

Spiroleiferthione A and Oleiferthione A: Two Isothiocyanate-derived Thioketone Alkaloids from *Moringa oleifera* Lam. Seeds

Yueping Jiang,^{a,b} Rong Liu,^{a,b} Lin Huang,^c Qi Huang,^{a,b} Min Liu,^{a,b} Shao Liu,^{*, a,b} and Jing Li^{*, a,b}

^a Department of Pharmacy, Xiangya Hospital, Central South University, Changsha, 410008, China

^b Institute for Rational and Safe Medication Practices, National Clinical Research Center for Geriatric Disorders, Xiangya Hospital, Central South University, Changsha, 410008, China

^c College of Pharmacy, Dali University, Dali, 671000, China

Corresponding Author

*E-mail: liushao999@csu.edu.cn (S. Liu)

*E-mail: lijingliyun@163.com (J. Li)

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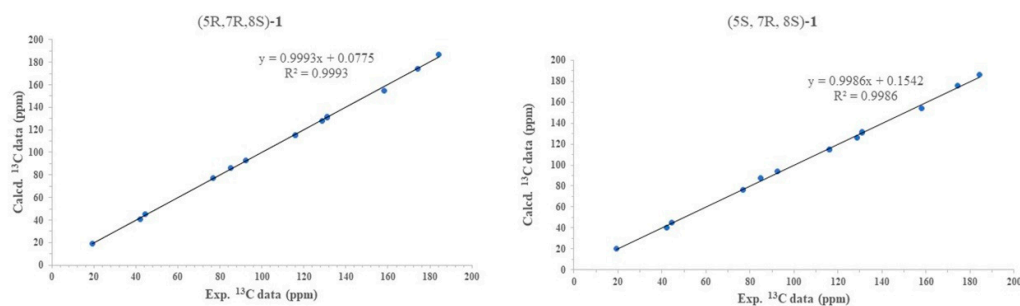
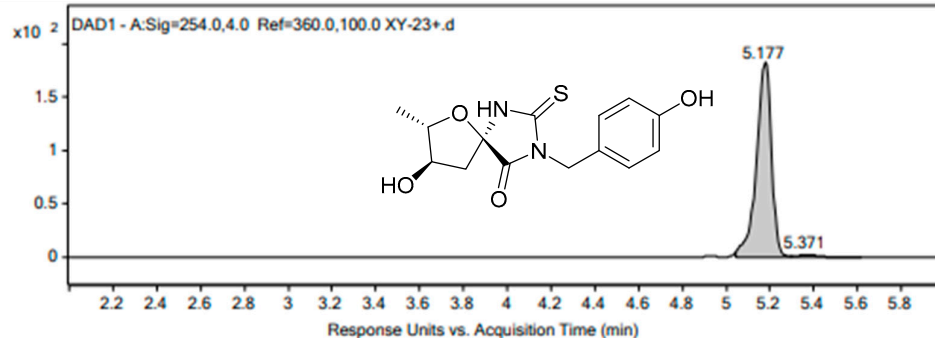
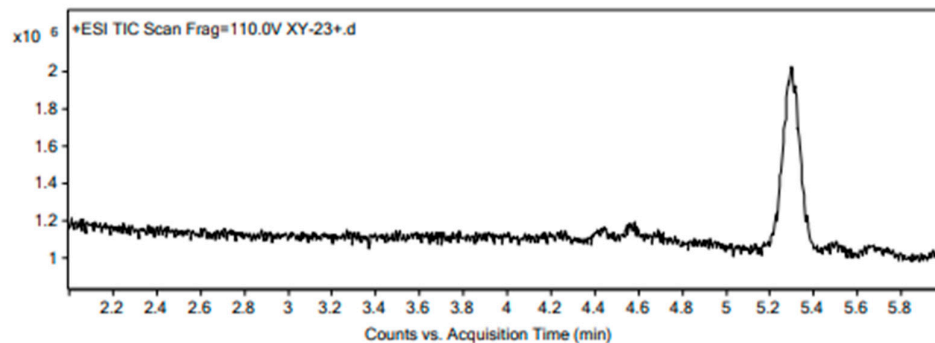


Figure S1. The linear correlation plots of predicted versus experimental ^{13}C NMR chemical shifts.
(Left (5R, 7R, 8S)-1, Right (5S, 7R, 8S)-1).

Qualitative Analysis Report

Chromatograms

Fragmentor Voltage 110 Collision Energy 0 Ionization Mode ESI

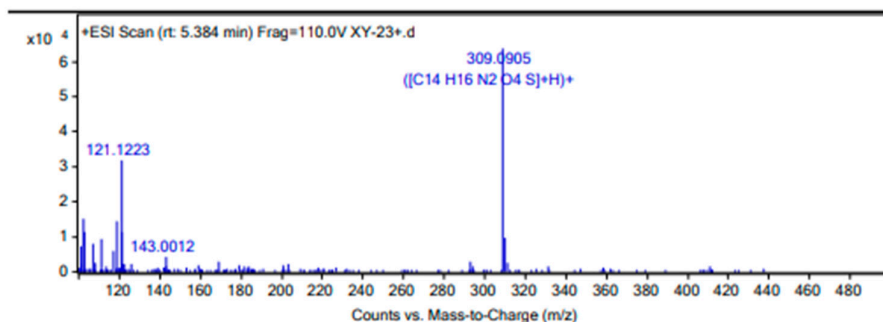


Spectra

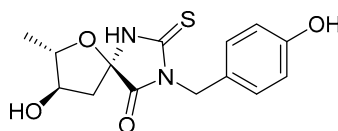
Fragmentor Voltage 110 Collision Energy 0 Ionization Mode ESI

Figure S2. (+)-HRESIMS spectrum of compound 1 (page 1).

Qualitative Analysis Report



Formula Calculator Element Limits		
Element	Min	Max
C	0	60
H	0	120
O	0	10
N	0	5
S	0	5



Formula Calculator Results						
Formula	Best	Mass	Tgt Mass	Diff (ppm)	Ion Species	Score
C14 H16 N2 O4 S	True	308.0832	308.0831	-0.28	C14 H17 N2 O4 S	97.22
C12 H14 N5 O3 S	False	308.0832	308.0817	-4.89	C12 H15 N5 O3 S	91.05
C8 H14 N5 O8	False	308.0831	308.0842	3.85	C8 H15 N5 O8	87.07
C20 H10 N3 O	False	308.0829	308.0824	-1.69	C20 H11 N3 O	82.1
C6 H20 N4 O6 S2	False	308.0834	308.0824	-3.02	C6 H21 N4 O6 S2	79.47
C9 H18 N5 O3 S2	False	308.0833	308.0851	5.75	C9 H19 N5 O3 S2	78.19
C22 H12 O2	False	308.0829	308.0837	2.84	C22 H13 O2	77.78
C11 H18 N O7 S	False	308.0832	308.0804	-8.94	C11 H19 N O7 S	76.14
C17 H14 N3 O S	False	308.0832	308.0858	8.42	C17 H15 N3 O S	75
C10 H16 N2 O9	False	308.083	308.0856	8.53	C10 H17 N2 O9	74.86

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Figure S3. (+)-HRESIMS spectrum of compound **1** (page 2).

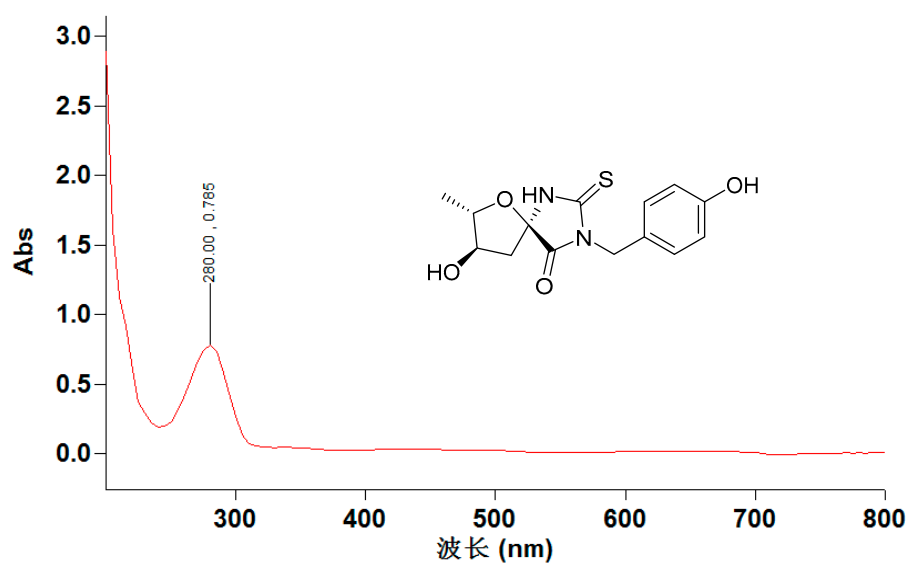


Figure S4. The UV spectrum of compound 1 in MeOH.

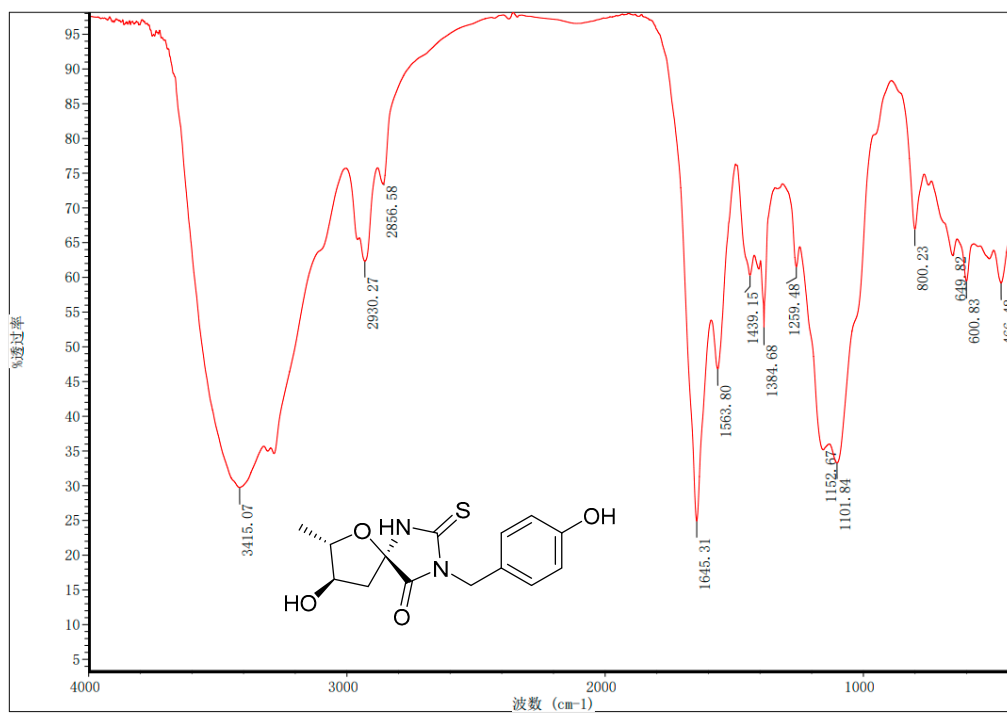


Figure S5. The IR spectrum of compound 1.

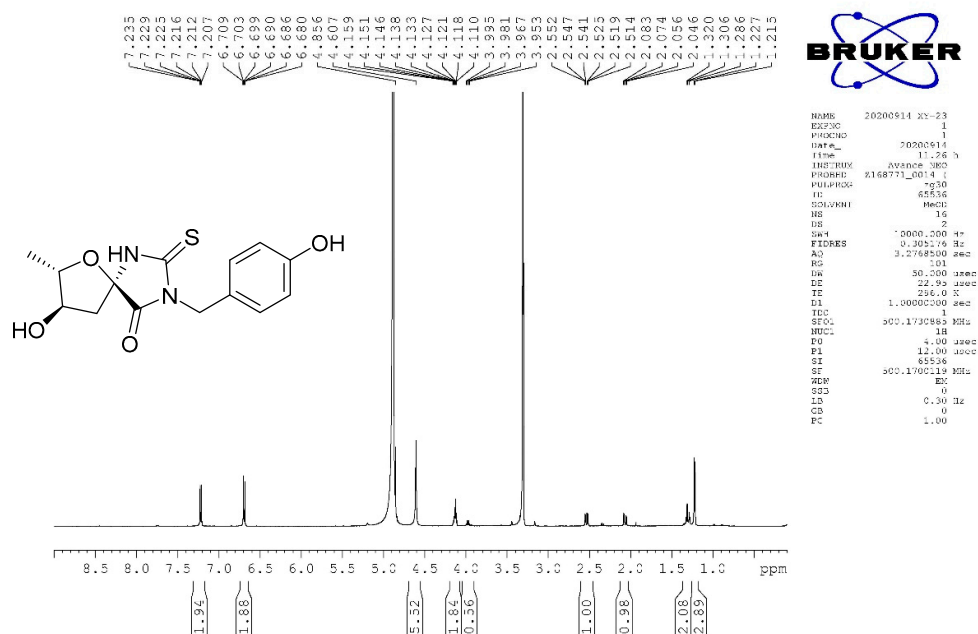


Figure S6. The ¹H NMR spectrum of compound **1** in MeOH-*d*₄ (500 MHz).

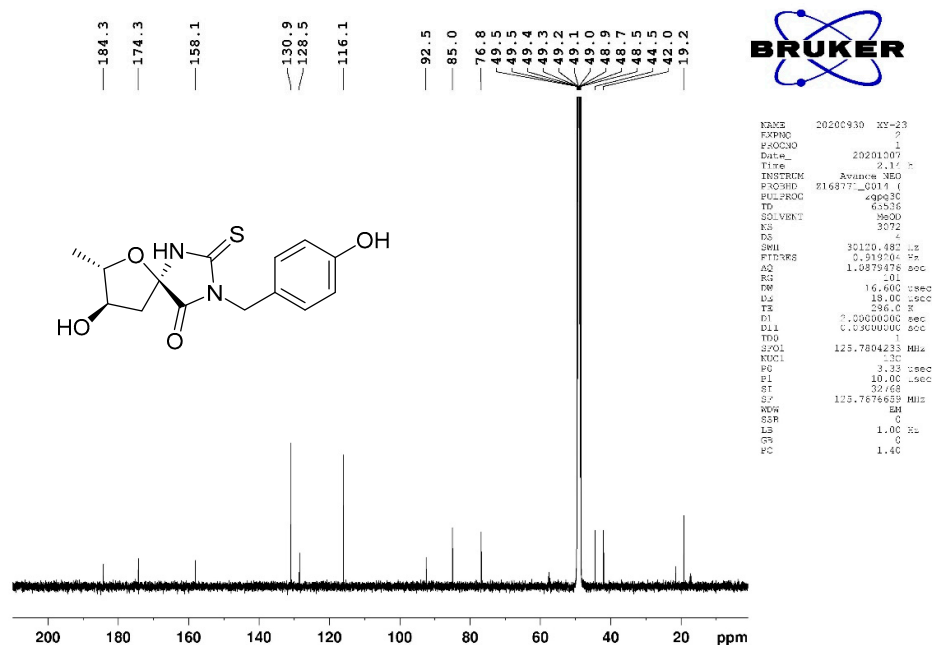


Figure S7. The ¹³C NMR spectrum of compound **1** in MeOH-*d*₄ (125 MHz).

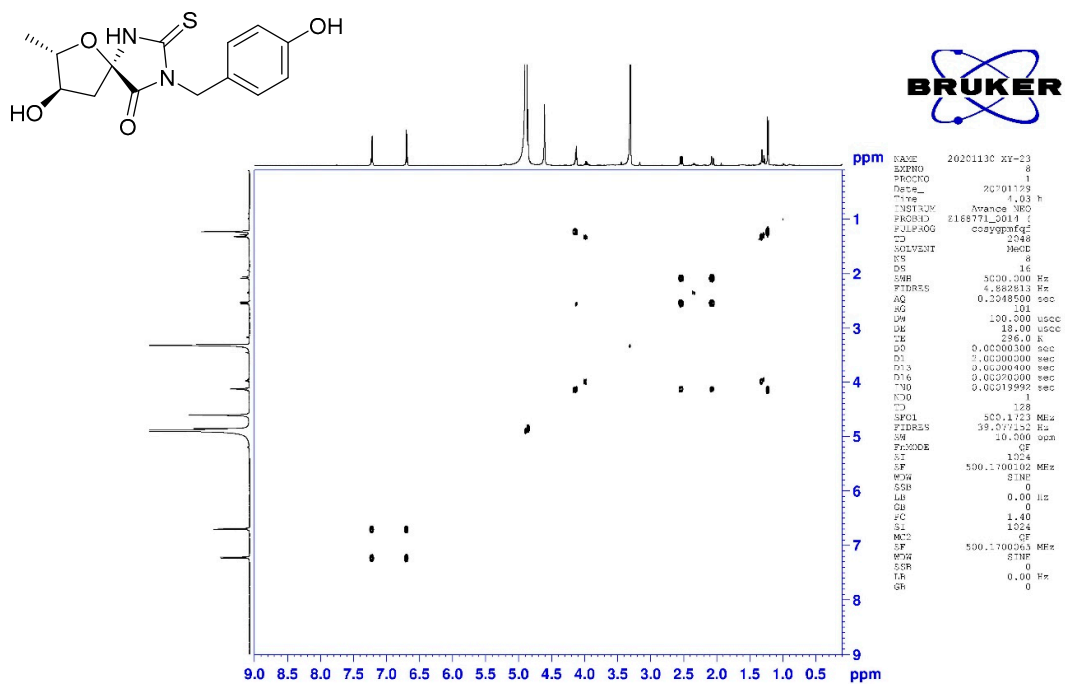


Figure S8. The ^1H - ^1H COSY spectrum of compound 1 in $\text{MeOH-}d_4$ (500 MHz).

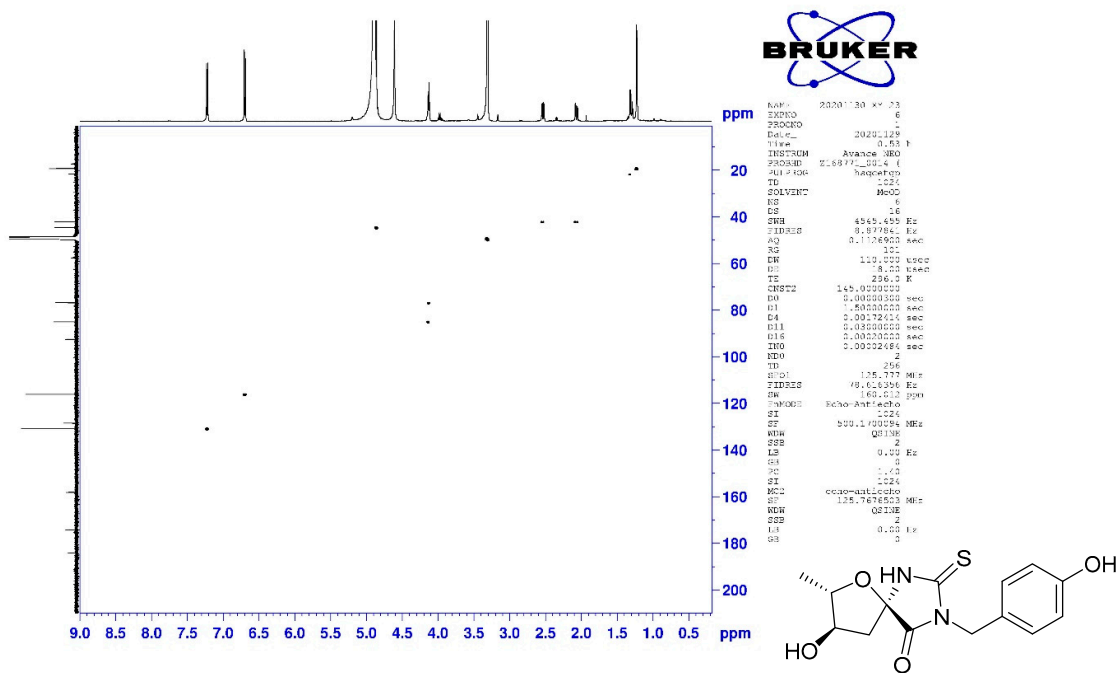


Figure S9. The HSQC spectrum of compound 1 in $\text{MeOH-}d_4$ (500 MHz for ^1H).

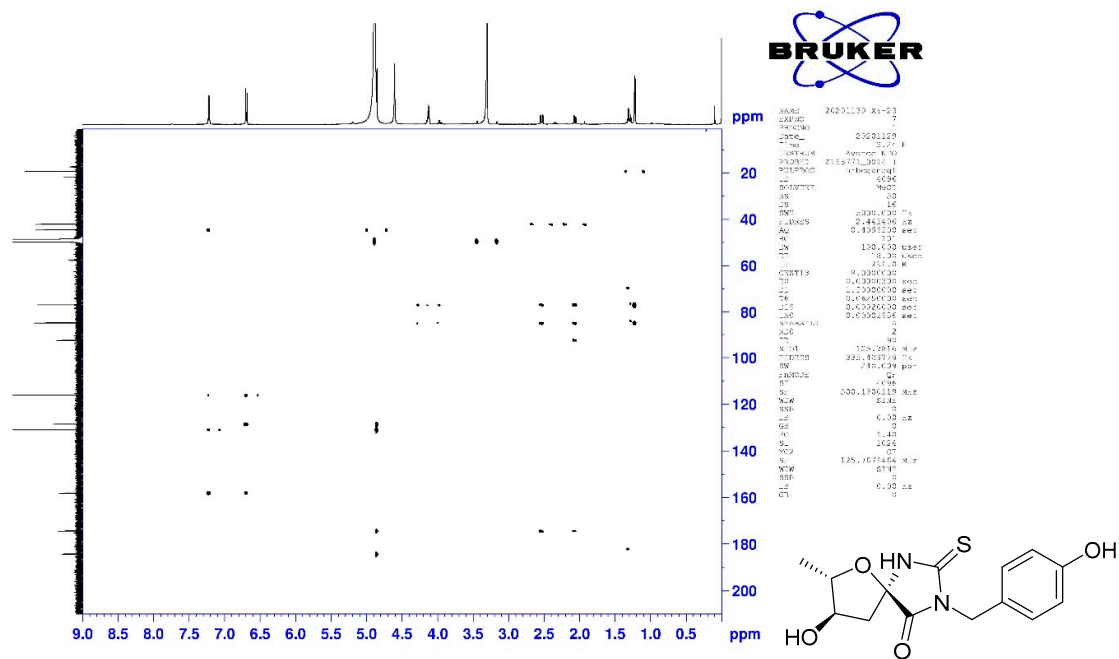


Figure S10. The HMBC spectrum of compound 1 in MeOH- d_4 (500 MHz for ^1H).

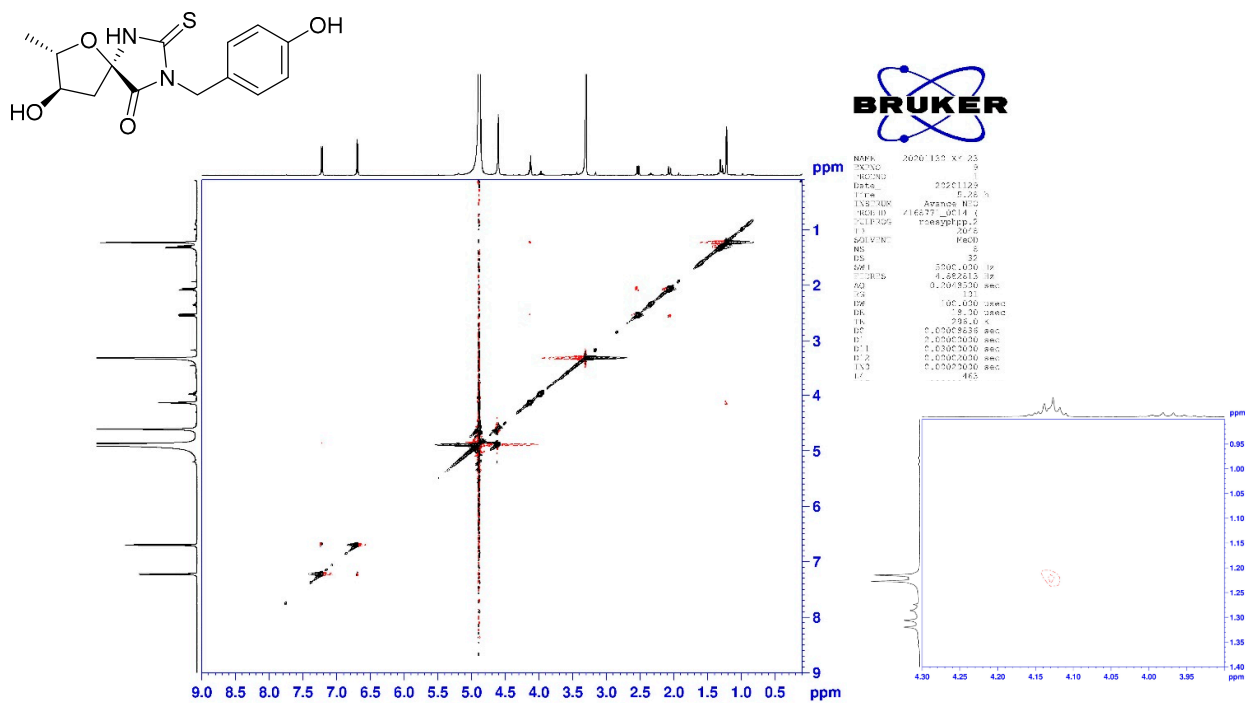


Figure S11. The ROESY spectrum and enlarged ROESY spectrum of compound 1 in MeOH- d_4 (500 MHz).

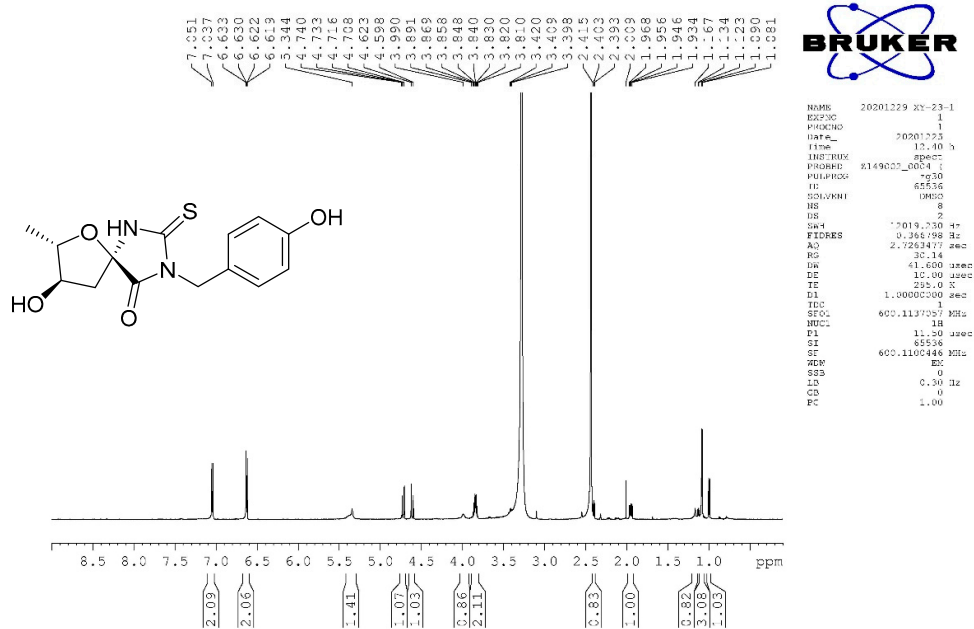


Figure S12. The ¹H NMR spectrum of compound **1** in DMSO-*d*₆ (600 MHz).

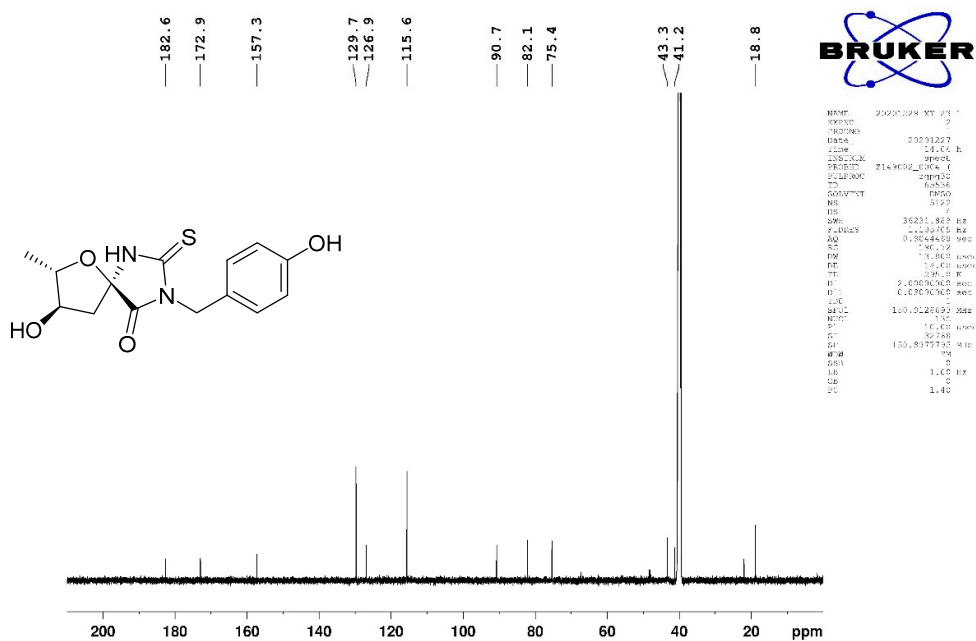


Figure S13. The ¹³C NMR spectrum of compound **1** in DMSO-*d*₆ (150 MHz).

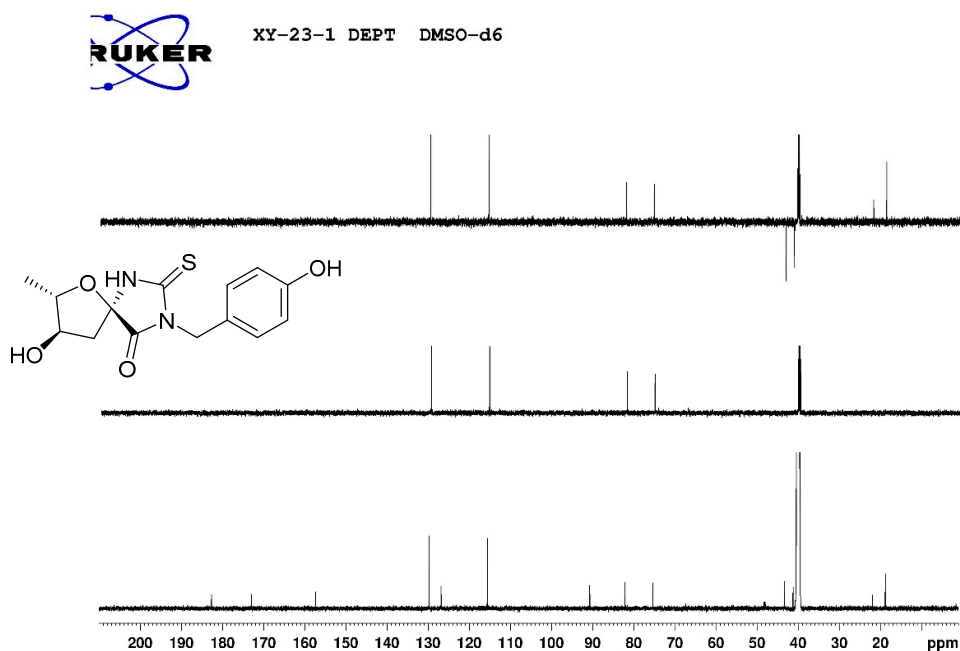


Figure S14. The DEPT spectrum of compound **1** in DMSO-*d*₆ (150 MHz).

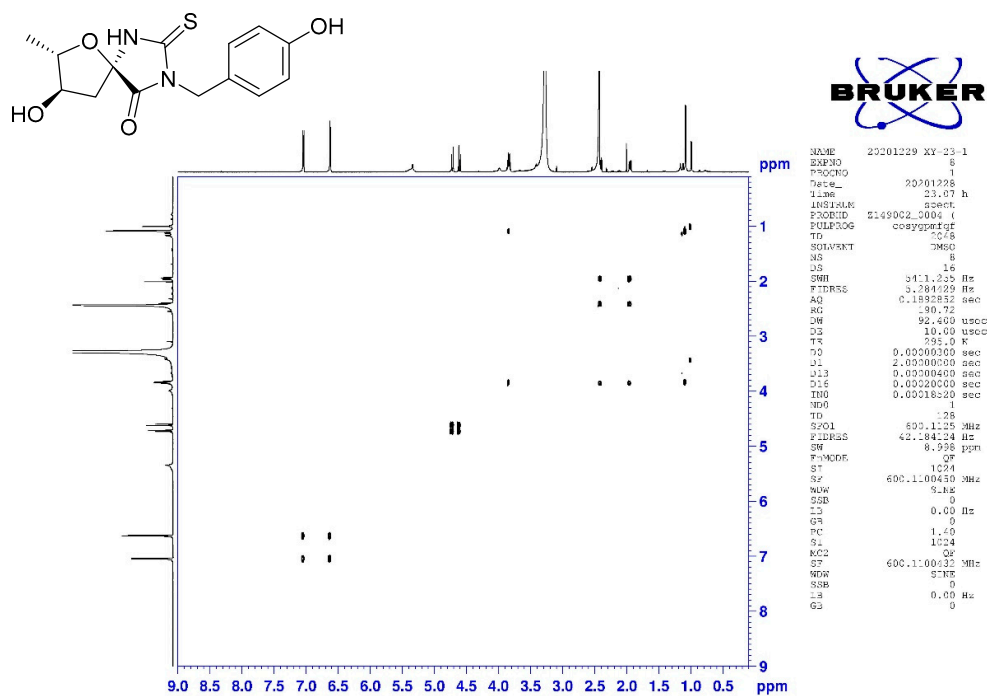


Figure S15. The ¹H-¹H COSY spectrum of compound **1** in DMSO-*d*₆ (600 MHz).

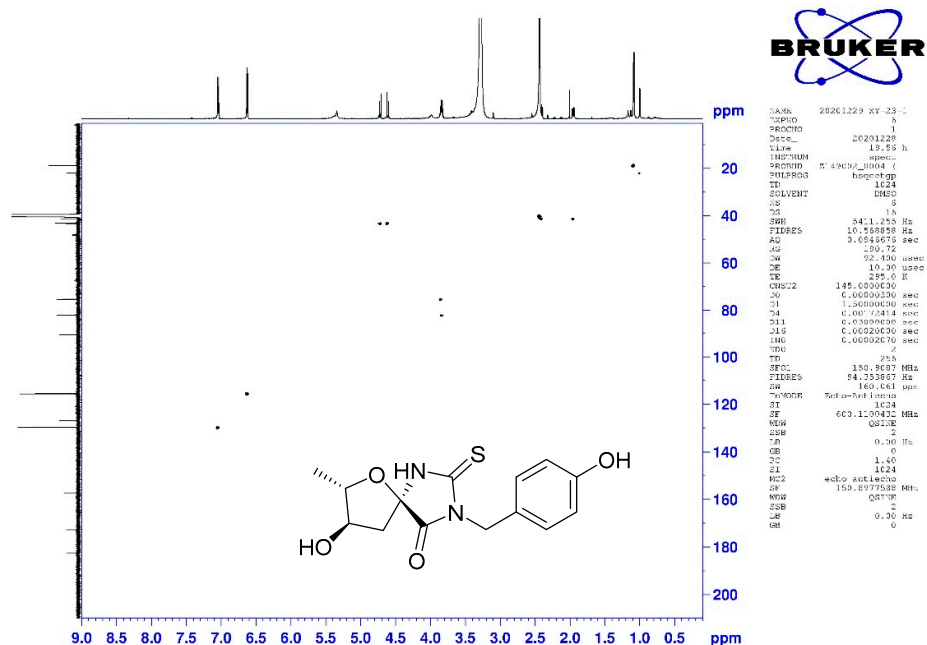


Figure S16. The HSQC spectrum of compound **1** in DMSO- d_6 (600 MHz for ^1H).

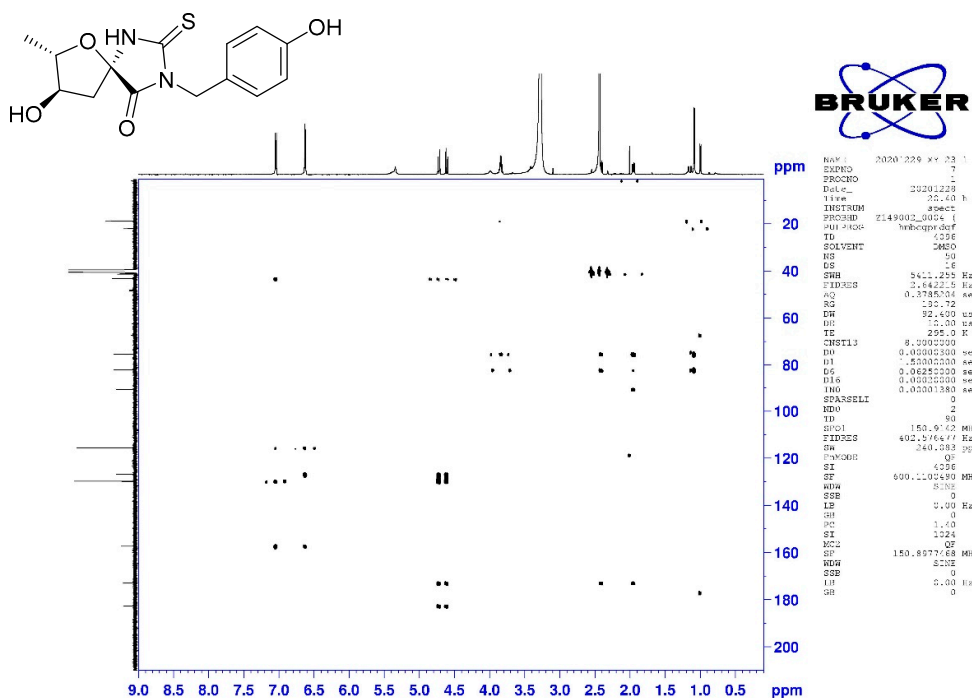


Figure S17. The HMBC spectrum of compound **1** in DMSO- d_6 (600 MHz for ^1H).

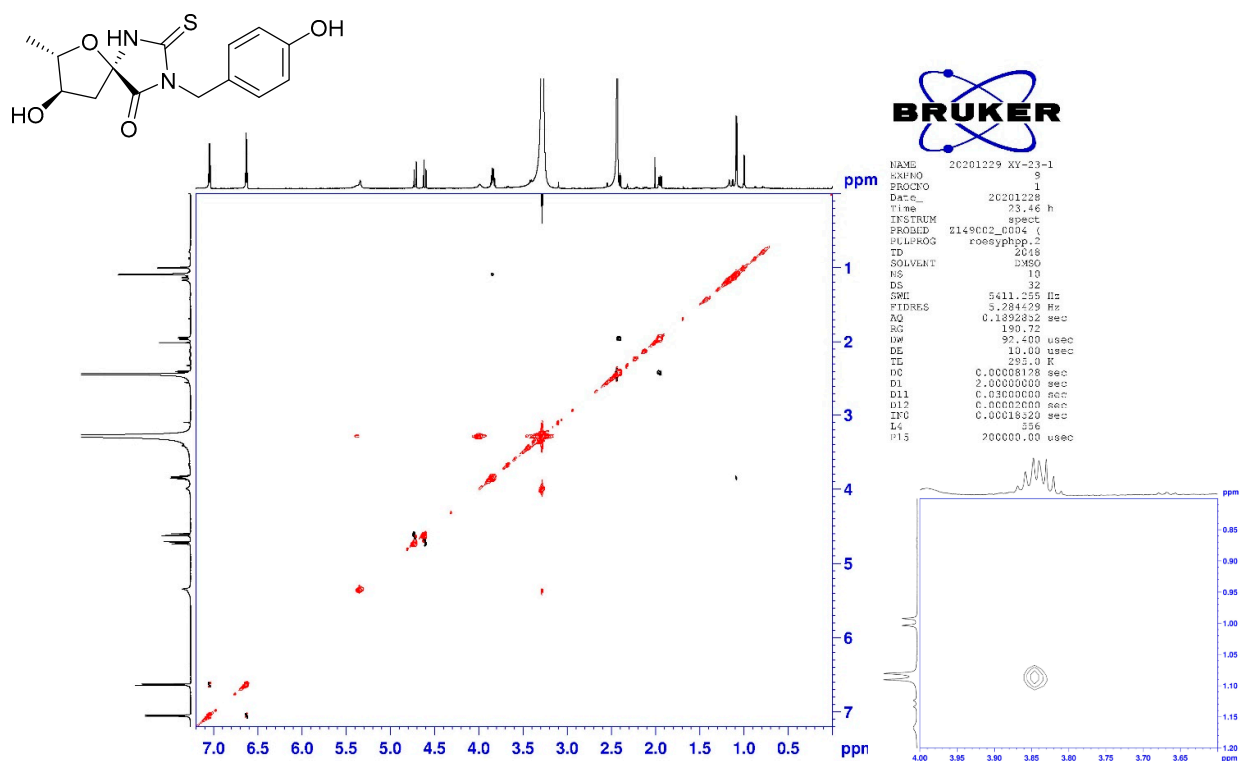
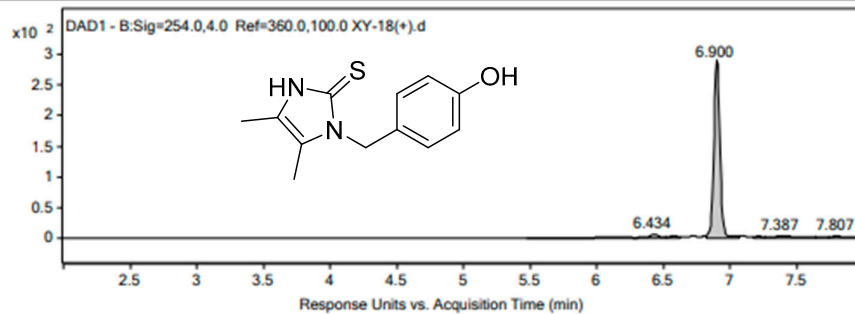
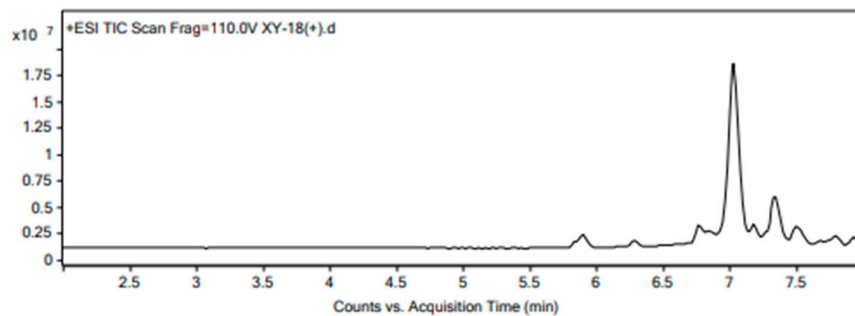


Figure S18. The NOESY spectrum and enlarged NOESY spectrum of compound **1** in DMSO- d_6 (600 MHz).

Qualitative Analysis Report

Chromatograms

Fragmentor Voltage 110 Collision Energy 0 Ionization Mode ESI

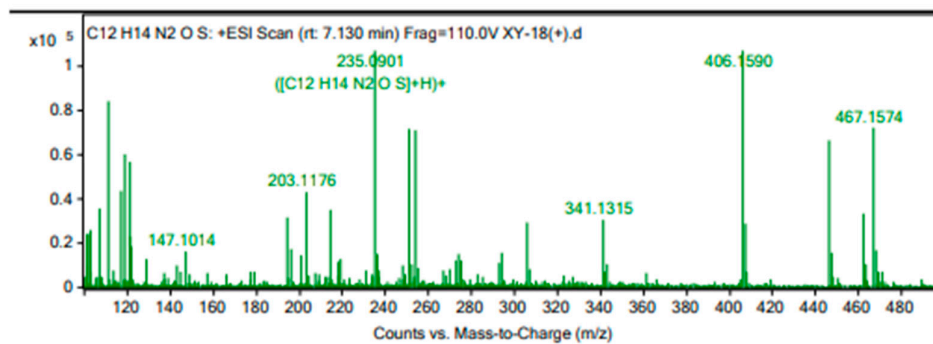


Spectra

Fragmentor Voltage 110 Collision Energy 0 Ionization Mode ESI

Figure S19. (+)-HRESIMS spectrum of compound 2 (page 1).

Qualitative Analysis Report



Formula Calculator Element Limits

Element	Min	Max
C	0	60
H	0	120
O	0	10
N	0	5
S	0	5

Formula Calculator Results

Formula	Best	Mass	Tgt Mass	Diff (ppm)	Ion Species	Score
C12 H14 N2 O S	True	234.083	234.0827	-1.17	C12 H15 N2 O S	97.49
C10 H12 N5 S	False	234.0831	234.0813	-7.34	C10 H13 N5 S	85.26
C7 H16 N5 S2	False	234.0832	234.0847	6.58	C7 H17 N5 S2	80.16
C6 H12 N5 O5	False	234.0827	234.0838	4.92	C6 H13 N5 O5	76.2
C9 H16 N O4 S	False	234.0829	234.08	-12.56	C9 H17 N O4 S	70.08
C9 H18 N2 O S2	False	234.0831	234.0861	12.76	C9 H19 N2 O S2	65.82
C8 H14 N2 O6	False	234.0826	234.0852	11.2	C8 H15 N2 O6	61.79
C10 H22 N O S2	True	236.1143	236.1143	0.04	C10 H23 N O S2	47.62
C10 H14 N5 O2	False	236.1143	236.1147	2.03	C10 H15 N5 O2	46.64
C9 H18 N O6	False	236.1143	236.1134	-3.64	C9 H19 N O6	44.55
C8 H20 N4 S2	False	236.1143	236.1129	-5.65	C8 H21 N4 S2	40.56
C12 H16 N2 O3	False	236.1143	236.1161	7.71	C12 H17 N2 O3	35.29

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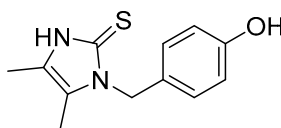


Figure S20. (+)-HRESIMS spectrum of compound 2 (page 2).

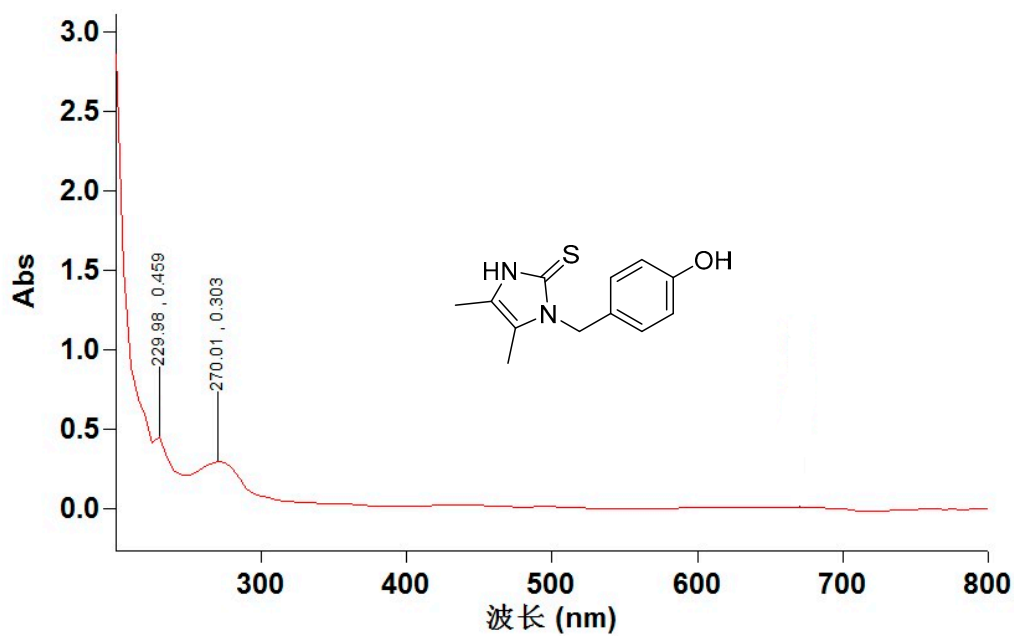


Figure S21. The UV spectrum of compound 2 in MeOH.

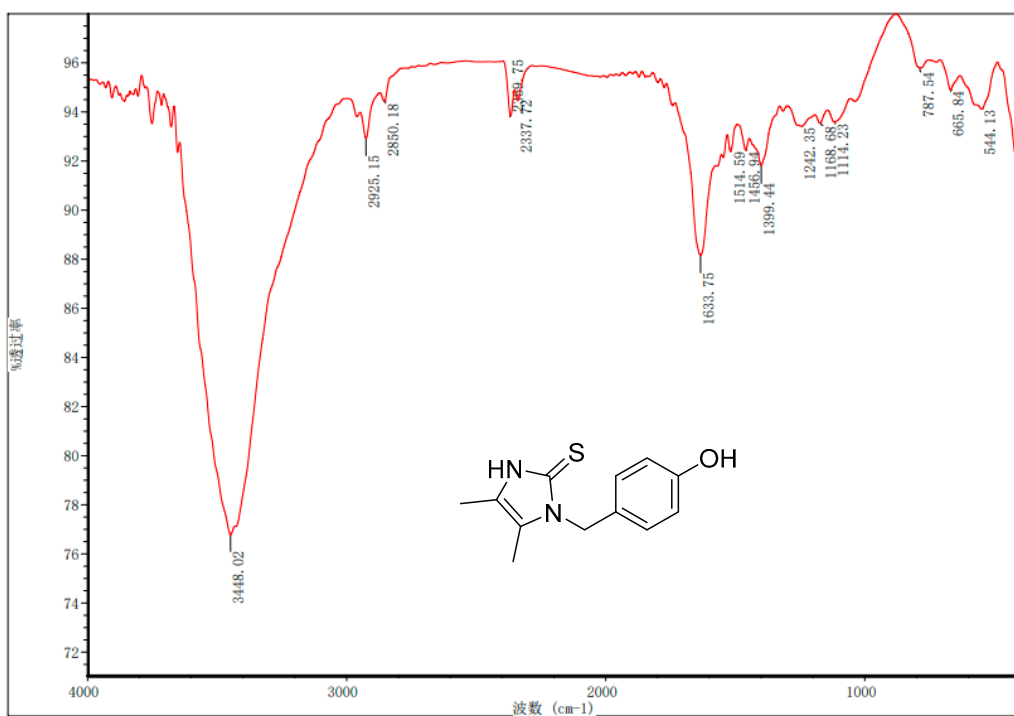


Figure S22. The IR spectrum of compound 2.

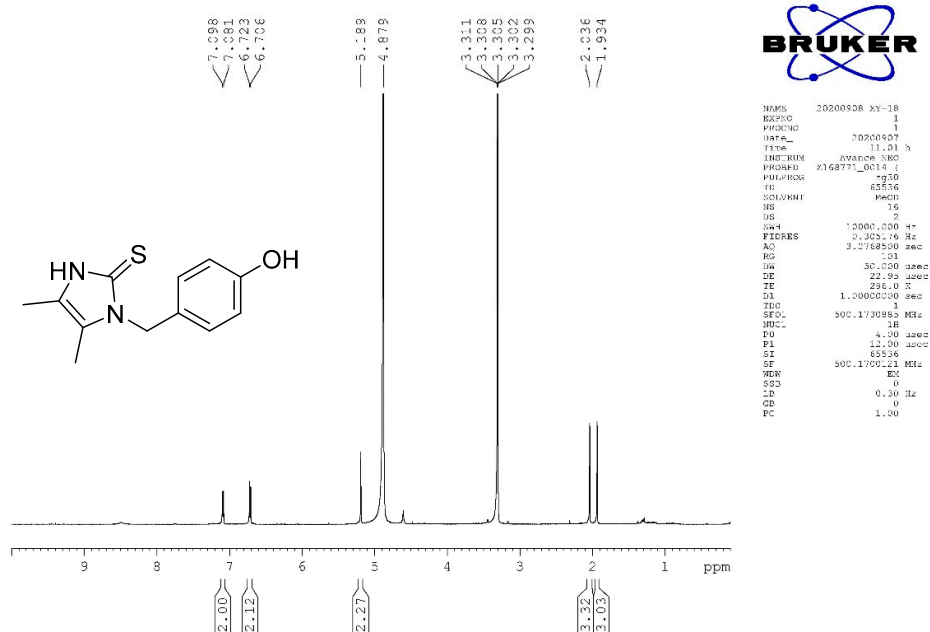


Figure S23. The ¹H NMR spectrum of compound 2 in MeOH-d₄ (500 MHz).

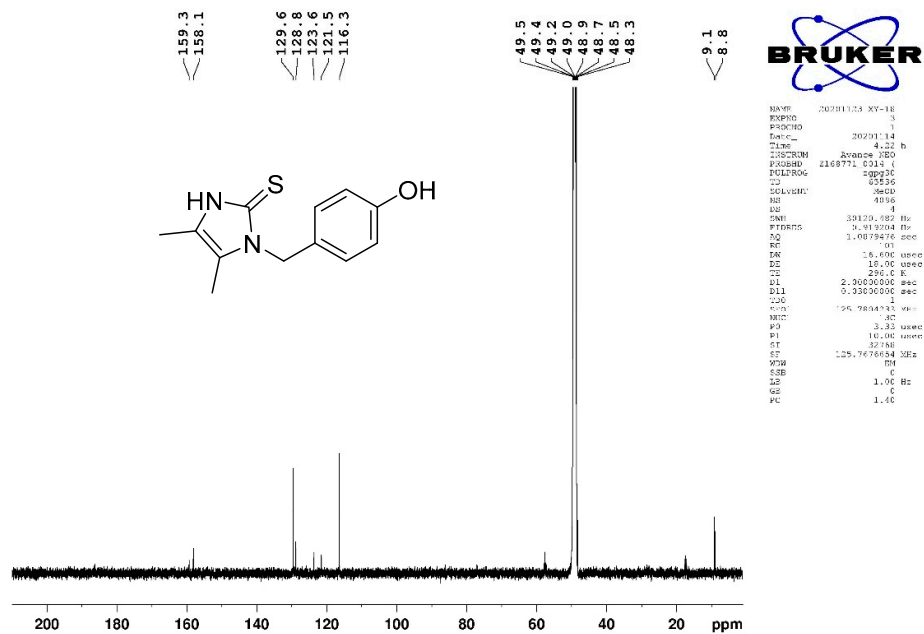


Figure S24. The ¹³C NMR spectrum of compound 2 in MeOH-d₄ (125 MHz).

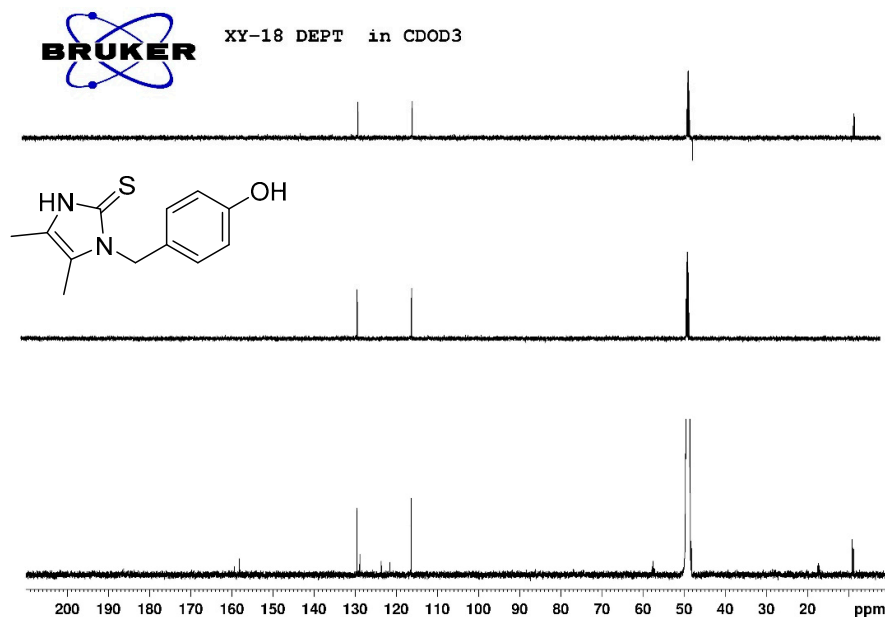


Figure S25. The DEPT spectrum of compound **2** in MeOH-*d*₄ (125 MHz).

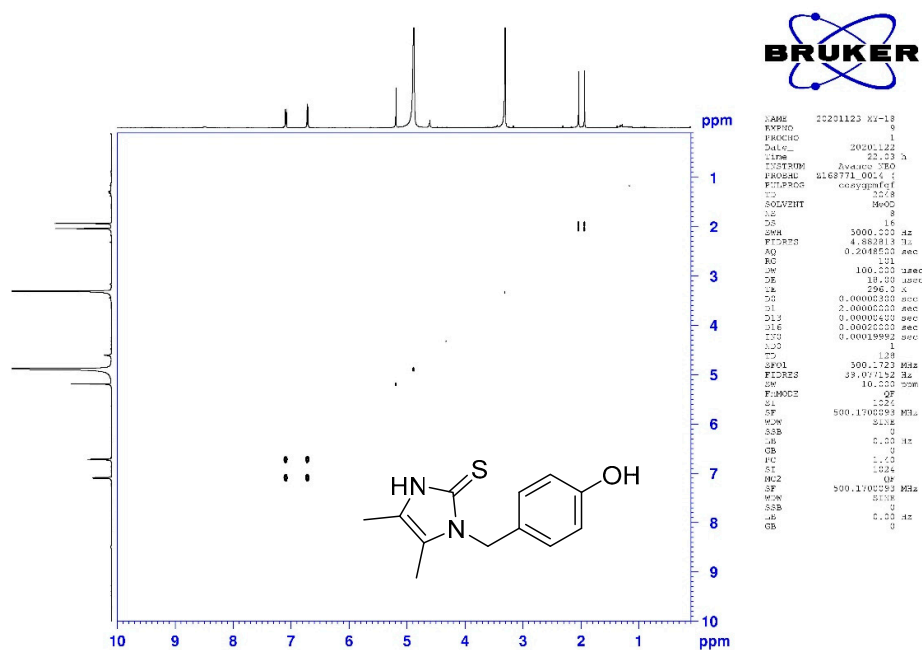


Figure S26. The ¹H-¹H COSY spectrum of compound **2** in MeOH-*d*₄ (500 MHz).

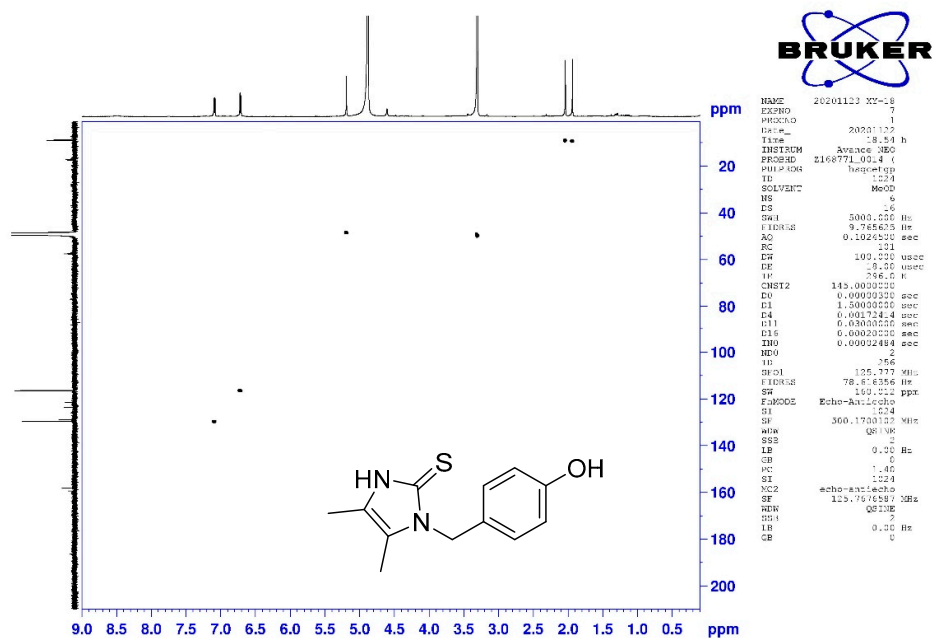


Figure S27. The HSQC spectrum of compound **2** in MeOH-*d*₄ (500 MHz for ¹H).

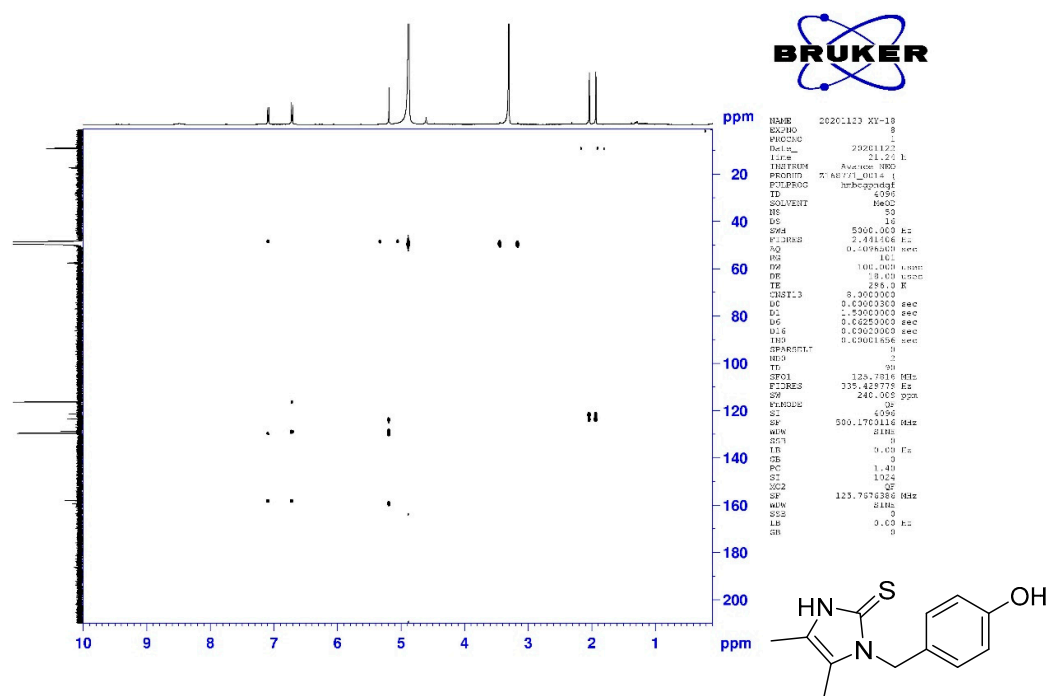


Figure S28. The HMBC spectrum of compound **2** in MeOH-*d*₄ (500 MHz for ¹H).

Table S1. Geometry data of conformers of isomer **1a** and isomer **1b**.

1a-c2 , $\Delta G = 0.0000$ kcal/mol, population = 21.81 %

N -1.562738 1.393339 -0.024114
C -1.881717 -0.000459 -0.285641
C -0.612855 -0.442888 -1.034619
N 0.206789 0.659427 -1.112470
C -0.377431 1.777798 -0.514903
O -2.016498 -0.747598 0.903472
C -3.416463 -1.089686 1.137137
C -4.193588 -0.290982 0.083633
C -3.188700 -0.201082 -1.054247
C 1.547383 0.612104 -1.700638
C 2.561277 -0.019893 -0.780158
C 3.156502 -1.237389 -1.105952
C 4.091099 -1.827700 -0.265239
C 4.438431 -1.199513 0.927978
C 3.849613 0.017710 1.270925
C 2.921483 0.598888 0.417631
S 0.288885 3.308855 -0.448185
O -0.379737 -1.547086 -1.467611
C -3.601535 -2.591293 1.043534
O -4.448668 1.052938 0.511585
O 5.361344 -1.820164 1.724742
H -2.234895 2.033134 0.371372
H -3.661176 -0.736790 2.140502
H -5.121121 -0.787769 -0.205518
H -3.140226 -1.142927 -1.599169
H -3.401196 0.608148 -1.747689
H 1.471234 0.047667 -2.628302
H 1.809126 1.641256 -1.938475
H 2.883731 -1.736037 -2.027895
H 4.551925 -2.772772 -0.521377
H 4.119827 0.509105 2.198460
H 2.472881 1.546867 0.687404
H -2.920848 -3.094272 1.730551
H -3.400534 -2.954265 0.034209
H -4.624254 -2.860246 1.313954
H -5.036197 1.029967 1.276555
H 5.520782 -1.293044 2.517850

1a-c10 , $\Delta G = 0.0489$ kcal/mol, population = 20.08 %

N -1.595382 1.296291 -0.352961
C -1.981071 -0.015906 0.136261

C -0.770561 -0.351721 1.024010
N 0.094198 0.714196 0.936508
C -0.401299 1.709816 0.092654
O -3.152579 0.030066 0.921093
C -4.272293 -0.574089 0.205248
C -3.745894 -0.807211 -1.215810
C -2.261726 -1.031781 -0.973185
C 1.390852 0.751404 1.623632
C 2.486422 0.082986 0.832177
C 2.679641 -1.298369 0.908682
C 3.673203 -1.924413 0.170158
C 4.497520 -1.167236 -0.660918
C 4.320887 0.212525 -0.745879
C 3.320510 0.826294 -0.001461
S 0.365871 3.146886 -0.276805
O -0.617229 -1.357622 1.677764
C -4.718331 -1.833921 0.920824
O -3.854698 0.369336 -2.027287
O 5.463734 -1.831426 -1.365255
H -2.133867 1.792449 -1.046413
H -5.075082 0.165329 0.198261
H -4.231561 -1.656723 -1.698574
H -2.083552 -2.035664 -0.589859
H -1.654776 -0.869101 -1.859690
H 1.619784 1.798441 1.803568
H 1.243621 0.254143 2.580762
H 2.041125 -1.890541 1.551677
H 3.823069 -2.994406 0.232761
H 4.963093 0.804202 -1.388068
H 3.181833 1.896884 -0.076451
H -5.611130 -2.241120 0.442890
H -4.957998 -1.606925 1.959743
H -3.936469 -2.595100 0.907909
H -4.788825 0.574967 -2.153693
H 5.972679 -1.207115 -1.897674

1a-c5, $\Delta G = 0.0998$ kcal/mol, population = 18.43 %

N -1.570422 1.403864 -0.037794
C -1.891367 0.009821 -0.294642
C -0.616599 -0.440867 -1.028534
N 0.211069 0.656030 -1.096622
C -0.374961 1.779531 -0.510347
O -2.037732 -0.730502 0.897734
C -3.440747 -1.065201 1.123317

C -4.206980 -0.271414 0.058028
C -3.192507 -0.191945 -1.072249
C 1.561423 0.597765 -1.661284
C 2.550538 -0.048636 -0.724197
C 3.134102 -1.271874 -1.040878
C 4.043432 -1.877700 -0.180415
C 4.372523 -1.257637 1.022120
C 3.795786 -0.031666 1.354386
C 2.895600 0.563185 0.483981
S 0.300511 3.306152 -0.436122
O -0.385073 -1.546982 -1.457506
C -3.631006 -2.566710 1.039517
O -4.462045 1.076127 0.474518
O 5.254075 -1.802695 1.915032
H -2.242909 2.047532 0.350716
H -3.691648 -0.703982 2.122195
H -5.133387 -0.767749 -0.235429
H -3.142297 -1.137589 -1.610434
H -3.397125 0.613203 -1.772773
H 1.496838 0.038247 -2.592826
H 1.837796 1.625290 -1.889381
H 2.874127 -1.765705 -1.969009
H 4.489899 -2.830484 -0.440537
H 4.062054 0.442666 2.290007
H 2.454237 1.517008 0.745234
H -4.656557 -2.829812 1.304963
H -2.956987 -3.067165 1.734909
H -3.424567 -2.937857 0.034270
H -5.058365 1.060325 1.232828
H 5.580571 -2.647763 1.580996

1a -c11 , delta G = 0.2102 kcal/mol, population = 15.29 %

N -1.603791 1.263402 0.348397
C -1.953486 -0.004581 -0.269689
C -0.686964 -0.270814 -1.101220
N 0.153578 0.798917 -0.898252
C -0.411361 1.739708 -0.035544
O -2.126553 -1.031675 0.681179
C -3.537716 -1.384810 0.802880
C -4.277934 -0.318899 -0.014240
C -3.252120 0.037996 -1.077956
C 1.499735 0.877785 -1.477446
C 2.525333 0.128660 -0.665340
C 3.204531 0.754526 0.382344

C 4.134449 0.063562 1.145514
C 4.400089 -1.276098 0.866151
C 3.732636 -1.915184 -0.177011
C 2.803728 -1.210832 -0.933360
S 0.276370 3.196664 0.406128
O -0.474077 -1.236324 -1.797543
C -3.754851 -2.805179 0.320121
O -4.509806 0.873393 0.746715
O 5.327498 -1.911473 1.645417
H -2.268902 1.801228 0.883190
H -3.791903 -1.298139 1.860774
H -5.211449 -0.698474 -0.432925
H -3.215749 -0.730300 -1.849185
H -3.433821 1.005462 -1.538244
H 1.427173 0.467457 -2.482984
H 1.744967 1.934617 -1.545329
H 2.997802 1.793525 0.604789
H 4.662849 0.550696 1.954721
H 3.939531 -2.955847 -0.398151
H 2.284156 -1.713324 -1.739101
H -3.540899 -2.899160 -0.745829
H -4.788582 -3.107637 0.497076
H -3.099789 -3.487126 0.862508
H -5.106676 0.666067 1.475894
H 5.430890 -2.826801 1.355797

1a-c9, $\Delta G = 0.4512$ kcal/mol, population = 10.18 %

N -1.596117 1.385555 -0.178536
C -1.897073 0.007552 0.173224
C -0.634040 -0.361058 0.969815
N 0.179517 0.748226 0.959881
C -0.397118 1.802499 0.248972
O -3.032418 -0.097138 1.003256
C -4.158662 -0.656019 0.260950
C -3.682398 -0.700853 -1.196036
C -2.181464 -0.886597 -1.035265
C 1.494346 0.773587 1.606217
C 2.544785 0.044141 0.807266
C 2.986673 0.547727 -0.419091
C 3.945744 -0.122981 -1.162107
C 4.484565 -1.316646 -0.681462
C 4.057130 -1.830442 0.540343
C 3.090311 -1.149119 1.272163
S 0.296981 3.299756 -0.013636

O -0.407026 -1.417853 1.510979
C -4.533078 -2.007574 0.835842
O -3.871442 0.555323 -1.860365
O 5.429088 -1.936081 -1.453042
H -2.180161 1.919491 -0.804086
H -4.985114 0.048371 0.369525
H -4.153563 -1.509721 -1.756680
H -1.947691 -1.918704 -0.777069
H -1.618292 -0.597534 -1.918548
H 1.747859 1.823756 1.734747
H 1.378804 0.319541 2.588906
H 2.574607 1.476528 -0.793566
H 4.289251 0.268257 -2.110907
H 4.473490 -2.757822 0.916784
H 2.754342 -1.559805 2.216204
H -4.727861 -1.917389 1.904578
H -3.732010 -2.734593 0.692466
H -5.436461 -2.383379 0.351888
H -4.817390 0.735344 -1.921936
H 5.731536 -2.743927 -1.019430

1a-c1 , delta G = 0.6081 kcal/mol, population = 7.81 %

N -1.599778 1.402660 -0.141104
C -1.898513 0.013153 0.164531
C -0.651313 -0.369377 0.979354
N 0.153971 0.745273 1.019549
C -0.413854 1.815189 0.325311
O -3.051700 -0.122796 0.964770
C -4.156121 -0.669112 0.181489
C -3.646667 -0.668830 -1.264872
C -2.148333 -0.848093 -1.075132
C 1.453064 0.761705 1.697190
C 2.528122 0.062351 0.903918
C 3.073155 -1.140684 1.349687
C 4.062279 -1.793154 0.625560
C 4.516649 -1.243076 -0.570383
C 3.979057 -0.041712 -1.032898
C 2.994874 0.602316 -0.295158
S 0.275480 3.323717 0.120430
O -0.428762 -1.439546 1.495432
C -4.532028 -2.039417 0.709139
O -3.830628 0.604414 -1.897474
O 5.491058 -1.922018 -1.249363
H -2.173423 1.950216 -0.764488

H -4.990742 0.025421 0.291112
H -4.098555 -1.464784 -1.858874
H -1.912193 -1.885437 -0.841254
H -1.567637 -0.529657 -1.936704
H 1.695281 1.809615 1.860936
H 1.317980 0.279582 2.663883
H 2.716617 -1.578807 2.273690
H 4.484661 -2.726175 0.975131
H 4.333074 0.388856 -1.962490
H 2.584738 1.537428 -0.655741
H -3.721705 -2.755711 0.563823
H -5.420842 -2.408391 0.193972
H -4.751978 -1.981266 1.775205
H -4.776353 0.779649 -1.974464
H 5.724266 -1.445338 -2.055936

1a-c12 , $\Delta G = 1.6893$ kcal/mol, population = 1.26 %

N -1.389125 1.568540 -0.274120
C -1.923117 0.244986 -0.048688
C -0.783999 -0.374268 0.786798
N 0.161469 0.609163 0.965986
C -0.207403 1.791448 0.328015
O -3.105373 0.274235 0.742011
C -4.183951 -0.417485 0.066581
C -3.473097 -1.371378 -0.890735
C -2.256957 -0.546184 -1.317350
C 1.418233 0.396845 1.694036
C 2.527832 -0.104281 0.804765
C 3.530068 0.755497 0.360696
C 4.547711 0.301865 -0.470785
C 4.568206 -1.032067 -0.871994
C 3.574192 -1.906292 -0.433357
C 2.567648 -1.441116 0.399411
S 0.665456 3.212227 0.319063
O -0.741673 -1.506114 1.211654
C -5.079282 -1.068772 1.092102
O -4.351673 -1.714804 -1.951463
O 5.538755 -1.541077 -1.690274
H -1.869199 2.289170 -0.789757
H -4.747142 0.308169 -0.531051
H -3.154660 -2.265150 -0.346785
H -1.415779 -1.142021 -1.665077
H -2.551803 0.142864 -2.110043
H 1.683803 1.346344 2.151213

H 1.192303 -0.320846 2.480867
H 3.513419 1.794936 0.661280
H 5.322598 0.981971 -0.805347
H 3.604584 -2.942138 -0.745335
H 1.800164 -2.124910 0.739181
H -5.879749 -1.609003 0.583869
H -5.531730 -0.321614 1.744910
H -4.510939 -1.772816 1.702194
H -3.986673 -2.473120 -2.421613
H 6.167389 -0.847767 -1.927793

1a-c16, $\Delta G = 1.8179$ kcal/mol, population = 1.01 %

N -1.388031 1.546205 -0.334486
C -1.920661 0.231283 -0.061150
C -0.773941 -0.361672 0.782993
N 0.170776 0.628205 0.926482
C -0.203673 1.789785 0.254548
O -3.094440 0.287901 0.741202
C -4.180924 -0.424147 0.100572
C -3.481355 -1.409527 -0.832889
C -2.269424 -0.599949 -1.299551
C 1.429879 0.441124 1.657203
C 2.539675 -0.085015 0.782609
C 2.585613 -1.432980 0.424498
C 3.597127 -1.922240 -0.391930
C 4.588554 -1.058902 -0.857221
C 4.559202 0.288441 -0.504313
C 3.539480 0.764588 0.308185
S 0.666415 3.211006 0.197402
O -0.726467 -1.480388 1.240929
C -5.065312 -1.040708 1.156611
O -4.371832 -1.786588 -1.872040
O 5.613933 -1.480119 -1.658351
H -1.873773 2.250903 -0.866580
H -4.750103 0.282320 -0.514140
H -3.157541 -2.285327 -0.263454
H -1.432748 -1.207693 -1.637370
H -2.572662 0.063544 -2.110666
H 1.694378 1.404899 2.084201
H 1.207262 -0.252194 2.466479
H 1.821362 -2.109142 0.786070
H 3.620983 -2.971976 -0.661423
H 5.335695 0.948872 -0.867764
H 3.516161 1.813623 0.572991

H -5.509772 -0.272202 1.789831
H -4.490699 -1.725216 1.782860
H -5.871878 -1.596218 0.675202
H -4.012527 -2.560204 -2.321177
H 5.532636 -2.427103 -1.827949

1a-c15, delta G = 1.9089 kcal/mol, population = 0.87 %

N -1.387946 1.537528 -0.260448
C -1.924940 0.216488 -0.026257
C -0.776858 -0.407241 0.794270
N 0.169058 0.576172 0.970540
C -0.204266 1.760252 0.338472
O -3.093116 0.249312 0.785695
C -4.192405 -0.405922 0.106118
C -3.500473 -1.376921 -0.858616
C -2.281994 -0.572074 -1.290140
C 1.429015 0.363734 1.692701
C 2.541717 -0.115245 0.795179
C 3.552620 0.752016 0.387356
C 4.575012 0.318998 -0.449374
C 4.591100 -1.001402 -0.892980
C 3.587974 -1.883031 -0.491304
C 2.577079 -1.438659 0.347455
S 0.666268 3.182081 0.331952
O -0.730295 -1.540987 1.213116
C -5.104832 -1.032776 1.131745
O -4.286575 -1.720060 -1.990360
O 5.565728 -1.490001 -1.718779
H -1.875529 2.262539 -0.762779
H -4.733462 0.337716 -0.489656
H -3.191569 -2.274279 -0.314456
H -1.454728 -1.182186 -1.644907
H -2.572226 0.119383 -2.082794
H 1.688327 1.308306 2.163551
H 1.209665 -0.367098 2.469285
H 3.539250 1.781582 0.720330
H 5.356487 1.004851 -0.755683
H 3.614808 -2.908451 -0.836286
H 1.803244 -2.128767 0.658985
H -4.563044 -1.770517 1.726088
H -5.938658 -1.528420 0.630316
H -5.517308 -0.276050 1.799779
H -4.903587 -2.417372 -1.739610
H 6.200028 -0.793106 -1.929198

1a-c13 , delta G = 1.9421 kcal/mol, population = 0.82 %

N -1.459361 1.374538 0.869365
C -1.946188 0.326518 0.001833
C -0.764289 0.210583 -0.982422
N 0.181690 1.126205 -0.582371
C -0.241190 1.837964 0.537650
O -2.092640 -0.909405 0.688444
C -3.437073 -1.423095 0.528016
C -3.934956 -0.766453 -0.757628
C -3.287417 0.618044 -0.680322
C 1.492465 1.264738 -1.229414
C 2.522654 0.322530 -0.660675
C 3.433033 0.755811 0.301475
C 4.371180 -0.114943 0.843416
C 4.404299 -1.443121 0.423159
C 3.502800 -1.891061 -0.541587
C 2.574294 -1.010498 -1.076201
S 0.602768 3.058456 1.298859
O -0.685863 -0.548346 -1.920966
C -3.398143 -2.931732 0.518168
O -5.354373 -0.751887 -0.759735
O 5.300373 -2.350281 0.917784
H -1.990393 1.768350 1.629945
H -4.053594 -1.059958 1.358200
H -3.552098 -1.318192 -1.620817
H -3.162262 1.103493 -1.645880
H -3.891361 1.260924 -0.038691
H 1.329088 1.072266 -2.288330
H 1.796977 2.300521 -1.104062
H 3.405210 1.784110 0.637672
H 5.075412 0.236640 1.588784
H 3.542292 -2.923072 -0.865019
H 1.876092 -1.362784 -1.824757
H -2.767337 -3.292336 -0.296059
H -4.408670 -3.319733 0.379445
H -3.010453 -3.317062 1.461747
H -5.659591 -0.536154 -1.648415
H 5.865899 -1.929386 1.577444

1a-c18 , delta G = 2.0350 kcal/mol, population = 0.70 %

N -1.460522 1.376139 0.822021
C -1.941406 0.302164 -0.016999
C -0.760880 0.170443 -1.001610

N 0.180645 1.100336 -0.624895
 C -0.244738 1.837036 0.477977
 O -2.073468 -0.918990 0.698366
 C -3.425254 -1.426601 0.578909
 C -3.934358 -0.810371 -0.730572
 C -3.286984 0.567616 -0.700993
 C 1.490496 1.229346 -1.275836
 C 2.526845 0.310633 -0.680398
 C 3.440075 0.779494 0.262107
 C 4.383907 -0.069057 0.828881
 C 4.419829 -1.410634 0.453972
 C 3.515519 -1.894249 -0.490742
 C 2.581453 -1.035592 -1.050665
 S 0.594127 3.079309 1.208483
 O -0.679824 -0.610424 -1.921539
 C -3.393039 -2.934623 0.629975
 O -5.347476 -0.683994 -0.794839
 O 5.321340 -2.297377 0.975049
 H -1.991730 1.784591 1.574720
 H -4.027586 -1.024854 1.401488
 H -3.558118 -1.391548 -1.577455
 H -3.170549 1.019458 -1.683270
 H -3.888738 1.232125 -0.079174
 H 1.328230 1.005658 -2.328770
 H 1.788252 2.270246 -1.180257
 H 3.410066 1.818482 0.563408
 H 5.090240 0.310104 1.558576
 H 3.557286 -2.936513 -0.779107
 H 1.881377 -1.415574 -1.783780
 H -2.976565 -3.282669 1.575739
 H -2.790532 -3.332636 -0.188373
 H -4.407575 -3.329166 0.544308
 H -5.723960 -1.529761 -1.064275
 H 5.888740 -1.852168 1.616899

1a-c14, $\Delta G = 2.0563$ kcal/mol, population = 0.68 %

N -1.461410 1.379693 0.879500
 C -1.942805 0.333792 0.006277
 C -0.753100 0.218035 -0.968657
 N 0.188704 1.135073 -0.562365
 C -0.242116 1.845484 0.555490
 O -2.097790 -0.902773 0.689471
 C -3.441739 -1.413762 0.516115
 C -3.926938 -0.753675 -0.772571

C -3.277752 0.629520 -0.686696
C 1.503848 1.272622 -1.201061
C 2.522070 0.311118 -0.643227
C 3.385582 0.699491 0.382608
C 4.308685 -0.188637 0.915942
C 4.378956 -1.490613 0.423932
C 3.527227 -1.893650 -0.603598
C 2.608932 -0.993471 -1.129327
S 0.594701 3.066889 1.323337
O -0.666611 -0.540741 -1.906602
C -3.405315 -2.922416 0.503107
O -5.346227 -0.736566 -0.787930
O 5.304518 -2.327616 0.983668
H -1.998202 1.773269 1.636134
H -4.064891 -1.051322 1.341603
H -3.537094 -1.304305 -1.633372
H -3.143358 1.116825 -1.650071
H -3.886040 1.272210 -0.048878
H 1.345159 1.099484 -2.263904
H 1.815940 2.303661 -1.056276
H 3.328267 1.707305 0.772899
H 4.978762 0.114719 1.709818
H 3.585554 -2.903684 -0.992794
H 1.947900 -1.312207 -1.925114
H -2.767962 -3.282154 -0.306407
H -4.415208 -3.308401 0.354431
H -3.026693 -3.310713 1.449148
H -5.642497 -0.516591 -1.678627
H 5.256238 -3.197966 0.568631

1a-c19, $\Delta G = 2.1593$ kcal/mol, population = 0.57 %

N -1.386186 1.518993 -0.308418
C -1.921887 0.204420 -0.037887
C -0.768095 -0.399440 0.789451
N 0.177125 0.588998 0.938559
C -0.200535 1.757535 0.280576
O -3.083615 0.258221 0.782510
C -4.189384 -0.409888 0.126560
C -3.506407 -1.406231 -0.818455
C -2.289730 -0.614742 -1.278923
C 1.439232 0.395300 1.662124
C 2.550891 -0.105010 0.774863
C 3.557985 0.755612 0.337634
C 4.580402 0.303692 -0.485332

C 4.604758 -1.030005 -0.886811
C 3.606069 -1.904281 -0.458847
C 2.592096 -1.439463 0.368657
S 0.667732 3.180013 0.237378
O -0.717482 -1.523430 1.233484
C -5.096743 -1.008392 1.173370
O -4.301180 -1.776412 -1.935487
O 5.632516 -1.427572 -1.696919
H -1.877918 2.232095 -0.823589
H -4.732228 0.320537 -0.483789
H -3.195069 -2.290117 -0.253953
H -1.466199 -1.235136 -1.624410
H -2.584624 0.057211 -2.086492
H 1.698889 1.351474 2.108790
H 1.222457 -0.316099 2.457210
H 3.538308 1.794643 0.639562
H 5.362300 0.972769 -0.820238
H 3.626381 -2.943751 -0.765798
H 1.822693 -2.124583 0.701380
H -5.501885 -0.234145 1.825635
H -4.553363 -1.733408 1.781765
H -5.935825 -1.512997 0.689974
H -4.918719 -2.464790 -1.662320
H 5.545680 -2.366740 -1.903215

1a-c20 , $\Delta G = 2.2283$ kcal/mol, population = 0.51 %

N -1.448304 1.513381 0.564351
C -1.934393 0.297315 -0.047084
C -0.758721 -0.025893 -0.992510
N 0.182821 0.961067 -0.812974
C -0.236542 1.899526 0.127013
O -2.065624 -0.760585 0.892798
C -3.419809 -1.275674 0.882185
C -3.934339 -0.925943 -0.520096
C -3.282683 0.428453 -0.764521
C 1.488424 0.957993 -1.485285
C 2.522663 0.155362 -0.737844
C 2.604042 -1.227596 -0.901708
C 3.536855 -1.978236 -0.197243
C 4.409168 -1.343634 0.686039
C 4.344945 0.038097 0.855382
C 3.406975 0.775235 0.146648
S 0.603587 3.262454 0.593413
O -0.681108 -0.972765 -1.740841

C -3.392654 -2.744636 1.227252
O -5.347337 -0.808879 -0.601087
O 5.349618 -2.024933 1.408507
H -1.976095 2.062440 1.224301
H -4.015993 -0.717867 1.613092
H -3.564446 -1.663374 -1.238413
H -3.169468 0.677945 -1.816906
H -3.879495 1.204703 -0.283188
H 1.317394 0.546290 -2.478287
H 1.792928 1.996703 -1.583872
H 1.927488 -1.725500 -1.584519
H 3.590591 -3.051921 -0.336332
H 5.030957 0.520633 1.539348
H 3.354371 1.846991 0.287396
H -2.972599 -2.902967 2.220999
H -2.795930 -3.297784 0.499864
H -4.409053 -3.143693 1.224732
H -5.728053 -1.689593 -0.696293
H 5.294492 -2.969152 1.214860

1b-c5 , $\Delta G = 0.0000$ kcal/mol, population = 31.84 %

N -1.501573 1.513260 0.676728
C -2.003601 0.241106 0.214456
C -0.868459 -0.167046 -0.744167
N 0.036762 0.856091 -0.764785
C -0.347482 1.888932 0.097281
O -3.202178 0.383148 -0.530488
C -4.204983 -0.580451 -0.087955
C -3.414384 -1.635944 0.698510
C -2.288406 -0.797759 1.306678
C 1.280286 0.818604 -1.548056
C 2.387285 0.085715 -0.834531
C 2.539233 -1.292486 -0.984140
C 3.540955 -1.979671 -0.309787
C 4.411787 -1.284710 0.527825
C 4.275973 0.093839 0.683754
C 3.270627 0.767243 0.005248
S 0.483147 3.309380 0.348695
O -0.812803 -1.204920 -1.375347
C -5.284527 0.120640 0.715171
O -2.938006 -2.694432 -0.124872
O 5.419030 -1.901374 1.216824
H -1.996430 2.111401 1.319679
H -4.622308 -1.025757 -0.990614

H -4.032467 -2.101775 1.463552
H -2.631172 -0.282046 2.203077
H -1.413382 -1.390349 1.564240
H 1.034091 0.332671 -2.490199
H 1.552308 1.852017 -1.745896
H 1.863723 -1.838054 -1.630547
H 3.647977 -3.050742 -0.436510
H 4.962016 0.623974 1.331457
H 3.165449 1.836861 0.132556
H -5.709618 0.940590 0.135939
H -4.888129 0.527722 1.647340
H -6.085004 -0.581084 0.956779
H -2.248764 -2.343058 -0.716640
H 5.417256 -2.848258 1.027693

1b-c1 , $\Delta G = 0.1525$ kcal/mol, population = 24.61 %

N -1.494548 1.553039 0.619806
C -2.007367 0.263123 0.223401
C -0.889992 -0.190794 -0.735578
N 0.016038 0.828608 -0.818855
C -0.351340 1.900152 0.002230
O -3.218256 0.376037 -0.506559
C -4.215140 -0.565254 -0.006297
C -3.414026 -1.586136 0.814532
C -2.276165 -0.724874 1.365534
C 1.244634 0.754403 -1.622746
C 2.368146 0.062804 -0.893968
C 3.269397 0.790480 -0.117776
C 4.291843 0.155082 0.575855
C 4.423963 -1.230251 0.496711
C 3.533834 -1.971310 -0.278873
C 2.517596 -1.323924 -0.966527
S 0.484806 3.329331 0.173243
O -0.846971 -1.256351 -1.319749
C -5.281699 0.172959 0.780741
O -2.953911 -2.682757 0.032850
O 5.409052 -1.913797 1.153953
H -1.977726 2.181319 1.242587
H -4.646676 -1.049768 -0.881688
H -4.020631 -2.014686 1.609949
H -2.602702 -0.168363 2.243406
H -1.398307 -1.307949 1.634866
H 0.982108 0.219807 -2.533619
H 1.509021 1.776943 -1.878818

H 3.167653 1.865720 -0.049230
H 4.987000 0.733240 1.173574
H 3.649775 -3.045645 -0.338208
H 1.826956 -1.904248 -1.565002
H -6.079460 -0.515784 1.064912
H -5.714184 0.967220 0.171946
H -4.871184 0.620254 1.688036
H -2.274028 -2.361038 -0.585942
H 5.963545 -1.297911 1.649508

1b-c2 , $\Delta G = 0.1845$ kcal/mol, population = 23.31 %

N -1.567580 1.668398 -0.106005
C -2.038359 0.318034 0.086751
C -0.873946 -0.260937 0.914199
N 0.062708 0.724973 1.046512
C -0.356874 1.907652 0.428186
O -2.122310 -0.391138 -1.139026
C -3.393943 -1.100111 -1.242803
C -3.943837 -1.132540 0.190419
C -3.407012 0.179930 0.765424
C 1.367017 0.521283 1.693421
C 2.393154 -0.050130 0.748783
C 3.241710 0.786525 0.025282
C 4.169321 0.265123 -0.868206
C 4.256484 -1.114379 -1.047289
C 3.418594 -1.964457 -0.327236
C 2.497840 -1.430441 0.562332
S 0.485024 3.343323 0.397333
O -0.807084 -1.395286 1.347309
C -4.295100 -0.407666 -2.247703
O -3.512477 -2.276100 0.919053
O 5.147015 -1.689467 -1.910903
H -2.082664 2.378006 -0.603105
H -3.156400 -2.111833 -1.570420
H -5.031646 -1.162294 0.195096
H -4.035701 1.018550 0.467540
H -3.341142 0.168208 1.851057
H 1.676929 1.489721 2.077277
H 1.190377 -0.149678 2.531927
H 3.172263 1.858564 0.155731
H 4.824705 0.926948 -1.422563
H 3.499688 -3.034179 -0.469584
H 1.846712 -2.094305 1.116660
H -5.203934 -0.992826 -2.400040

H -3.783568 -0.312335 -3.205762
H -4.578196 0.590677 -1.909017
H -2.553975 -2.201090 1.075967
H 5.668044 -1.006132 -2.351241

1b-c6 , $\Delta G = 0.2679$ kcal/mol, population = 20.24 %

N -1.573284 1.626617 -0.365574
C -2.039538 0.325405 0.049094
C -0.860904 -0.115402 0.939080
N 0.076011 0.878125 0.897540
C -0.355116 1.947390 0.105136
O -2.144011 -0.571376 -1.045085
C -3.418038 -1.283023 -1.013293
C -3.942751 -1.084818 0.415958
C -3.396300 0.301204 0.764416
C 1.389700 0.779249 1.549826
C 2.401632 0.057348 0.697361
C 2.512233 -1.331973 0.749527
C 3.422958 -2.008015 -0.052823
C 4.242901 -1.290701 -0.922419
C 4.147426 0.098601 -0.982499
C 3.232705 0.760794 -0.176573
S 0.483369 3.359333 -0.166964
O -0.785314 -1.166118 1.546598
C -4.335810 -0.755960 -2.100180
O -3.497989 -2.098421 1.310255
O 5.160900 -1.895968 -1.735118
H -2.097905 2.248904 -0.960116
H -3.187118 -2.334831 -1.179727
H -5.030296 -1.110898 0.444339
H -4.030141 1.083075 0.347068
H -3.311676 0.463050 1.836669
H 1.705735 1.796718 1.764791
H 1.225428 0.255676 2.489693
H 1.875721 -1.894270 1.420756
H 3.499378 -3.087909 -0.000826
H 4.792970 0.645381 -1.657409
H 3.157222 1.839054 -0.230265
H -5.248131 -1.353927 -2.141402
H -3.841168 -0.817046 -3.069823
H -4.611270 0.284882 -1.920544
H -2.536993 -2.001377 1.436874
H 5.138234 -2.852284 -1.603845

