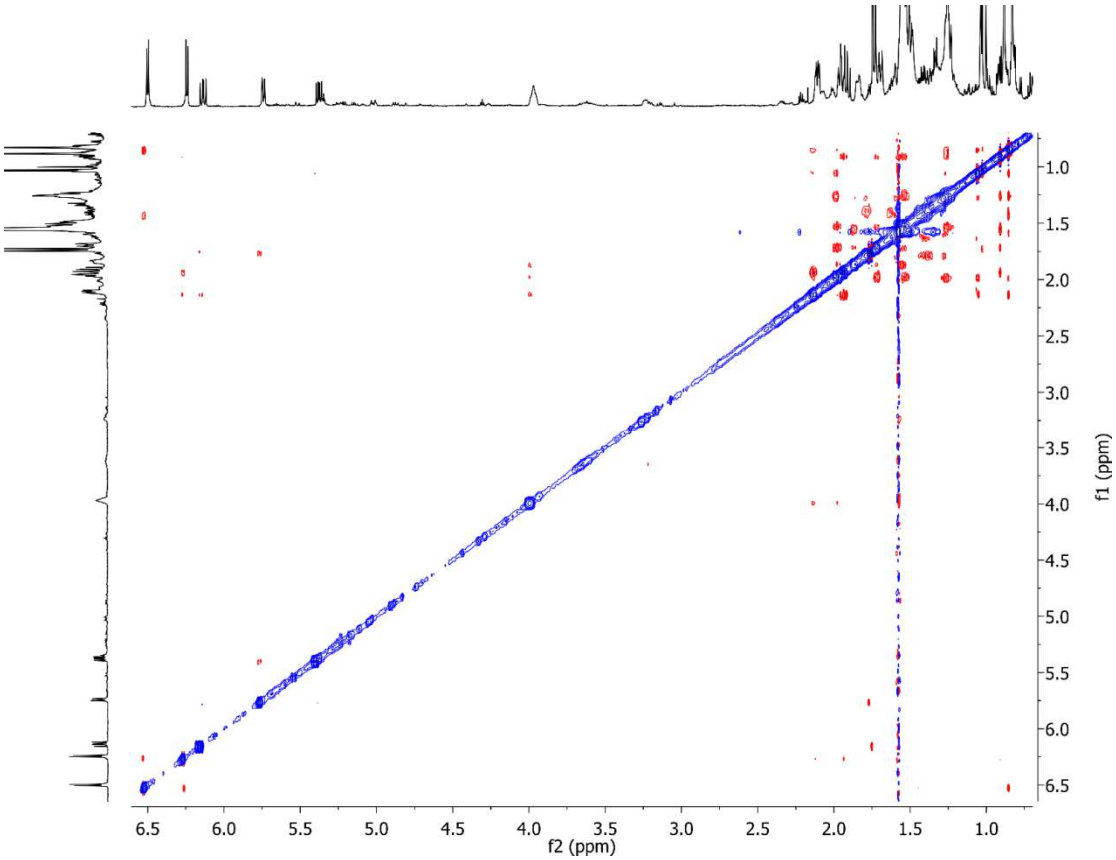
S4 COSY spectrum of aspergorakhins A (**1**).



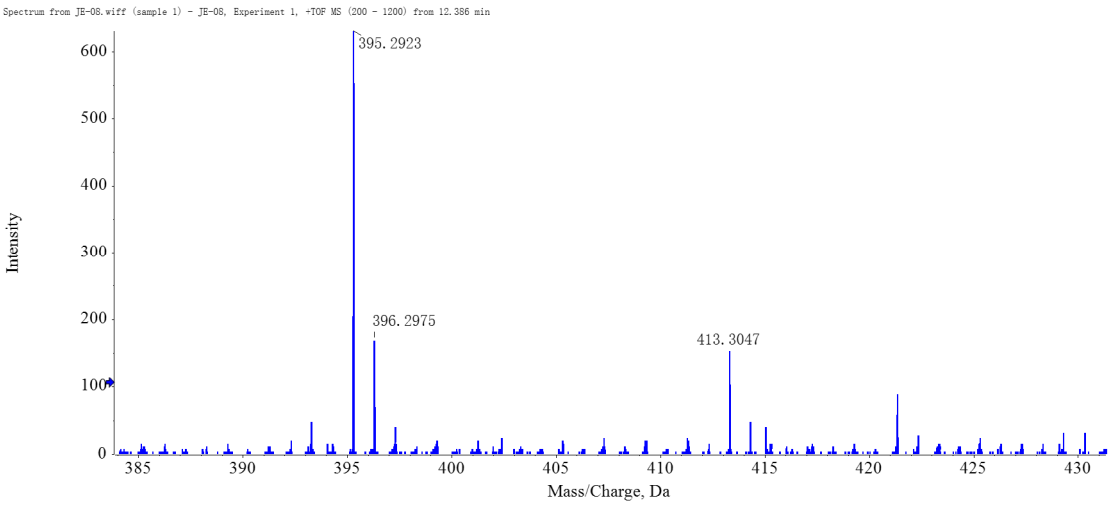
S5 HMBC spectrum of aspergorakhins A (**1**).



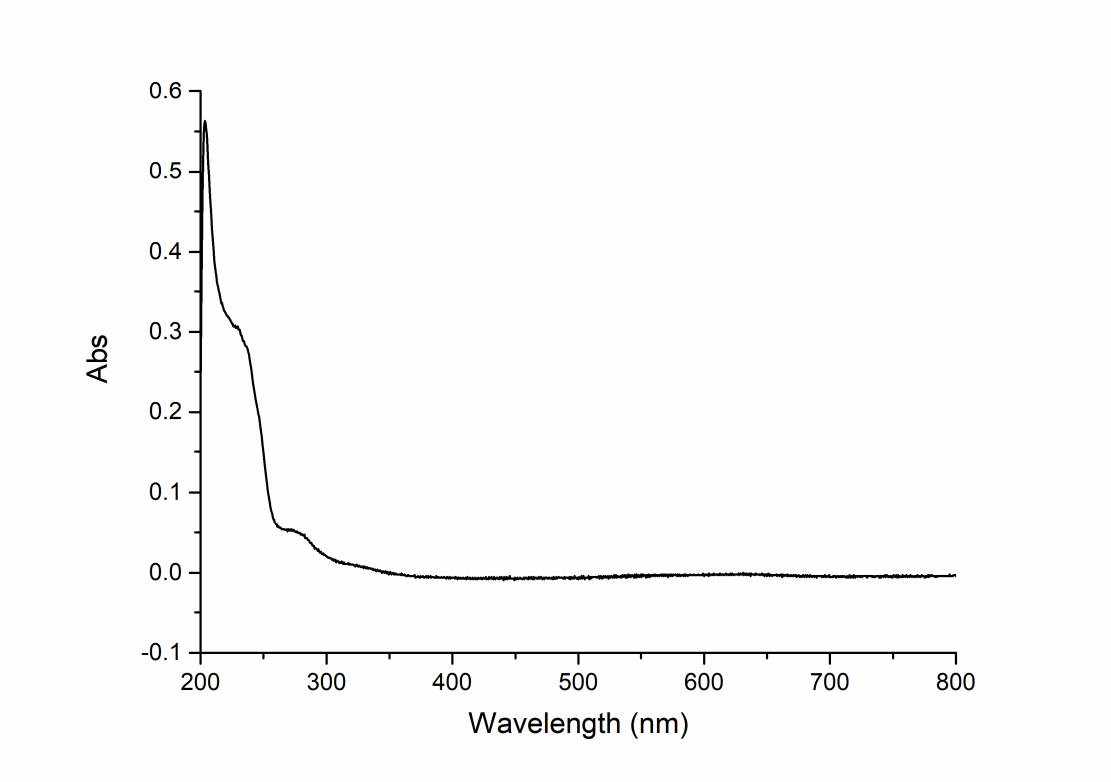
S6 NOESY spectrum of aspergorakhins A (**1**).



S7 (+)-HRESIMS spectrum of aspergorakhins A (**1**).



S8 UV spectrum of aspergorakhins A (**1**).



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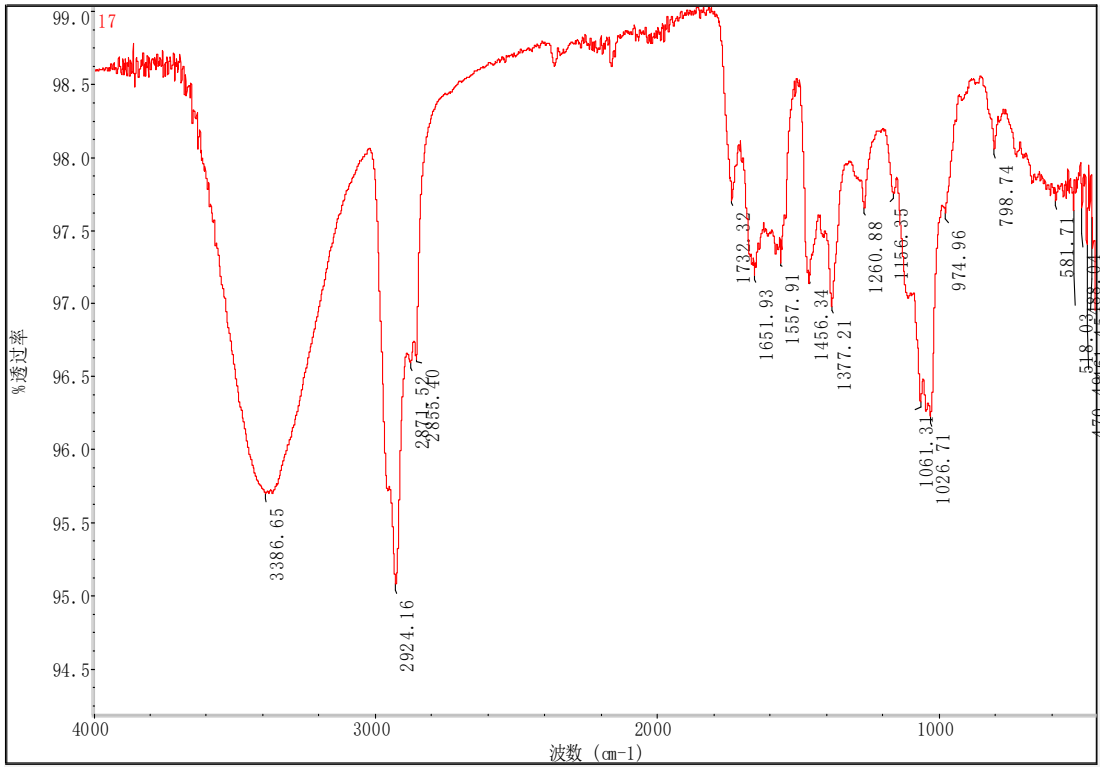
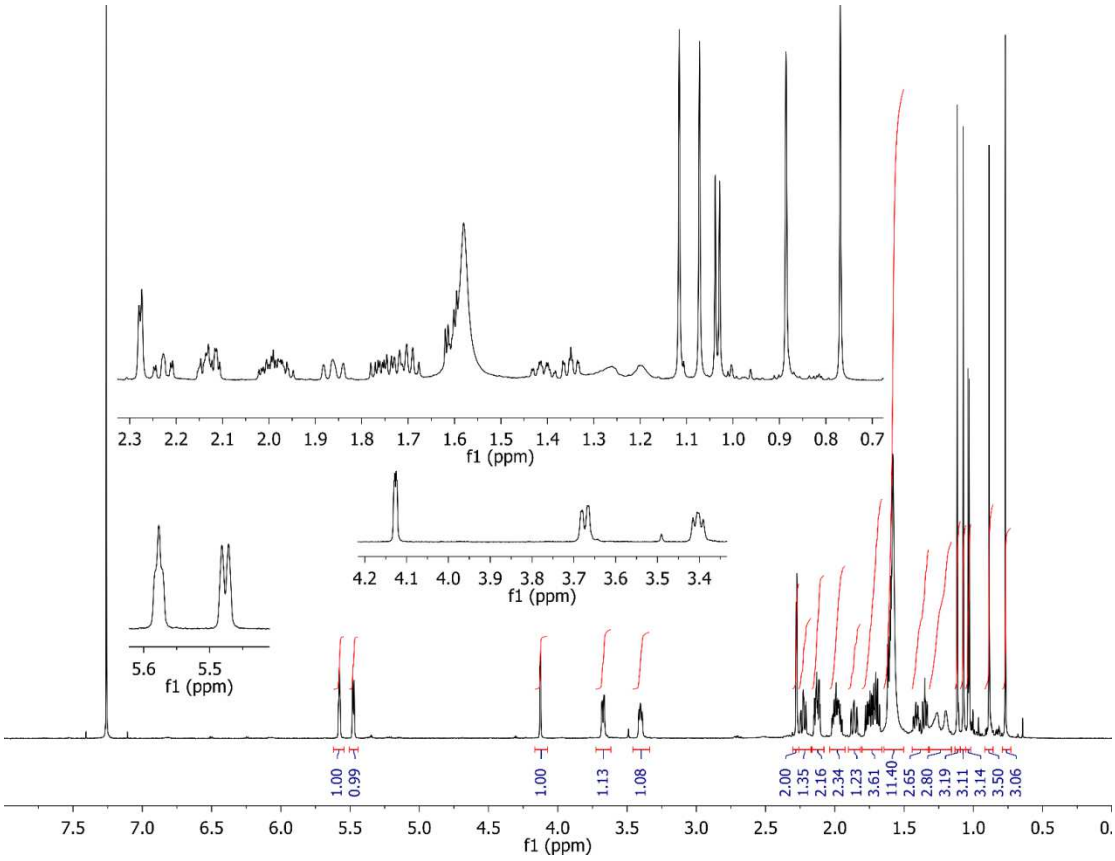
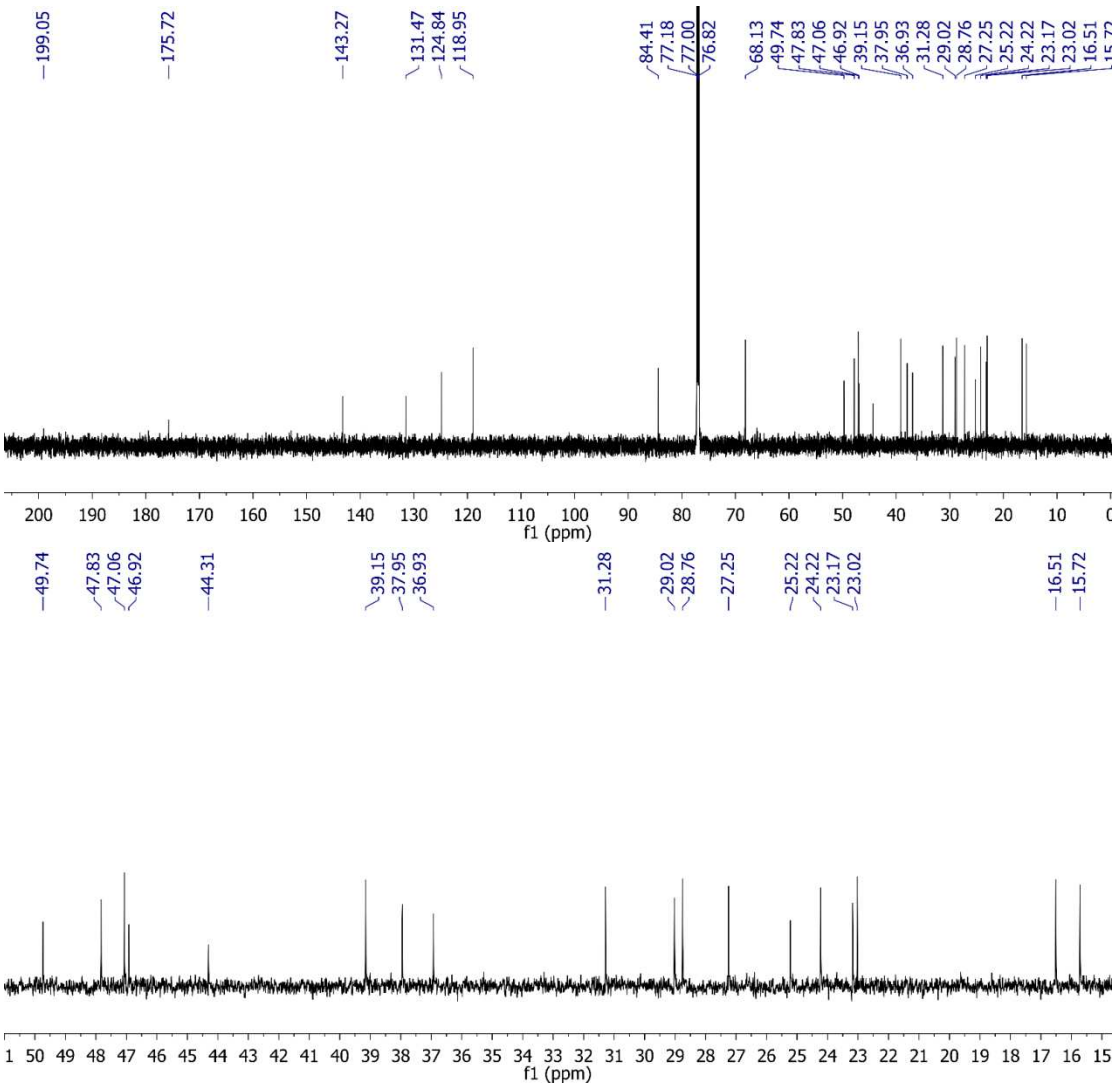


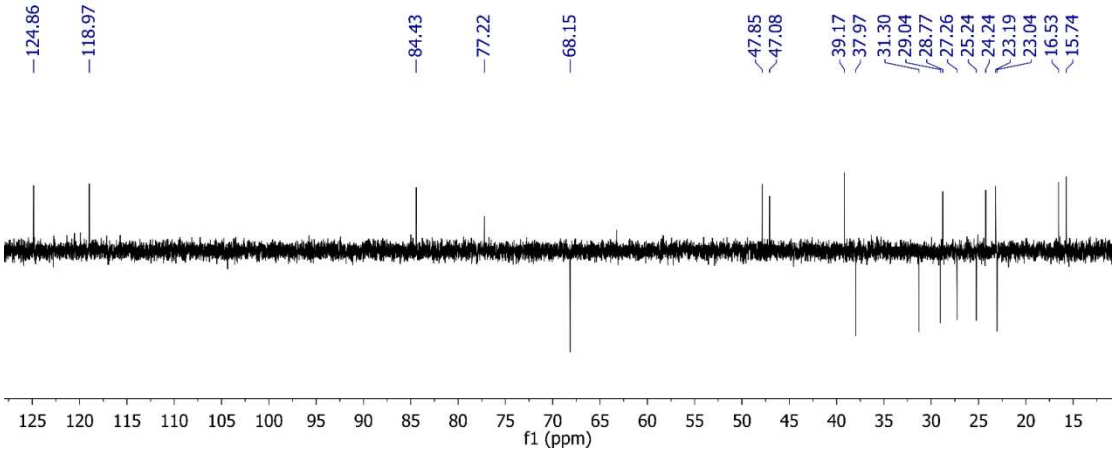
S10 ^{1}H NMR (700 MHz, CDCl3) spectrum of aspergorakhins B (**2**).



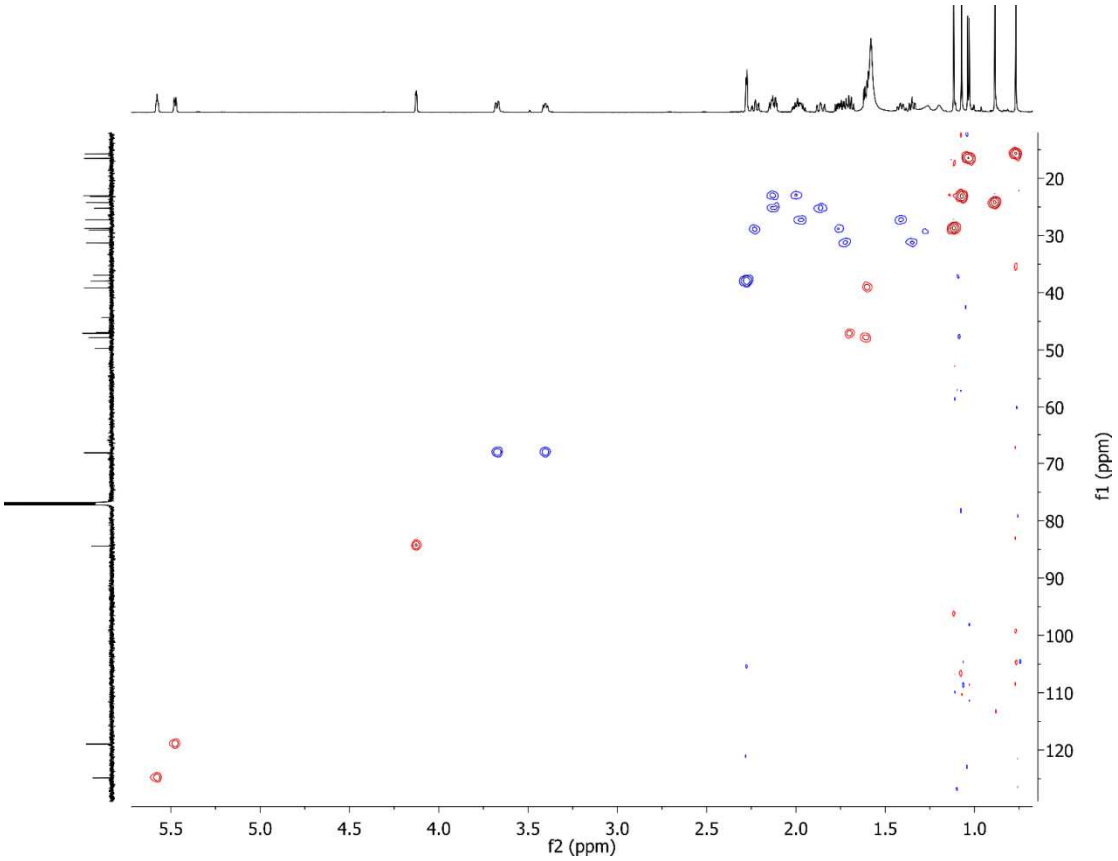
S11 ^{13}C NMR (175 MHz, CDCl3) spectrum of aspergorakhins B (**2**).



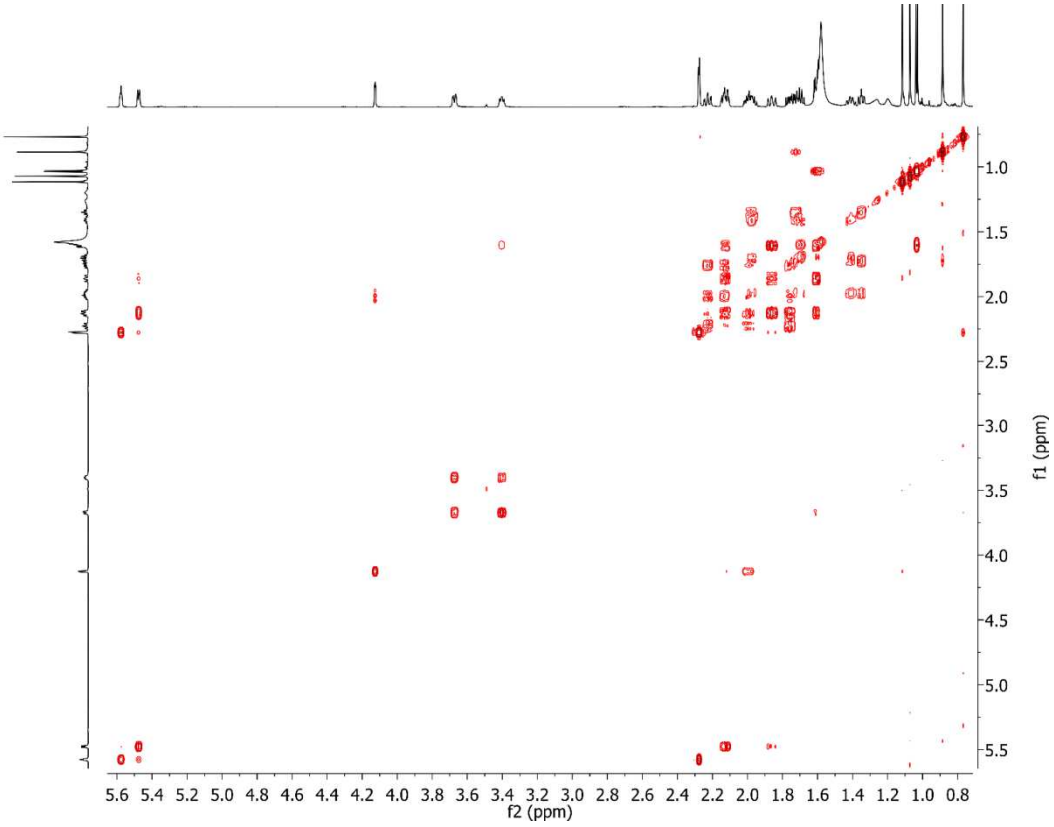
S12 DEPT135 spectrum of aspergorakhins B (**2**).



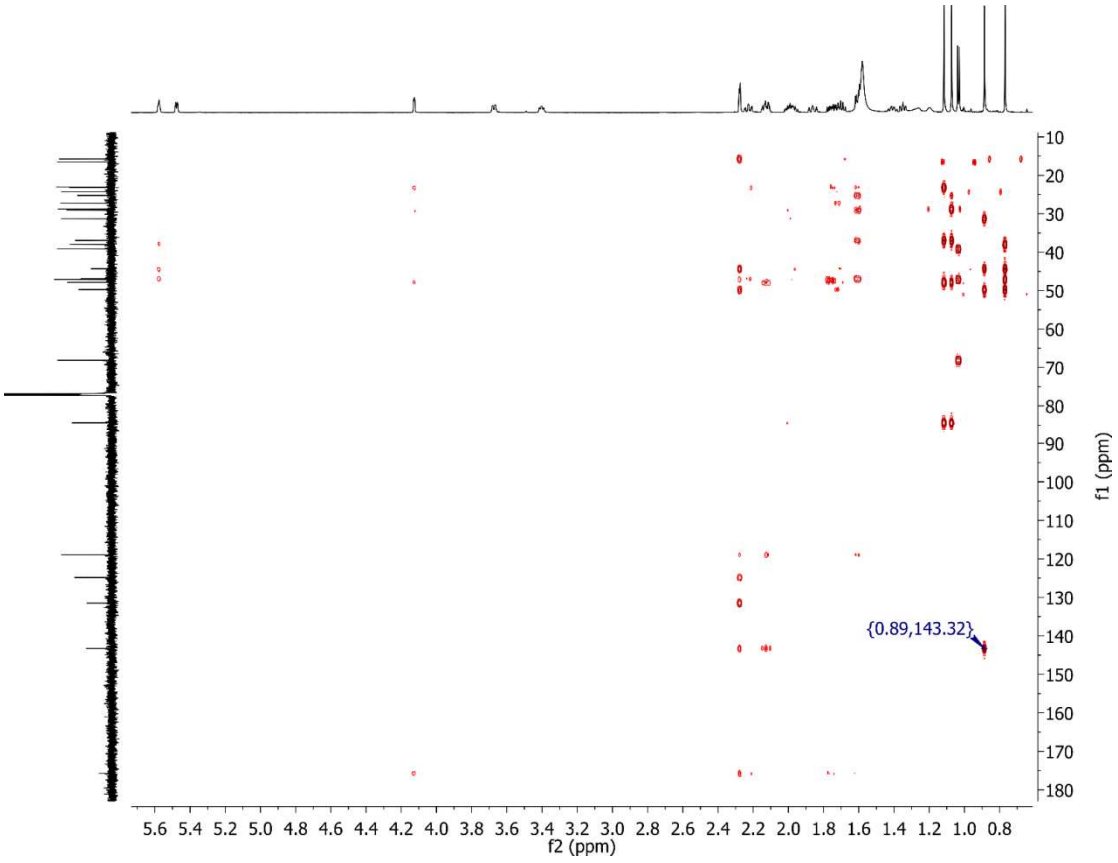
S13 HSQC spectrum of aspergorakhins B (**2**).



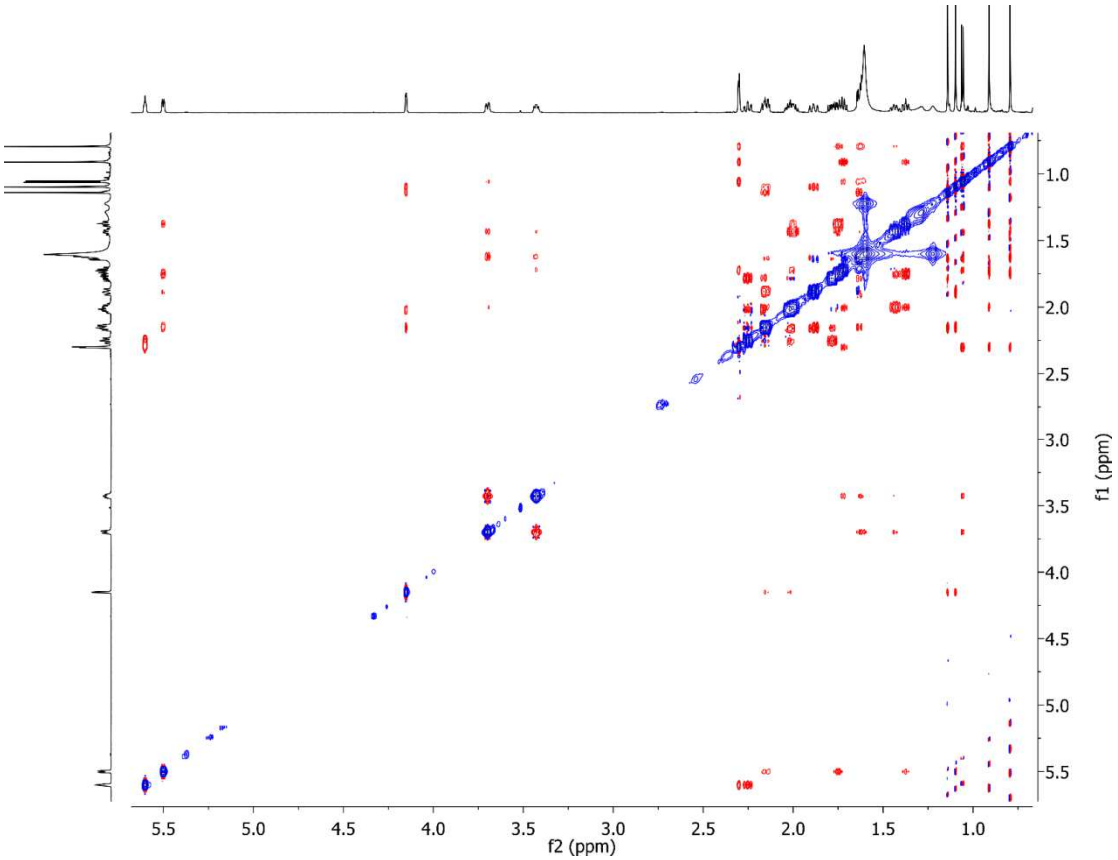
S14 COSY spectrum of aspergorakhins B (**2**).



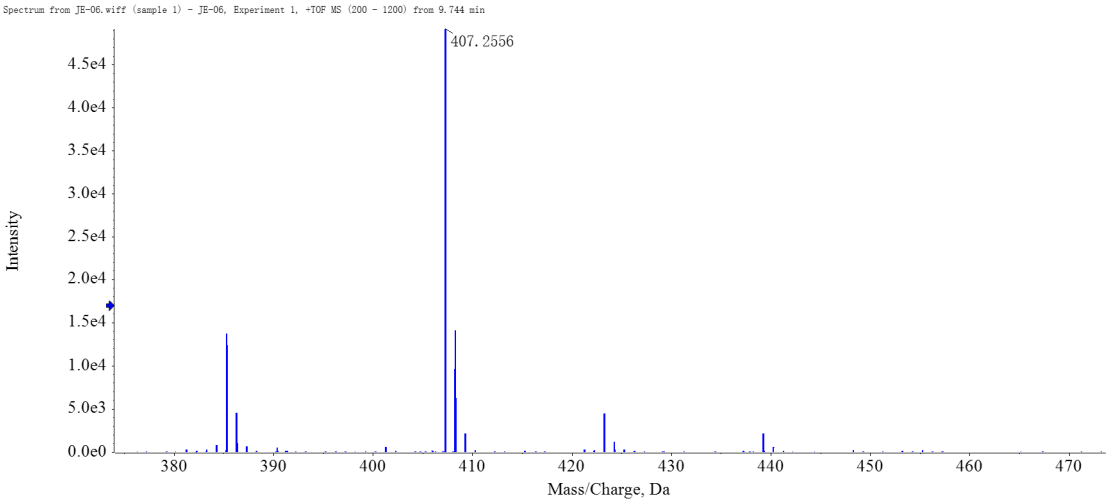
S15 HMBC spectrum of aspergorakhins B (**2**).



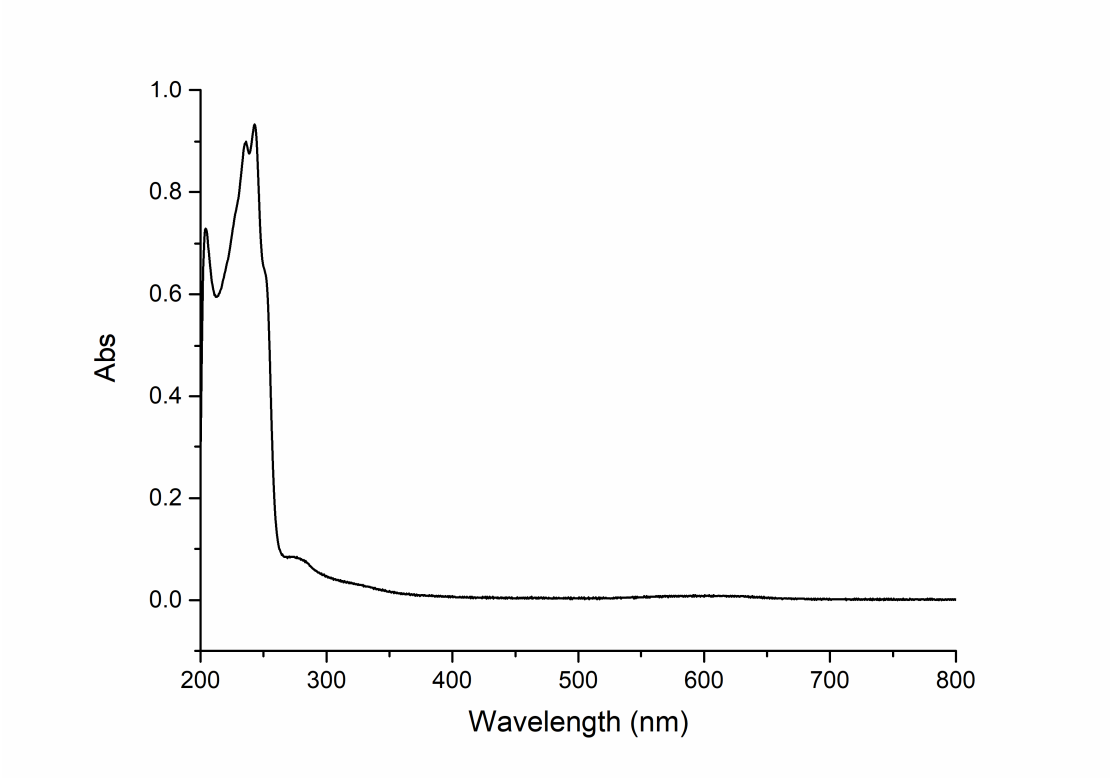
S16 NOESY spectrum of aspergorakhins B (**2**).



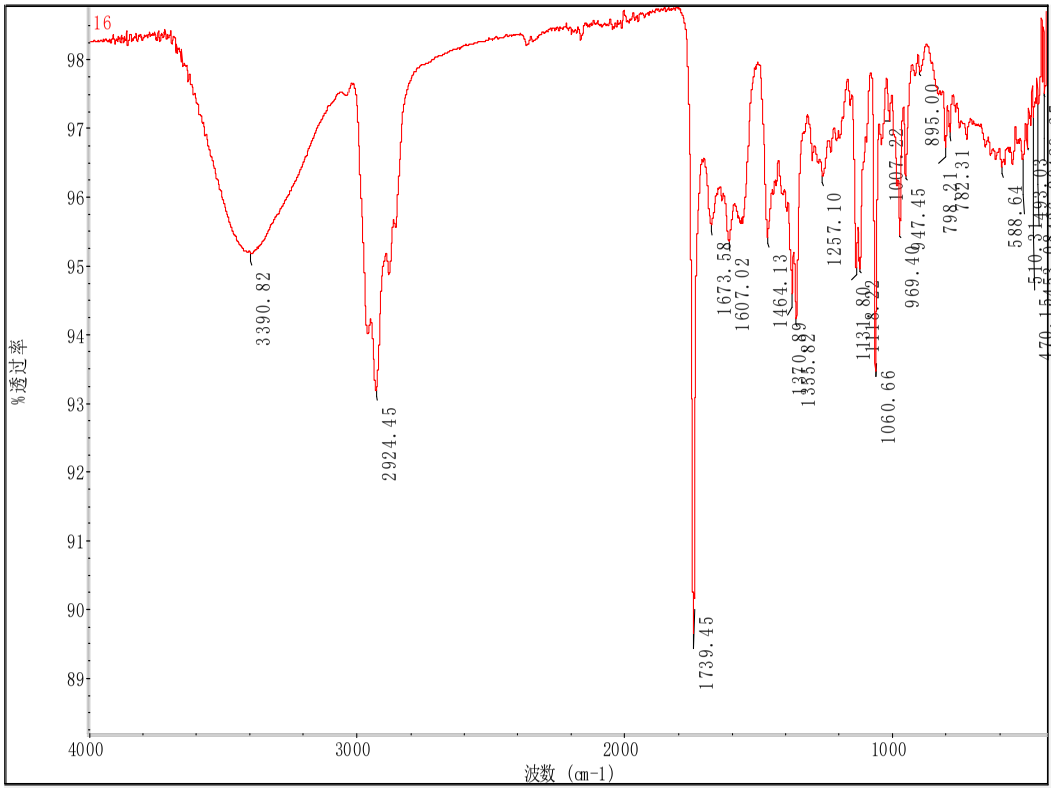
S17 (+)-HRESIMS spectrum of aspergorakhins B (**2**).



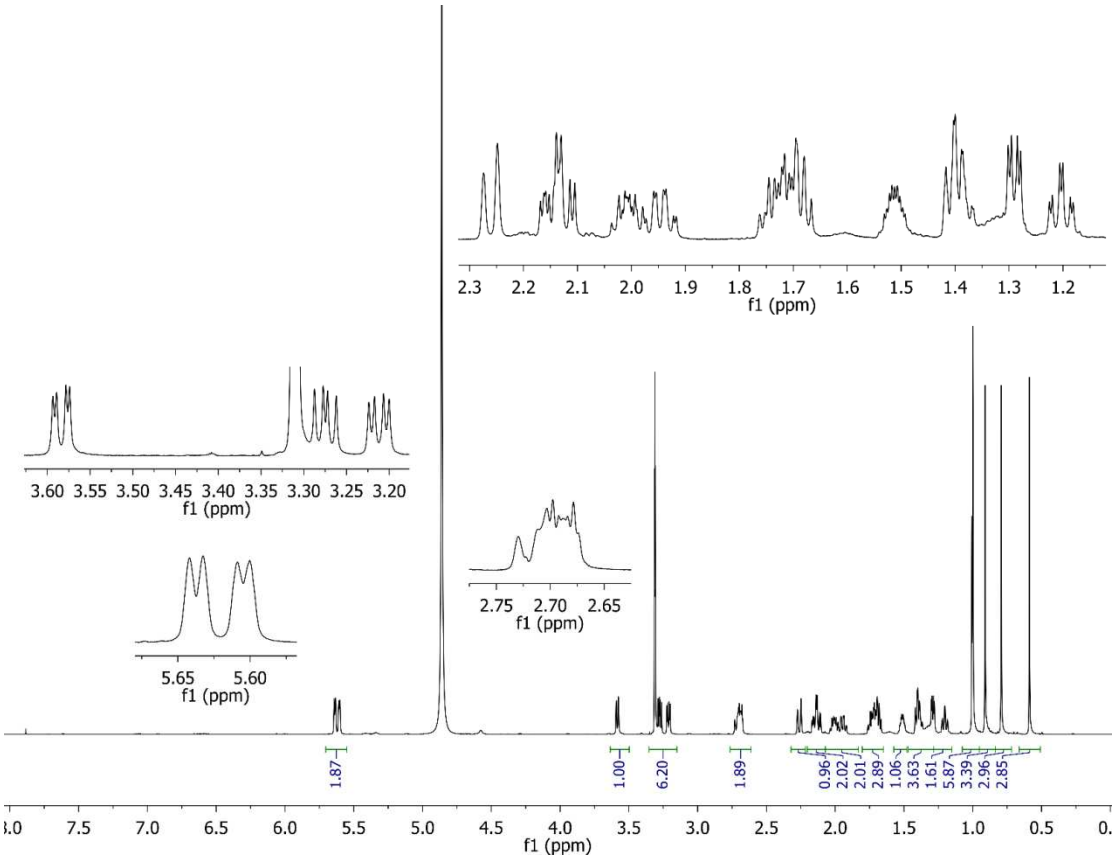
S18 UV spectrum of aspergorakhins B (**2**).



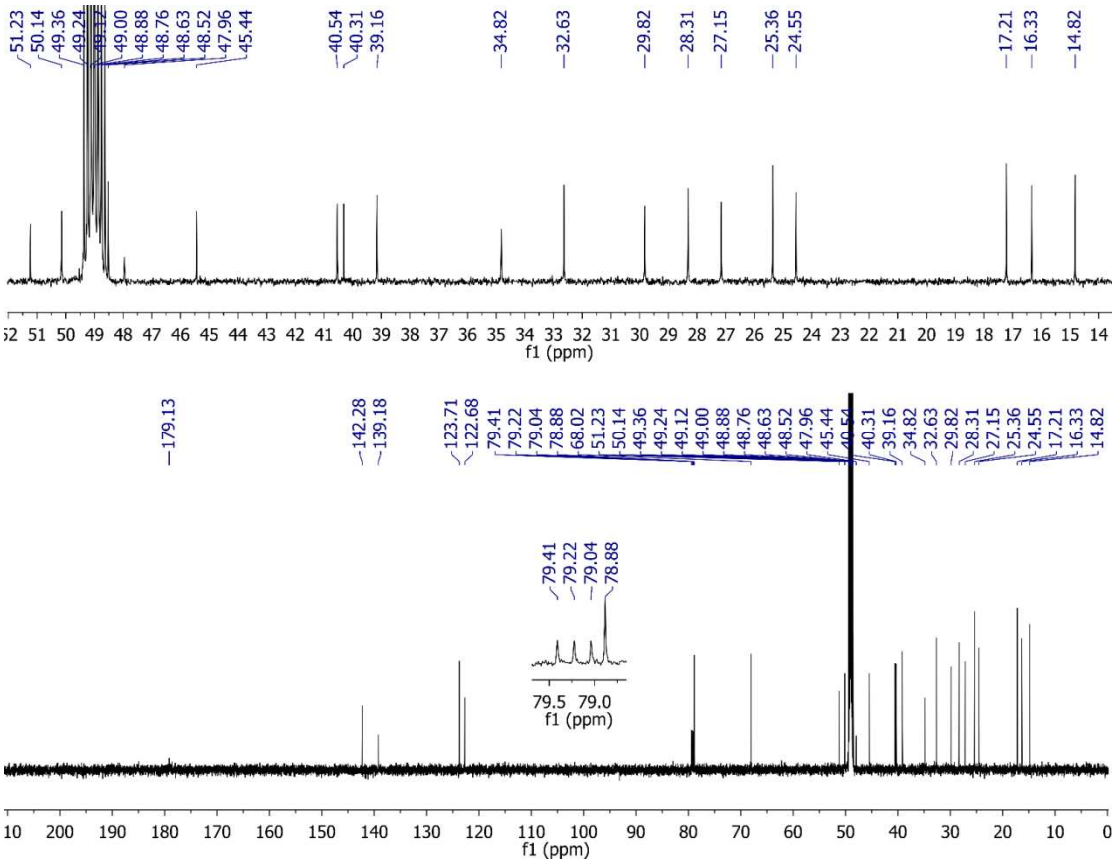
S19 IR spectrum of aspergorakhins B (**2**).



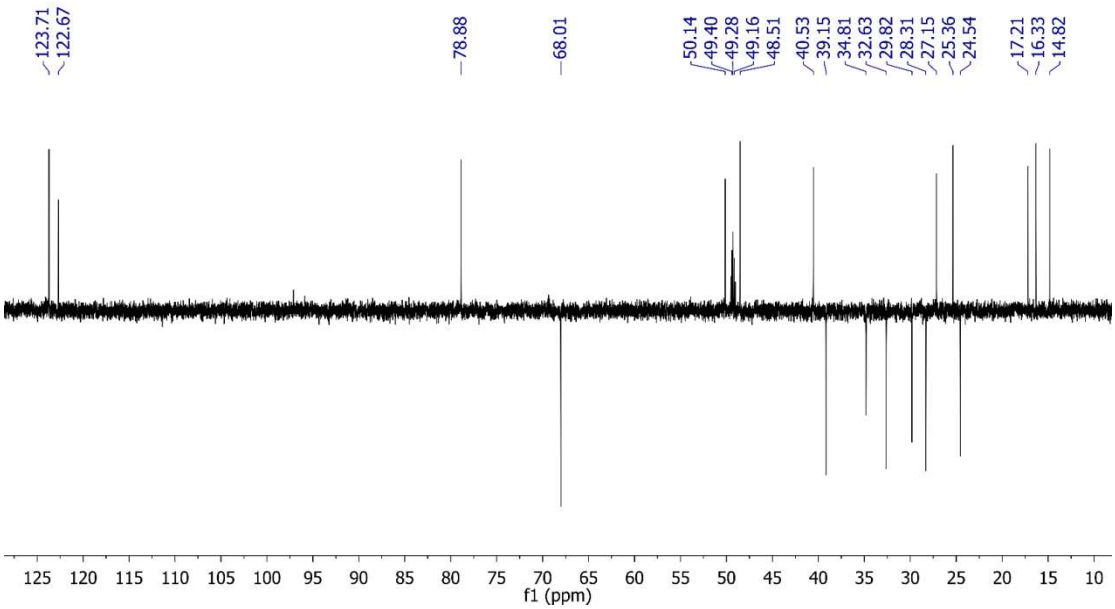
S20 ^{1}H NMR (700 MHz, CD_3OD) spectrum of aspergorakhins C (**3**).



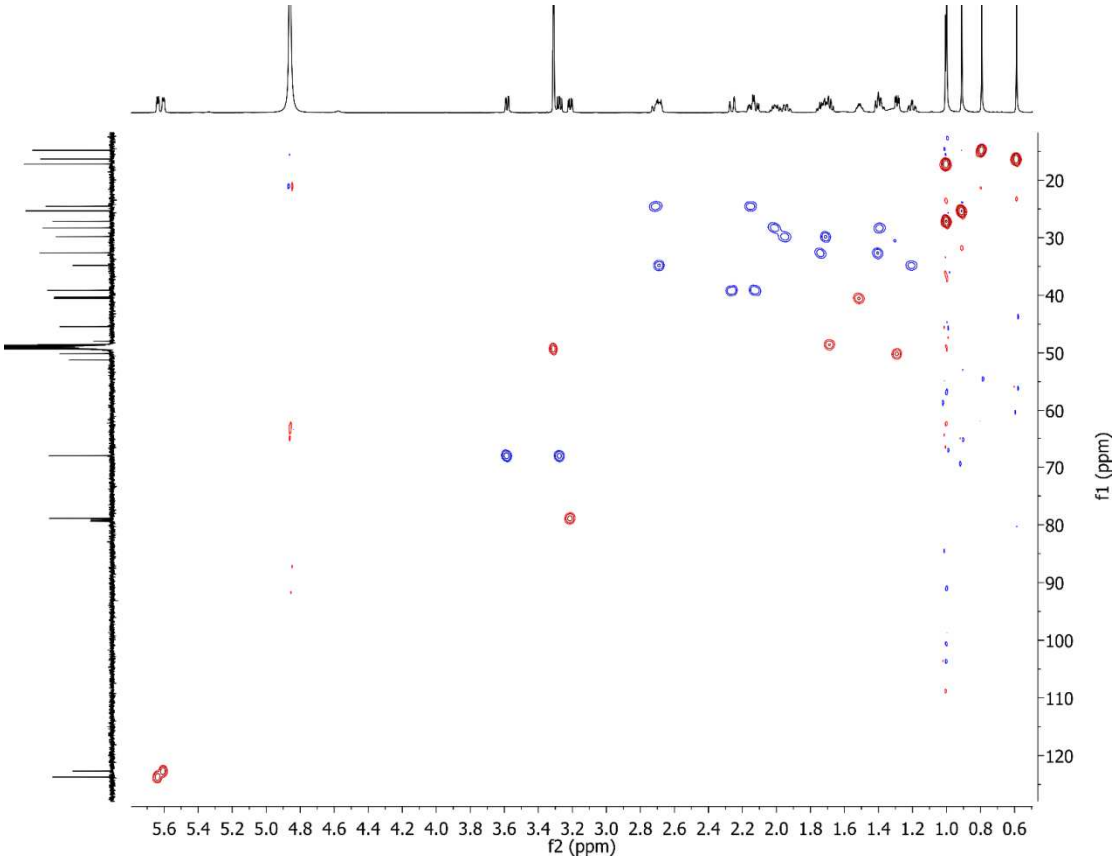
S21 ^{13}C NMR (175 MHz, CD_3OD) spectrum of aspergorakhins C (**3**).



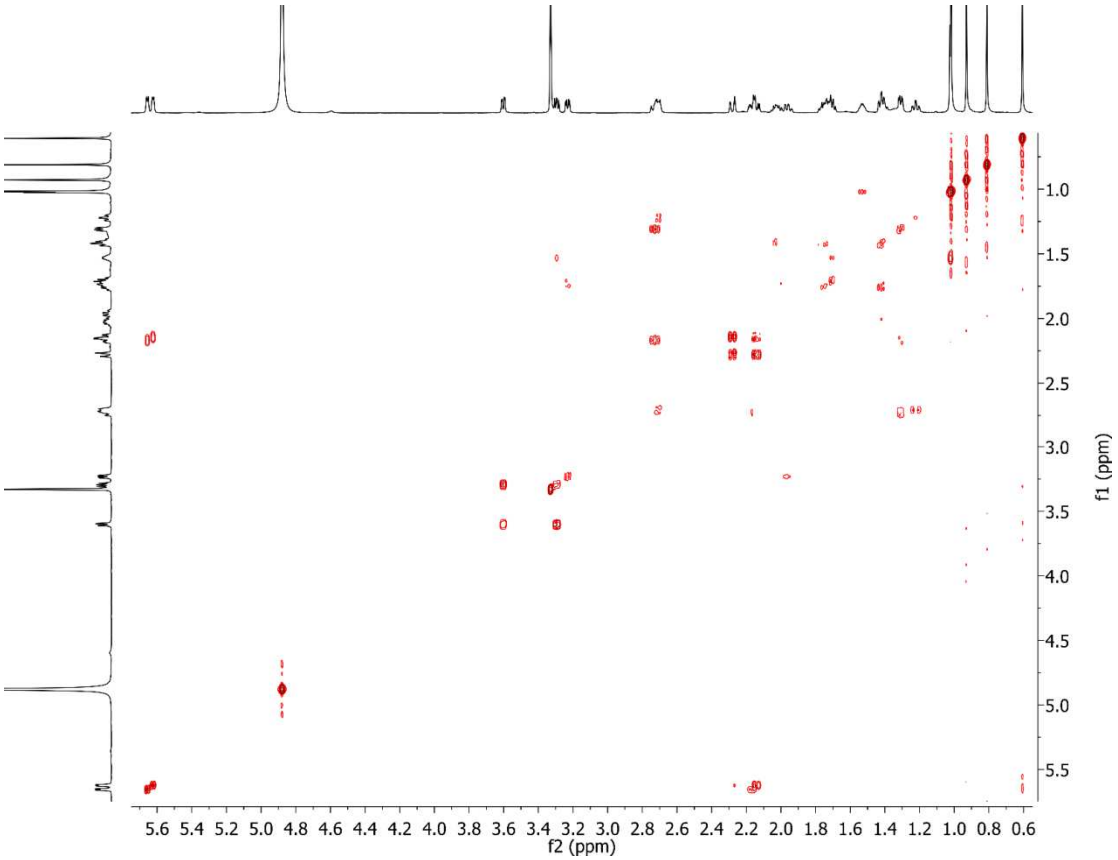
S22 DEPT135 spectrum of aspergorakhins C (**3**).



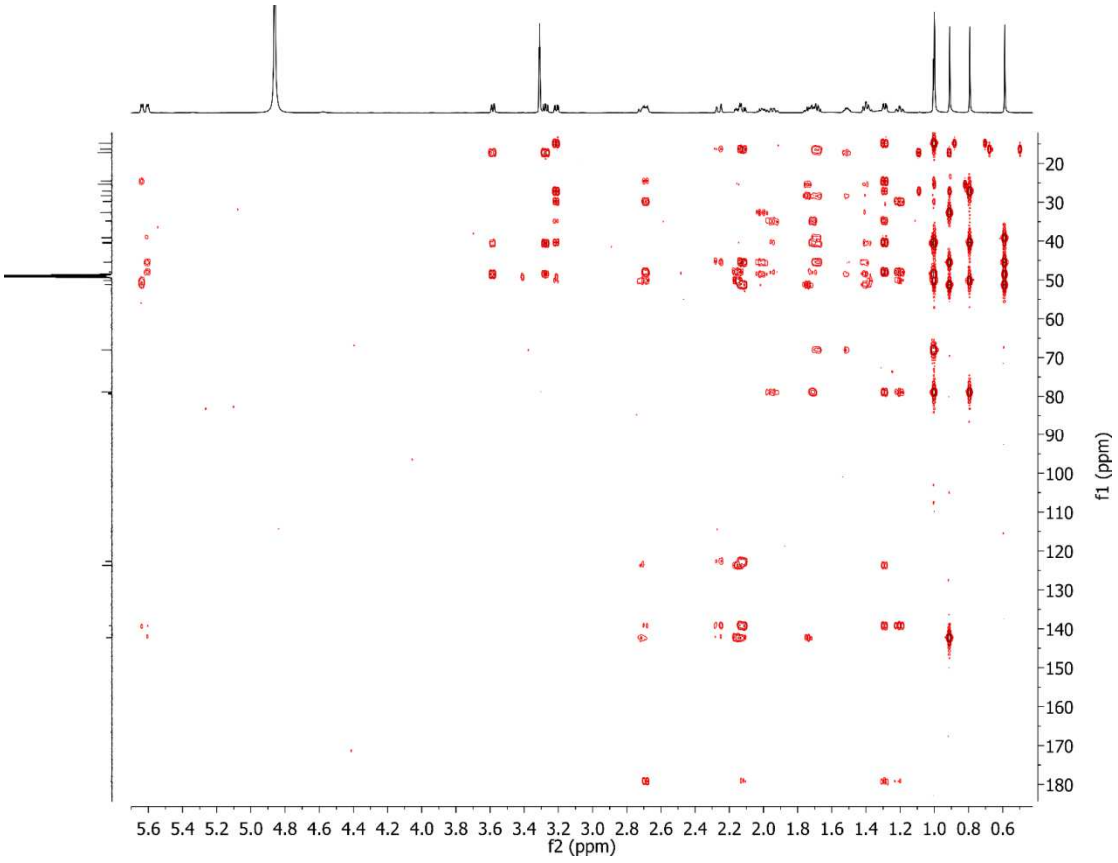
S23 HSQC spectrum of aspergorakhins C (**3**).



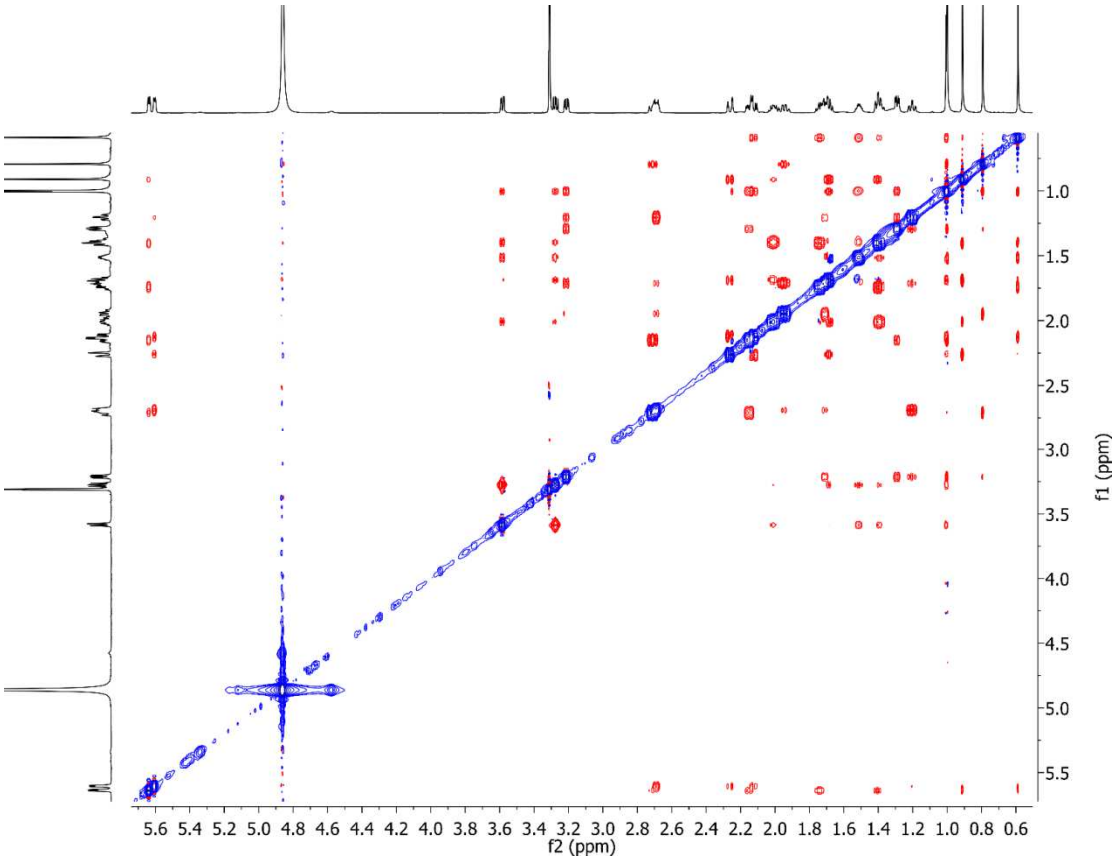
S24 COSY spectrum of aspergorakhins C (**3**).



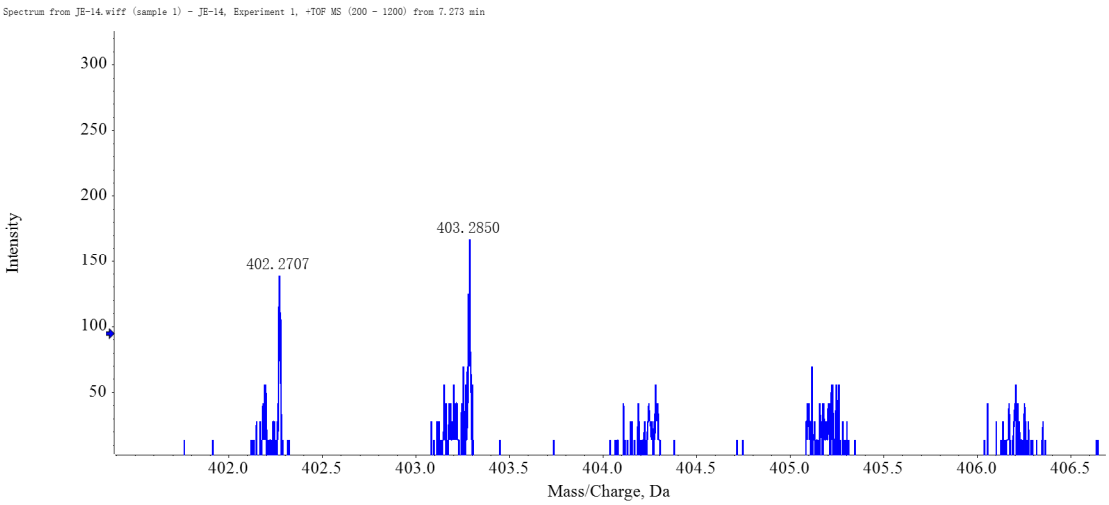
S25 HMBC spectrum of aspergorakhins C (**3**).



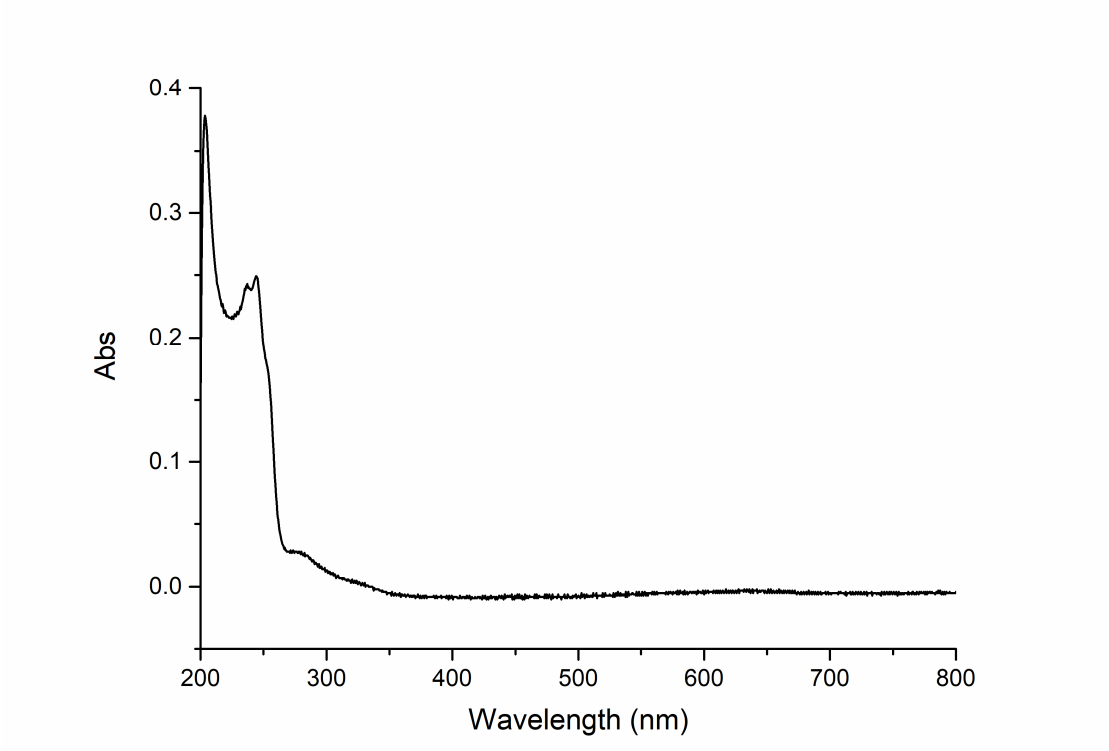
S26 NOESY spectrum of aspergorakhins C (**3**).



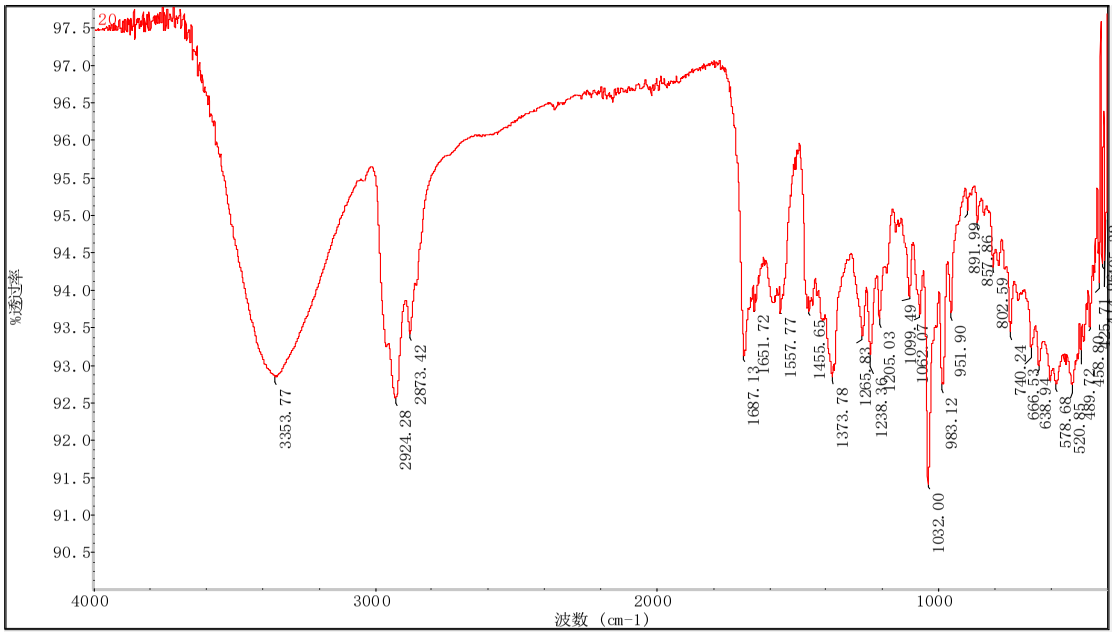
S27 (+)-HRESIMS spectrum of aspergorakhins C (**3**).



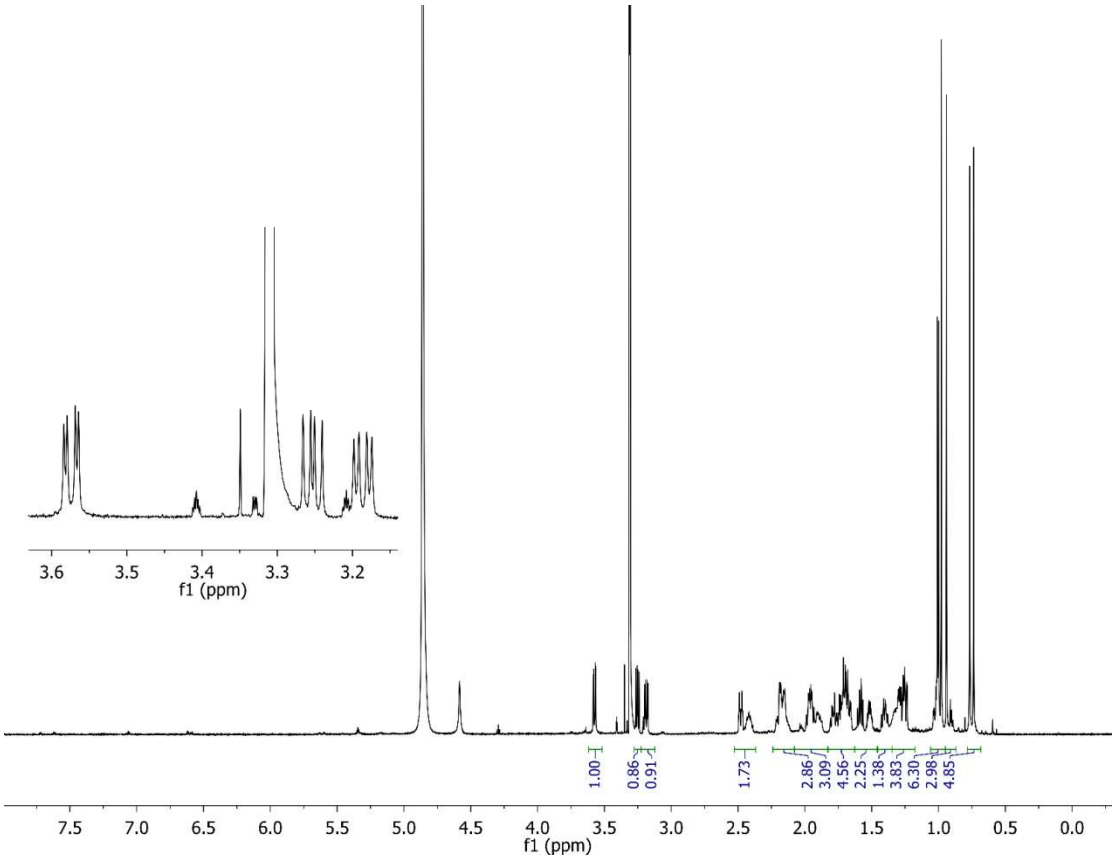
S28 UV spectrum of aspergorakhins C (**3**).

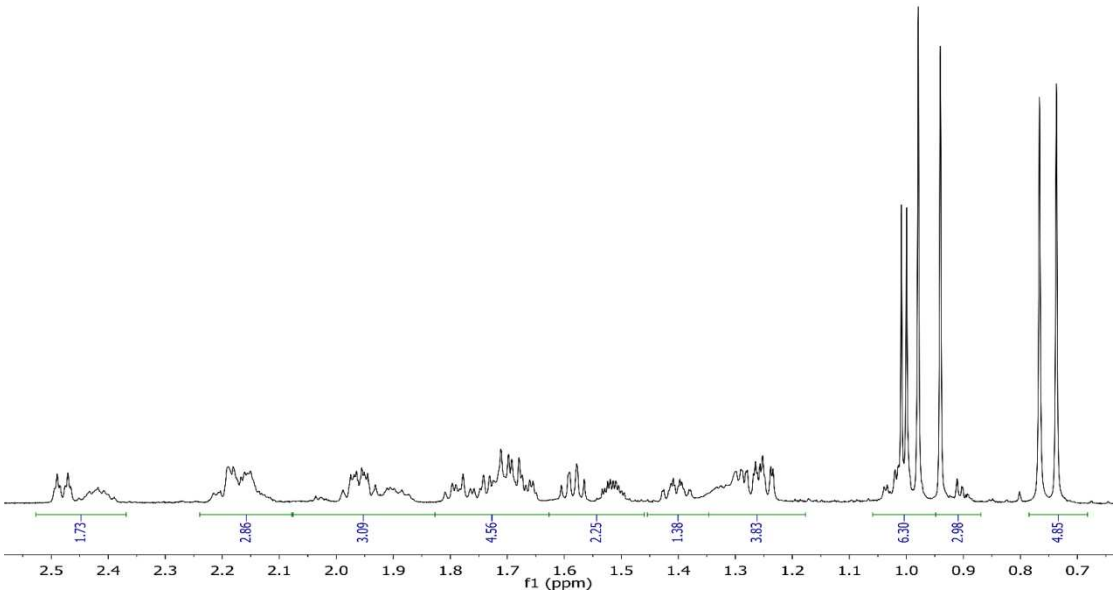


S29 IR spectrum of aspergorakhins C (**3**).

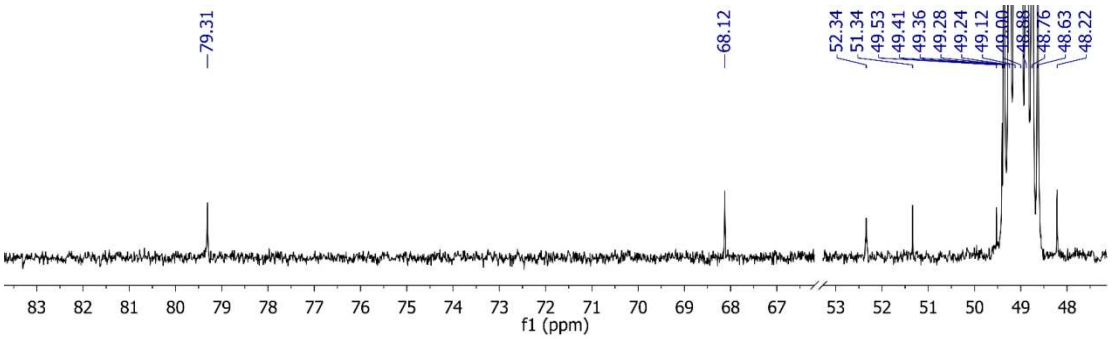


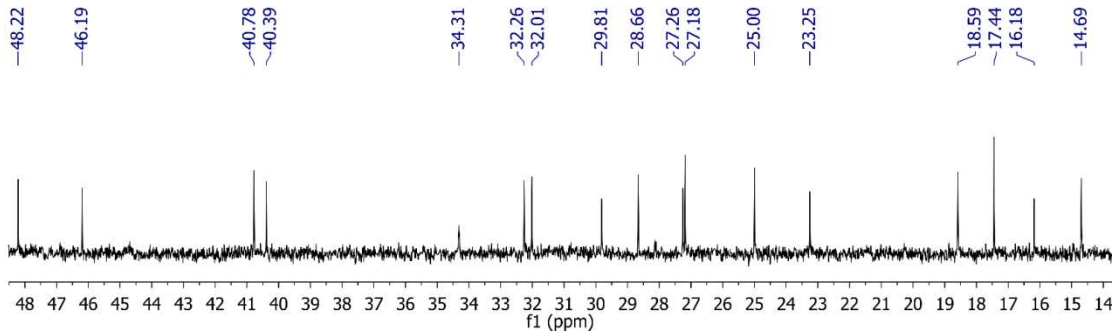
S30 ^{1}H NMR (700 MHz, CD_3OD) spectrum of aspergorakhins D (**4**).



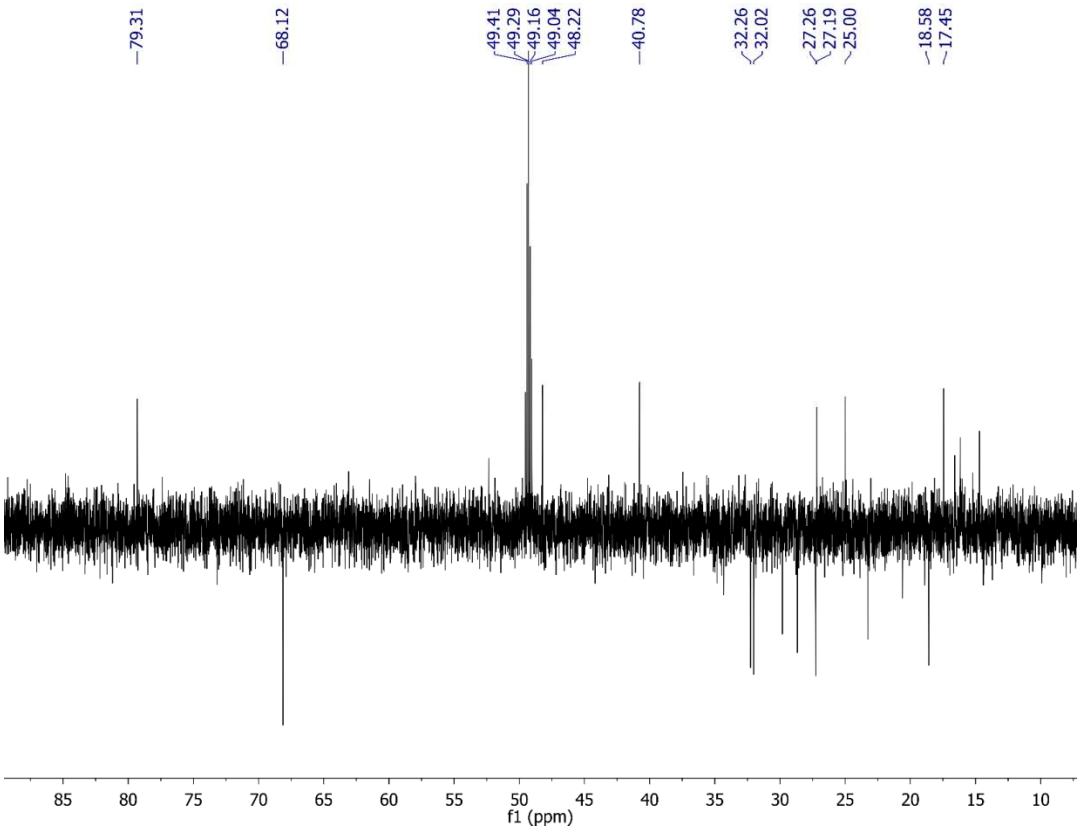


S31 ^{13}C NMR (175 MHz, CD_3OD)spectrum of aspergorakhins D (**4**).

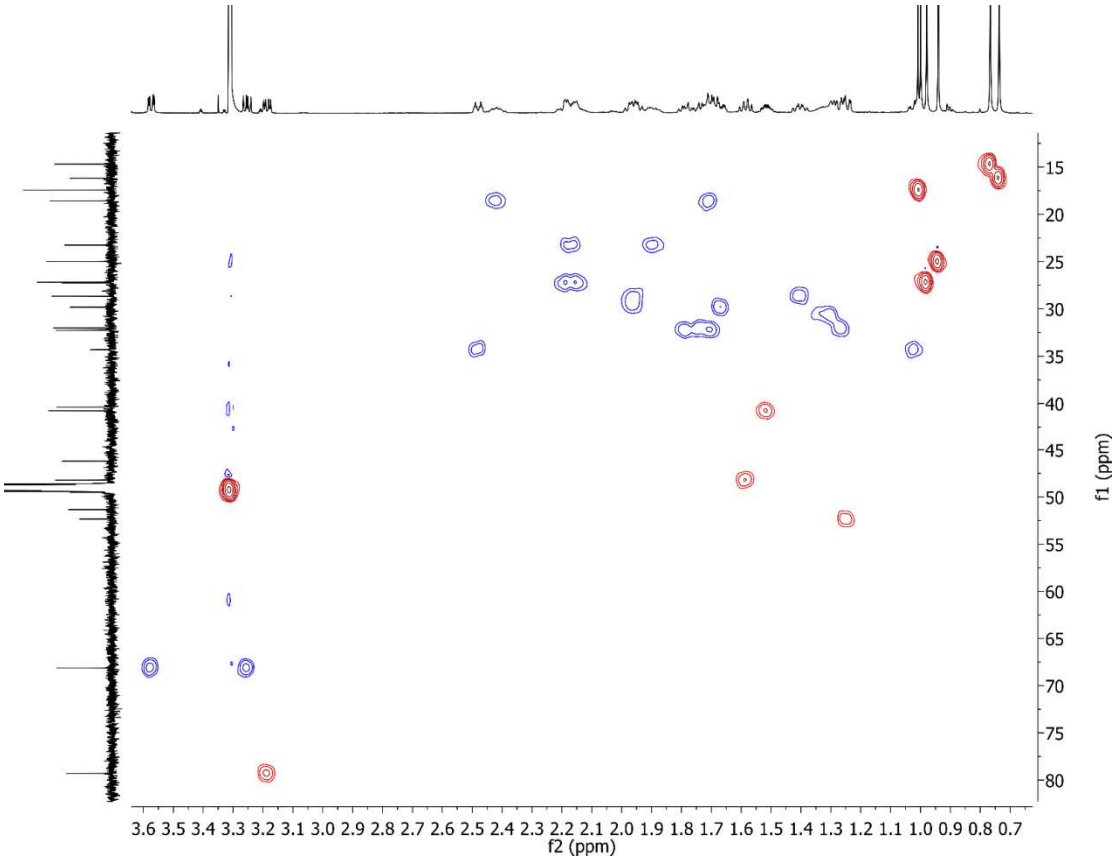




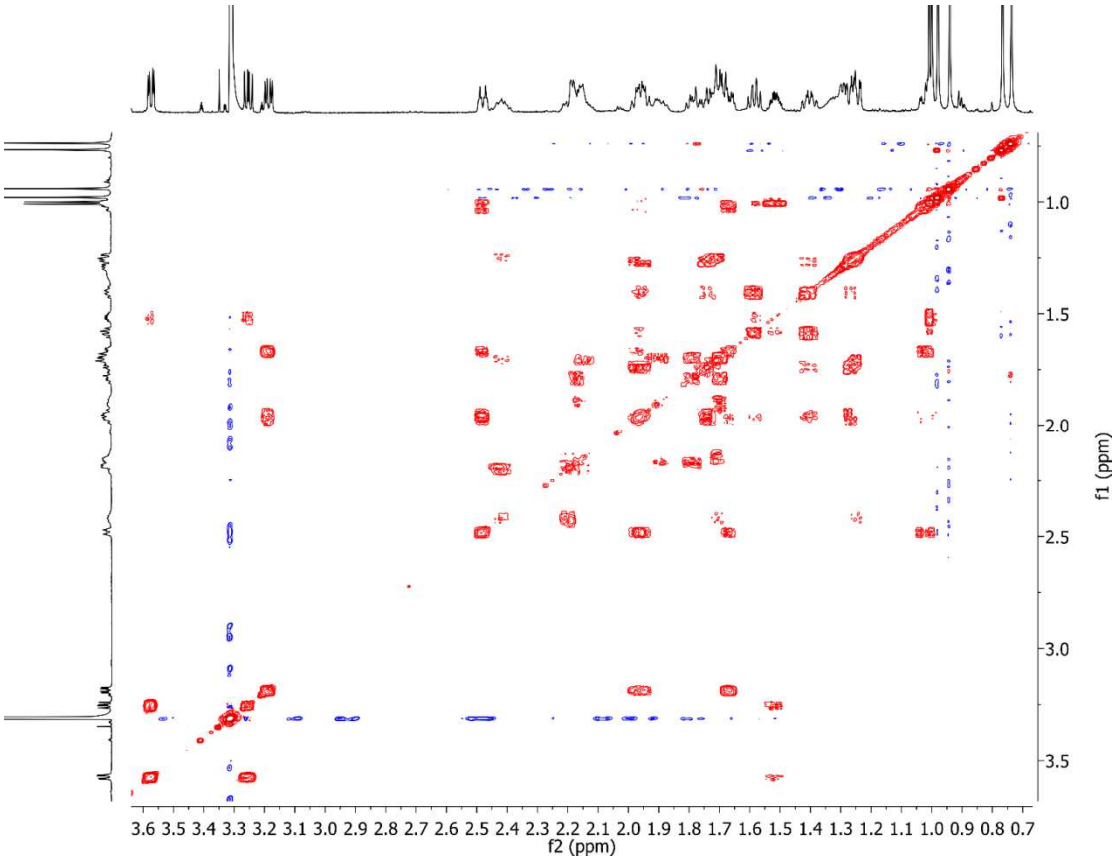
S32 DEPT135 spectrum of aspergorakhins D (**4**).



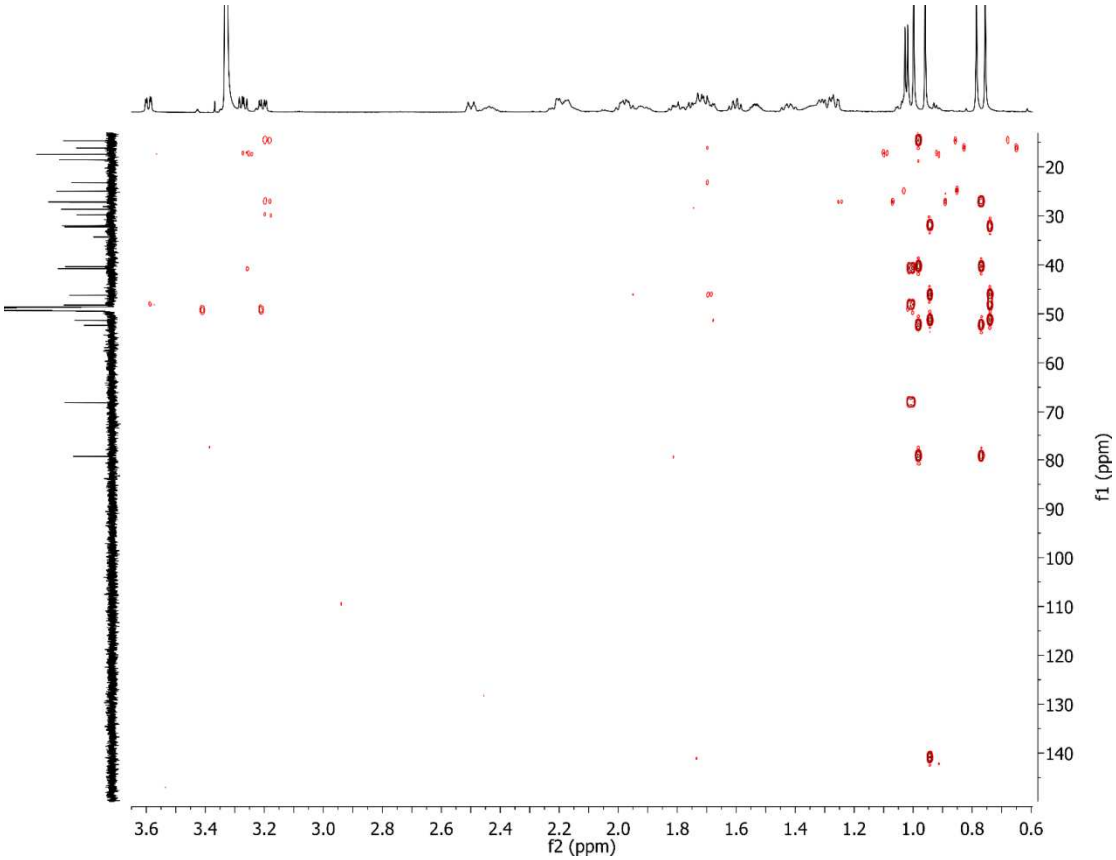
S33 HSQC spectrum of aspergorakhins D (**4**).



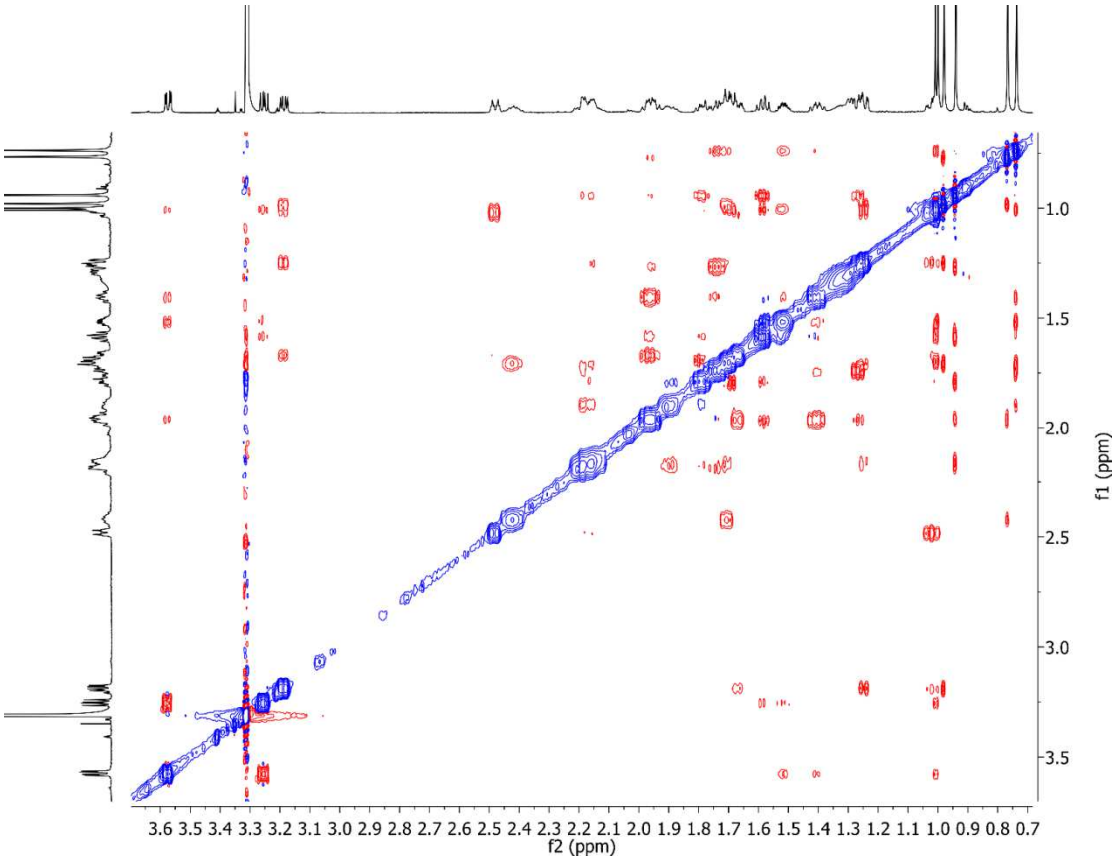
S34 COSY spectrum of aspergorakhins D (**4**).



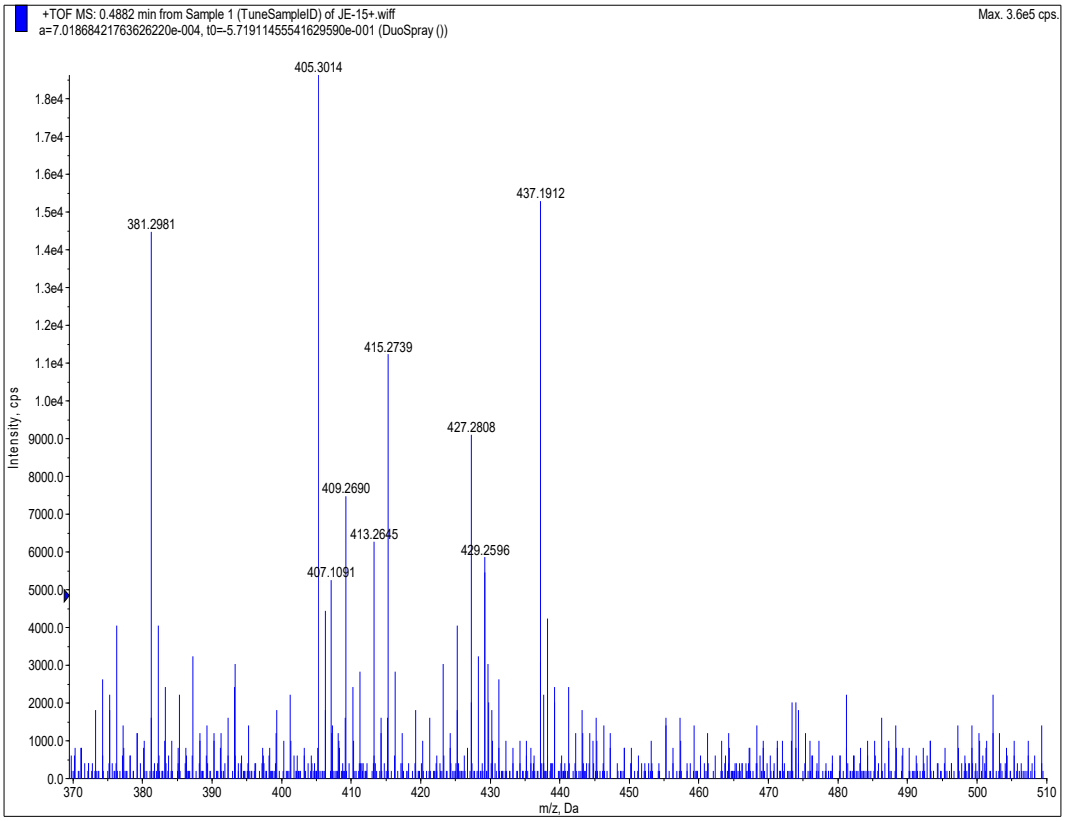
S35 HMBC spectrum of aspergorakhins D (**4**).



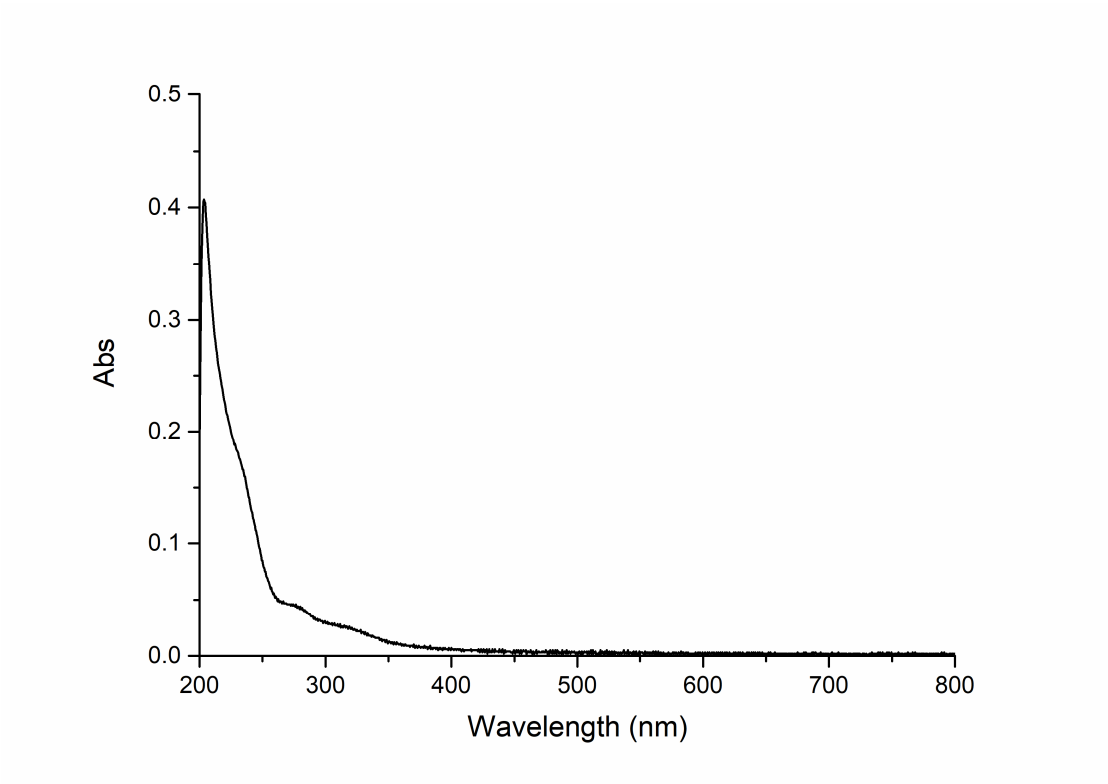
S36 NOESY spectrum of aspergorakhins D (**4**).



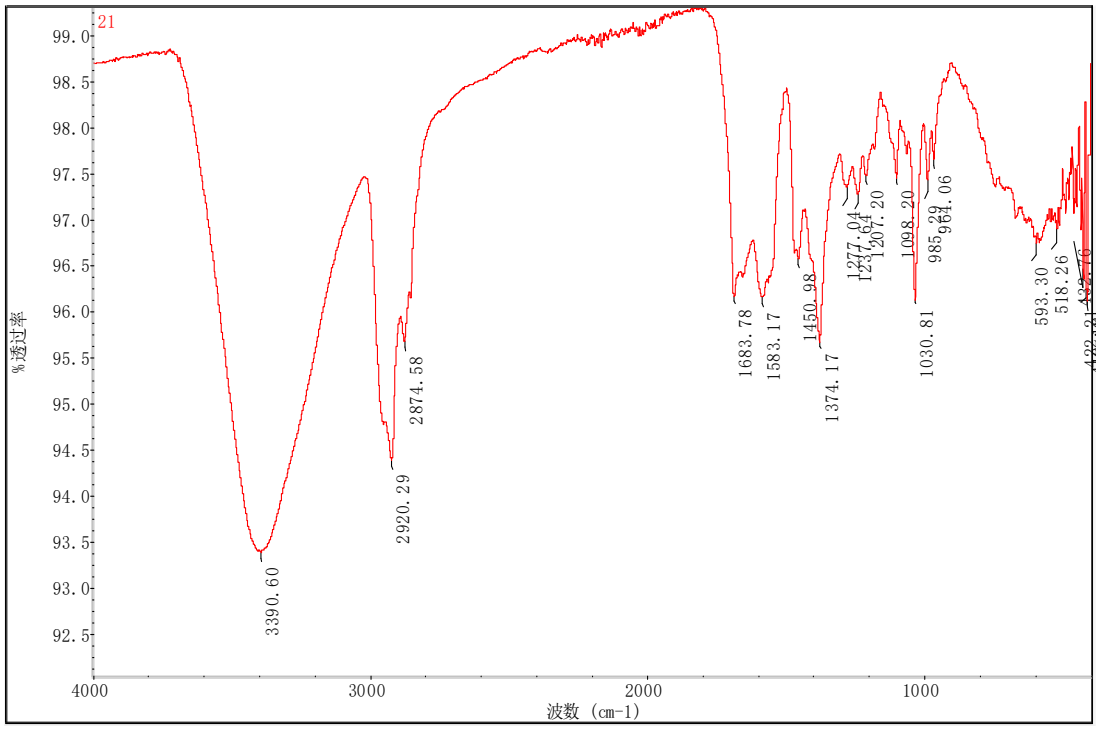
S37 (+)-HRESIMS spectrum of aspergorakhins D (**4**).



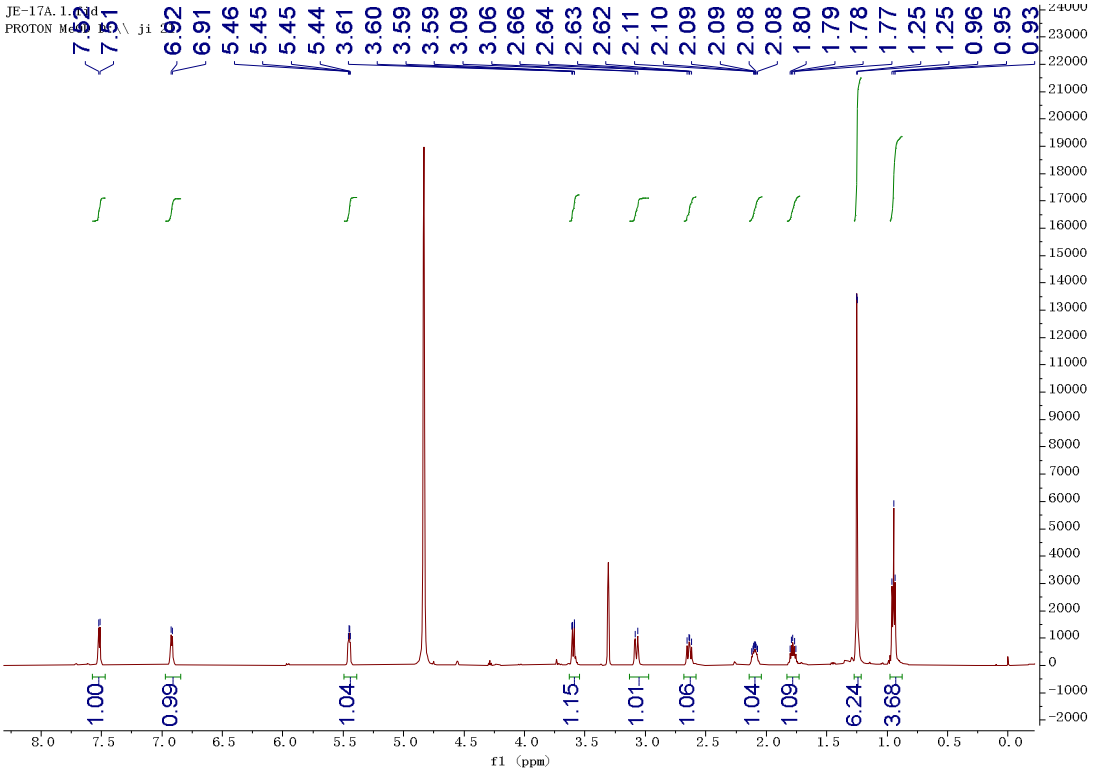
S38 UV spectrum of aspergorakhins D (**4**).



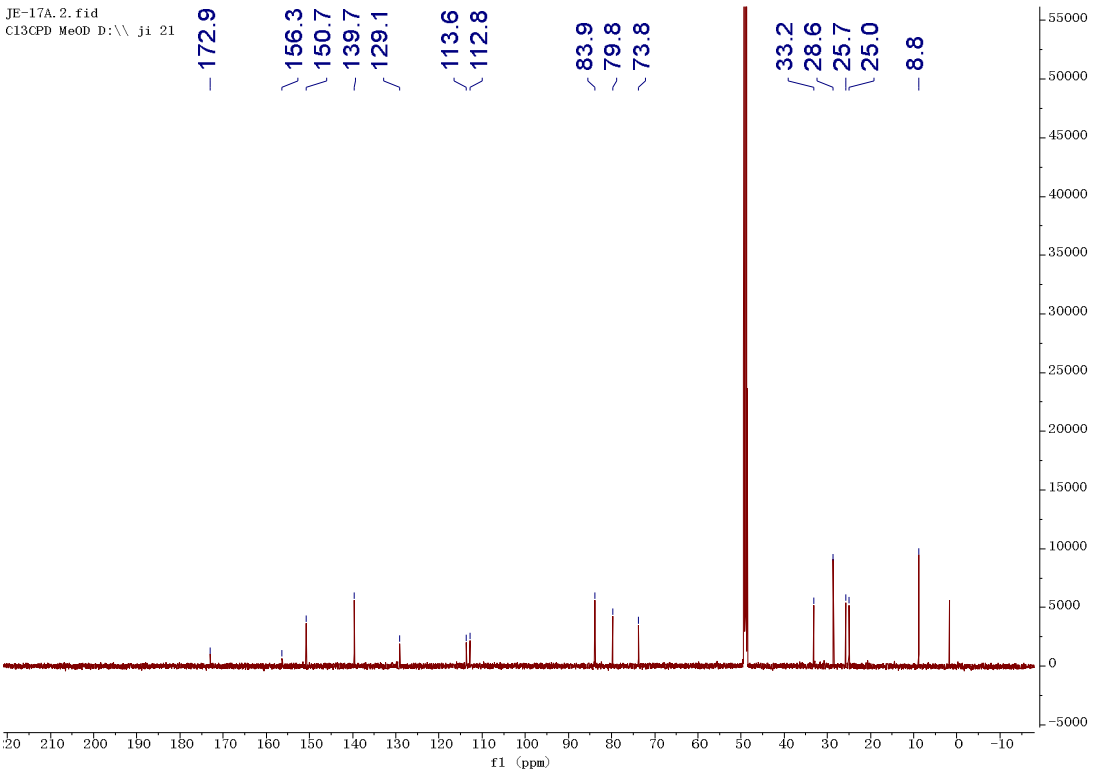
S39 IR spectrum of aspergorakhins D (**4**).



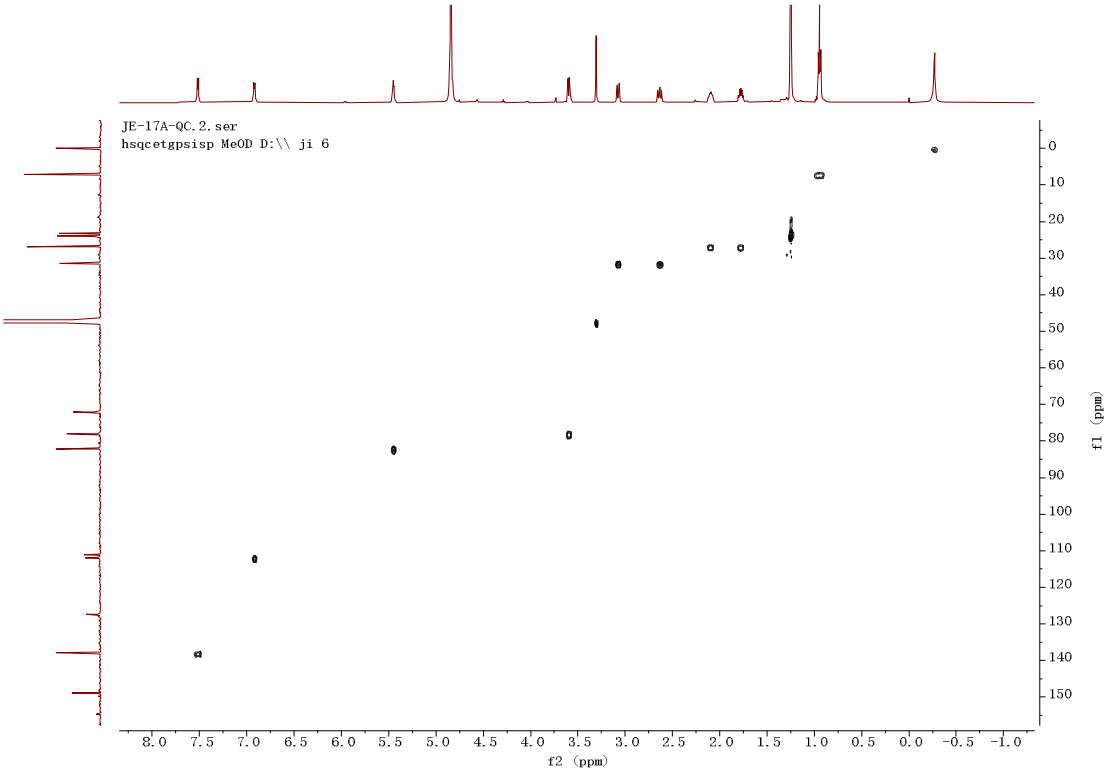
S40 ^{1}H NMR (600 MHz, CD_3OD) spectrum of aspergorakhins E (**5**).



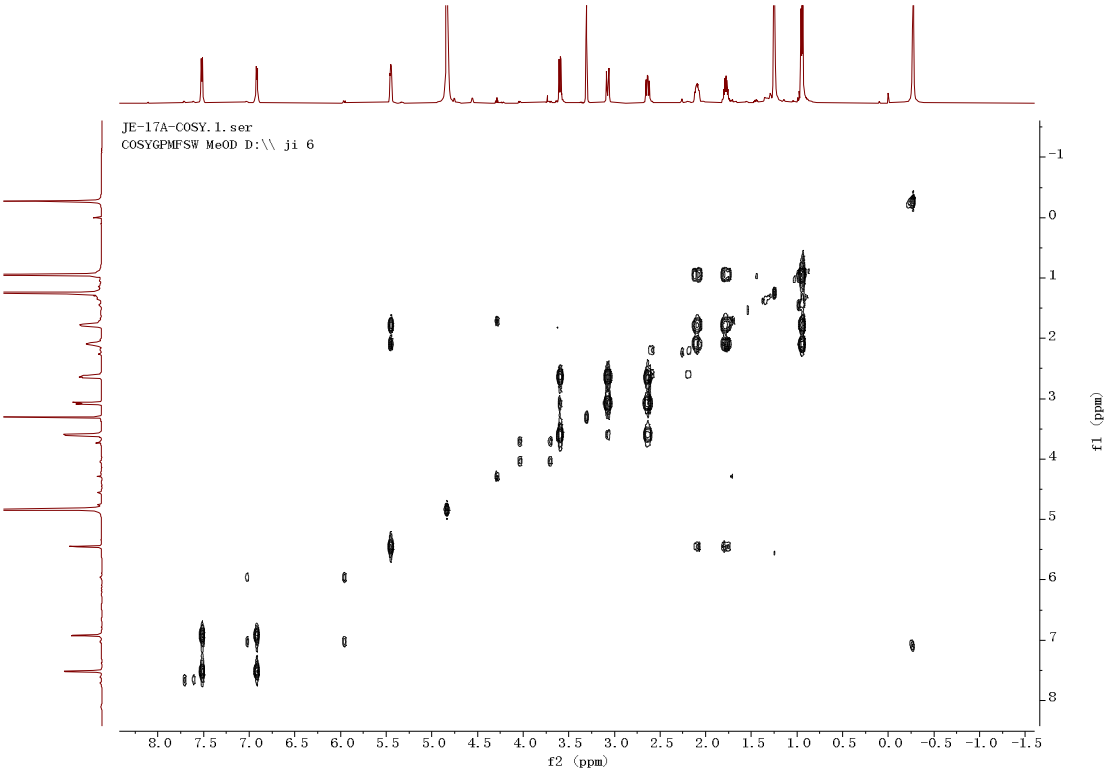
S41 ^{13}C NMR (150 MHz, CD_3OD) spectrum of aspergorakhins E (**5**).



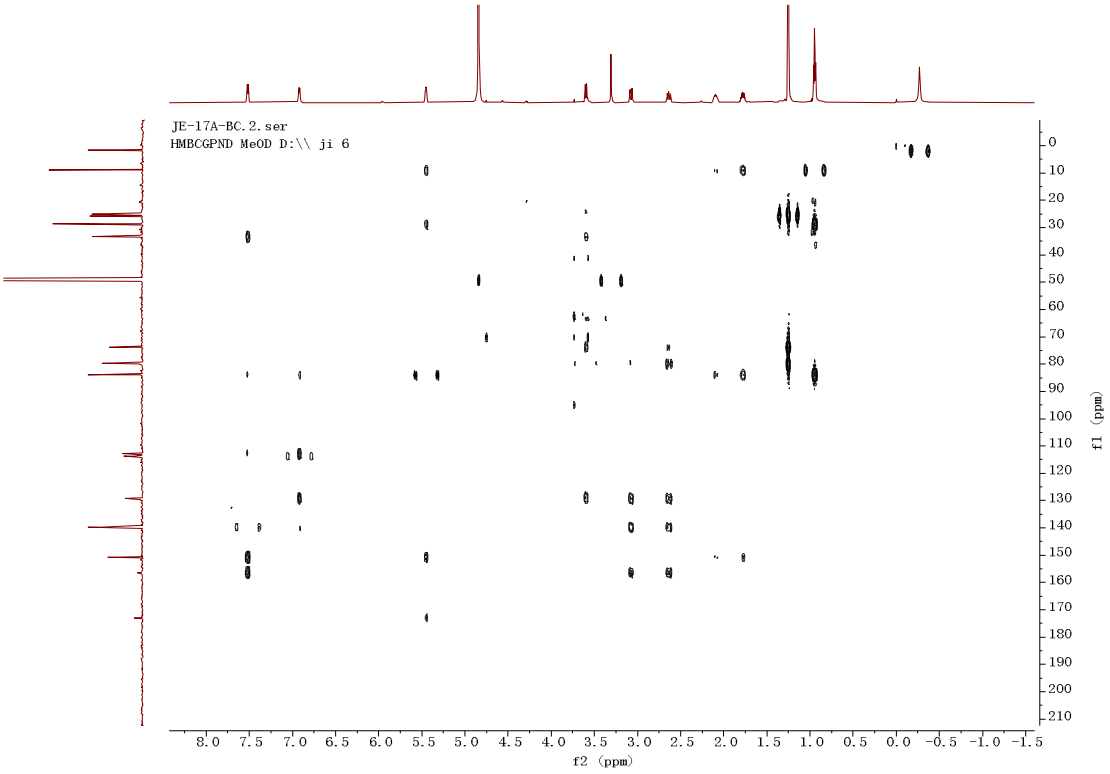
S42 HSQC spectrum of aspergorakhins E (**5**).



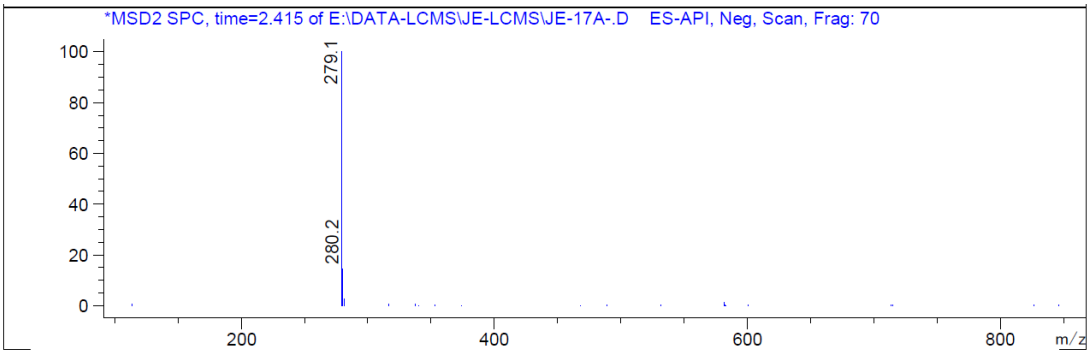
S43 COSY spectrum of aspergorakhins E (**5**).



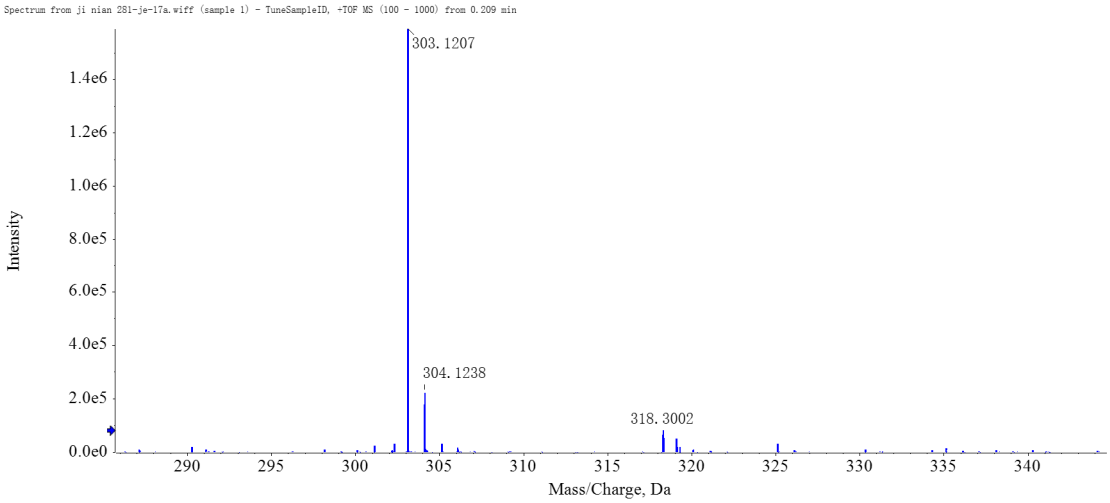
S44 HMBC spectrum of aspergorakhins E (**5**).



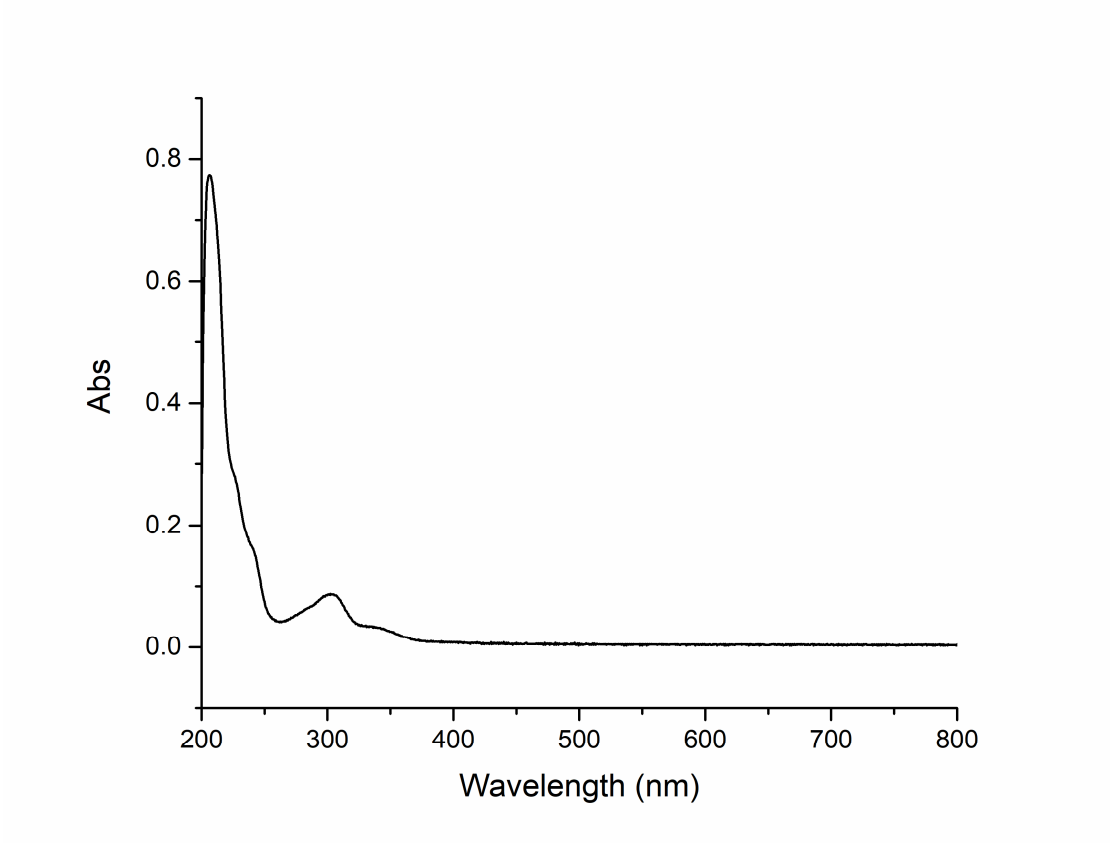
S45 ESIMS spectrum of aspergorakhins E (**5**).



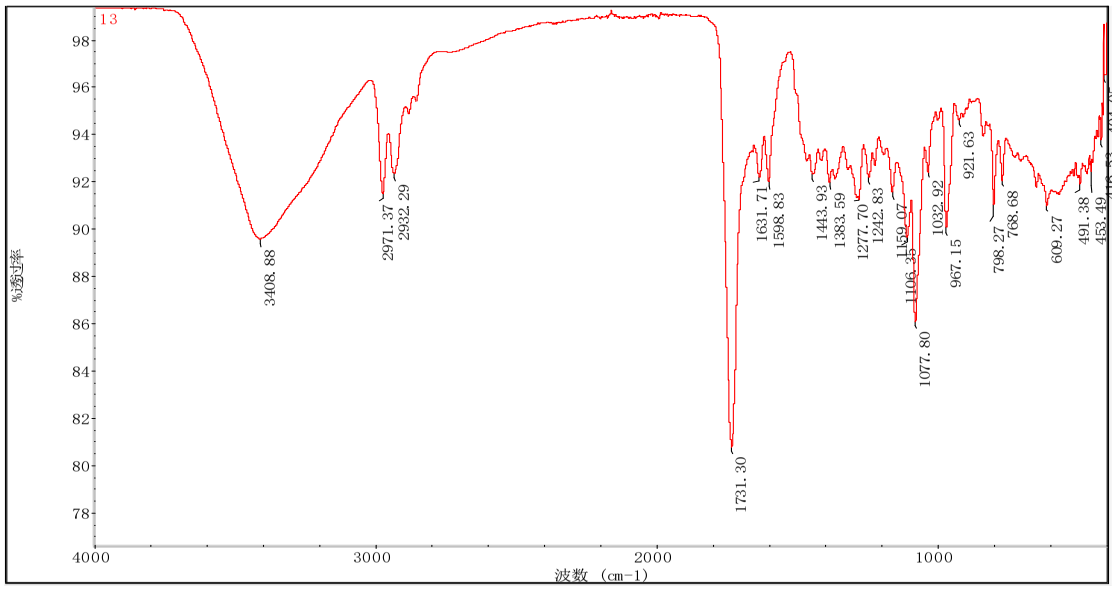
S46 (+)-HRESIMS spectrum of aspergorakhins E (**5**).



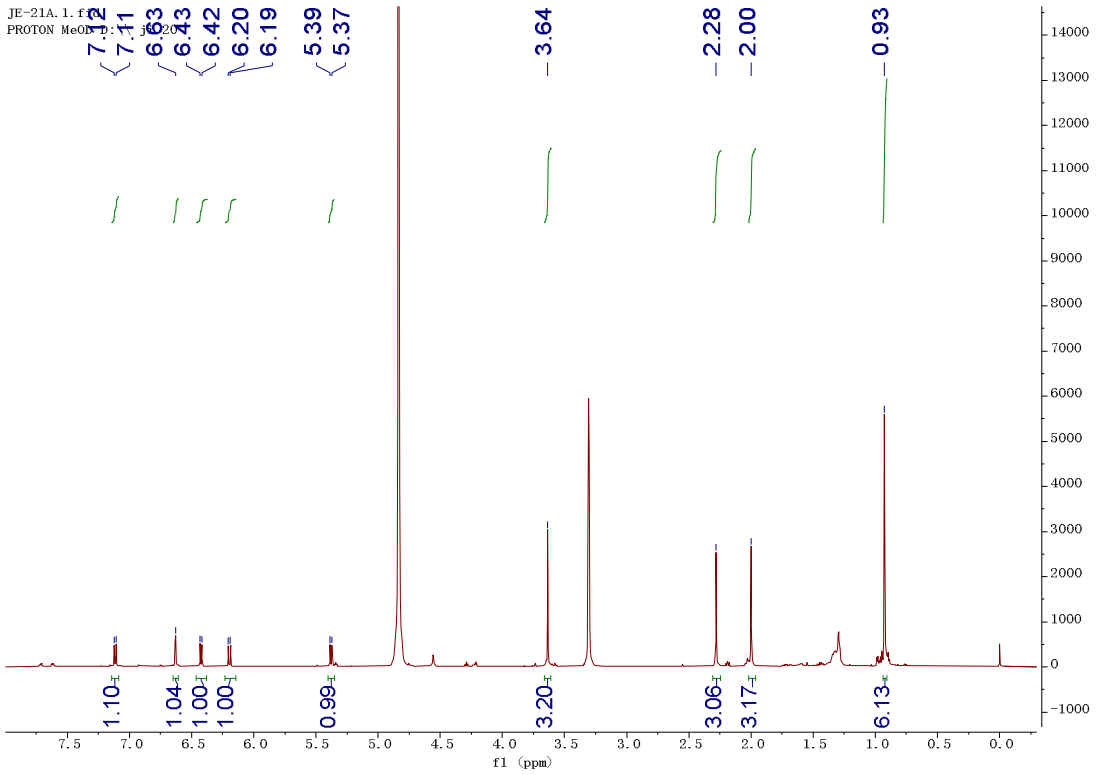
S47 UV spectrum of aspergorakhins E (**5**).



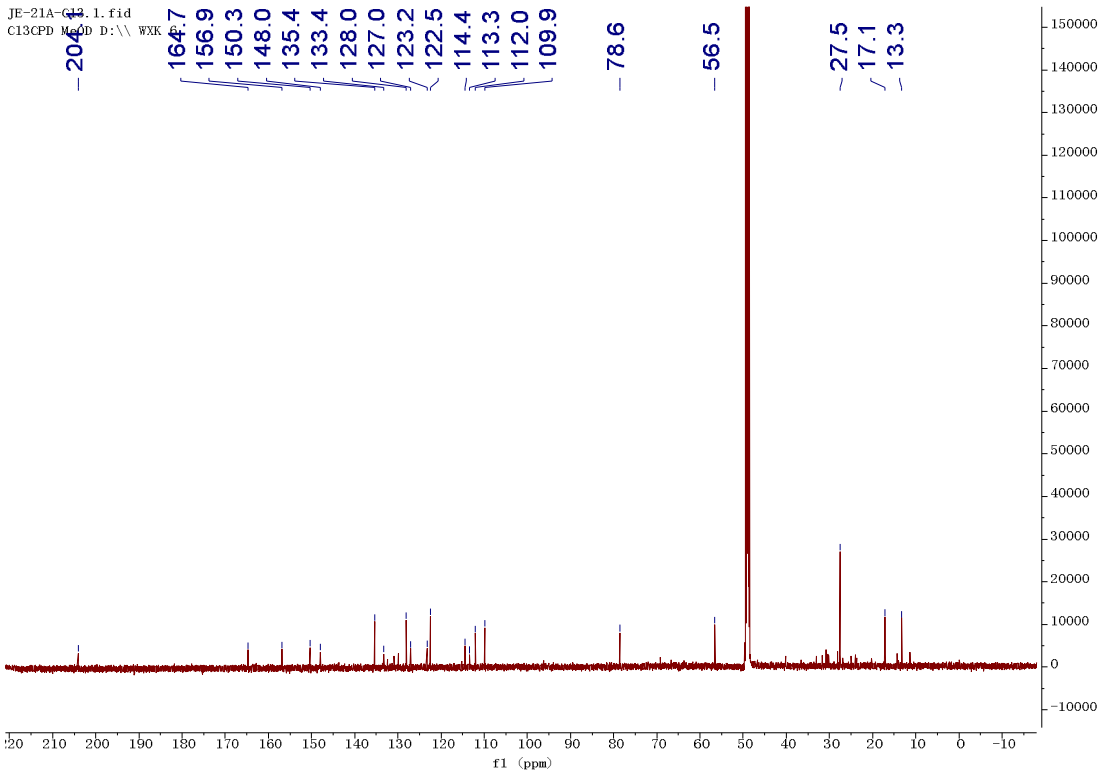
S48 IR spectrum of aspergorakhins E (**5**).



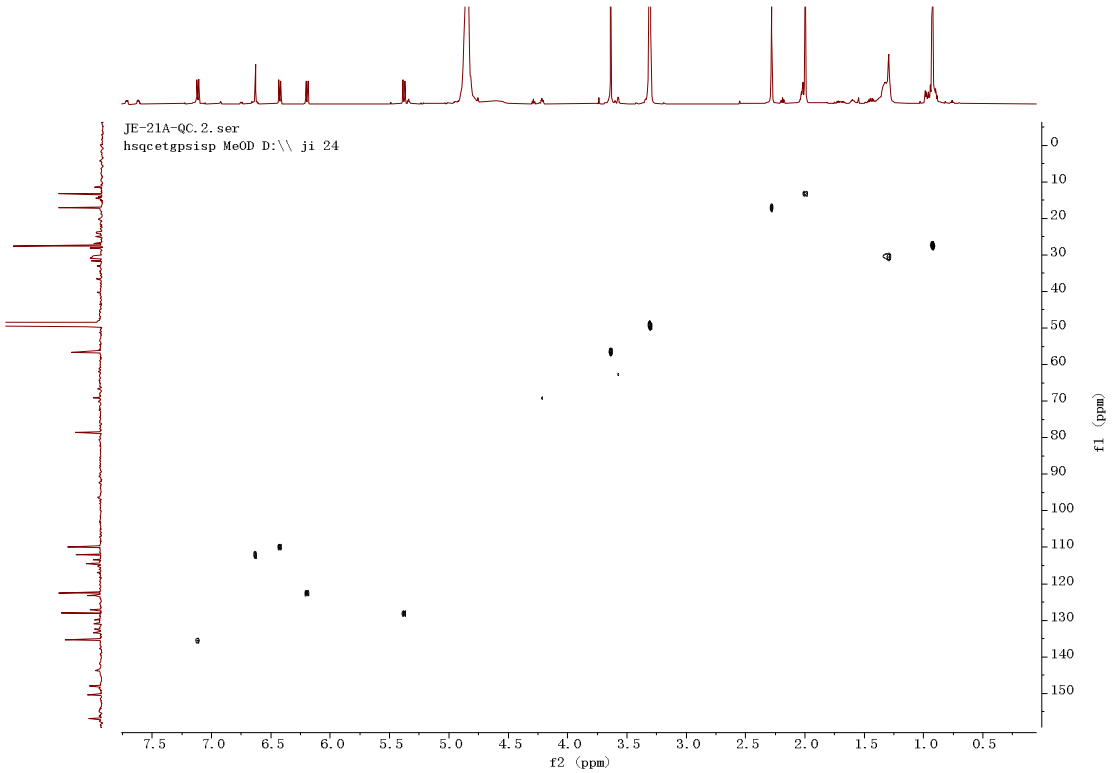
S49 ^{1}H NMR (600 MHz, CD_3OD) spectrum of aspergorakhins F (**6**).



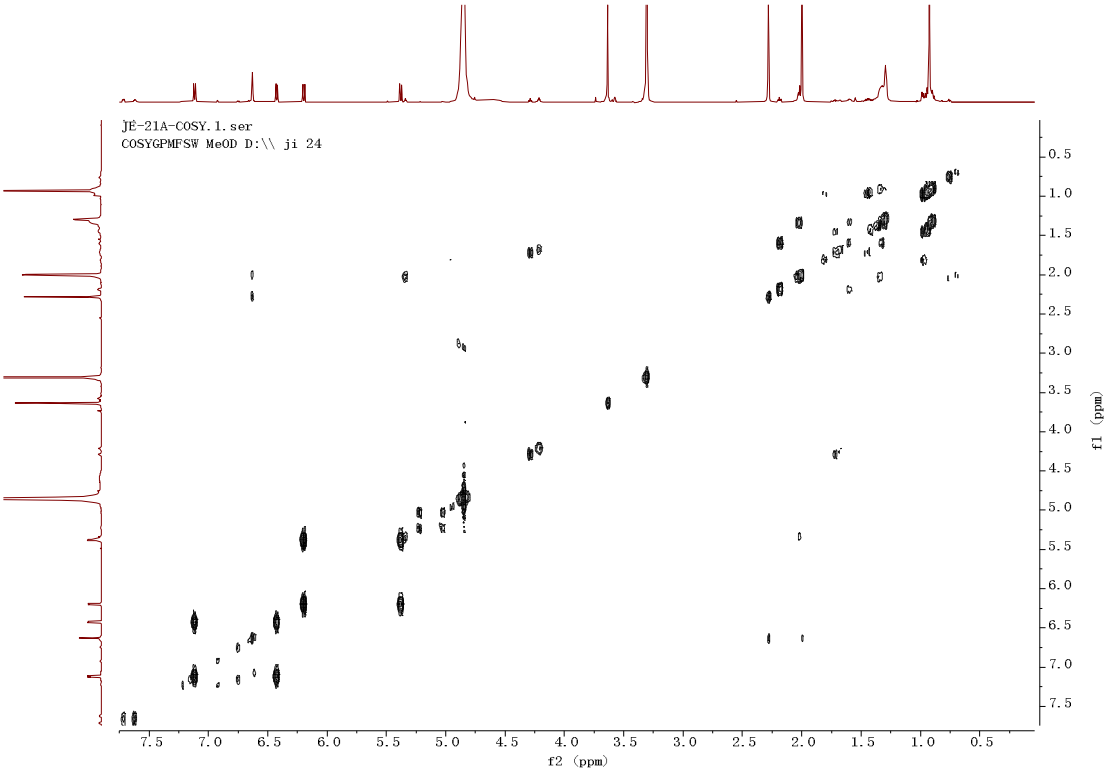
S50 ^{13}C NMR (150 MHz, CD_3OD) spectrum of aspergorakhins F (**6**).



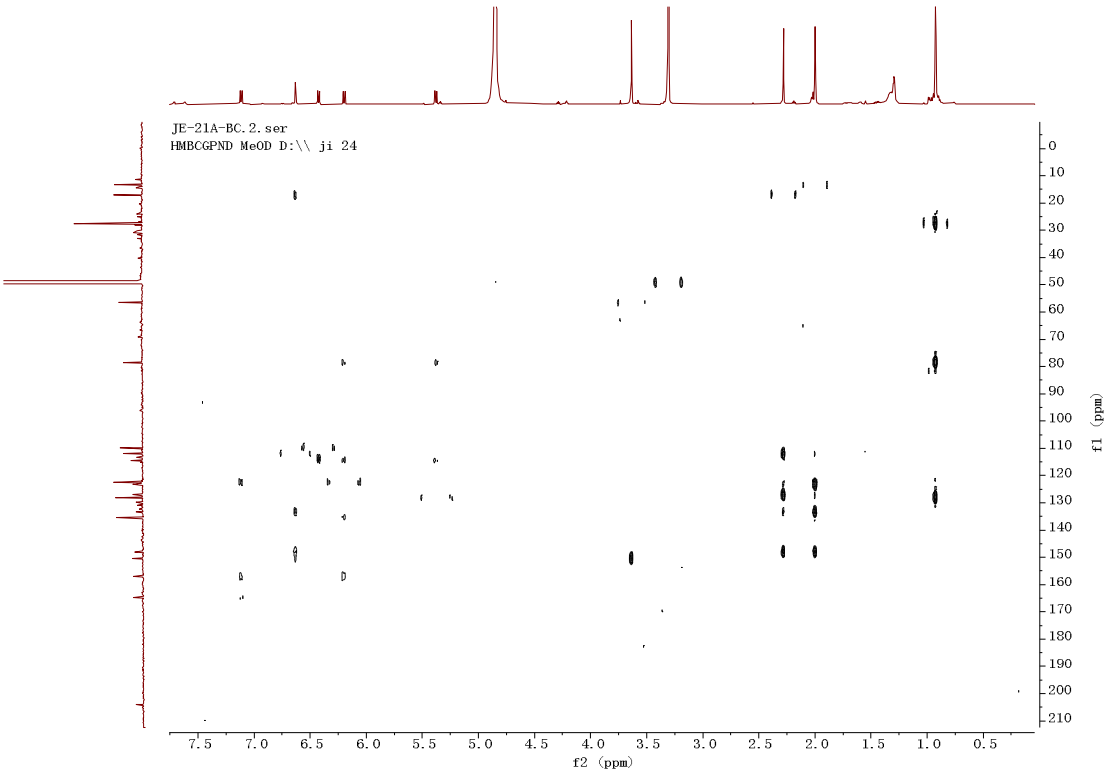
S51 HSQC spectrum of aspergorakhins F (**6**).



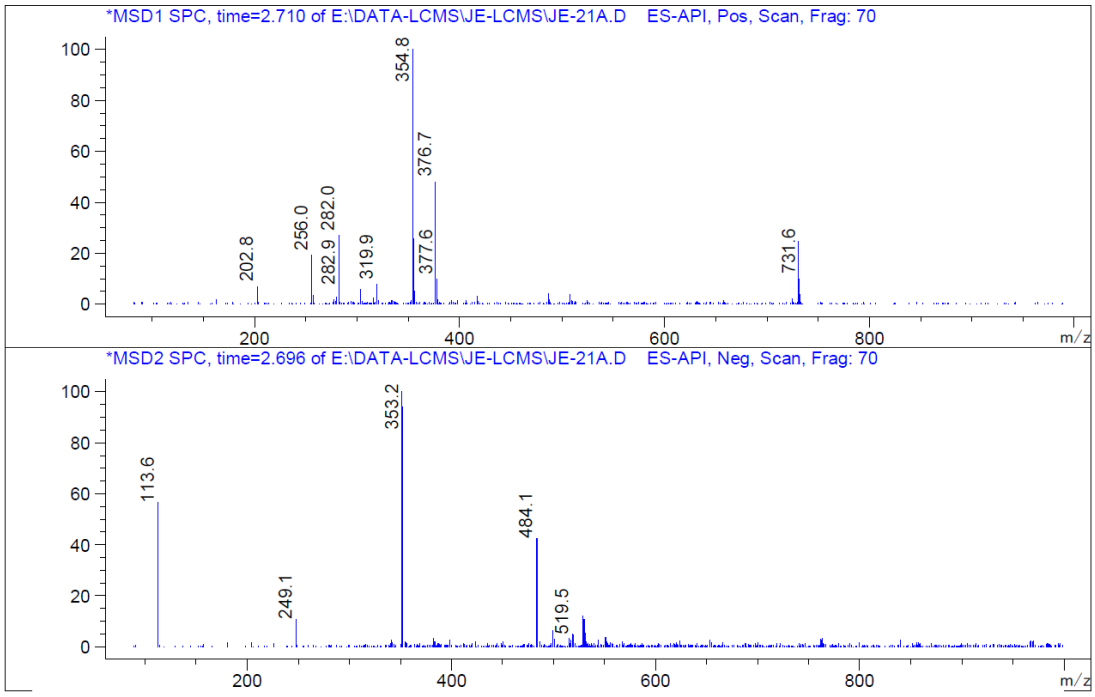
S52 COSY spectrum of aspergorakhins F (**6**).



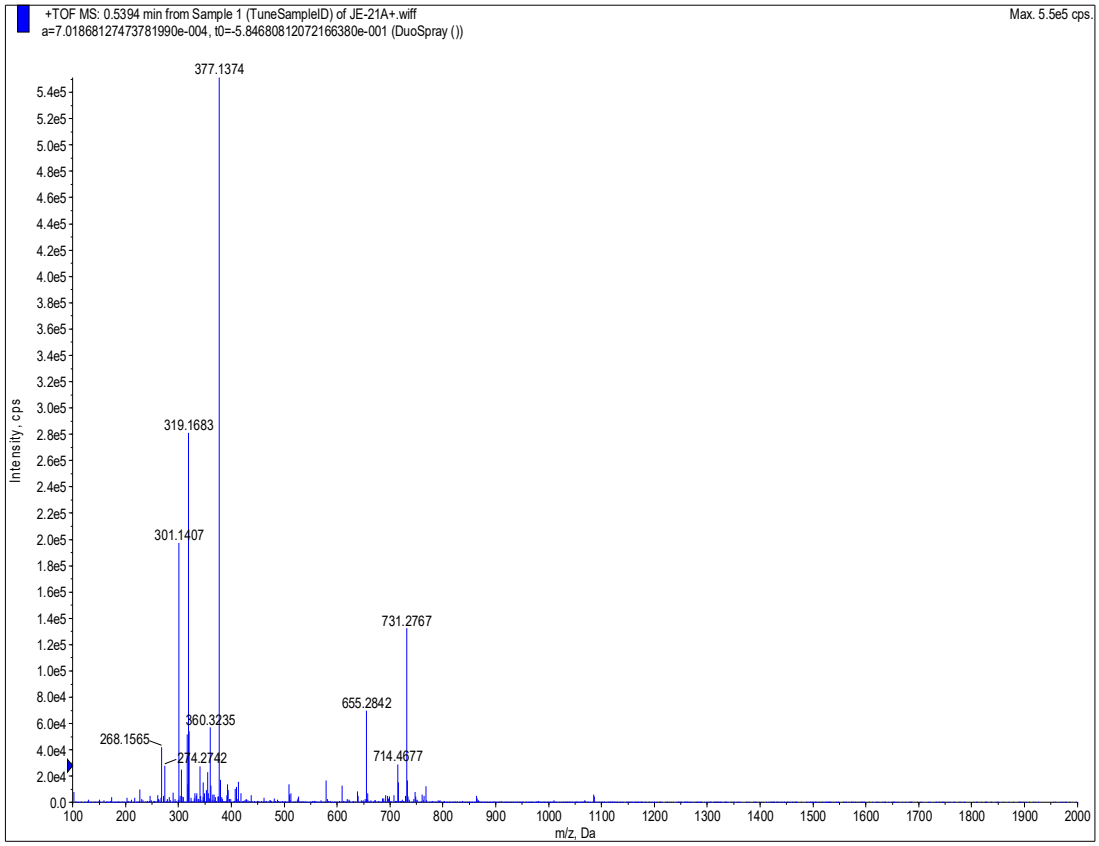
S53 HMBC spectrum of aspergorakhins F (**6**).



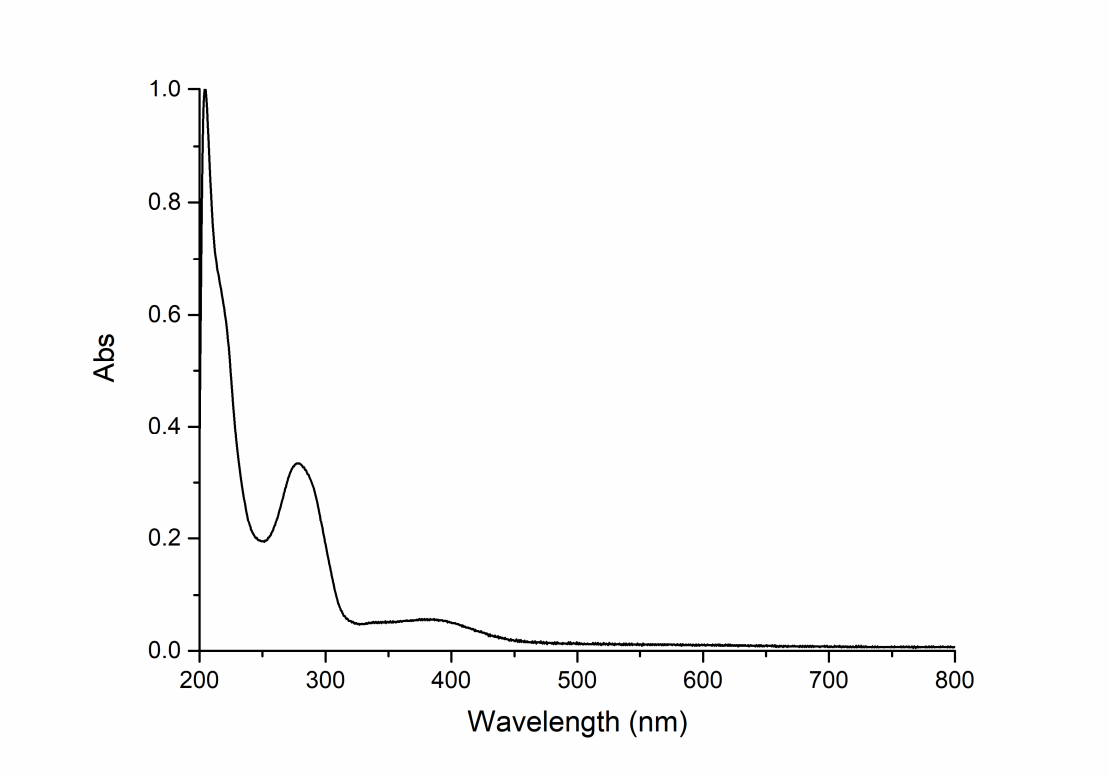
S54 ESIMS spectrum of aspergorakhins F (**6**).



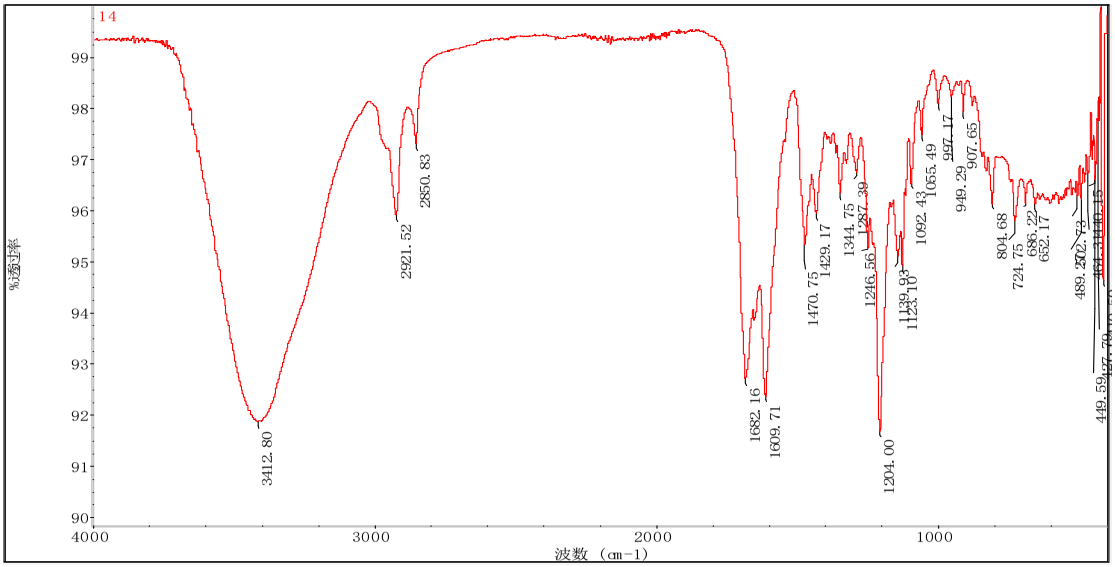
S55 (+)-HRESIMS spectrum of aspergorakhins F (**6**).



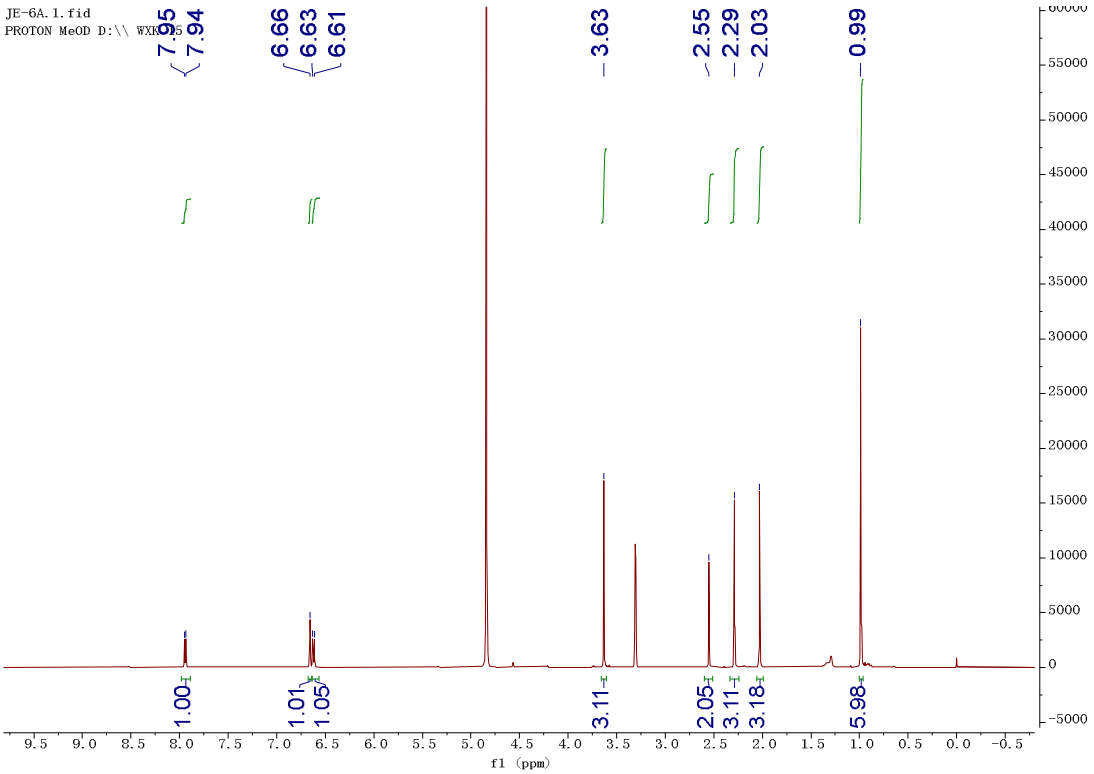
S56 UV spectrum of aspergorakhins F (**6**).



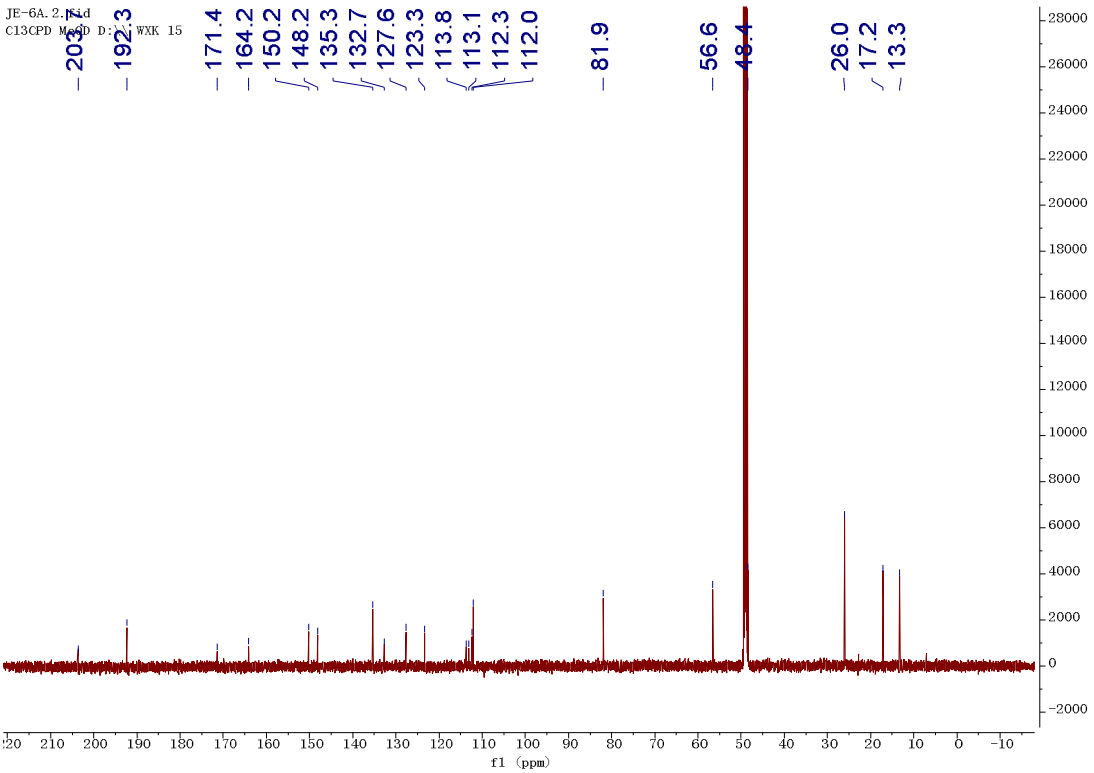
S57 IR spectrum of aspergorakhins F (**6**).



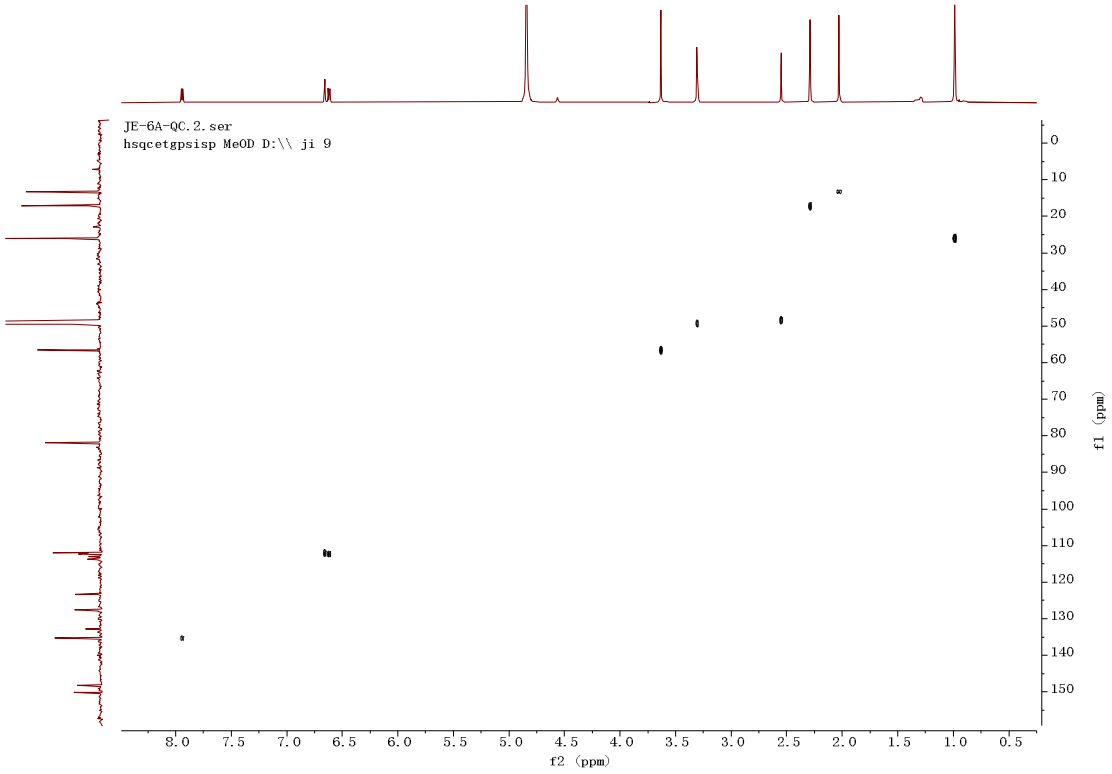
S58 ^{1}H NMR (600 MHz, CD_3OD) spectrum of aspergorakhins G (**7**).



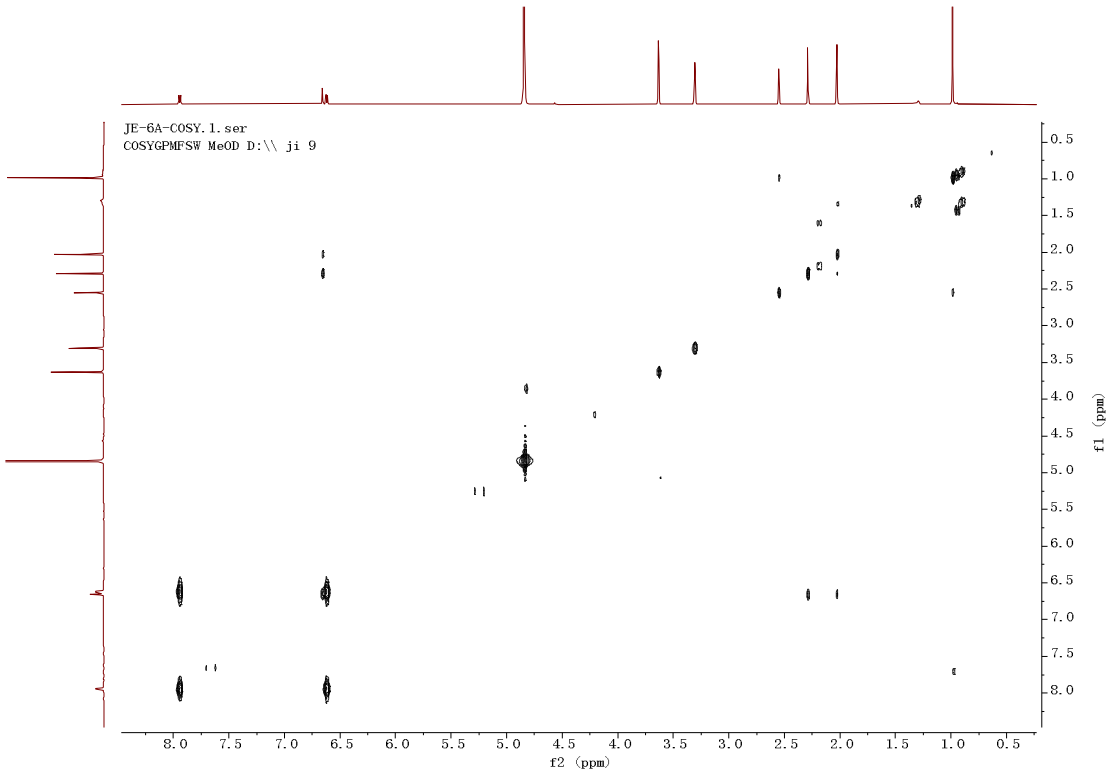
S59 ^{13}C NMR (150 MHz, CD_3OD) spectrum of aspergorakhins G (**7**).



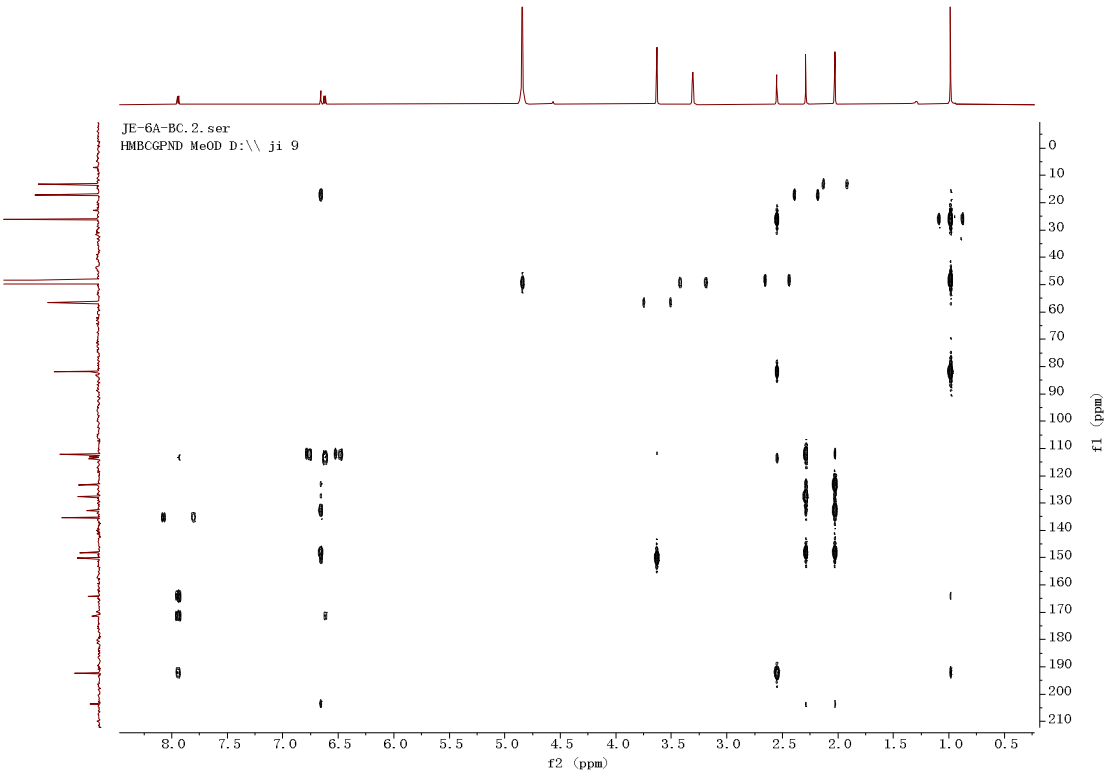
S60 HSQC spectrum of aspergorakhins G (**7**).



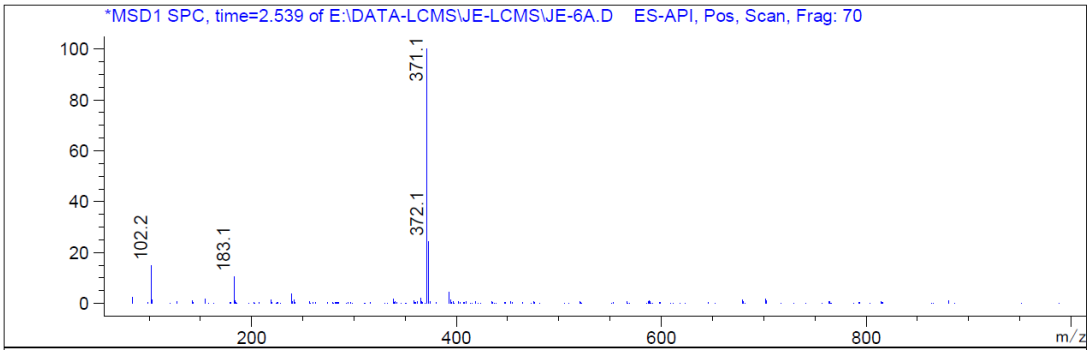
S61 COSY spectrum of aspergorakhins G (**7**).



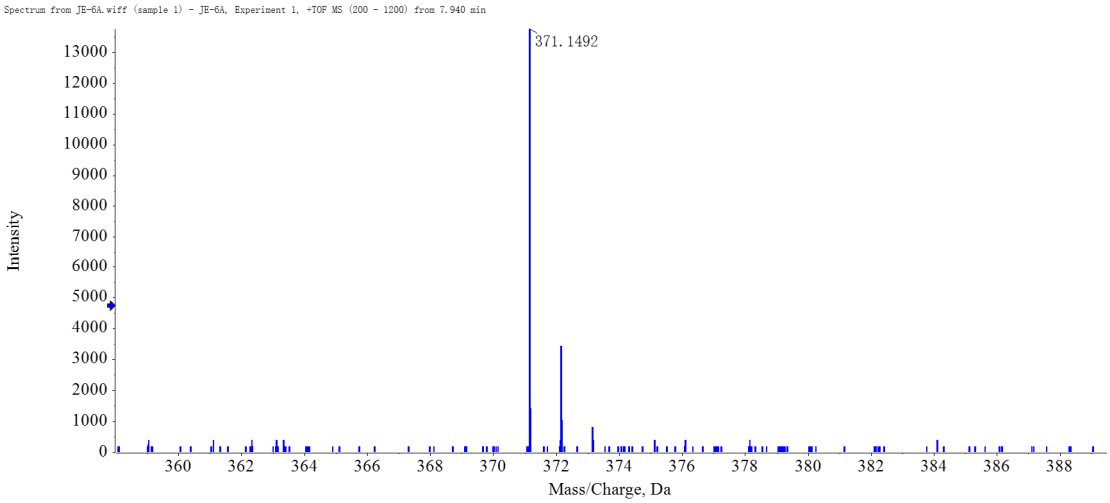
S62 HMBC spectrum of aspergorakhins G (**7**).



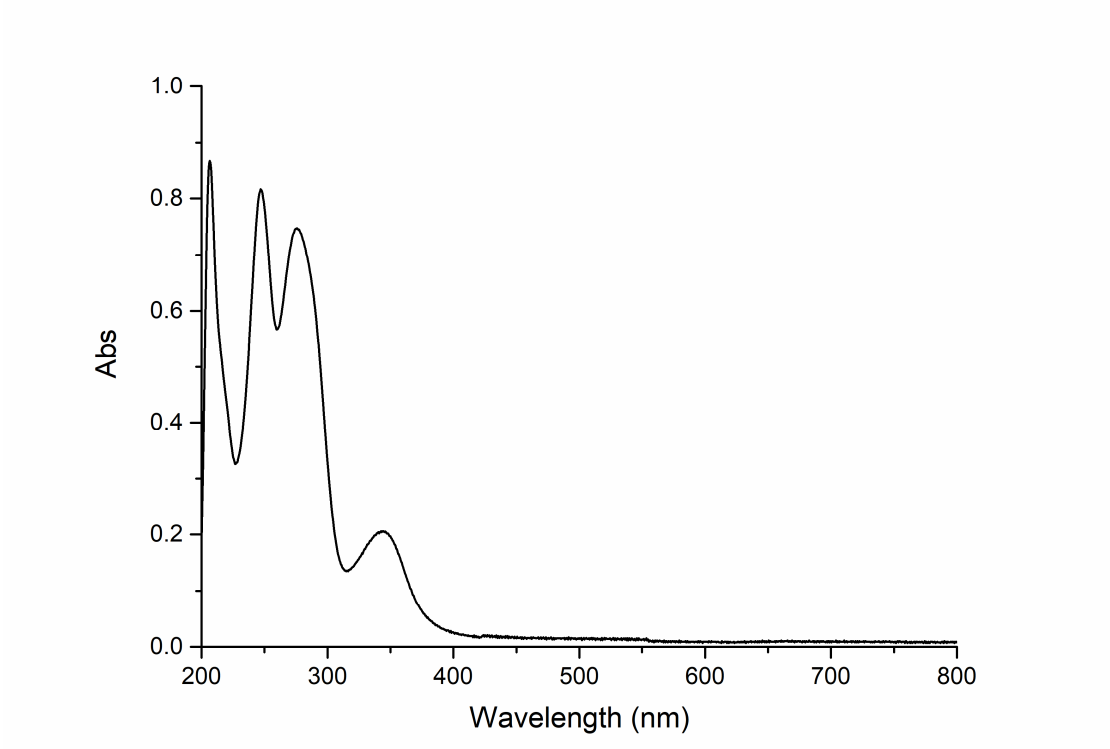
S63 ESIMS spectrum of aspergorakhins G (**7**).



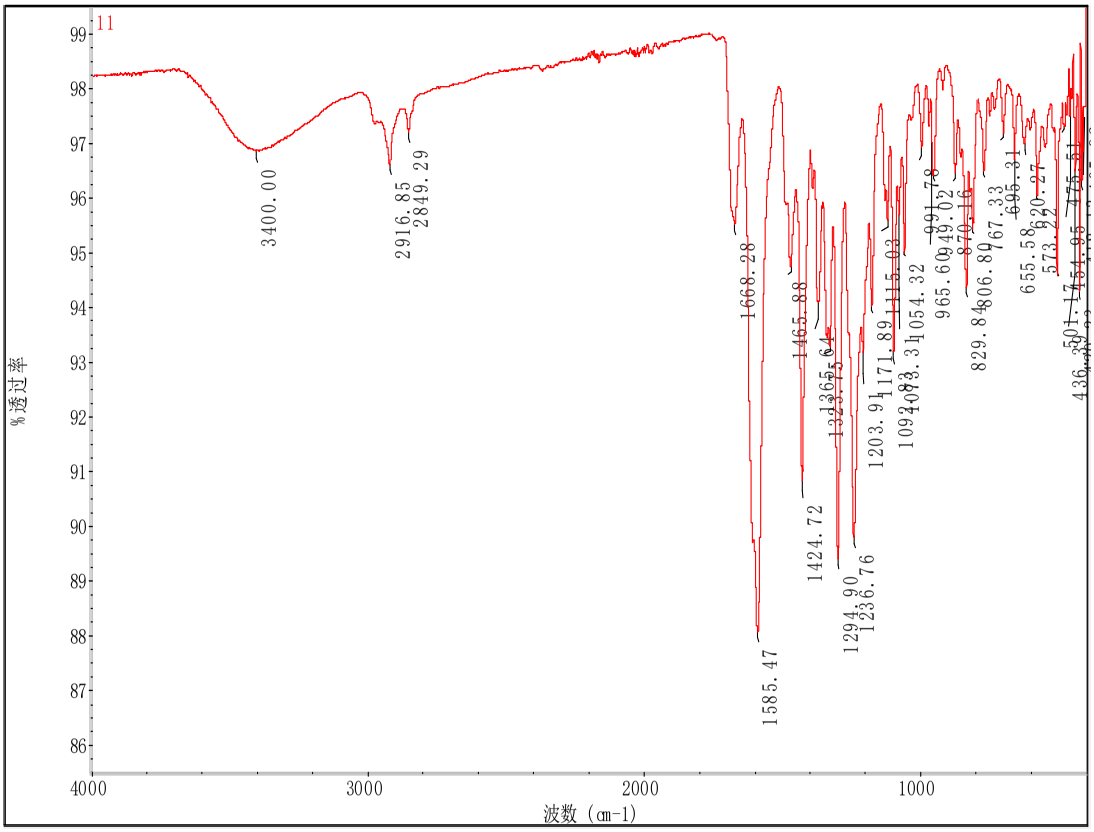
S64 (+)-HRESIMS spectrum of aspergorakhins G (**7**).



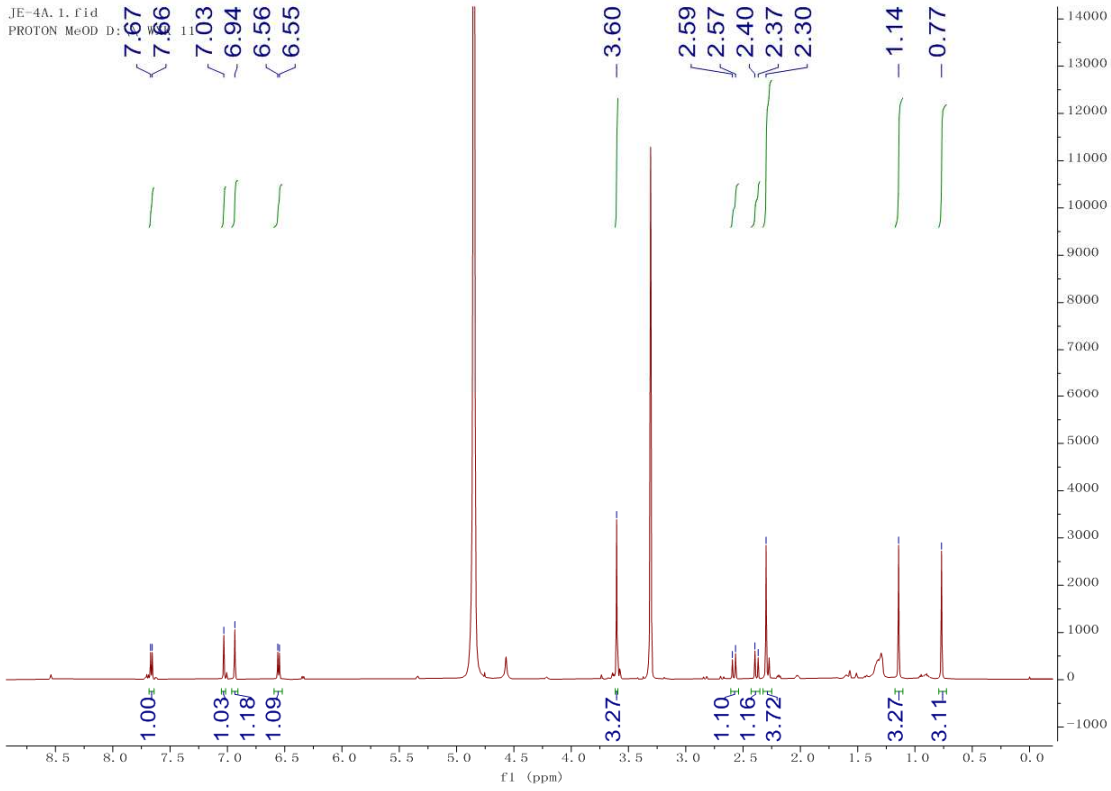
S65 UV spectrum of aspergorakhins G (**7**).



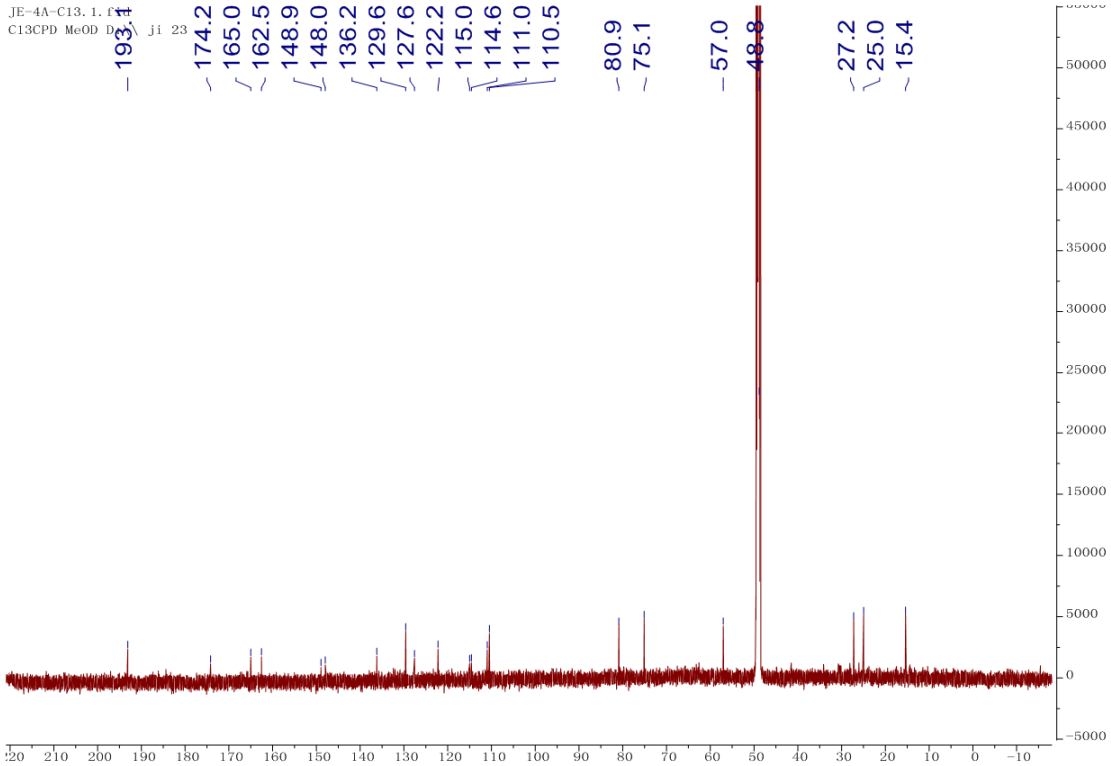
S66 IR spectrum of aspergorakhins G (**7**).



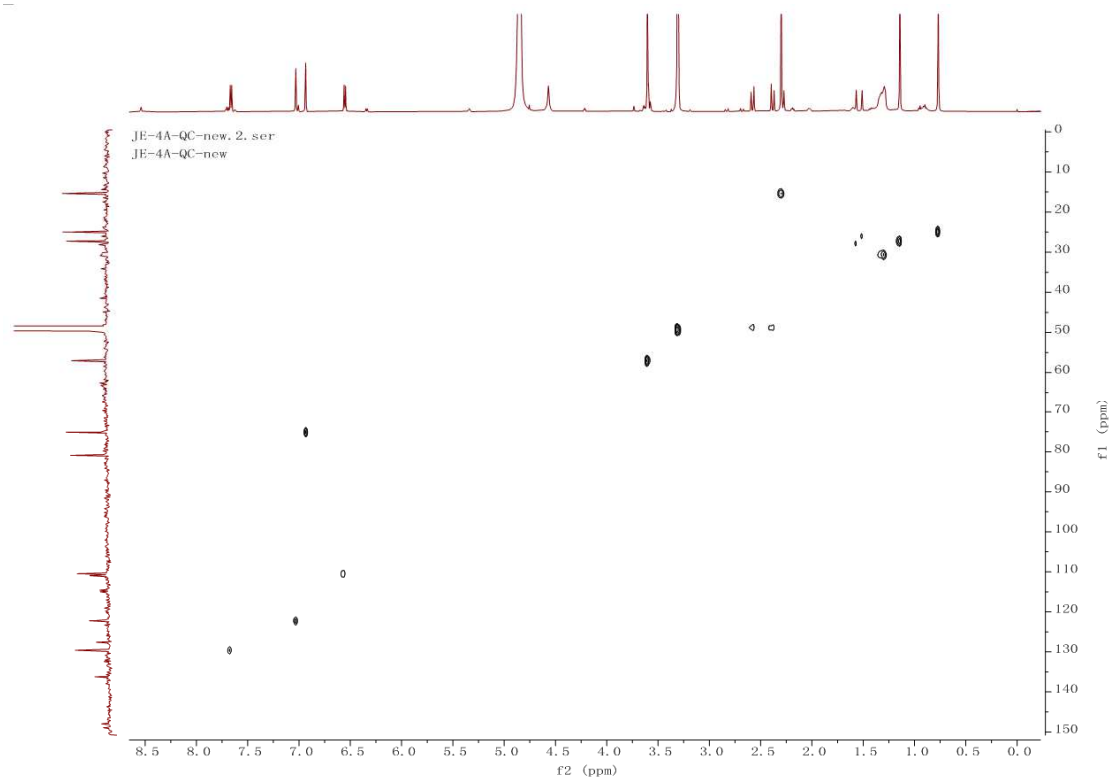
S67 ^{1}H NMR (600 MHz, CD_3OD) spectrum of aspergorakhins H (**8**).



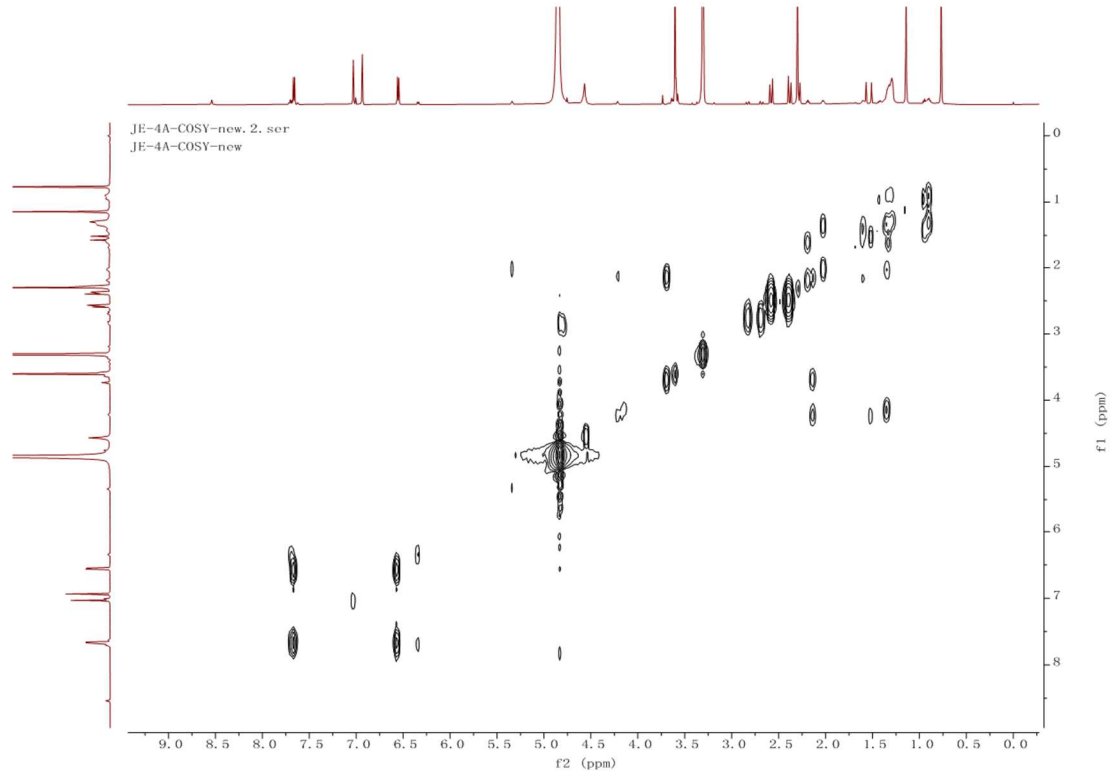
S68 ^{13}C NMR (150 MHz, CD_3OD) spectrum of aspergorakhins H (**8**).



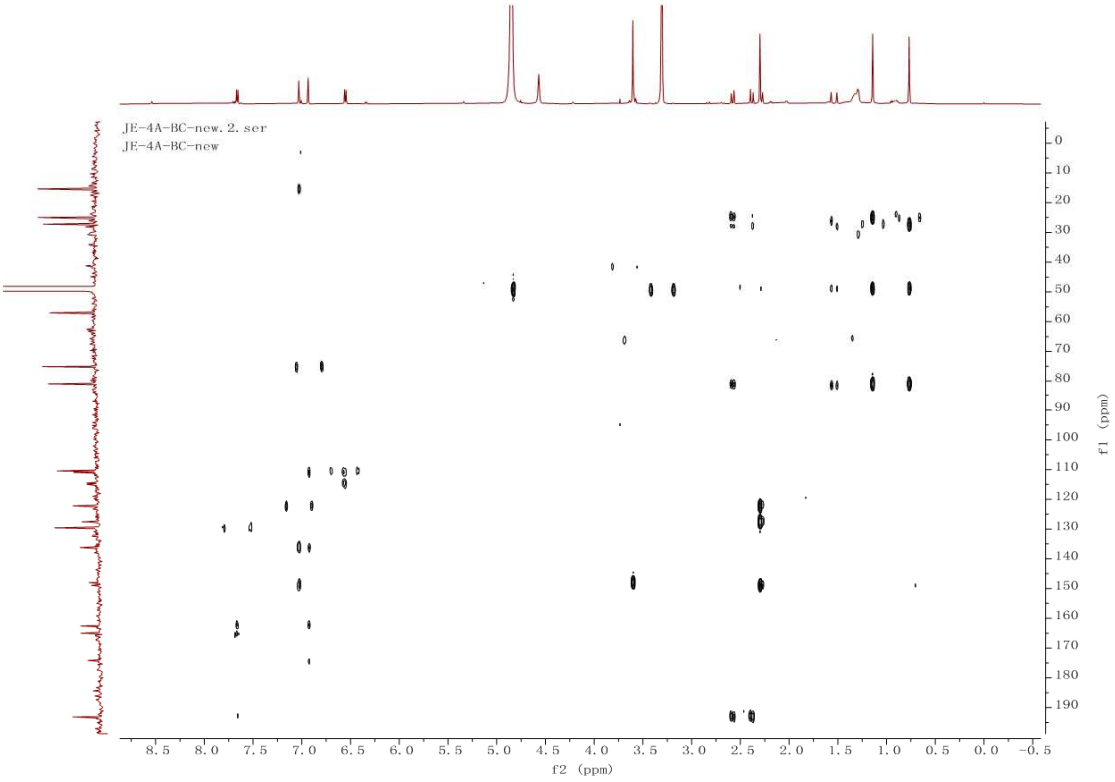
S69 HSQC spectrum of aspergorakhins H (**8**).



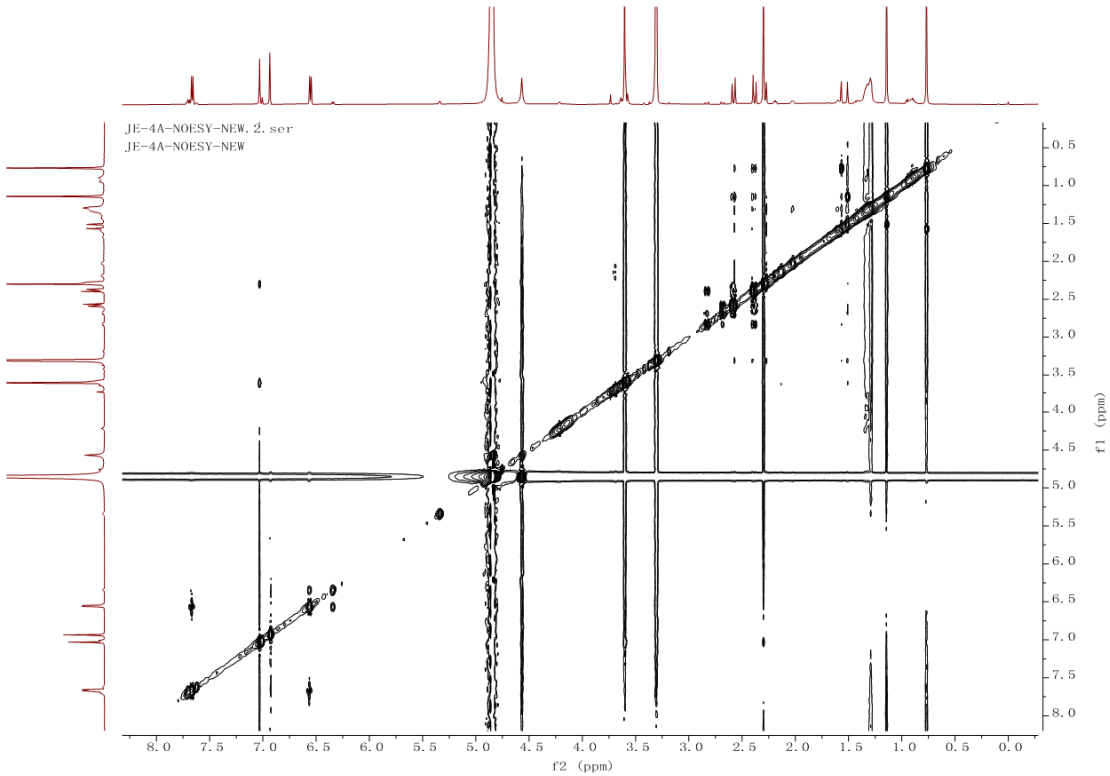
S70 COSY spectrum of aspergorakhins H (**8**).



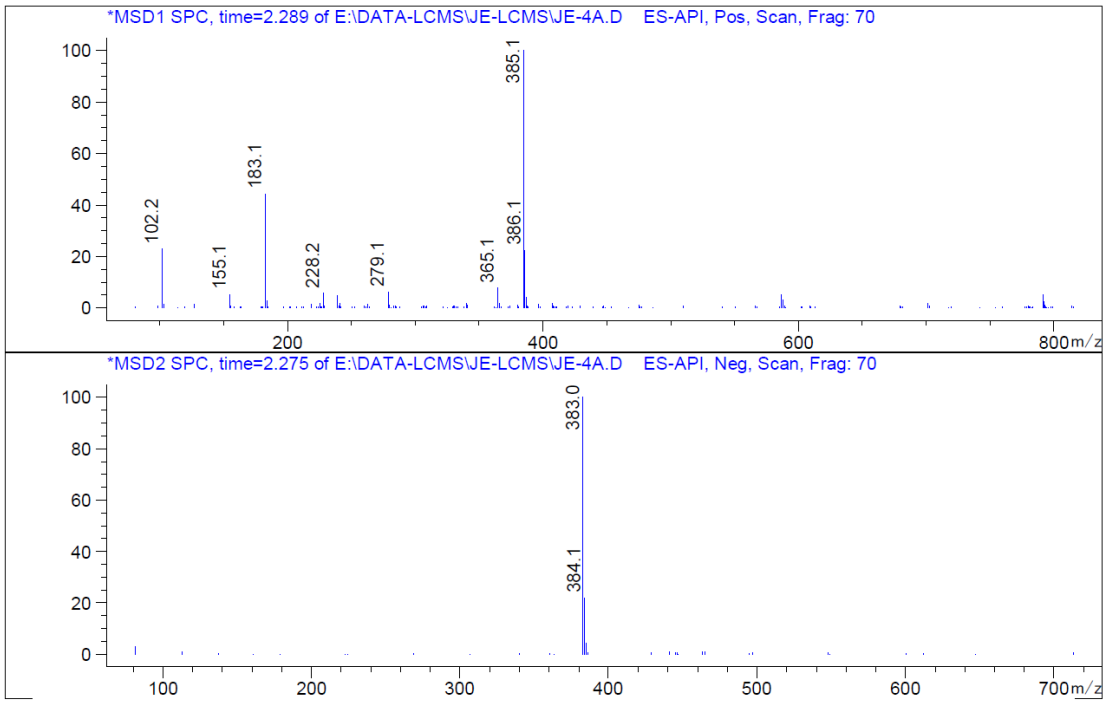
S71 HMBC spectrum of aspergorakhins H (**8**).



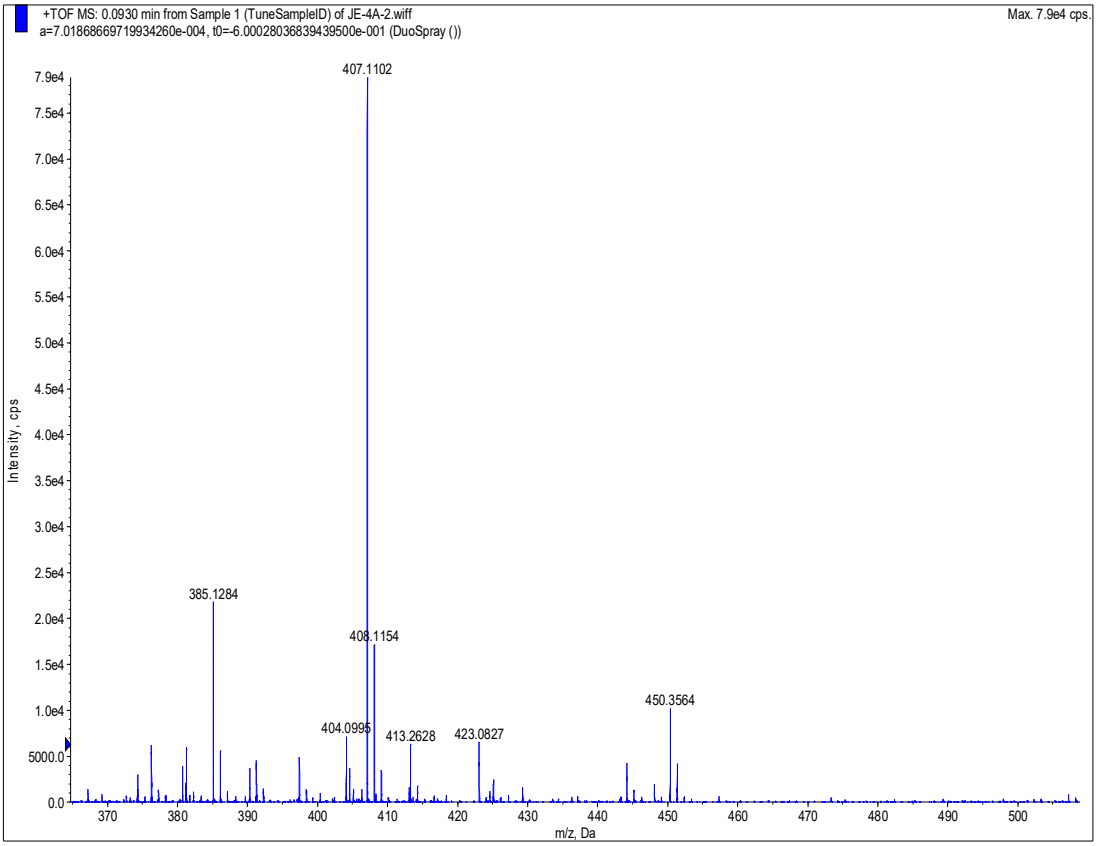
S72 NOESY spectrum of aspergorakhins H (**8**).



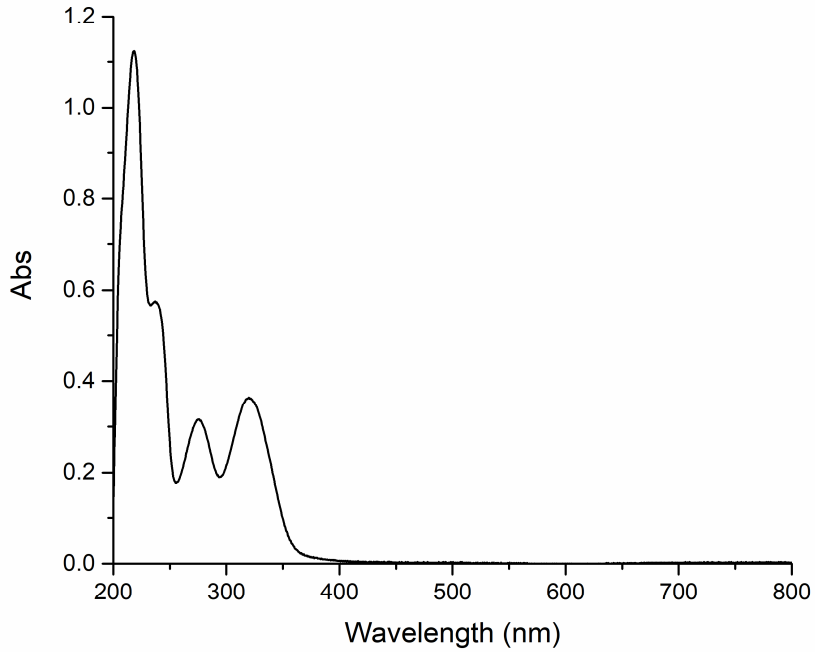
S73 ESIMS spectrum of aspergorakhins H (**8**).



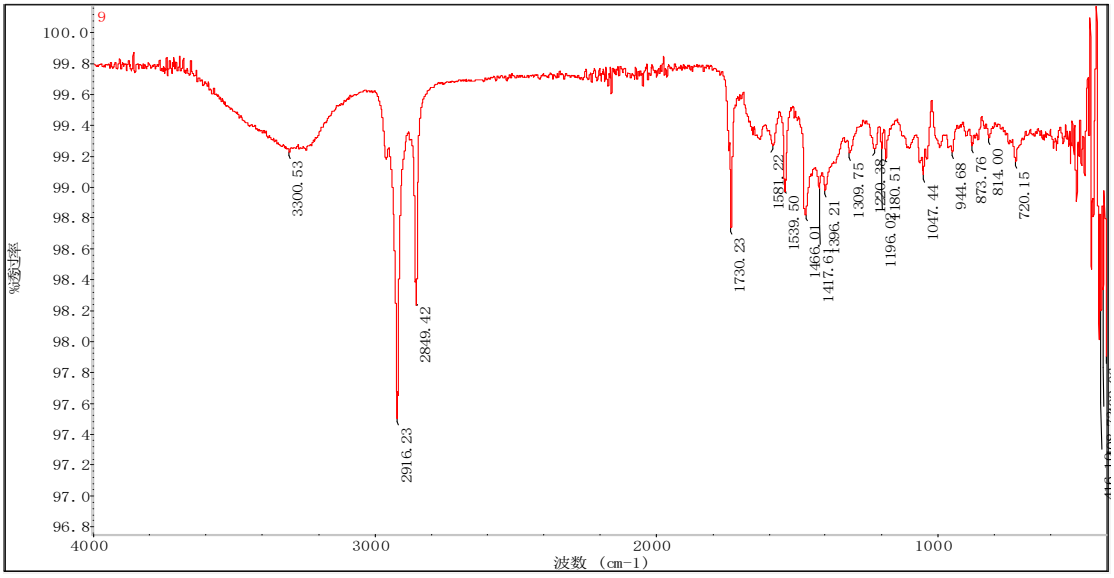
S74 (+)-HRESIMS spectrum of aspergorakhins H (**8**).



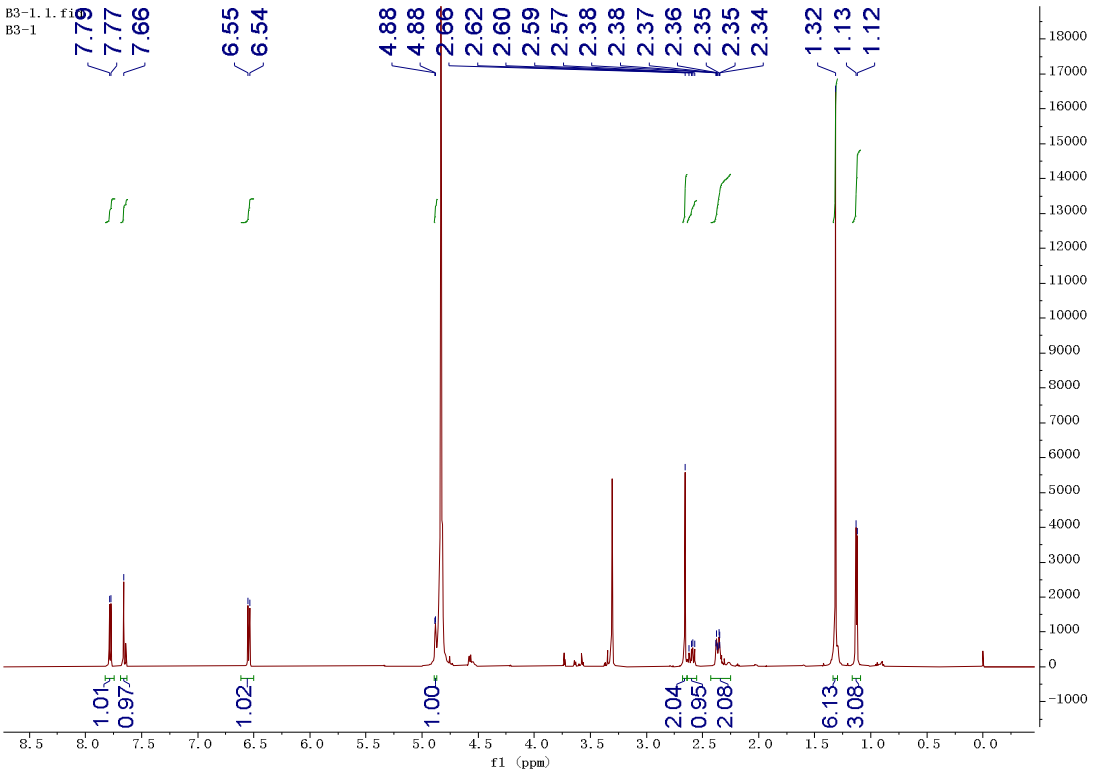
S75 UV spectrum of aspergorakhins H (**8**).



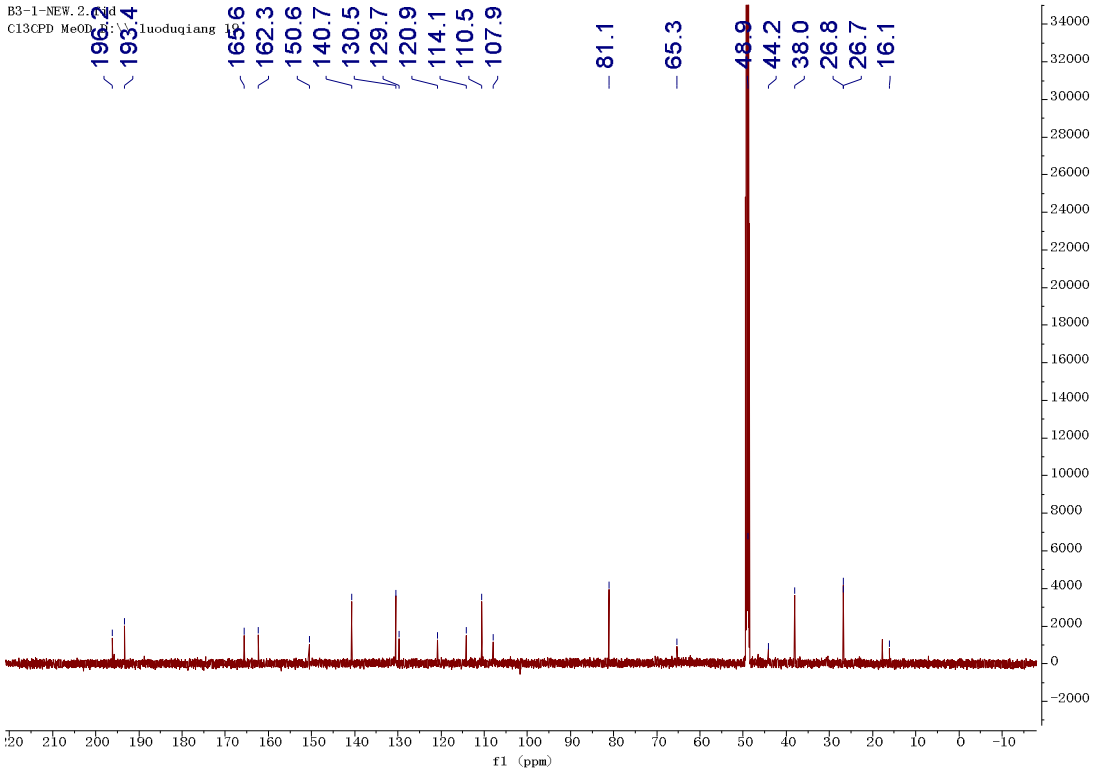
S76 IR spectrum of aspergorakhins H (**8**).



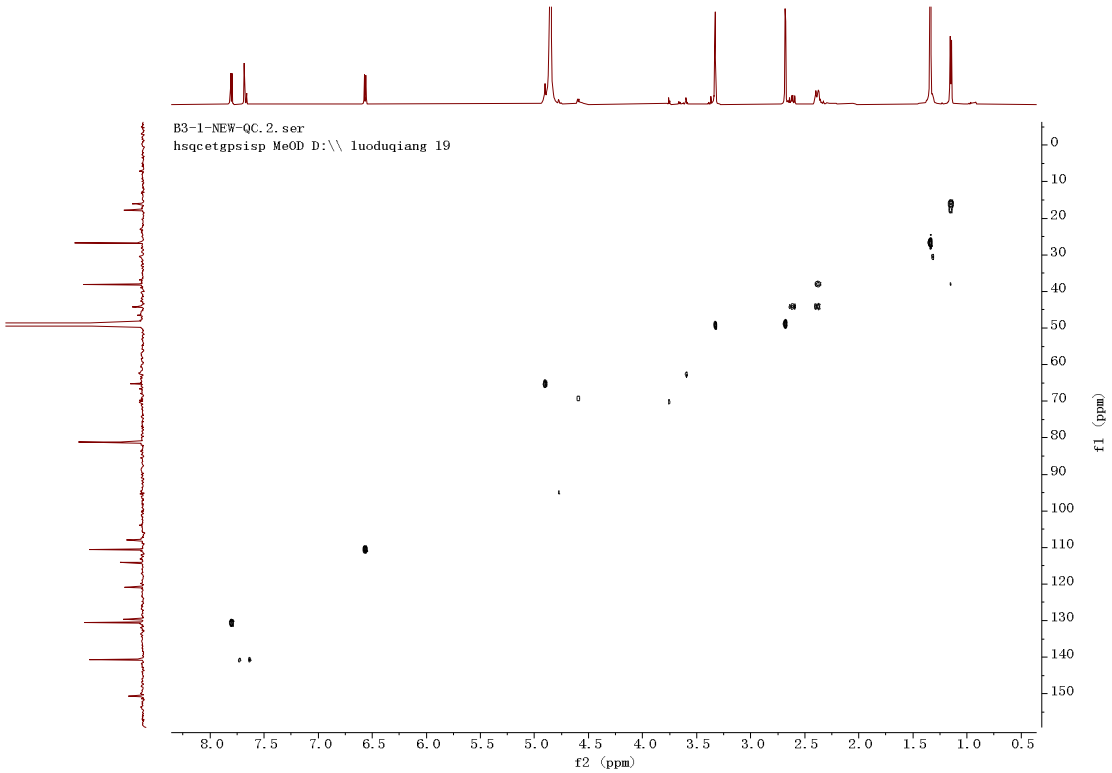
S77 ^{1}H NMR (600 MHz, CD_3OD) spectrum of aspergorakhins I (**9**).



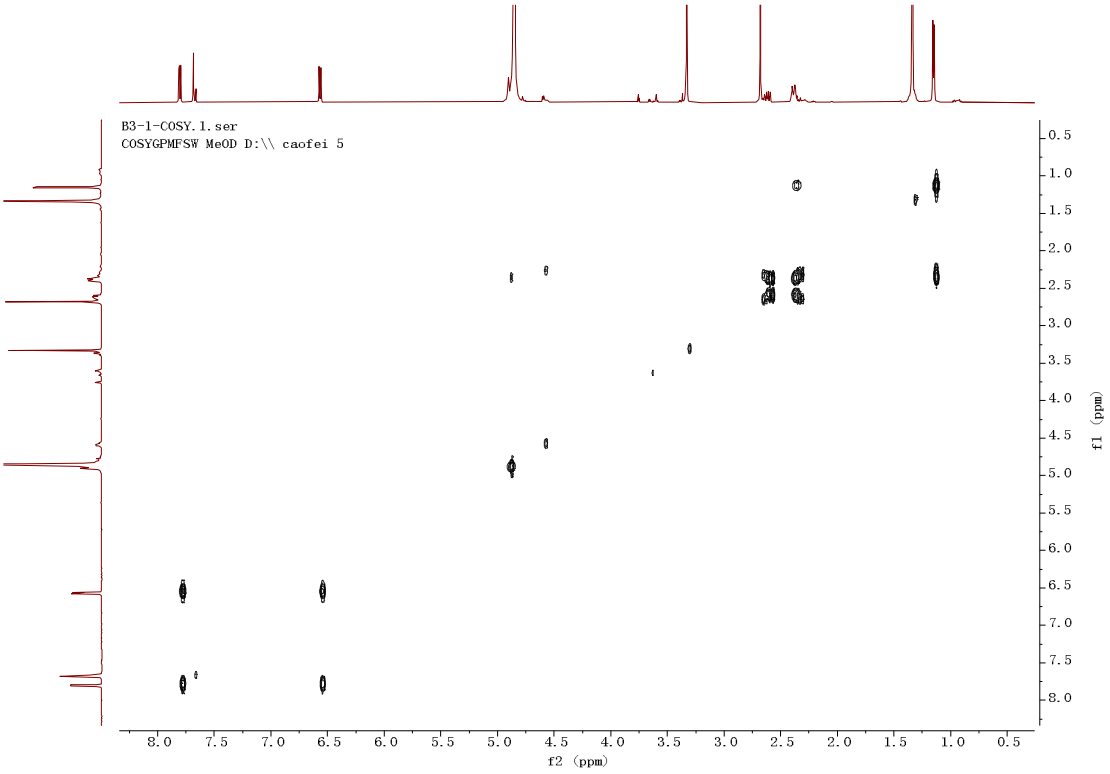
S78 ^{13}C NMR (150 MHz, CD_3OD) spectrum of aspergorakhins I (**9**).



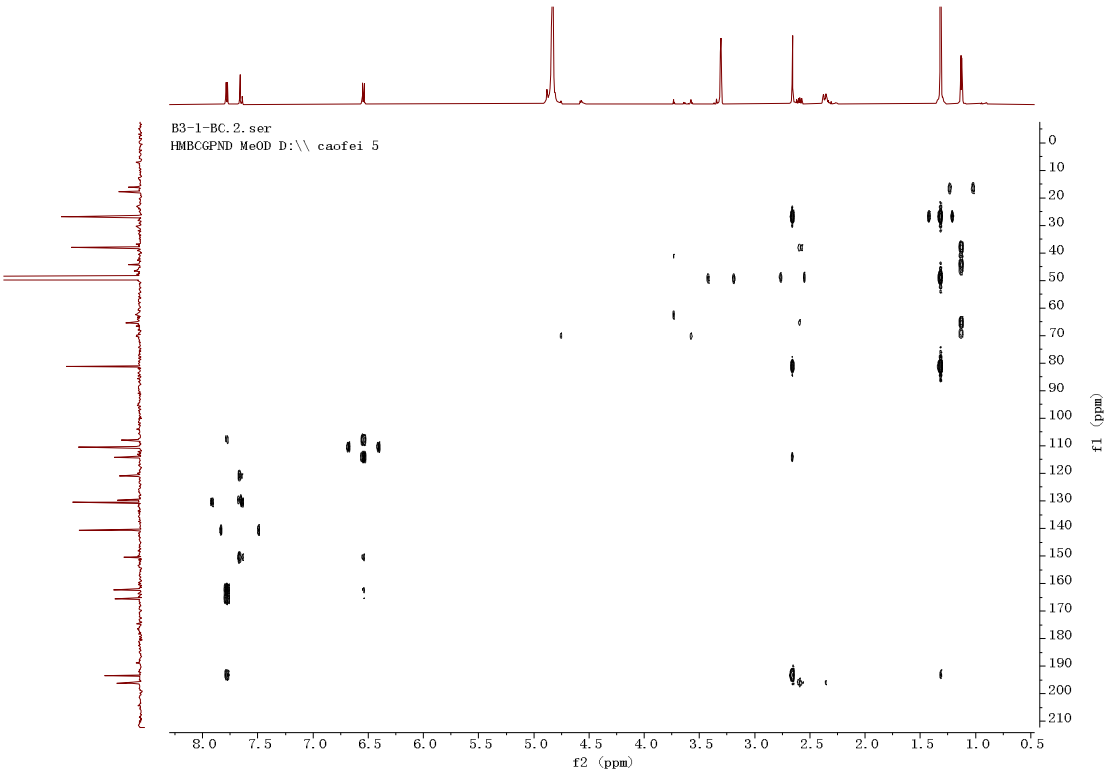
S79 HSQC spectrum of aspergorakhins I (**9**).



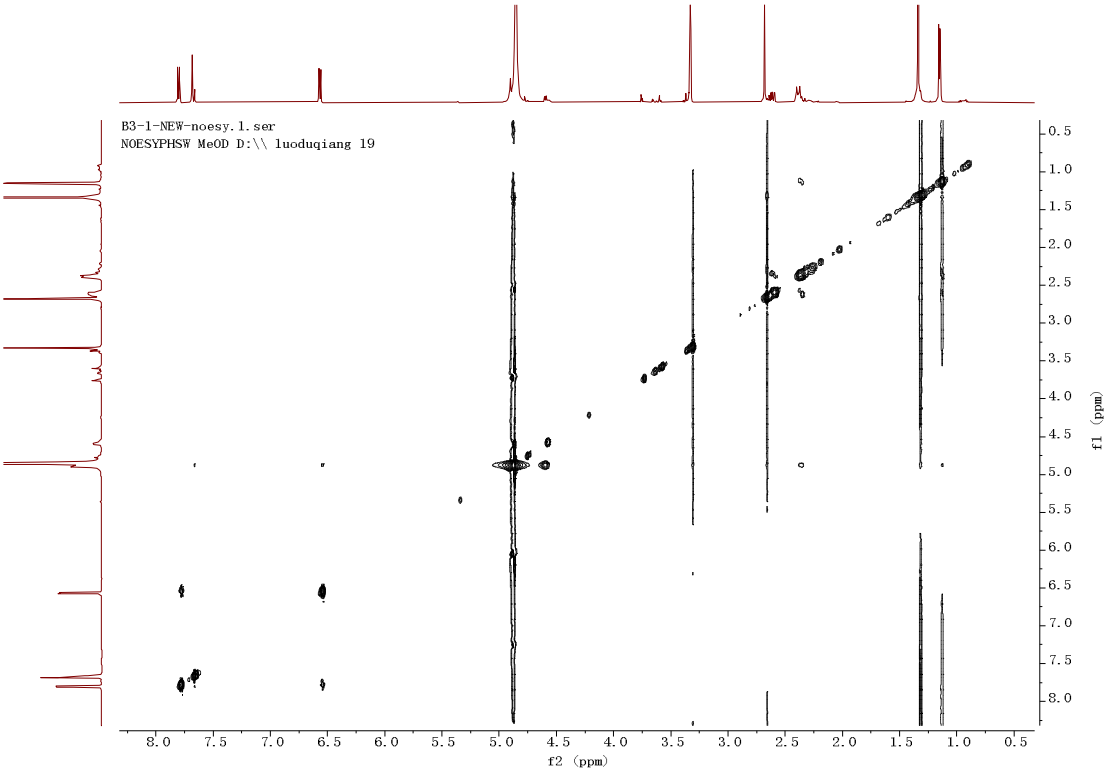
S80 COSY spectrum of aspergorakhins I (**9**).



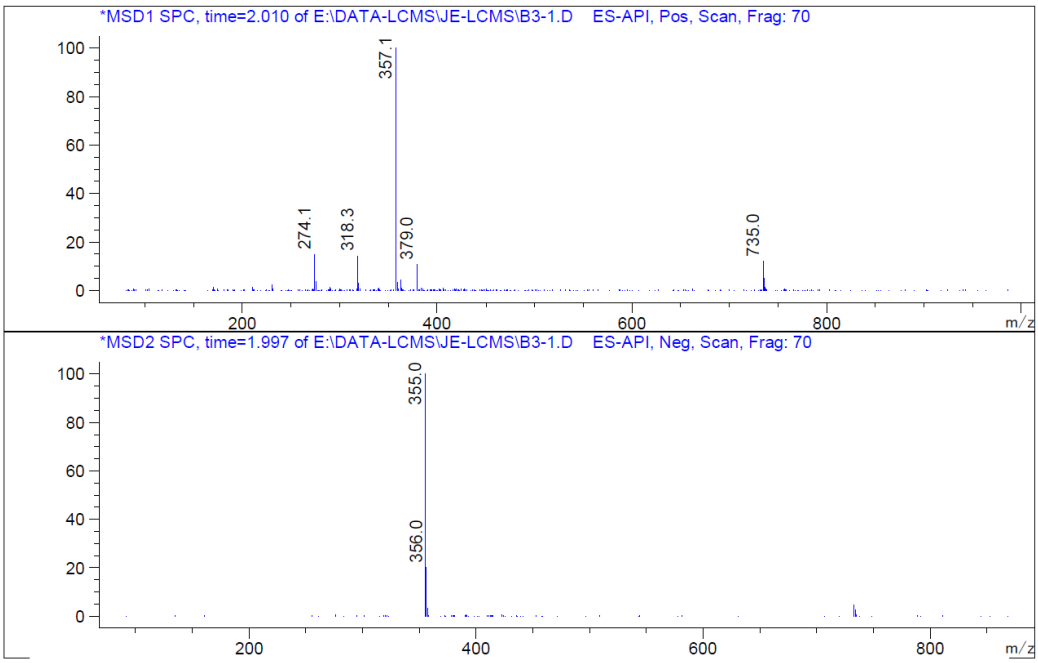
S81 HMBC spectrum of aspergorakhins I (**9**).



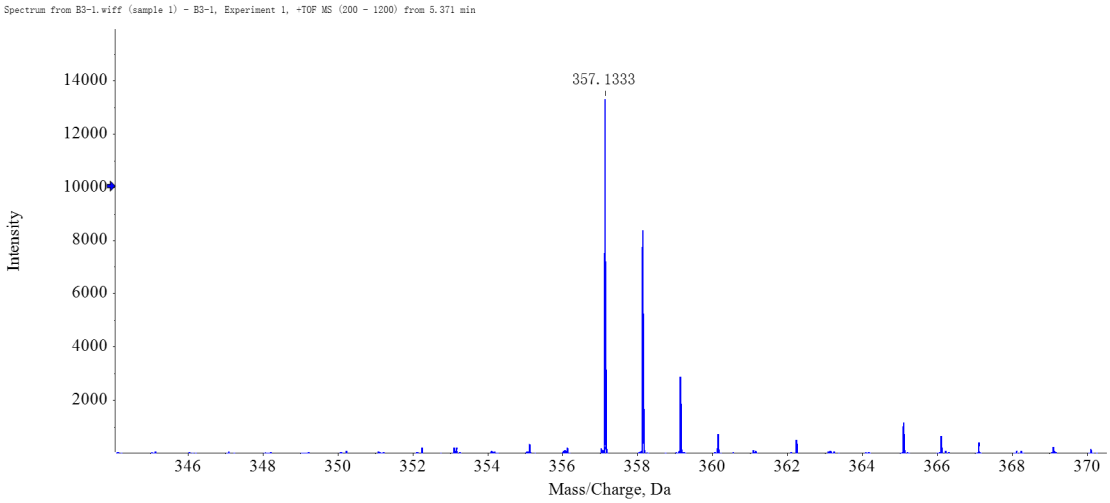
S82 NOESY spectrum of aspergorakhins I (**9**).



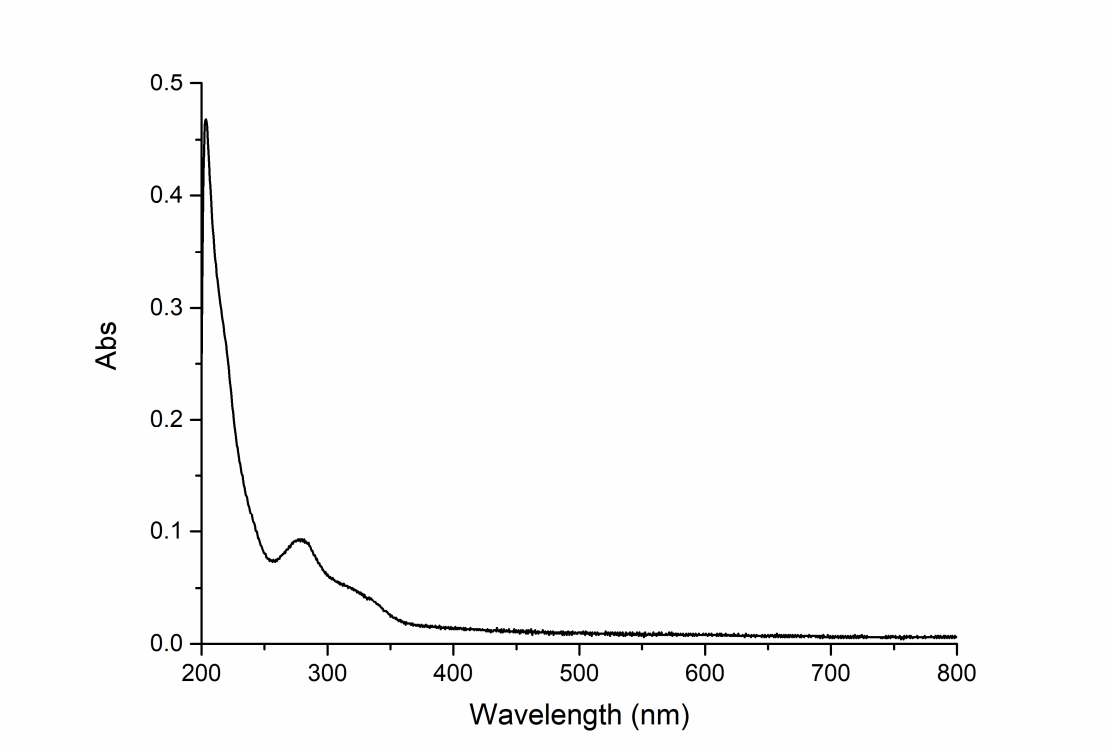
S83 ESIMS spectrum of aspergorakhins I (**9**).



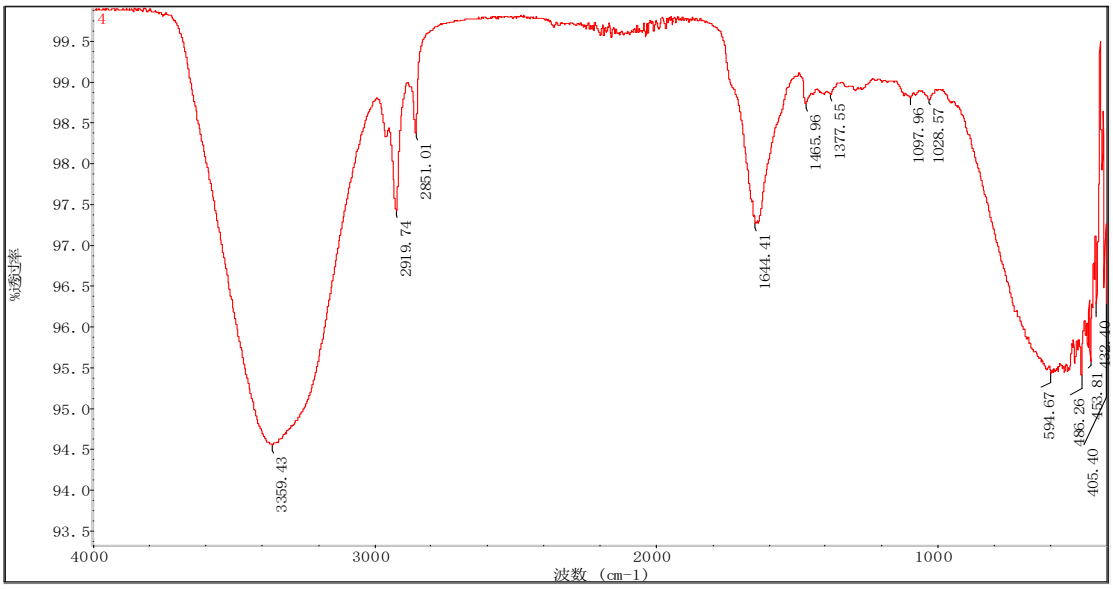
S84 (+)-HRESIMS spectrum of aspergorakhins I (**9**).



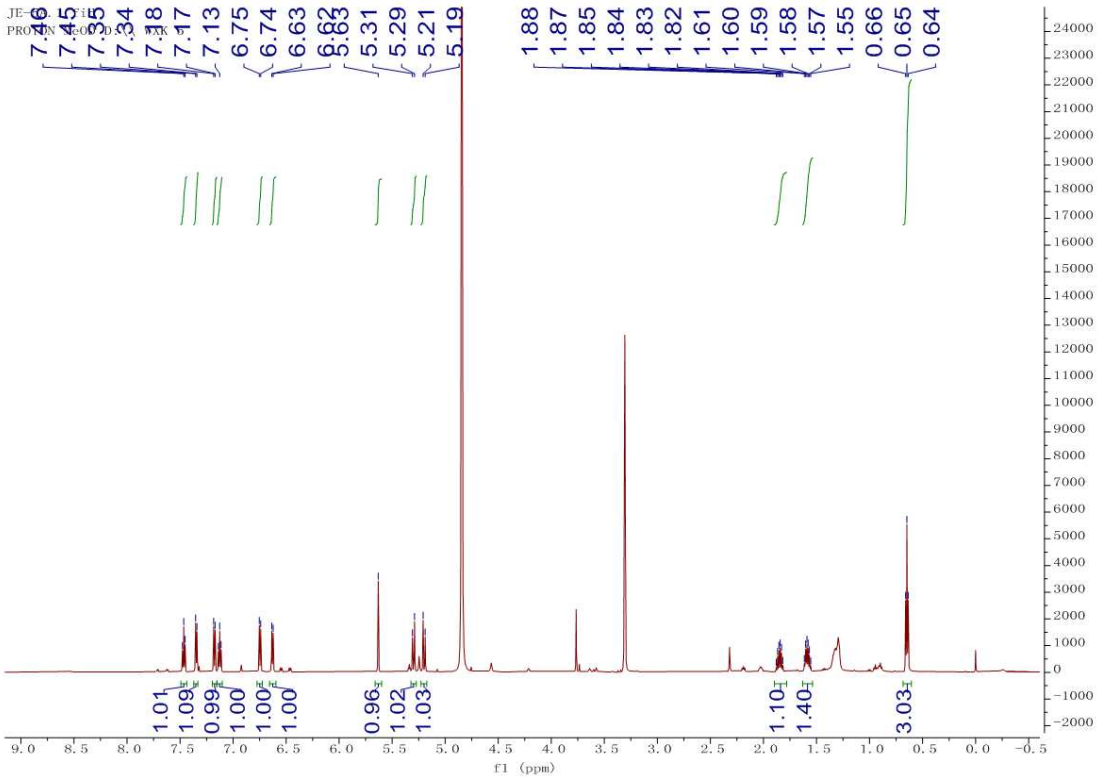
S85 UV spectrum of aspergorakhins I (**9**).



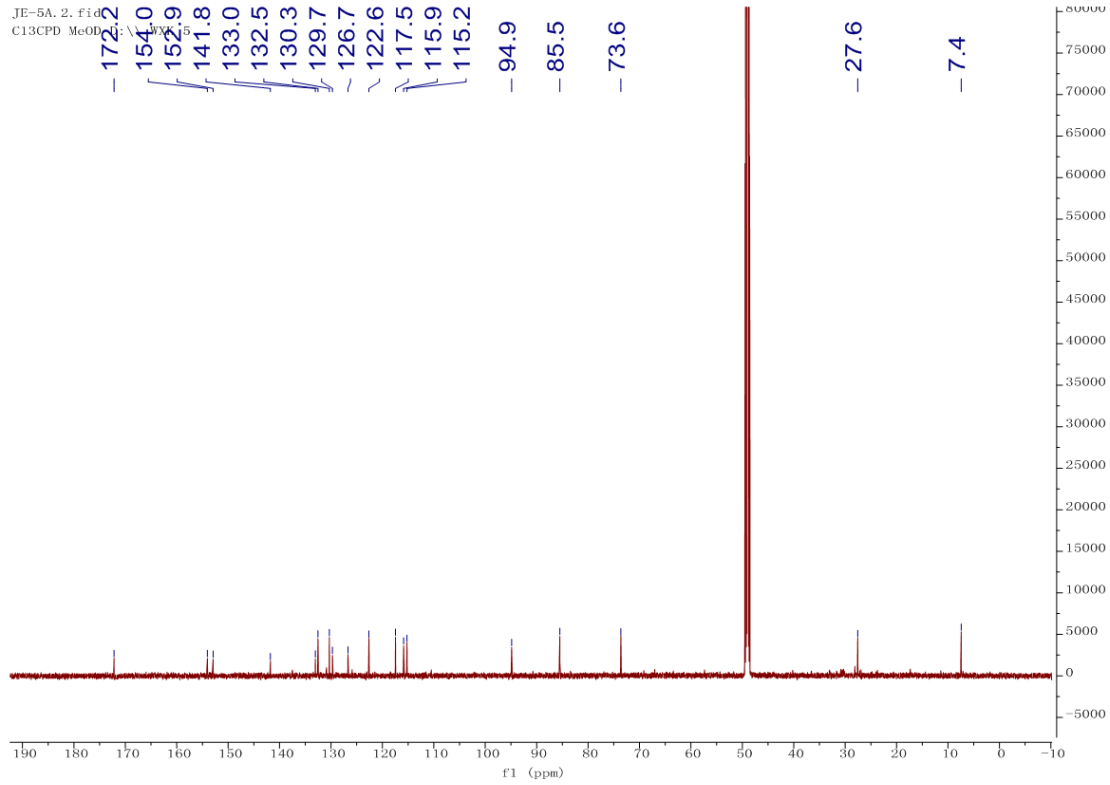
S86 IR spectrum of aspergorakhins I (**9**).



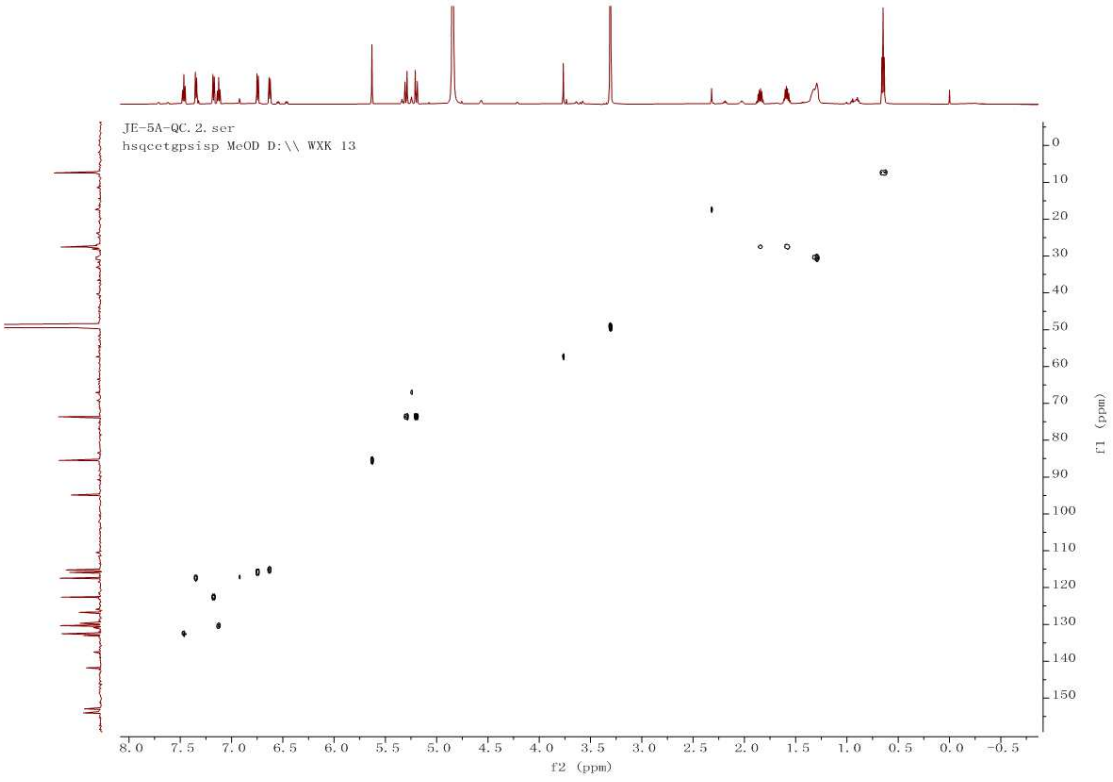
S87 ^{1}H NMR (600 MHz, CD_3OD) spectrum of aspergorakhins J (**10**).



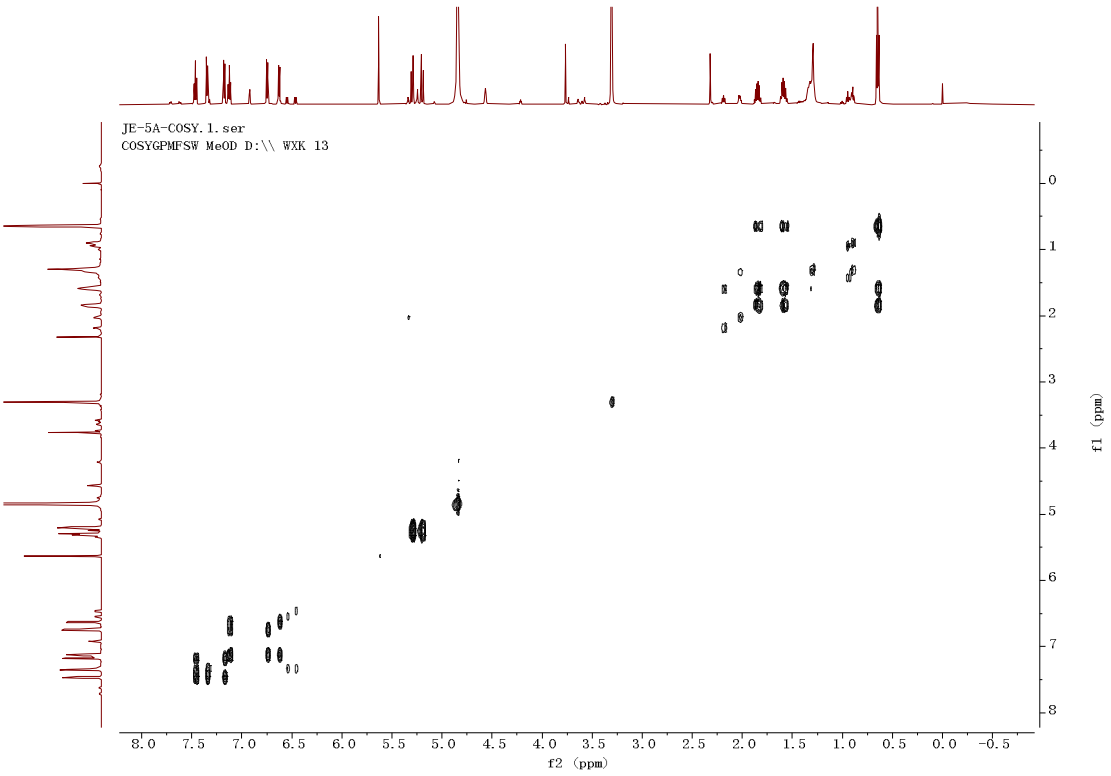
S88 ^{13}C NMR (150 MHz, CD_3OD) spectrum of aspergorakhins J (**10**).



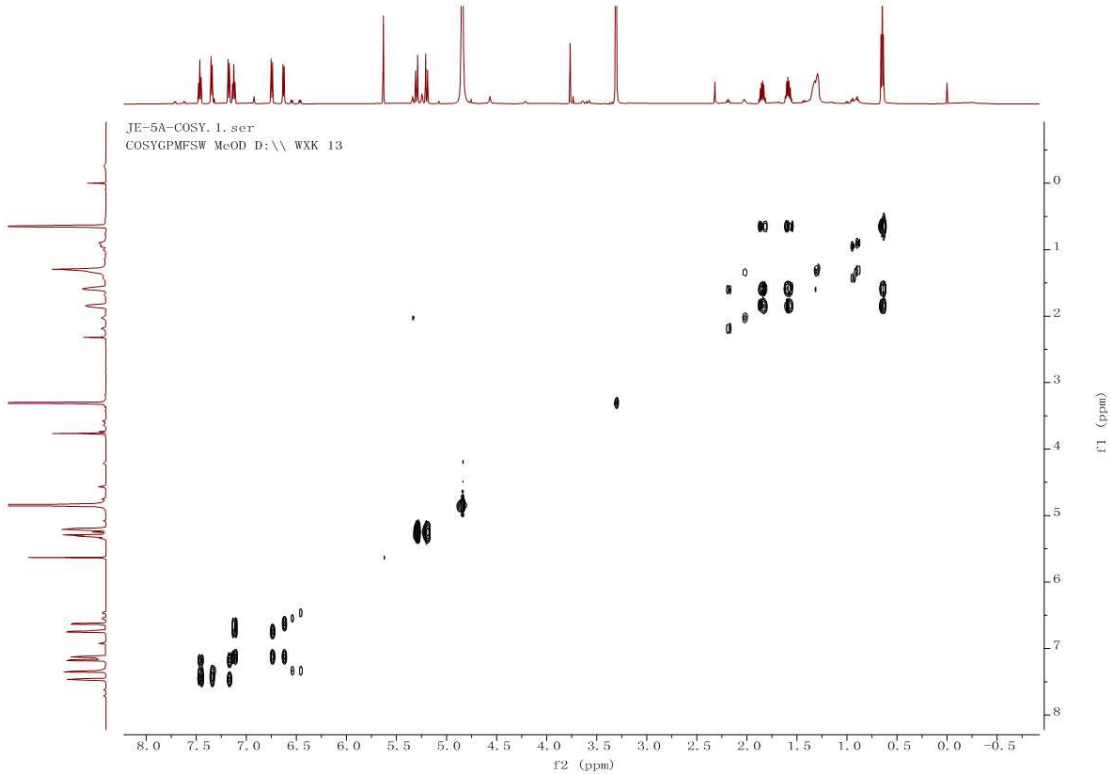
S89 HSQC spectrum of aspergorakhins J (**10**).



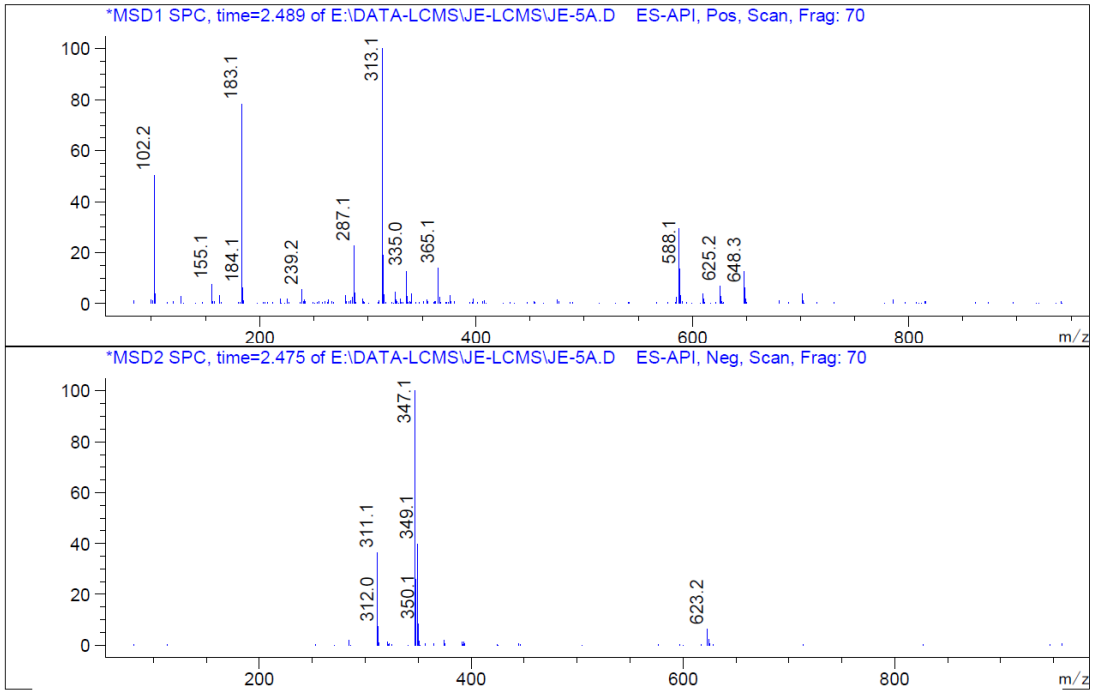
S90 COSY spectrum of aspergorakhins J (**10**).



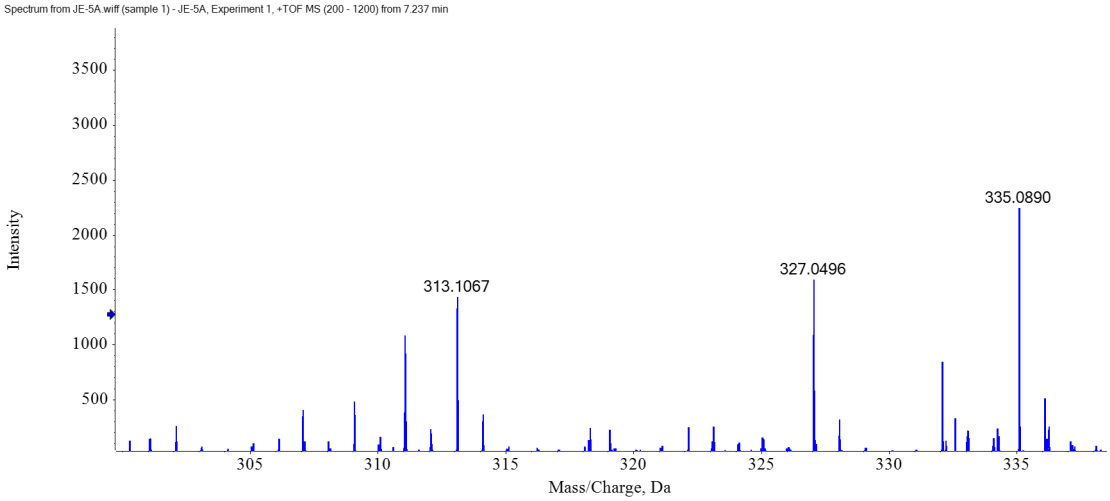
S91 HMBC spectrum of aspergorakhins J (**10**).



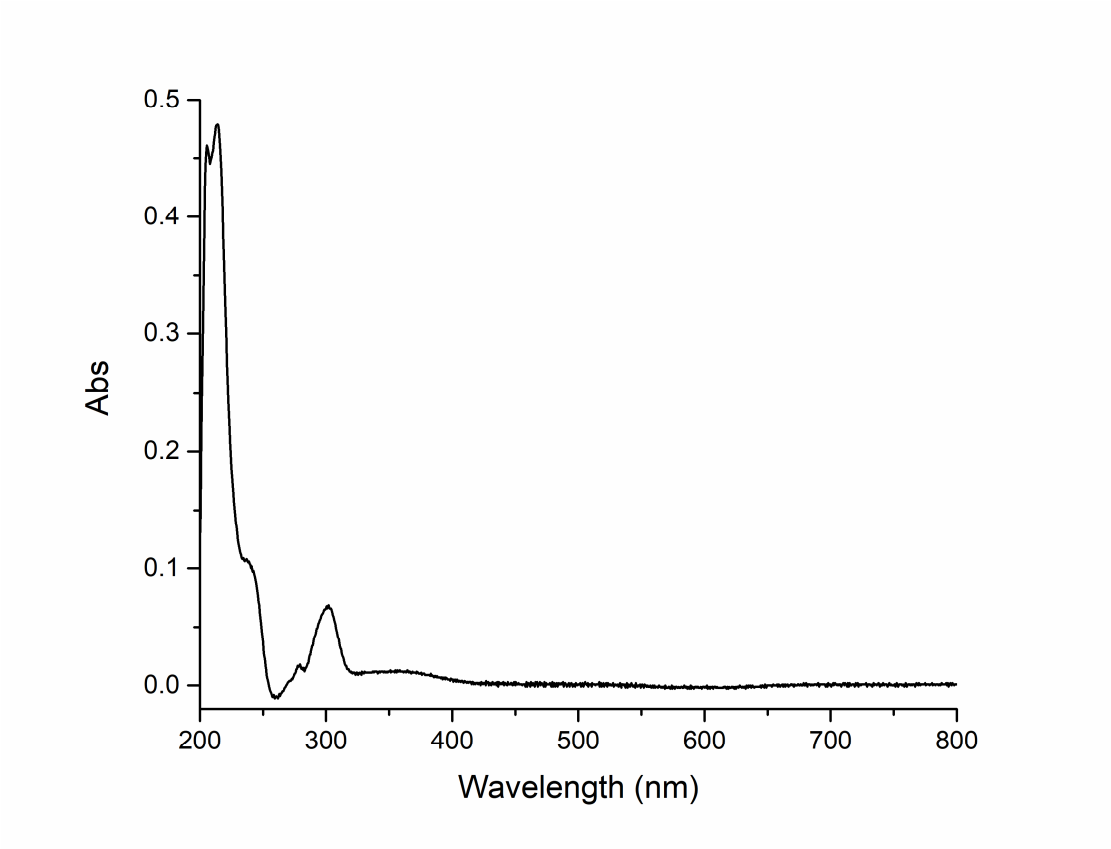
S92 ESIMS spectrum of aspergorakhins J (**10**).



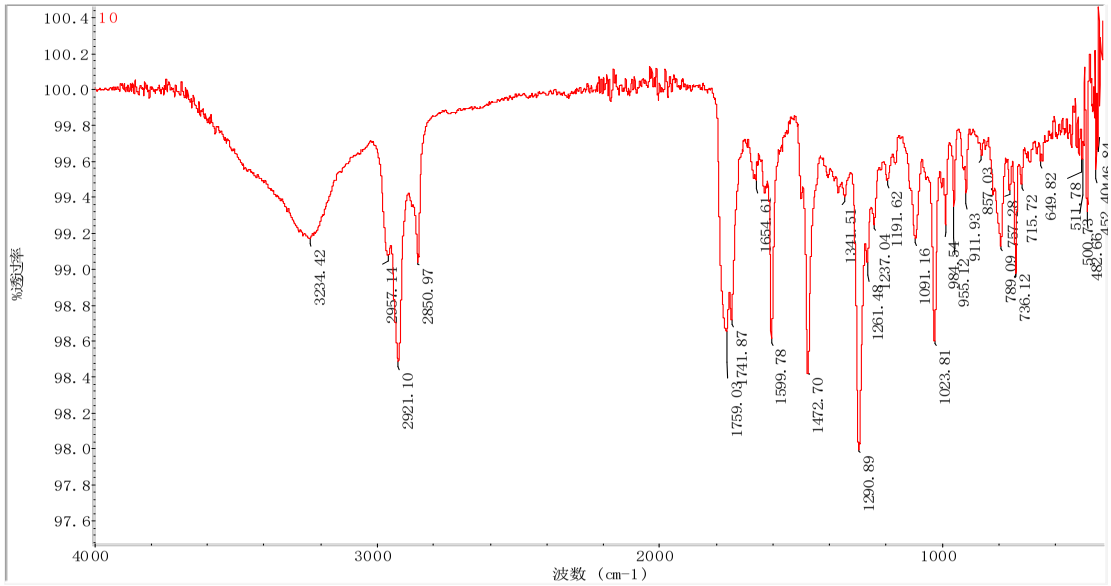
S93 (+)-HRESIMS spectrum of aspergorakhins J (**10**).



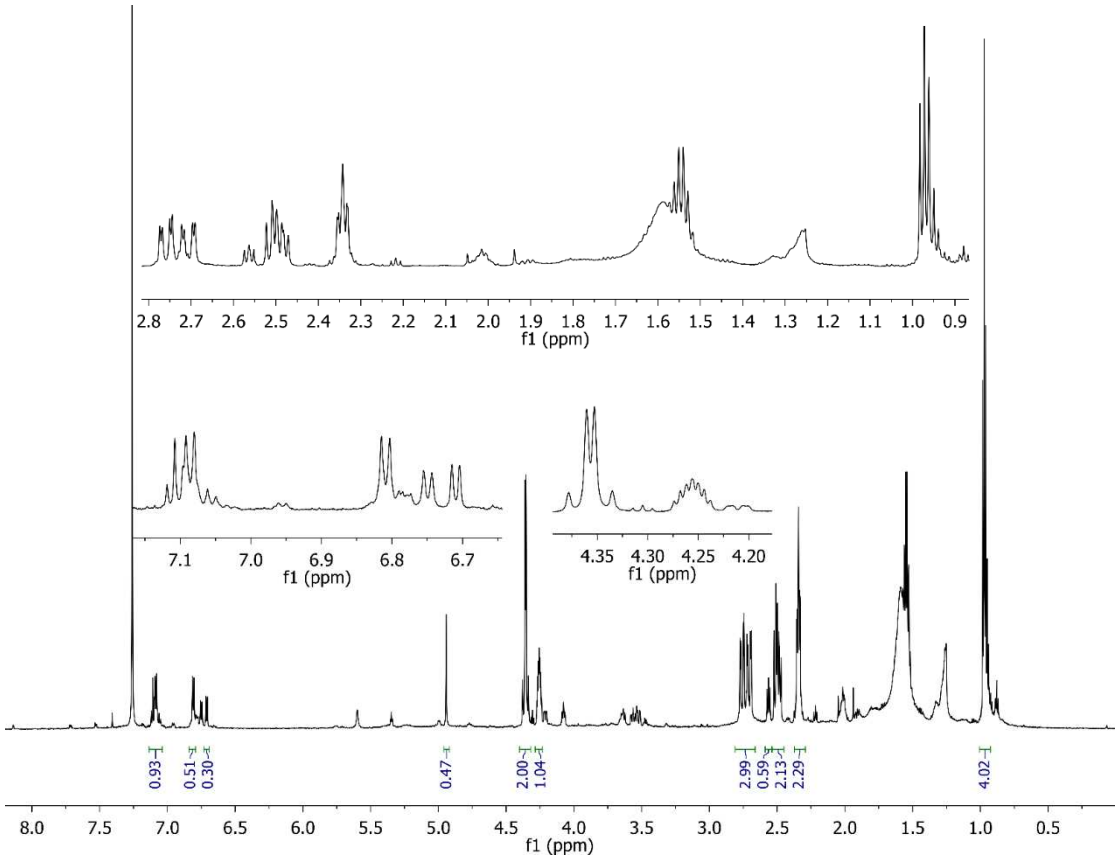
S94 UV spectrum of aspergorakhins J (**10**).



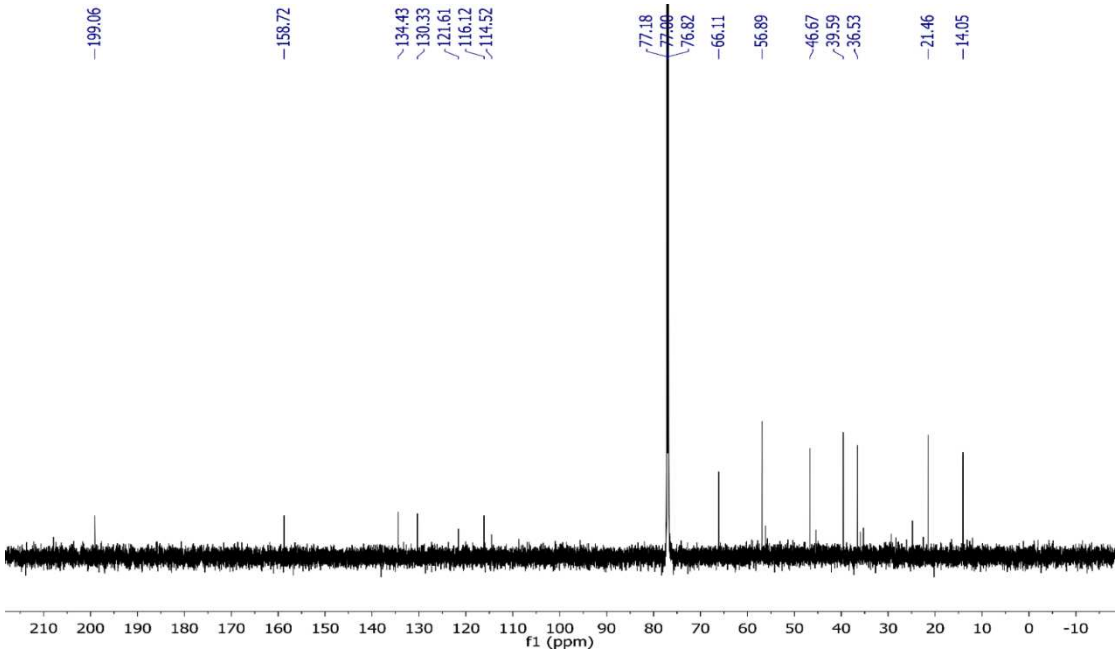
S95 IR spectrum of aspergorakhins J (**10**).



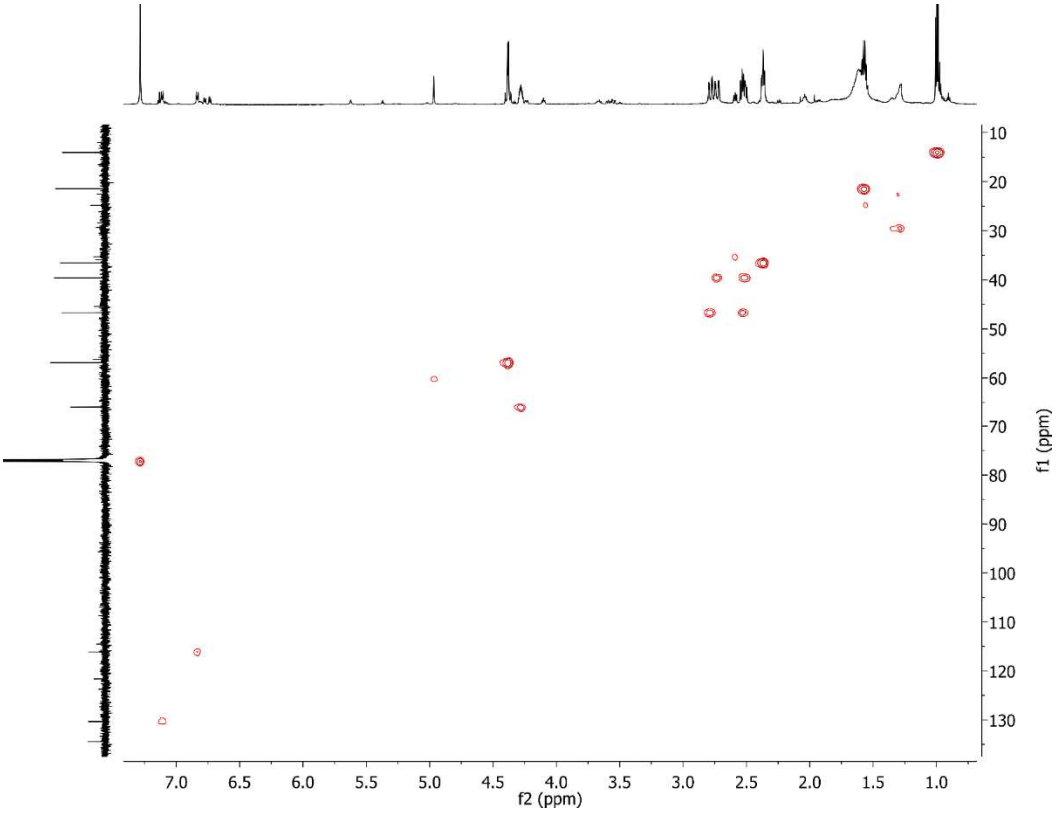
S96 ^{1}H NMR (700 MHz, $CDCl_3$) spectrum of aspergorakhins K (**11**).



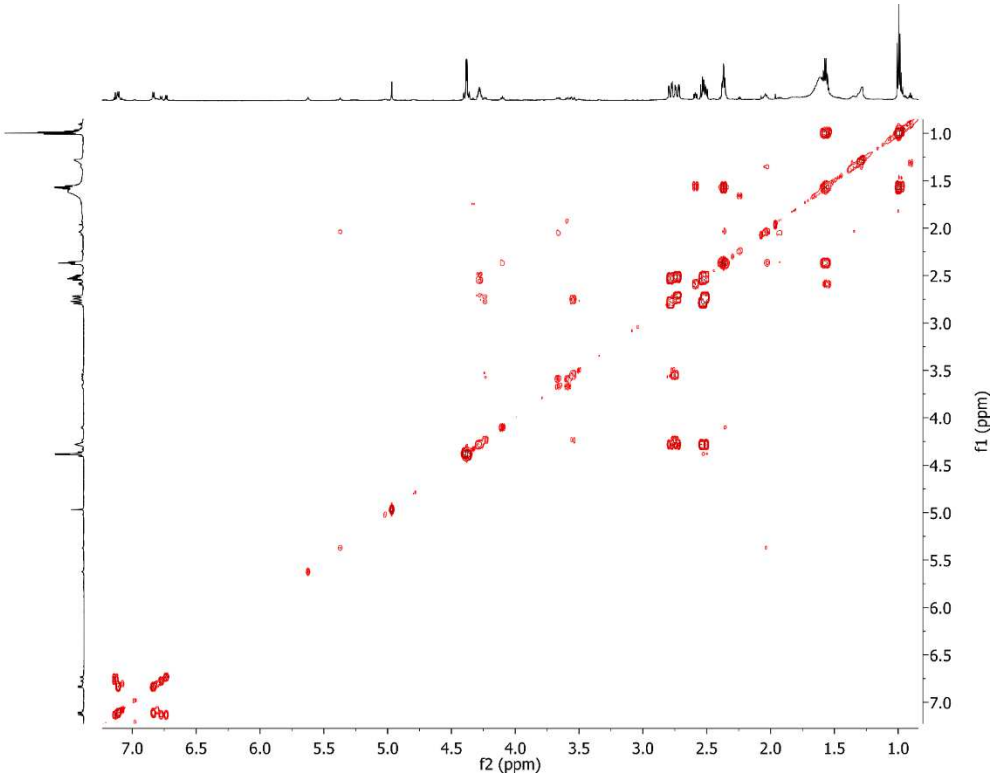
S97 ^{13}C NMR (175 MHz, $CDCl_3$) spectrum of aspergorakhins K (**11**).



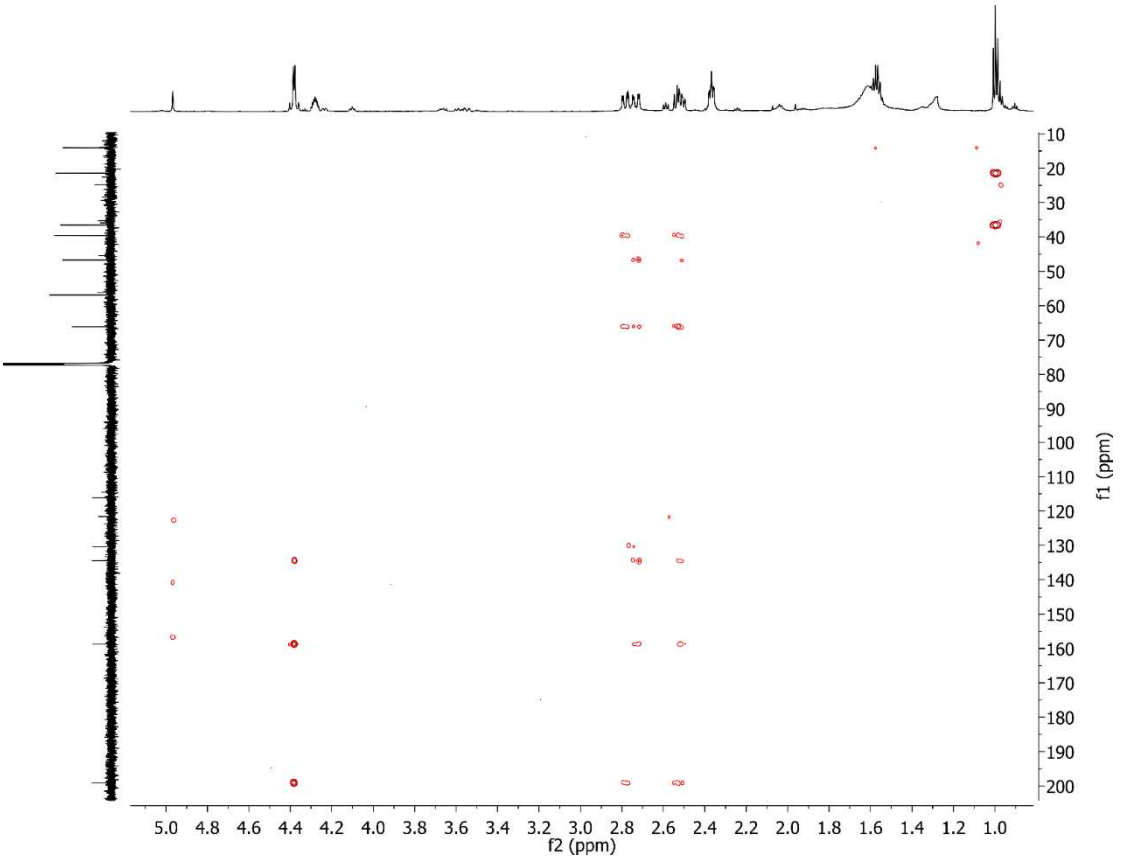
S98 HSQC spectrum of aspergorakhins K (**11**).



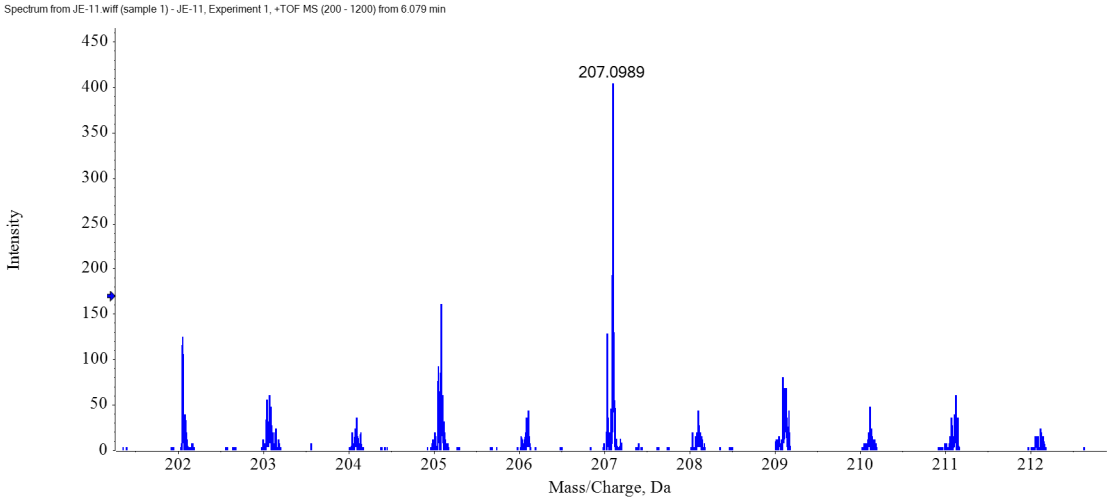
S99 COSY spectrum of aspergorakhins K (**11**).



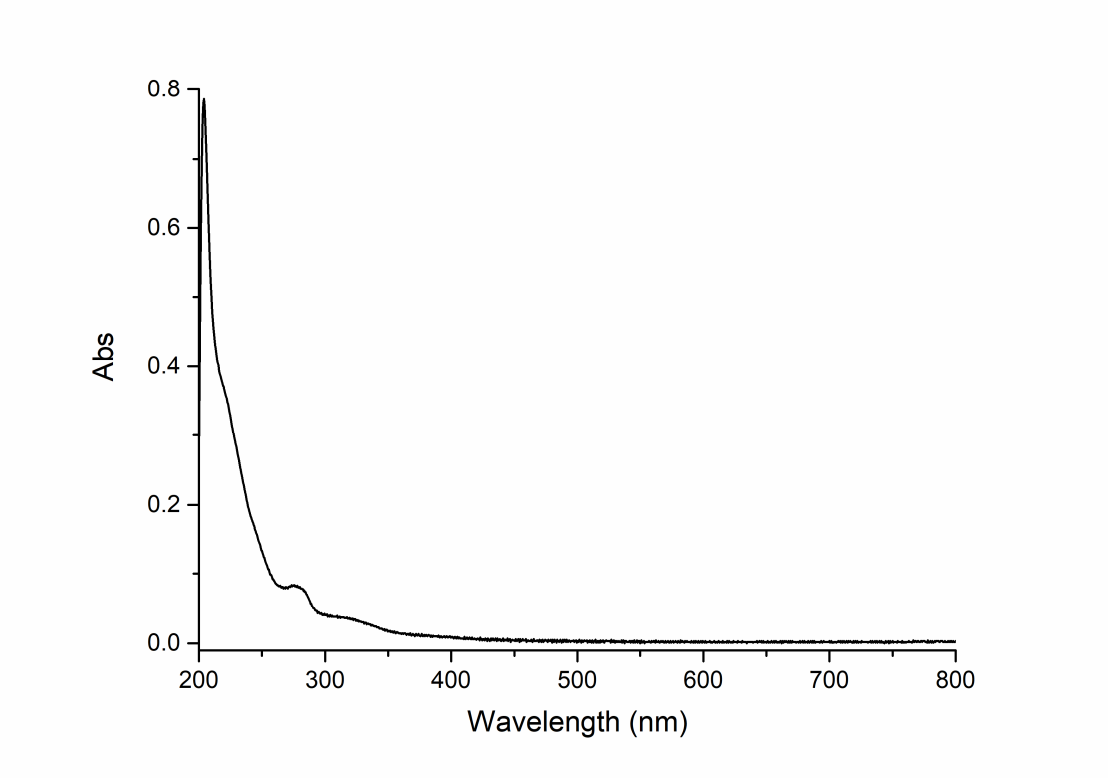
S100 HMBC spectrum of aspergorakhins K (**11**).



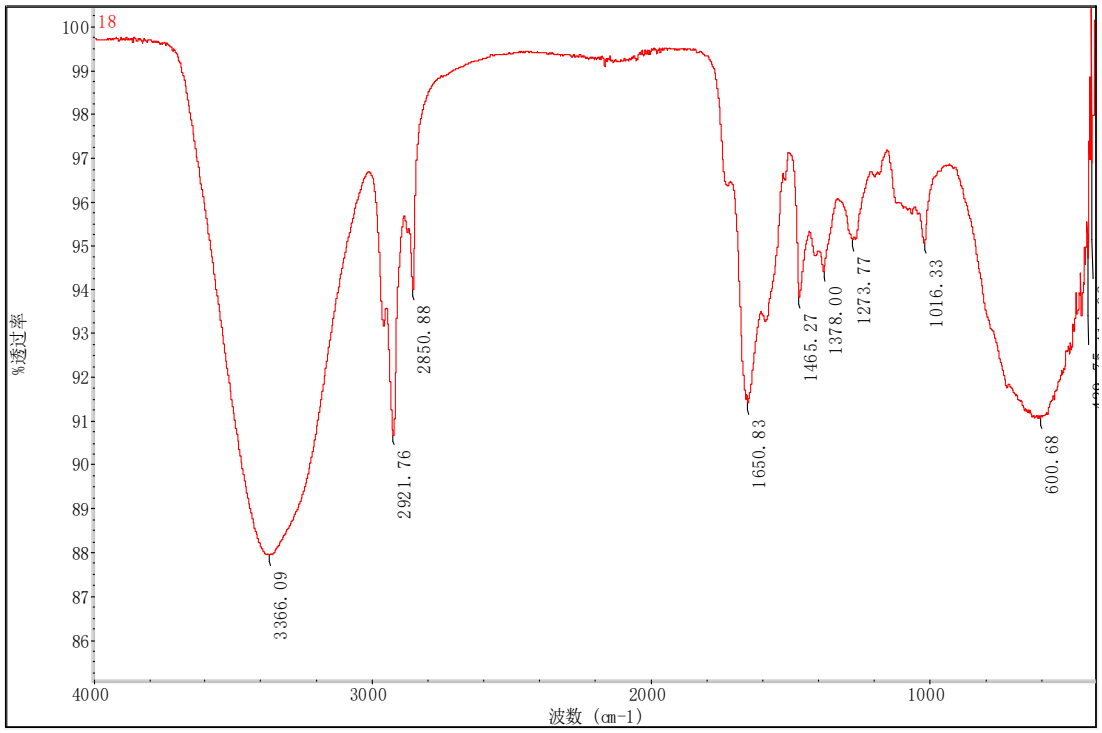
S101 (+)-HRESIMS spectrum of aspergorakhins K (**11**).



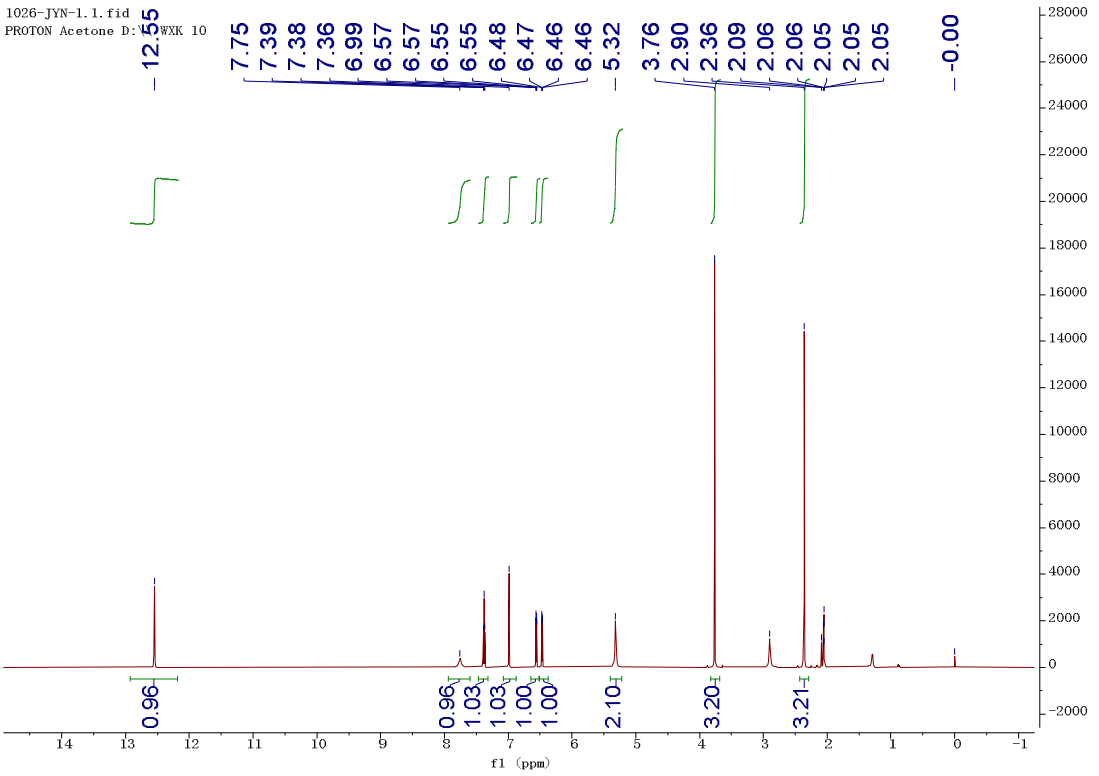
S102 UV spectrum of aspergorakhins K (**11**).



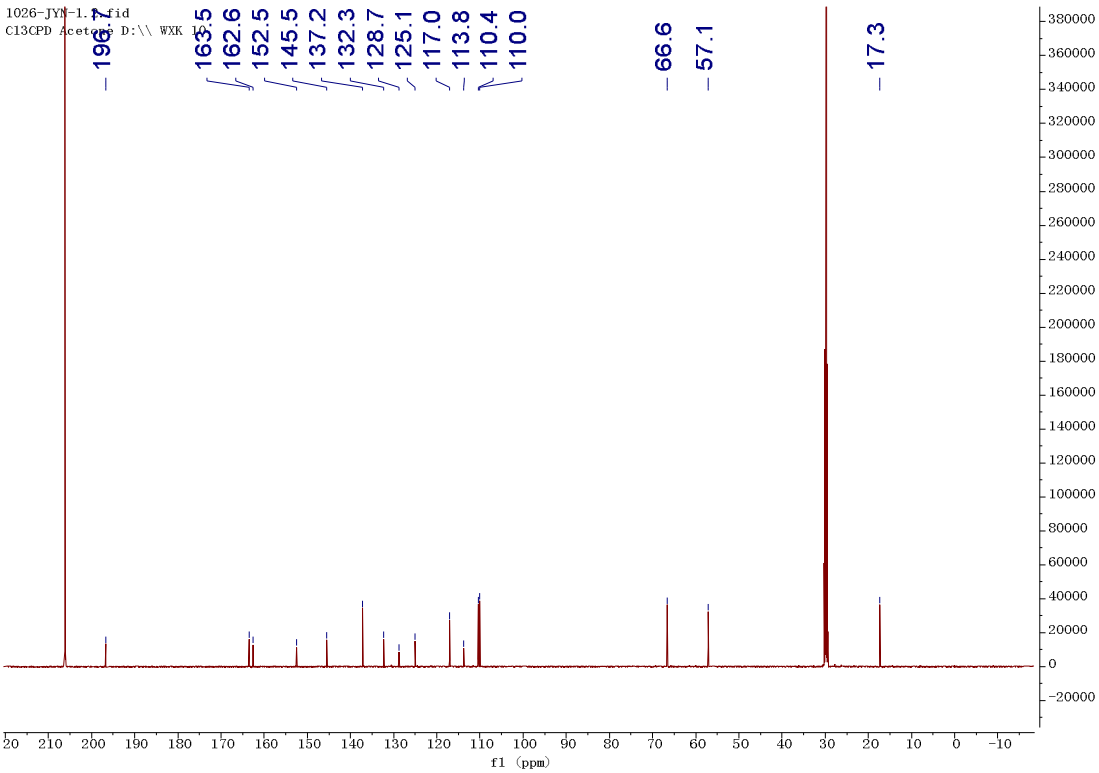
S103 IR spectrum of aspergorakhins K (**11**).



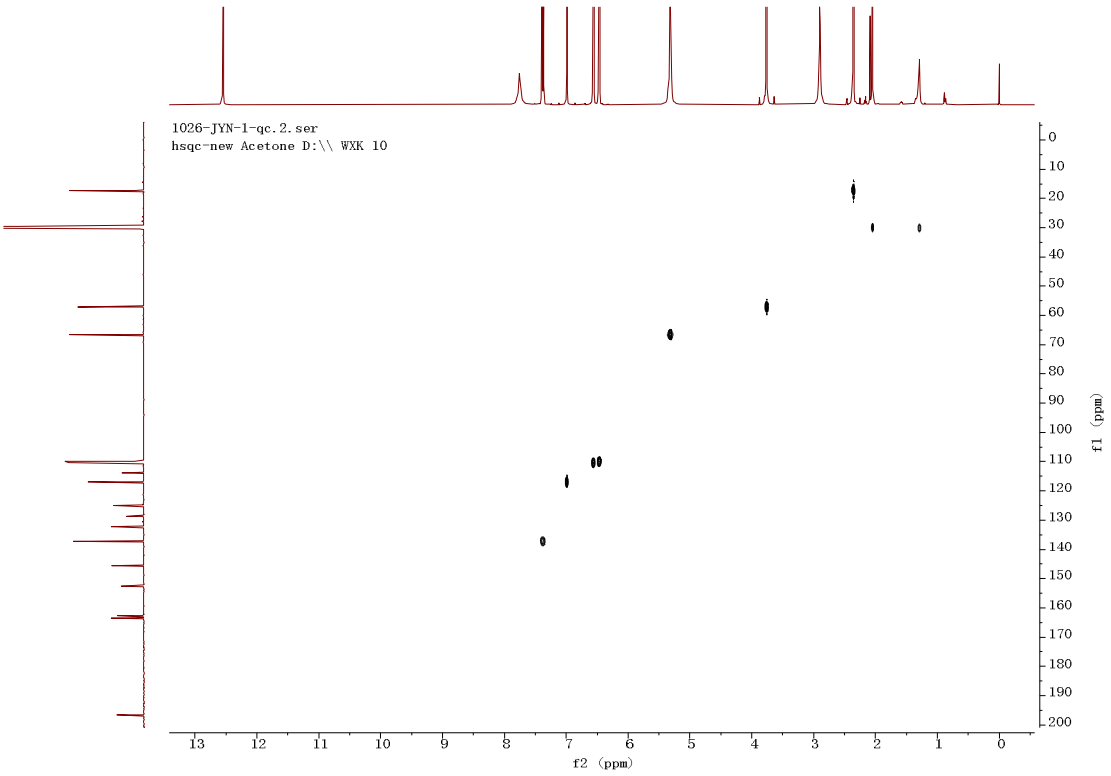
S104 ^{1}H NMR (600 MHz, Acetone-d_6) spectrum of aspergorakhins L (**12**).



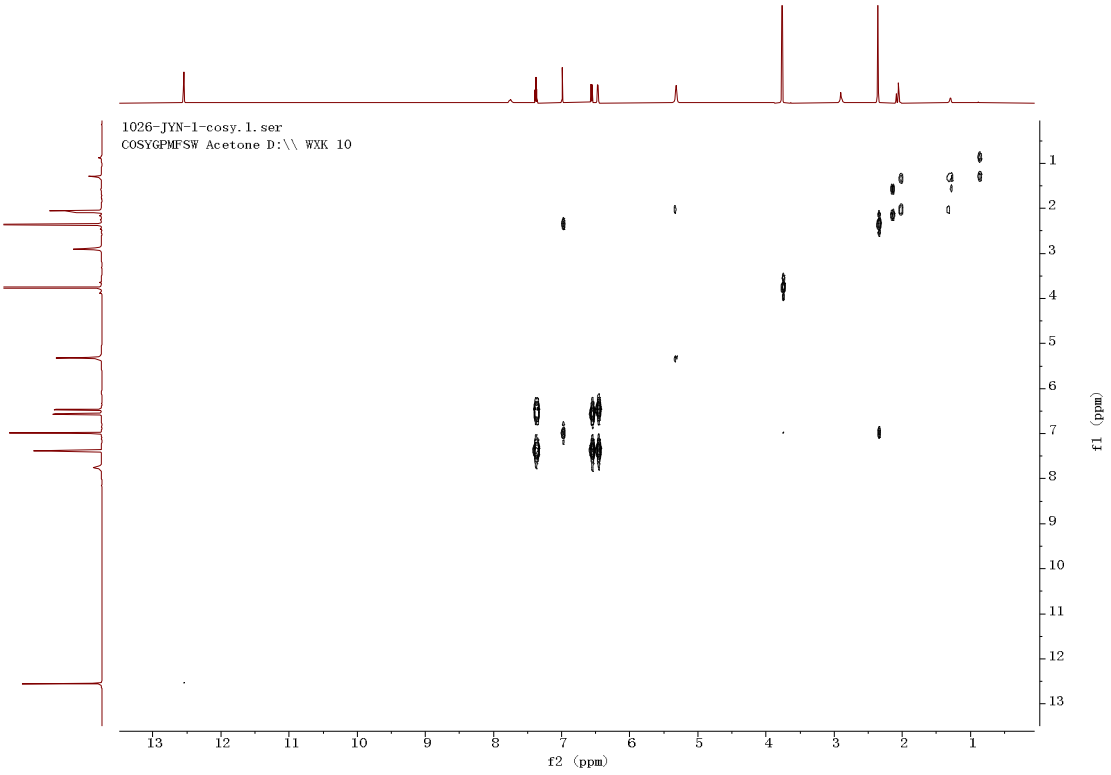
S105 ^{13}C NMR (150 MHz, Acetone-d_6) spectrum of aspergorakhins L (**12**).



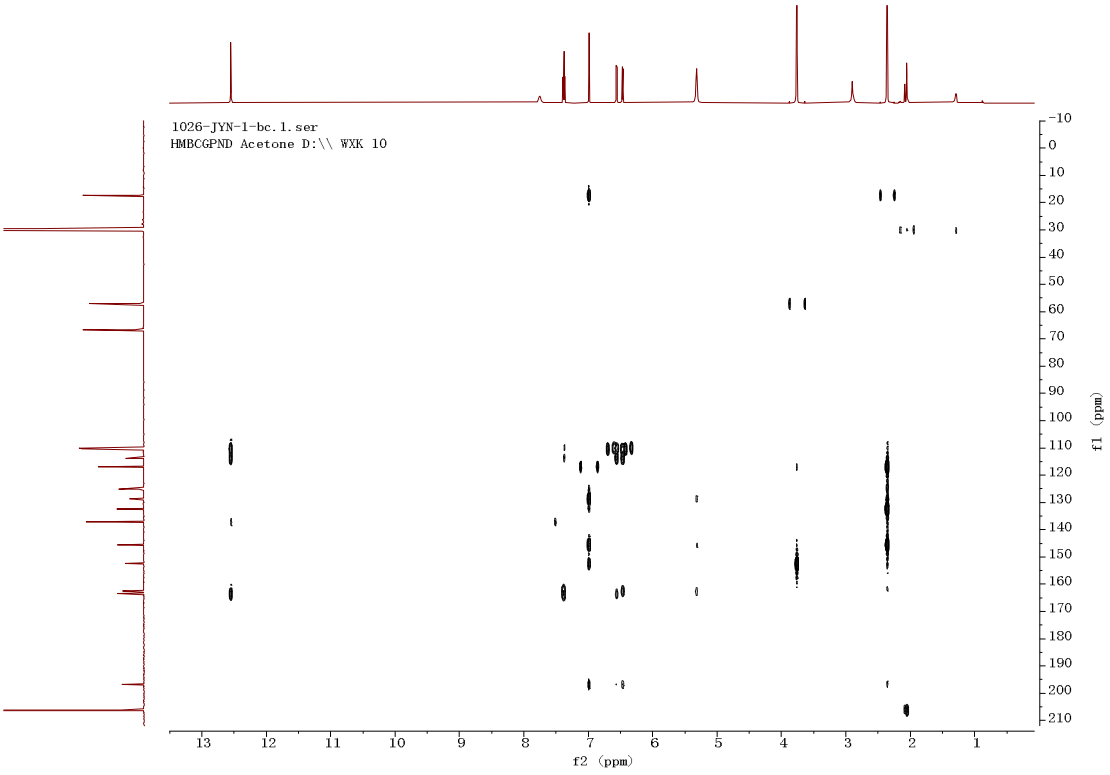
S106 HSQC spectrum of aspergorakhins L (**12**).



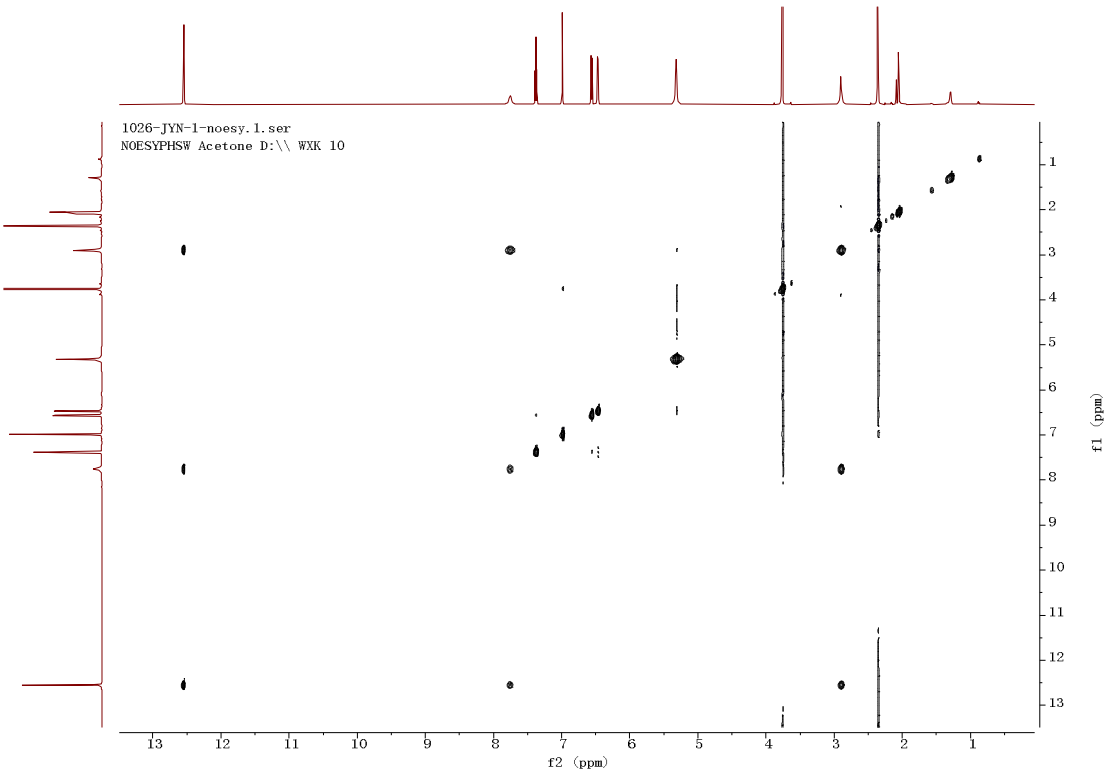
S107 COSY spectrum of aspergorakhins L (**12**).



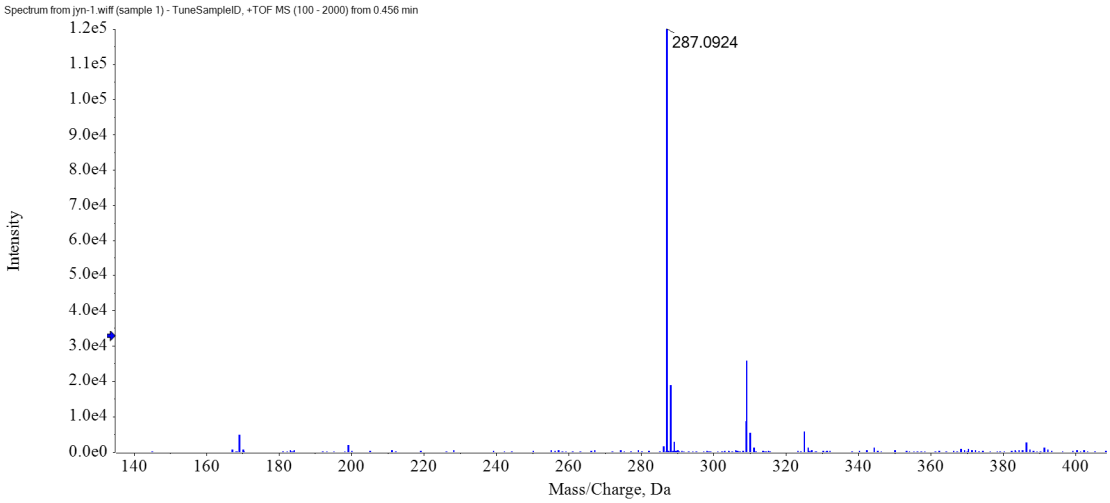
S108 HMBC spectrum of aspergorakhins L (**12**).



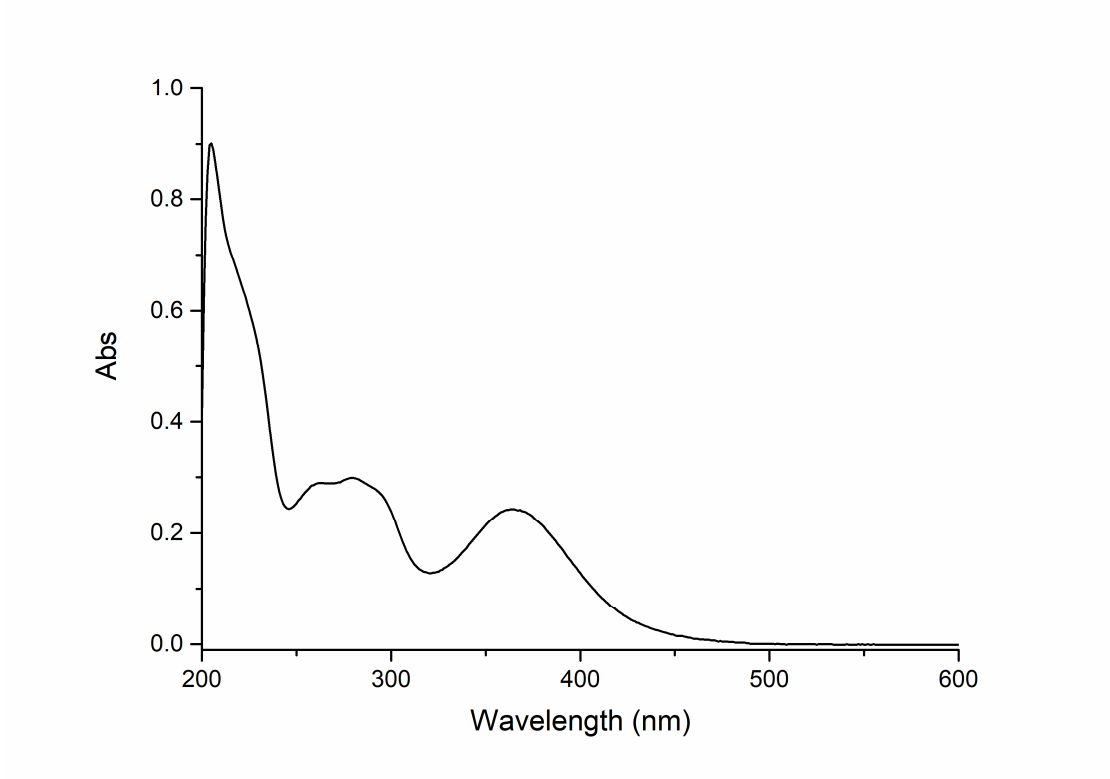
S109 NOESY spectrum of aspergorakhins L (**12**).



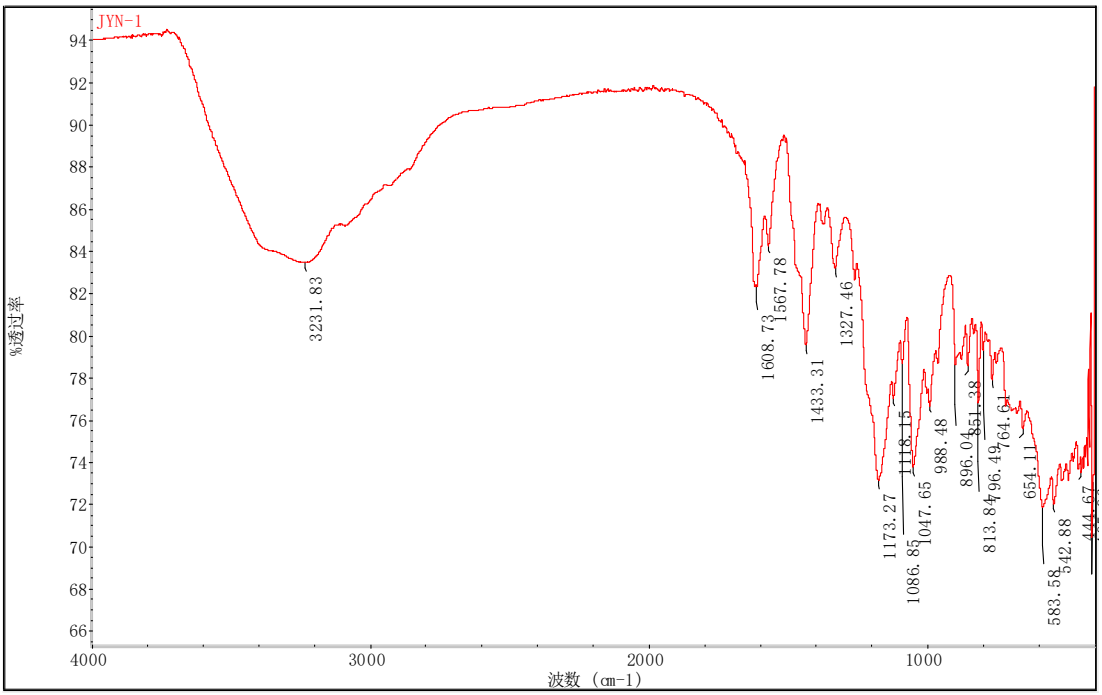
S110 (+)-HRESIMS spectrum of aspergorakhins L (**12**).



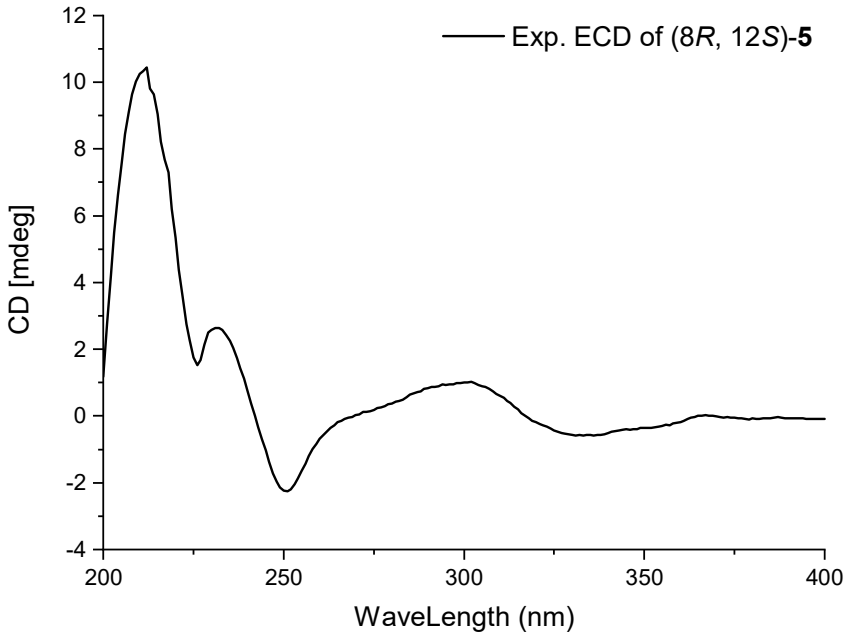
S111 UV spectrum of aspergorakhins L (**12**).

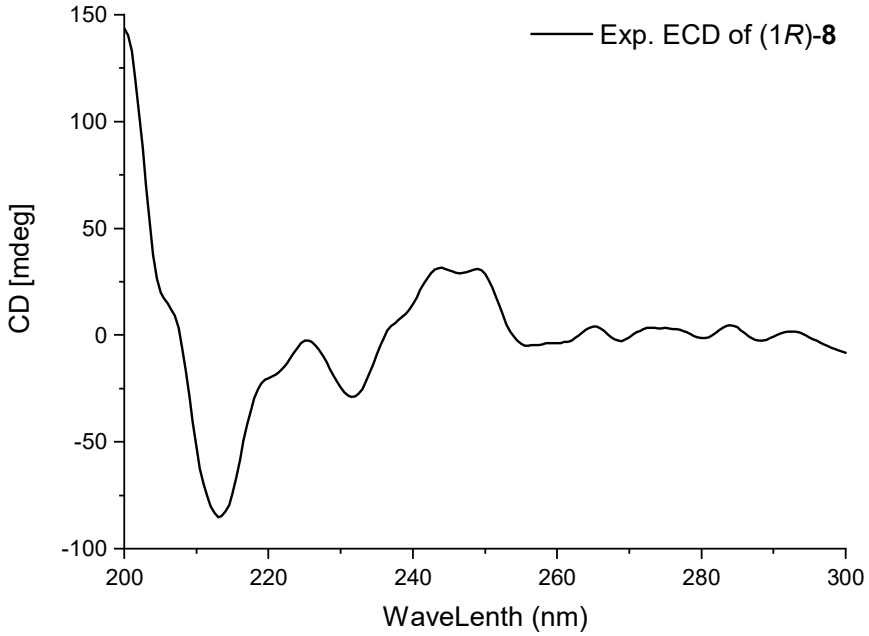


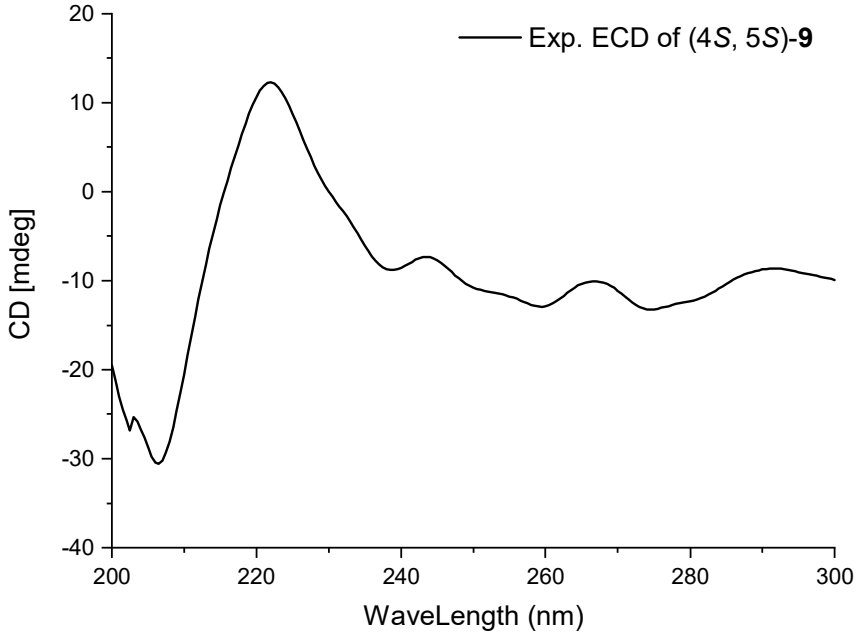
S112 IR spectrum of aspergorakhins L (**12**).

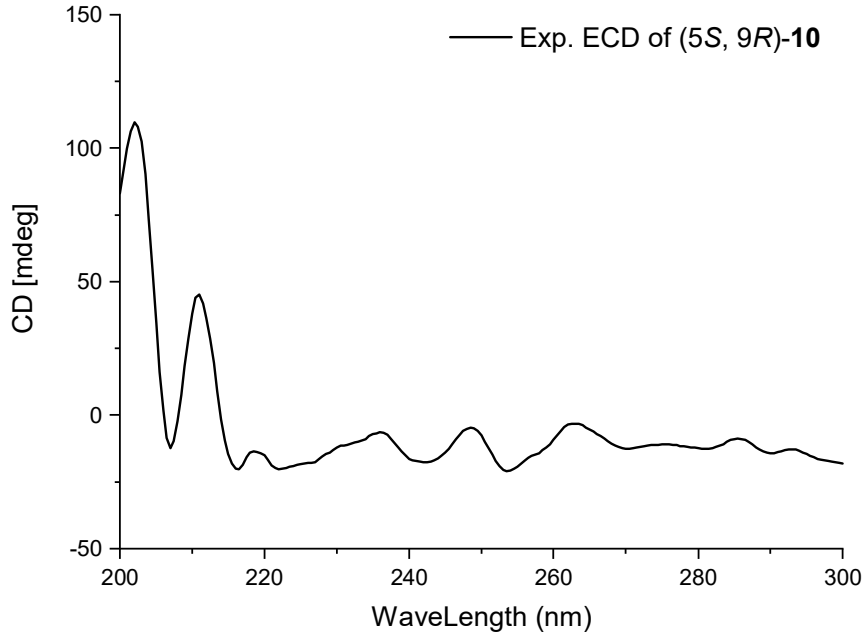


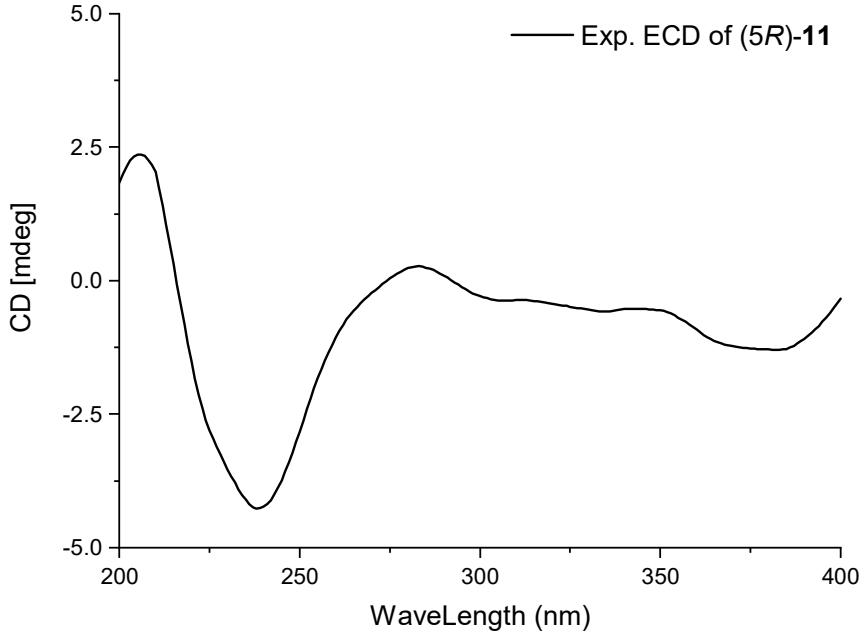
S113. Experimental ECD spectra of **5**, **8**-**11**.




Exp. ECD of (1R)-8
150
100
50
0
-50
-100
CD [mdeg]
200
220
240
260
280
300
WaveLenth (nm)


Exp. ECD of (4S, 5S)-9
20
10
0
-10
-20
-30
-40
CD [mdeg]
200
220
240
260
280
300
WaveLength (nm)





S114. Quantum chemical CD and OR calculation of models **5**, **8**-**11**.

ECD and OR calculation details

1. Methods

Monte Carlo conformational searches were performed by means of the BARISTA software (CONFLEX Corporation) using Merck Molecular Force Field (MMFF94S). The conformers with energy from 0-5 kcal/mol were used for optimization at the B3LYP/6-31G(d) level in the gas phase using the Gaussian 09 package. These

conformations with 0-2.5 kcal/mol were further optimized at the B3LYP/6-311+G(d) level in the gas phase. Calculation of ECD and OR were performed at the B3LYP/6-311++G(2d,p) level. Compounds **5**, **8-11** was selected for the calculations. The Boltzmann sums were performed to simulate the ECD curves and OR values for the selected chiral compounds. ECD spectra were generated using the program SpecDis 1.6 (University of Würzburg, Würzburg, Germany) and GraphPad Prism 5 (University of California San Diego, San Diego, CA, USA) from dipole-length rotational strengths by applying Gaussian band shapes with sigma = 0.3 eV.

2. Results

Table S114.2.1. Gibbs Free Energies[a] and Equilibrium Populations[b] of Low-energy conformers of model (8*R*,12*S*)-**5** in MeOH (PCM).

Conformers	ΔG^a	P (%)[b]
A	0.33	26.21
B	1.08	7.43
C	1.41	4.25
D	0.00	45.92
E	0.62	16.20

[a]B3LYP/6-311++G(2d,p), in kcal/mol. [b]From *G* values at 298.15K.

Table S114.2.2. Cartesian Coordinates, Relative Thermal Free Energies (B3LYP/6-311++G(2d,p) PCM/MeOH), and Equilibrium Populations of Low-energy Conformers of model **5** in MeOH (PCM).

Conformation A

ΔG = 0.33 kcal/mol P(%) = 26.21%

1	C	-1.759502	1.396434	0.812176
2	C	-0.671861	2.021614	1.406137
3	C	0.603876	1.772688	0.920270
4	C	0.868066	0.913678	-0.144630
5	C	-0.213030	0.268284	-0.771657
6	C	-1.497331	0.535244	-0.265314
7	C	0.338739	-3.183655	-2.569438
8	C	0.667003	-2.017074	-1.597534
9	C	-0.017807	-0.671870	-1.945125
10	C	-0.526677	2.986971	2.563468
11	O	0.915147	3.233870	2.648059
12	C	1.580734	2.523477	1.697720
13	O	2.791729	2.539495	1.553731
14	C	-1.033231	2.468537	3.909589
15	C	-0.824013	3.459360	5.057220
16	O	2.089098	-1.907475	-1.620544
17	O	2.149058	0.714680	-0.557775
18	O	1.132530	-4.299256	-2.154738
19	C	-1.113139	-3.645842	-2.432411

20	C	0.679596	-2.826514	-4.025284
21	H	-0.986115	3.958065	2.338764
22	H	-2.778542	1.556526	1.148959
23	H	-2.337510	0.041826	-0.747160
24	H	0.333448	-2.338820	-0.597820
25	H	0.583210	-0.185012	-2.721722
26	H	-1.001941	-0.867524	-2.380132
27	H	-2.100195	2.240401	3.791753
28	H	-0.530004	1.518430	4.122803
29	H	-1.352476	4.400800	4.870310
30	H	0.237061	3.688184	5.184570
31	H	-1.199806	3.046054	5.997539
32	H	2.351594	-1.099995	-1.152366
33	H	2.735778	1.256893	0.014362
34	H	2.014147	-3.934648	-1.979222
35	H	-1.823236	-2.896415	-2.794721
36	H	-1.345861	-3.881011	-1.389391
37	H	-1.254168	-4.556573	-3.021074
38	H	0.032040	-2.037000	-4.422071
39	H	0.558729	-3.714981	-4.651020
40	H	1.716860	-2.488843	-4.097281

Conformation B

ΔG = 1.08 kcal/mol P(%) = 7.43%

1	C	-0.102310	2.225025	1.270923
2	C	-0.787580	2.648705	0.140497
3	C	-1.359242	1.704478	-0.700379
4	C	-1.283017	0.330491	-0.480877
5	C	-0.598108	-0.131297	0.657695
6	C	-0.027986	0.841300	1.498062
7	C	1.062779	-3.691895	0.629011
8	C	0.433008	-2.411935	0.014287
9	C	-0.474666	-1.607951	0.978781
10	C	-1.093619	4.011647	-0.446302
11	O	-1.847872	3.715559	-1.666879
12	C	-2.011534	2.373654	-1.818240
13	O	-2.608274	1.856969	-2.748102
14	C	0.111937	4.891829	-0.789806
15	C	1.120478	4.250286	-1.745264
16	O	-0.286125	-2.868606	-1.129897
17	O	-1.863551	-0.532161	-1.358305
18	O	1.772400	-4.347437	-0.426167
19	C	2.120585	-3.354992	1.681499

20	C	-0.007884	-4.640641	1.191957
21	H	-1.778149	4.572183	0.202109
22	H	0.361447	2.918801	1.964629
23	H	0.500877	0.491608	2.380991
24	H	1.271819	-1.771565	-0.302713
25	H	-1.464213	-2.079256	0.971849
26	H	-0.088013	-1.694321	1.998129
27	H	-0.270057	5.826109	-1.215974
28	H	0.597353	5.157144	0.158188
29	H	0.646747	3.989311	-2.695610
30	H	1.557107	3.341833	-1.319550
31	H	1.936837	4.945965	-1.958859
32	H	-0.814838	-2.136357	-1.482663
33	H	-2.279440	0.001040	-2.071379
34	H	1.178585	-4.313912	-1.192547
35	H	1.684359	-2.908859	2.580320
36	H	2.867468	-2.668743	1.270884
37	H	2.635382	-4.273542	1.976667
38	H	0.465424	-5.580208	1.489720
39	H	-0.759281	-4.856453	0.427811
40	H	-0.516835	-4.220805	2.066501

Conformation C

ΔG = 1.41 kcal/mol P(%) = 4.25%

1	C	1.060077	2.080484	-0.456305
2	C	-0.046296	2.647062	0.164430
3	C	-0.839184	1.852090	0.982089
4	C	-0.601660	0.498201	1.211162
5	C	0.505595	-0.105114	0.587999
6	C	1.302513	0.716322	-0.227582
7	C	0.438304	-3.949629	-0.208059
8	C	-0.162447	-2.566084	0.163190
9	C	0.844535	-1.568738	0.789833
10	C	-0.649851	4.038829	0.183119
11	O	-1.783797	3.926020	1.103435
12	C	-1.912289	2.651407	1.556794
13	O	-2.788400	2.280479	2.320528
14	C	-1.181614	4.575555	-1.150110
15	C	-0.082451	4.946360	-2.149554
16	O	-1.238031	-2.858688	1.053488
17	O	-1.428320	-0.208940	2.027720
18	O	-0.647843	-4.758203	-0.669612
19	C	1.402001	-3.850301	-1.391885

20	C	1.101906	-4.626849	1.001993
21	H	0.036902	4.768121	0.630863
22	H	1.732581	2.652739	-1.085284
23	H	2.166630	0.260655	-0.704253
24	H	-0.557414	-2.135353	-0.770923
25	H	0.910506	-1.796017	1.860095
26	H	1.838017	-1.740538	0.366249
27	H	-1.856131	3.827173	-1.581102
28	H	-1.789513	5.456880	-0.919350
29	H	0.483366	4.069812	-2.477737
30	H	0.623478	5.666992	-1.721668
31	H	-0.520995	5.404202	-3.040550
32	H	-1.582794	-2.026897	1.413381
33	H	-2.119193	0.406676	2.359732
34	H	-1.370027	-4.597618	-0.042077
35	H	2.317794	-3.308442	-1.137475
36	H	0.919873	-3.354858	-2.240049
37	H	1.683068	-4.858707	-1.707931
38	H	1.391214	-5.645477	0.729444
39	H	0.399388	-4.676698	1.838074
40	H	1.998503	-4.093908	1.336892

Conformation D

ΔG = 0.00 kcal/mol P(%) = 45.92%

1	C	1.121008	1.981383	-0.879238
2	C	0.152998	2.591896	-0.093039
3	C	-0.466634	1.863217	0.912228
4	C	-0.174908	0.528282	1.182237
5	C	0.802762	-0.118282	0.406909
6	C	1.421629	0.637943	-0.603960
7	C	0.725314	-4.064948	0.138091
8	C	0.205136	-2.598868	0.060329
9	C	1.186460	-1.563847	0.650587
10	C	-0.451302	3.980024	-0.072786
11	O	-1.428291	3.932182	1.017938
12	C	-1.448976	2.697954	1.591122
13	O	-2.181413	2.383740	2.513855
14	C	-1.152375	4.400749	-1.364623
15	C	-1.788737	5.790354	-1.283053
16	O	-1.043502	-2.608560	0.758916
17	O	-0.830016	-0.133676	2.174943
18	O	0.811230	-4.426226	1.518272
19	C	-0.270461	-4.990660	-0.584663

20	C	2.125940	-4.243661	-0.449256
21	H	0.287899	4.737826	0.217008
22	H	1.639845	2.506011	-1.674946
23	H	2.184150	0.145721	-1.202378
24	H	0.026053	-2.346679	-0.997516
25	H	1.283401	-1.765539	1.722905
26	H	2.171950	-1.726278	0.208141
27	H	-0.405165	4.369364	-2.167752
28	H	-1.907158	3.643872	-1.607194
29	H	-1.036905	6.559947	-1.075807
30	H	-2.537947	5.828628	-0.488259
31	H	-2.278342	6.046987	-2.226834
32	H	-1.125863	-1.811650	1.304742
33	H	-1.472480	0.490085	2.578378
34	H	-0.044053	-4.152345	1.888333
35	H	-0.291046	-4.791631	-1.662219
36	H	-1.280823	-4.850158	-0.193564
37	H	0.025594	-6.031945	-0.429640
38	H	2.376645	-5.307632	-0.483994
39	H	2.881093	-3.748932	0.166195
40	H	2.181287	-3.848649	-1.469410

Conformation E

ΔG = 0.62 kcal/mol P(%) = 16.20%

1	C	-1.951804	1.430200	0.997992
2	C	-0.914631	2.257098	1.408893
3	C	0.312827	2.178992	0.766485
4	C	0.574720	1.300832	-0.282410
5	C	-0.454491	0.451885	-0.724043
6	C	-1.691646	0.548271	-0.063132
7	C	0.507406	-2.884492	-2.621187
8	C	0.488868	-1.819076	-1.485454
9	C	-0.249504	-0.519111	-1.869090
10	C	-0.789160	3.321129	2.480388
11	O	0.597548	3.779752	2.370544
12	C	1.245285	3.121539	1.370898
13	O	2.409917	3.314559	1.065836
14	C	-1.068998	2.875409	3.918844
15	C	-0.210422	1.705569	4.404329
16	O	1.864970	-1.577739	-1.176261
17	O	1.806242	1.265263	-0.861163
18	O	1.280174	-2.358861	-3.702602
19	C	1.160230	-4.173856	-2.090183

20	C	-0.880195	-3.194417	-3.184297
21	H	-1.414132	4.190714	2.242753
22	H	-2.932649	1.453484	1.461788
23	H	-2.494301	-0.100678	-0.404518
24	H	-0.008155	-2.256157	-0.604158
25	H	0.305841	-0.044879	-2.685563
26	H	-1.233415	-0.779990	-2.265717
27	H	-0.924696	3.744861	4.569759
28	H	-2.134556	2.617981	3.974375
29	H	0.852842	1.957196	4.361824
30	H	-0.373724	0.807935	3.800426
31	H	-0.454392	1.460360	5.441835
32	H	2.015099	-0.629233	-1.043985
33	H	2.373757	1.920633	-0.399579
34	H	2.090946	-2.033159	-3.278363
35	H	0.542744	-4.645754	-1.317371
36	H	2.140658	-3.959939	-1.658202
37	H	1.285373	-4.881607	-2.914433
38	H	-1.580602	-3.463909	-2.386321
39	H	-0.815402	-4.037939	-3.877343
40	H	-1.282571	-2.343866	-3.739596

Table S114.2.3. Gibbs Free Energies[a] and Equilibrium Populations[b] of Low-energy conformers of model (1*R*)-**8** in MeOH (PCM).

Conformers	ΔG^a	P (%)[b]
A	0.16	23.52
B	0.06	27.71
C	0.92	6.53
D	1.09	4.91
E	0.00	30.74
F	0.91	6.59

[a] B3LYP/6-311++G(2d,p), in kcal/mol. [b]From *G* values at 298.15K.

Table S114.2.4. Cartesian Coordinates, Relative Thermal Free Energies (B3LYP/6-311++G(2d,p) PCM/MeOH), and Equilibrium Populations of Low-energy Conformers of model **8** in MeOH (PCM).

Conformation A

ΔG = 0.16 kcal/mol P(%) = 23.52%

1	C	3.085911	2.458186	-0.066079
2	C	1.814968	2.416949	0.534081
3	C	1.104700	1.214602	0.667251
4	C	1.713598	0.031534	0.207037

5	C	3.000332	0.054540	-0.374560
6	C	3.659080	1.288730	-0.511053
7	O	1.015446	-1.109790	0.375850
8	C	1.399664	-2.315586	-0.390156
9	C	2.923043	-2.458250	-0.355518
10	C	3.649259	-1.197740	-0.758057
11	O	4.746831	-1.242045	-1.317657
12	C	0.860081	-2.168427	-1.812823
13	C	0.722266	-3.464634	0.341321
14	C	-1.911470	0.906738	-0.739901
15	C	-1.416949	0.628195	0.523545
16	C	-2.037385	-0.340512	1.306152
17	C	-3.145231	-1.061782	0.860513
18	C	-3.651704	-0.815484	-0.411408
19	C	-3.017740	0.169627	-1.199027
20	O	-3.501040	0.398439	-2.446734
21	O	-1.345536	1.811820	-1.613092
22	C	-1.661612	3.200686	-1.358576
23	C	-4.834889	-1.562818	-0.962782
24	O	1.228338	3.550843	0.993515
25	C	-0.264960	1.219900	1.299171
26	O	-0.266323	0.433911	2.542716
27	C	-1.299153	-0.455428	2.560645
28	O	-1.481854	-1.180548	3.520984
29	H	3.601257	3.408545	-0.161017
30	H	4.646224	1.305097	-0.959191
31	H	3.245720	-2.691053	0.667980
32	H	3.241638	-3.285099	-0.992957
33	H	1.304865	-1.321562	-2.341698
34	H	1.081833	-3.072791	-2.385323
35	H	-0.223504	-2.031846	-1.795207
36	H	-0.363052	-3.338930	0.338778
37	H	0.956882	-4.409897	-0.154333
38	H	1.065782	-3.524476	1.376798
39	H	-3.603410	-1.814458	1.493807
40	H	-2.939130	1.056605	-2.889159
41	H	-1.169168	3.768956	-2.146327
42	H	-1.280923	3.513072	-0.384769
43	H	-2.741933	3.359709	-1.404971
44	H	-4.576233	-2.099939	-1.880870
45	H	-5.204783	-2.289140	-0.237103
46	H	-5.656370	-0.884173	-1.213797
47	H	1.804091	4.318573	0.863431

48	H	-0.507544	2.237597	1.602601

Conformation B

ΔG = 0.06 kcal/mol P(%) = 27.71%

1	C	2.809359	2.702624	0.212790
2	C	1.564719	2.438265	0.810996
3	C	0.967621	1.171630	0.736123
4	C	1.649552	0.159632	0.035494
5	C	2.891816	0.414600	-0.586477
6	C	3.453921	1.698240	-0.473144
7	O	1.049033	-1.046877	-0.017833
8	C	1.860078	-2.237071	-0.352571
9	C	2.743020	-1.903148	-1.556645
10	C	3.536002	-0.630157	-1.380526
11	O	4.630485	-0.479219	-1.927735
12	C	0.840537	-3.312787	-0.694888
13	C	2.674471	-2.619515	0.883187
14	C	-2.083074	0.939440	-0.584716
15	C	-1.504961	0.427961	0.564970
16	C	-2.004056	-0.743289	1.125337
17	C	-3.074104	-1.439448	0.562645
18	C	-3.661674	-0.959877	-0.603436
19	C	-3.147207	0.227792	-1.167362
20	O	-3.708443	0.682204	-2.317243
21	O	-1.635781	2.069867	-1.235794
22	C	-2.089275	3.323296	-0.672388
23	C	-4.810403	-1.665256	-1.271070
24	O	0.900405	3.410461	1.484402
25	C	-0.359495	0.927239	1.411401
26	O	-0.236664	-0.110076	2.445166
27	C	-1.193460	-1.069402	2.295410
28	O	-1.266687	-2.002898	3.072897
29	H	3.238565	3.696260	0.293968
30	H	4.407542	1.893249	-0.950902
31	H	3.422423	-2.729907	-1.772673
32	H	2.112313	-1.759133	-2.443964
33	H	0.214011	-3.004826	-1.535528
34	H	1.354746	-4.236899	-0.970291
35	H	0.197461	-3.524147	0.163052
36	H	2.010856	-2.798423	1.732268
37	H	3.234428	-3.537216	0.685623
38	H	3.392025	-1.844534	1.164344
39	H	-3.440316	-2.351496	1.022305

40	H	-3.219092	1.461259	-2.631201
41	H	-1.655975	4.105569	-1.293886
42	H	-1.742077	3.433079	0.356198
43	H	-3.180144	3.383309	-0.705274
44	H	-4.559209	-1.957852	-2.295515
45	H	-5.085105	-2.565148	-0.717878
46	H	-5.693748	-1.021572	-1.333222
47	H	1.406681	4.235535	1.487413
48	H	-0.654471	1.830577	1.943487

Conformation C

ΔG = 0.92 kcal/mol P(%) = 6.53%

1	C	2.811706	2.642876	0.608851
2	C	1.551774	2.314139	1.139329
3	C	0.957356	1.067357	0.897772
4	C	1.650392	0.148585	0.088811
5	C	2.913161	0.466709	-0.456963
6	C	3.475212	1.723535	-0.172184
7	O	1.038637	-1.030701	-0.144536
8	C	1.848778	-2.184681	-0.590142
9	C	2.795629	-1.720988	-1.700086
10	C	3.584868	-0.484540	-1.340696
11	O	4.702428	-0.280689	-1.819511
12	C	0.831321	-3.187541	-1.112096
13	C	2.595981	-2.736761	0.623912
14	C	-2.193600	1.129798	-0.335457
15	C	-1.545911	0.394117	0.643704
16	C	-2.041582	-0.851782	1.013325
17	C	-3.175889	-1.406616	0.421278
18	C	-3.859142	-0.682654	-0.549746
19	C	-3.364735	0.592603	-0.901886
20	O	-4.071548	1.310148	-1.813121
21	O	-1.799673	2.398325	-0.710156
22	C	-0.914525	2.459659	-1.856409
23	C	-5.106754	-1.204870	-1.208636
24	O	0.869060	3.197933	1.909370
25	C	-0.371096	0.734735	1.529992
26	O	-0.241036	-0.458444	2.378574
27	C	-1.197292	-1.381372	2.080645
28	O	-1.251320	-2.440540	2.677931
29	H	3.241597	3.616315	0.821359
30	H	4.444610	1.967563	-0.592138
31	H	3.481982	-2.524529	-1.973996

32	H	2.213933	-1.470562	-2.597352
33	H	0.248076	-2.761252	-1.931890
34	H	1.344706	-4.078480	-1.481979
35	H	0.147743	-3.493589	-0.316298
36	H	1.888859	-3.006799	1.411732
37	H	3.150891	-3.634000	0.337958
38	H	3.310890	-2.019295	1.034588
39	H	-3.534464	-2.384221	0.726514
40	H	-3.708259	2.207674	-1.883487
41	H	-0.735675	3.518220	-2.038997
42	H	-1.386303	2.006954	-2.731993
43	H	0.027026	1.953152	-1.639659
44	H	-4.989355	-1.269697	-2.294993
45	H	-5.353489	-2.199693	-0.833968
46	H	-5.962392	-0.548235	-1.021442
47	H	1.374731	4.014166	2.034209
48	H	-0.651412	1.544208	2.203520

Conformation D

ΔG = 1.09 kcal/mol P(%) = 4.91%

1	C	2.963435	2.549866	0.316455
2	C	1.688020	2.372645	0.881445
3	C	1.044954	1.126986	0.863911
4	C	1.713245	0.043906	0.261980
5	C	3.006268	0.200672	-0.283989
6	C	3.604152	1.472712	-0.252464
7	O	1.062815	-1.137252	0.259260
8	C	1.520620	-2.218503	-0.640027
9	C	3.048293	-2.295015	-0.585688
10	C	3.721469	-0.961984	-0.806247
11	O	4.830093	-0.885041	-1.339787
12	C	1.000974	-1.920809	-2.046629
13	C	0.885124	-3.479728	-0.073800
14	C	-2.059347	1.123514	-0.488383
15	C	-1.484324	0.545754	0.631992
16	C	-2.064516	-0.583257	1.201081
17	C	-3.210145	-1.177719	0.672689
18	C	-3.816510	-0.613623	-0.444324
19	C	-3.236800	0.547392	-1.001054
20	O	-3.864775	1.118392	-2.061317
21	O	-1.591856	2.286869	-1.065253
22	C	-0.651779	2.110223	-2.154002
23	C	-5.069120	-1.185616	-1.050452

24	O	1.030552	3.414306	1.450672
25	C	-0.319483	0.980757	1.490073
26	O	-0.285689	-0.042623	2.544142
27	C	-1.289914	-0.949107	2.383637
28	O	-1.432033	-1.869002	3.167612
29	H	3.428737	3.529862	0.345300
30	H	4.596166	1.591735	-0.673685
31	H	3.362307	-2.644323	0.406860
32	H	3.417917	-3.017585	-1.315613
33	H	1.423298	-1.002805	-2.462880
34	H	1.265848	-2.742753	-2.716780
35	H	-0.087180	-1.825725	-2.036213
36	H	-0.204852	-3.405684	-0.090387
37	H	1.176934	-4.344670	-0.674594
38	H	1.208721	-3.650871	0.955613
39	H	-3.636106	-2.060611	1.137755
40	H	-3.440370	1.963974	-2.279497
41	H	-0.430743	3.111095	-2.521836
42	H	-1.095691	1.511164	-2.952863
43	H	0.261210	1.633335	-1.795766
44	H	-4.917082	-1.462680	-2.098463
45	H	-5.388783	-2.076282	-0.506636
46	H	-5.889661	-0.461321	-1.030274
47	H	1.562918	4.222359	1.414931
48	H	-0.574126	1.912182	1.995178

Conformation E

ΔG = 0.00 kcal/mol P(%) = 30.74%

1	C	-1.322099	-1.744344	2.435068
2	C	-0.350528	-1.547215	1.439668
3	C	-0.619893	-0.792430	0.288107
4	C	-1.903089	-0.231133	0.149833
5	C	-2.881510	-0.397603	1.156043
6	C	-2.564799	-1.170095	2.286249
7	O	-2.141621	0.488764	-0.969499
8	C	-3.540666	0.732083	-1.381295
9	C	-4.336081	1.186486	-0.155795
10	C	-4.177087	0.268658	1.032855
11	O	-5.076384	0.145865	1.867246
12	C	-4.091781	-0.555630	-1.993239
13	C	-3.444855	1.837691	-2.421782
14	C	2.107150	1.125631	0.267680
15	C	1.757099	-0.036501	-0.399523

16	C	2.752314	-0.909038	-0.829153
17	C	4.106826	-0.662742	-0.604251
18	C	4.486109	0.488026	0.078998
19	C	3.471188	1.368462	0.511794
20	O	3.841230	2.482923	1.192949
21	O	1.201771	2.032641	0.776033
22	C	0.621747	2.936668	-0.193116
23	C	5.926631	0.812308	0.366239
24	O	0.882913	-2.093078	1.550174
25	C	0.411415	-0.595146	-0.794376
26	O	0.759425	-1.882762	-1.416226
27	C	2.110388	-2.060089	-1.457579
28	O	2.593404	-3.058386	-1.959117
29	H	-1.077618	-2.340749	3.308442
30	H	-3.318165	-1.301021	3.054955
31	H	-3.983922	2.176346	0.163851
32	H	-5.395044	1.283659	-0.402577
33	H	-4.133817	-1.375863	-1.272339
34	H	-5.106295	-0.382951	-2.361611
35	H	-3.471120	-0.869803	-2.835747
36	H	-2.845188	1.513454	-3.276203
37	H	-4.443032	2.094209	-2.784903
38	H	-2.992711	2.737106	-1.996832
39	H	4.858706	-1.365113	-0.948893
40	H	3.046359	2.970112	1.468930
41	H	0.035398	2.388055	-0.931898
42	H	1.404829	3.513597	-0.691523
43	H	-0.028418	3.603650	0.371176
44	H	6.110236	0.898399	1.441961
45	H	6.583672	0.035990	-0.029503
46	H	6.219196	1.767097	-0.082315
47	H	0.965541	-2.601164	2.370481
48	H	-0.025384	0.002968	-1.592487

Conformation F

ΔG = 0.91 kcal/mol P(%) = 6.59%

1	C	1.475630	-2.063343	-2.127928
2	C	0.446235	-1.806404	-1.207095
3	C	0.653948	-0.997434	-0.080272
4	C	1.934438	-0.448085	0.114275
5	C	2.983496	-0.708381	-0.796100
6	C	2.721306	-1.515193	-1.916415
7	O	2.110819	0.319644	1.212567

8	C	3.252404	1.256356	1.259547
9	C	4.508235	0.519010	0.789106
10	C	4.324840	-0.188769	-0.532289
11	O	5.272449	-0.357271	-1.302447
12	C	3.357581	1.654114	2.723955
13	C	2.917036	2.461326	0.380726
14	C	-1.963707	1.146409	-0.188096
15	C	-1.726375	-0.074417	0.423095
16	C	-2.797540	-0.892159	0.769562
17	C	-4.120589	-0.536847	0.508573
18	C	-4.390067	0.687142	-0.093896
19	C	-3.299910	1.523415	-0.419660
20	O	-3.578133	2.736173	-0.963560
21	O	-0.966492	2.050309	-0.493141
22	C	-0.428584	1.958517	-1.835077
23	C	-5.793202	1.146861	-0.381212
24	O	-0.792417	-2.325935	-1.376982
25	C	-0.446850	-0.713438	0.910500
26	O	-0.914933	-1.971691	1.511051
27	C	-2.270287	-2.082381	1.431013
28	O	-2.844909	-3.056474	1.880695
29	H	1.275559	-2.693762	-2.988468
30	H	3.526584	-1.713805	-2.614724
31	H	5.352523	1.207748	0.720658
32	H	4.775960	-0.252636	1.523057
33	H	3.532051	0.779087	3.354791
34	H	4.189331	2.349130	2.862666
35	H	2.441378	2.148857	3.056440
36	H	1.988029	2.927078	0.716991
37	H	3.717893	3.201873	0.452081
38	H	2.806953	2.190542	-0.672092
39	H	-4.934145	-1.198688	0.786851
40	H	-2.765448	3.263159	-1.028622
41	H	-1.228144	2.037746	-2.575977
42	H	0.106777	1.017946	-1.969036
43	H	0.255161	2.798851	-1.942073
44	H	-5.942291	1.336544	-1.448952
45	H	-6.517574	0.394268	-0.065348
46	H	-6.022585	2.081122	0.141138
47	H	-0.838889	-2.863669	-2.181272
48	H	-0.038429	-0.127216	1.732565

Table S114.2.5. Gibbs Free Energies[a] and Equilibrium Populations[b] of Low energy conformers of model (4*S*,5*S*)-**9** in MeOH (PCM).

Conformers	ΔG^a	P (%)[b]
A	0.88	6.85
B	0.00	30.34
C	0.33	17.41
D	0.04	28.20
E	0.34	17.20

[a] B3LYP/6-311++G(2d,p), in kcal/mol. [b]From *G* values at 298.15K.

Table S114.2.6. Cartesian Coordinates, Relative Thermal Free Energies (B3LYP/6-311++G(2d,p) PCM/MeOH), and Equilibrium Populations of Low energy Conformers of model **9** in MeOH (PCM).

Conformation A

ΔG = 0.88 kcal/mol P(%) = 6.85%

1	C	3.061722	-1.031467	-1.488335
2	C	4.254332	-0.235561	-0.917256
3	C	4.074207	0.034717	0.585900
4	C	2.730601	0.664078	0.812127
5	C	1.589662	0.393343	-0.028927
6	C	1.696550	-0.419982	-1.241074
7	O	0.757908	-0.608625	-2.012779
8	C	2.310453	1.541865	1.751175
9	O	0.978537	1.828106	1.562518
10	C	0.537302	1.122697	0.475257
11	C	-0.861700	1.319047	0.092154
12	C	-1.747410	0.220735	0.008507
13	C	-3.089226	0.407154	-0.382259
14	C	-3.543228	1.711653	-0.649859
15	C	-2.705773	2.798938	-0.550482
16	C	-1.365245	2.604840	-0.181371
17	O	-1.241808	-0.986358	0.322007
18	C	-2.167632	-2.097283	0.636515
19	C	-3.299544	-2.099377	-0.393172
20	C	-3.964525	-0.752750	-0.547690
21	O	-5.155311	-0.656555	-0.849919
22	C	5.583782	-0.920646	-1.236285
23	O	4.178261	-1.224272	1.287288
24	C	-2.674860	-1.900778	2.065018
25	C	-1.310946	-3.349018	0.523376
26	O	-0.599549	3.721461	-0.124386
27	H	3.175462	-1.180275	-2.565031
28	H	3.037246	-2.032875	-1.037233

29	H	4.258058	0.751987	-1.394426
30	H	4.868930	0.700231	0.937931
31	H	2.782455	2.047088	2.579071
32	H	-4.576293	1.849257	-0.948823
33	H	-3.050123	3.804817	-0.761059
34	H	-2.896119	-2.364868	-1.379316
35	H	-4.047953	-2.850469	-0.133997
36	H	5.628930	-1.931056	-0.821934
37	H	6.426159	-0.351549	-0.830491
38	H	5.725976	-0.997562	-2.318283
39	H	4.076404	-1.061600	2.234652
40	H	-3.256837	-0.982724	2.178530
41	H	-3.316789	-2.739702	2.345897
42	H	-1.834967	-1.864134	2.762817
43	H	-0.482836	-3.314781	1.235831
44	H	-1.913743	-4.233377	0.743903
45	H	-0.902313	-3.453025	-0.484448
46	H	0.302910	3.541337	0.178646

Conformation B

ΔG = 0.00 kcal/mol P(%) = 30.34%

1	C	-3.944292	0.786662	-1.158258
2	C	-4.329033	-0.691885	-0.960676
3	C	-3.974329	-1.173510	0.456162
4	C	-2.523135	-0.890984	0.706694
5	C	-1.845433	0.248603	0.135750
6	C	-2.547896	1.177687	-0.729215
7	O	-2.070198	2.269950	-1.071911
8	C	-1.594167	-1.561954	1.420839
9	O	-0.382760	-0.923710	1.329096
10	C	-0.520169	0.176147	0.535414
11	C	0.714801	0.928583	0.292245
12	C	1.905785	0.228409	-0.036341
13	C	3.144309	0.895405	-0.098389
14	C	3.191008	2.272474	0.185144
15	C	2.044016	2.982138	0.455033
16	C	0.801958	2.326332	0.472875
17	O	1.780134	-1.083358	-0.319350
18	C	2.975553	-1.952058	-0.272143
19	C	4.121780	-1.244944	-0.998292
20	C	4.344485	0.168730	-0.518610
21	O	5.463012	0.683844	-0.539935
22	C	-5.795794	-0.935452	-1.318533

23	O	-4.813889	-0.473205	1.399518
24	C	2.554409	-3.218314	-1.002020
25	C	3.299767	-2.238776	1.194013
26	O	-0.286238	3.089713	0.723540
27	H	-4.063973	1.081919	-2.204926
28	H	-4.623772	1.433137	-0.586931
29	H	-3.709742	-1.294433	-1.635802
30	H	-4.168210	-2.247558	0.539274
31	H	-1.604090	-2.458531	2.020484
32	H	4.148884	2.778922	0.147939
33	H	2.065951	4.051035	0.633238
34	H	5.047036	-1.815560	-0.899231
35	H	3.890637	-1.178730	-2.069806
36	H	-6.469213	-0.337990	-0.698464
37	H	-6.061603	-1.989035	-1.187636
38	H	-5.984887	-0.672735	-2.363592
39	H	-4.607547	-0.787734	2.289962
40	H	2.262005	-2.996759	-2.031353
41	H	3.386042	-3.926723	-1.025765
42	H	1.713466	-3.696935	-0.493733
43	H	2.443557	-2.704154	1.687507
44	H	4.146244	-2.927646	1.254751
45	H	3.566104	-1.334401	1.747104
46	H	-1.039115	2.818281	0.139154

Conformation C

ΔG = 0.33 kcal/mol P(%) = 17.41%

1	C	3.944175	0.787253	-1.122911
2	C	4.713034	0.051859	-0.000965
3	C	3.956167	-1.205563	0.455385
4	C	2.520927	-0.859126	0.736904
5	C	1.840932	0.264238	0.135163
6	C	2.553984	1.203924	-0.713876
7	O	2.078015	2.295960	-1.056002
8	C	1.597925	-1.492917	1.493541
9	O	0.387772	-0.856806	1.388289
10	C	0.521453	0.213013	0.553521
11	C	-0.715838	0.960370	0.299522
12	C	-1.899688	0.249598	-0.029122
13	C	-3.142128	0.907981	-0.106167
14	C	-3.198898	2.287492	0.163261
15	C	-2.057956	3.006693	0.434232
16	C	-0.812432	2.358102	0.467103

17	O	-1.762681	-1.064644	-0.296078
18	C	-2.952902	-1.940491	-0.251770
19	C	-4.097981	-1.247141	-0.993041
20	C	-4.334404	0.168903	-0.527005
21	O	-5.456636	0.675370	-0.559701
22	C	6.154863	-0.242820	-0.415041
23	O	4.041482	-2.192739	-0.596750
24	C	-3.287622	-2.216819	1.213961
25	C	-2.517471	-3.209823	-0.967889
26	O	0.270600	3.129702	0.718408
27	H	4.487555	1.676355	-1.449394
28	H	3.847006	0.128320	-1.995898
29	H	4.739197	0.714018	0.873061
30	H	4.431717	-1.611896	1.353860
31	H	1.614362	-2.358613	2.137069
32	H	-4.159349	2.788042	0.114532
33	H	-2.087530	4.077108	0.601993
34	H	-3.858646	-1.188105	-2.063178
35	H	-5.019988	-1.823438	-0.896694
36	H	6.201537	-0.850278	-1.322371
37	H	6.687889	-0.777691	0.377285
38	H	6.694921	0.688459	-0.608838
39	H	3.574348	-2.989390	-0.311237
40	H	-3.565512	-1.309432	1.756391
41	H	-4.129474	-2.911446	1.273637
42	H	-2.432201	-2.671280	1.718896
43	H	-1.677605	-3.678661	-0.448811
44	H	-3.344149	-3.923995	-0.992853
45	H	-2.217887	-2.994450	-1.996452
46	H	1.028544	2.853272	0.144852

Conformation D

ΔG = 0.04 kcal/mol P(%) = 28.20%

1	C	3.869988	0.652902	1.258876
2	C	4.275715	-0.784970	0.885000
3	C	3.984365	-1.076092	-0.596825
4	C	2.543208	-0.762910	-0.871557
5	C	1.829355	0.282639	-0.177796
6	C	2.483964	1.085763	0.837696
7	O	1.975697	2.111345	1.315905
8	C	1.653582	-1.330827	-1.713918
9	O	0.433116	-0.716903	-1.587995
10	C	0.523032	0.260887	-0.642356

11	C	-0.734603	0.953942	-0.347680
12	C	-1.924052	0.192082	-0.180202
13	C	-3.178881	0.823549	-0.078656
14	C	-3.239332	2.228649	-0.100360
15	C	-2.096826	2.987459	-0.197244
16	C	-0.844174	2.360049	-0.300784
17	O	-1.785596	-1.147071	-0.121135
18	C	-2.881181	-1.965553	0.443340
19	C	-4.208367	-1.475316	-0.137291
20	C	-4.398394	0.015642	-0.003763
21	O	-5.521018	0.511056	0.101651
22	C	5.728698	-1.068681	1.268154
23	O	4.861107	-0.259916	-1.403023
24	C	-2.828028	-1.847340	1.966392
25	C	-2.566890	-3.383222	-0.010278
26	O	0.234759	3.172727	-0.394036
27	H	3.953488	0.811617	2.338073
28	H	4.560357	1.371738	0.797581
29	H	3.634474	-1.473191	1.448533
30	H	4.186449	-2.130179	-0.811465
31	H	1.698697	-2.135252	-2.431303
32	H	-4.208501	2.708778	-0.026137
33	H	-2.131520	4.070732	-0.188309
34	H	-4.246195	-1.701803	-1.211248
35	H	-5.045230	-1.994623	0.333414
36	H	6.421617	-0.393661	0.759311
37	H	6.008587	-2.095406	1.012524
38	H	5.873286	-0.943841	2.345422
39	H	4.716321	-0.476612	-2.333850
40	H	-3.015618	-0.828205	2.313820
41	H	-3.586713	-2.496205	2.411397
42	H	-1.849312	-2.161563	2.336663
43	H	-1.599483	-3.708663	0.380659
44	H	-3.332208	-4.070193	0.359081
45	H	-2.543841	-3.448296	-1.100758
46	H	0.973770	2.833012	0.171170

Conformation E

ΔG = 0.34 kcal/mol P(%) = 17.20%

1	C	-3.885868	0.685404	1.198746
2	C	-4.697764	0.084552	0.028126
3	C	-3.969710	-1.121860	-0.584347
4	C	-2.541591	-0.756363	-0.876679

5	C	-1.827645	0.286330	-0.177251
6	C	-2.499460	1.125947	0.800690
7	O	-1.993733	2.159304	1.262140
8	C	-1.654473	-1.307547	-1.734000
9	O	-0.434631	-0.696076	-1.603125
10	C	-0.524141	0.273441	-0.648583
11	C	0.733853	0.972009	-0.362872
12	C	1.921255	0.210666	-0.183822
13	C	3.177433	0.840985	-0.091136
14	C	3.240739	2.245506	-0.133744
15	C	2.099785	3.004821	-0.243355
16	C	0.846344	2.377729	-0.339172
17	O	1.779799	-1.127505	-0.106705
18	C	2.872686	-1.938444	0.474218
19	C	4.201768	-1.460914	-0.112484
20	C	4.395149	0.031732	-0.003680
21	O	5.518905	0.526153	0.093648
22	C	-6.128871	-0.242674	0.454257
23	O	-4.029374	-2.213938	0.360206
24	C	2.556725	-3.363233	0.045078
25	C	2.816868	-1.793501	1.994836
26	O	-0.231331	3.190583	-0.447624
27	H	-4.404911	1.541524	1.634838
28	H	-3.776064	-0.063318	1.994635
29	H	-4.742651	0.838180	-0.767368
30	H	-4.478936	-1.427307	-1.503959
31	H	-1.704472	-2.094979	-2.469789
32	H	4.210752	2.724847	-0.066096
33	H	2.136184	4.088065	-0.251170
34	H	5.036772	-1.973950	0.368296
35	H	4.241019	-1.705521	-1.182376
36	H	-6.152252	-0.951148	1.285953
37	H	-6.694620	-0.677247	-0.375827
38	H	-6.650300	0.664368	0.773257
39	H	-3.583498	-2.980072	-0.024918
40	H	2.536724	-3.447743	-1.044116
41	H	3.319663	-4.044884	0.428855
42	H	1.587678	-3.679658	0.439220
43	H	1.837032	-2.100081	2.368471
44	H	3.573881	-2.435472	2.452457
45	H	3.004933	-0.768803	2.325207
46	H	-0.972514	2.857514	0.117153

Table S114.2.7. Gibbs Free Energies[a] and Equilibrium Populations[b] of Low energy conformers of model (5*R*,9*S*)-**10** in MeOH (PCM).

Conformers	ΔG^a	P (%)[b]
A	0.00	81.19
B	2.67	0.90
C	2.37	1.47
D	0.95	16.43

[a]B3LYP/6-311++G(2d,p), in kcal/mol. [b]From *G* values at 298.15K.

Table S114.2.8. Cartesian Coordinates, Relative Thermal Free Energies (B3LYP/6-311++G(2d,p) PCM/MeOH), and Equilibrium Populations of Low energy Conformers of model **10** in MeOH (PCM).

Conformation A

ΔG = 0.00 kcal/mol P(%) = 81.19%

1	C	-1.796824	0.412465	0.195267
2	C	-2.270312	1.716078	0.327616
3	C	-3.585086	1.979125	-0.061998
4	C	-4.405648	0.969761	-0.571219
5	C	-3.914843	-0.331789	-0.696255
6	C	-2.605308	-0.599987	-0.305968
7	C	-0.431189	-0.156979	0.530402
8	C	0.043954	0.095654	1.964960
9	C	-0.937309	-0.343480	3.051381
10	C	0.624698	0.270201	-0.534190
11	C	2.033675	-0.248419	-0.379347
12	C	2.905031	0.838266	-0.346970
13	C	4.288481	0.703030	-0.277715
14	C	4.793351	-0.595071	-0.246289
15	C	3.937841	-1.699631	-0.270272
16	C	2.547423	-1.547345	-0.329377
17	O	0.790237	1.715125	-0.518553
18	O	1.772744	-2.665028	-0.340076
19	C	2.102311	2.064966	-0.420015
20	O	2.442445	3.229774	-0.406634
21	O	-0.607117	-1.592281	0.328815
22	C	-1.861775	-1.897306	-0.332316
23	O	-4.659992	-1.373808	-1.183873
24	H	-1.645608	2.507729	0.724058
25	H	-3.983366	2.984274	0.032430
26	H	-5.427811	1.187175	-0.867600
27	H	0.256679	1.165056	2.063286
28	H	0.997490	-0.423597	2.102439
29	H	-0.503633	-0.160652	4.038782

30	H	-1.162865	-1.411227	2.984977
31	H	-1.881376	0.205288	3.000447
32	H	0.222896	0.013008	-1.518466
33	H	4.938859	1.569995	-0.257054
34	H	5.864430	-0.760188	-0.198180
35	H	4.343523	-2.705647	-0.236657
36	H	0.832861	-2.423093	-0.167090
37	H	-2.352054	-2.698195	0.227397
38	H	-1.661258	-2.255469	-1.348044
39	H	-5.556117	-1.081948	-1.404311

Conformation B

ΔG = 2.67 kcal/mol P(%) = 0.90%

1	C	-1.854599	0.359394	0.235742
2	C	-2.312742	1.676706	0.195886
3	C	-3.637211	1.904273	-0.183440
4	C	-4.487123	0.850148	-0.522923
5	C	-4.011505	-0.461980	-0.493626
6	C	-2.692170	-0.694952	-0.114299
7	C	-0.483135	-0.190136	0.595358
8	C	-0.016920	0.068150	2.040965
9	C	0.289343	1.502426	2.478359
10	C	0.552829	0.120654	-0.526685
11	C	1.968339	-0.373204	-0.348649
12	C	2.834990	0.707741	-0.500686
13	C	4.220688	0.585654	-0.459348
14	C	4.734098	-0.693744	-0.258983
15	C	3.884880	-1.792193	-0.104147
16	C	2.492191	-1.653544	-0.143895
17	O	0.711419	1.554993	-0.710095
18	O	1.730286	-2.769739	0.008804
19	C	2.024638	1.911090	-0.724141
20	O	2.360765	3.063757	-0.901581
21	O	-0.669982	-1.640273	0.502934
22	C	-1.965004	-1.997571	-0.036879
23	O	-4.779014	-1.548326	-0.824626
24	H	-1.668073	2.510887	0.438433
25	H	-4.017287	2.920199	-0.219075
26	H	-5.515718	1.041790	-0.814929
27	H	0.865771	-0.557274	2.209654
28	H	-0.804682	-0.339223	2.682365
29	H	0.567109	1.494077	3.536632
30	H	-0.573796	2.163592	2.378860

31	H	1.122469	1.947615	1.931938
32	H	0.128580	-0.261337	-1.459724
33	H	4.866044	1.447626	-0.583727
34	H	5.807061	-0.848846	-0.220618
35	H	4.297620	-2.783482	0.053480
36	H	0.784603	-2.523781	0.133321
37	H	-2.427423	-2.722306	0.639077
38	H	-1.834034	-2.471856	-1.015696
39	H	-5.675565	-1.274437	-1.065136

Conformation C

ΔG = 2.37 kcal/mol P(%) = 1.47%

1	C	-1.901344	0.434241	0.270204
2	C	-2.386614	1.739215	0.331906
3	C	-3.710441	1.965528	-0.050699
4	C	-4.529402	0.919888	-0.482885
5	C	-4.027413	-0.382294	-0.535630
6	C	-2.708343	-0.613589	-0.153818
7	C	-0.524524	-0.103309	0.627398
8	C	-0.146020	0.232861	2.079863
9	C	1.041196	-0.512854	2.693680
10	C	0.507999	0.315563	-0.463357
11	C	1.916335	-0.227859	-0.424770
12	C	2.804379	0.845218	-0.440720
13	C	4.186650	0.688239	-0.491557
14	C	4.670932	-0.616985	-0.539294
15	C	3.797942	-1.708420	-0.523110
16	C	2.411031	-1.534283	-0.457917
17	O	0.698129	1.756530	-0.421527
18	O	1.617757	-2.638874	-0.429927
19	C	2.019310	2.084451	-0.416864
20	O	2.378330	3.243630	-0.399316
21	O	-0.677768	-1.546612	0.475138
22	C	-1.955486	-1.903393	-0.114448
23	O	-4.769424	-1.459227	-0.945176
24	H	-1.764116	2.560410	0.666255
25	H	-4.116548	2.971244	-0.012376
26	H	-5.558216	1.109573	-0.775195
27	H	-1.037351	0.029965	2.681780
28	H	0.019447	1.313295	2.138306
29	H	1.101669	-0.272622	3.759506
30	H	1.996051	-0.235157	2.245342
31	H	0.927258	-1.596655	2.611121

32	H	0.053368	0.090213	-1.432813
33	H	4.850676	1.545000	-0.502522
34	H	5.739439	-0.798421	-0.585874
35	H	4.188312	-2.720609	-0.552291
36	H	0.703908	-2.386088	-0.159781
37	H	-2.419896	-2.664731	0.518092
38	H	-1.786972	-2.333214	-1.107725
39	H	-5.670341	-1.189078	-1.173236

Conformation D

ΔG = 0.95 kcal/mol P(%) = 16.43%

1	C	-1.802666	0.405045	0.211102
2	C	-2.276035	1.704108	0.363272
3	C	-3.588190	1.975168	-0.033760
4	C	-4.399338	0.976620	-0.571022
5	C	-3.909830	-0.323563	-0.718790
6	C	-2.604690	-0.603825	-0.317086
7	C	-0.435803	-0.161213	0.544710
8	C	0.045387	0.093050	1.976391
9	C	-0.929817	-0.345834	3.068308
10	C	0.615046	0.265447	-0.525842
11	C	2.027067	-0.246411	-0.374911
12	C	2.893936	0.844281	-0.357790
13	C	4.278443	0.715779	-0.298484
14	C	4.789445	-0.579737	-0.260343
15	C	3.938670	-1.688099	-0.267598
16	C	2.547191	-1.542465	-0.316753
17	O	0.774100	1.710943	-0.519173
18	O	1.778340	-2.664452	-0.309916
19	C	2.085478	2.067029	-0.433817
20	O	2.420727	3.233251	-0.431743
21	O	-0.611780	-1.596519	0.347179
22	C	-1.843918	-1.896062	-0.351621
23	O	-4.756415	-1.262585	-1.254633
24	H	-1.653786	2.487168	0.780220
25	H	-3.987515	2.978239	0.076673
26	H	-5.417803	1.192402	-0.877321
27	H	0.257470	1.162806	2.071882
28	H	1.000423	-0.424500	2.109793
29	H	-0.492385	-0.158206	4.053138
30	H	-1.152009	-1.414532	3.006463
31	H	-1.875923	0.199539	3.019572
32	H	0.210961	0.001510	-1.507451

33	H	4.925003	1.585785	-0.290077
34	H	5.861592	-0.739774	-0.219779
35	H	4.348995	-2.692032	-0.228219
36	H	0.838455	-2.426536	-0.133901
37	H	-2.338026	-2.714939	0.178793
38	H	-1.614511	-2.229719	-1.370087
39	H	-4.332967	-2.128220	-1.339198

Table S114.2.9. Gibbs Free Energies[a] and Equilibrium Populations[b] of Low energy conformers of model (5*R*)-**11** in MeOH (PCM).

Conformers	ΔG^a	P (%)[b]
A	1.39	4.02
B	0.74	12.03
C	0.93	8.85
D	1.03	7.47
E	1.23	5.31
F	0.00	42.28
G	0.44	20.02

[a]B3LYP/6-311++G(2d,p), in kcal/mol. [b]From *G* values at 298.15K.

Table S114.2.10. Cartesian Coordinates, Relative Thermal Free Energies (B3LYP/6-311++G(2d,p) PCM/MeOH), and Equilibrium Populations of Low energy Conformers of model **11** in MeOH (PCM).

Conformation A

ΔG = 1.39 kcal/mol P(%) = 4.02%

1	C	-0.701081	0.193433	0.106836
2	C	0.120129	1.235167	-0.153481
3	C	-2.123018	0.302185	0.617783
4	C	-0.242223	-1.199462	-0.111732
5	O	-1.006484	-2.142017	0.050822
6	C	1.168365	-1.442878	-0.617494
7	C	2.140056	-0.33848	-0.239111
8	O	2.371313	-0.469855	1.167229
9	C	1.551306	1.027604	-0.599662
10	C	-0.27399	2.682824	-0.044658
11	O	-3.084596	-0.226024	-0.290163
12	H	-2.186977	-0.220977	1.580703
13	H	-2.412462	1.336056	0.792691
14	H	1.507703	-2.411475	-0.246636
15	H	1.109781	-1.518906	-1.711069
16	H	3.087627	-0.477419	-0.776758
17	H	3.00745	0.196152	1.454578
18	H	1.606998	1.166457	-1.689515

19	H	2.178885	1.825716	-0.181483
20	H	-1.349414	2.844324	-0.009959
21	H	0.16564	3.131687	0.854771
22	H	0.123684	3.246563	-0.895125
23	H	-2.918041	-1.177366	-0.346189

Conformation B

ΔG = 0.74 kcal/mol P(%) = 12.03%

1	C	-0.708158	0.197992	0.091978
2	C	0.119106	1.242601	-0.142582
3	C	-2.13527	0.30233	0.590036
4	C	-0.239523	-1.189649	-0.11511
5	O	-0.977942	-2.144986	0.093343
6	C	1.159486	-1.413532	-0.661186
7	C	2.141	-0.321579	-0.248669
8	O	2.398786	-0.343561	1.159613
9	C	1.560688	1.051287	-0.561463
10	C	-0.276652	2.687949	-0.017698
11	O	-3.084353	-0.267506	-0.305841
12	H	-2.199784	-0.189837	1.569327
13	H	-2.439815	1.337103	0.729238
14	H	1.493649	-2.410076	-0.357186
15	H	1.082248	-1.436339	-1.756984
16	H	3.087422	-0.447469	-0.791448
17	H	2.712711	-1.21905	1.416929
18	H	1.64007	1.241403	-1.641063
19	H	2.18189	1.813026	-0.079151
20	H	-1.352354	2.851986	-0.015483
21	H	0.134745	3.112907	0.905958
22	H	0.15246	3.268837	-0.840646
23	H	-2.909232	-1.218461	-0.328242

Conformation C

ΔG = 0.93 kcal/mol P(%) = 8.85%

1	C	-0.716962	0.244091	-0.283862
2	C	0.17584	1.263465	-0.251249
3	C	-2.221588	0.382078	-0.152947
4	C	-0.258062	-1.157847	-0.463622
5	O	-1.062453	-2.081284	-0.467629
6	C	1.222397	-1.421677	-0.664122
7	C	2.102531	-0.389262	0.039264
8	O	2.102077	-0.560803	1.457279
9	C	1.666686	1.020079	-0.364895

10	C	-0.185609	2.71707	-0.122608
11	O	-2.729848	-0.309385	0.983764
12	H	-2.524703	1.418462	-0.0268
13	H	-2.698351	0.006266	-1.067324
14	H	1.447357	-2.435844	-0.329494
15	H	1.414578	-1.386499	-1.745552
16	H	3.146941	-0.541922	-0.240524
17	H	1.208593	-0.439426	1.806056
18	H	1.973471	1.215247	-1.402974
19	H	2.205863	1.750603	0.246702
20	H	-1.251305	2.922793	-0.187501
21	H	0.1782	3.109498	0.834148
22	H	0.320094	3.298445	-0.901602
23	H	-2.610352	-1.25382	0.811796

Conformation D

ΔG = 1.03 kcal/mol P(%) = 7.47%

1	C	-0.691603	0.183133	0.116675
2	C	0.127179	1.228724	-0.155266
3	C	-2.11482	0.290241	0.627517
4	C	-0.239031	-1.21093	-0.120919
5	O	-1.009927	-2.149949	0.033093
6	C	1.178871	-1.450893	-0.607833
7	C	2.144835	-0.333018	-0.222028
8	O	2.488781	-0.374992	1.165015
9	C	1.553425	1.021052	-0.619367
10	C	-0.272496	2.674488	-0.052305
11	O	-3.074623	-0.199136	-0.302476
12	H	-2.191539	-0.262188	1.573006
13	H	-2.394084	1.321206	0.832959
14	H	1.517738	-2.419871	-0.235931
15	H	1.128324	-1.529851	-1.702676
16	H	3.10053	-0.477102	-0.730096
17	H	1.695529	-0.250782	1.702822
18	H	1.582399	1.129142	-1.713513
19	H	2.188475	1.820569	-0.224128
20	H	-1.346638	2.832873	0.016161
21	H	0.199012	3.139249	0.822154
22	H	0.095724	3.224607	-0.924431
23	H	-2.927476	-1.152015	-0.380239

Conformation E

ΔG = 1.23 kcal/mol P(%) = 5.31%

1	C	-0.740965	0.206637	-0.293995
2	C	0.094097	1.2693	-0.225611
3	C	-2.254185	0.260364	-0.208148
4	C	-0.196405	-1.163015	-0.433964
5	O	-0.924402	-2.144784	-0.352638
6	C	1.283384	-1.325063	-0.726177
7	C	2.131819	-0.274663	-0.014003
8	O	2.091651	-0.435723	1.40656
9	C	1.598981	1.122045	-0.305526
10	C	-0.34812	2.697755	-0.069506
11	O	-2.762979	-0.390982	0.951058
12	H	-2.620714	1.282666	-0.156713
13	H	-2.678347	-0.1971	-1.111878
14	H	1.581628	-2.344902	-0.466126
15	H	1.422895	-1.225146	-1.811347
16	H	3.172707	-0.344675	-0.357903
17	H	2.333314	-1.340641	1.639108
18	H	1.924643	1.431841	-1.308639
19	H	2.069761	1.825624	0.388577
20	H	-1.418266	2.850491	-0.186753
21	H	-0.062402	3.064352	0.923333
22	H	0.168313	3.337341	-0.793853
23	H	-2.539334	-1.3281	0.863939

Conformation F

ΔG = 0.00 kcal/mol P(%) = 42.28%

1	C	0.861764	0.176488	-0.215067
2	C	0.049683	1.257155	-0.130095
3	C	2.377177	0.209664	-0.267816
4	C	0.289256	-1.191191	-0.267007
5	O	1.013823	-2.178428	-0.263016
6	C	-1.219638	-1.337017	-0.352138
7	C	-1.933191	-0.23255	0.422107
8	O	-3.348773	-0.264765	0.243176
9	C	-1.456349	1.126036	-0.062972
10	C	0.521712	2.684307	-0.101825
11	O	2.975978	-0.452424	0.841302
12	H	2.712574	-0.250679	-1.206483
13	H	2.760812	1.2266	-0.245977
14	H	-1.512648	-1.270845	-1.408417
15	H	-1.488462	-2.336823	-0.001101
16	H	-1.695998	-0.332386	1.491244
17	H	-3.70383	-1.073922	0.630907

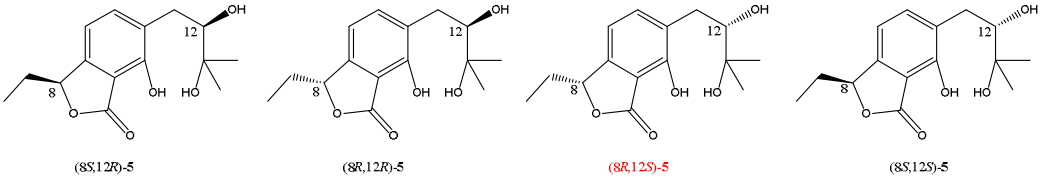
18	H	-1.86944	1.911762	0.577489
19	H	-1.879569	1.306634	-1.061301
20	H	1.582304	2.810922	-0.305474
21	H	-0.038241	3.279155	-0.831782
22	H	0.311167	3.126823	0.878739
23	H	2.750634	-1.389659	0.759332

Conformation G

ΔG = 0.44 kcal/mol P(%) = 20.02%

1	C	0.861212	0.182322	-0.20964
2	C	0.048336	1.262251	-0.137446
3	C	2.376761	0.217714	-0.254407
4	C	0.290517	-1.188732	-0.265521
5	O	1.023337	-2.169188	-0.2861
6	C	-1.216346	-1.349937	-0.324039
7	C	-1.93159	-0.238188	0.422535
8	O	-3.332766	-0.429231	0.230747
9	C	-1.459184	1.119131	-0.095221
10	C	0.515829	2.691009	-0.107721
11	O	2.971213	-0.452904	0.851513
12	H	2.716384	-0.234	-1.195666
13	H	2.759143	1.234906	-0.222208
14	H	-1.52337	-1.319584	-1.37834
15	H	-1.484763	-2.334593	0.061091
16	H	-1.692849	-0.314216	1.493241
17	H	-3.823063	0.162693	0.814197
18	H	-1.881339	1.927407	0.514904
19	H	-1.864947	1.2659	-1.106031
20	H	1.582739	2.817758	-0.2751
21	H	-0.018022	3.276963	-0.864276
22	H	0.270567	3.144446	0.859785
23	H	2.752046	-1.390512	0.757888

S115 Possible isomers, experimental and calculated ECD of compound **5**, **8-11**.



(8*S*,12*R*)-5 (8*R*,12*R*)-5 (8*R*,12*S*)-5 (8*S*,12*S*)-5

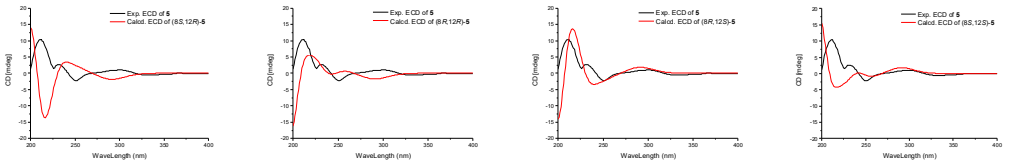


Figure S115.1 Possible isomers, experimental and calculated ECD of **5**.

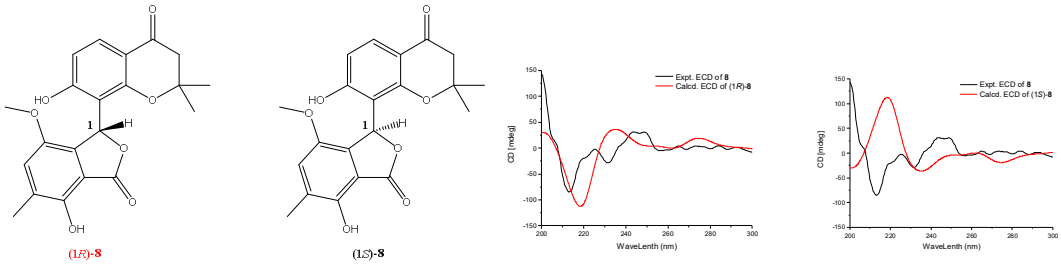


Figure S115.2 Possible isomers, experimental and calculated ECD of **8**.

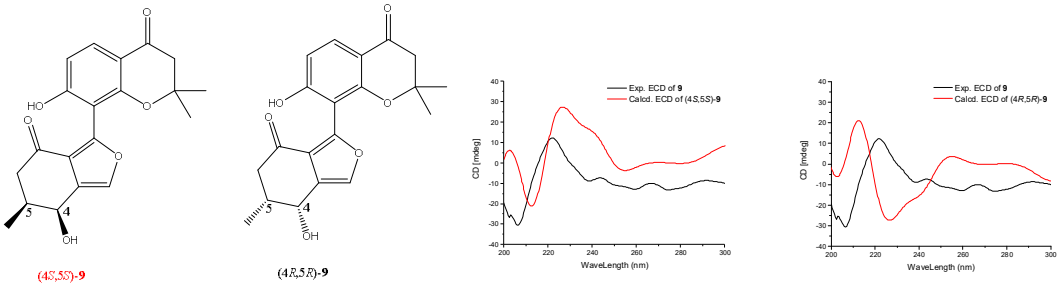


Figure S115.3 Possible isomers, experimental and calculated ECD of **9**.

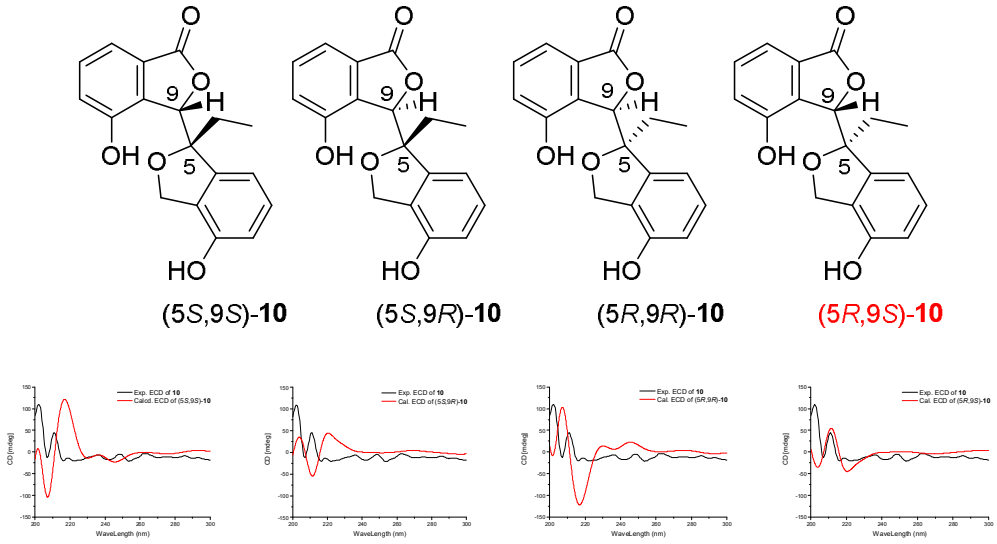


Figure S115.4 Possible isomers, experimental and calculated ECD of **10**.

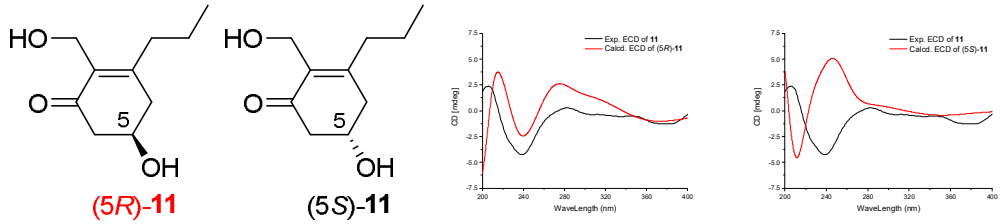


Figure S115.5. Possible isomers, experimental and calculated ECD of **11**.

S116 Detailed procedure of inhibitory activity of enzymes assay.

Phosphatase Enzyme Inhibition Assays. Recombinant human phosphatase TCPTP, SHP1, PTP1B were expressed in Escherichia coli and purified. The enzyme inhibition assays were measured using *p*-nitrophenyl phosphate (pNPP) as a substrate in a 96-well plate with a final volume of 100 μL. Human recombinant TCPTP, SHP1, PTP1B (0.05 μg) in 50 μL reaction buffer (pH 6.5) containing 50 mM HEPES, 100mM NaCl, 1 mM EDTA, and 1 mM dithiothreitol (DTT) and test compounds were added to each well of a 96-well plate. Na3VO4 was used as the positive control and DMSO as the negative control to evaluate the high-throughput screening (HTS) system. After preincubation for 15 min at room temperature, 50 μL of reaction buffer containing 50 mM pNPP was added and incubated at 37°C for 60 min. The phosphatase activity was determined by measuring the absorbance at 405 nm for the amount of produced *p*-nitrophenol. Each compound was assayed in triplicate.

The cathepsin B assays were carried out in triplicate according to a published method[1] with modification: 50 μL of reaction buffer (100 mMAcONa, 1 mM EDTA, 4 mM dithiothreitol, pH 5.5) containing 0.0025 units of cathepsin B and 2 μL of compounds dissolved in DMSO were added to each well of a 96 well plate. After pre-incubation for 15 min at r.t., 50 μL of reaction buffer (100 μM Z-Arg-Arg-7-amido-4-methylcoumarin) was added and incubated for 30 min at r.t. Fluorescence was measured using a microplate reader (Wallac 1420 Victor2, Perkin-Elmer Ex 355, Em 460 nm). The IC_{50} value was defined as the concentration of sample necessary to inhibit the cathepsin B activity to 50% of the control. Leupeptin was used as a positive control substance.

S117 ITS gene sequences of *Aspergillus gorakhpurensis* F07ZB1707.

GenBank accession No. MT994887

AGTGAAGGGCCCTCTGGGTCCGACCTCCCACCCTTGTCTATCGTACCT
TGTTGCTTCGGCGGGCCCGCCATTCGTGGCCGCCGGGGGGCATCTGCCCCC
GGGCCCGCGCCCGCCGGAGACAAATACGAACACTGTCTGAAGTTGCAGTC
TGAGTTGATTTATTCAATCATTAAAACTTTCAACAACGGATCTCTTGGTTCC
GGCATCGATGAAGAACGCAGCGAAATGCGATAACTAATGTGAATTGCAGAA
TTCAGTGAATCATCGAGTCTTTGAACGCACATTGCGCCCCTTGGTATTCCGG
GGGGCATGCCTGTCCGAGCGTCATTGCTGCCCTCAAGCACGGCTTGTGTGT
TGGGCCCTCGTCCCCTCCCCGGGGGACGGGCCCGAAAGGCAGCGGCGGCA
CCGAGTCCGGTCCTCGAGCGTATGGGATAACACCCGCTTTCGTAGGCCCGG
CCGGCGCTTGCCGACCCCAACCTATTTTTTAACCAGGTTGACCTCGGATCA
GGTAGGGATACCCGCTGAACTTAAGCATATCAATAAGCGGAGGA

References

1 W. Halangk, M.M. Lerch, B. Brandt-Nedelev, W. Roth, M. Ruthenbuerger, T. Reinheckel, W. Domschke, H. Lippert, C. Peters and J. Deussing, *J. Clin. Invest.*, 2000, **106**, 773-781.