Supplementary Material

Hyalangium ruber sp. nov, characterization of a novel myxobacterium strain s54d21 and their secondary metabolites

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Table S1. Genomic features of strain s54d21^T and the closely type strains.

Genomic features	s54d21^T	*H. minutum* DSM 14724^T	*H. gracilis* DSM 14753^T	*H. versicolor* H56D21^T
Size (Mbp)	10.77	11.19	11.73	13.56
Number of contigs	43	44	82	101
DNA G+C content (mol%)	68.5	68.0	69.5	67.1
N50 (bp)	586569	504291	346585	364296
L50	7	7	11	12
Number of genes	8727	8967	9333	10609
Number of CDSs	8621	8882	9176	10522
Number of rRNAs genes	3	3	3	3
Number of tRNAs genes	70	81	89	83
Completeness (%)	99.76%	98.94%	98.94%	99.57%
GenBank accession number	JAXIVS000000000	JMCB000000 00	JAHXBG000000000	JAHXBF000000000

Table S2. ANI and dDDH values between strain s54d21^T and the closely type strains.

Type strain	ANI values (%)	dDDH values (%)
H. minutum DSM 14724^T	81.7	24.5
H. gracilis DSM 14753^T	82.7	25.7
H. versicolor H56D21^T	81.3	24.4

Table S3. Cellular fatty acid profiles of strain s54d21^T and the closely related type strains.

Fatty acids	1	2	3	4
$C_{16:0}$	2.8	7.8	8.8	6.9
$C_{16:1}\omega5c$	6.6	22.1	24.3	14.3
$C_{16:1}\omega7c$	1.5	7.1	6.6	3.7
$C_{18:1}\omega9c$	–	1.3	0.4	1.1
$C_{16:0}$-2OH	–	1.5	–	0.9
iso-$C_{15:0}$	17.4	11.7	19.2	27.9
iso-$C_{16:0}$	6.8	10.7	1.5	3.3
iso-$C_{17:0}$	3.7	6.0	17.9	11.3
iso-$C_{17:1}\omega5c$	0.9	1.1	1.4	0.5
iso-$C_{15:0}$-3 OH	6.2	8.1	2.6	3.8
iso-$C_{17:0}$-2 OH	27.8	8.0	1.0	3.6
iso-$C_{15:0}$ OAG	0.5	1.7	0.4	0.6
iso-$C_{15:0}$ DMA	8.2	7.3	11.2	18.4

1. s54d21^T; 2. *H. minutum* DSM 14724^T; 3. *H. gracilis* DSM 14753^T; 4. *H. versicolor* H56D21^T. All data are obtained from this study. Values are percentages of total fatty acids detected. Fatty acids percentages less than 1% of the total amounts in all the strains are not shown. Components in bold represent major fatty acid profiles. −, not detected.

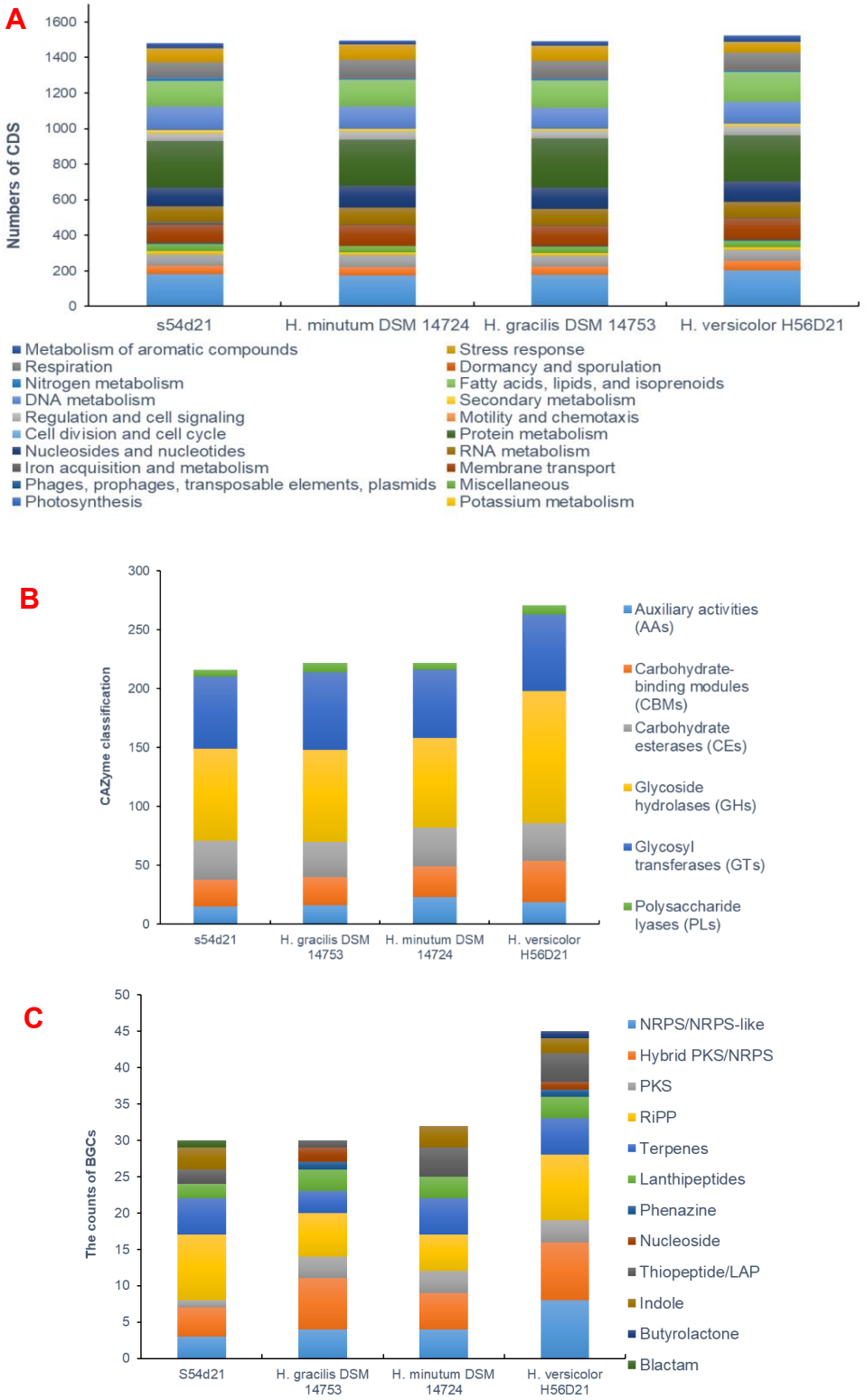

Figure S1. Distribution of genes in strain s54d21^{T} and its closely related type strains. (A) RAST annotation; (B) dbCAN annotation; (C) antiSMASH annotation.

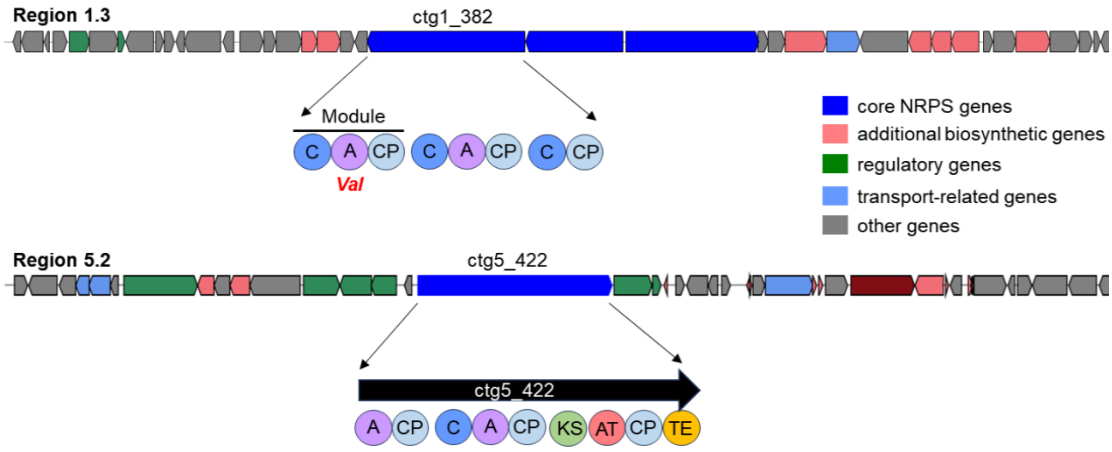

Figure S2. The NRPS-like (Region 1.3) and PKS-NRPS (Region 5.2) gene clusters within strain s54d21^{T}. The analyses of the gene cluster on the website of antiSMASH predicted the gene containing a *Val* module that were potent BGCs involved in the biosynthesis of those new pyrazinones.

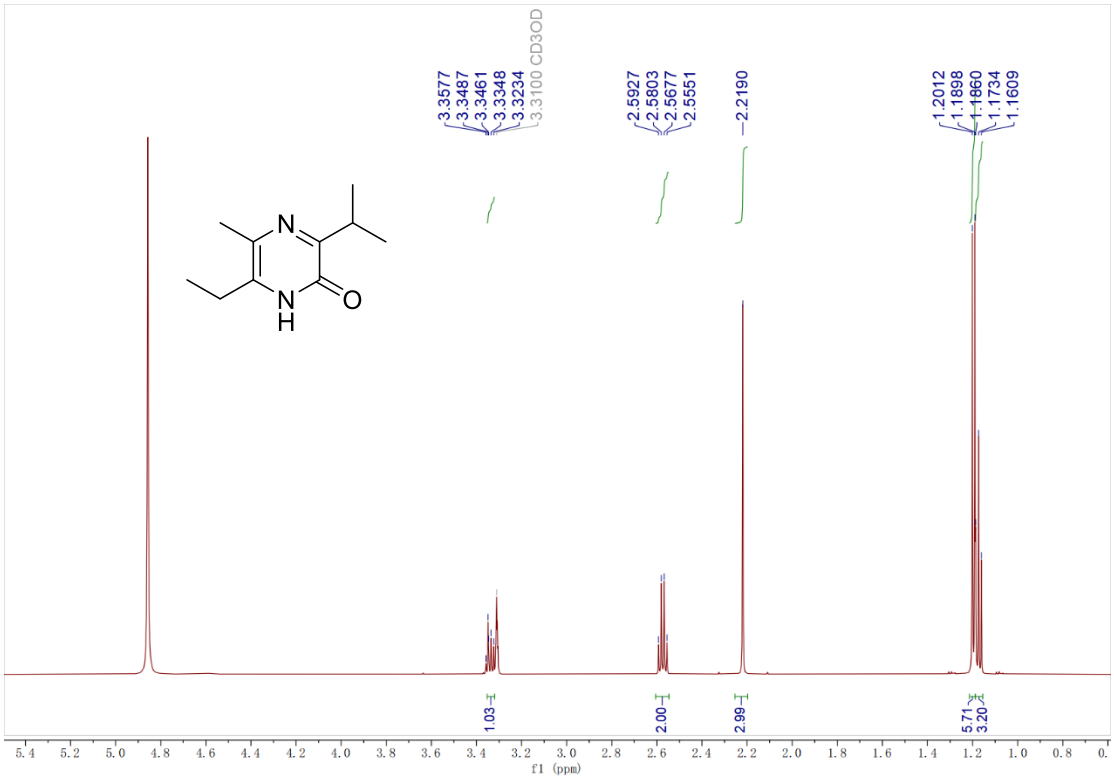

Figure S3. ^{1}H NMR spectrum of **1** in methanol-d_4.

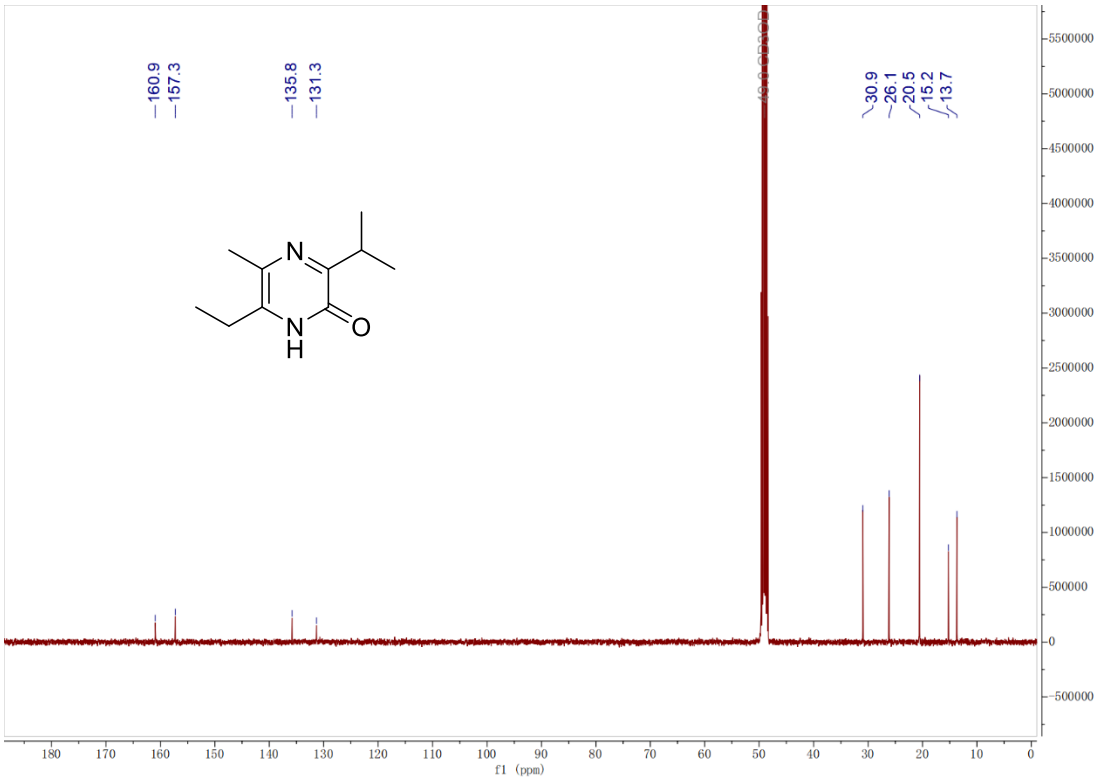

Figure S4. ^{13}C NMR spectrum of **1** in methanol-d_4.

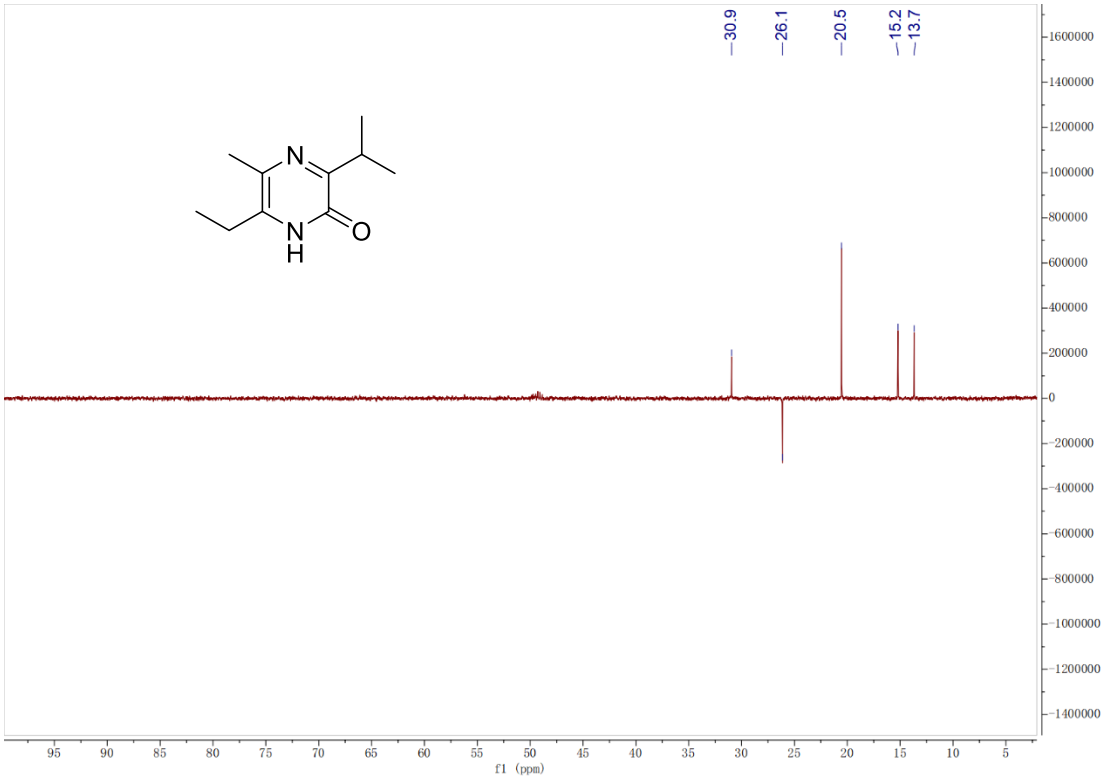

Figure S5. DEPT-135° spectrum of **1** in methanol-d_4.

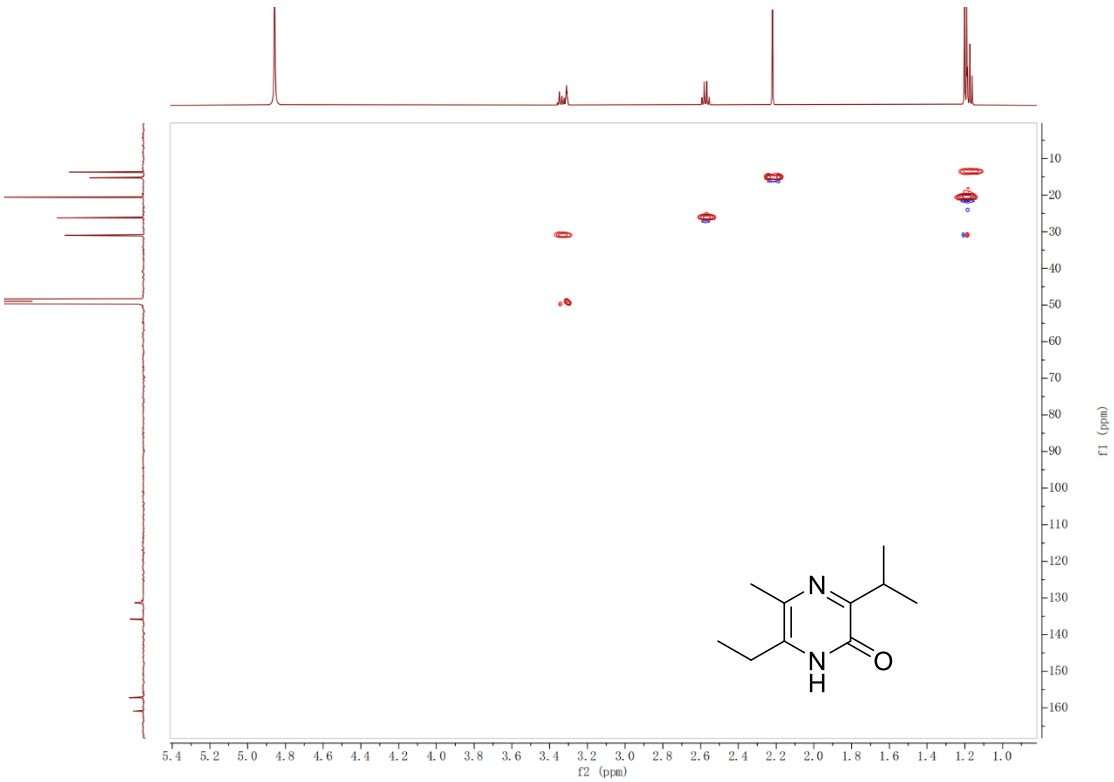

Figure S6. HSQC spectrum of **1** in methanol-d_4.

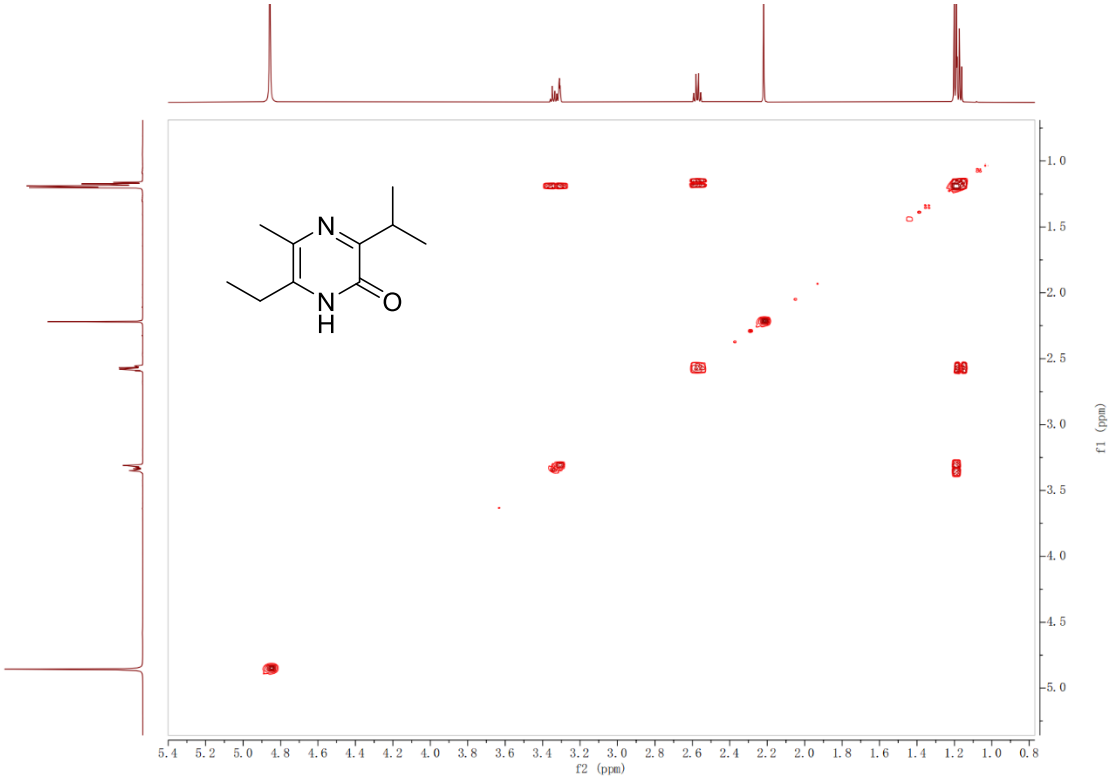

Figure S7. ^{1}H–^{1}H COSY spectrum of **1** in methanol-d_4.

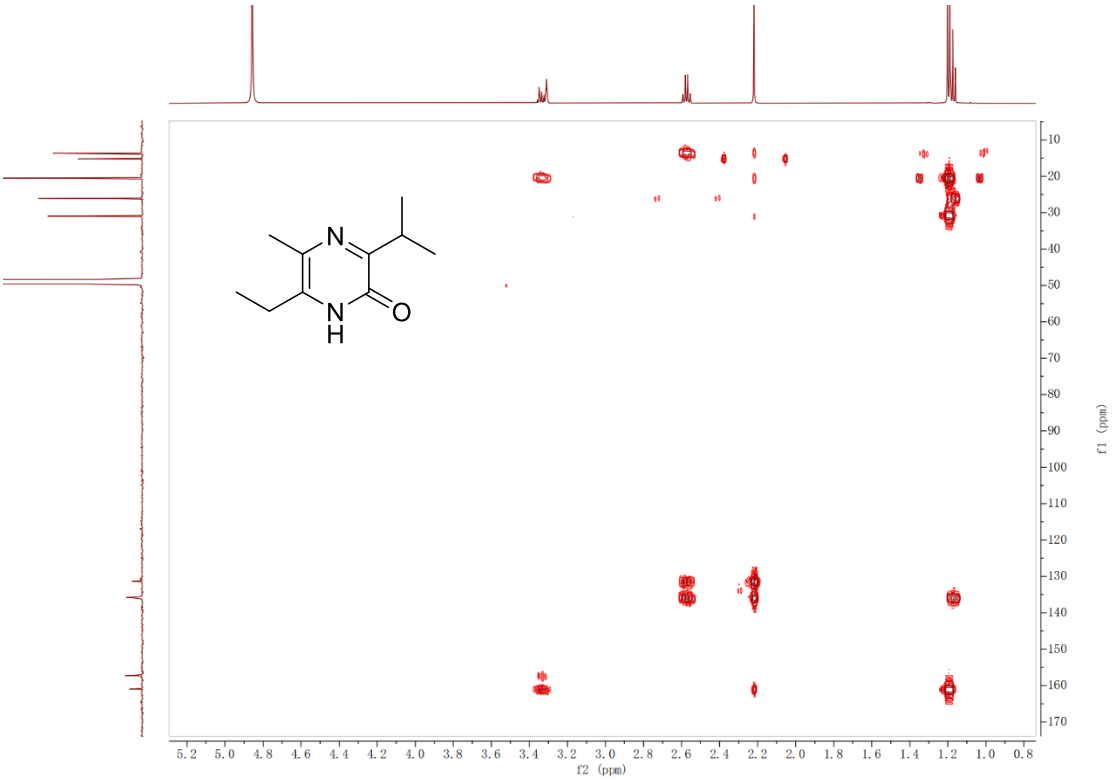

Figure S8. HMBC spectrum of **1** in methanol-d_4.

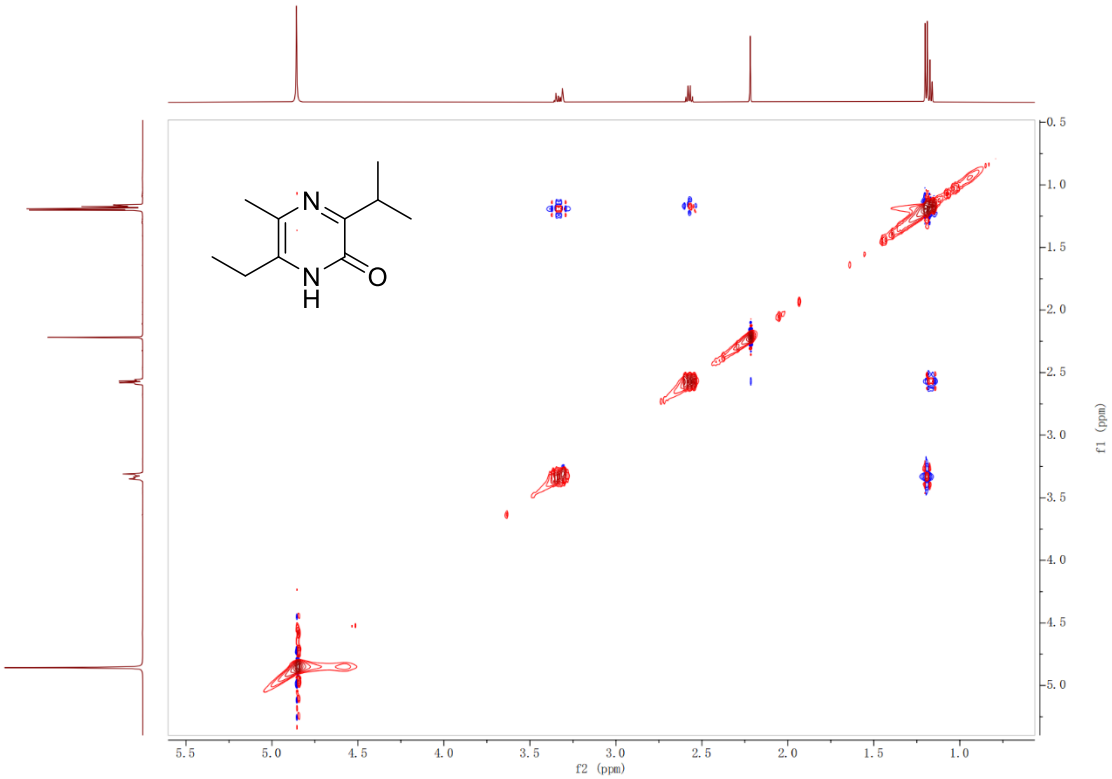

Figure S9. NOESY spectrum of **1** in methanol-d_4.

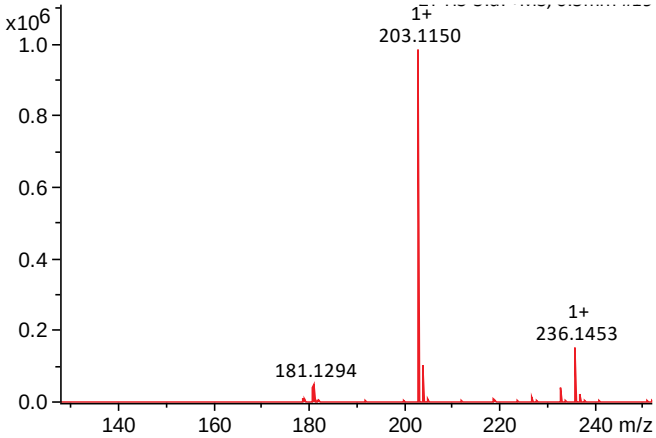

Figure S10. (+) HRESIMS spectrum of **1**.

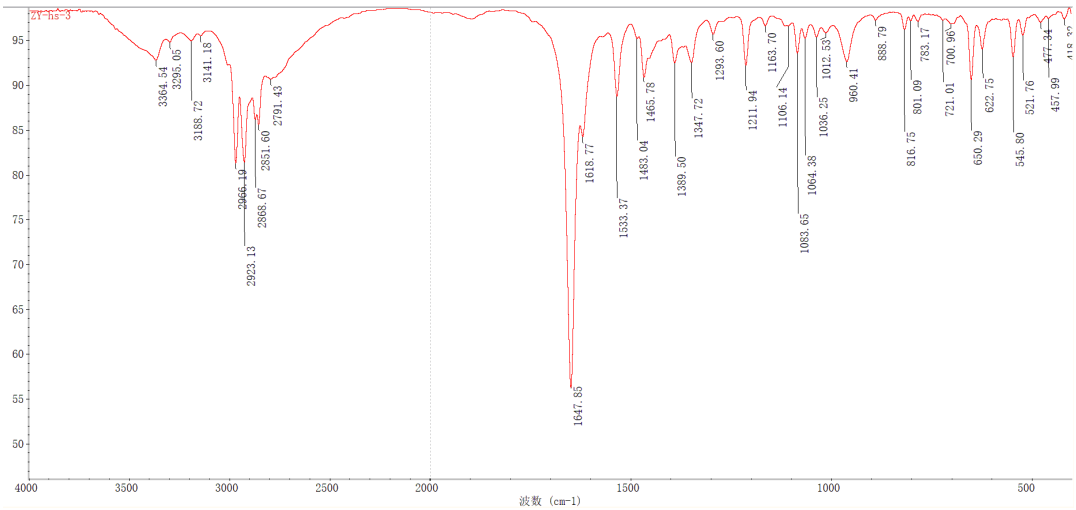

Figure S11. IR spectrum of **1**.

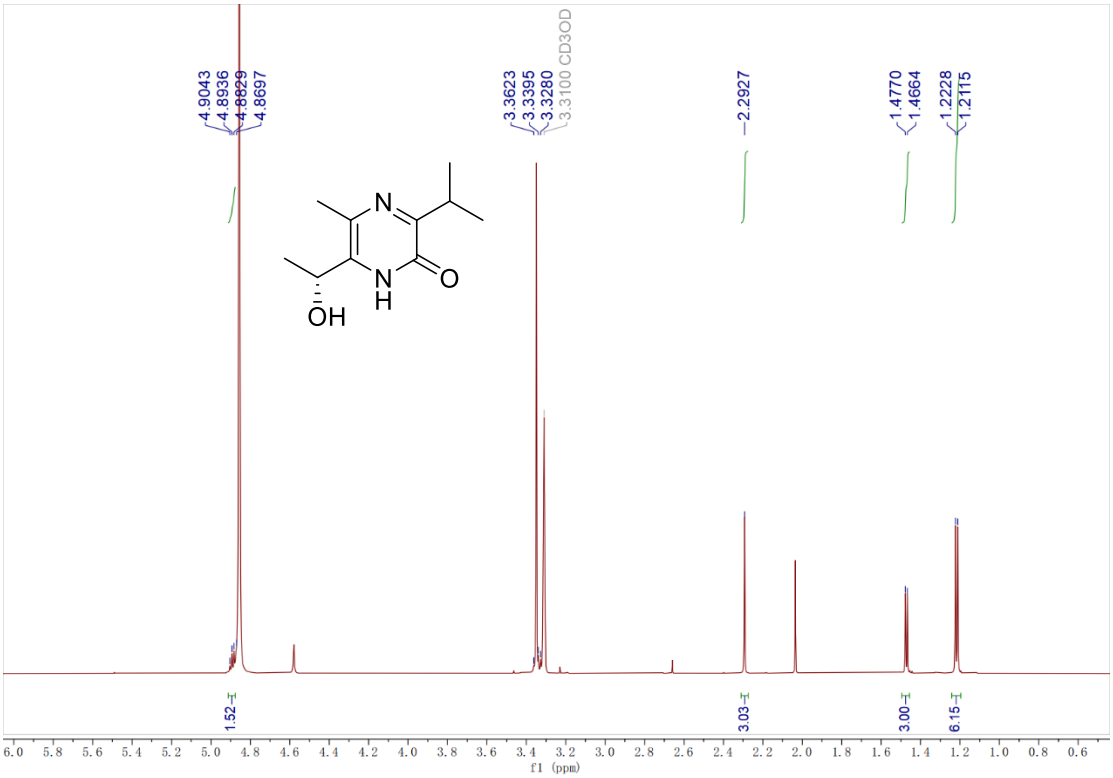

Figure S12. ^{1}H NMR spectrum of **2** in methanol-d_4.

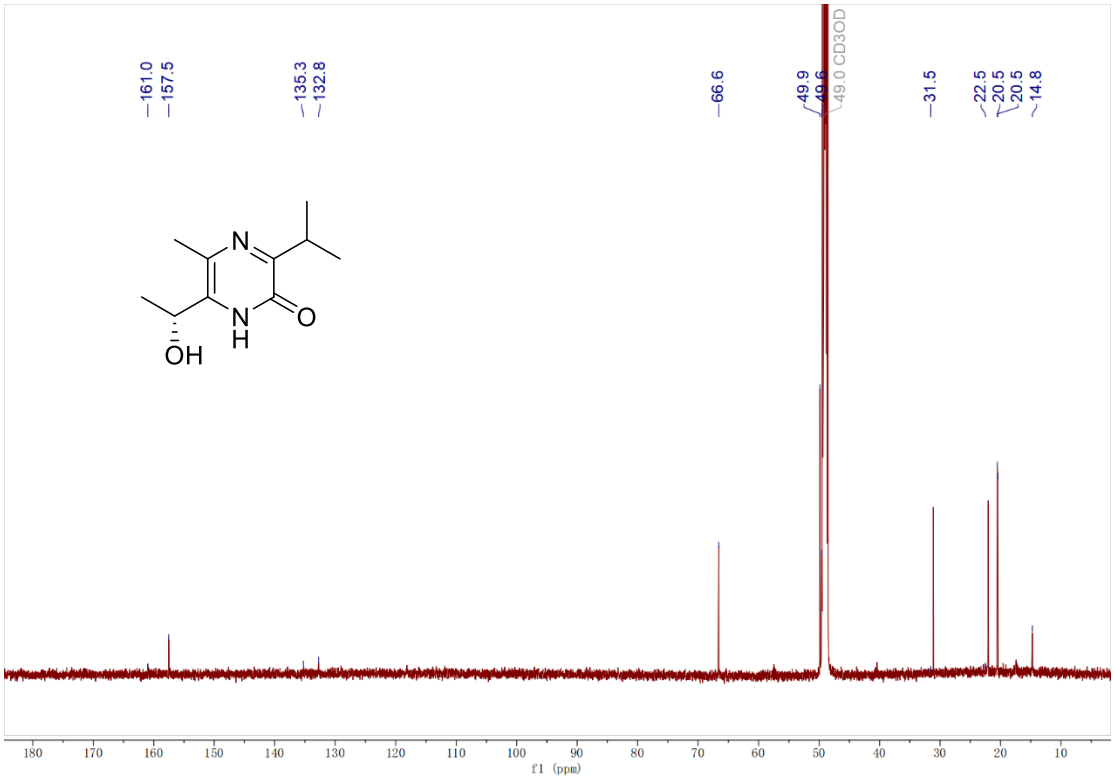

Figure S13. ^{13}C NMR spectrum of **2** in methanol-d_4.

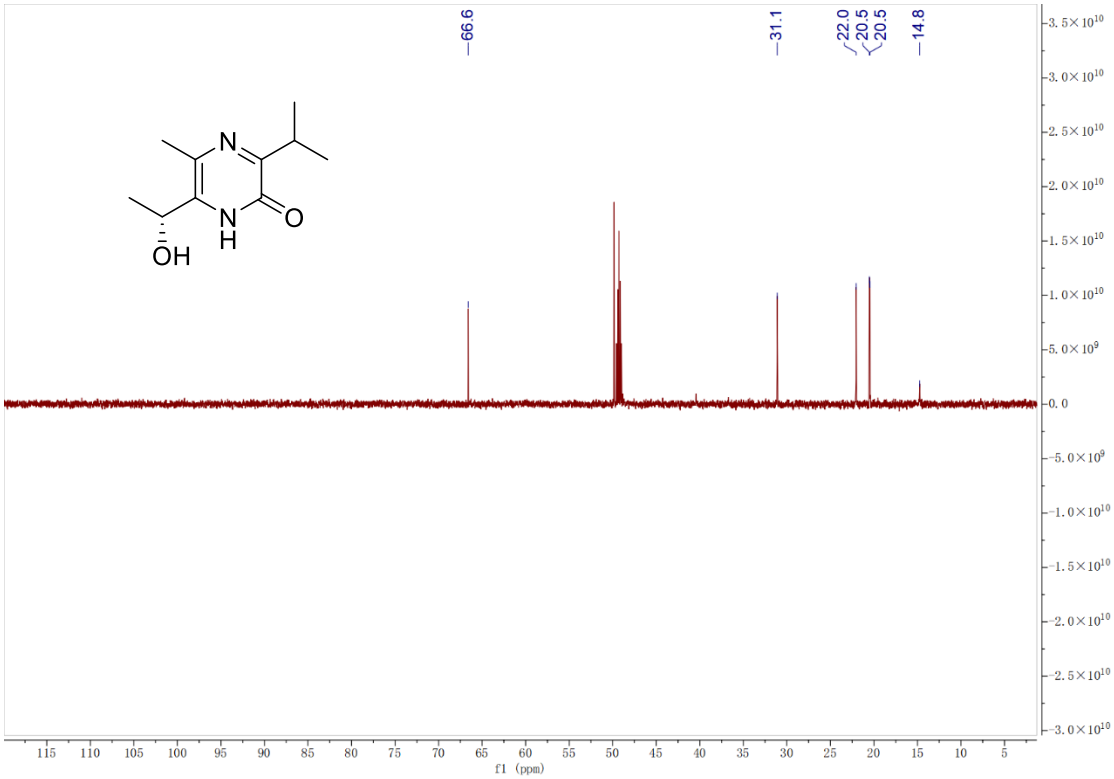

Figure S14. DEPT-135° spectrum of **2** in methanol-d_4.

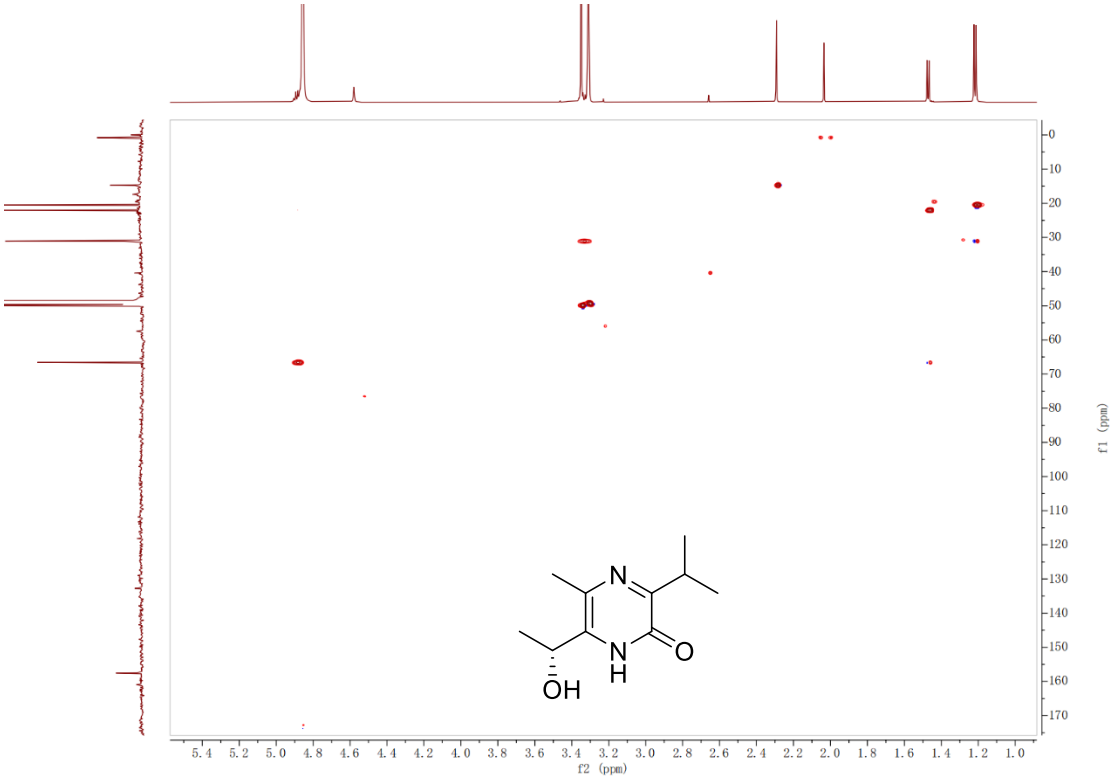

Figure S15. HSQC spectrum of **2** in methanol-d_4.

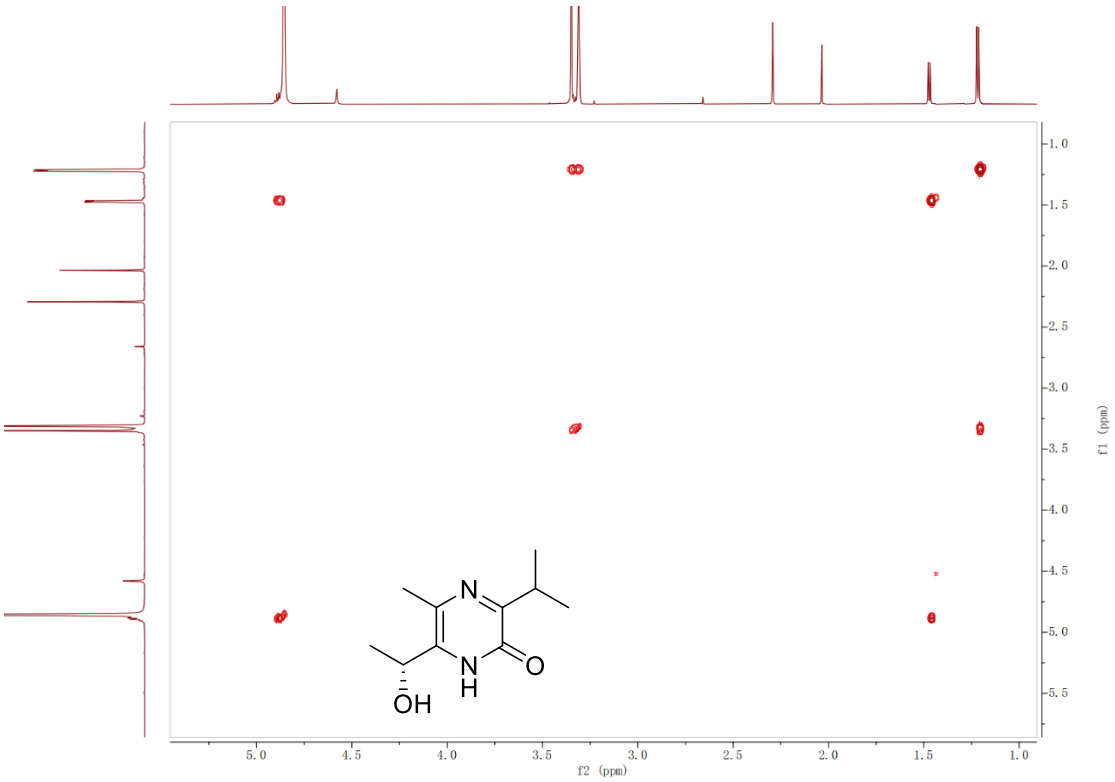

Figure S16. ^{1}H–^{1}H COSY spectrum of **2** in methanol-d_4.

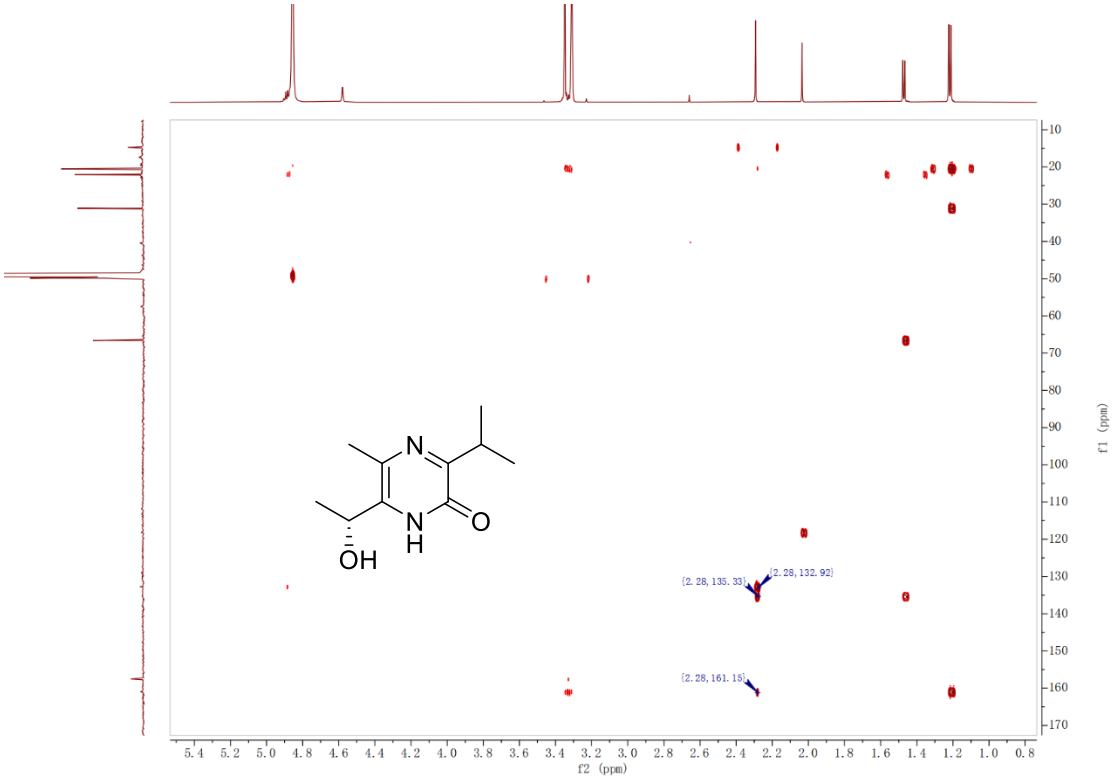

Figure S17. HMBC spectrum of **2** in methanol-d_4.

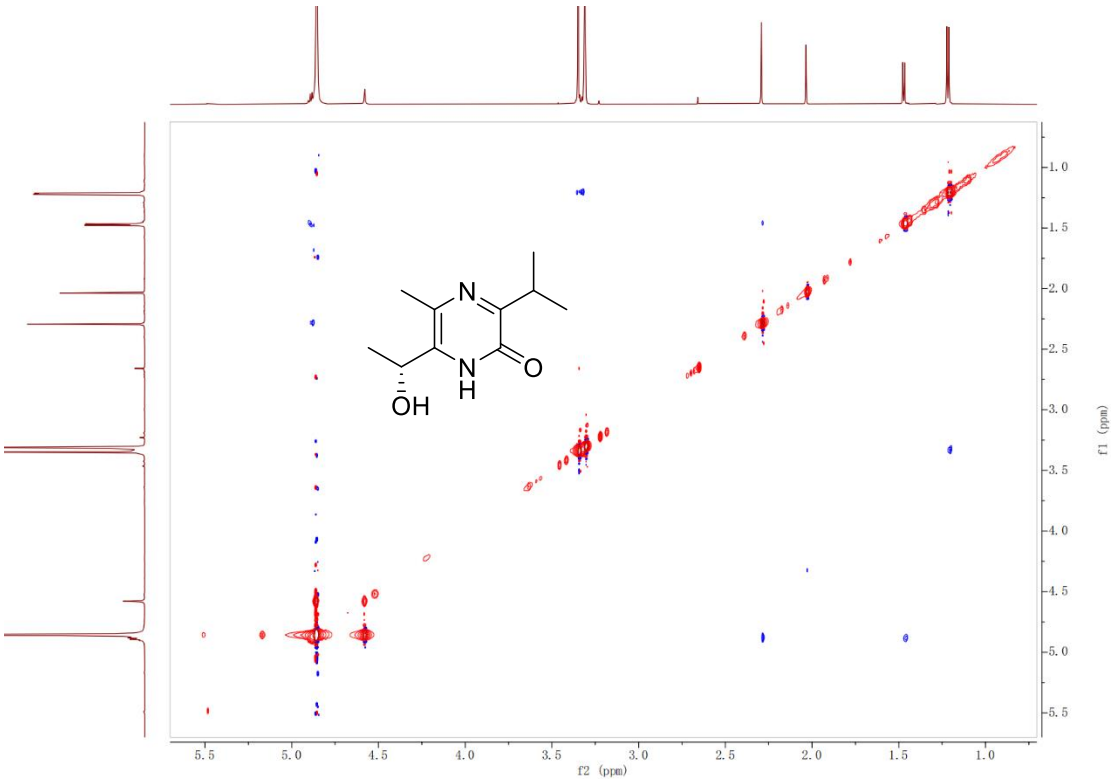

Figure S18. NOESY spectrum of **2** in methanol-d_4.

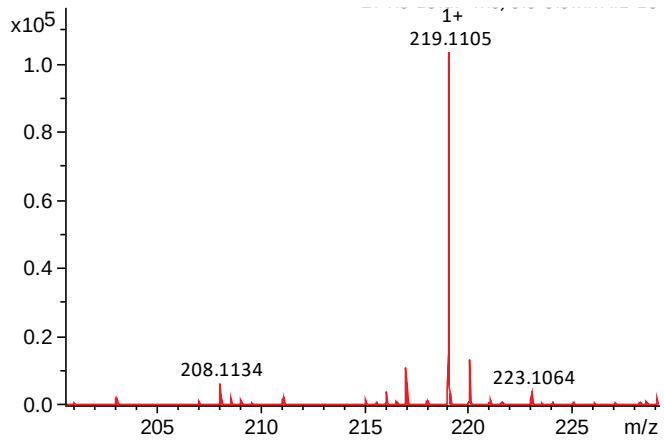

Figure S19. (+)-HRESIMS spectrum of **2**.

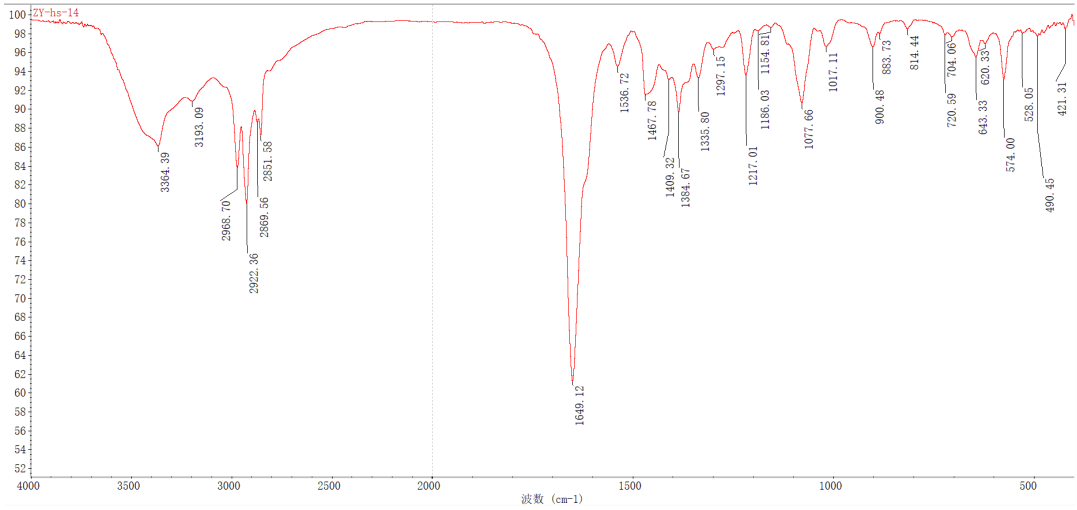

Figure S20. IR spectrum of **2**.

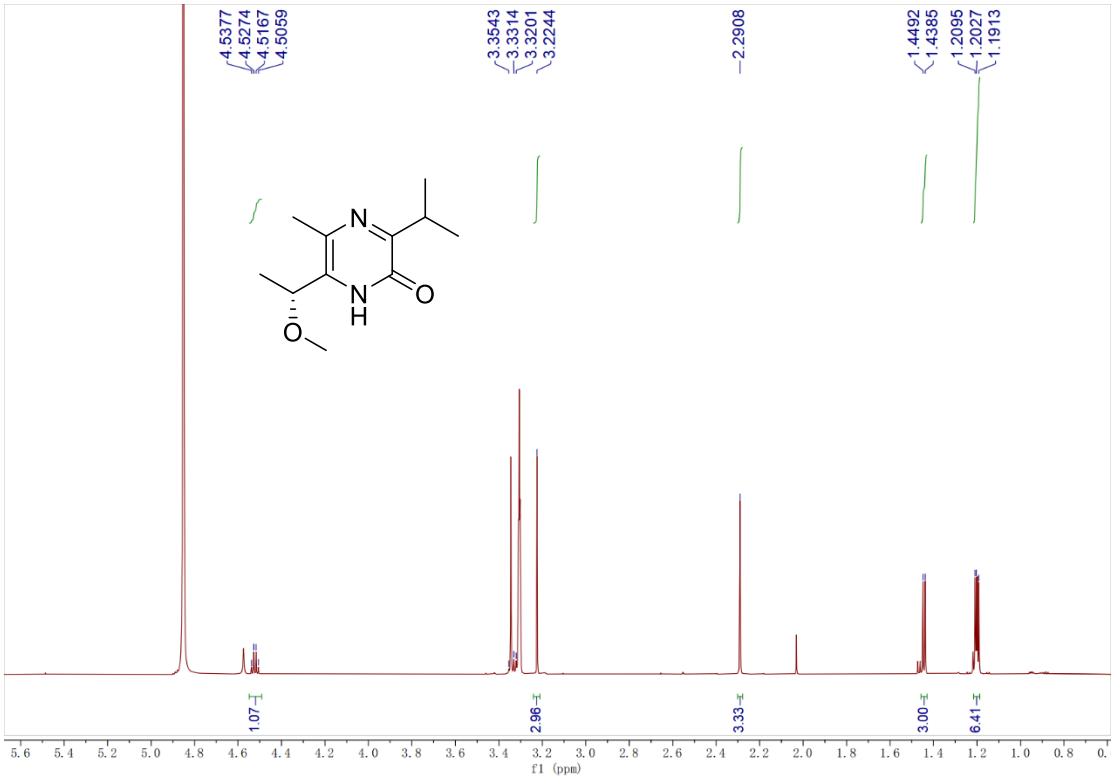

Figure S21. [1]H NMR spectrum of **3** in methanol-d_4.

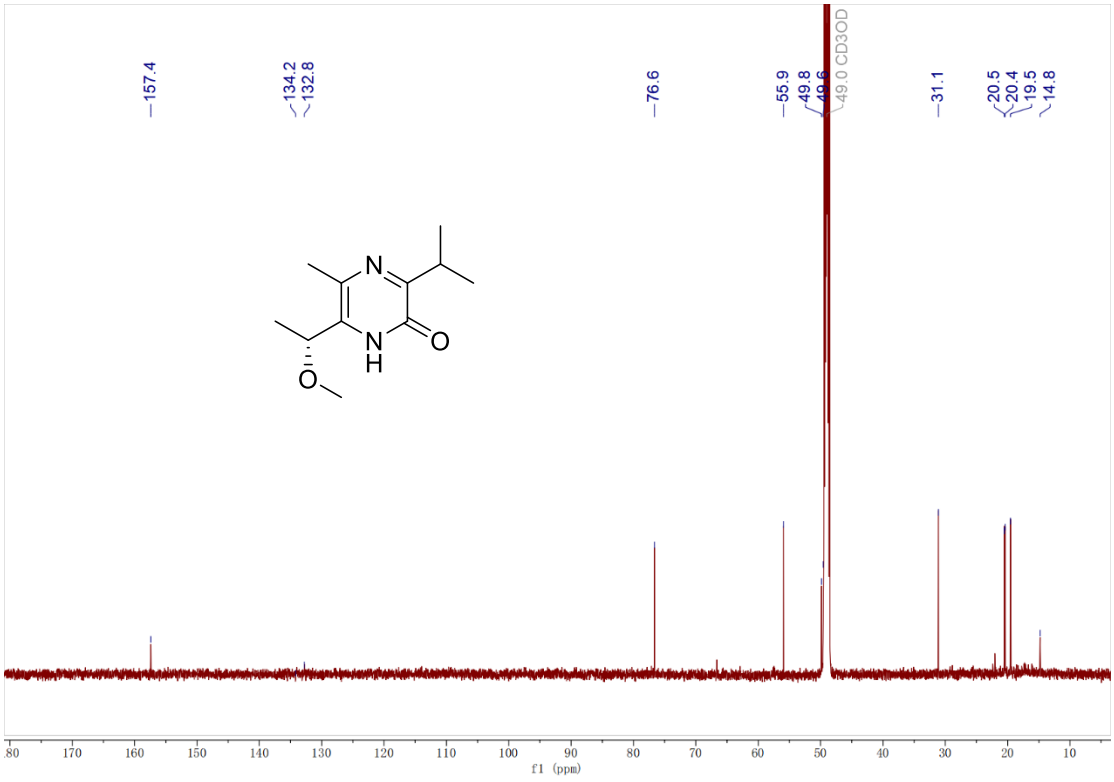

Figure S22. [13]C NMR spectrum of **3** in methanol-d_4.

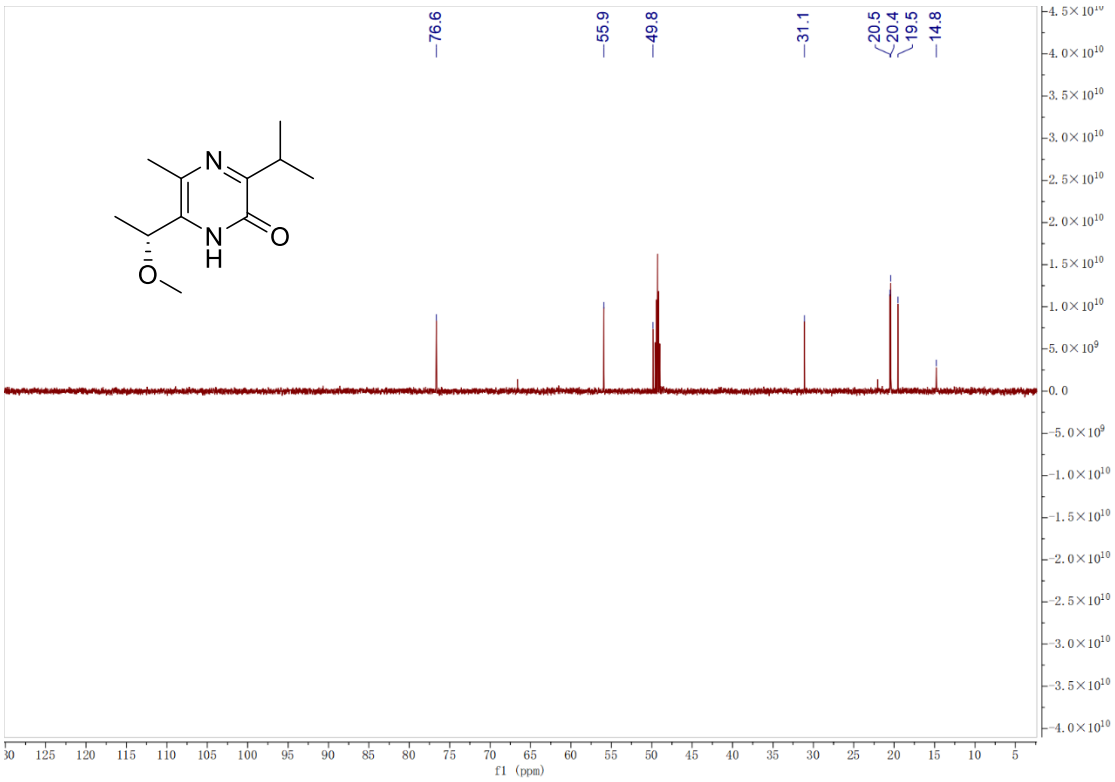

Figure S23. DEPT-135° spectrum of **3** in methanol-d_4.

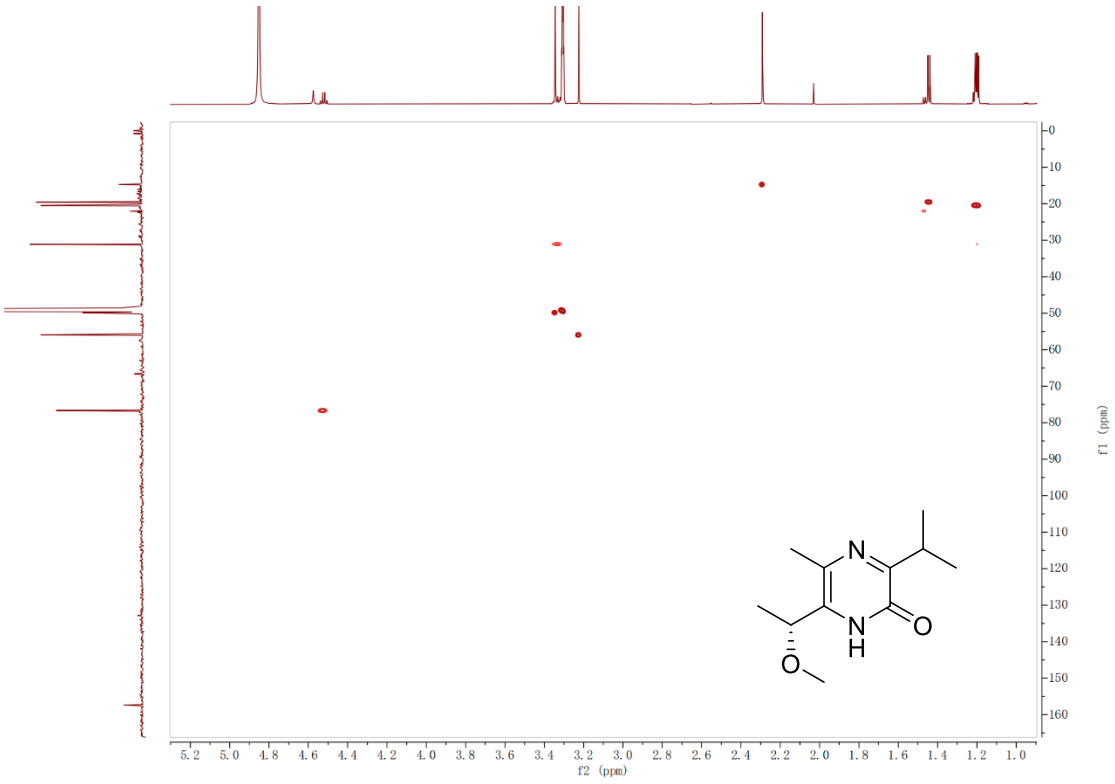

Figure S24. HSQC spectrum of **3** in methanol-d_4.

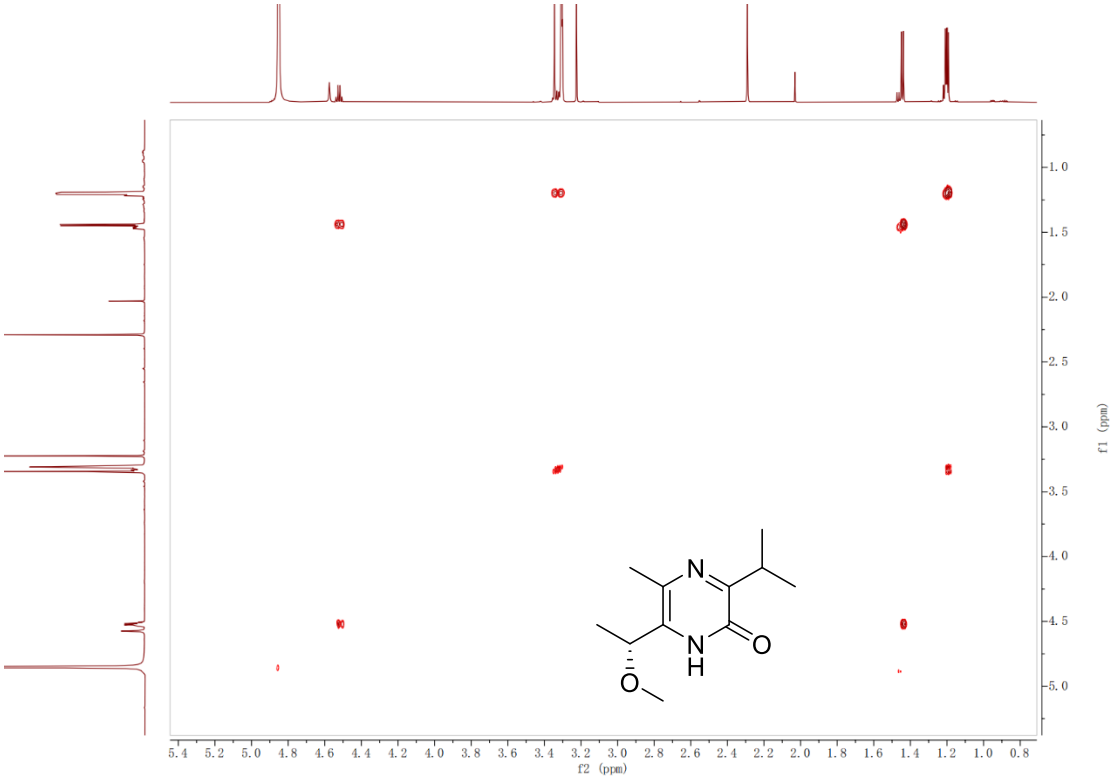

Figure S25. ^{1}H–^{1}H COSY spectrum of **3** in methanol-d_4.

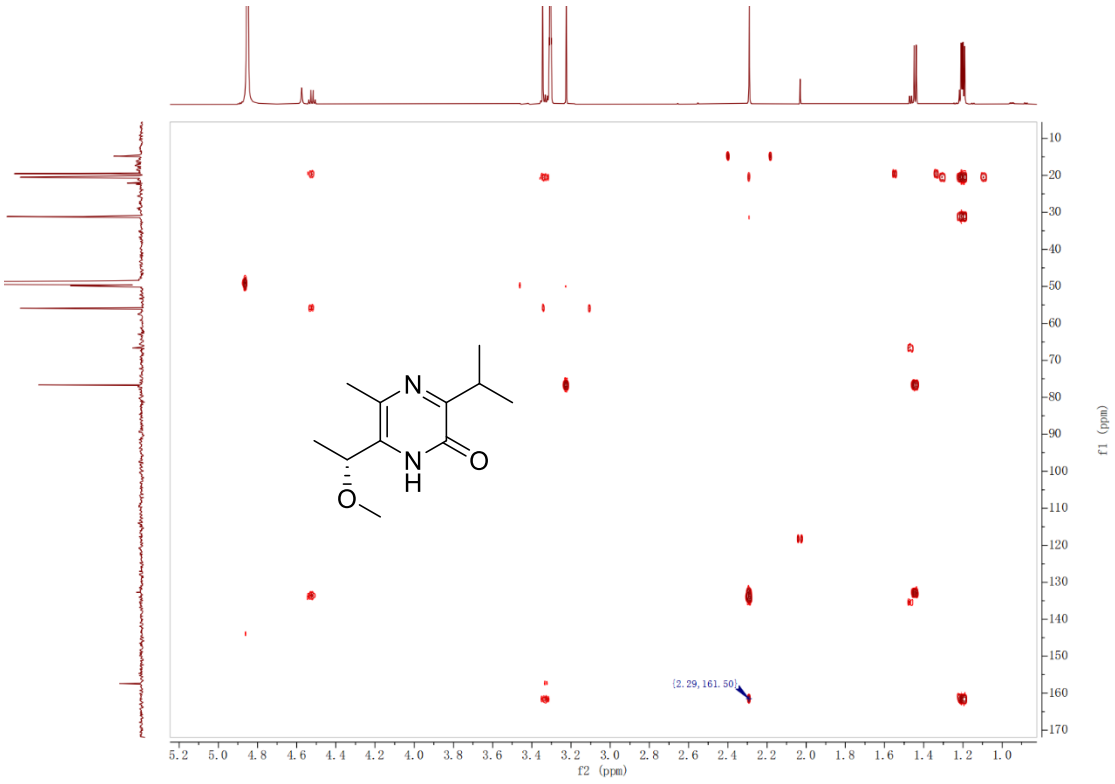

Figure S26. HMBC spectrum of **3** in methanol-d_4.

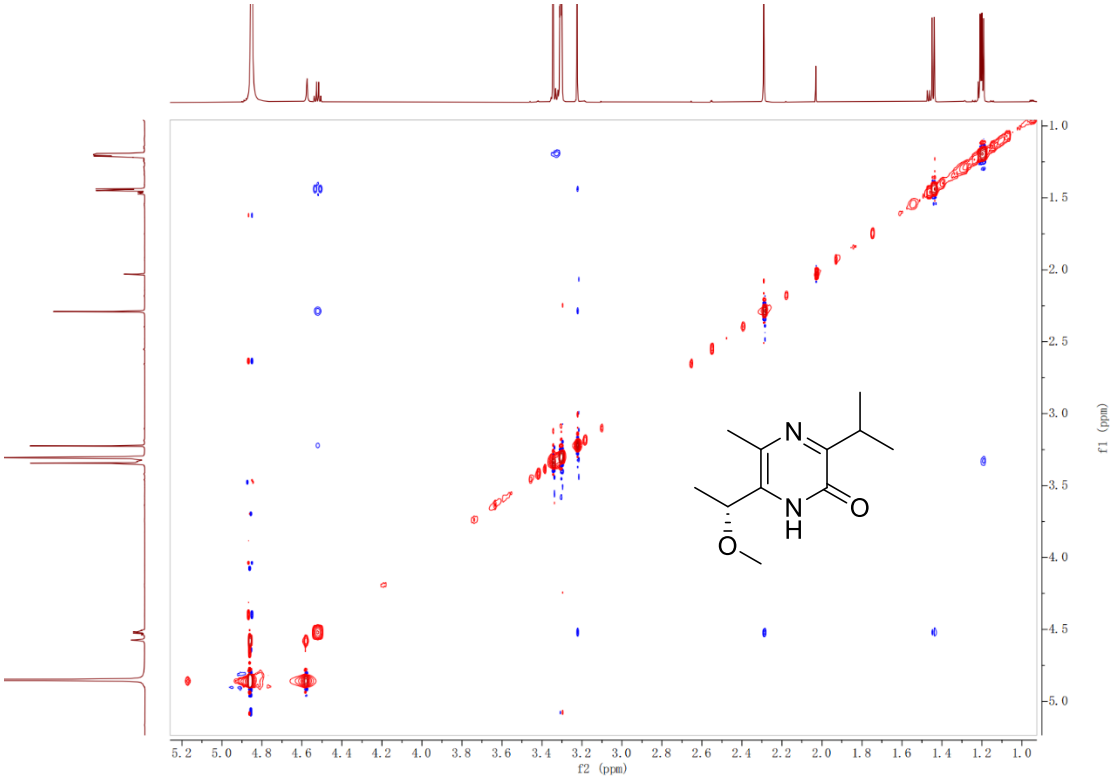

Figure S27. NOESY spectrum of **3** in methanol-d_4.

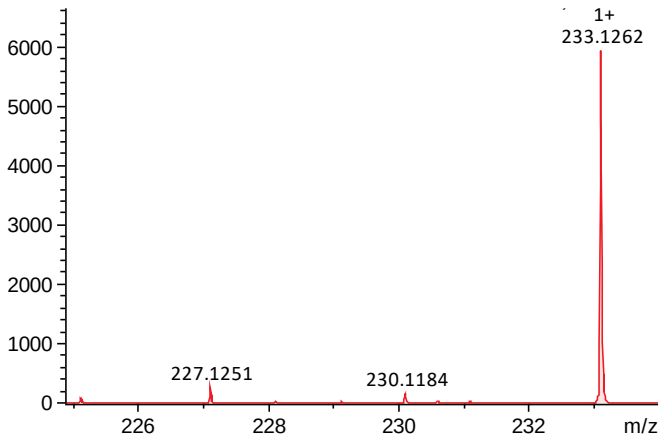

Figure S28. (+)-HR-ESI-MS spectrum of **3**.

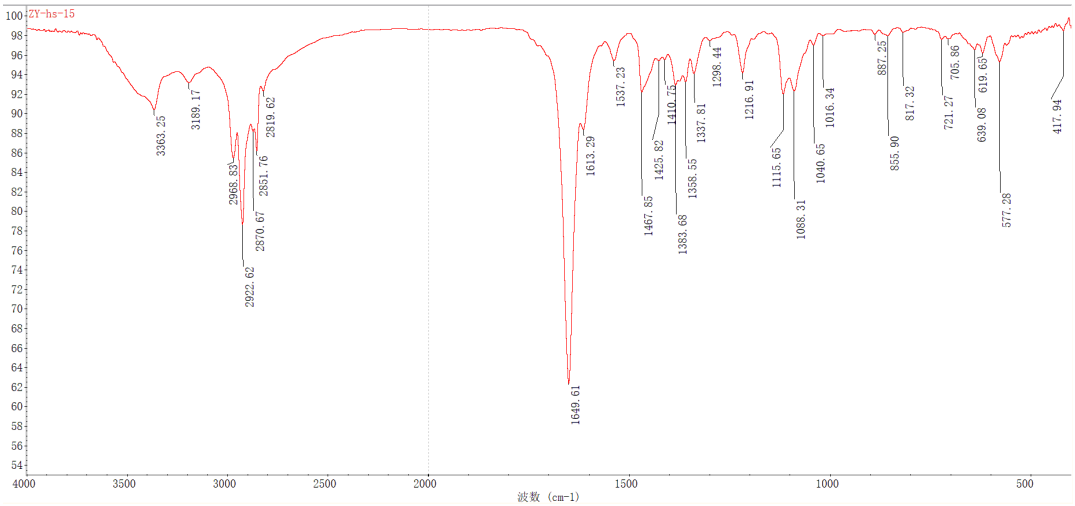

Figure S29. IR spectrum of **3**.

Details of theoretical computation for compound 2:

Table S1. Gibbs free energies[a] and equilibrium populations[b] of low-energy conformers of **2**.

Conformers	ΔG(a.u.)	P(%)/100	G(a.u.)
2A000001_tddft_	0.0	44.77	-650.469226
2A000002_tddft_	0.00056	24.88	-650.468671
2A000003_tddft_	0.00046	27.62	-650.46877
2A000005_tddft_	0.00613	0.07	-650.463099
2A000006_tddft_	0.00744	0.02	-650.461787
2A000008_tddft_	0.00477	0.29	-650.464453
2A000010_tddft_	0.00446	0.4	-650.464767
2A000011_tddft_	0.00437	0.44	-650.464855
2A000012_tddft_	0.00426	0.49	-650.464968
2A000013_tddft_	0.00461	0.34	-650.464616
2A000014_tddft_	0.00686	0.03	-650.462369
2A000016_tddft_	0.00646	0.05	-650.462768
2A000017_tddft_	0.00532	0.16	-650.463903
2A000018_tddft_	0.00476	0.29	-650.464469
2A000019_tddft_	0.00534	0.16	-650.463888

[a] wB97M-V/def2-TZVP, in a.u.

[b] From ΔG values at 298.15K.

Table S2. Cartesian coordinates for the low-energy reoptimized random research conformers of **2** at B3LYP-D3(BJ)/6-31G* level of theory in acetonitrile.

2A000001_en_		Standard Orientation (A.U.)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	-13.758314	0.843825	-2.001674
1	6	0	-12.60436	0.056902	0.181202
2	7	0	-13.893548	-1.560645	1.728043

3	6	0	-16.29929	-2.477843	1.286652
4	6	0	-17.37562	-1.528858	-1.091279
5	7	0	-16.14647	0.00723	-2.584121
6	6	0	-10.037067	0.895876	1.16108
7	6	0	-12.580413	2.665861	-3.840209
8	8	0	-17.345651	-3.948777	2.773691
9	6	0	-20.024685	-2.376229	-1.741823
10	6	0	-21.946457	-0.907278	-0.113726
11	6	0	-10.222689	3.447592	2.498033
12	6	0	-20.620731	-2.117678	-4.557991
13	8	0	-9.092266	-0.877132	2.967962
14	1	0	-12.971466	-2.166422	3.303415
15	1	0	-8.727519	1.048424	-0.436122
16	1	0	-13.214917	4.609377	-3.488009
17	1	0	-10.51601	2.660598	-3.744575
18	1	0	-13.147163	2.170366	-5.765214
19	1	0	-20.158463	-4.371955	-1.19364
20	1	0	-21.540478	-1.140928	1.899345
21	1	0	-21.883966	1.112937	-0.568783
22	1	0	-23.866718	-1.592361	-0.47513
23	1	0	-11.517437	3.313397	4.106141
24	1	0	-8.356919	4.012431	3.185192
25	1	0	-10.92818	4.89618	1.204194
26	1	0	-22.522501	-2.836641	-4.947159
27	1	0	-19.271917	-3.178638	-5.714607
28	1	0	-20.537296	-0.138906	-5.152609
29	1	0	-8.477517	-2.346715	2.055313

2A000002_en_		Standard Orientation (A.U.)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	-12.90799	-1.903924	0.229734
1	6	0	-12.86278	0.68002	0.431715
2	7	0	-15.025834	1.985106	-0.104007
3	6	0	-17.292353	0.912492	-0.836291
4	6	0	-17.149473	-1.853971	-1.015996
5	7	0	-15.085997	-3.110712	-0.502862
6	6	0	-10.57894	2.281825	1.070515
7	6	0	-10.649559	-3.565688	0.702963
8	8	0	-19.185084	2.218113	-1.266519
9	6	0	-19.541034	-3.2305	-1.754769
10	6	0	-19.030381	-5.890397	-2.763069
11	6	0	-8.868084	2.612571	-1.241518
12	6	0	-21.376782	-3.291277	0.509255
13	8	0	-11.520948	4.652969	1.956785
14	1	0	-14.965714	3.891902	0.130888
15	1	0	-9.513369	1.343548	2.583248
16	1	0	-9.267986	-2.681005	1.959482
17	1	0	-11.266043	-5.34413	1.557397
18	1	0	-9.673004	-4.034558	-1.066331
19	1	0	-20.439903	-2.096045	-3.240389
20	1	0	-17.749381	-5.847901	-4.387961
21	1	0	-18.160999	-7.076781	-1.309393
22	1	0	-20.805758	-6.776359	-3.353317
23	1	0	-9.914408	3.519991	-2.778226

24	1	0	-7.231823	3.786435	-0.756357
25	1	0	-8.16788	0.784605	-1.905522
26	1	0	-21.772461	-1.380025	1.188861
27	1	0	-20.566802	-4.391727	2.066733
28	1	0	-23.168059	-4.172056	-0.041459
29	1	0	-10.156885	5.872921	1.859092

2A000003_en_		Standard Orientation (A.U.)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	-13.35888	-1.077306	1.500968
1	6	0	-13.200304	1.292643	0.462592
2	7	0	-15.192429	2.148192	-0.940844
3	6	0	-17.381009	0.807147	-1.426804
4	6	0	-17.371581	-1.704866	-0.245235
5	7	0	-15.477904	-2.524653	1.112038
6	6	0	-10.944045	3.045418	0.601354
7	6	0	-11.284781	-2.269359	3.03908
8	8	0	-19.115062	1.711663	-2.709858
9	6	0	-19.656453	-3.358072	-0.697625
10	6	0	-19.539751	-4.467122	-3.391665
11	6	0	-8.92989	2.291981	-1.337816
12	6	0	-19.937637	-5.442729	1.284335
13	8	0	-11.875653	5.539418	0.147225
14	1	0	-15.064094	3.940032	-1.624361
15	1	0	-10.134987	2.935782	2.508405
16	1	0	-10.104356	-0.866761	3.993759
17	1	0	-12.11545	-3.508398	4.469284
18	1	0	-10.03735	-3.433141	1.858534
19	1	0	-21.31242	-2.111831	-0.620773
20	1	0	-21.247185	-5.568511	-3.790428
21	1	0	-19.390355	-2.964604	-4.80313
22	1	0	-17.901427	-5.720207	-3.586764
23	1	0	-7.314633	3.584079	-1.230531
24	1	0	-8.24081	0.377089	-0.975556
25	1	0	-9.719965	2.362734	-3.248205
26	1	0	-21.663454	-6.528928	0.928192
27	1	0	-20.043452	-4.656325	3.195627
28	1	0	-18.327734	-6.739306	1.227205
29	1	0	-10.445985	6.605895	-0.2736

2A000005_en_		Standard Orientation (A.U.)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	-13.872888	0.798349	-2.446902
1	6	0	-13.083831	1.248567	-0.014827
2	7	0	-14.297422	-0.032392	1.886746
3	6	0	-16.244513	-1.75623	1.582491
4	6	0	-16.950545	-2.092722	-1.080302
5	7	0	-15.810662	-0.87089	-2.901979
6	6	0	-10.936297	2.962824	0.834754
7	6	0	-12.722574	1.9909	-4.759033
8	8	0	-17.205989	-2.815724	3.432803
9	6	0	-19.061573	-3.896402	-1.762873
10	6	0	-18.41966	-6.63306	-1.014566

11	6	0	-8.354634	1.814199	0.253257
12	6	0	-21.604521	-3.053801	-0.629249
13	8	0	-11.012364	5.389709	-0.326497
14	1	0	-13.767078	0.270193	3.707012
15	1	0	-11.107812	3.182167	2.897245
16	1	0	-14.225206	2.634651	-6.028347
17	1	0	-11.526498	3.594726	-4.274715
18	1	0	-11.592413	0.604091	-5.808094
19	1	0	-19.204274	-3.801052	-3.82654
20	1	0	-18.23138	-6.802065	1.035154
21	1	0	-19.92285	-7.909861	-1.645974
22	1	0	-16.645934	-7.246469	-1.889543
23	1	0	-6.866656	3.079505	0.931983
24	1	0	-8.153785	-0.014507	1.196299
25	1	0	-8.118689	1.539269	-1.781284
26	1	0	-22.084664	-1.13047	-1.227763
27	1	0	-21.532452	-3.098669	1.434308
28	1	0	-23.115553	-4.320107	-1.263029
29	1	0	-12.668333	6.115484	-0.00976

2A000006_en_		Standard Orientation (A.U.)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	-12.809766	-0.907566	0.839088
1	6	0	-13.278289	1.468674	-0.09744
2	7	0	-15.605814	1.898714	-1.144541
3	6	0	-17.550308	0.150158	-1.346609
4	6	0	-16.855416	-2.323212	-0.30812
5	7	0	-14.631097	-2.747554	0.690867
6	6	0	-11.510214	3.736601	-0.03366
7	6	0	-10.348305	-1.691432	2.043561
8	8	0	-19.589905	0.743033	-2.325603
9	6	0	-18.744609	-4.468683	-0.379321
10	6	0	-21.118561	-3.862961	1.188698
11	6	0	-11.661736	5.114349	2.506298
12	6	0	-19.435077	-5.204054	-3.10763
13	8	0	-8.987031	3.087667	-0.701514
14	1	0	-16.00781	3.632235	-1.866477
15	1	0	-12.130812	5.034546	-1.524697
16	1	0	-10.604701	-3.548314	2.906958
17	1	0	-8.82038	-1.830895	0.653993
18	1	0	-9.737547	-0.385517	3.530422
19	1	0	-17.772661	-6.071006	0.501705
20	1	0	-22.129041	-2.251216	0.38452
21	1	0	-22.391444	-5.496359	1.20642
22	1	0	-20.620973	-3.414503	3.148091
23	1	0	-13.598925	5.728529	2.889457
24	1	0	-11.067916	3.877255	4.056805
25	1	0	-10.432061	6.776337	2.470991
26	1	0	-20.701719	-6.842364	-3.100502
27	1	0	-17.744296	-5.703235	-4.193809
28	1	0	-20.389083	-3.641011	-4.062906
29	1	0	-8.110102	2.558226	0.818076

2A000008_en_		Standard Orientation (A.U.)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	-12.835003	-0.940583	0.050803
1	6	0	-13.364173	1.585017	-0.223434
2	7	0	-15.835414	2.252752	-0.655816
3	6	0	-17.851776	0.59748	-0.835079
4	6	0	-17.083309	-2.049508	-0.524888
5	7	0	-14.739539	-2.701309	-0.117214
6	6	0	-11.524784	3.770663	0.001183
7	6	0	-10.247656	-1.994886	0.584749
8	8	0	-20.027189	1.36072	-1.223777
9	6	0	-19.127097	-4.029884	-0.764198
10	6	0	-19.836102	-4.36872	-3.572382
11	6	0	-10.666357	4.17226	2.735998
12	6	0	-18.386793	-6.549196	0.443054
13	8	0	-9.455248	3.303642	-1.664331
14	1	0	-16.27986	4.105897	-0.883377
15	1	0	-12.525097	5.486311	-0.619953
16	1	0	-8.76949	-0.609074	0.22246
17	1	0	-10.108109	-2.62996	2.55429
18	1	0	-9.916487	-3.650548	-0.61192
19	1	0	-20.799031	-3.271598	0.201297
20	1	0	-21.401326	-5.711094	-3.759202
21	1	0	-20.416803	-2.571139	-4.410626
22	1	0	-18.221354	-5.105055	-4.641201
23	1	0	-9.664277	2.511943	3.448025
24	1	0	-9.403266	5.810229	2.849726
25	1	0	-12.295879	4.537089	3.957117
26	1	0	-17.907432	-6.315204	2.442428
27	1	0	-16.742424	-7.369501	-0.505443
28	1	0	-19.958269	-7.888853	0.300291
29	1	0	-8.189385	4.588399	-1.32456

2A000010_en_		Standard Orientation (A.U.)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	-14.025867	0.480404	-2.405294
1	6	0	-13.24242	1.420341	-0.117707
2	7	0	-14.400087	0.519049	2.014374
3	6	0	-16.318503	-1.262054	2.054261
4	6	0	-17.033096	-2.119789	-0.484114
5	7	0	-15.929303	-1.275841	-2.527048
6	6	0	-11.146113	3.351889	0.149196
7	6	0	-12.885666	1.314127	-4.877226
8	8	0	-17.26718	-1.981761	4.066736
9	6	0	-19.085586	-4.09782	-0.654575
10	6	0	-20.341921	-4.180951	-3.256272
11	6	0	-11.126411	4.77835	2.658584
12	6	0	-17.995391	-6.700899	0.079471
13	8	0	-8.823513	2.000424	-0.227181
14	1	0	-13.862553	1.169869	3.735607
15	1	0	-11.405724	4.725317	-1.383986
16	1	0	-13.324202	-0.086697	-6.329307

17	1	0	-13.659029	3.134903	-5.504098
18	1	0	-10.834656	1.510802	-4.733021
19	1	0	-20.503245	-3.602349	0.775727
20	1	0	-18.978081	-4.705851	-4.719098
21	1	0	-21.870895	-5.576257	-3.257867
22	1	0	-21.136723	-2.340273	-3.768874
23	1	0	-9.649299	6.224919	2.609905
24	1	0	-12.932118	5.727673	3.007575
25	1	0	-10.697396	3.513921	4.241286
26	1	0	-17.146385	-6.642512	1.962913
27	1	0	-16.545677	-7.285743	-1.279953
28	1	0	-19.493058	-8.130522	0.083416
29	1	0	-7.493259	3.255998	-0.386714

2A000011_en_		Standard Orientation (A.U.)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	-13.00286	-0.777176	-1.706351
1	6	0	-13.087646	1.369165	-0.246783
2	7	0	-15.305206	1.89525	0.983362
3	6	0	-17.480522	0.440295	0.874622
4	6	0	-17.1939	-1.788407	-0.747564
5	7	0	-15.083928	-2.305683	-1.926041
6	6	0	-10.837294	3.120705	0.114718
7	6	0	-10.67337	-1.559563	-3.143907
8	8	0	-19.408538	1.050334	2.049077
9	6	0	-19.446066	-3.529831	-0.970943
10	6	0	-19.339076	-5.195449	-3.330707
11	6	0	-11.485381	5.72139	1.185334
12	6	0	-19.682503	-5.136998	1.450622
13	8	0	-8.915286	1.905666	1.587404
14	1	0	-15.443976	3.472767	2.064055
15	1	0	-9.963522	3.37346	-1.74088
16	1	0	-8.97546	-1.380606	-1.981474
17	1	0	-10.87914	-3.524581	-3.742247
18	1	0	-10.397876	-0.404702	-4.845991
19	1	0	-21.124364	-2.315022	-1.065465
20	1	0	-19.193587	-4.055927	-5.051975
21	1	0	-17.70138	-6.456438	-3.271896
22	1	0	-21.050425	-6.353129	-3.45605
23	1	0	-9.765933	6.863179	1.24231
24	1	0	-12.88156	6.701927	0.013651
25	1	0	-12.208887	5.598081	3.124492
26	1	0	-19.811225	-3.934278	3.126482
27	1	0	-18.038222	-6.380479	1.655453
28	1	0	-21.380409	-6.318751	1.36442
29	1	0	-9.625794	1.556218	3.24458

2A000012_en_		Standard Orientation (A.U.)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	-12.695025	-1.129563	-0.742345
1	6	0	-13.122306	1.385742	-0.271779
2	7	0	-15.557683	2.125154	0.198563
3	6	0	-17.643041	0.542448	0.20448

4	6	0	-16.983186	-2.097494	-0.328716
5	7	0	-14.660403	-2.821004	-0.759239
6	6	0	-11.034948	3.344776	-0.201808
7	6	0	-10.099277	-2.17234	-1.270378
8	8	0	-19.790609	1.363073	0.631461
9	6	0	-19.132033	-3.976048	-0.418678
10	6	0	-20.613376	-3.648436	-2.908952
11	6	0	-11.925071	6.077728	-0.466335
12	6	0	-18.244153	-6.704794	-0.075642
13	8	0	-9.725219	2.968161	2.144569
14	1	0	-15.939793	3.968799	0.558922
15	1	0	-9.762737	2.913478	-1.783076
16	1	0	-9.541571	-1.87606	-3.247173
17	1	0	-8.672581	-1.288803	-0.066849
18	1	0	-10.105762	-4.207243	-0.919868
19	1	0	-20.419052	-3.474243	1.128735
20	1	0	-22.252166	-4.913409	-2.939851
21	1	0	-21.28627	-1.705519	-3.117118
22	1	0	-19.410108	-4.108788	-4.531354
23	1	0	-13.062057	6.661073	1.163194
24	1	0	-10.277929	7.325769	-0.544315
25	1	0	-13.015219	6.360028	-2.202871
26	1	0	-17.210594	-6.943836	1.701046
27	1	0	-16.985647	-7.271668	-1.615379
28	1	0	-19.873796	-7.980954	-0.060925
29	1	0	-8.19887	3.986496	2.074093

2A000013_en_		Standard Orientation (A.U.)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	-14.62495	2.06902	0.081818
1	6	0	-12.635042	0.400851	0.117161
2	7	0	-13.117392	-2.054476	-0.55152
3	6	0	-15.459901	-3.0057	-1.235866
4	6	0	-17.448473	-1.075555	-1.200333
5	7	0	-17.001454	1.274728	-0.580303
6	6	0	-9.94599	1.168301	0.780145
7	6	0	-14.331471	4.817789	0.76245
8	8	0	-15.737628	-5.257806	-1.800763
9	6	0	-20.093845	-1.927885	-1.856614
10	6	0	-21.230338	-3.402416	0.387766
11	6	0	-8.186566	-1.022094	1.441056
12	6	0	-21.806748	0.260253	-2.650549
13	8	0	-8.893112	2.718458	-1.176668
14	1	0	-11.697904	-3.343317	-0.537436
15	1	0	-10.062659	2.429778	2.412553
16	1	0	-12.636332	5.63018	-0.093317
17	1	0	-15.987215	5.856038	0.097075
18	1	0	-14.196583	5.090272	2.815305
19	1	0	-19.909928	-3.261809	-3.434413
20	1	0	-23.099922	-4.139086	-0.111076
21	1	0	-20.021705	-4.994584	0.912609
22	1	0	-21.441683	-2.162397	2.033893
23	1	0	-6.356648	-0.254059	2.011372
24	1	0	-8.934833	-2.154949	3.003313

25	1	0	-7.853509	-2.264835	-0.184864
26	1	0	-23.669011	-0.461849	-3.193837
27	1	0	-21.012825	1.295073	-4.257113
28	1	0	-22.055625	1.60433	-1.098959
29	1	0	-8.84622	1.714363	-2.713832

2A000014_en_		Standard Orientation (A.U.)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	-14.352952	1.689837	0.966899
1	6	0	-12.638507	0.108506	-0.171534
2	7	0	-13.579546	-1.867913	-1.56133
3	6	0	-16.112527	-2.411005	-1.943141
4	6	0	-17.784557	-0.617275	-0.646039
5	7	0	-16.900435	1.262169	0.69492
6	6	0	-9.783666	0.355191	-0.16118
7	6	0	-13.657852	3.971726	2.51642
8	8	0	-16.7597	-4.243818	-3.244784
9	6	0	-20.619448	-0.933134	-0.845411
10	6	0	-21.539512	-0.655246	-3.590933
11	6	0	-8.898327	2.598436	-1.761315
12	6	0	-21.506966	-3.444636	0.323374
13	8	0	-8.963353	0.539048	2.401298
14	1	0	-12.359434	-3.08186	-2.410686
15	1	0	-9.009124	-1.383557	-1.002275
16	1	0	-14.025993	5.71668	1.457391
17	1	0	-14.833241	4.034452	4.218392
18	1	0	-11.677765	3.93647	3.077774
19	1	0	-21.413638	0.621147	0.268891
20	1	0	-20.967061	1.169183	-4.385765
21	1	0	-20.761512	-2.158149	-4.774739
22	1	0	-23.6063	-0.765738	-3.659099
23	1	0	-9.626641	4.378416	-1.006971
24	1	0	-6.828658	2.680924	-1.778469
25	1	0	-9.545092	2.392127	-3.715483
26	1	0	-23.573895	-3.559479	0.267549
27	1	0	-20.907939	-3.597681	2.299629
28	1	0	-20.731554	-5.048322	-0.721787
29	1	0	-7.174538	0.948516	2.366247

2A000016_en_		Standard Orientation (A.U.)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	-14.391432	2.363819	-0.845819
1	6	0	-12.813335	0.67927	0.344697
2	7	0	-13.771264	-1.656851	0.908176
3	6	0	-16.211652	-2.472074	0.399314
4	6	0	-17.743553	-0.527799	-0.848294
5	7	0	-16.834056	1.708095	-1.404643
6	6	0	-10.073966	1.26253	0.992579
7	6	0	-13.5624	4.9869	-1.577438
8	8	0	-16.892054	-4.630626	0.992624
9	6	0	-20.465222	-1.091848	-1.518903
10	6	0	-20.672353	-3.264145	-3.442361
11	6	0	-8.873445	-0.539473	2.900682

12	6	0	-22.067744	-1.61678	0.851507
13	8	0	-8.582305	1.444199	-1.260865
14	1	0	-12.669493	-2.949233	1.798337
15	1	0	-10.032318	3.173434	1.778308
16	1	0	-13.542363	6.26781	0.055316
17	1	0	-11.665843	4.97622	-2.394453
18	1	0	-14.889473	5.75305	-2.961014
19	1	0	-21.170171	0.638652	-2.411634
20	1	0	-22.651096	-3.540383	-3.987146
21	1	0	-19.586448	-2.846519	-5.155343
22	1	0	-19.962373	-5.025173	-2.629928
23	1	0	-6.962172	0.117858	3.32286
24	1	0	-9.947586	-0.60236	4.668892
25	1	0	-8.71255	-2.464826	2.148207
26	1	0	-24.049675	-1.893797	0.318889
27	1	0	-21.974518	-0.029669	2.178257
28	1	0	-21.403068	-3.31721	1.817134
29	1	0	-8.630869	-0.192739	-2.092167

2A000017_en_		Standard Orientation (A.U.)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	-13.588182	-0.810511	1.161787
1	6	0	-13.034206	1.164049	-0.430412
2	7	0	-14.797873	1.788849	-2.222779
3	6	0	-17.100228	0.592287	-2.580351
4	6	0	-17.4963	-1.494851	-0.801854
5	7	0	-15.827586	-2.098273	0.915453
6	6	0	-10.679638	2.816191	-0.385481
7	6	0	-11.852071	-1.728636	3.227628
8	8	0	-18.584992	1.283572	-4.248104
9	6	0	-19.917009	-2.987383	-1.067395
10	6	0	-19.731281	-4.751629	-3.381474
11	6	0	-10.919193	4.939438	1.565663
12	6	0	-20.586669	-4.46225	1.326291
13	8	0	-8.426971	1.381165	-0.068202
14	1	0	-14.437077	3.234213	-3.43409
15	1	0	-10.498028	3.667444	-2.265882
16	1	0	-11.183828	-0.195432	4.449235
17	1	0	-12.892071	-3.062993	4.409757
18	1	0	-10.192399	-2.702811	2.464462
19	1	0	-21.41767	-1.611963	-1.466344
20	1	0	-19.306113	-3.679008	-5.096204
21	1	0	-18.239824	-6.161242	-3.09749
22	1	0	-21.521293	-5.75268	-3.665761
23	1	0	-12.581712	6.106314	1.176424
24	1	0	-11.115012	4.169167	3.477631
25	1	0	-9.235689	6.138259	1.499963
26	1	0	-20.744758	-3.208462	2.96495
27	1	0	-19.138927	-5.875676	1.754199
28	1	0	-22.395156	-5.436685	1.0721
29	1	0	-8.137856	1.160551	1.727992

2A000018_en_		Standard Orientation (A.U.)			
Center	Atomic	Atomic	X	Y	Z

number	number	Type			
0	6	0	-13.001051	-0.780999	-0.806964
1	6	0	-13.499608	1.728992	-0.37704
2	7	0	-15.987682	2.439209	-0.164767
3	6	0	-18.047295	0.83494	-0.314862
4	6	0	-17.310778	-1.796561	-0.790459
5	7	0	-14.952868	-2.484398	-1.0172
6	6	0	-11.588122	3.830069	0.000469
7	6	0	-10.390689	-1.886115	-1.042755
8	8	0	-20.233766	1.629297	-0.081613
9	6	0	-19.413708	-3.72126	-0.961447
10	6	0	-18.607791	-6.136313	-2.329057
11	6	0	-10.21427	3.584434	2.535986
12	6	0	-20.423467	-4.302366	1.711648
13	8	0	-9.887448	3.808235	-2.092626
14	1	0	-16.413286	4.28728	0.130726
15	1	0	-12.638456	5.626431	0.007194
16	1	0	-9.887735	-2.950193	0.665151
17	1	0	-10.348103	-3.220464	-2.623936
18	1	0	-8.972439	-0.429368	-1.36449
19	1	0	-20.95601	-2.818825	-2.01465
20	1	0	-17.095319	-7.099954	-1.29955
21	1	0	-20.216691	-7.429101	-2.486462
22	1	0	-17.909832	-5.726464	-4.233495
23	1	0	-8.906298	5.170512	2.789871
24	1	0	-11.57051	3.619549	4.097782
25	1	0	-9.143151	1.820394	2.628857
26	1	0	-21.047411	-2.573839	2.657282
27	1	0	-18.94845	-5.190492	2.863836
28	1	0	-22.030543	-5.603314	1.603884
29	1	0	-8.534791	4.985234	-1.70108

2A000019_en_		Standard Orientation (A.U.)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	-14.37447	1.848785	-0.546694
1	6	0	-12.72839	0.142574	0.511677
2	7	0	-13.563419	-2.289704	0.828241
3	6	0	-15.938377	-3.18427	0.180329
4	6	0	-17.550408	-1.213474	-0.912103
5	7	0	-16.766824	1.107236	-1.225433
6	6	0	-10.010707	0.630634	1.3189
7	6	0	-13.745569	4.588276	-1.020414
8	8	0	-16.535094	-5.41701	0.530467
9	6	0	-20.215311	-1.958323	-1.620244
10	6	0	-21.836802	-2.205036	0.790548
11	6	0	-8.193561	0.43349	-0.924237
12	6	0	-21.418033	-0.134562	-3.512534
13	8	0	-9.739849	2.947754	2.657565
14	1	0	-12.392102	-3.591712	1.615211
15	1	0	-9.514089	-0.832887	2.699111
16	1	0	-11.957061	4.832925	-2.035796
17	1	0	-15.241548	5.410711	-2.180232
18	1	0	-13.629417	5.669107	0.741476
19	1	0	-20.094106	-3.846222	-2.471144

20	1	0	-23.739891	-2.864575	0.310635
21	1	0	-20.995215	-3.552611	2.112447
22	1	0	-22.007614	-0.370229	1.737331
23	1	0	-6.25128	0.715741	-0.273423
24	1	0	-8.331886	-1.427208	-1.816278
25	1	0	-8.630341	1.861592	-2.358475
26	1	0	-23.30692	-0.802121	-4.033326
27	1	0	-20.282334	0.021705	-5.235316
28	1	0	-21.596189	1.760344	-2.70358
29	1	0	-9.4711	4.286284	1.43499