ЖУРНАЛ СТРУКТУРНОЙ ХИМИИ

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SUPPLEMENTARY MATERIALS TO: SYNTHESIS, CHARACTERIZATION, CRYSTAL STRUCTURE, AND DFT STUDY OF N-(2-METHOXY-5-(4,4,5,5-TETRAMETHYL-1,3,2-DIOXABOROLAN-2-YL)PYRIDIN-3-YL)CYCLOPROPANESULFONAMIDE

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Contents:

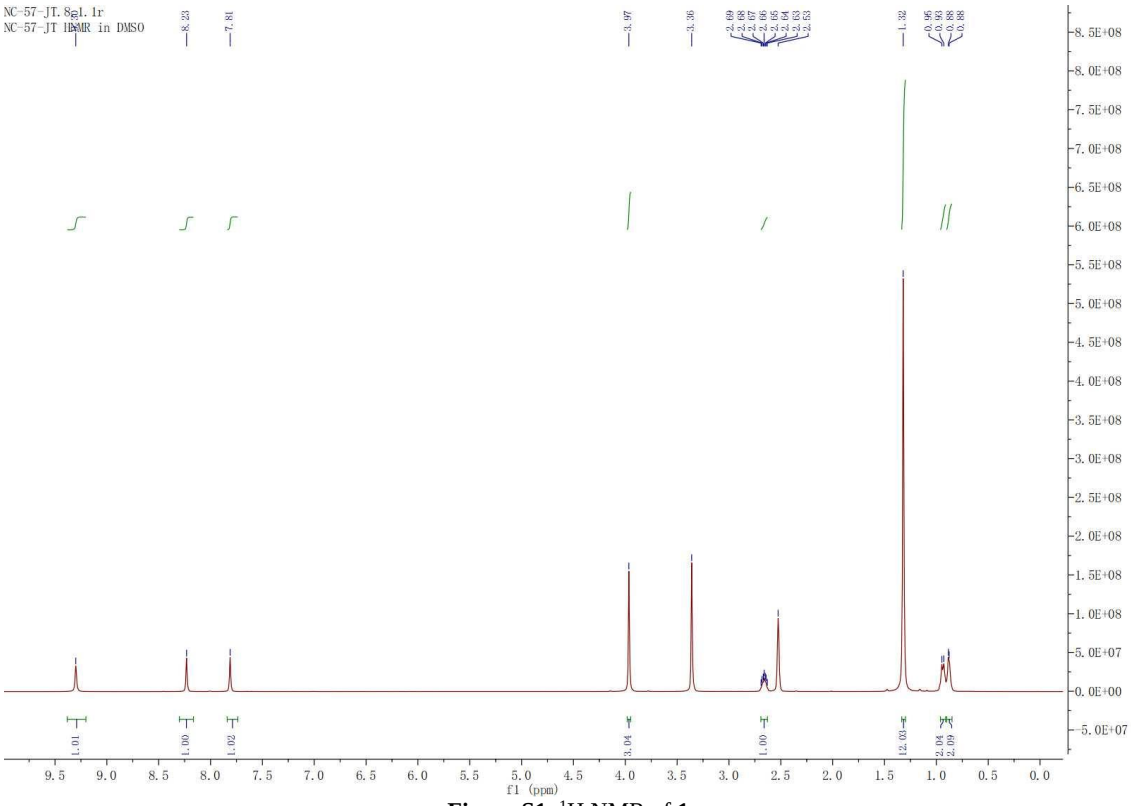

Figure S1. ^{1}H NMR of **1**.

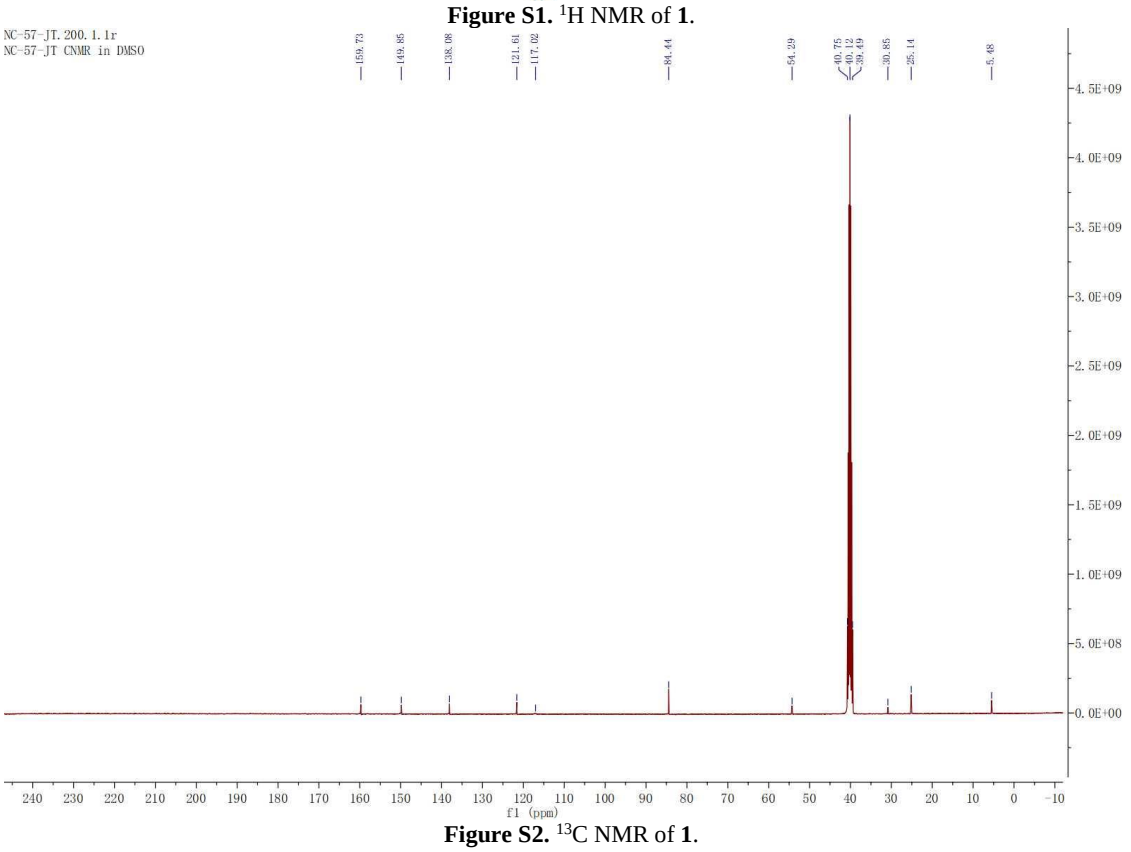

Figure S2. ^{13}C NMR of **1**.

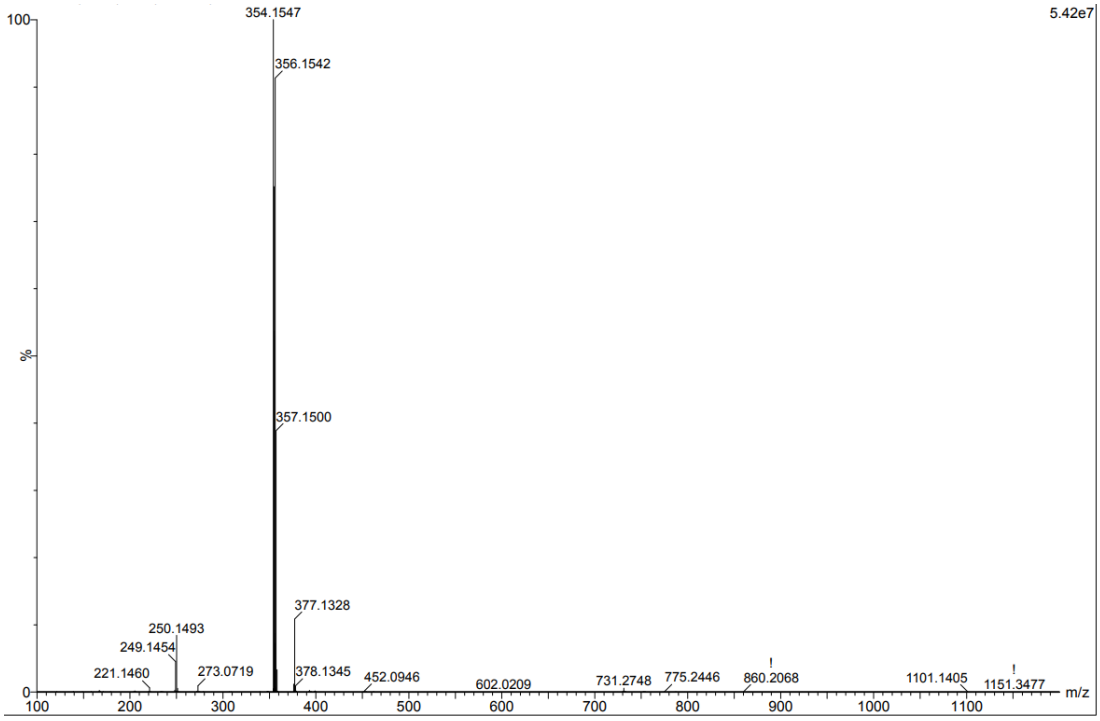

Figure S3. MS of **1**.

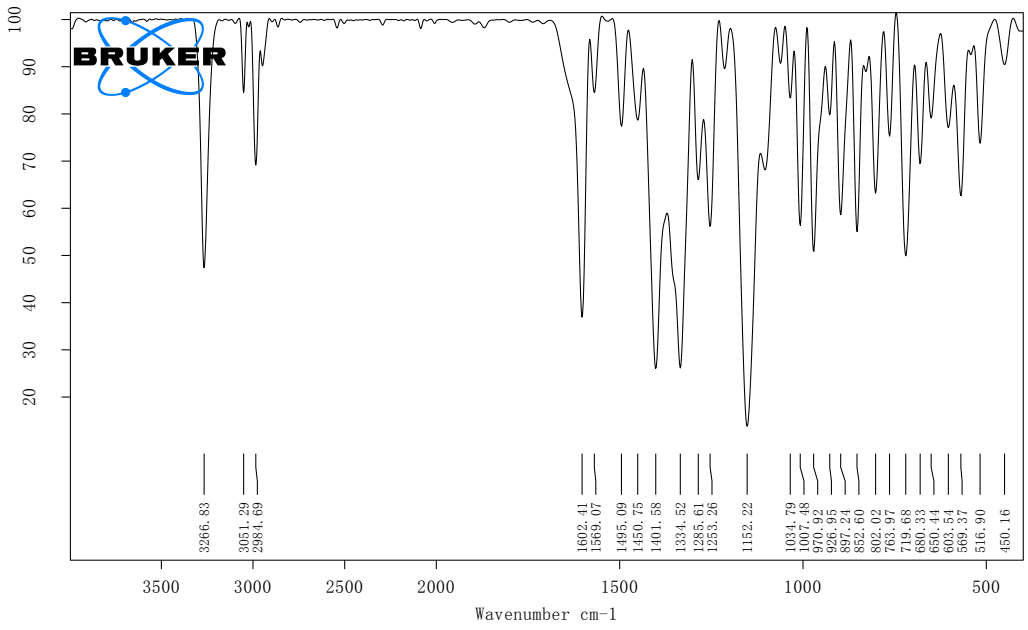

Figure S4. IR of **1**.

Table S1. Crystallographic characteristics, the X-ray data collection and structure-refinement parameters for **1**.

Compound	**1**
CCDC	2062825
Molecular formula	$C_{15}H_{23}B_2N_4O_{10}S$
Molecular weight	354.23
Crystal system	Orthorhombic
Space group	$Pca2_1$
a(Å)	19.5181(13)
b(Å)	9.2162(8)
c(Å)	19.7357(19)
α (°)	90
β (°)	90
γ (°)	90
V (Å^3)	3550.1(5)
Z	4
N(param)refined	483
μ (mm^{-1})	0.209
Radiation λ (Å)	0.71073
Ranges/indices (*h, k, l*)	$-21 \le h \le 24$, $-11 \le k \le 11$, $-24 \le l \le 19$
θ limit (°)	2.328 - 26.409
$N(hkl)_{measured}$, $N(hkl)_{unique}$	23302 / 6406 [R(int) = 0.0671]
$N(hkl)_{gt}$	4405
Diffractometer	Bruker D8 VENTURE
Scan mode	φ - ω
Programs	SHELXL-2014/7

Table S2. Bond distances, bond angles and torsion angles for compound **1** and conformer **1-1**.

Bond distance (Å)	**Exp.[a]**	**Calcd.[b]**	**Difference**
S(1)-O(4)	1.411(4)	1.45903	0.04803
S(1)-O(5)	1.420(4)	1.45762	0.03762
S(1)-N(2)	1.626(5)	1.69813	0.07213
S(1)-C(1)	1.745(7)	1.78459	0.03959
O(1)-C(11)	1.458(7)	1.45907	0.00107
O(1)-B(1)	1.353(7)	1.37167	0.01867
O(3)-C(5)	1.364(6)	1.35352	-0.01048
O(3)-C(4)	1.414(8)	1.43560	0.0216
O(2)-B(1)	1.344(8)	1.36986	0.02586
O(2)-C(10)	1.452(7)	1.45896	0.00696
N(1)-C(9)	1.320(8)	1.34214	0.02214
N(1)-C(5)	1.318(7)	1.31928	0.00128
N(2)-C(6)	1.437(6)	1.41771	-0.01929
C(8)-B(1)	1.571(9)	1.54564	-0.02536
Bond angle (°)	**Exp.[a]**	**Calcd.[b]**	**Difference**
O(4)-S(1)-O(5)	119.6(3)	121.94096	2.34096
O(4)-S(1)-N(2)	107.8(2)	107.28627	-0.51373
O(4)-S(1)-C(1)	108.5(3)	107.51871	-0.98129
O(5)-S(1)-N(2)	106.1(3)	104.79902	-1.30098
O(5)-S(1)-C(1)	108.3(3)	108.84225	0.54225
N(2)-S(1)-C(1)	105.6(3)	105.26401	-0.33599
B(1)-O(1)-C(11)	107.4(5)	107.29280	-0.1072
C(5)-O(3)-C(4)	117.5(5)	117.31965	-0.18035
B(1)-O(2)-C(10)	106.5(4)	107.38173	0.88173
C(5)-N(1)-C(9)	117.4(5)	117.68393	0.28393

C(6)-N(2)-S(1)	122.6(4)	119.40526	-3.19474
C(9)-C(8)-B(1)	121.2(5)	121.31134	0.11134
C(7)-C(8)-B(1)	121.8(5)	121.58109	-0.21891
N(1)-C(9)-C(8)	124.8(5)	123.98606	-0.81394
C(7)-C(6)-N(2)	122.2(5)	122.77798	0.57798
C(5)-C(6)-N(2)	120.2(5)	119.67015	-0.52985
O(3)-C(5)-C(6)	116.6(5)	115.97813	-0.62187
N(1)-C(5)-O(3)	120.0(5)	120.15579	0.15579
O(1)-C(11)-C(10)	102.1(4)	102.17521	0.07521
O(1)-C(11)-C(13)	109.2(5)	108.66320	-0.5368
O(1)-C(11)-C(12)	106.0(5)	106.67067	0.67067
C(3)-C(1)-S(1)	119.5(5)	119.43246	-0.06754
C(2)-C(1)-S(1)	118.8(6)	118.13173	-0.66827
O(1)-B(1)-C(8)	122.6(6)	123.58225	0.98225
O(2)-B(1)-O(1)	114.1(5)	113.21670	-0.8833
O(2)-B(1)-C(8)	123.3(5)	123.20102	-0.09898
O(2)-C(10)-C(11)	103.1(5)	102.11046	-0.98954
O(2)-C(10)-C(15)	105.5(5)	106.57820	1.0782
O(2)-C(10)-C(14)	110.7(5)	108.65676	-2.04324
Torsion angle (°)	**Exp.[a]**	**Calcd.[b]**	**Difference**
C(1)-C(2)-S(1)-O(4)	-30.4(6)	-38.44544	-8.04544
C(1)-C(2)-S(1)-O(5)	100.9(6)	94.90282	-5.99718
C(1)-C(3)-S(1)-O(4)	38.8(6)	31.18520	-7.6148
C(1)-C(3)-S(1)-O(5)	170.1(5)	164.53346	-5.56654
C(1)-C(2)-C(3)-S(1)	109.2(6)	106.81738	-2.38262
N(1)-C(5)-C(6)-C(7)	3.8(9)	0.88766	-2.91234
O(3)-C(4)-C(5)-C(6)	-178.8(6)	-177.56091	1.23909
N(1)-C(5)-O(3)-C(4)	-1.8(8)	-1.40869	0.39131
N(1)-C(5)-C(8)-C(9)	1.1(9)	-1.08036	-2.18036
C(6)-C(7)-C(8)-C(9)	-2.0(9)	1.34421	3.34421
N(1)-C(9)-C(8)-B(1)	179.8(5)	178.80886	-0.99114
C(8)-C(9)-B(1)-O(1)	-7.9(9)	-7.79469	0.10531
C(8)-C(9)-B(1)-O(2)	170.2(6)	178.22828	8.02828
C(8)-B(1)-O(1)-C(11)	173.6(5)	170.83586	-2.76414
C(8)-B(1)-O(2)-C(10)	168.9(6)	170.60874	1.70874

a: Experimental geometry parameters for compound **1**; b: Calculated geometry parameters for conformer **1-1**.

Table S3. Bond distances, bond angles and torsion angles for compound **1** and conformer **1-2**.

Bond distance (Å)	**Exp.[a]**	**Calcd.[b]**	**Difference**
S(2)-O(7)	1.426(4)	1.45903	0.03303
S(2)-O(8)	1.432(4)	1.45762	0.02562
S(2)-N(3)	1.635(4)	1.69813	0.06313
S(2)-C(18)	1.727(7)	1.78459	0.05759
O(8)-C(20)	1.345(6)	1.45907	0.11407
O(8)-C(19)	1.407(8)	1.37167	-0.03533
O(9)-C(26)	1.408(8)	1.35352	-0.05448
O(9)-B(2)	1.346(7)	1.43560	0.0896

N(3)-C(21)	1.435(6)	1.36986	-0.06514
O(10)-C(25)	1.465(8)	1.45896	-0.00604
O(10)-B(2)	1.336(9)	1.34214	0.00614
C(20)-N(4)	1.314(7)	1.31928	0.00528
N(4)-C(24)	1.382(8)	1.41771	0.03571
C(23)-B(2)	1.551(9)	1.54564	-0.00536
Bond angle (°)	**Exp.[a]**	**Calcd.[b]**	**Difference**
O(7)-S(2)-O(6)	119.4(3)	121.94099	2.54099
O(7)-S(2)-N(3)	108.7(3)	107.28635	-1.41365
O(7)-S(2)-C(18)	109.2(3)	107.53133	-1.66867
O(6)-S(2)-N(3)	104.8(3)	104.79915	-0.00085
O(6)-S(2)-C(18)	107.8(3)	108.84218	1.04218
N(3)-S(2)-C(18)	106.1(3)	105.26397	-0.83603
C(20)-O(8)-C(19)	117.6(4)	117.31963	-0.28037
B(2)-O(9)-C(26)	108.0(5)	107.29284	-0.70716
C(21)-N(3)-S(2)	119.7(4)	119.40534	-0.29466
B(2)-O(10)-C(25)	107.7(5)	107.38171	-0.31829
O(8)-C(20)-C(21)	117.9(4)	115.97803	-1.92197
N(4)-C(20)-O(8)	117.7(5)	120.15581	2.45581
N(4)-C(20)-C(21)	124.4(5)	123.86323	-0.53677
C(16)-C(18)-S(2)	118.8(5)	119.43248	0.63248
C(17)-C(18)-S(2)	118.5(6)	118.13176	-0.36824
C(20)-C(21)-N(3)	119.3(5)	119.67014	0.37014
C(20)-N(4)-C(24)	115.7(5)	117.68389	1.98389
C(23)-C(24)-N(4)	125.3(5)	123.98609	-1.31391
C(22)-C(23)-B(2)	122.9(5)	121.58112	-1.31888
C(24)-C(23)-B(2)	120.7(5)	121.31130	0.6113
O(10)-C(25)-C(26)	103.3(5)	102.11051	-1.18949
O(10)-C(25)-C(29)	98.7(8)	108.65670	9.9567
O(10)-C(25)-C(30)	110.7(7)	106.57817	-4.12183
O(9)-C(26)-C(25)	106.6(5)	102.17530	-4.4247
O(9)-C(26)-C(28)	100.3(7)	106.67080	6.3708
O(9)-C(26)-C(27)	110.8(7)	108.66309	-2.13691
O(9)-B(2)-C(23)	123.0(6)	123.58216	0.58216
O(10)-B(2)-O(9)	113.7(6)	113.21678	-0.48322
O(10)-B(2)-C(23)	123.3(5)	123.20104	-0.09896
Torsion angle (°)	**Exp.[a]**	**Calcd.[b]**	**Difference**
C(17)-C(18)-S(2)-O(6)	101.6(6)	101.92405	0.32405
C(16)-C(18)-S(2)-O(6)	169.0(5)	164.55200	-4.448
C(16)-C(18)-S(2)-O(7)	37.8(6)	37.20563	-0.59437
C(17)-C(18)-S(2)-O(7)	-29.5(6)	-28.42232	1.07768
C(16)-C(17)-C(18)-S(2)	-107.4(6)	-106.81539	0.58461
S(2)-N(3)-C(21)-C(22)	69.0(6)	66.02821	-2.97179
S(2)-N(3)-C(20)-C(21)	-112.8(5)	-112.15739	0.64261
N(4)-C(20)-C(21)-C(22)	2.5(8)	2.88917	0.38917
O(8)-C(19)-C(20)-C(21)	172.0(5)	177.54789	5.54789

N(4)-C(20)-O(8)-C(19)	-6.9(7)	-7.42396	-0.52396
C(21)-C(22)-C(23)-C(24)	-1.6(8)	-1.34600	0.254
N(4)-C(24)-C(23)-B(2)	-176.7(6)	-178.80849	-2.10849
C(23)-C(24)-B(2)-O(9)	-7.8(9)	-7.79752	0.00248
C(23)-C(24)-B(2)-O(10)	169.7(6)	178.21543	8.51543
C(23)-B(2)-O(9)-C(26)	175.0(6)	170.82936	-4.17064
C(23)-B(2)-O(10)-C(25)	179.8(6)	178.61615	-1.18385

a: Experimental geometry parameters for compound **1**; b: Calculated geometry parameters for conformer **1-2**.

Table S4. Cartesian Coordinates for conformer **1-1**, conformer **1-2** and conformer **1-3**.

Cartesian Coordinates

1-1

S	3.27518900	-1.43610700	-0.62265800
O	-3.25268900	1.11181800	0.37070000
O	2.13360600	-2.34025200	-0.72200500
O	3.02567000	2.60732900	-0.23452300
O	4.51314700	-1.67344700	-1.35563400
O	-2.47849900	-0.87701000	-0.45428900
N	0.78055200	2.81837200	0.29766400
N	2.76328600	0.08903400	-1.15432300
H	3.56452800	0.69292300	-1.30377300
C	-0.72229600	0.97122000	-0.10798700
C	-0.44112400	2.26366400	0.33464300
H	-1.23110200	2.89058100	0.73493700
C	0.35487200	0.22019700	-0.61742900
H	0.19926300	-0.78451600	-0.99008800
C	1.62926400	0.76202000	-0.63631400
C	1.77548500	2.08830800	-0.16620100
C	-4.37655900	0.18469300	0.47618000
C	3.68104900	-1.26906000	1.11354000
H	4.51477200	-0.59098300	1.24953100
C	-4.35650500	-0.76935500	-1.94574800
H	-4.07499800	0.22424300	-2.30075000
H	-5.43474300	-0.89144500	-2.07323900
H	-3.85071700	-1.50704600	-2.57194500
B	-2.16252400	0.39866000	-0.06293200
C	-3.93436600	-0.98612100	-0.48824200
C	-5.64827600	0.91972800	0.06570700
H	-5.84735900	1.72615000	0.77488300
H	-6.50695800	0.24235700	0.07375600
H	-5.55839300	1.35842800	-0.92763200
C	2.60246000	-1.36310100	2.16224500
H	1.58952000	-1.53234500	1.82159800
H	2.70032400	-0.70448500	3.01645600
C	-4.46181900	-0.23687200	1.94721000
H	-3.55418400	-0.75177300	2.26893500
H	-5.31599100	-0.89400800	2.12666400
H	-4.58018400	0.65645400	2.56398200
C	3.20403000	3.96981300	0.18343500
H	2.92990100	4.09043900	1.23248900
H	2.59378800	4.64098800	-0.42261400
H	4.26254800	4.17600500	0.03654200
C	3.57711600	-2.49430400	1.98783200
H	3.20241700	-3.40006500	1.52848900
H	4.36695000	-2.63434800	2.71509500
C	-4.32293600	-2.38813500	-0.03088900
H	-3.94392100	-3.12133500	-0.74602900
H	-5.41052400	-2.49304200	0.01760300
H	-3.90446300	-2.62428500	0.94703000

1-2

S	-3.27509800	-1.43616100	-0.62265500
O	-3.02562200	2.60711300	-0.23463900
O	-2.13330700	-2.34013000	-0.72116100
O	-4.51266800	-1.67392000	-1.35614900
O	3.25281200	1.11183800	0.37056200
N	-2.76315000	0.08883900	-1.15448600
H	-3.56435500	0.69281100	-1.30396200
O	2.47862100	-0.87709700	-0.45417400
C	-1.77541300	2.08815600	-0.16634100
C	-0.35472800	0.22010800	-0.61758600
H	-0.19907900	-0.78459900	-0.99024300
C	-3.68188800	-1.26880800	1.11323900
H	-4.51605700	-0.59120100	1.24870700
C	-1.62913700	0.76187000	-0.63646300
C	-2.60378700	-1.36196600	2.16254700
H	-1.59056300	-1.53065300	1.82251300
H	-2.70256600	-0.70316500	3.01650300
N	-0.78052600	2.81825300	0.29754700
C	0.44117100	2.26357300	0.33453600
H	1.23111400	2.89053900	0.73483200
C	0.72240700	0.97116400	-0.10809900
C	-3.20397300	3.96967700	0.18305900
H	-2.59300300	4.64064300	-0.42244700
H	-2.93074900	4.09027300	1.23236600
H	-4.26230300	4.17615200	0.03525300
C	3.93453200	-0.98622700	-0.48803800
C	-3.57768600	-2.49374700	1.98798100
H	-4.36782100	-2.63394200	2.71488300
H	-3.20232300	-3.39945300	1.52910700
C	4.37666300	0.18472100	0.47621000
B	2.16265100	0.39864000	-0.06304000
C	4.46197900	-0.23658800	1.94728100
H	4.58067700	0.65680100	2.56388000
H	5.31598600	-0.89391300	2.12676700
H	3.55427200	-0.75118200	2.26930700
C	4.35668400	-0.76982800	-1.94555700
H	3.85093600	-1.50769800	-2.57155100
H	5.43491200	-0.89194000	-2.07304500
H	4.07516100	0.22363700	-2.30089500
C	4.32300400	-2.38819400	-0.03040300
H	3.90482600	-2.62397000	0.94772900
H	5.41059000	-2.49336000	0.01770900
H	3.94355300	-3.12150900	-0.74518500
C	5.64837800	0.91975500	0.06561200
H	5.55869900	1.35772900	-0.92806500
H	6.50721600	0.24259100	0.07443800
H	5.84700800	1.72672000	0.77429000

1-3

C	-0.84002000	0.95429200	-0.10110800
C	-0.58895300	2.27787600	0.25670800
N	0.62232700	2.85326800	0.18700000
C	1.63238000	2.11644100	-0.22705200
C	1.51701700	0.75854900	-0.61166500
C	0.25380100	0.19195300	-0.55788500
B	-2.26850300	0.35651700	-0.02044400
N	2.67679300	0.09502200	-1.08054300
O	2.87287000	2.65452500	-0.32678600
C	3.02502100	4.04282800	0.00763700
S	3.12354100	-1.46518600	-0.59910800
C	3.31784900	-1.40565500	1.18128500

O	2.00359100	-2.35022300	-0.89221900
O	4.44174400	-1.66830700	-1.19350500
C	4.32025100	-2.33702700	1.81370700
C	4.58764400	-0.85604700	1.77351000
O	-3.37146500	1.07325500	0.37365100
C	-4.47675700	0.13295100	0.53789500
C	-4.01452200	-1.08417400	-0.35750400
O	-2.56102100	-0.94536800	-0.33578300
C	-4.54990300	-0.20329700	2.03157300
C	-5.76374200	0.81826500	0.09011000
C	-4.44540400	-0.96180300	-1.82304400
C	-4.37463700	-2.46361100	0.18417100
H	-1.39300200	2.91307100	0.61315000
H	0.11610000	-0.83671400	-0.86597800
H	3.49160700	0.69737000	-1.13229000
H	4.07988600	4.25954400	-0.14996300
H	2.40404900	4.66404000	-0.63940000
H	2.74578100	4.22165800	1.04697200
H	2.36758400	-1.23524300	1.67170200
H	4.02771700	-2.79982000	2.74794300
H	4.90734000	-2.95992000	1.15093800
H	5.35262800	-0.51849100	1.08518300
H	4.48931700	-0.27355600	2.68134300
H	-4.68006700	0.72241300	2.59591500
H	-5.39281700	-0.86238900	2.25251200
H	-3.63307500	-0.68474500	2.37816200
H	-6.60855400	0.12530900	0.13817700
H	-5.97835800	1.65908900	0.75338700
H	-5.68430300	1.20265400	-0.92643000
H	-3.92871000	-1.72612900	-2.40694400
H	-5.52184600	-1.10981400	-1.93771800
H	-4.18232600	0.01416200	-2.23615400
H	-5.45989600	-2.58584400	0.24364200
H	-3.98379400	-3.23114100	-0.48720000
H	-3.94915100	-2.63345600	1.17288200