Supporting Information

Induction of Cryptic Metabolites of the Endophytic Fungus *Trichocladium* sp. through OSMAC and Co-Cultivation

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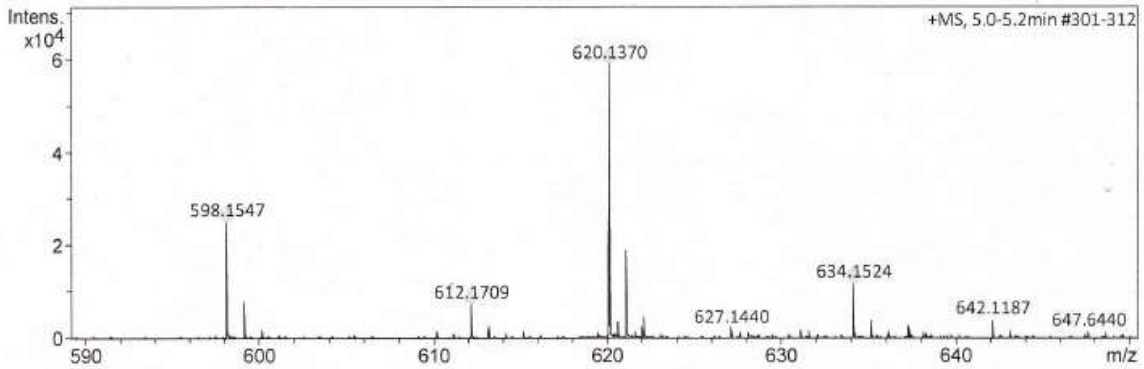
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	600.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e⁻ Conf	N-Rule
598.1547	1	C29H28NO13	598.1555	1.4	5.5	1	79.18	16.5	even	ok
	2	C28H25N5NaO9	598.1544	-0.4	7.9	2	100.00	18.5	even	ok
	3	C26H20N11O7	598.1542	-0.9	9.2	3	85.80	22.5	even	ok
	4	C29H21N9NaO5	598.1558	1.8	18.2	4	53.46	23.5	even	ok
	5	C27H16N15O3	598.1555	1.3	18.5	5	62.10	27.5	even	ok
	6	C42H20N3O2	598.1550	0.5	77.5	6	13.51	34.5	even	ok
612.1709	1	C30H30NO13	612.1712	0.4	101.9	1	100.00	16.5	even	ok
	2	C29H27N5NaO9	612.1701	-1.3	103.9	2	68.12	18.5	even	ok
	3	C30H23N9NaO5	612.1714	0.8	104.6	3	77.28	23.5	even	ok
	4	C27H22N11O7	612.1698	-1.8	105.2	4	54.64	22.5	even	ok
	5	C28H18N15O3	612.1712	0.4	105.9	5	82.58	27.5	even	ok
	6	C43H22N3O2	612.1707	-0.4	117.2	6	45.44	34.5	even	ok
620.1370	1	C29H27NNaO13	620.1375	0.8	2.1	1	89.08	16.5	even	ok
	2	C27H22N7O11	620.1372	0.3	2.8	2	100.00	20.5	even	ok
	3	C26H19N11NaO7	620.1361	-1.4	6.8	3	67.71	22.5	even	ok
	4	C24H14N17O5	620.1358	-1.8	8.8	4	55.64	26.5	even	ok
	5	C26H26N3O15	620.1358	-1.8	10.3	5	54.47	15.5	even	ok
	6	C27H15N15NaO3	620.1375	0.8	15.8	6	69.74	27.5	even	ok
	7	C25H10N21O	620.1372	0.3	16.4	7	78.09	31.5	even	ok
	8	C40H14N9	620.1367	-0.5	74.4	8	13.70	38.5	even	ok
	9	C42H19N3NaO2	620.1369	-0.0	75.4	9	14.85	34.5	even	ok

Figure S1. The HRESIMS of compound **1**

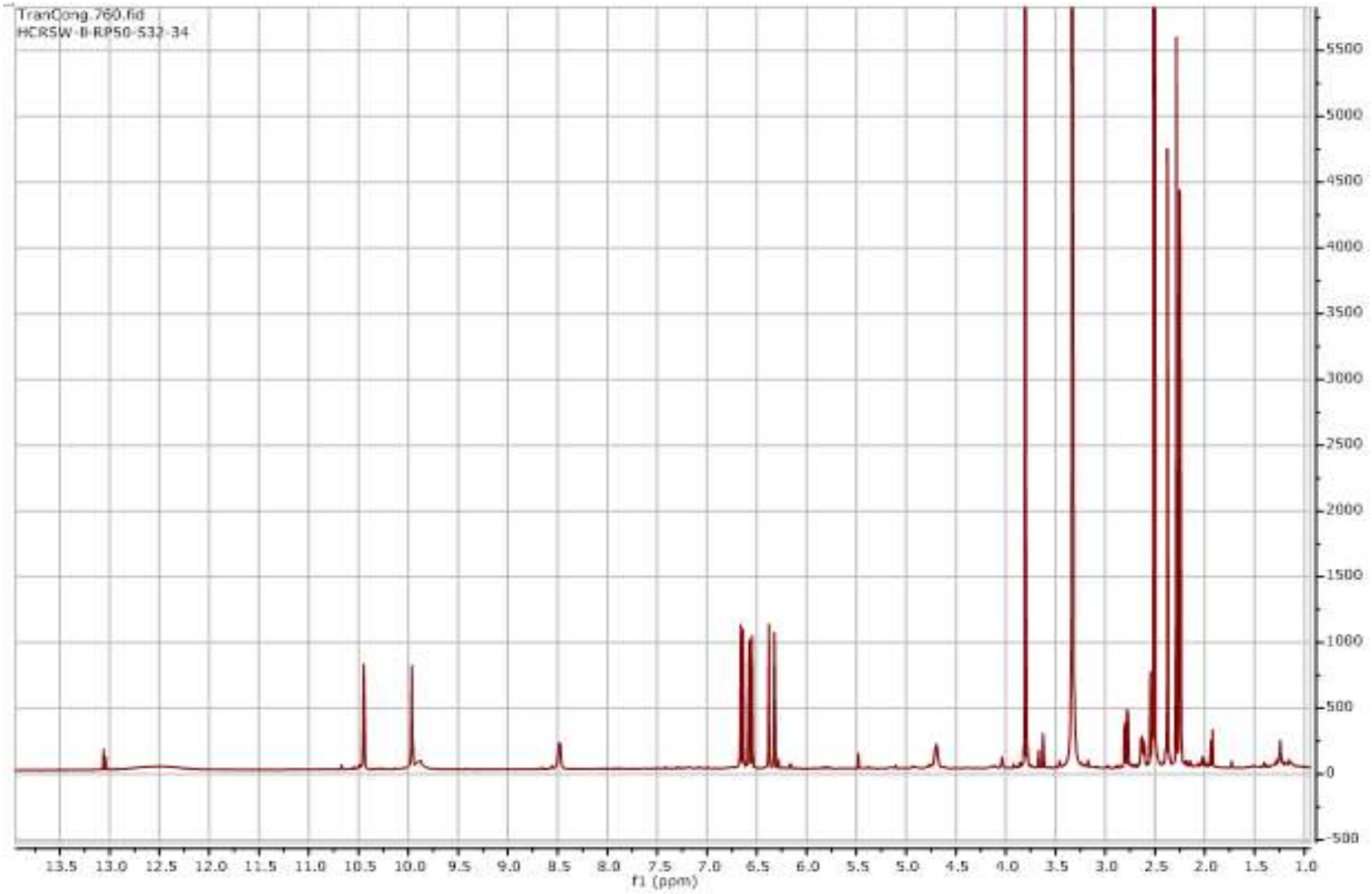


Figure S2. The ^{1}H NMR (600 MHz, DMSO-d_6) spectrum of compound **1**

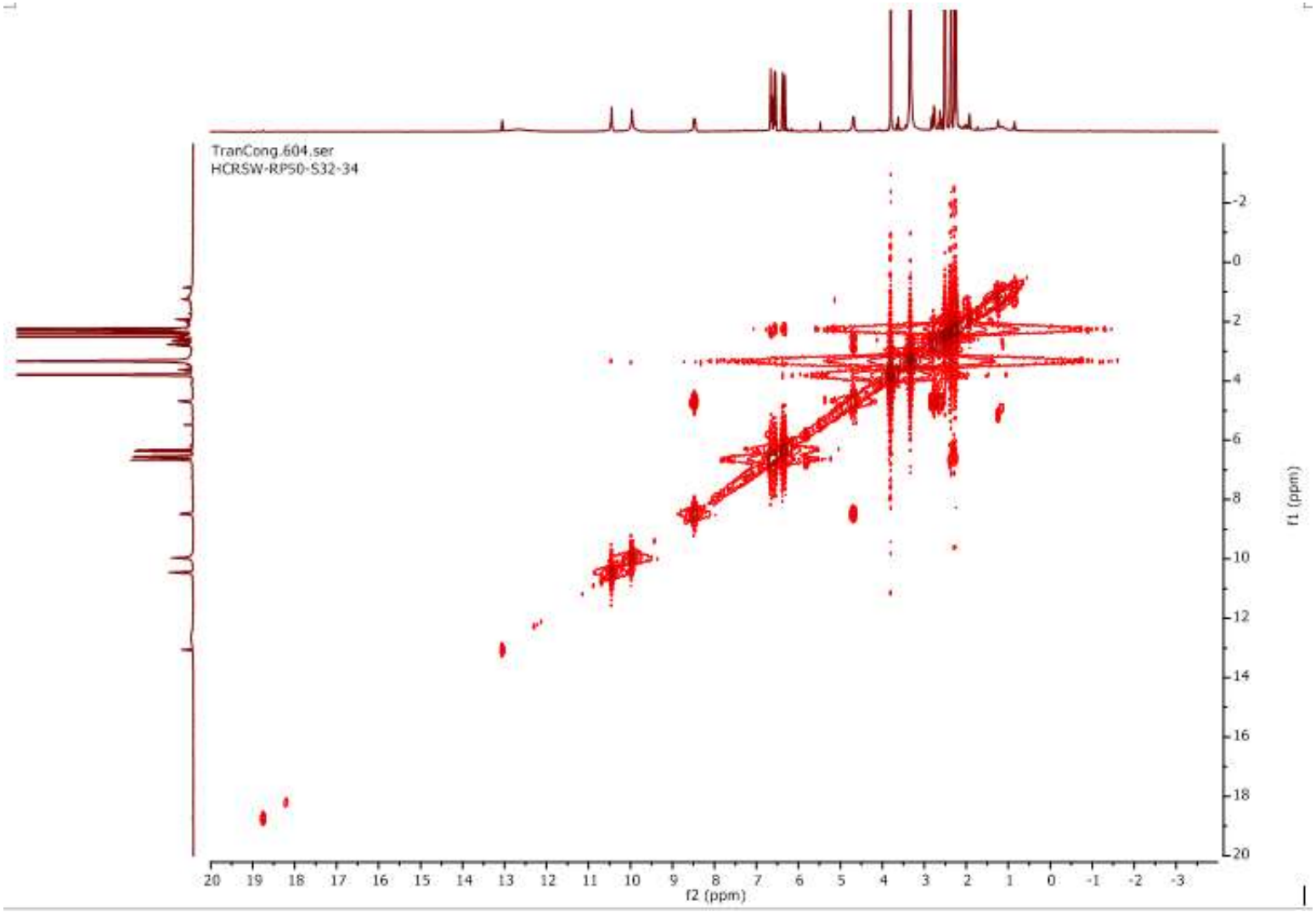


Figure S3. The COSY (300 MHz, DMSO-d_6) spectrum of compound **1**

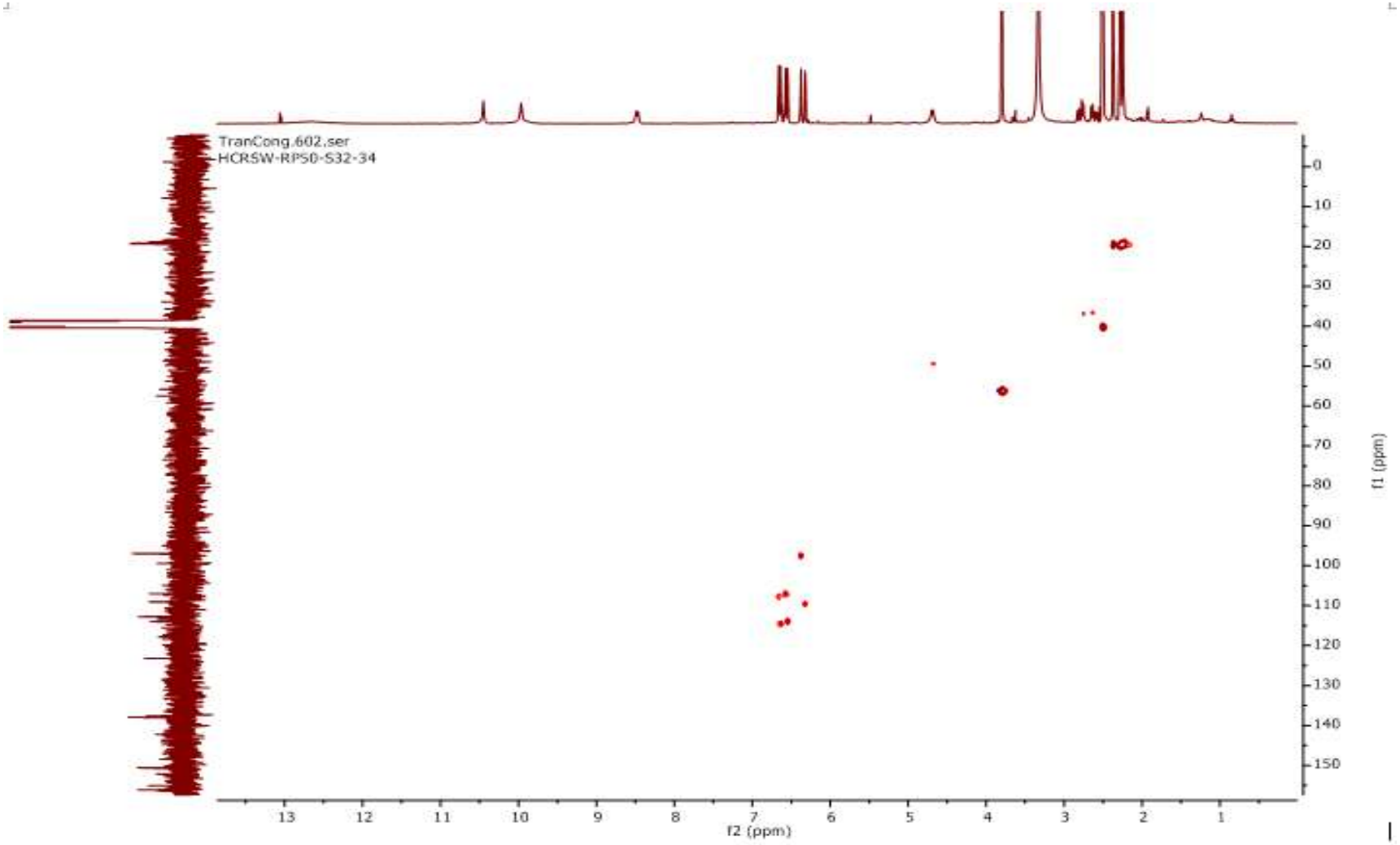


Figure S4. The HSQC (300 MHz, DMSO-d_6) spectrum of compound **1**

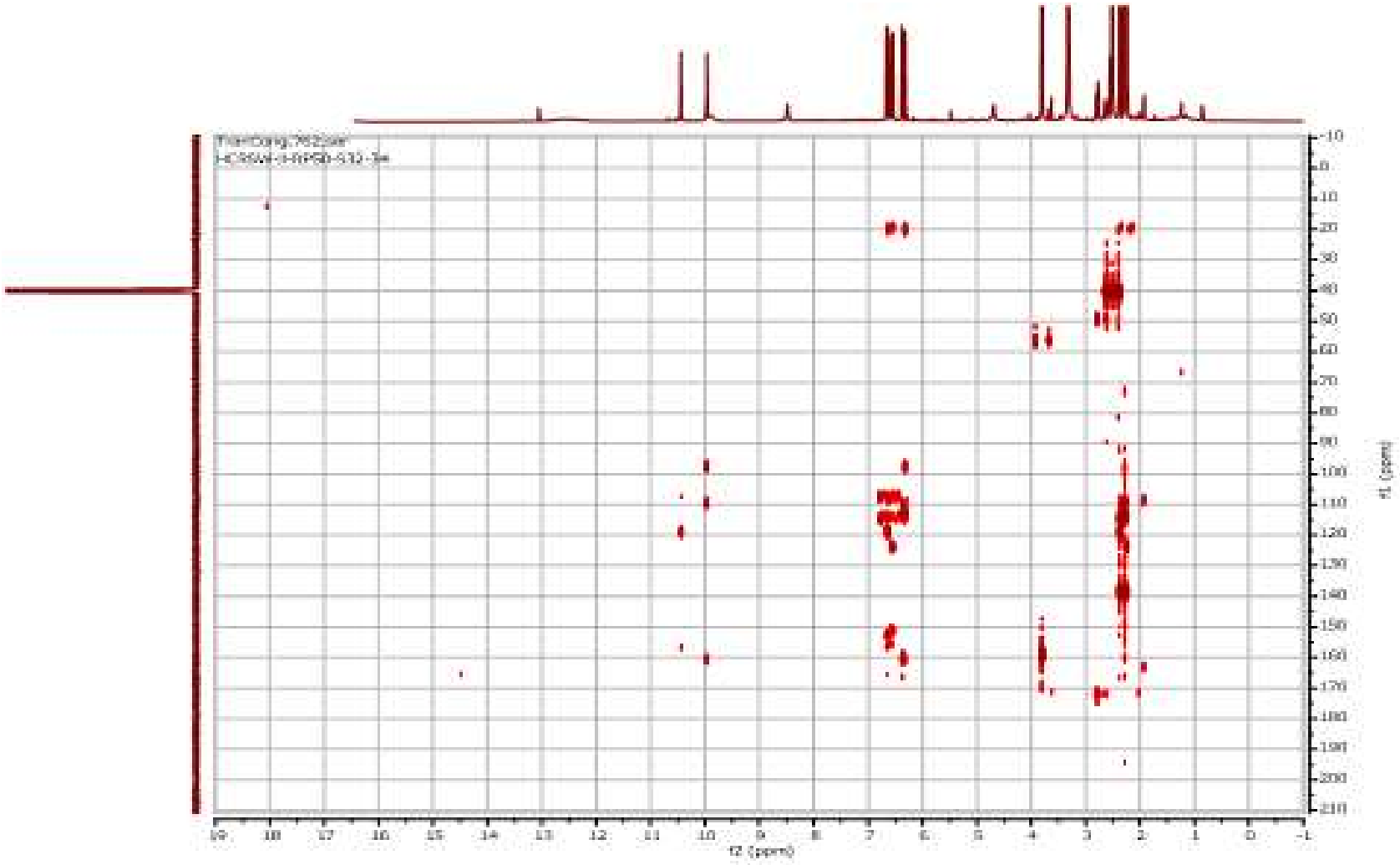


Figure S5. The HMBC (600MHz, DMSO-d_6) spectrum of compound **1**

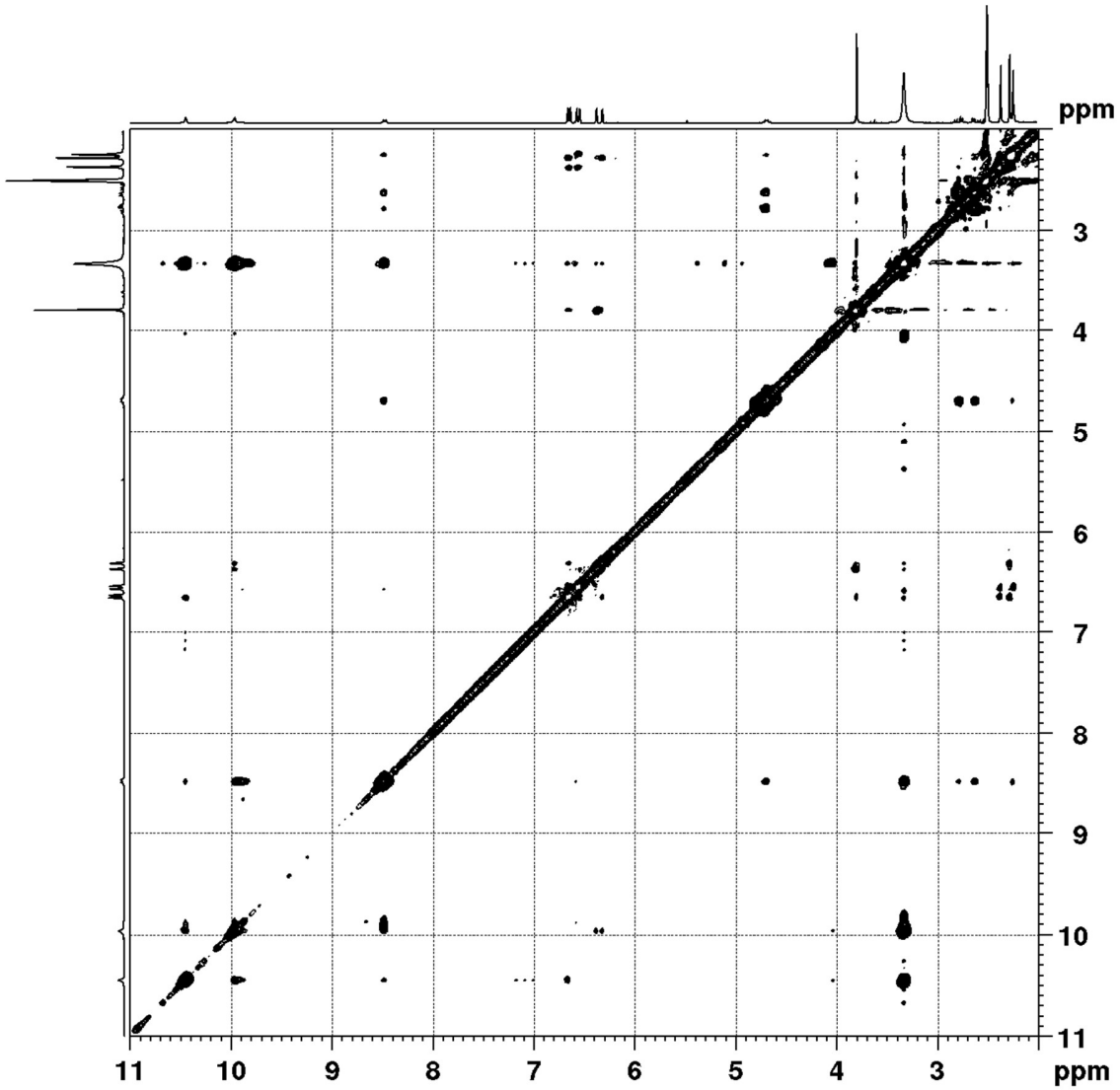


Figure S6. The ROESY (600MHz, DMSO-d_6) spectrum of compound **1**

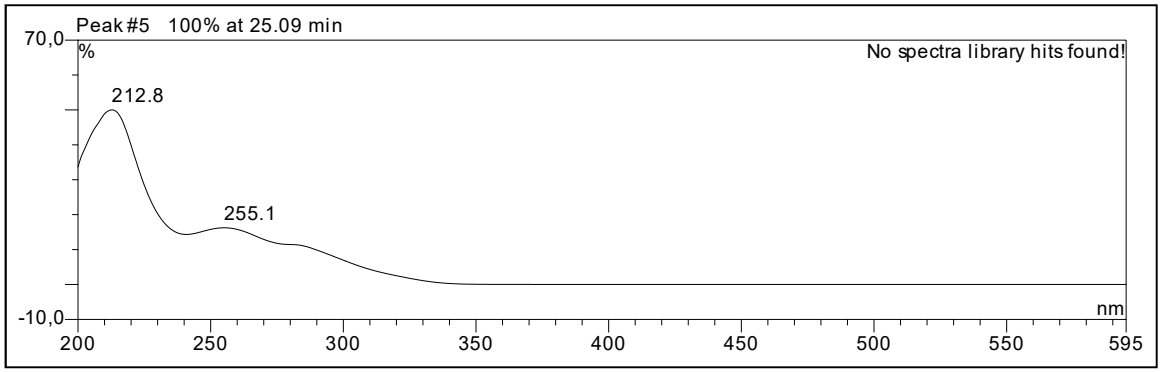


Figure S7. The UV spectrum of compound **1**

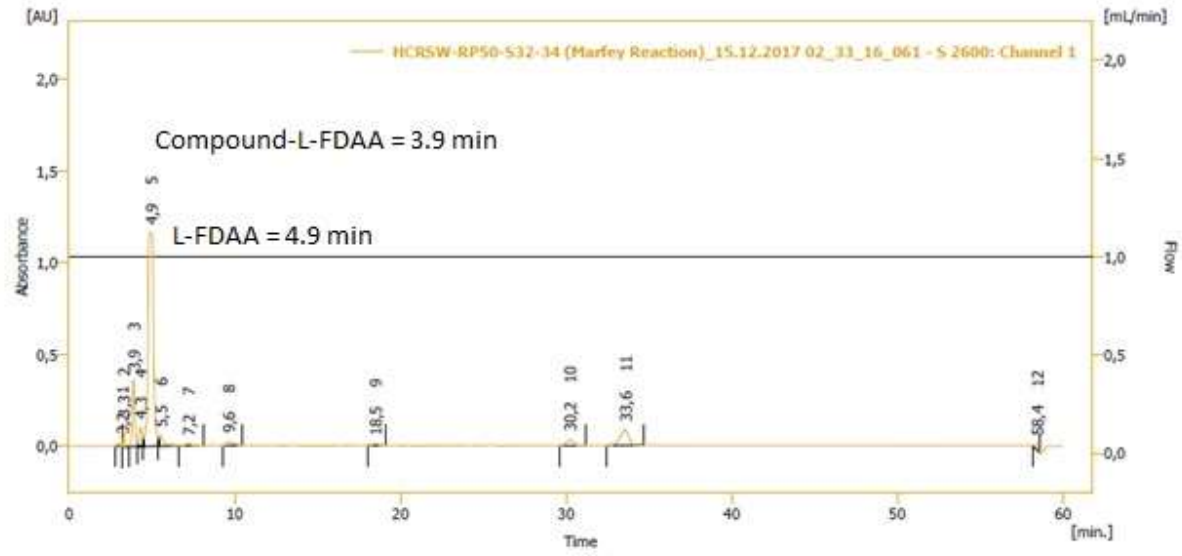


Figure S8. The HPLC chromatogram of compound **1** with L-FDAA for Marfey's method

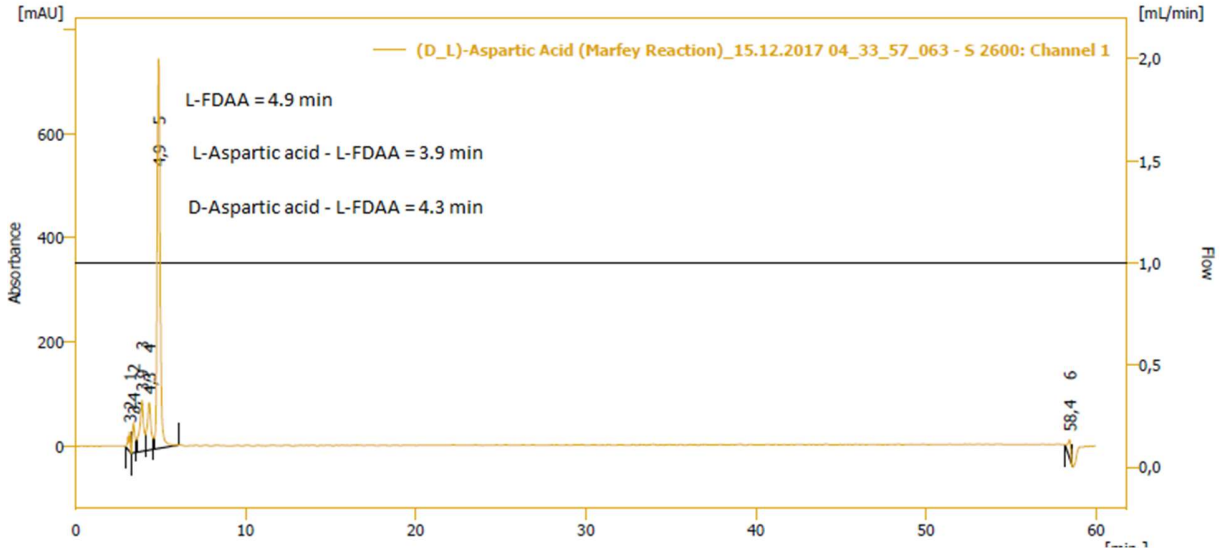


Figure S9. The HPLC chromatogram of DL-aspartic acid with L-FDAA for Marfey's method

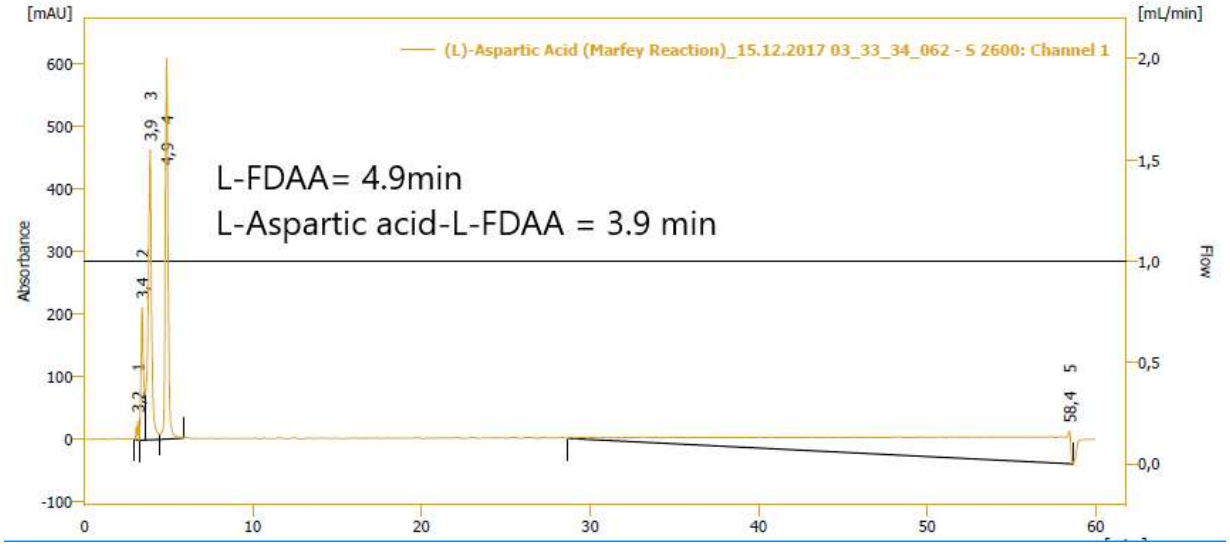


Figure S10. The HPLC chromatogram of L-aspartic acid with L-FDAA for Marfey's method

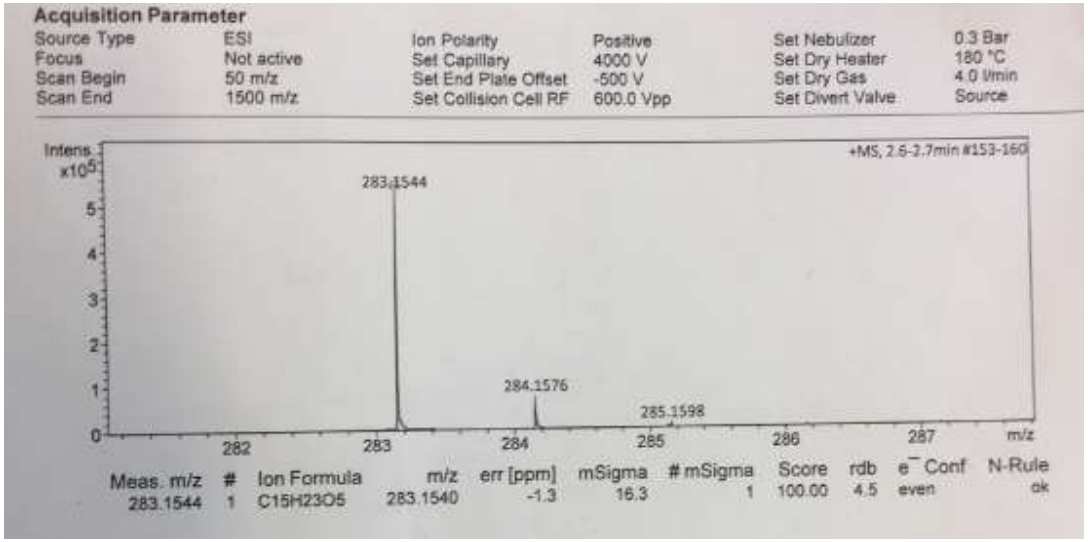


Figure S11. The HRESIMS of compound **2**

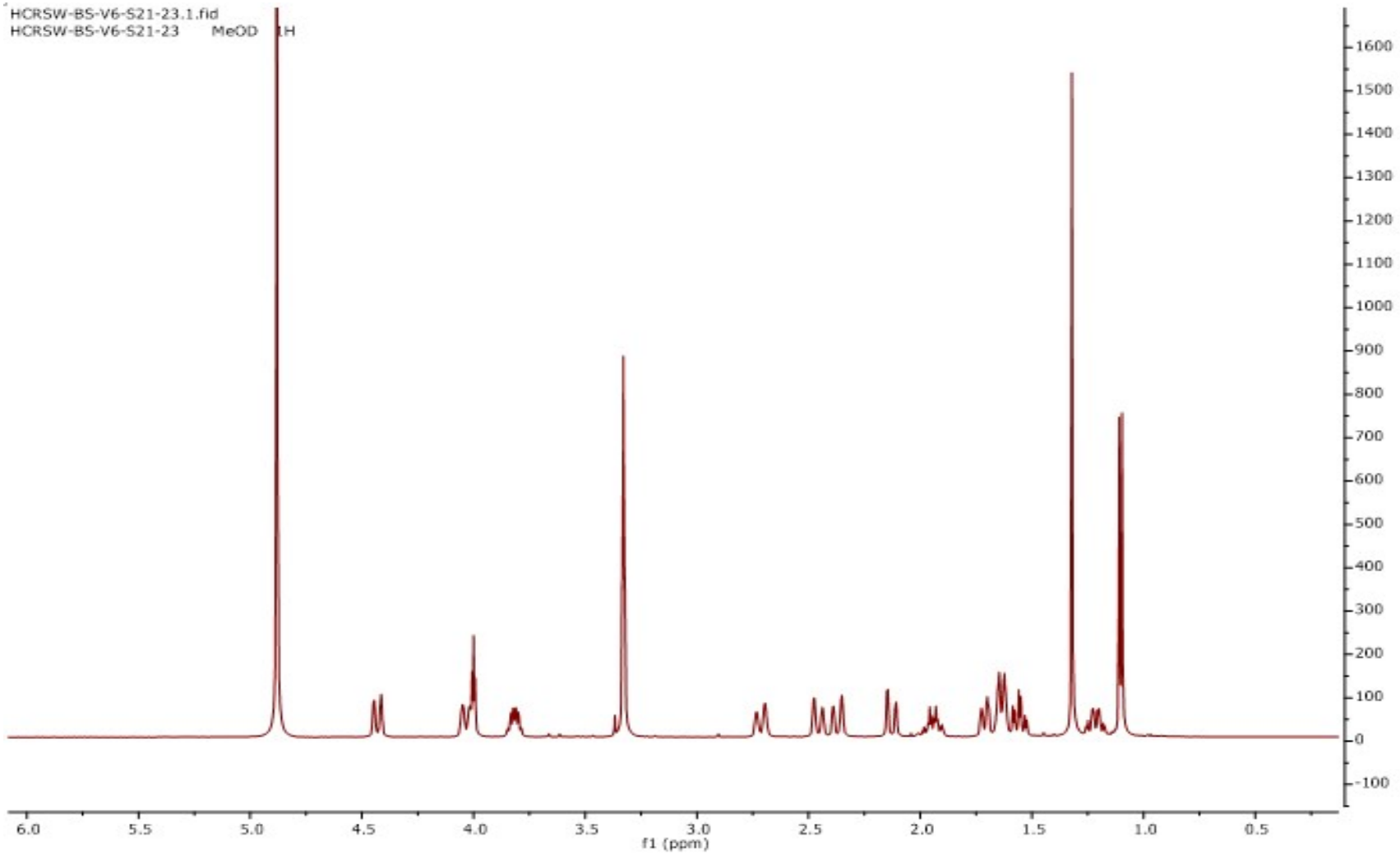


Figure S12. The ^{1}H NMR (500 MHz, CD_3OD) spectrum of compound **2**

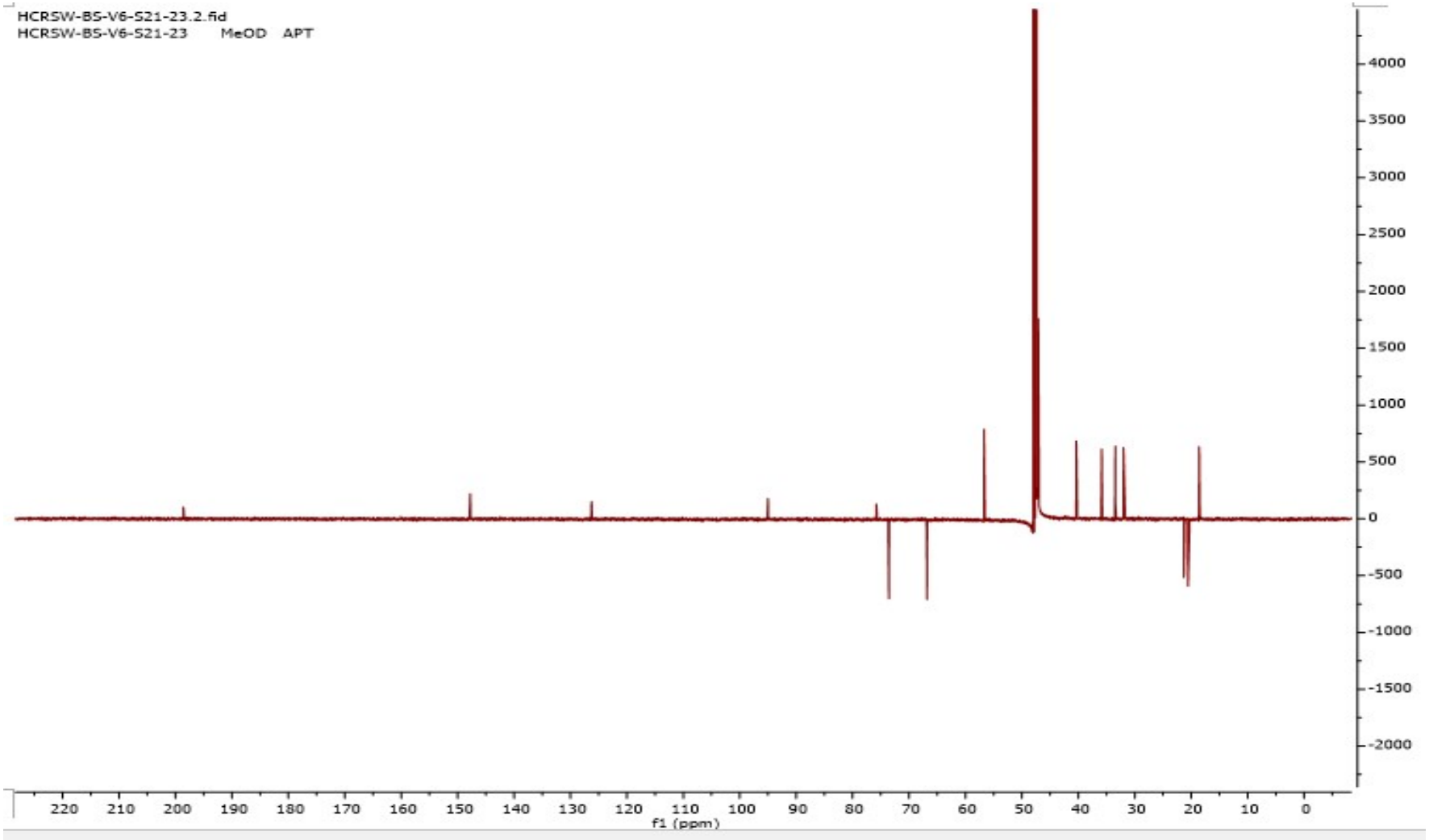


Figure S13. The ^{13}C NMR (125 MHz, CD_3OD) spectrum of compound **2**

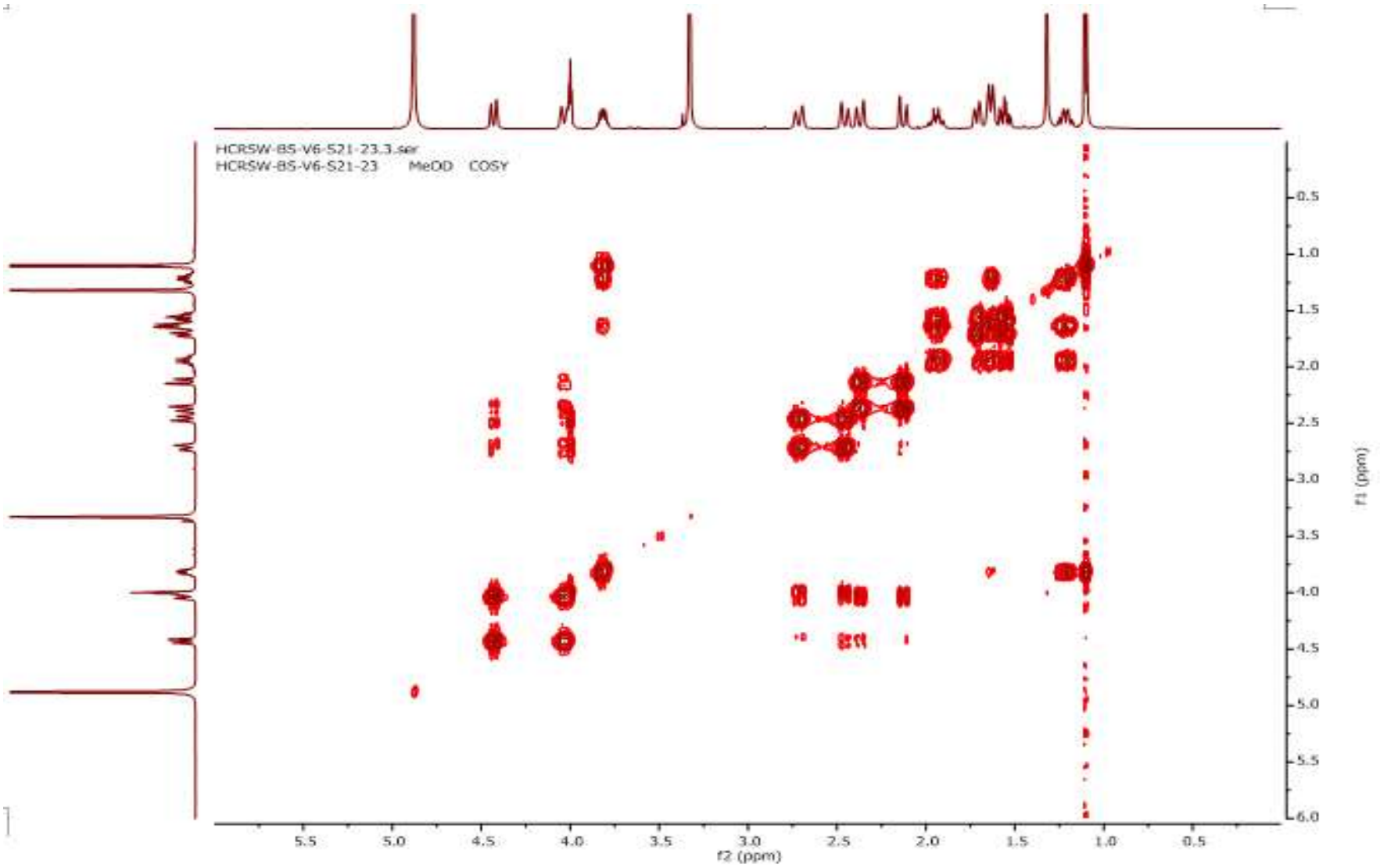


Figure S14. The COSY (500 MHz, CD_3OD) spectrum of compound **2**

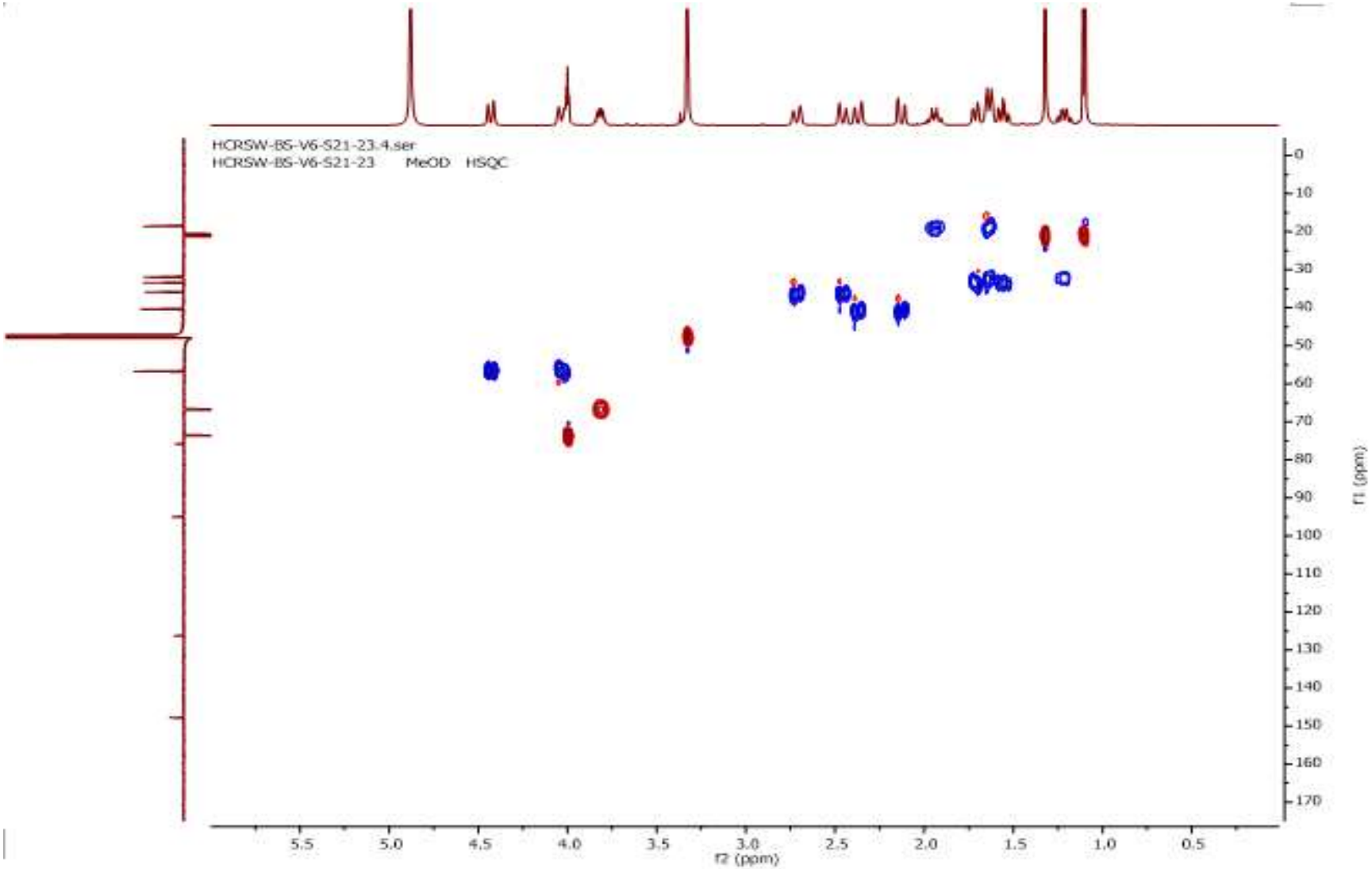


Figure S15. The HSQC (500 MHz, CD_3OD) spectrum of compound **2**

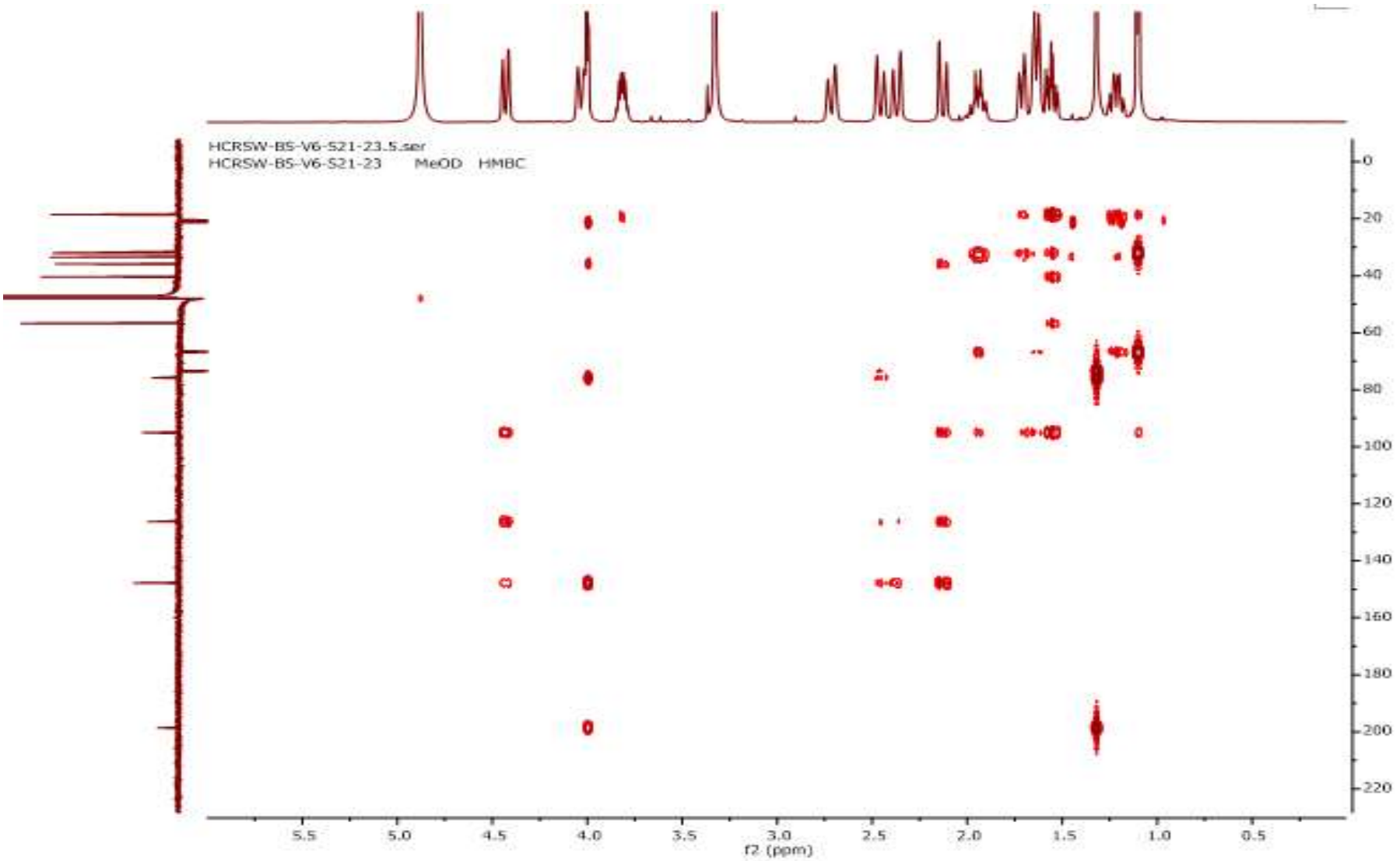


Figure S16. The HMBC (500 MHz, CD_3OD) spectrum of compound **2**

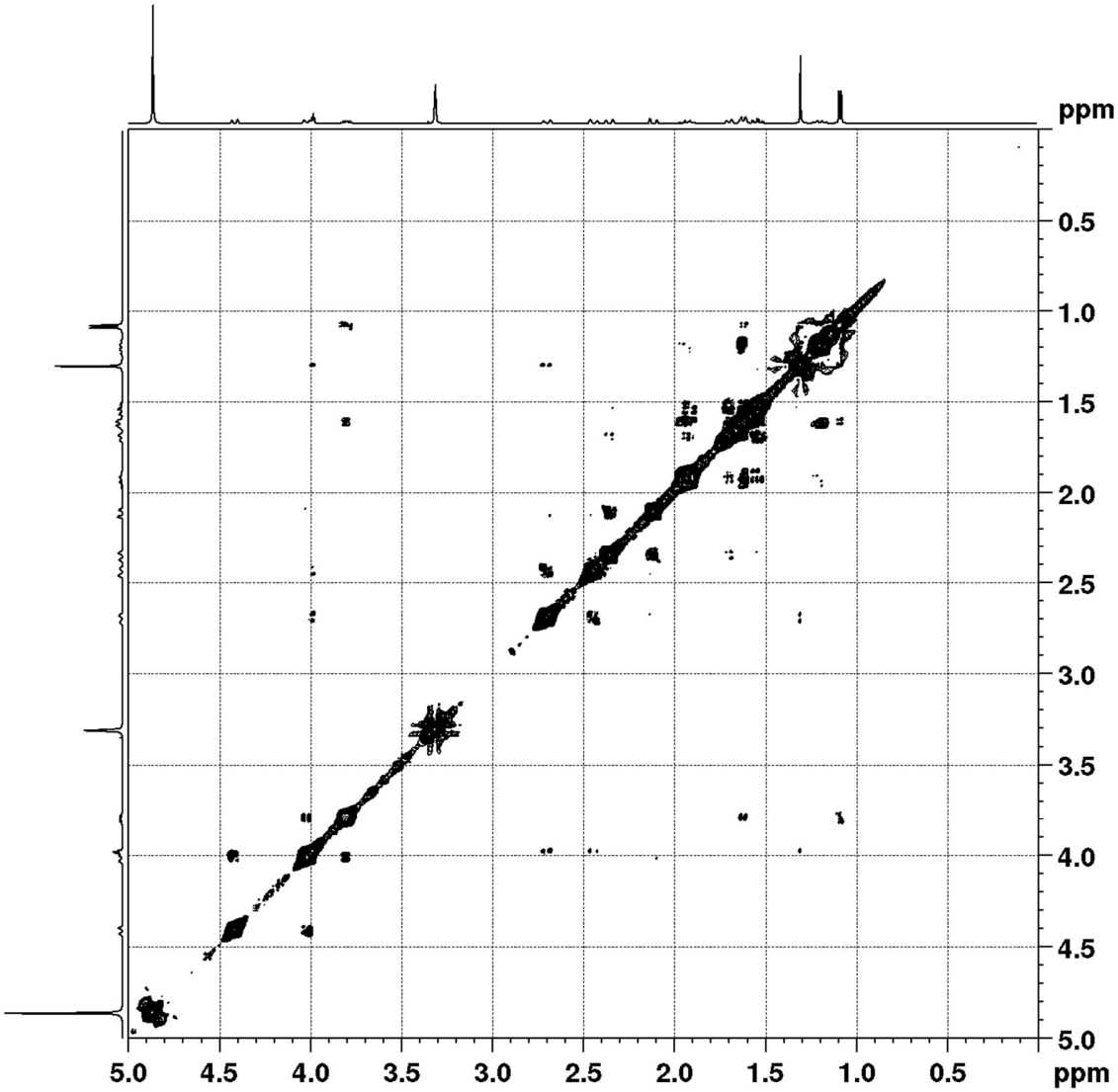


Figure S17. The ROESY (500 MHz, CD_3OD) spectrum of compound **2**

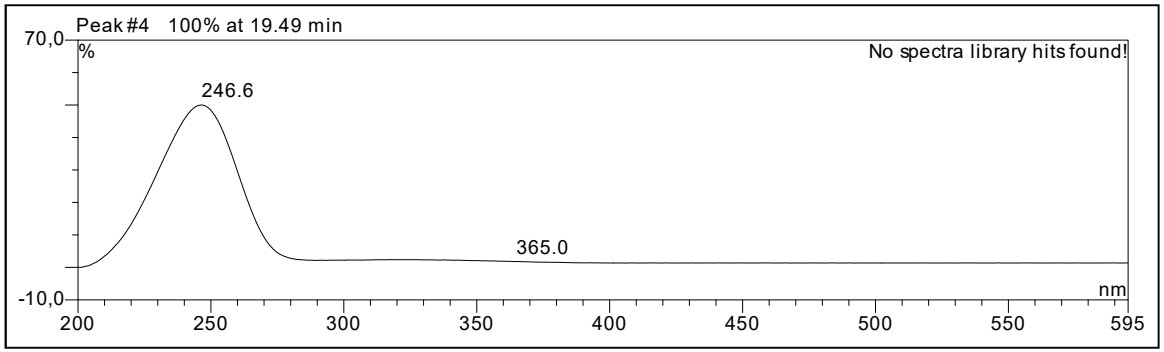


Figure S18. The UV spectrum of compound **2**

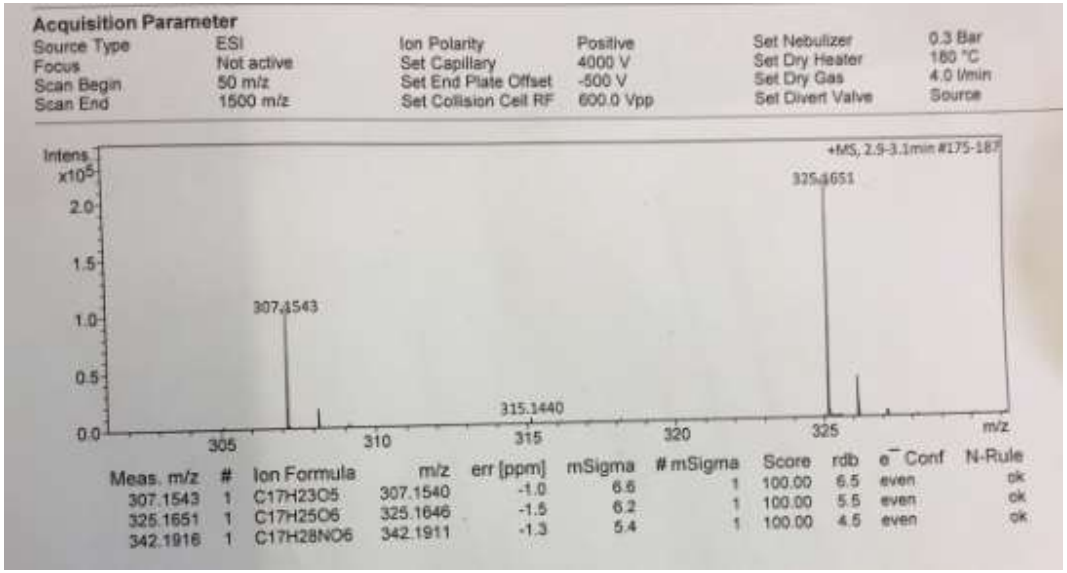


Figure S19. The HRESIMS of compound **3**

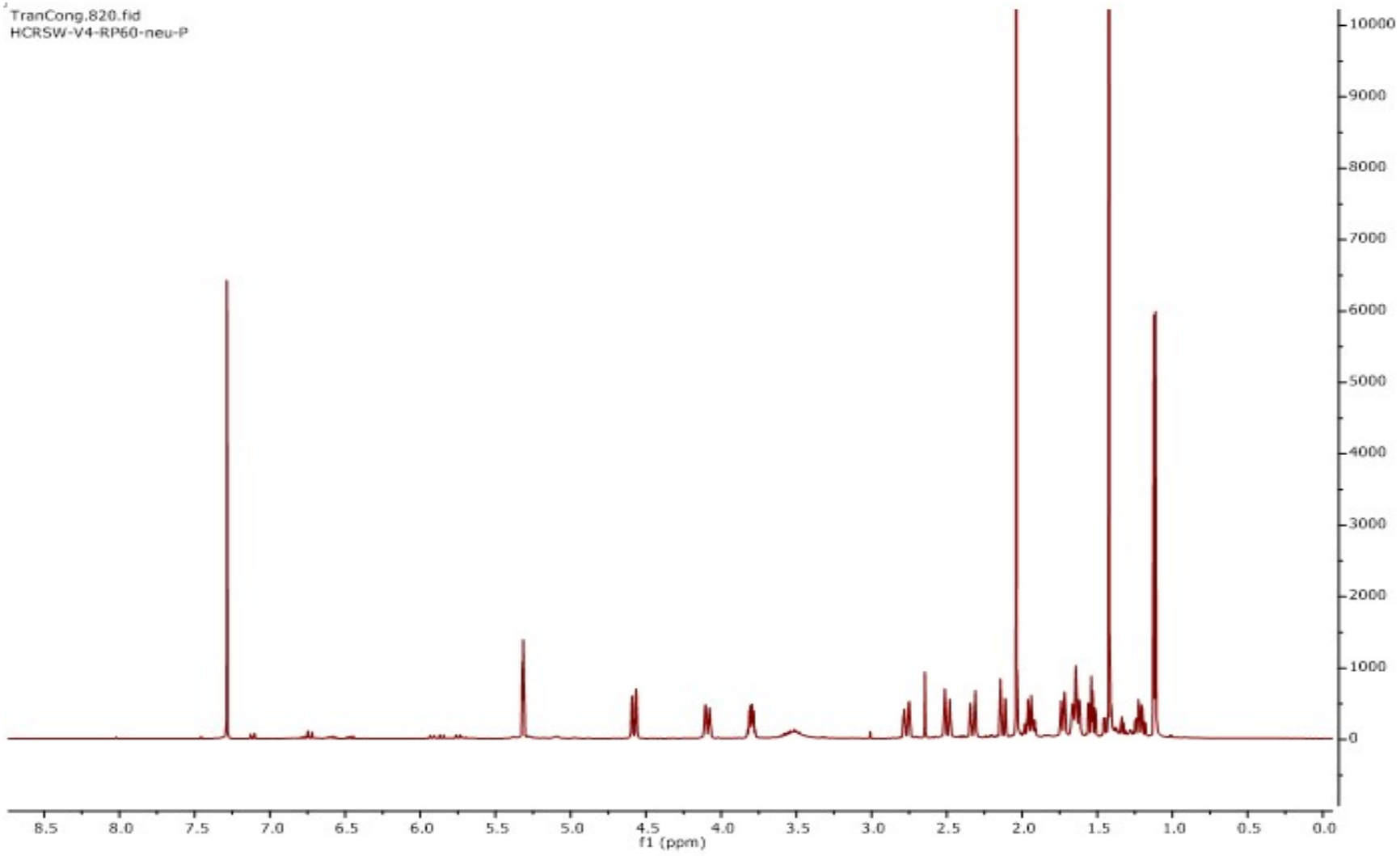


Figure S20. The ^{1}H NMR (600 MHz, $CDCl_3$) spectrum of compound **3**

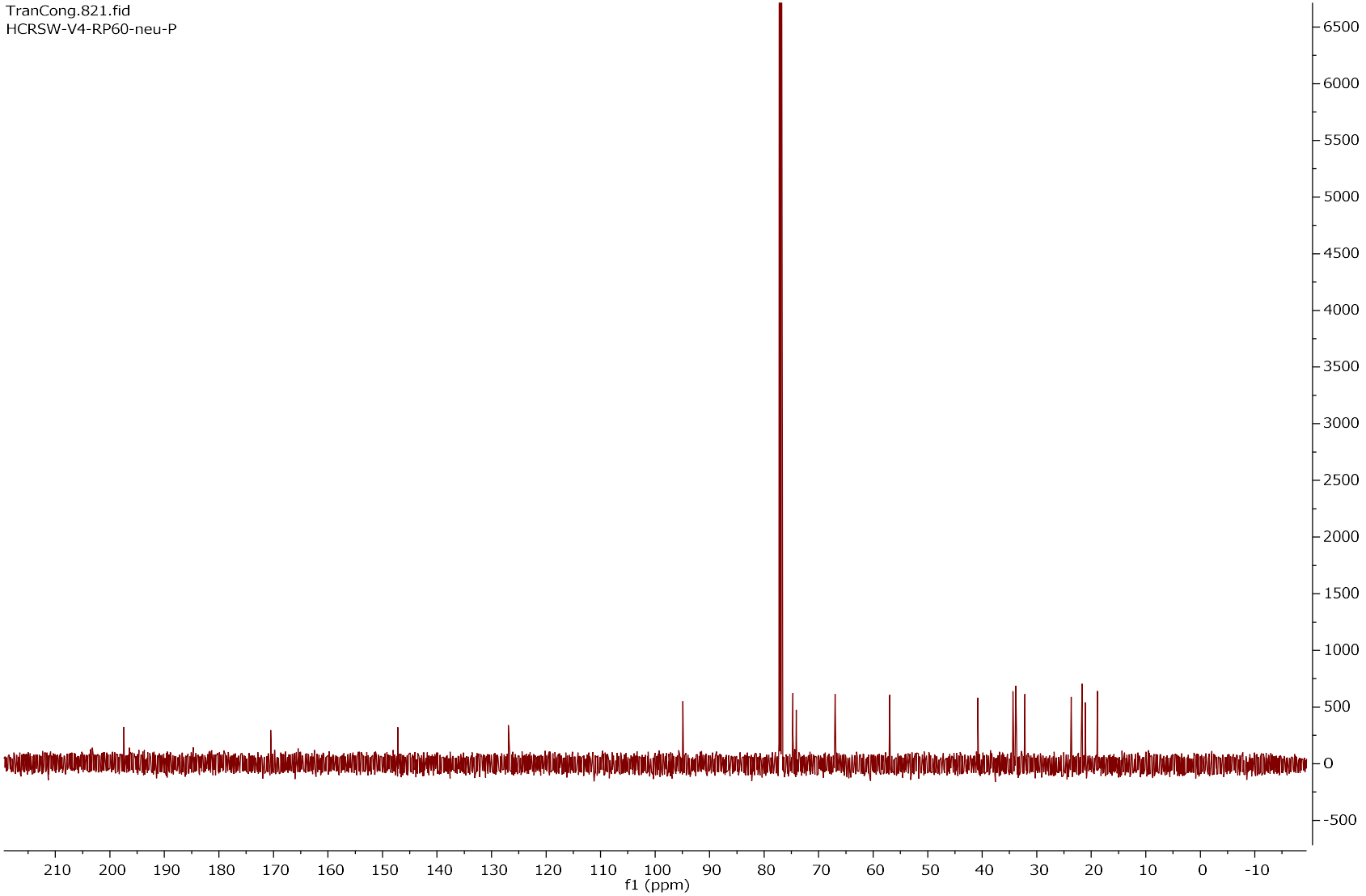


Figure S21. The ^{13}C NMR (150 MHz, $CDCl_3$) spectrum of compound **3**

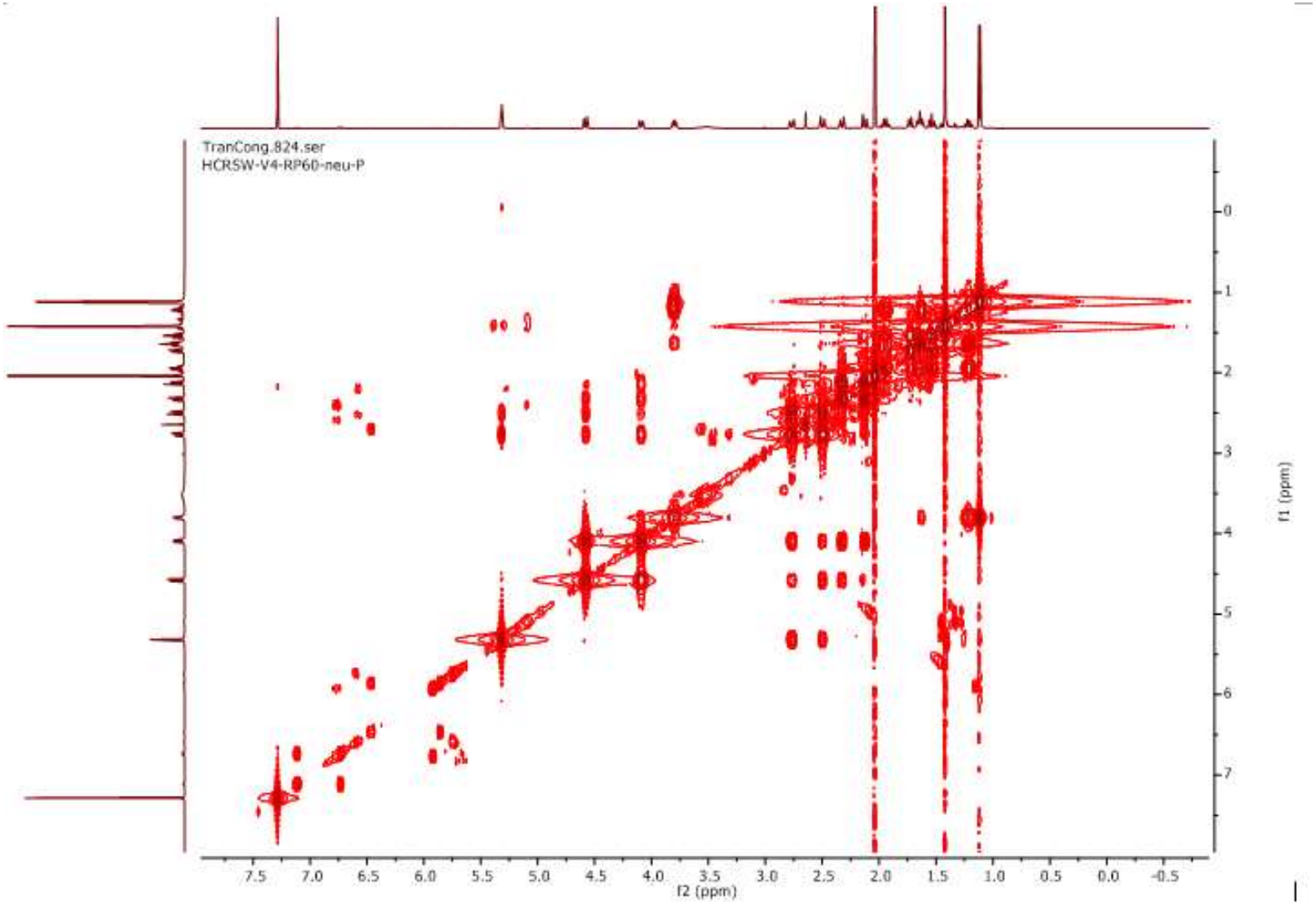


Figure S22. The COSY (600 MHz, $CDCl_3$) spectrum of compound **3**

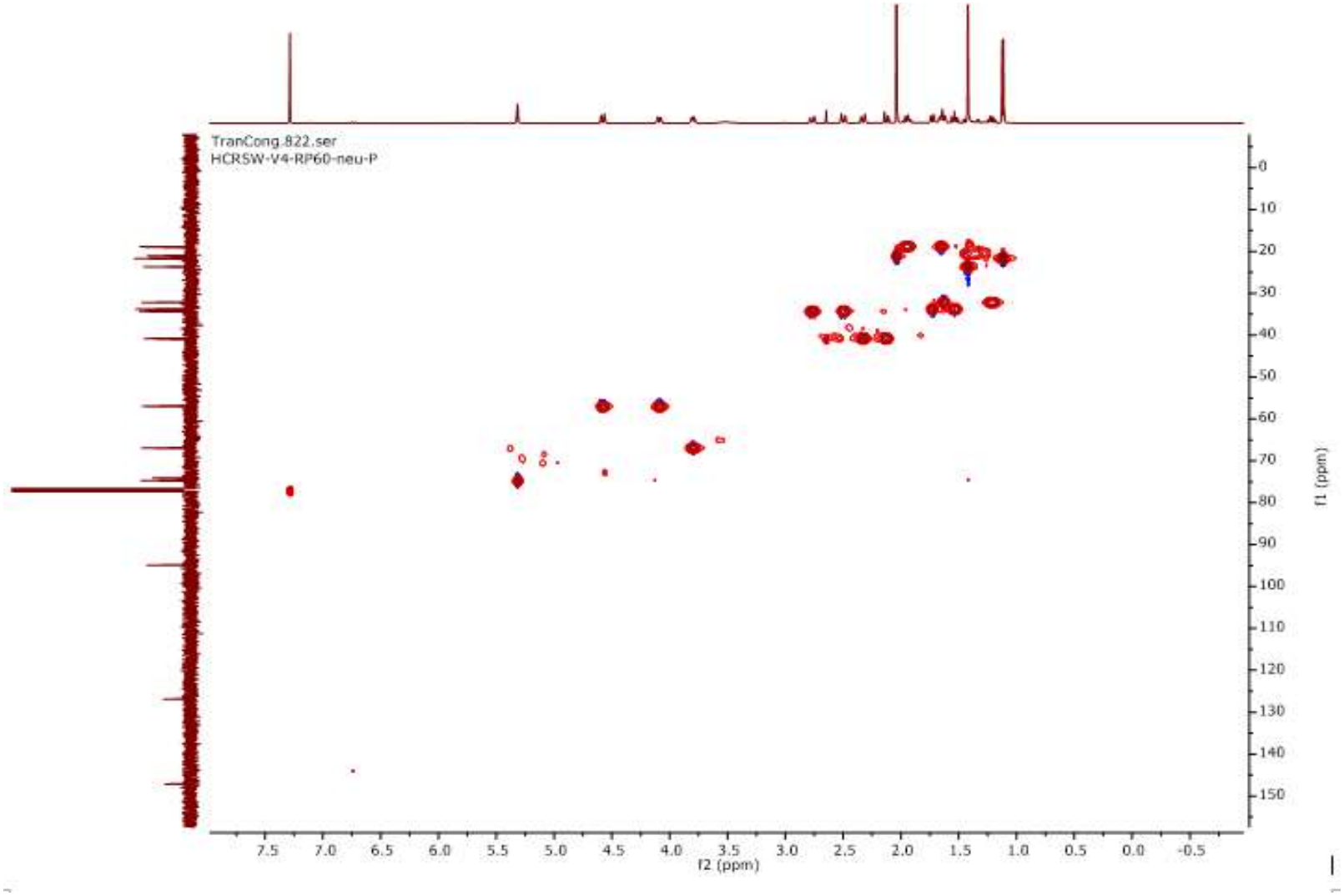


Figure S23. The HSQC (600 MHz, $CDCl_3$) spectrum of compound **3**

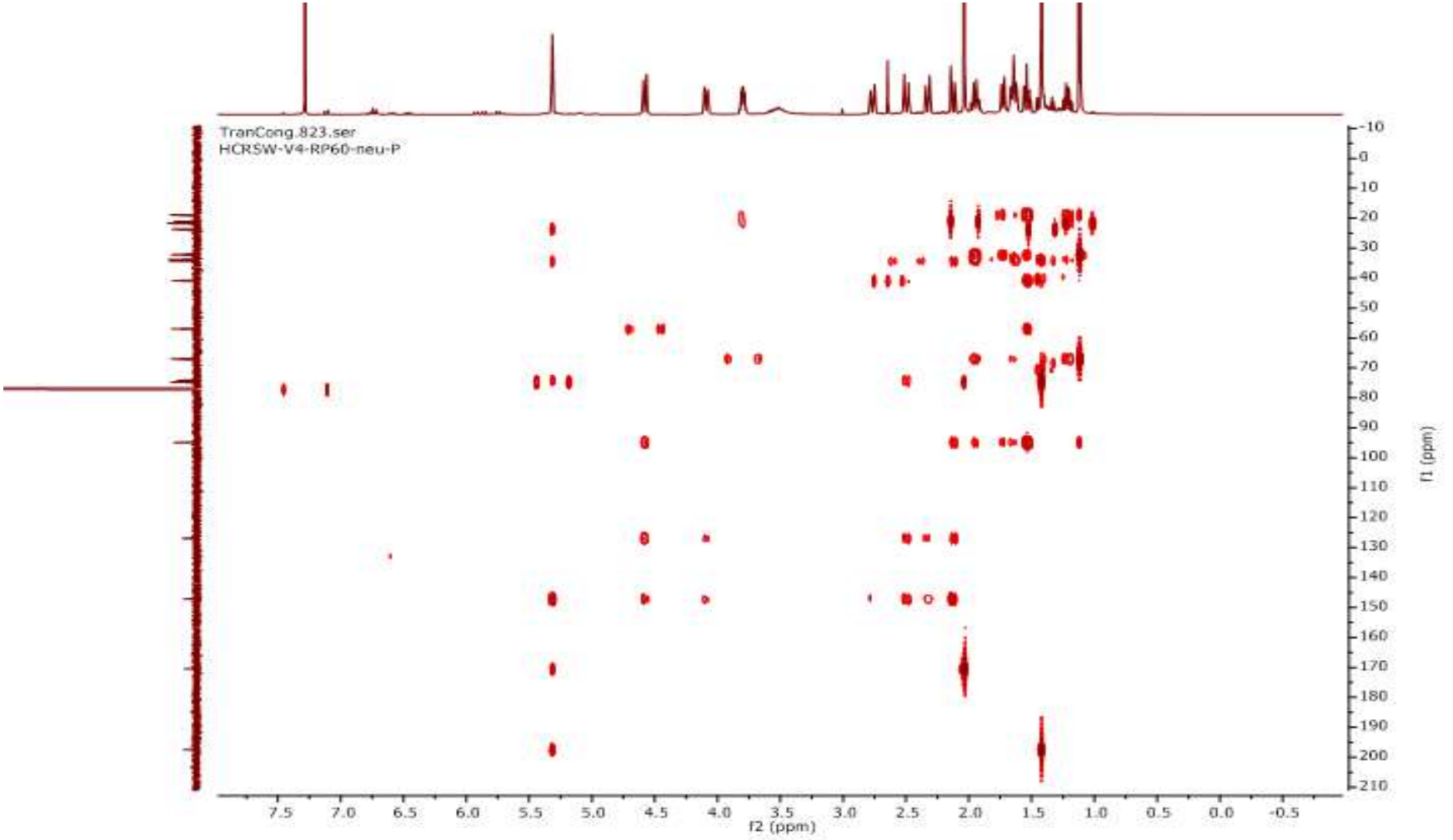


Figure S24. The HMBC (600 MHz, $CDCl_3$) spectrum of compound **3**

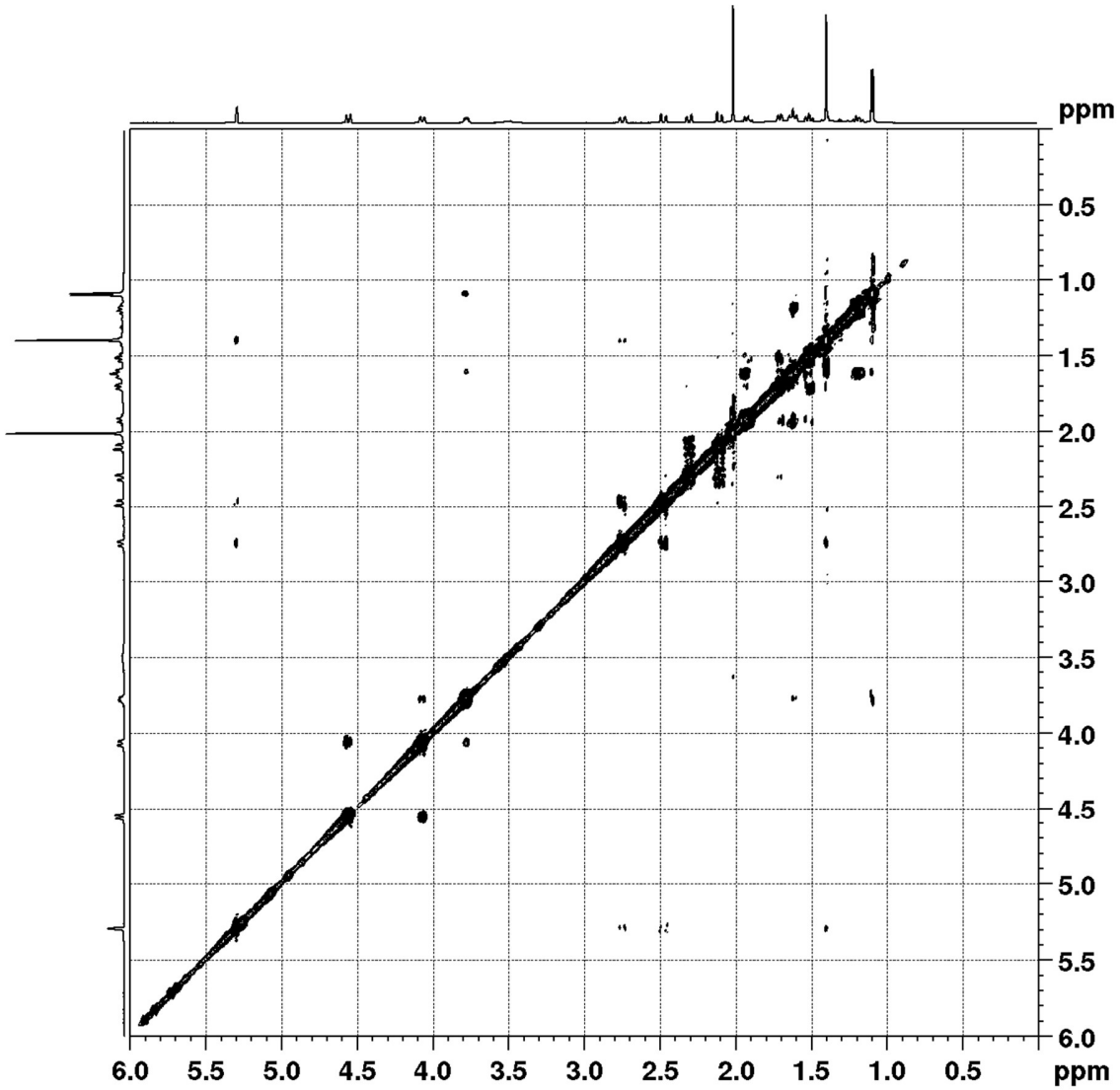


Figure S25. The ROESY (600 MHz, $CDCl_3$) spectrum of compound **3**

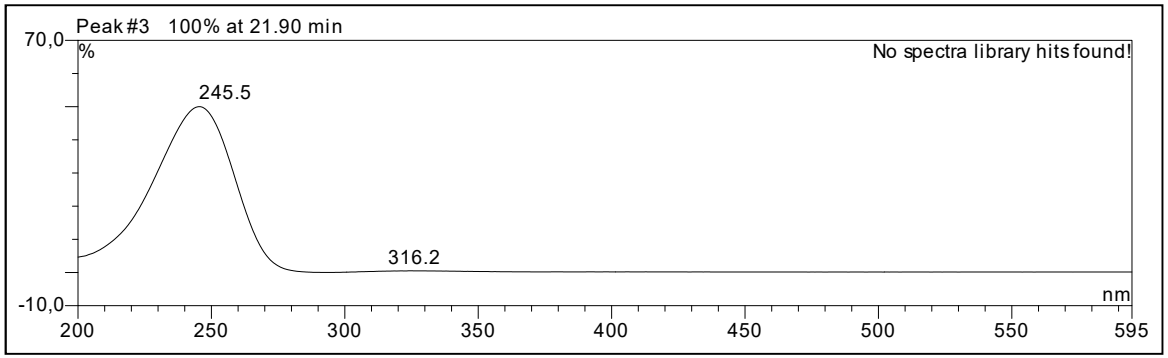


Figure S26. The UV spectrum of compound **3**

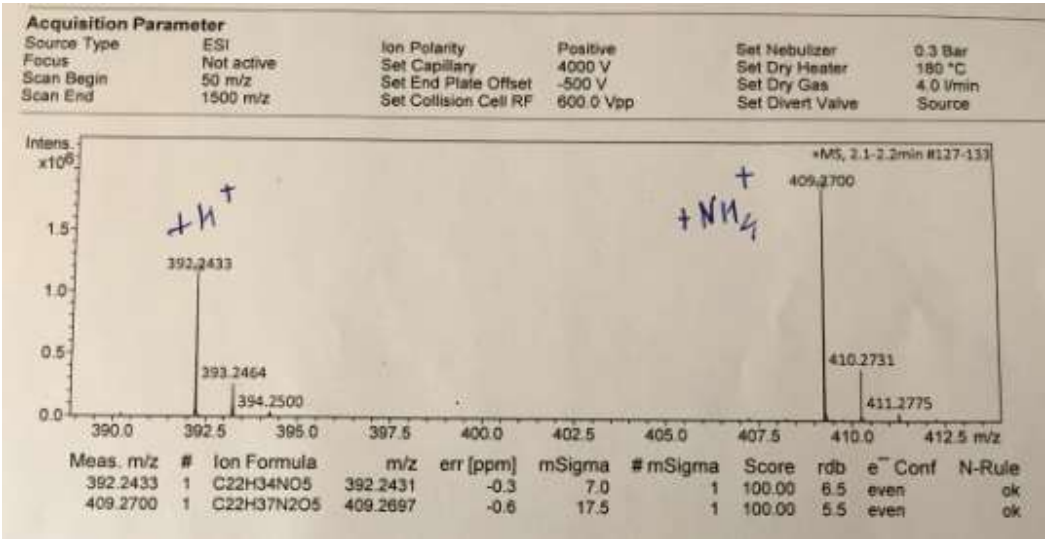


Figure S27. The HRESIMS of compound **13**

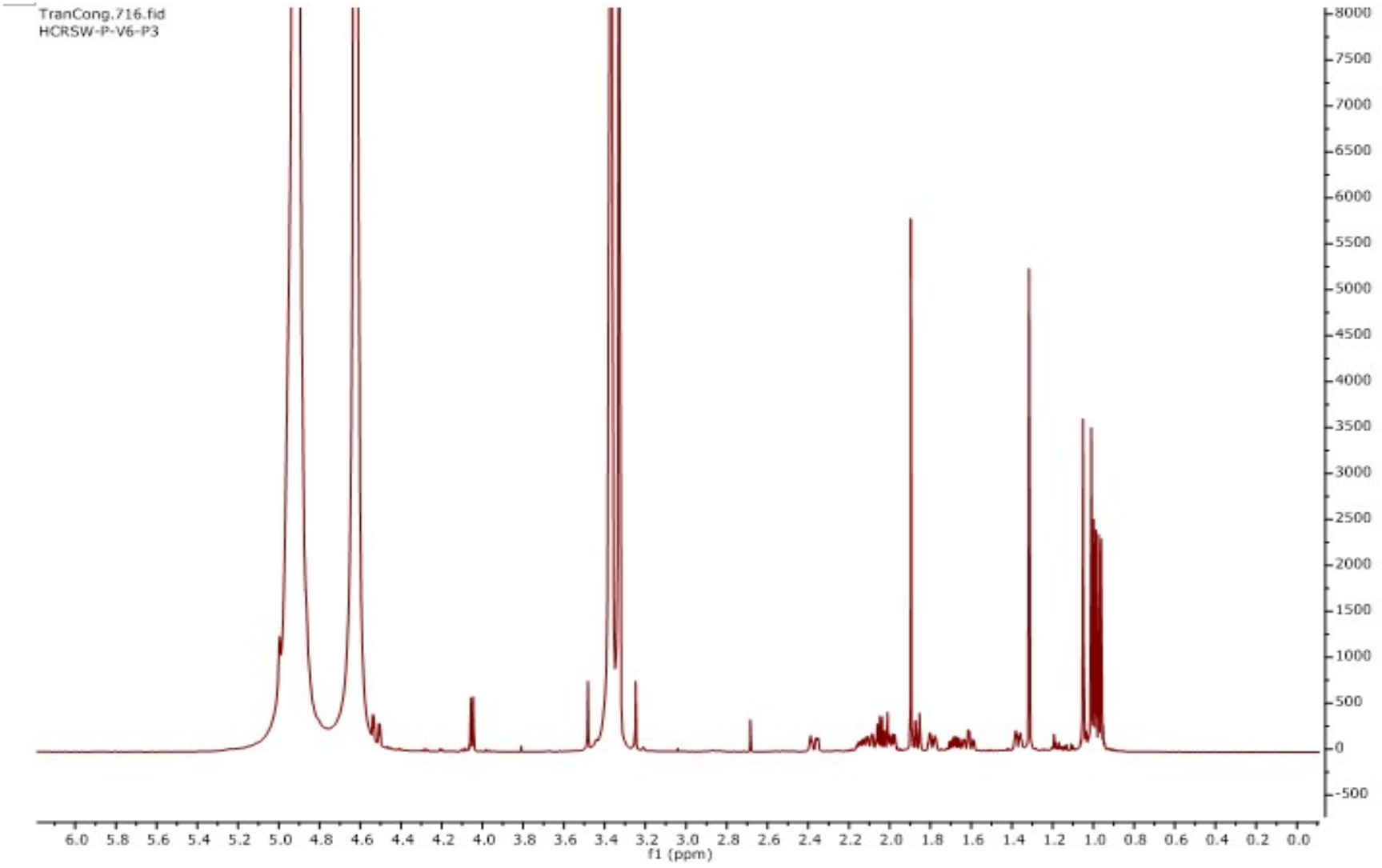


Figure S28. The ^{1}H NMR (600 MHz, CD_3OD) spectrum of compound **13**

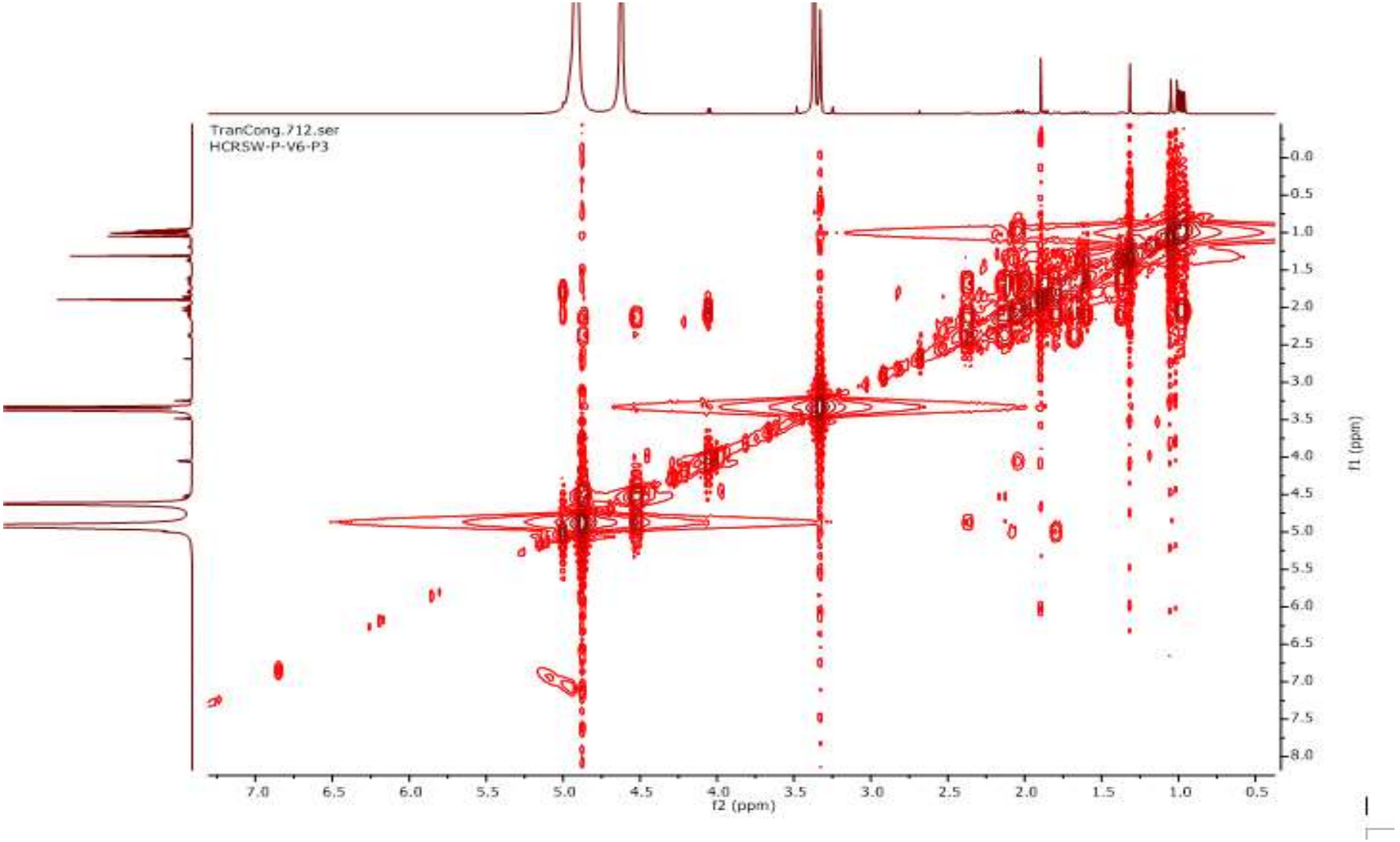


Figure S29. The COSY (600 MHz, CH_3OD) spectrum of compound **13**

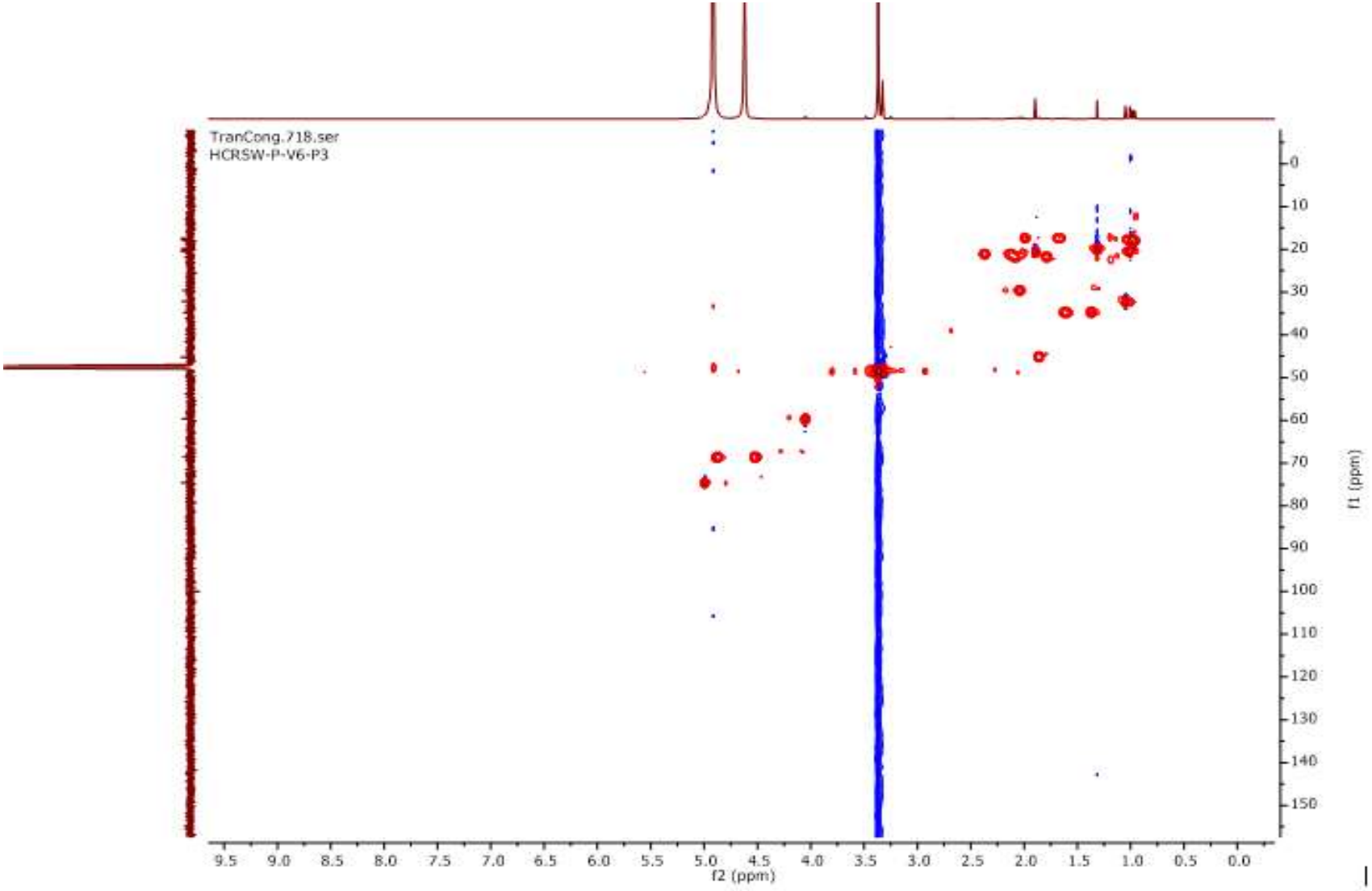


Figure S30. The HSQC (600 MHz, CD_3OD) spectrum of compound **13**

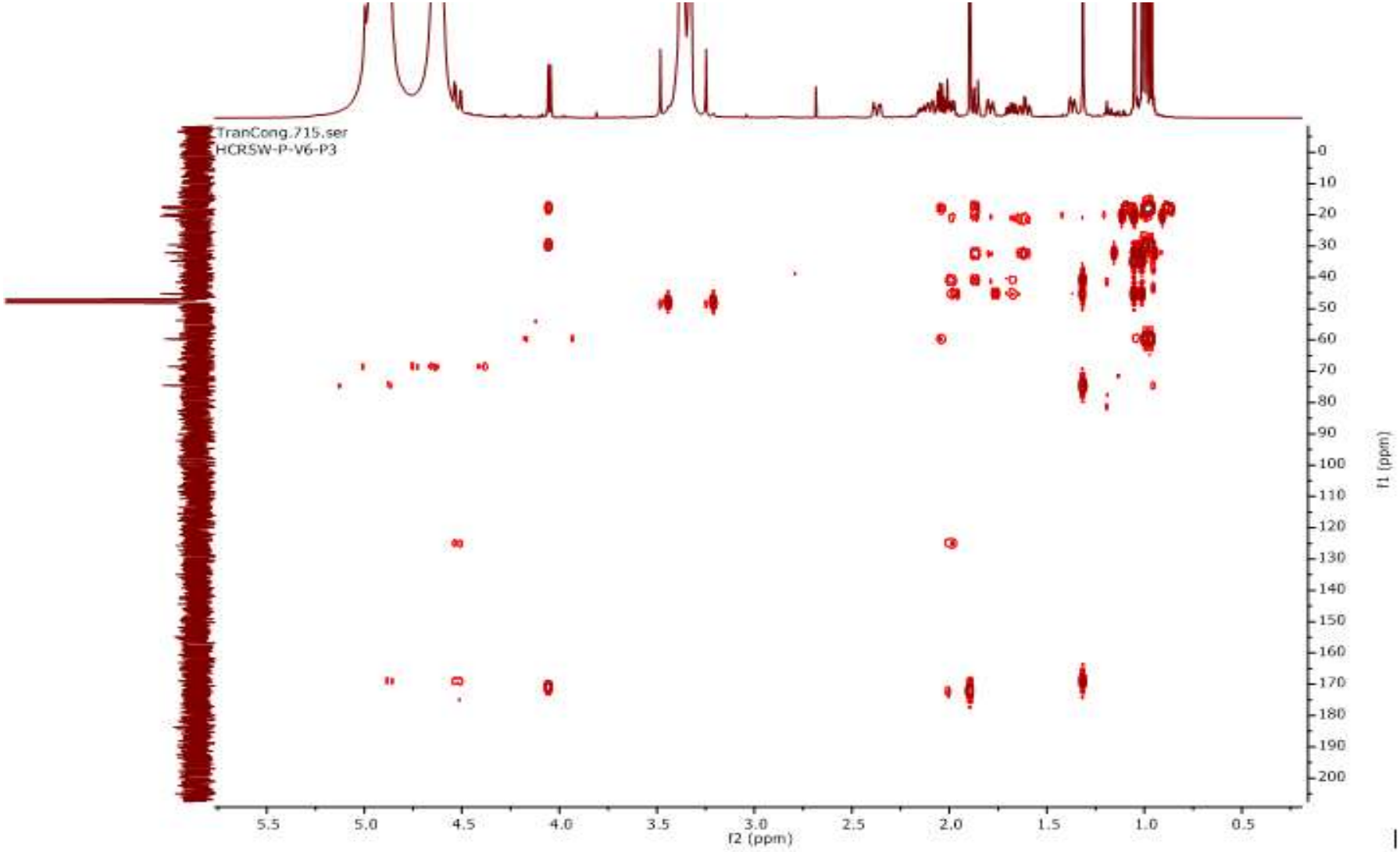


Figure S31. The HMBC (600 MHz, CD_3OD) spectrum of compound **13**

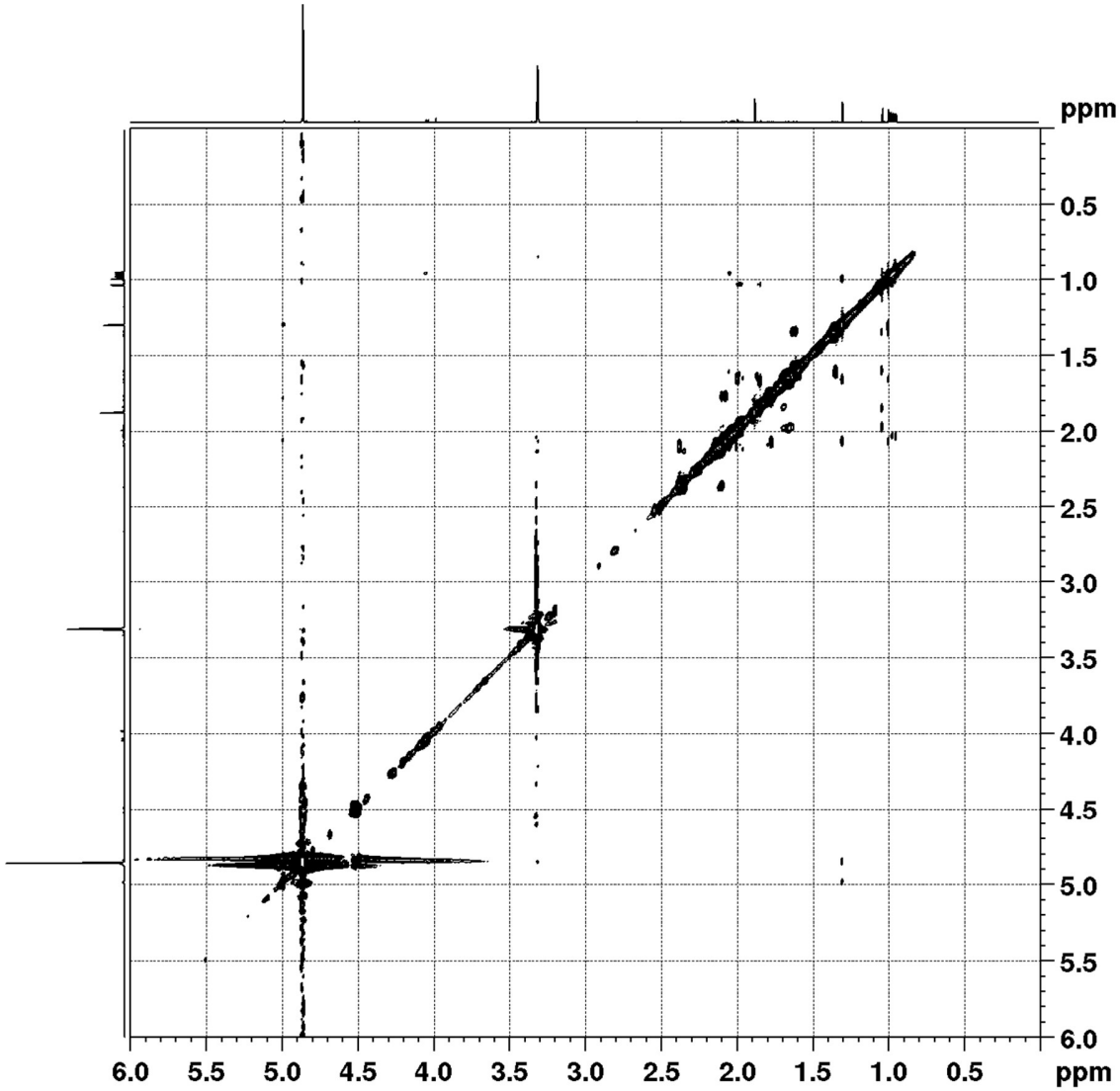


Figure S32. The ROESY (600 MHz, CD_3OD) spectrum of compound **13**

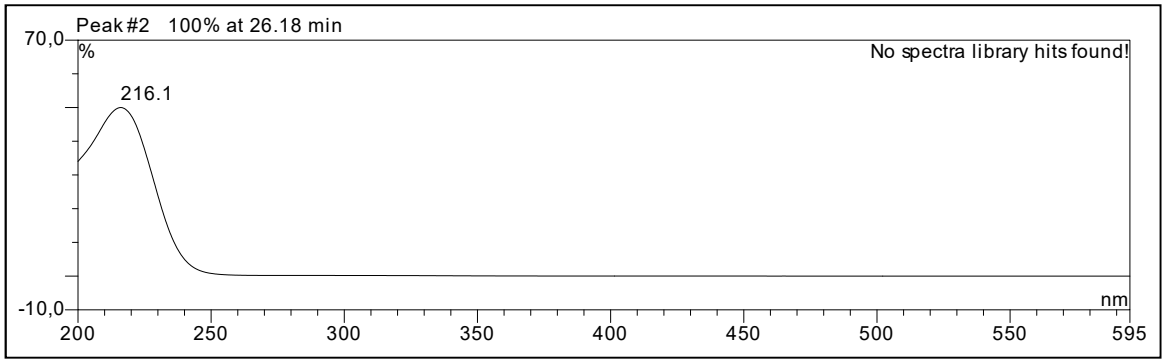


Figure S33. The UV spectrum of compound **13**

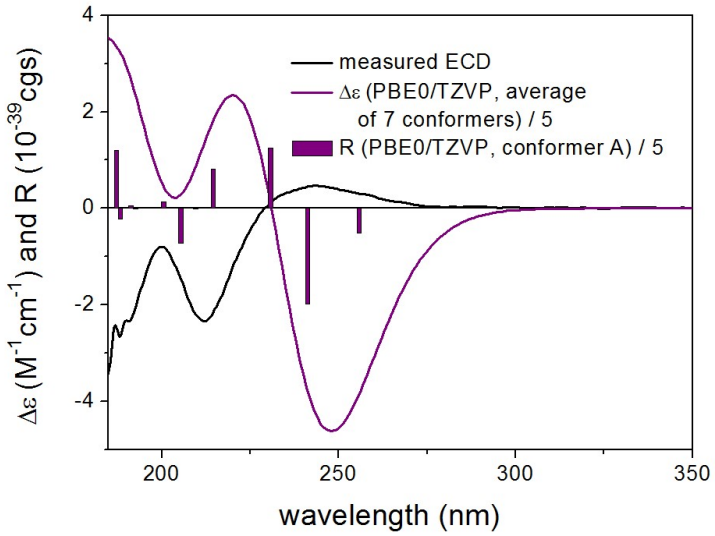


Figure S34. Experimental ECD spectrum of **13** in MeCN compared with the Boltzmann-weighted PBE0/TZVP SMD/MeCN ECD spectrum of (1*S*,5*S*,9*S*,17*S*)-**13**. Level of optimization: SOGGA11-X/TZVP SMD/MeCN. Bars represent the rotatory strength values of the lowest-energy conformer.

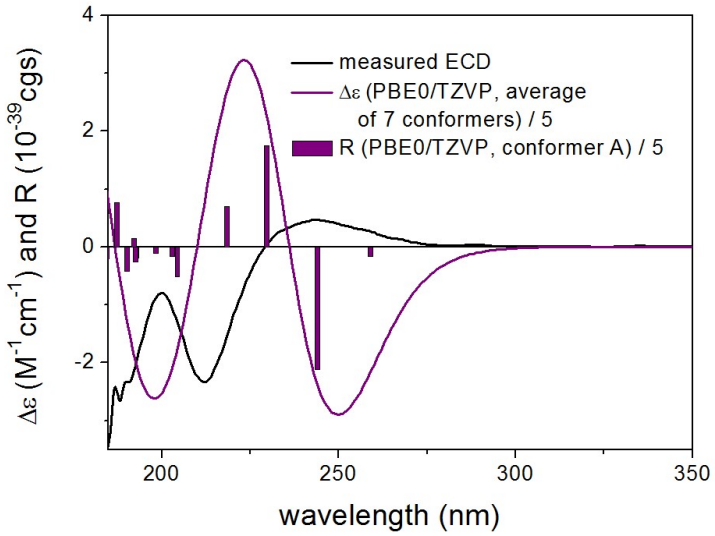


Figure S35. Experimental ECD spectrum of **13** in MeCN compared with the Boltzmann-weighted PBE0/TZVP SMD/MeCN ECD spectrum of (1*R*,5*R*,9*R*,17*S*)-**13**. Level of optimization: SOGGA11-X/TZVP SMD/MeCN. Bars represent the rotatory strength values of the lowest-energy conformer.

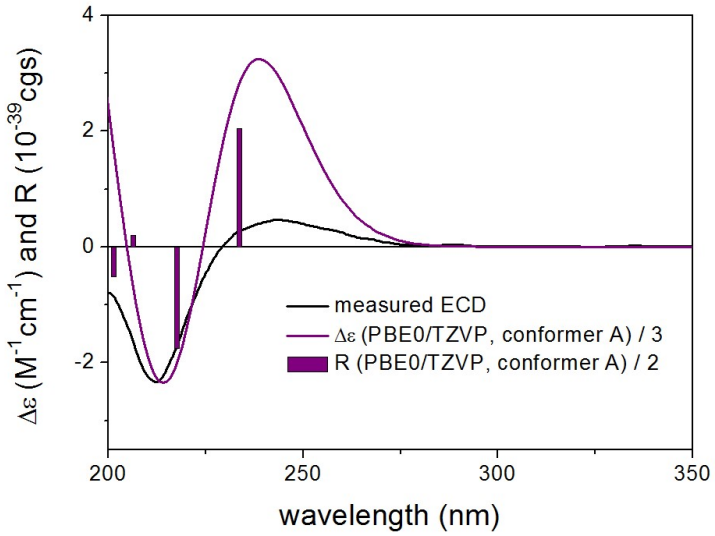


Figure S36. Experimental ECD spectrum of **13** in MeCN compared with the lowest-energy PBE0/TZVP PCM/MeCN ECD spectrum of (1*R*,5*R*,9*R*,17*S*)-**13**. Level of optimization: ωB97X/TZVP PCM/MeCN. Bars represent the rotatory strength values of the lowest-energy conformer.

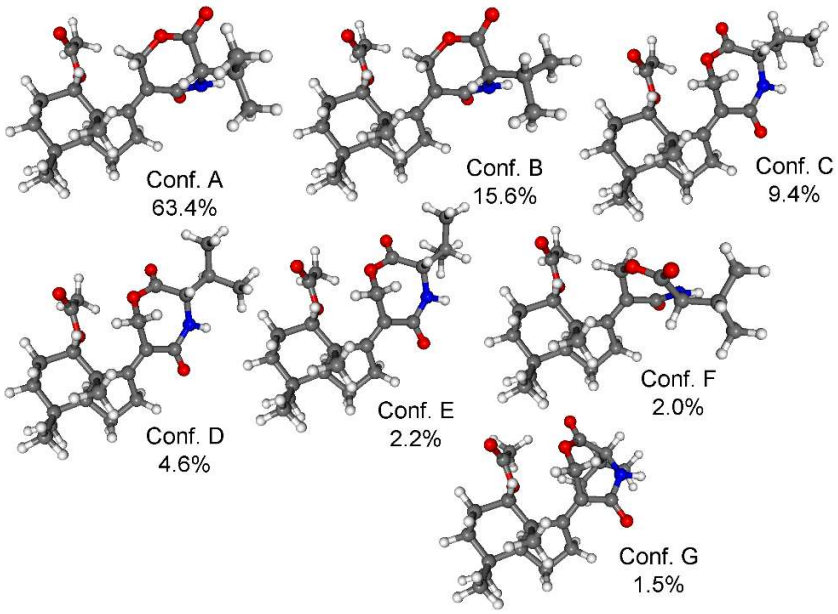


Figure S37. Structure and population of the low-energy SOGGA11-X/TZVP SMD/MeCN conformers (>1%) of (1*S*,5*S*,9*S*,17*S*)-**13**.

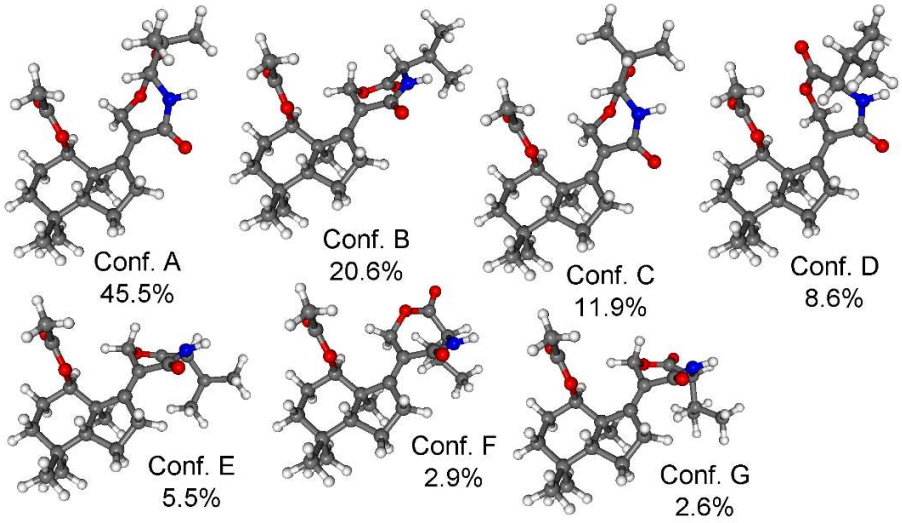


Figure S38. Structure and population of the low-energy SOGGA11-X/TZVP SMD/MeCN conformers (>1%) of (1*R*,5*R*,9*R*,17*S*)-**13**.

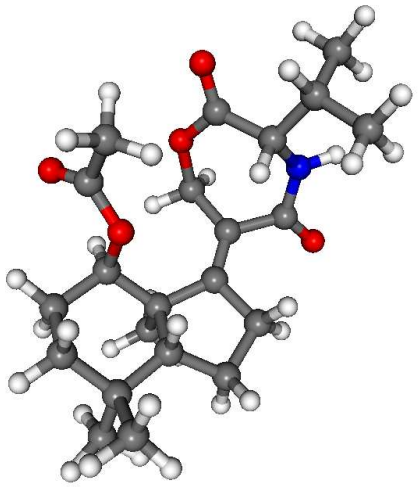


Figure S39. Structure and population of the lowest-energy (24.5%) ωB97X/TZVP PCM/MeCN conformer of (1*R*,5*R*,9*R*,17*S*)-**13** giving moderate normal agreement with the experimental spectrum.

Table S1. Boltzmann populations and specific optical rotations of the low-energy conformers of (1*S*,5*S*,9*S*,17*S*)-**13** computed at various levels for the CAM-B3LYP/TZVP PCM/MeOH conformers.

Conformer	Boltzmann population	B3LYP/TZVP PCM/acetone	BH&HLYP/TZVP PCM/acetone	CAM-B3LYP/TZVP PCM/acetone	PBE0/TZVP PCM/acetone
Conf. A	40.93	-187.33	-147.95	-162.42	-186.18
Conf. B	19.22	-151.15	-125.76	-134.37	-147.79
Conf. C	11.88	-121.90	-103.53	-108.98	-120.47
Conf. D	10.01	-203.98	-158.23	-176.23	-200.78
Conf. E	6.80	-103.16	-83.91	-90.43	-99.13
Conf. F	4.68	150.48	108.11	116.47	149.72
Conf. G	2.39	-191.12	-146.17	-162.36	-188.44
Conf. H	1.38	-36.76	-13.57	-23.89	-31.78
Conf. I	1.14	-83.09	-50.83	-62.13	-77.51
Average	N/A	-148.95	-119.64	-130.55	-146.88

Table S2. Boltzmann populations and specific optical rotations of the low-energy conformers of (1*R*,5*R*,9*R*,17*S*)-**13** computed at various levels for the CAM-B3LYP/TZVP PCM/MeOH conformers.

Conformer	Boltzmann population	B3LYP/TZVP PCM/acetone	BH&HLYP/TZVP PCM/acetone	CAM-B3LYP/TZVP PCM/acetone	PBE0/TZVP PCM/acetone
Conf. A	27.71	-232.94	-173.86	-189.03	-233.36
Conf. B	26.26	-226.28	-179.97	-188.62	-224.40
Conf. C	17.71	61.33	36.20	45.85	57.12
Conf. D	7.84	-109.95	-74.11	-82.49	-109.60
Conf. E	6.68	-215.93	-157.75	-171.23	-216.53
Conf. F	6.16	-156.34	-113.01	-121.56	-155.20
Conf. G	2.44	45.40	27.45	38.13	42.88
Conf. H	1.78	61.30	38.97	49.17	57.60
Conf. I	1.72	57.21	33.29	42.28	47.30
Conf. J	1.38	165.66	128.77	143.60	162.51
Average	N/A	-140.76	-108.97	-115.04	-141.41

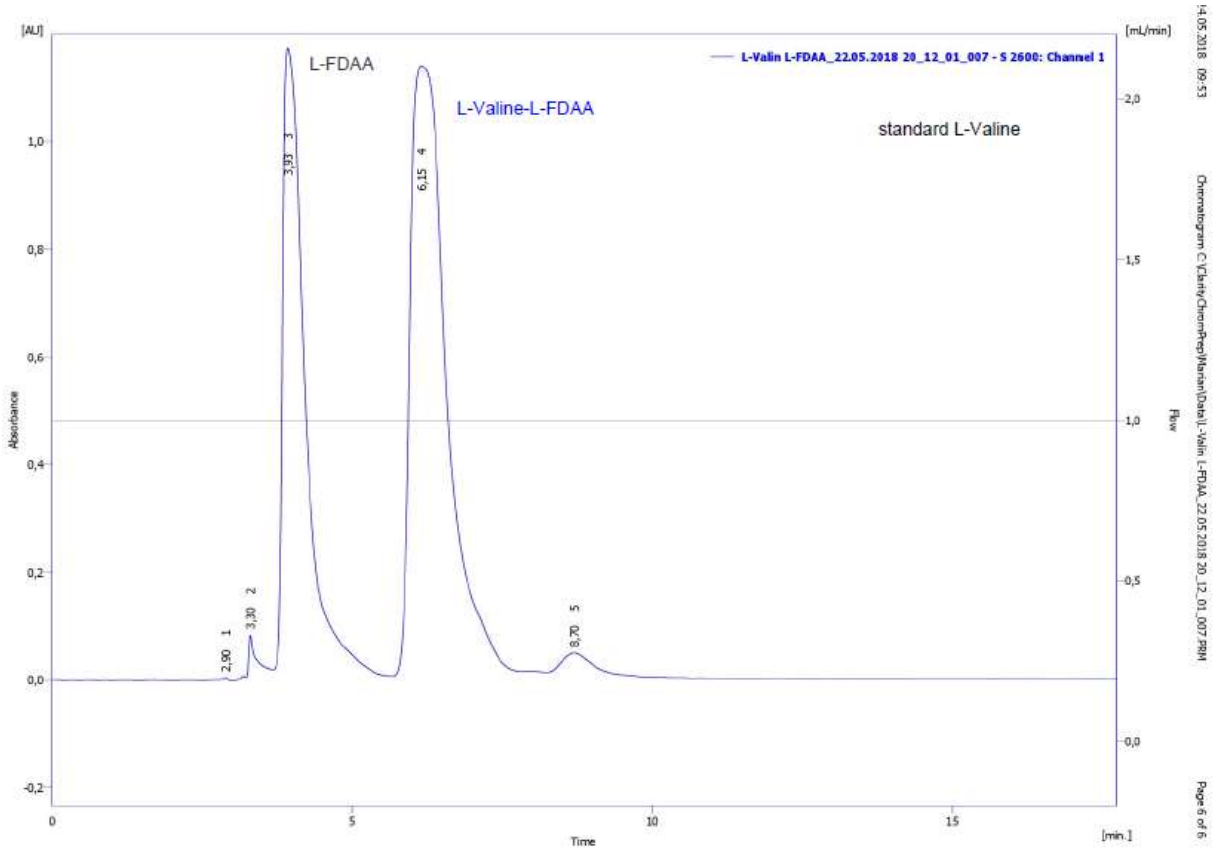


Figure S40. The HPLC chromatogram of L-Valin L-FDAA for Marfey's method

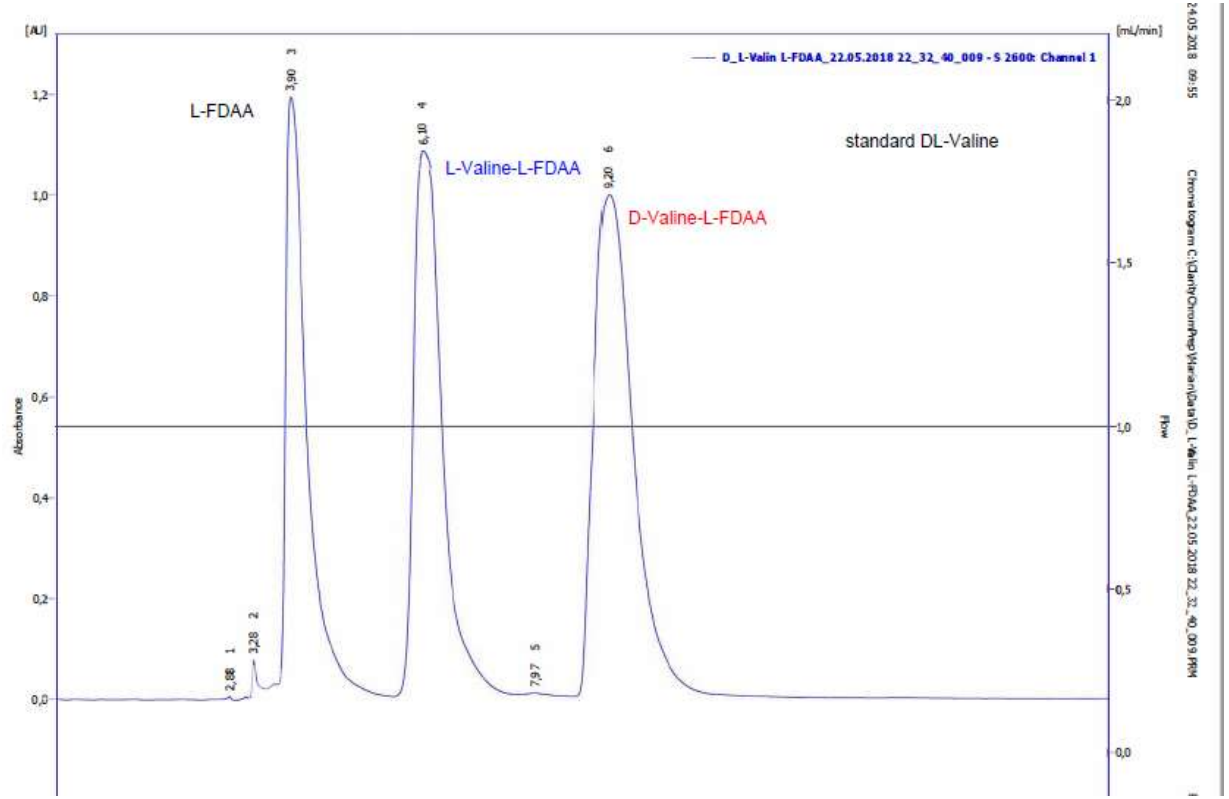


Figure S41. The HPLC chromatogram of DL-Valin L-FDAA for Marfey's method

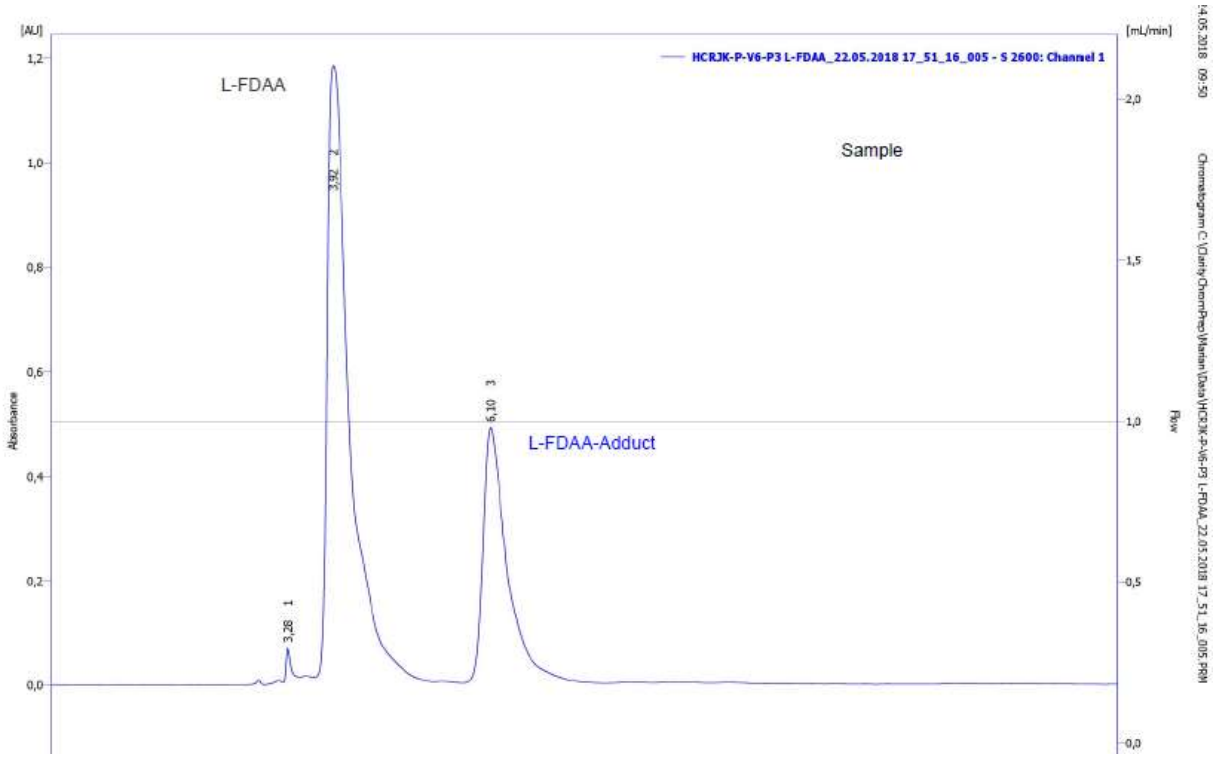


Figure S42. The HPLC chromatogram of compound **13** with L-FDAA for Marfey's method

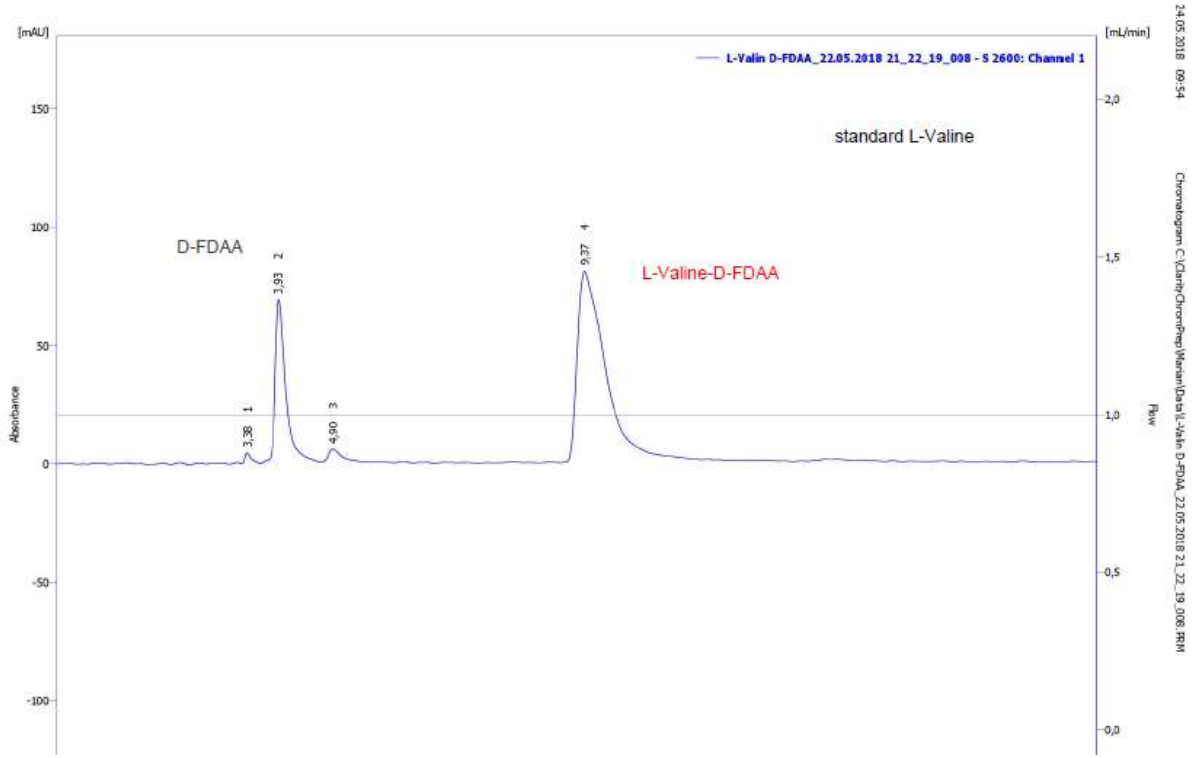


Figure S43. The HPLC chromatogram of L-Valin D-FDAA for Marfey's method

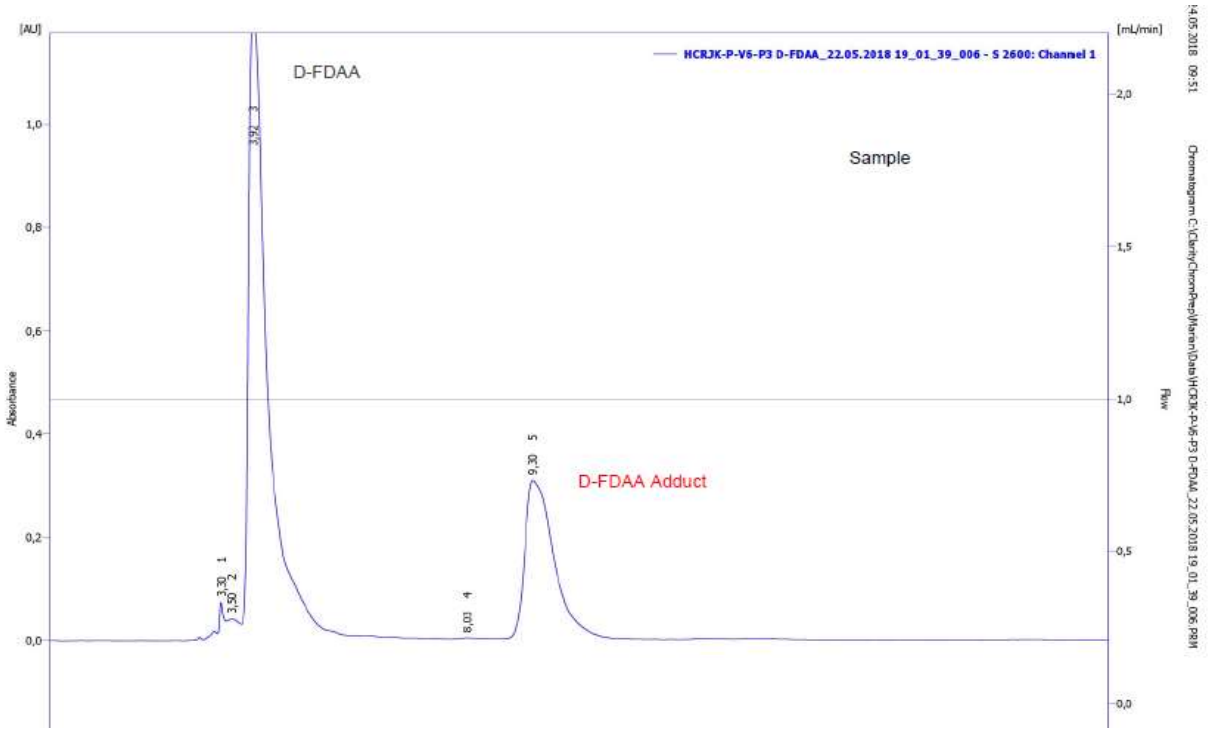


Figure S44. The HPLC chromatogram of compound **13** with D-FDAA for Marfey's method

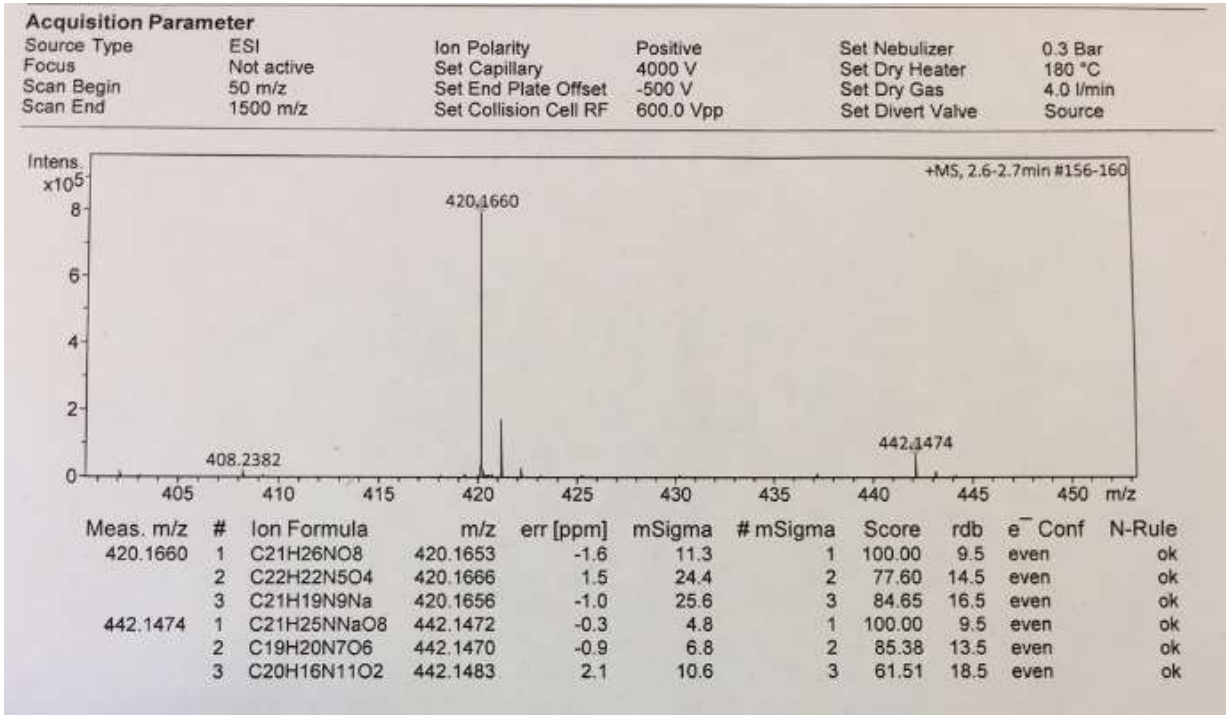


Figure S45. The HRESIMS of compound **15**

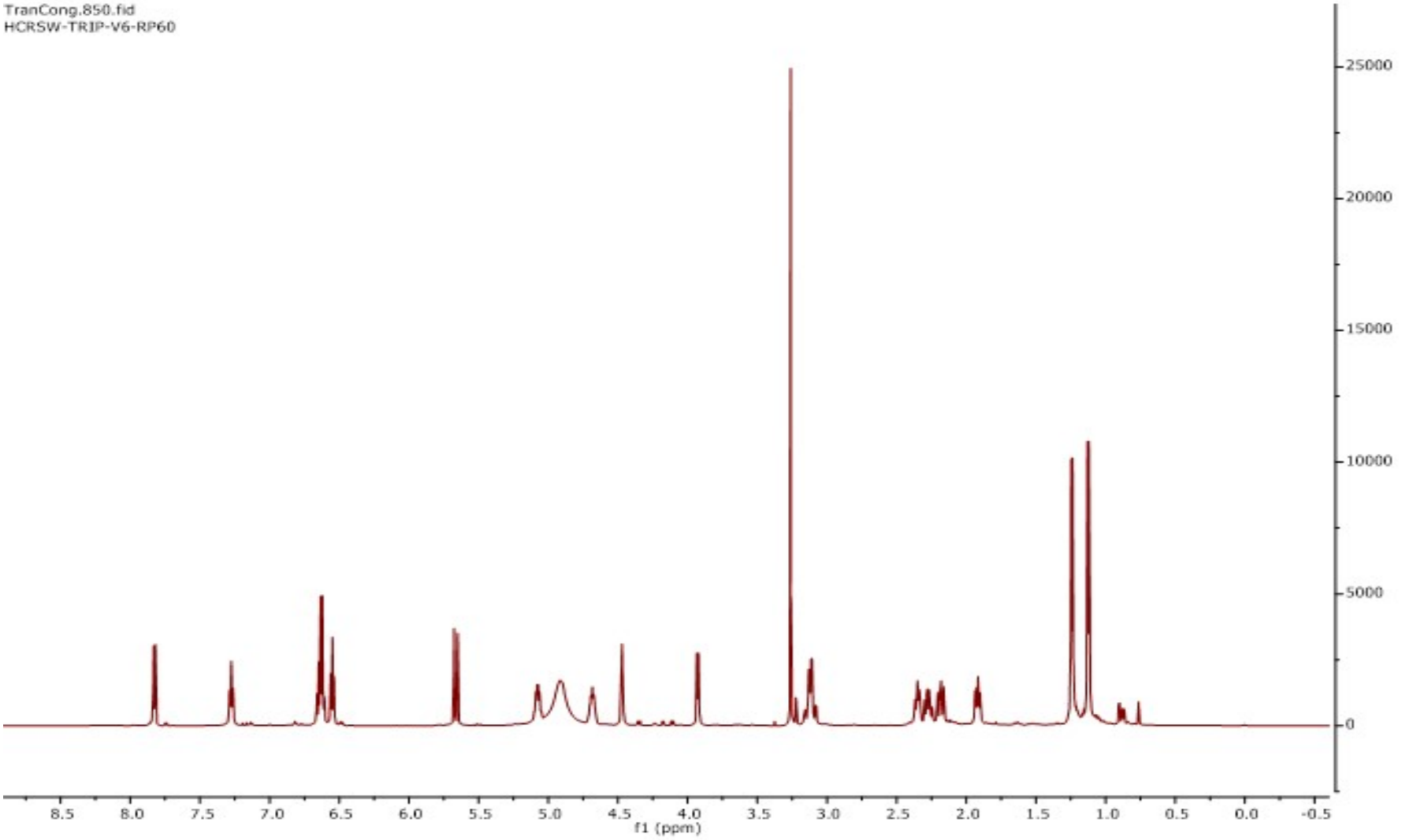


Figure S46. The ^{1}H NMR (600 MHz, CD_3OD) of compound **15**

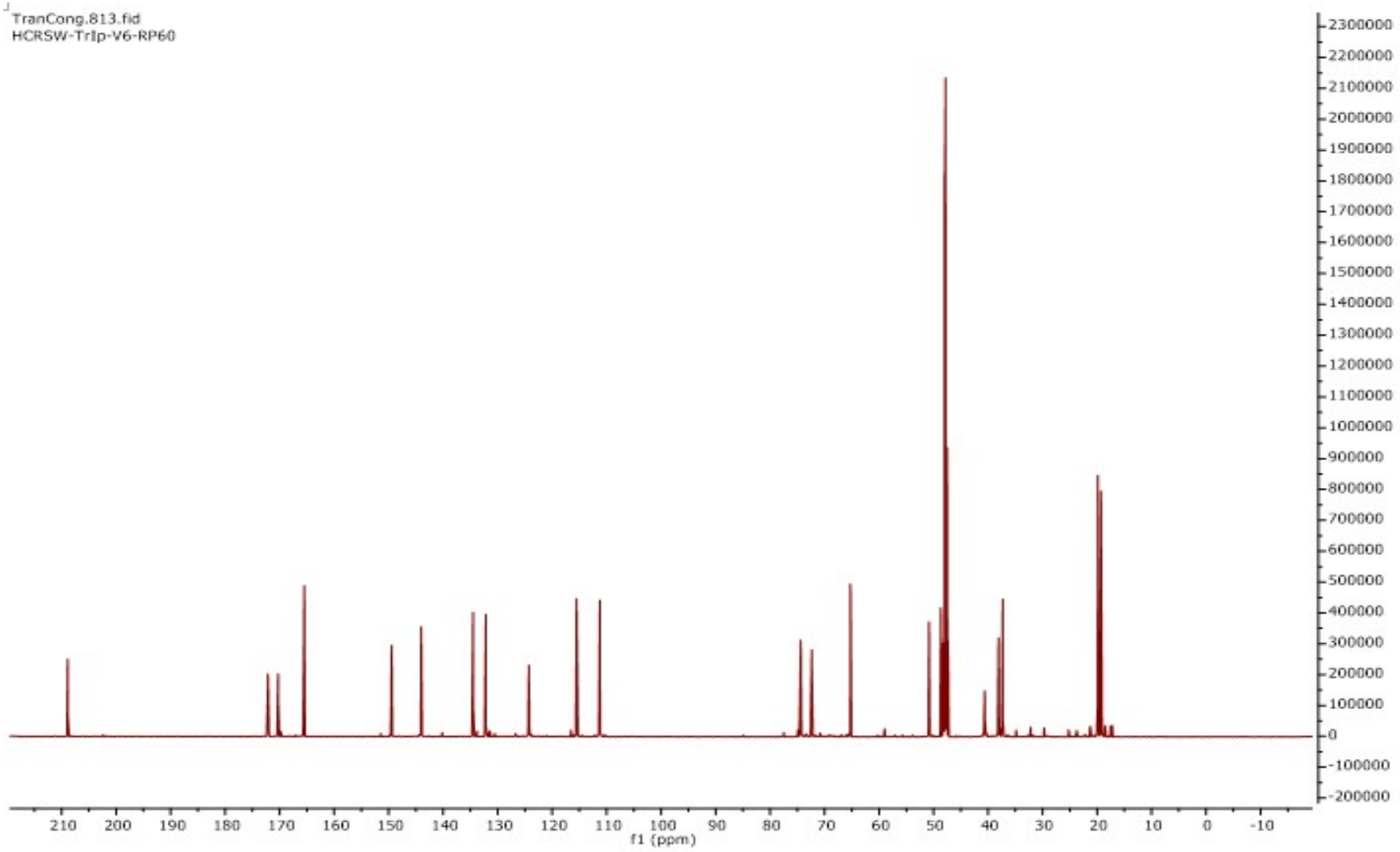


Figure S47. The ^{13}C NMR (150 MHz, CD_3OD) of compound **15**

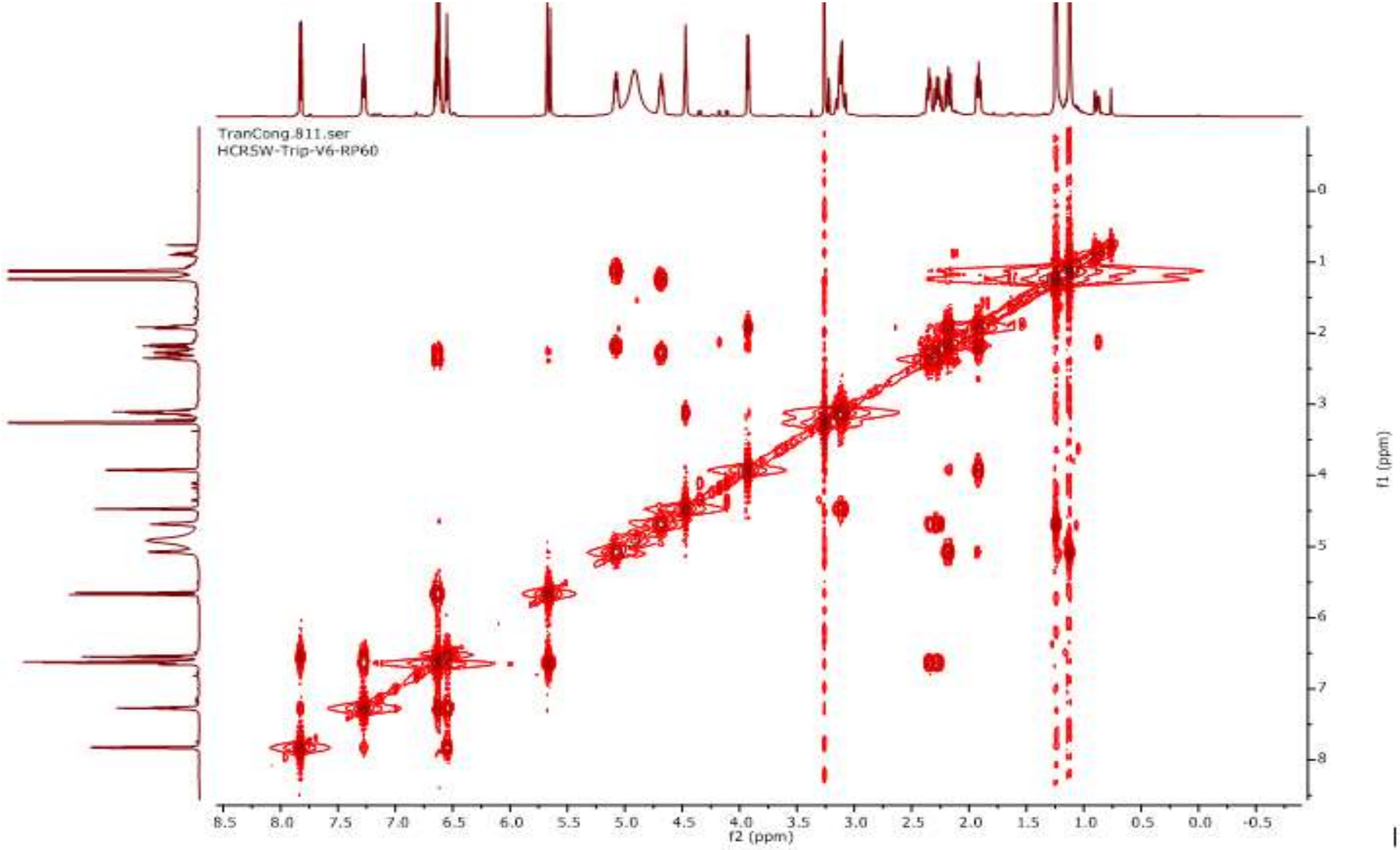


Figure S48. The COSY (600 MHz, CD_3OD) of compound **15**

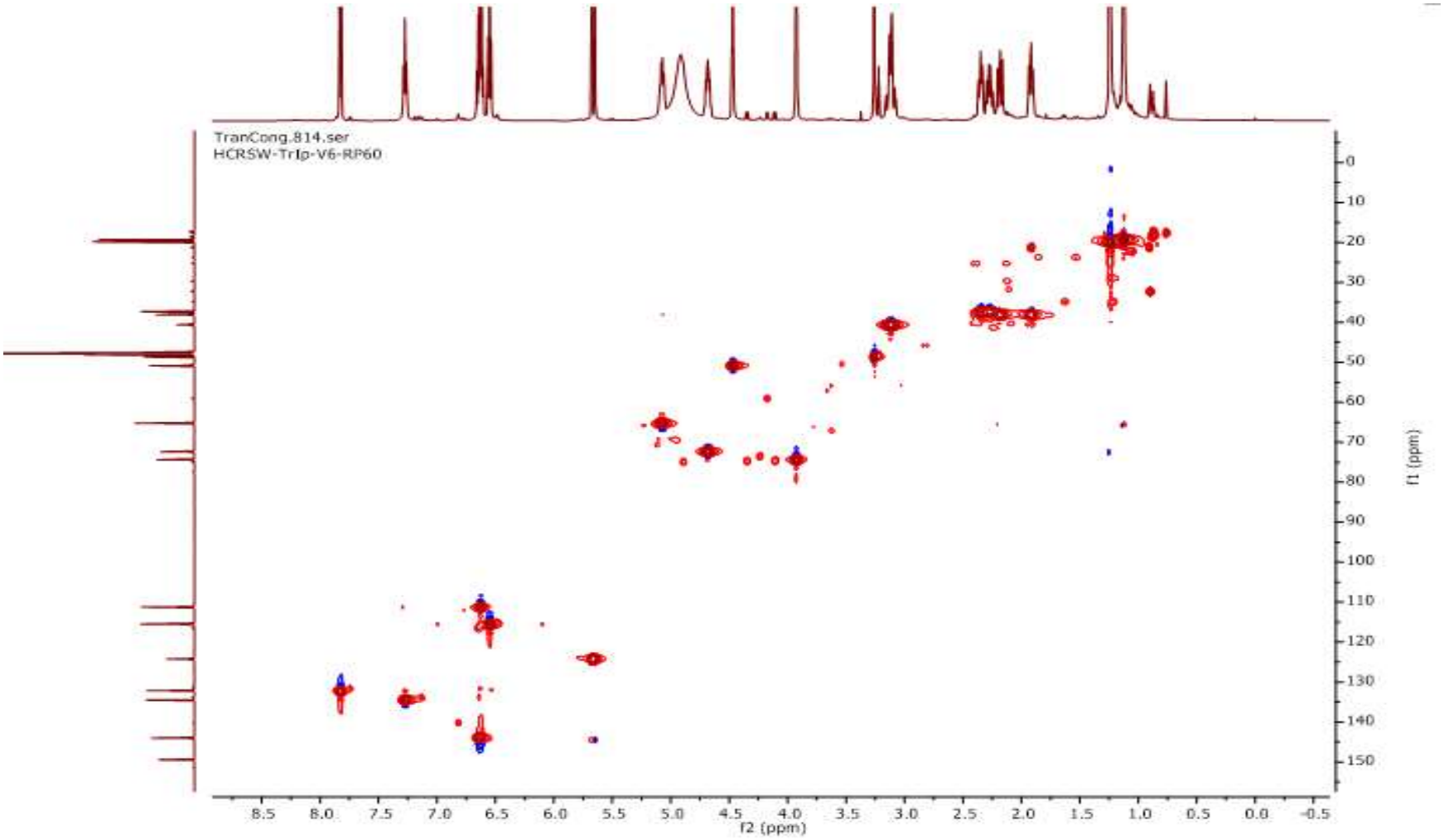


Figure S49. The HSQC (600 MHz, CD_3OD) of compound **15**

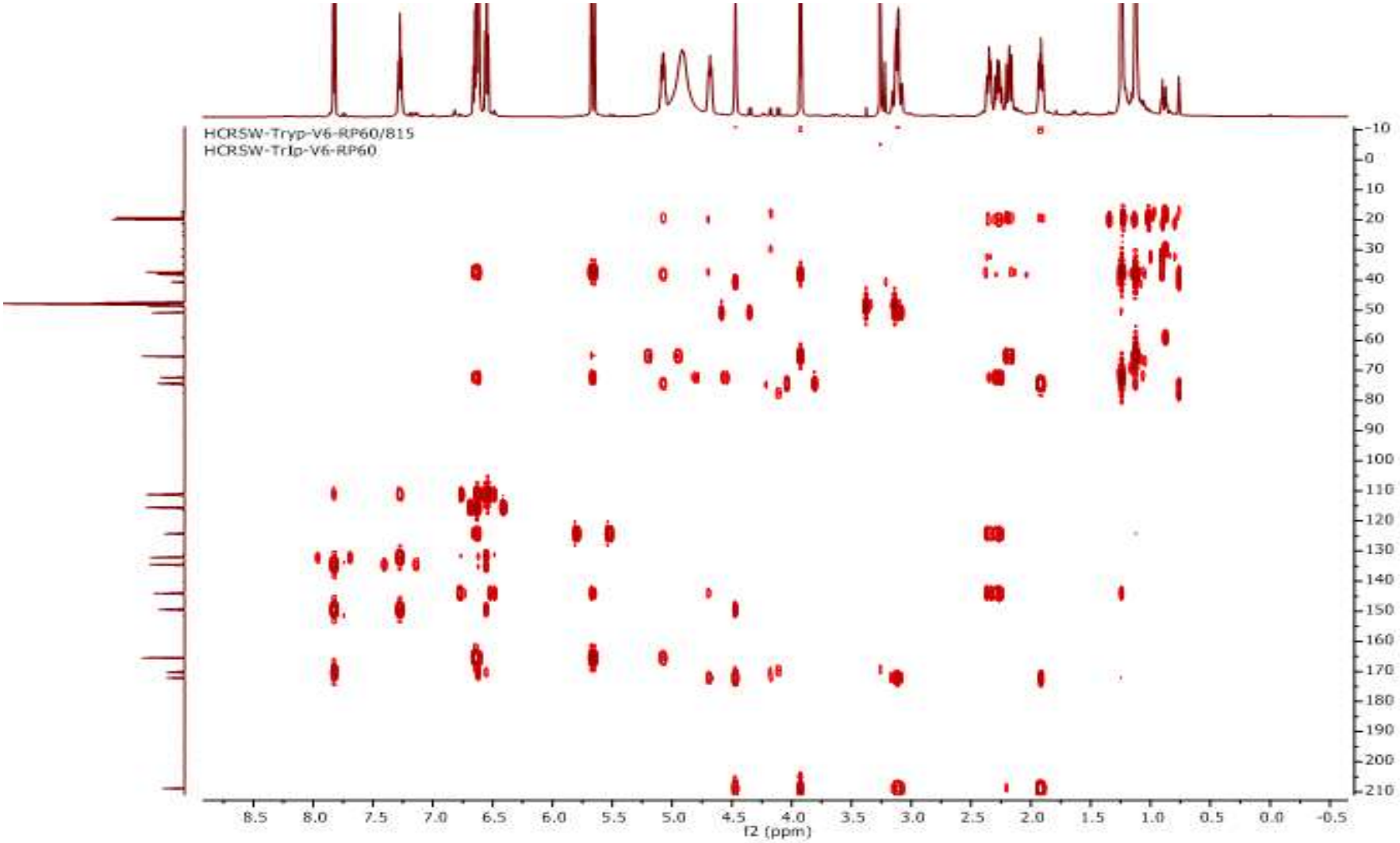


Figure S50. The HMBC (600 MHz, CD_3OD) of compound **15**

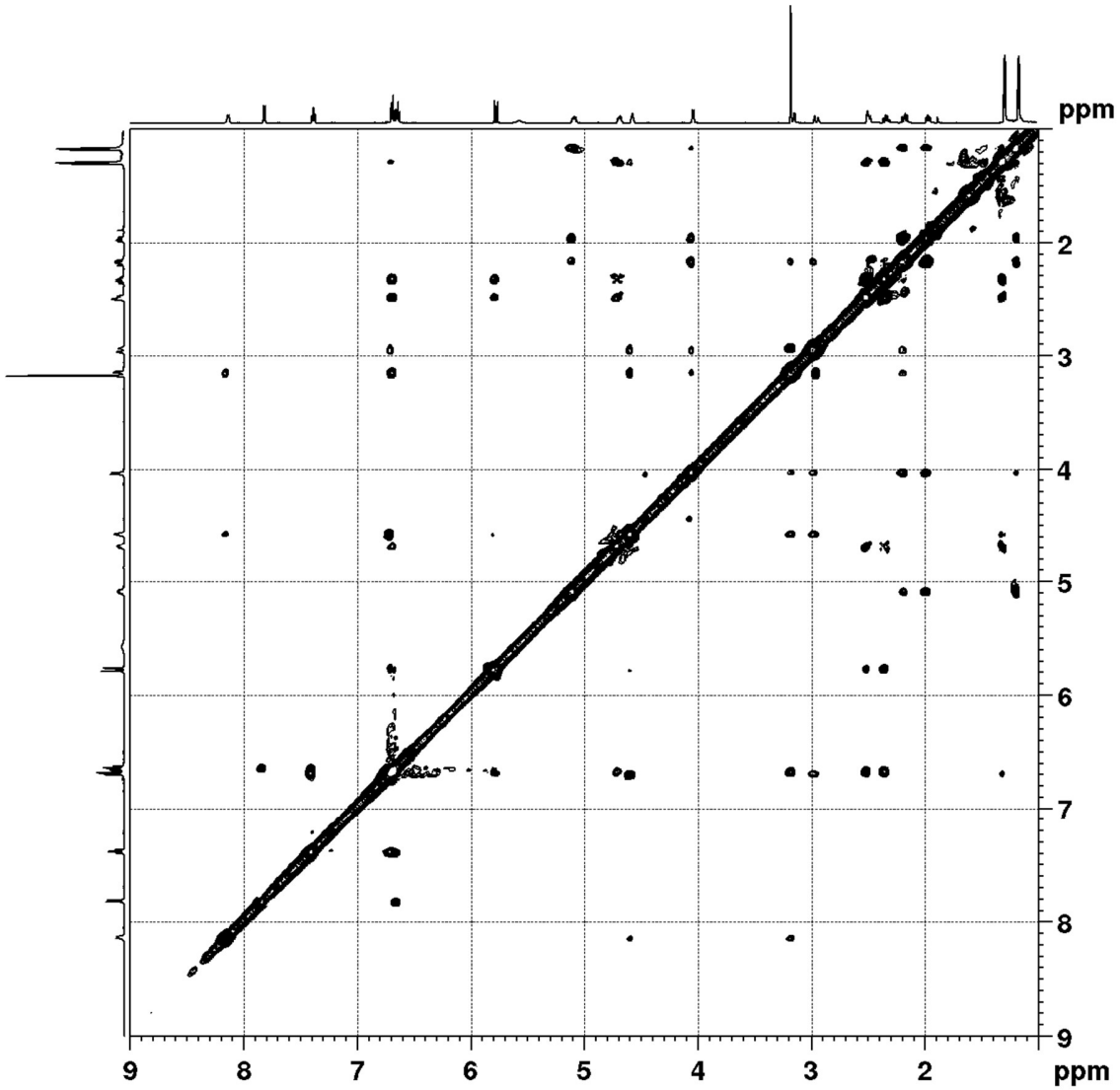


Figure S51. The ROESY (600 MHz, CD_3OD) of compound **15**

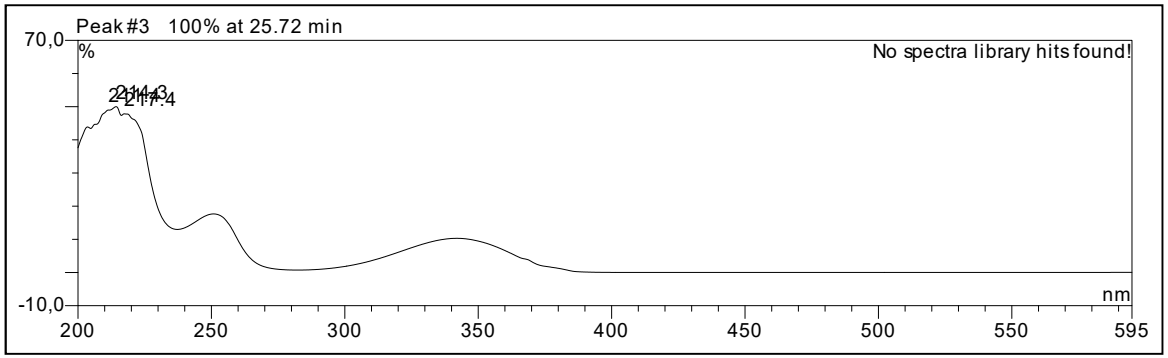


Figure S52. The UV spectrum of compound **15**

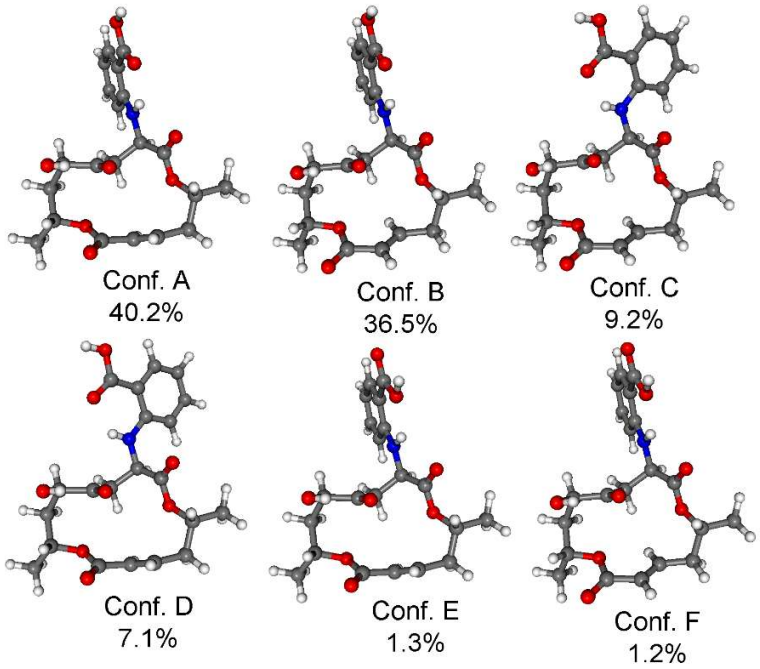


Figure S53. Structure and population of the low-energy ωB97X/TZVP PCM/MeCN conformers (>1%) of (2*R*,8*R*,10*R*,13*R*)-**15**.

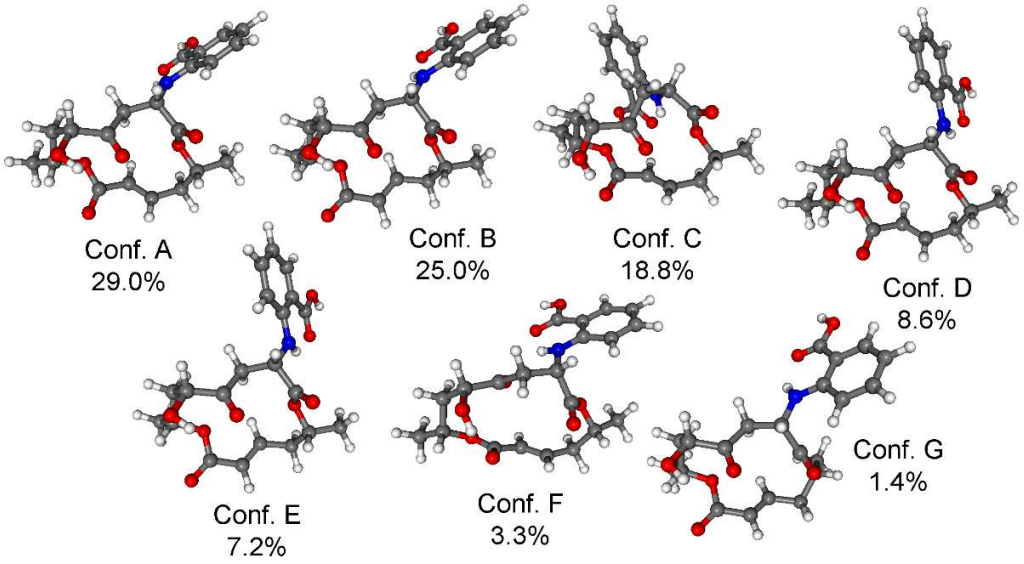


Figure S54. Structure and population of the low-energy ωB97X/TZVP PCM/MeCN conformers (>1%) of (2*R*,8*R*,10*R*,13*S*)-**15**.

Table S3. Comparison of the experimental and the mPW1PW91/6-311+(2d,p) // mPW1PW91/6-311+(2d,p) ^{13}C NMR data of (2*R*,8*R*,10*R*,13*R*)-**15** and (2*R*,8*R*,10*R*,13*S*)-**15**. For a better comparison Δδ values over 2.5 were marked with yellow and those over 5.0 with red.

Carbon	Exp.	calcd (2*R*,8*R*,10*R*,13*R*)-**15**	calcd (2*R*,8*R*,10*R*,13*S*)-**15**	Δδ (2*R*,8*R*,10*R*,13*R*)-**15**	Δδ (2*R*,8*R*,10*R*,13*S*)-**15**
C-2	71.2	72.60	75.77	1.40	4.57
C-3	37.1	40.37	41.11	3.27	4.01
C-4	143.6	151.29	153.11	7.69	9.51
C-5	125.1	125.68	127.42	0.58	2.32
C-6	164.5	165.97	168.99	1.47	4.49
C-8	65.2	64.45	68.31	0.75	3.11
C-9	38.4	39.82	41.32	1.42	2.92
C-10	73.0	76.04	77.86	3.04	4.86
C-11	209.1	212.93	216.57	3.83	7.47
C-12	41.8	41.47	43.92	0.33	2.12
C-13	49.8	50.90	55.79	1.10	5.99
C-14	172.3	172.06	173.68	0.24	1.38
C-15	20.0	19.89	20.31	0.11	0.31
C-16	20.5	20.06	20.72	0.44	0.22
C-17	149.2	149.65	152.29	0.45	3.09
C-18	111.4	109.11	113.10	2.29	1.70
C-19	134.5	136.70	139.34	2.20	4.84
C-20	115.5	113.53	116.62	1.97	1.12
C-21	131.9	133.99	135.79	2.09	3.89
C-22	111.2	106.80	109.53	4.40	1.67
C-23	169.7	168.29	172.23	1.41	2.53
CMAE	N/A	N/A	N/A	1.95	3.48

Table S4. Cartesian coordinates and energies of the low-energy conformers calculated at the ωB97X/TZVP PCM/MeCN level.

(1*S*,5*S*,9*S*,17*S*)-**13**, Conf A

C	2.931575	1.715313	-0.642850
C	3.568226	1.284267	0.675608
C	3.686482	-0.241213	0.843030
C	2.294039	-0.827242	0.549119
C	1.599686	-0.430697	-0.784092
C	1.551663	1.098583	-0.884551
C	2.076414	-2.331369	0.641914
C	0.643276	-2.504880	0.120013
C	0.305800	-1.241777	-0.664861
C	4.038409	-0.543756	2.304006
C	4.818550	-0.798358	-0.028118
C	2.266194	-0.973340	-2.067707
O	0.628038	1.585792	0.115486
C	0.086967	2.795740	-0.078514
O	0.301181	3.471677	-1.057697
C	-0.803716	3.210811	1.052981
C	-0.918197	-1.004232	-1.146792
C	-2.005911	-2.027588	-1.018093
N	-3.223094	-1.522580	-0.674009
C	-3.442366	-0.364573	0.184269
C	-3.174082	0.988070	-0.474221
O	-2.111474	1.200269	-1.255363
C	-1.358169	0.176944	-1.957614
O	-3.876897	1.935197	-0.214460
O	-1.868530	-3.208893	-1.301819
C	-2.728485	-0.458038	1.561472
C	-3.218230	0.623833	2.521387
C	-2.959557	-1.834901	2.181251
H	1.644163	-0.384522	1.317681
H	2.826017	2.801483	-0.672262
H	3.576141	1.455668	-1.485786
H	2.967248	1.677398	1.502775
H	4.558721	1.740823	0.767109
H	1.198434	1.426250	-1.862144
H	2.787980	-2.877328	0.018544
H	2.184340	-2.705460	1.660263
H	-0.063260	-2.613235	0.947946
H	0.520257	-3.387891	-0.505555
H	4.207520	-1.612217	2.460115
H	4.953612	-0.017557	2.589296
H	3.239777	-0.223203	2.978786
H	5.779104	-0.463828	0.372928
H	4.825325	-1.890981	-0.025500
H	4.770644	-0.467201	-1.064443
H	3.206327	-0.476853	-2.294509
H	1.595941	-0.818171	-2.915982
H	2.463296	-2.043317	-1.995927
H	-0.812451	2.470999	1.850501
H	-1.814131	3.348700	0.664197
H	-0.456166	4.168443	1.440885
H	-3.954123	-2.218064	-0.646180
H	-4.515533	-0.347695	0.377540
H	-0.519783	0.725402	-2.370971
H	-1.980301	-0.153790	-2.791517
H	-1.653638	-0.322490	1.397251
H	-3.055290	1.632055	2.142138
H	-4.288988	0.507650	2.713033

H	-2.695080	0.532453	3.475115
H	-2.556528	-2.646732	1.573958
H	-4.028978	-2.017950	2.323881
H	-2.478897	-1.882693	3.159892

ωB97X Energy = -1289.26754192 a.u.

(1*S*,5*S*,9*S*,17*S*)-**13**, Conf B

C	3.214951	0.736334	-1.595029
C	4.300811	0.027379	-0.786230
C	3.901826	-1.368875	-0.269798
C	2.537034	-1.200788	0.418081
C	1.391307	-0.538273	-0.394025
C	1.871133	0.838811	-0.869434
C	1.860265	-2.379071	1.103770
C	0.552244	-1.745041	1.591640
C	0.243309	-0.611095	0.620412
C	4.924726	-1.803847	0.785989
C	3.939550	-2.405335	-1.399483
C	0.905277	-1.342563	-1.618101
O	2.016431	1.674098	0.305053
C	1.982815	3.003427	0.145922
O	1.784298	3.541415	-0.918295
C	2.211266	3.713856	1.445709
C	-0.894483	0.088350	0.635640
C	-1.930905	-0.251473	1.671148
N	-3.170673	-0.528944	1.190223
C	-3.586656	-0.273306	-0.182842
C	-3.636064	1.251001	-0.290465
O	-2.457120	1.880902	-0.137568
C	-1.211535	1.192311	-0.357905
O	-4.640141	1.906367	-0.363363
O	-1.687868	-0.311895	2.867713
C	-4.912101	-0.954118	-0.520058
C	-5.263612	-0.726082	-1.988534
C	-4.842446	-2.449618	-0.219759
H	2.732817	-0.478176	1.222439
H	3.541255	1.746534	-1.851063
H	3.048963	0.227853	-2.547579
H	4.558972	0.650705	0.076953
H	5.208046	-0.052273	-1.393290
H	1.148998	1.312512	-1.535319
H	1.671708	-3.199845	0.407449
H	2.447939	-2.778488	1.930901
H	0.691752	-1.322623	2.588160
H	-0.275896	-2.452515	1.665261
H	4.736941	-2.825984	1.124516
H	5.934914	-1.772224	0.368422
H	4.898275	-1.145661	1.658995
H	3.477298	-3.347102	-1.092835
H	4.979959	-2.618692	-1.659105
H	3.445153	-2.070766	-2.310271
H	-0.033223	-0.926812	-1.990778
H	0.718830	-2.384899	-1.358653
H	1.613909	-1.326496	-2.441923
H	1.508881	3.350489	2.196025
H	2.089783	4.784533	1.305130
H	3.219976	3.500042	1.801830
H	-3.897912	-0.615036	1.887115
H	-2.822143	-0.671679	-0.855994
H	-0.480596	1.993356	-0.280398
H	-1.199305	0.827668	-1.388344
H	-5.689608	-0.497352	0.101078
H	-5.352255	0.333517	-2.228277

H	-4.501717	-1.167549	-2.638008
H	-6.216236	-1.204661	-2.221820
H	-4.654374	-2.655964	0.834465
H	-4.047335	-2.922844	-0.803665
H	-5.786131	-2.925956	-0.491207

ωB97X Energy = -1289.26731511 a.u.

(1*S*,5*S*,9*S*,17*S*)-**13**, Conf C

C	2.950419	1.577548	-0.736224
C	3.701920	1.152064	0.523659
C	3.775405	-0.371926	0.733522
C	2.340250	-0.902957	0.575685
C	1.564768	-0.532269	-0.720733
C	1.534073	1.001091	-0.831513
C	2.041237	-2.380599	0.773447
C	0.543592	-2.449017	0.455454
C	0.254846	-1.299608	-0.497573
C	4.233591	-0.641804	2.171464
C	4.809760	-1.006103	-0.204348
C	2.144652	-1.117242	-2.026608
O	0.729492	1.507562	0.260825
C	0.284643	2.769503	0.175206
O	0.469100	3.479179	-0.784840
C	-0.418606	3.197586	1.428500
C	-0.941132	-1.089087	-1.059190
C	-2.117402	-1.965455	-0.776077
N	-3.313648	-1.306368	-0.723850
C	-3.593392	0.011219	-0.163465
C	-2.788569	1.229345	-0.641149
O	-1.797165	1.183623	-1.525264
C	-1.260452	-0.038884	-2.078768
O	-3.100340	2.313198	-0.208416
O	-2.073447	-3.186648	-0.720425
C	-3.656735	0.008113	1.384461
C	-4.774357	-0.906053	1.876254
C	-2.327336	-0.366970	2.030949
H	1.776792	-0.388965	1.366956
H	2.880133	2.665386	-0.778134
H	3.500185	1.281736	-1.632316
H	3.206638	1.595054	1.394693
H	4.713946	1.568079	0.497824
H	1.079148	1.339050	-1.762365
H	2.617733	-3.006923	0.088077
H	2.255242	-2.721597	1.786786
H	-0.040835	-2.306437	1.370314
H	0.225529	-3.397218	0.028096
H	4.386039	-1.709905	2.346205
H	5.182433	-0.134622	2.367182
H	3.499596	-0.279383	2.896637
H	4.716965	-0.674452	-1.237280
H	5.814987	-0.736583	0.130755
H	4.741776	-2.096874	-0.194469
H	2.332738	-2.187043	-1.929780
H	3.074245	-0.641470	-2.326138
H	1.430266	-0.985741	-2.841512
H	0.334540	3.528467	2.147133
H	-0.975697	2.374817	1.872563
H	-1.086244	4.025346	1.204305
H	-4.095405	-1.941556	-0.643655
H	-4.598423	0.260200	-0.515448
H	-0.379229	0.289827	-2.618862
H	-1.975223	-0.420880	-2.808275
H	-3.905510	1.033741	1.664161

H	-5.733302	-0.651620	1.418082
H	-4.558163	-1.956396	1.661240
H	-4.884235	-0.813494	2.958246
H	-1.491845	0.224741	1.647270
H	-2.094863	-1.422875	1.865588
H	-2.382608	-0.214110	3.110309

ωB97X Energy = -1289.26725973 a.u.

(1*S*,5*S*,9*S*,17*S*)-**13**, Conf D

C	3.220631	1.557225	-0.883289
C	4.124844	1.148920	0.275472
C	4.215949	-0.372538	0.485887
C	2.769528	-0.894987	0.532327
C	1.817042	-0.540622	-0.646614
C	1.800789	0.991300	-0.789692
C	2.508611	-2.368773	0.784733
C	0.984945	-2.457308	0.661606
C	0.542809	-1.288490	-0.206249
C	4.866327	-0.634449	1.849300
C	5.106227	-1.020392	-0.581486
C	2.190245	-1.163301	-2.007909
O	1.132081	1.528992	0.372827
C	0.606454	2.757276	0.281671
O	0.693137	3.447242	-0.707536
C	-0.117449	3.151631	1.532208
C	-0.734995	-1.040940	-0.543421
C	-1.851146	-1.872647	0.000613
N	-3.115897	-1.355211	-0.002037
C	-3.730888	-0.119017	-0.477013
C	-2.887865	1.131302	-0.209073
O	-1.685706	1.193891	-0.787595
C	-1.160376	0.042819	-1.484749
O	-3.273678	2.081164	0.422226
O	-1.693867	-2.996546	0.466357
C	-5.142262	0.021416	0.120244
C	-6.098448	-0.994129	-0.503667
C	-5.172542	-0.058465	1.645161
H	2.321924	-0.370230	1.387983
H	3.144918	2.644631	-0.936037
H	3.650138	1.241620	-1.836990
H	3.744904	1.603102	1.197160
H	5.126941	1.559641	0.116594
H	1.254778	1.319786	-1.673077
H	3.001565	-2.999346	0.040640
H	2.853900	-2.693800	1.766653
H	0.508023	-2.375277	1.641418
H	0.635539	-3.398416	0.242971
H	5.039363	-1.701410	2.010923
H	5.833704	-0.128176	1.909020
H	4.239228	-0.263787	2.664956
H	4.879053	-0.687971	-1.593476
H	5.027540	-2.110148	-0.560596
H	6.150732	-0.762781	-0.386586
H	2.352134	-2.238435	-1.921576
H	3.086762	-0.725936	-2.439684
H	1.374680	-1.012936	-2.718579
H	-1.177847	2.931305	1.382801
H	-0.006242	4.222209	1.693358
H	0.242675	2.595615	2.395231
H	-3.775298	-2.028850	0.358587
H	-3.854861	-0.156779	-1.567312
H	-0.337453	0.429541	-2.070709
H	-1.906304	-0.322062	-2.192926

H	-5.477870	1.018374	-0.173245
H	-6.108086	-0.917712	-1.593179
H	-5.842039	-2.024630	-0.239918
H	-7.113445	-0.817145	-0.143735
H	-4.481418	0.651453	2.099004
H	-4.924377	-1.059898	2.006273
H	-6.178298	0.171999	2.001716

ωB97X Energy = -1289.26710765 a.u.

(1*S*,5*S*,9*S*,17*S*)-**13**, Conf E

C	-3.172550	1.630916	0.929539
C	-4.162850	1.210816	-0.151150
C	-4.298368	-0.313511	-0.304516
C	-2.868977	-0.865778	-0.441845
C	-1.824731	-0.503614	0.654527
C	-1.773528	1.030908	0.763384
C	-2.654275	-2.349743	-0.674502
C	-1.127760	-2.460096	-0.672916
C	-0.598591	-1.284822	0.135644
C	-5.054213	-0.605101	-1.606119
C	-5.116880	-0.910073	0.847065
C	-2.106793	-1.088821	2.053820
O	-1.159189	1.533707	-0.443702
C	-0.581835	2.741882	-0.396804
O	-0.579836	3.439978	0.590404
C	0.076951	3.095989	-1.694173
C	0.705960	-1.054448	0.374005
C	1.762626	-1.911038	-0.254001
N	3.052552	-1.456061	-0.298222
C	3.728715	-0.287715	0.258718
C	2.936687	0.969017	-0.109564
O	1.768394	1.138877	0.518812
C	1.199607	0.041840	1.269946
O	3.295050	1.794200	-0.908738
O	1.527660	-2.998389	-0.770398
C	5.180286	-0.209018	-0.235470
C	5.913598	0.923818	0.482197
C	5.929741	-1.520536	0.005496
H	-2.476125	-0.371283	-1.341522
H	-3.069678	2.717459	0.944790
H	-3.543749	1.353186	1.919050
H	-3.838146	1.627910	-1.110743
H	-5.142642	1.649148	0.063136
H	-1.175830	1.367028	1.609345
H	-3.095478	-2.951761	0.123768
H	-3.082416	-2.693442	-1.616529
H	-0.732508	-2.399323	-1.689616
H	-0.757264	-3.400823	-0.271399
H	-5.256626	-1.673014	-1.720358
H	-6.014840	-0.082670	-1.608663
H	-4.485307	-0.271417	-2.478512
H	-5.055892	-2.001104	0.858357
H	-6.168986	-0.641206	0.720198
H	-4.810305	-0.547825	1.827454
H	-1.236876	-0.941280	2.697432
H	-2.297358	-2.161484	2.005289
H	-2.958916	-0.620913	2.540267
H	-0.411497	2.606862	-2.534630
H	1.114815	2.755547	-1.641862
H	0.070659	4.176342	-1.823300
H	3.655069	-2.119566	-0.759943
H	3.774168	-0.358158	1.351339
H	0.404148	0.490877	1.847190

H	1.931523	-0.331094	1.986862
H	5.158793	0.003979	-1.308131
H	5.426673	1.887705	0.339007
H	5.975357	0.720355	1.555477
H	6.933094	1.004559	0.101598
H	5.580397	-2.349367	-0.613076
H	5.858195	-1.823464	1.054105
H	6.986126	-1.381555	-0.229553

ωB97X Energy = -1289.26651114 a.u.

(1*S*,5*S*,9*S*,17*S*)-**13**, Conf F

C	3.129714	1.695729	-0.860692
C	4.048381	1.329753	0.300484
C	4.232725	-0.185544	0.491221
C	2.822368	-0.800927	0.517450
C	1.853543	-0.485098	-0.659201
C	1.746062	1.044430	-0.782020
C	2.660052	-2.294639	0.734405
C	1.148249	-2.487746	0.588603
C	0.627958	-1.320901	-0.238443
C	4.886980	-0.424783	1.857127
C	5.172333	-0.760355	-0.575640
C	2.267869	-1.062880	-2.028622
O	1.042445	1.528886	0.382907
C	0.441934	2.723490	0.301232
O	0.471774	3.417058	-0.688848
C	-0.284166	3.070798	1.564061
C	-0.665905	-1.145108	-0.560387
C	-1.718072	-2.079108	-0.050879
N	-3.017996	-1.657922	-0.030738
C	-3.715714	-0.451183	-0.469763
C	-2.959560	0.825948	-0.097895
O	-1.780719	1.019848	-0.699965
C	-1.169232	-0.051505	-1.452353
O	-3.374095	1.680913	0.640929
O	-1.476821	-3.208323	0.363157
C	-5.160176	-0.500771	0.061304
C	-5.277811	-0.510209	1.584184
C	-6.022297	0.593038	-0.563033
H	2.337548	-0.325143	1.381545
H	2.989432	2.777279	-0.902918
H	3.583218	1.416452	-1.814573
H	3.632919	1.746943	1.224347
H	5.024352	1.803758	0.156084
H	1.187727	1.350392	-1.665641
H	3.205103	-2.871578	-0.016726
H	3.015972	-2.617085	1.713335
H	0.655326	-2.483743	1.563560
H	0.875420	-3.433981	0.126556
H	5.119029	-1.481826	2.009654
H	5.823614	0.134782	1.929972
H	4.233504	-0.098940	2.671166
H	6.193842	-0.426159	-0.375055
H	5.175603	-1.852994	-0.559982
H	4.925337	-0.441311	-1.587293
H	2.484747	-2.129559	-1.959999
H	3.142873	-0.571665	-2.446380
H	1.449412	-0.942427	-2.741766
H	-0.304419	4.151748	1.686877
H	0.173920	2.595524	2.429204
H	-1.311746	2.710625	1.465255
H	-3.632636	-2.392531	0.288949
H	-3.796689	-0.443638	-1.563650

H	-0.376452	0.425949	-2.011859
H	-1.882523	-0.435398	-2.183466
H	-5.543643	-1.458838	-0.310254
H	-6.312409	-0.716718	1.865383
H	-4.652364	-1.279459	2.042311
H	-4.994226	0.454366	2.004033
H	-5.741672	1.578481	-0.189268
H	-7.071324	0.423034	-0.314108
H	-5.934906	0.597492	-1.652420

ωB97X Energy = -1289.26623278 a.u.

(1*S*,5*S*,9*S*,17*S*)-**13**, Conf G

C	3.319196	0.759671	-1.492311
C	4.358930	0.019894	-0.650965
C	3.925248	-1.386210	-0.192305
C	2.530689	-1.223233	0.434334
C	1.430875	-0.530719	-0.415565
C	1.942965	0.854889	-0.829284
C	1.811532	-2.410124	1.059689
C	0.488485	-1.772970	1.501608
C	0.235681	-0.616326	0.541132
C	4.893509	-1.858557	0.898388
C	4.008792	-2.392293	-1.346606
C	1.000034	-1.299413	-1.682391
O	2.038834	1.655884	0.373887
C	2.024525	2.989226	0.250815
O	1.881186	3.558615	-0.805919
C	2.199353	3.661332	1.579086
C	-0.893001	0.096839	0.520354
C	-1.976905	-0.243373	1.502690
N	-3.194997	-0.502038	0.963404
C	-3.548984	-0.263260	-0.427582
C	-3.570923	1.250678	-0.634006
O	-2.424999	1.890696	-0.327379
C	-1.150984	1.229439	-0.456038
O	-4.531013	1.895470	-0.956406
O	-1.789758	-0.315910	2.709005
C	-4.856967	-0.957957	-0.821749
C	-4.631983	-2.461434	-0.960264
C	-6.019017	-0.667659	0.127380
H	2.693765	-0.521559	1.264040
H	3.665890	1.772965	-1.705704
H	3.195483	0.277092	-2.464532
H	4.578718	0.617328	0.240655
H	5.294368	-0.051373	-1.214685
H	1.256339	1.353691	-1.513985
H	1.646914	-3.212737	0.336501
H	2.355870	-2.835326	1.903483
H	0.586786	-1.372906	2.512277
H	-0.348877	-2.473176	1.522104
H	4.684682	-2.889405	1.195634
H	5.923169	-1.820465	0.531945
H	4.827298	-1.227102	1.788816
H	3.530079	-3.339649	-1.085807
H	5.058876	-2.603530	-1.565977
H	3.555818	-2.031126	-2.268667
H	0.076450	-0.876055	-2.082502
H	0.807076	-2.349423	-1.461666
H	1.742921	-1.257184	-2.474629
H	3.194475	3.439521	1.967290
H	1.470321	3.274956	2.291481
H	2.080696	4.735495	1.465102
H	-3.948950	-0.591917	1.629385

H	-2.756485	-0.677103	-1.058165
H	-0.444175	2.039433	-0.289974
H	-1.043000	0.901389	-1.493199
H	-5.114292	-0.553456	-1.804144
H	-3.863624	-2.684423	-1.703958
H	-4.322228	-2.900504	-0.008175
H	-5.555209	-2.954406	-1.270202
H	-6.147356	0.400412	0.304602
H	-5.892099	-1.173133	1.089567
H	-6.945006	-1.050743	-0.304700

ωB97X Energy = -1289.26614415 a.u.

(1*S*,5*S*,9*S*,17*S*)-**13**, Conf H

C	3.341127	0.663451	-1.425355
C	4.300022	-0.222094	-0.632456
C	3.722551	-1.600112	-0.256601
C	2.356621	-1.331744	0.396242
C	1.330287	-0.468660	-0.388635
C	1.986210	0.869954	-0.745115
C	1.520556	-2.478728	0.946889
C	0.271227	-1.741030	1.442579
C	0.150461	-0.485530	0.587638
C	4.641758	-2.239813	0.790423
C	3.690584	-2.533845	-1.472486
C	0.778927	-1.096185	-1.686181
O	2.166692	1.609379	0.485766
C	2.222747	2.945657	0.419274
O	2.099763	3.566292	-0.610825
C	2.433807	3.550977	1.774041
C	-0.891837	0.341952	0.683789
C	-1.996549	0.081452	1.661371
N	-3.219513	0.052133	1.070273
C	-3.431912	-0.339760	-0.318027
C	-3.116616	0.749459	-1.355552
O	-2.004111	1.484809	-1.255220
C	-1.148266	1.602837	-0.088258
O	-3.786508	0.890732	-2.348199
O	-1.852883	0.004129	2.872221
C	-4.849921	-0.900491	-0.506187
C	-5.012777	-2.222538	0.240456
C	-5.942470	0.096051	-0.122722
H	2.598942	-0.710084	1.270058
H	3.790280	1.644638	-1.593993
H	3.160924	0.243321	-2.417812
H	4.576525	0.297606	0.291442
H	5.224582	-0.355841	-1.202627
H	1.355231	1.460232	-1.410054
H	1.271637	-3.207462	0.171741
H	2.020011	-3.014339	1.754628
H	0.401621	-1.440291	2.484226
H	-0.638938	-2.343588	1.401653
H	4.324663	-3.258262	1.029027
H	5.666421	-2.291435	0.412027
H	4.651686	-1.660268	1.717769
H	3.118359	-3.441387	-1.263729
H	4.710850	-2.838636	-1.720605
H	3.270281	-2.070117	-2.363708
H	-0.044721	-0.482562	-2.058585
H	0.389816	-2.100061	-1.511790
H	1.525723	-1.159822	-2.473320
H	3.341528	3.146237	2.222139
H	1.597239	3.289122	2.423321
H	2.510243	4.631331	1.685714

H	-3.998630	-0.064076	1.701237
H	-2.729397	-1.145564	-0.567540
H	-1.607353	2.349431	0.562839
H	-0.239296	2.032044	-0.492845
H	-4.941400	-1.101317	-1.574325
H	-4.255182	-2.947784	-0.065101
H	-4.939245	-2.095698	1.324153
H	-5.994181	-2.651003	0.029736
H	-5.823766	1.045890	-0.646019
H	-5.960748	0.297261	0.952382
H	-6.919972	-0.312728	-0.384662

ωB97X Energy = -1289.26480747 a.u.

(1*R*,5*R*,9*R*,17*S*)-**13**, Conf A

C	-3.136310	1.674780	-0.509904
C	-3.777079	1.195917	0.790516
C	-3.879363	-0.335379	0.913138
C	-2.477625	-0.892099	0.610109
C	-1.789140	-0.456303	-0.714057
C	-1.751662	1.076184	-0.769820
C	-2.224310	-2.392033	0.679433
C	-0.773738	-2.509334	0.192475
C	-0.481298	-1.243991	-0.606222
C	-4.999530	-0.881542	0.019714
C	-4.234012	-0.683352	2.363220
C	-2.450377	-0.972860	-2.009451
O	-0.824985	1.534284	0.242066
C	-0.297883	2.756979	0.095353
O	-0.535075	3.476714	-0.846078
C	0.592793	3.130916	1.242287
C	0.727648	-0.987074	-1.108620
C	1.857470	-1.958291	-0.932894
N	2.976395	-1.379021	-0.430053
C	2.955686	-0.174703	0.388756
C	2.838216	1.124276	-0.418039
O	1.899864	1.239595	-1.363707
C	1.131735	0.168638	-1.976172
O	3.486144	2.106745	-0.154637
O	1.831876	-3.126193	-1.291733
C	4.152470	-0.145839	1.350364
C	4.023305	-1.248090	2.399342
C	5.501959	-0.211666	0.637279
H	-1.838192	-0.451095	1.388080
H	-3.774791	1.438070	-1.364324
H	-3.039667	2.762069	-0.502602
H	-4.773096	1.639109	0.888267
H	-3.186562	1.570714	1.633677
H	-1.399121	1.436617	-1.736298
H	-2.347276	-2.789734	1.687080
H	-2.903358	-2.944767	0.026199
H	-0.592321	-3.396125	-0.414246
H	-0.084340	-2.566143	1.039925
H	-4.970205	-0.491468	-0.996724
H	-4.970055	-1.972331	-0.038566
H	-5.967830	-0.601684	0.443228
H	-5.153186	-0.171072	2.660670
H	-4.397275	-1.756919	2.487232
H	-3.439442	-0.378212	3.049861
H	-1.785877	-0.784022	-2.855437
H	-3.399638	-0.486683	-2.220115
H	-2.628570	-2.047835	-1.966586
H	1.499488	3.591990	0.853355

H	0.069581	3.865620	1.856905
H	0.842438	2.269266	1.858496
H	3.783409	-1.980094	-0.354325
H	2.045511	-0.188030	1.001732
H	1.734354	-0.196474	-2.810644
H	0.271974	0.682255	-2.392578
H	4.089848	0.817065	1.860128
H	3.070623	-1.182157	2.929867
H	4.094038	-2.244878	1.955463
H	4.825756	-1.160695	3.133988
H	5.593267	0.561290	-0.126609
H	6.305674	-0.066767	1.361386
H	5.673751	-1.183701	0.165753

ωB97X Energy = -1289.26657503 a.u.

(1*R*,5*R*,9*R*,17*S*)-**13**, Conf B

C	-3.136895	1.593009	-0.962390
C	-4.035795	1.278527	0.232450
C	-4.159600	-0.223032	0.552951
C	-2.725960	-0.778003	0.609902
C	-1.799428	-0.523934	-0.610827
C	-1.733943	0.991838	-0.846973
C	-2.485169	-2.238338	0.957859
C	-0.966491	-2.376336	0.789956
C	-0.534397	-1.270415	-0.166774
C	-5.087113	-0.922460	-0.448157
C	-4.789600	-0.370905	1.942933
C	-2.225887	-1.216891	-1.922095
O	-1.052915	1.578776	0.290614
C	-0.520614	2.799502	0.150364
O	-0.504656	3.403397	-0.896713
C	0.036911	3.307842	1.445987
C	0.728756	-1.060841	-0.554144
C	1.818582	-1.932651	0.002868
N	2.947265	-1.303053	0.424843
C	3.285186	0.090767	0.180543
C	3.503444	0.238580	-1.324821
O	2.446427	-0.097937	-2.089527
C	1.113836	0.014436	-1.553845
O	4.537805	0.540188	-1.854607
O	1.716981	-3.147676	0.105067
C	4.478266	0.552987	1.024422
C	4.047591	0.755505	2.474979
C	5.690097	-0.374306	0.940781
H	-2.248044	-0.207081	1.417760
H	-3.586646	1.233150	-1.890394
H	-3.035923	2.673659	-1.080580
H	-5.030670	1.699607	0.057032
H	-3.635405	1.786486	1.116592
H	-1.169647	1.241846	-1.745531
H	-2.804668	-2.483322	1.971259
H	-3.016984	-2.908203	0.277846
H	-0.664374	-3.350635	0.413104
H	-0.458072	-2.244858	1.749400
H	-6.119620	-0.616922	-0.258606
H	-4.867350	-0.678895	-1.486605
H	-5.042060	-2.009176	-0.341690
H	-5.744977	0.159568	1.983734
H	-4.981646	-1.419853	2.182671
H	-4.138993	0.042248	2.718799
H	-3.094546	-0.754147	-2.383251
H	-2.458260	-2.268893	-1.753897
H	-1.411031	-1.176471	-2.648000

H	0.703074	4.145430	1.255486
H	-0.790582	3.643270	2.074276
H	0.560133	2.514409	1.978895
H	3.709272	-1.926452	0.650448
H	2.429412	0.708614	0.465270
H	0.485798	-0.057790	-2.439324
H	0.997467	1.020583	-1.147043
H	4.766415	1.522492	0.609633
H	3.243079	1.490721	2.553610
H	3.696275	-0.181846	2.914460
H	4.888653	1.110400	3.073384
H	6.547694	0.104405	1.416321
H	5.520354	-1.312839	1.477124
H	5.961222	-0.601404	-0.090566

ωB97X Energy = -1289.26642191 a.u.

(1*R*,5*R*,9*R*,17*S*)-**13**, Conf C

C	-3.239430	0.581984	-1.406941
C	-4.163880	-0.319406	-0.591816
C	-3.532762	-1.664066	-0.183907
C	-2.177726	-1.326917	0.460429
C	-1.184120	-0.446846	-0.346380
C	-1.892077	0.855744	-0.735405
C	-1.298464	-2.426132	1.036949
C	-0.085771	-1.624940	1.519870
C	0.006281	-0.400177	0.621643
C	-3.466109	-2.625401	-1.377064
C	-4.424622	-2.313761	0.880530
C	-0.615284	-1.088321	-1.630241
O	-2.097536	1.617402	0.478184
C	-2.212098	2.948153	0.379241
O	-2.117293	3.547887	-0.666029
C	-2.450558	3.576037	1.719014
C	1.030099	0.461813	0.662513
C	2.161236	0.277921	1.618682
N	3.388317	0.627717	1.128506
C	3.932277	0.440056	-0.213070
C	3.153875	0.941474	-1.438140
O	1.936453	1.476867	-1.395482
C	1.198636	1.696673	-0.169492
O	3.685116	0.846525	-2.518140
O	2.024318	-0.037848	2.792700
C	4.401315	-1.013798	-0.479862
C	5.397011	-1.464786	0.583697
C	3.244571	-1.999226	-0.598617
H	-2.443566	-0.693372	1.318657
H	-3.044699	0.145942	-2.389686
H	-3.724376	1.541800	-1.597818
H	-5.082744	-0.502190	-1.157669
H	-4.460136	0.211448	0.319529
H	-1.287428	1.453126	-1.417792
H	-1.776754	-2.964379	1.855662
H	-1.017100	-3.160008	0.277861
H	0.845500	-2.193741	1.534406
H	-0.248367	-1.282310	2.543546
H	-3.085229	-2.161364	-2.285768
H	-2.841081	-3.494384	-1.155893
H	-4.470940	-2.992560	-1.602386
H	-5.447370	-2.412581	0.506374
H	-4.068743	-3.313795	1.141267
H	-4.454331	-1.713941	1.794474
H	0.176571	-0.450237	-2.028979
H	-1.366219	-1.209932	-2.406398

H	-0.180401	-2.068557	-1.430039
H	-3.361076	3.167969	2.158811
H	-1.622651	3.336791	2.387451
H	-2.540896	4.653305	1.609032
H	4.102268	0.600242	1.843069
H	4.829136	1.064610	-0.240623
H	0.257615	2.105602	-0.514678
H	1.710759	2.473788	0.398300
H	4.920535	-0.974402	-1.439459
H	6.218189	-0.751964	0.694935
H	4.915730	-1.590637	1.557526
H	5.826227	-2.429178	0.306569
H	3.625584	-2.990984	-0.848907
H	2.701797	-2.090449	0.346313
H	2.533102	-1.710812	-1.376895

ωB97X Energy = -1289.26601086 a.u.

(1*R*,5*R*,9*R*,17*S*)-**13**, Conf D

C	-3.101507	0.475551	-1.544630
C	-4.054381	-0.395541	-0.729159
C	-3.425193	-1.699725	-0.203233
C	-2.114170	-1.297297	0.493276
C	-1.093589	-0.444896	-0.310236
C	-1.800737	0.817360	-0.815242
C	-1.249715	-2.344665	1.180260
C	-0.068608	-1.499657	1.670101
C	0.034067	-0.313627	0.719793
C	-3.274576	-2.731439	-1.327710
C	-4.366343	-2.299144	0.848184
C	-0.439636	-1.148299	-1.518946
O	-2.091186	1.643903	0.336719
C	-2.220398	2.964183	0.152609
O	-2.071116	3.504161	-0.918555
C	-2.550201	3.664207	1.436055
C	1.034700	0.569610	0.779847
C	2.108776	0.442259	1.816093
N	3.374205	0.550264	1.321940
C	3.798055	0.148449	-0.015855
C	3.363123	1.072482	-1.156276
O	2.120274	1.559544	-1.242213
C	1.247930	1.763725	-0.101026
O	4.121084	1.295845	-2.067662
O	1.897998	0.348379	3.016518
C	3.470162	-1.334854	-0.335679
C	3.903932	-1.740060	-1.741068
C	4.127997	-2.237821	0.704980
H	-2.437192	-0.620067	1.296566
H	-2.843183	-0.012955	-2.487155
H	-3.592606	1.411562	-1.819557
H	-4.935658	-0.631955	-1.333719
H	-4.412401	0.183263	0.129208
H	-1.167313	1.386751	-1.495377
H	-1.761501	-2.838752	2.006509
H	-0.923279	-3.120130	0.483213
H	0.872419	-2.052305	1.728144
H	-0.265500	-1.120356	2.674562
H	-2.838811	-2.320158	-2.237120
H	-2.659247	-3.578124	-1.013102
H	-4.260078	-3.122881	-1.593808
H	-5.363206	-2.444688	0.422943
H	-4.008095	-3.271537	1.195819
H	-4.460978	-1.640961	1.716326
H	0.366793	-0.521459	-1.907259

H	-1.140473	-1.326761	-2.330205
H	-0.005193	-2.109109	-1.238477
H	-3.467258	3.250422	1.856299
H	-1.749645	3.498415	2.158116
H	-2.670622	4.728707	1.254023
H	4.094026	0.521954	2.028735
H	4.883943	0.247621	-0.018631
H	0.329080	2.116796	-0.552388
H	1.668588	2.586963	0.479398
H	2.385373	-1.458313	-0.266669
H	3.366619	-1.193592	-2.517816
H	4.973766	-1.567392	-1.886638
H	3.710882	-2.804209	-1.888240
H	3.875953	-3.281001	0.506459
H	5.217229	-2.141856	0.663988
H	3.803588	-2.005205	1.720982

ωB97X Energy = -1289.26597356 a.u.

(1*R*,5*R*,9*R*,17*S*)-**13**, Conf E

C	-3.011012	1.754301	-0.467756
C	-3.557003	1.319821	0.889843
C	-3.715322	-0.203887	1.040863
C	-2.366028	-0.823938	0.638362
C	-1.763335	-0.431778	-0.739968
C	-1.678522	1.096431	-0.834303
C	-2.176946	-2.334375	0.705783
C	-0.784880	-2.531472	0.087172
C	-0.480602	-1.264138	-0.705168
C	-4.923413	-0.708398	0.242611
C	-3.972140	-0.521698	2.518125
C	-2.535536	-0.945362	-1.973433
O	-0.650407	1.548747	0.079048
C	-0.077531	2.733939	-0.170146
O	-0.346860	3.415032	-1.131473
C	0.918293	3.118618	0.882796
C	0.721459	-1.039260	-1.234588
C	1.821041	-2.055968	-1.087602
N	2.910627	-1.562865	-0.454952
C	2.884198	-0.333518	0.326690
C	3.036060	0.867812	-0.612691
O	2.070069	1.093423	-1.515227
C	1.149452	0.119519	-2.086320
O	3.941696	1.658724	-0.545712
O	1.785264	-3.183681	-1.558070
C	3.923527	-0.346425	1.454320
C	3.710342	0.841103	2.392573
C	3.844692	-1.643367	2.259831
H	-1.650252	-0.404162	1.360061
H	-3.729709	1.532588	-1.260211
H	-2.870996	2.836961	-0.488126
H	-4.520869	1.807688	1.065488
H	-2.879340	1.675959	1.673467
H	-1.404609	1.418807	-1.838971
H	-2.224561	-2.713773	1.726741
H	-2.941181	-2.859336	0.128467
H	-0.725417	-3.409334	-0.556982
H	-0.027762	-2.664794	0.865216
H	-4.952001	-1.800099	0.205503
H	-5.843233	-0.372364	0.728732
H	-4.949881	-0.338681	-0.781542
H	-4.844769	0.030399	2.877874
H	-4.167607	-1.586461	2.668508
H	-3.115772	-0.241970	3.138194

H	-1.927680	-0.794877	-2.868323
H	-3.479433	-0.427433	-2.124454
H	-2.749333	-2.011834	-1.896680
H	1.096474	2.309732	1.588654
H	1.850591	3.411541	0.399637
H	0.533377	3.985008	1.422478
H	3.727691	-2.152834	-0.409196
H	1.893407	-0.248032	0.786743
H	1.650262	-0.259144	-2.980642
H	0.308688	0.721872	-2.411558
H	4.916231	-0.262641	1.001243
H	3.761693	1.795219	1.869678
H	2.737426	0.763551	2.888416
H	4.476039	0.841751	3.170139
H	4.110970	-2.529314	1.682390
H	4.532277	-1.588940	3.105566
H	2.836033	-1.790723	2.657650

ωB97X Energy = -1289.26545843 a.u.

(1*R*,5*R*,9*R*,17*S*)-**13**, Conf F

C	3.058348	1.651661	1.008831
C	3.992459	1.406243	-0.174816
C	4.196184	-0.080451	-0.522202
C	2.792711	-0.703734	-0.618307
C	1.831035	-0.517911	0.587935
C	1.688111	0.987473	0.853387
C	2.627519	-2.167419	-0.996938
C	1.113362	-2.376732	-0.866789
C	0.611722	-1.313521	0.104353
C	5.138630	-0.753786	0.482466
C	4.858128	-0.169439	-1.902269
C	2.262638	-1.215712	1.895134
O	1.000021	1.566203	-0.284381
C	0.412478	2.759752	-0.129045
O	0.356148	3.342013	0.928751
C	-0.154796	3.264951	-1.421708
C	-0.666580	-1.172842	0.471279
C	-1.702416	-2.086234	-0.123898
N	-2.837542	-1.494988	-0.583136
C	-3.216827	-0.110714	-0.343986
C	-3.514199	-0.006255	1.153139
O	-2.472468	-0.299976	1.957214
C	-1.123603	-0.135972	1.481662
O	-4.586861	0.205904	1.649018
O	-1.549651	-3.295482	-0.226397
C	-4.340647	0.343198	-1.282720
C	-5.628911	-0.472235	-1.185686
C	-4.612752	1.834984	-1.102324
H	2.303414	-0.141038	-1.425285
H	3.507538	1.292380	1.937299
H	2.904965	2.723498	1.148119
H	4.962126	1.871757	0.027148
H	3.582831	1.911990	-1.056011
H	1.096560	1.190756	1.746293
H	2.980409	-2.379831	-2.006612
H	3.174151	-2.824432	-0.316087
H	0.846536	-3.372538	-0.520333
H	0.621601	-2.243346	-1.834751
H	4.877707	-0.557157	1.521209
H	5.163852	-1.837305	0.341901
H	6.154602	-0.379544	0.330114
H	5.790451	0.402058	-1.913110
H	5.099358	-1.203709	-2.160560

H	4.204781	0.232619	-2.681636
H	1.430651	-1.228730	2.602465
H	3.096891	-0.720512	2.385235
H	2.550076	-2.251524	1.712756
H	-0.815742	4.105968	-1.228352
H	-0.689880	2.470878	-1.942385
H	0.665958	3.589765	-2.063923
H	-3.569789	-2.138151	-0.847679
H	-2.353108	0.518653	-0.570724
H	-0.530557	-0.213111	2.390880
H	-1.020149	0.882932	1.104667
H	-3.926748	0.198226	-2.286302
H	-6.093045	-0.362600	-0.205750
H	-6.334191	-0.119801	-1.940738
H	-5.472617	-1.536943	-1.376312
H	-5.302367	2.184134	-1.872657
H	-5.063646	2.038242	-0.129345
H	-3.692905	2.420191	-1.186216

ωB97X Energy = -1289.26513353 a.u.

(1*R*,5*R*,9*R*,17*S*)-**13**, Conf G

C	3.420100	1.037470	1.271728
C	4.465201	0.334873	0.410511
C	4.123694	-1.132559	0.095436
C	2.686755	-1.131003	-0.452565
C	1.569700	-0.469766	0.403683
C	1.997053	0.972065	0.712860
C	2.049382	-2.419591	-0.942641
C	0.660873	-1.931525	-1.362274
C	0.337880	-0.730788	-0.485947
C	4.353194	-2.026899	1.319751
C	5.061786	-1.621774	-1.013967
C	1.249553	-1.174788	1.738847
O	1.918991	1.724904	-0.519908
C	1.697315	3.043694	-0.444447
O	1.529427	3.631878	0.598167
C	1.674837	3.671348	-1.805286
C	-0.857390	-0.117795	-0.466117
C	-1.965920	-0.580403	-1.355609
N	-3.254916	-0.352044	-0.968534
C	-3.887462	0.330993	0.156679
C	-3.187468	0.100402	1.500378
O	-1.925790	0.528776	1.614029
C	-1.221340	1.012469	0.446633
O	-3.729691	-0.360831	2.470027
O	-1.774563	-1.157927	-2.420726
C	-5.376038	-0.052404	0.227599
C	-6.151182	0.572386	-0.931777
C	-5.618387	-1.558112	0.303959
H	2.743697	-0.485188	-1.340623
H	3.404022	0.610751	2.277504
H	3.681938	2.090207	1.400019
H	5.439105	0.388937	0.907019
H	4.567193	0.875680	-0.536753
H	1.341368	1.441419	1.444590
H	2.586876	-2.865696	-1.779918
H	1.990381	-3.170861	-0.151252
H	-0.117701	-2.691962	-1.303581
H	0.680445	-1.602505	-2.402618
H	5.427264	-2.147971	1.483908
H	3.933559	-1.618099	2.237838
H	3.928865	-3.023138	1.171500
H	6.104403	-1.470792	-0.720895

H	4.922713	-2.687789	-1.210618
H	4.890679	-1.078469	-1.947557
H	2.043747	-1.060909	2.472633
H	1.077401	-2.242105	1.596028
H	0.338277	-0.748761	2.163899
H	0.911267	3.191958	-2.418693
H	1.468780	4.734535	-1.715817
H	2.637976	3.519078	-2.293642
H	-3.903412	-0.662900	-1.676844
H	-3.853763	1.417288	-0.000496
H	-0.361286	1.523799	0.853148
H	-1.829438	1.762559	-0.061085
H	-5.741426	0.397717	1.153179
H	-5.993375	1.651896	-0.984682
H	-5.871876	0.142363	-1.898429
H	-7.219866	0.393286	-0.801945
H	-6.680690	-1.747815	0.469504
H	-5.340921	-2.062397	-0.625234
H	-5.061601	-2.013953	1.122329

ωB97X Energy = -1289.26509896 a.u.

(1*R*,5*R*,9*R*,17*S*)-**13**, Conf H

C	-3.037833	1.704260	-0.712614
C	-3.669361	1.444798	0.652213
C	-3.862859	-0.047450	0.978344
C	-2.508389	-0.731164	0.724971
C	-1.826348	-0.515566	-0.656002
C	-1.699109	0.991005	-0.915835
C	-2.355293	-2.224639	0.980956
C	-0.934164	-2.510599	0.476147
C	-0.568819	-1.366068	-0.462845
C	-5.039453	-0.632143	0.188264
C	-4.198979	-0.178213	2.468427
C	-2.547483	-1.154725	-1.861989
O	-0.720458	1.522197	0.008004
C	-0.123325	2.676756	-0.315522
O	-0.338882	3.272439	-1.344922
C	0.825429	3.145579	0.746989
C	0.650720	-1.242725	-0.989223
C	1.718289	-2.257395	-0.699233
N	2.866058	-1.701033	-0.237855
C	2.910219	-0.405300	0.432277
C	2.936827	0.765988	-0.556002
O	1.980166	0.851260	-1.490354
C	1.121335	-0.215344	-1.976072
O	3.711012	1.685909	-0.472702
O	1.619927	-3.453079	-0.932778
C	4.050370	-0.396344	1.464376
C	5.447559	-0.469248	0.849118
C	3.928815	0.767775	2.444087
H	-1.821435	-0.239569	1.428614
H	-3.713422	1.395301	-1.513585
H	-2.876752	2.774492	-0.855401
H	-4.633226	1.959992	0.709874
H	-3.032772	1.887606	1.426029
H	-1.353330	1.196600	-1.928791
H	-2.470618	-2.479848	2.034661
H	-3.094325	-2.803937	0.423078
H	-0.845625	-3.468752	-0.035645
H	-0.223950	-2.536245	1.307266
H	-4.999230	-0.410037	-0.877093
H	-5.097016	-1.717386	0.302323
H	-5.974037	-0.212241	0.569902

H	-5.077466	0.425490	2.712765
H	-4.422805	-1.213910	2.736490
H	-3.369124	0.163544	3.093360
H	-1.892603	-1.118683	-2.735521
H	-3.470916	-0.642519	-2.120655
H	-2.787420	-2.202069	-1.675319
H	0.938896	2.410467	1.541415
H	0.441219	4.075234	1.168923
H	1.792316	3.354971	0.289254
H	3.624551	-2.342644	-0.057394
H	1.972884	-0.275989	0.986428
H	1.678152	-0.708573	-2.776189
H	0.293616	0.316153	-2.432427
H	3.887942	-1.315942	2.037579
H	5.546632	-1.282918	0.126088
H	5.699425	0.463113	0.344167
H	6.184550	-0.643107	1.635443
H	4.668328	0.657601	3.239735
H	4.102177	1.722564	1.947272
H	2.939984	0.793242	2.909366

ωB97X Energy = -1289.26499493 a.u.

(1*R*,5*R*,9*R*,17*S*)-**13**, Conf I

C	-2.836357	1.617098	-1.165714
C	-3.891192	1.402967	-0.081581
C	-4.152978	-0.074547	0.266605
C	-2.775588	-0.718493	0.502277
C	-1.699449	-0.567066	-0.610881
C	-1.498026	0.937082	-0.859921
C	-2.669192	-2.174895	0.922253
C	-1.152254	-2.386536	0.967108
C	-0.549287	-1.390979	-0.012507
C	-5.012230	-0.748222	-0.810327
C	-4.940997	-0.129747	1.580643
C	-2.031044	-1.266303	-1.946040
O	-0.931096	1.498650	0.346247
C	-0.361120	2.708590	0.275214
O	-0.245563	3.334647	-0.751819
C	0.059400	3.193951	1.629957
C	0.755664	-1.338182	-0.315776
C	1.746924	-2.248176	0.331597
N	3.010939	-1.756836	0.474164
C	3.523416	-0.403229	0.678746
C	2.682837	0.804842	0.258250
O	1.860148	0.798298	-0.789793
C	1.370136	-0.440649	-1.347458
O	2.847558	1.846613	0.844096
O	1.512228	-3.410761	0.639600
C	4.938222	-0.306724	0.043929
C	4.916160	-0.400170	-1.478179
C	5.711839	0.920428	0.512968
H	-2.355649	-0.148816	1.342145
H	-3.194008	1.250744	-2.130706
H	-2.654788	2.684238	-1.302027
H	-4.827841	1.878331	-0.389369
H	-3.567165	1.917925	0.829418
H	-0.806206	1.135796	-1.677971
H	-3.133892	-2.368516	1.889536
H	-3.136584	-2.842967	0.194304
H	-0.842652	-3.400505	0.727150
H	-0.765693	-2.176166	1.969184
H	-4.663871	-0.557982	-1.824227
H	-5.056420	-1.830863	-0.667268

H	-6.034757	-0.366437	-0.745997
H	-5.858321	0.459615	1.496840
H	-5.226565	-1.155042	1.829326
H	-4.354894	0.271787	2.412013
H	-1.150056	-1.279400	-2.590375
H	-2.829164	-0.773355	-2.493763
H	-2.328632	-2.303091	-1.784189
H	-0.822180	3.585226	2.142820
H	0.470806	2.379911	2.223283
H	0.793490	3.988060	1.522444
H	3.634594	-2.455732	0.855190
H	3.646854	-0.248471	1.753614
H	2.190407	-0.945423	-1.858242
H	0.657679	-0.126784	-2.101641
H	5.462708	-1.188006	0.429263
H	4.427831	-1.314343	-1.820570
H	4.404253	0.458639	-1.923282
H	5.937117	-0.406982	-1.863857
H	5.706993	1.007244	1.601497
H	6.749347	0.842429	0.182654
H	5.295192	1.840969	0.100032

ωB97X Energy = -1289.26449372 a.u.

(1*R*,5*R*,9*R*,17*S*)-**13**, Conf J

C	-2.998429	0.737193	-1.628195
C	-4.113720	0.103649	-0.797434
C	-3.757259	-1.266208	-0.187396
C	-2.397170	-1.090138	0.508321
C	-1.224121	-0.502468	-0.322792
C	-1.666368	0.855024	-0.883932
C	-1.757057	-2.241262	1.270547
C	-0.446775	-1.603934	1.747690
C	-0.095687	-0.536256	0.717089
C	-3.810181	-2.372166	-1.248663
C	-4.804216	-1.604590	0.880394
C	-0.741702	-1.387813	-1.489428
O	-1.816514	1.757302	0.239011
C	-1.749740	3.074720	0.008681
O	-1.514802	3.549843	-1.077817
C	-1.994647	3.859273	1.262148
C	1.054094	0.144038	0.715150
C	2.042787	-0.122824	1.813831
N	3.312161	-0.424766	1.444111
C	3.892449	-0.328115	0.113331
C	3.847213	1.131833	-0.336078
O	2.690676	1.805760	-0.208279
C	1.409934	1.165328	-0.346305
O	4.827770	1.729322	-0.693218
O	1.729257	-0.105594	2.996926
C	3.373554	-1.357197	-0.910748
C	4.036169	-1.135136	-2.267158
C	3.635125	-2.767940	-0.394308
H	-2.585381	-0.317936	1.266972
H	-2.825993	0.167543	-2.544310
H	-3.297465	1.736299	-1.952195
H	-5.012239	0.006479	-1.414841
H	-4.372014	0.786053	0.019680
H	-0.922707	1.277087	-1.560680
H	-2.367102	-2.583468	2.107158
H	-1.571795	-3.102864	0.624290
H	0.366362	-2.321143	1.878186
H	-0.596422	-1.123277	2.715459
H	-3.306937	-2.105812	-2.177031

H	-3.366928	-3.300861	-0.880268
H	-4.853373	-2.582343	-1.499394
H	-5.807928	-1.575067	0.447382
H	-4.647633	-2.606310	1.288698
H	-4.771189	-0.890569	1.707980
H	0.186161	-0.989640	-1.906154
H	-1.457915	-1.440092	-2.304796
H	-0.539241	-2.406109	-1.156287
H	-3.017550	3.688035	1.600450
H	-1.321982	3.520021	2.050049
H	-1.843311	4.917924	1.069150
H	3.953842	-0.534226	2.214680
H	4.957499	-0.526635	0.239557
H	1.353778	0.740400	-1.351560
H	0.719784	2.005202	-0.304753
H	2.294391	-1.241964	-1.026979
H	3.807644	-0.152271	-2.686571
H	5.123684	-1.222223	-2.187352
H	3.690130	-1.886371	-2.978764
H	3.254773	-3.503758	-1.105133
H	4.708100	-2.941565	-0.269390
H	3.147203	-2.940297	0.566535

ωB97X Energy = -1289.26440523 a.u.

(2*R*,8*R*,10*R*,13*R*)-**15**, Conf A

C	0.689980	-2.389164	0.728934
C	0.667119	-0.886348	0.479008
C	0.233271	-0.370068	-0.869453
C	1.612582	-3.182074	-0.201154
C	1.857006	3.460799	-0.099800
C	3.312634	3.153380	-0.442714
C	3.731225	1.844043	0.143831
C	3.790781	0.720920	-0.558350
C	-0.710054	0.839382	-0.758752
C	-0.057772	2.036065	-0.066967
O	1.072453	2.377938	-0.672394
C	3.085404	-2.848070	-0.041646
C	3.934832	-0.590127	0.108895
O	3.255777	-1.514964	-0.588136
O	-0.538932	2.615059	0.874690
O	0.944937	-0.132300	1.388750
O	1.022133	-2.646113	2.071955
C	3.996090	-3.798387	-0.789134
O	4.508109	-0.807107	1.149998
C	1.383632	4.782379	-0.665603
N	-1.930970	0.529951	-0.063709
C	-3.013481	-0.073091	-0.631406
C	-2.967805	-0.558217	-1.954404
C	-4.056850	-1.177844	-2.527049
C	-5.243539	-1.353047	-1.817795
C	-5.311126	-0.884880	-0.524311
C	-4.225718	-0.246271	0.088095
C	-4.365526	0.250387	1.466717
O	-3.518409	0.865716	2.088336
O	-5.552793	-0.029786	2.027136
H	-0.341384	-2.718178	0.533854
H	-0.260300	-1.163438	-1.432552
H	1.134420	-0.092553	-1.421380
H	1.470350	-4.239269	0.032034
H	1.315030	-3.040387	-1.243933
H	1.709436	3.433200	0.981489
H	3.923306	3.967662	-0.045557

H	3.427488	3.142789	-1.529613
H	3.892517	1.803657	1.218895
H	3.581453	0.706973	-1.622777
H	-0.923266	1.181634	-1.777658
H	3.349277	-2.815521	1.015470
H	1.131230	-1.784863	2.500521
H	5.037923	-3.493528	-0.680578
H	3.890574	-4.806931	-0.386178
H	3.744442	-3.819908	-1.851628
H	1.967409	5.597545	-0.235124
H	0.332960	4.949489	-0.427247
H	1.509099	4.800168	-1.750093
H	-2.067116	0.960770	0.841287
H	-2.065871	-0.445793	-2.540886
H	-3.978728	-1.534475	-3.548219
H	-6.095010	-1.842881	-2.272498
H	-6.224168	-1.004002	0.044604
H	-5.546586	0.342038	2.919402

ωB97X Energy = -1472.05464606 a.u.

(2*R*,8*R*,10*R*,13*R*)-**15**, Conf B

C	0.851516	-2.379643	0.571453
C	0.605834	-0.886147	0.398092
C	0.095493	-0.390714	-0.932307
C	1.842935	-2.981791	-0.429238
C	1.792203	3.337013	-0.180683
C	3.206174	2.997110	-0.655747
C	3.459217	1.529557	-0.534522
C	4.171864	0.936617	0.414964
C	-0.860856	0.807264	-0.803565
C	-0.198218	2.013772	-0.142240
O	0.917680	2.342569	-0.784331
C	3.290630	-2.618481	-0.156013
C	4.255370	-0.535370	0.541280
O	3.366549	-1.173557	-0.233690
O	-0.645915	2.602092	0.808401
O	0.759664	-0.143498	1.344437
O	1.253541	-2.649855	1.891994
C	4.250823	-3.232874	-1.153030
O	5.021788	-1.101441	1.287935
C	1.353198	4.730516	-0.570978
N	-2.056700	0.491229	-0.071455
C	-3.152002	-0.121945	-0.600438
C	-3.151787	-0.598532	-1.927553
C	-4.256249	-1.224062	-2.462717
C	-5.413676	-1.415384	-1.710147
C	-5.435585	-0.958376	-0.411241
C	-4.333577	-0.313803	0.164180
C	-4.424320	0.167881	1.552003
O	-3.557826	0.781382	2.148408
O	-5.588435	-0.124916	2.153109
H	-0.129216	-2.841098	0.383547
H	-0.413987	-1.202912	-1.454313
H	0.961151	-0.119953	-1.542739
H	1.756741	-4.068874	-0.372403
H	1.567918	-2.694742	-1.448330
H	1.728062	3.199821	0.900681
H	3.911073	3.574016	-0.053717
H	3.317086	3.307330	-1.698685
H	2.959070	0.902582	-1.263682
H	4.721423	1.492620	1.166967
H	-1.108274	1.137029	-1.818708
H	3.555611	-2.908140	0.860432

H	1.229337	-1.805183	2.364912
H	4.006324	-2.915979	-2.169168
H	5.277004	-2.939486	-0.928771
H	4.188788	-4.321455	-1.104905
H	2.048641	5.462492	-0.156184
H	0.356406	4.944786	-0.186103
H	1.348216	4.836309	-1.657691
H	-2.155273	0.896575	0.849832
H	-2.273231	-0.474755	-2.546548
H	-4.213912	-1.573056	-3.488639
H	-6.277274	-1.909830	-2.136062
H	-6.324208	-1.091213	0.192277
H	-5.550876	0.236664	3.048777

ωB97X Energy = -1472.05455618 a.u.

(2*R*,8*R*,10*R*,13*R*)-**15**, Conf C

C	1.580896	-2.533494	-0.299107
C	0.903105	-1.191667	-0.052467
C	0.370374	-0.425849	-1.238695
C	2.776103	-2.486725	-1.254716
C	0.928247	3.309675	0.587662
C	2.404960	3.479846	0.226751
C	3.045597	2.144633	0.023902
C	3.791834	1.498064	0.910870
C	-0.871144	0.420727	-0.931436
C	-0.596187	1.536121	0.087225
O	0.400639	2.315535	-0.333583
C	4.018572	-1.851956	-0.659343
C	4.277517	0.118932	0.683877
O	3.660593	-0.483887	-0.343160
O	-1.212779	1.706122	1.105971
O	0.737176	-0.808511	1.086728
O	1.951318	-3.117386	0.925360
C	5.197731	-1.864016	-1.609808
O	5.119024	-0.417800	1.368433
C	0.137015	4.594132	0.483883
N	-1.961196	-0.422179	-0.526117
C	-3.276533	-0.038294	-0.550027
C	-3.692225	1.112404	-1.245998
C	-5.023328	1.460436	-1.318939
C	-6.006083	0.689927	-0.700106
C	-5.619638	-0.431683	-0.001474
C	-4.275377	-0.814039	0.092573
C	-3.921884	-2.009568	0.877429
O	-2.791359	-2.409238	1.093261
O	-4.981347	-2.665457	1.373609
H	0.800875	-3.144184	-0.777937
H	0.131710	-1.116030	-2.049758
H	1.177421	0.218502	-1.595998
H	3.024844	-3.515087	-1.525006
H	2.497230	-1.973763	-2.179626
H	0.845707	2.886903	1.590897
H	2.887129	4.033849	1.034714
H	2.485279	4.073165	-0.688216
H	2.820831	1.648726	-0.913556
H	4.084228	1.937110	1.858740
H	-1.120609	0.921681	-1.869426
H	4.273998	-2.351039	0.274985
H	1.618915	-2.534520	1.623151
H	6.063425	-1.382947	-1.153330
H	5.467402	-2.893437	-1.851909
H	4.950468	-1.342544	-2.536956
H	-0.903941	4.430927	0.762850

H	0.176904	4.984205	-0.535214
H	0.561487	5.341440	1.156869
H	-1.754019	-1.138022	0.157718
H	-2.962804	1.745244	-1.733515
H	-5.301634	2.354637	-1.865694
H	-7.050117	0.969508	-0.760599
H	-6.363114	-1.040423	0.496533
H	-4.646664	-3.419300	1.877822

ωB97X Energy = -1472.05325259 a.u.

(2*R*,8*R*,10*R*,13*R*)-**15**, Conf D

C	1.532461	-2.551302	0.043117
C	1.025163	-1.116984	0.144256
C	0.482346	-0.437129	-1.089487
C	2.676489	-2.765774	-0.951795
C	0.851290	3.450226	0.627540
C	2.339763	3.677222	0.371917
C	3.127897	2.450465	0.700615
C	3.526223	1.582893	-0.219605
C	-0.765347	0.416847	-0.832871
C	-0.528583	1.551600	0.176640
O	0.457819	2.347366	-0.232383
C	3.960977	-2.047372	-0.578142
C	4.057139	0.255001	0.152430
O	3.705794	-0.635589	-0.789066
O	-1.183992	1.728350	1.170725
O	1.017297	-0.568701	1.227182
O	1.909545	-3.015005	1.316545
C	5.143797	-2.459180	-1.428411
O	4.656130	-0.023731	1.163859
C	0.008805	4.666660	0.307504
N	-1.869751	-0.419357	-0.456492
C	-3.183701	-0.048697	-0.534128
C	-3.573581	1.135672	-1.188550
C	-4.902389	1.475023	-1.316946
C	-5.908995	0.663143	-0.796301
C	-5.548814	-0.490913	-0.137963
C	-4.207449	-0.867030	0.009709
C	-3.882639	-2.102612	0.741375
O	-2.759850	-2.513988	0.977492
O	-4.958438	-2.785078	1.160330
H	0.667427	-3.126821	-0.318542
H	0.249388	-1.172066	-1.861202
H	1.283248	0.198460	-1.474177
H	2.876484	-3.838815	-0.980826
H	2.367180	-2.469532	-1.958072
H	0.689079	3.134682	1.660043
H	2.656627	4.519098	0.991857
H	2.481629	3.954933	-0.675657
H	3.286686	2.219642	1.751704
H	3.336704	1.752926	-1.274145
H	-0.984789	0.906394	-1.785196
H	4.178032	-2.197340	0.479457
H	1.711337	-2.304206	1.943116
H	6.030597	-1.887266	-1.151459
H	5.358262	-3.518398	-1.277958
H	4.934672	-2.293111	-2.487311
H	0.305578	5.499709	0.946914
H	-1.047566	4.459760	0.481255
H	0.146802	4.961461	-0.734719
H	-1.688626	-1.194212	0.167089
H	-2.825251	1.801866	-1.596721
H	-5.160468	2.395372	-1.829154

H	-6.951284	0.936175	-0.900695
H	-6.311752	-1.132875	0.282966
H	-4.641288	-3.565873	1.633965

ωB97X Energy = -1472.05300750 a.u.

(2*R*,8*R*,10*R*,13*R*)-**15**, Conf E

C	0.699519	-2.389354	0.736594
C	0.669381	-0.887719	0.481075
C	0.227565	-0.378383	-0.867578
C	1.622272	-3.181683	-0.193865
C	1.837921	3.462377	-0.114164
C	3.293725	3.159553	-0.460118
C	3.719375	1.853931	0.129619
C	3.782994	0.729019	-0.569312
C	-0.720599	0.826891	-0.755673
C	-0.069469	2.028184	-0.070430
O	1.056071	2.373776	-0.680505
C	3.094234	-2.841337	-0.039950
C	3.934115	-0.579316	0.101719
O	3.257727	-1.509256	-0.591084
O	-0.550807	2.607166	0.871755
O	0.947836	-0.128905	1.386705
O	1.037291	-2.640024	2.079425
C	4.006489	-3.790399	-0.787092
O	4.510331	-0.790449	1.142402
C	1.357177	4.779527	-0.683925
N	-1.934212	0.514571	-0.046804
C	-3.027885	-0.082385	-0.609748
C	-2.969712	-0.566594	-1.932917
C	-4.047190	-1.189167	-2.524856
C	-5.240958	-1.370508	-1.832191
C	-5.320180	-0.905019	-0.538780
C	-4.249248	-0.262572	0.093173
C	-4.520210	0.178148	1.481117
O	-5.544315	-0.050909	2.084292
O	-3.529411	0.885314	2.058636
H	-0.331055	-2.723515	0.546334
H	-0.264429	-1.176345	-1.425457
H	1.124867	-0.098398	-1.424505
H	1.484868	-4.238666	0.043113
H	1.320835	-3.044432	-1.236120
H	1.693311	3.438122	0.967598
H	3.902097	3.977713	-0.067427
H	3.405628	3.145756	-1.547283
H	3.882736	1.817571	1.204518
H	3.571953	0.710839	-1.633336
H	-0.941401	1.166842	-1.773728
H	3.361157	-2.804333	1.016250
H	1.146075	-1.776867	2.504154
H	3.906409	-4.797950	-0.380293
H	3.751627	-3.816692	-1.848707
H	5.047360	-3.480803	-0.682825
H	1.939023	5.598795	-0.258671
H	0.306590	4.943397	-0.442933
H	1.479193	4.793293	-1.768851
H	-2.054766	0.987270	0.835537
H	-2.061804	-0.451240	-2.508961
H	-3.951595	-1.541370	-3.546053
H	-6.086393	-1.861701	-2.296578
H	-6.234052	-1.024909	0.030239
H	-3.812425	1.122771	2.952409

ωB97X Energy = -1472.05141225 a.u.

(2*R*,8*R*,10*R*,13*R*)-**15**, Conf F

C	0.858767	-2.378545	0.588040
C	0.607190	-0.887160	0.405656
C	0.089197	-0.402419	-0.925759
C	1.848976	-2.983648	-0.412145
C	1.776415	3.336245	-0.201274
C	3.188967	2.998664	-0.682046
C	3.447928	1.532782	-0.553026
C	4.168313	0.948443	0.395930
C	-0.870539	0.793004	-0.800190
C	-0.208380	2.004696	-0.147362
O	0.902527	2.335008	-0.795340
C	3.296278	-2.613457	-0.146375
C	4.257390	-0.522424	0.531489
O	3.366891	-1.168789	-0.234659
O	-0.655124	2.594950	0.803143
O	0.763067	-0.137480	1.346153
O	1.266204	-2.638639	1.908959
C	4.255325	-3.231859	-1.142011
O	5.029432	-1.080862	1.278103
C	1.329671	4.725660	-0.597058
N	-2.060690	0.478248	-0.056251
C	-3.164954	-0.133916	-0.578077
C	-3.148158	-0.619843	-1.902091
C	-4.239440	-1.253800	-2.454941
C	-5.406314	-1.446766	-1.720354
C	-5.444113	-0.981887	-0.424971
C	-4.358257	-0.327723	0.168446
C	-4.584050	0.110244	1.565102
O	-5.583442	-0.129531	2.204536
O	-3.580535	0.827434	2.107645
H	-0.120867	-2.844837	0.406623
H	-0.419497	-1.220092	-1.439818
H	0.950922	-0.132541	-1.542146
H	1.766850	-4.070612	-0.347713
H	1.569491	-2.704452	-1.432196
H	1.718309	3.204383	0.881087
H	3.895027	3.581853	-0.087481
H	3.292974	3.302778	-1.727486
H	2.945521	0.899388	-1.275054
H	4.720595	1.511196	1.140871
H	-1.122945	1.118158	-1.815604
H	3.565646	-2.894706	0.871292
H	1.243960	-1.790427	2.375552
H	5.281084	-2.932643	-0.923642
H	4.197818	-4.320256	-1.085005
H	4.006020	-2.924035	-2.159766
H	2.024632	5.462605	-0.190387
H	0.334265	4.938338	-0.207723
H	1.318097	4.825222	-1.684293
H	-2.146729	0.929277	0.840919
H	-2.261890	-0.497066	-2.509637
H	-4.176318	-1.606512	-3.478487
H	-6.262494	-1.946811	-2.154611
H	-6.335365	-1.111318	0.176912
H	-3.833746	1.060889	3.011331

ωB97X Energy = -1472.05131062 a.u.

(2*R*,8*R*,10*R*,13*S*)-**15**, Conf A

C	2.870385	-1.859834	1.570981
C	1.831209	-0.771522	1.322029

C	0.608513	-1.103341	0.507874
C	3.495558	-2.452621	0.304972
C	-0.201358	3.065593	-0.152267
C	0.766871	3.332192	-1.303329
C	2.092135	2.692319	-1.040097
C	2.432429	1.510600	-1.535949
C	-0.677443	-0.452781	1.027601
C	-0.595335	1.078404	1.114016
O	-0.336117	1.622470	-0.070013
C	4.321887	-1.464913	-0.499558
C	3.619132	0.782431	-1.041091
O	3.375477	-0.537190	-1.088687
O	-0.800841	1.702270	2.126185
O	1.991275	0.321708	1.823936
O	3.876290	-1.369992	2.424179
C	5.116238	-2.119649	-1.609456
O	4.631537	1.271903	-0.599141
C	-1.563839	3.688022	-0.372255
N	-1.756131	-0.870064	0.163891
C	-3.084612	-0.698688	0.441318
C	-3.512428	-0.243908	1.703470
C	-4.853235	-0.113467	1.994739
C	-5.831396	-0.417894	1.049937
C	-5.432605	-0.852134	-0.194597
C	-4.079733	-0.997988	-0.525012
C	-3.713134	-1.448538	-1.877997
O	-2.577058	-1.576285	-2.299453
O	-4.765359	-1.720326	-2.663708
H	2.320295	-2.666493	2.076099
H	0.458631	-2.183678	0.471364
H	0.808670	-0.767181	-0.514686
H	4.148115	-3.268156	0.623508
H	2.721550	-2.890373	-0.331718
H	0.228063	3.409372	0.790904
H	0.872175	4.414589	-1.405397
H	0.330350	2.945147	-2.227661
H	2.754311	3.177632	-0.326543
H	1.773412	0.968534	-2.205708
H	-0.861312	-0.797871	2.047660
H	4.979222	-0.900382	0.161754
H	3.632528	-0.459989	2.647821
H	5.845702	-2.812312	-1.186679
H	4.456923	-2.675528	-2.279461
H	5.654010	-1.367963	-2.189057
H	-2.006669	3.315616	-1.298305
H	-1.468099	4.772651	-0.444021
H	-2.231728	3.455284	0.457817
H	-1.536785	-1.072811	-0.801943
H	-2.782434	0.019412	2.457129
H	-5.142936	0.238745	2.978663
H	-6.882494	-0.308787	1.284688
H	-6.173235	-1.087953	-0.947745
H	-4.422411	-1.997210	-3.524077

ωB97X Energy = -1472.05179791 a.u.

(2*R*,8*R*,10*R*,13*S*)-**15**, Conf B

C	-2.671799	-2.041254	-1.444845
C	-1.641034	-0.924230	-1.327286
C	-0.414145	-1.169607	-0.487784
C	-3.252784	-2.517005	-0.109241
C	-0.101681	2.960240	0.248520
C	-1.114177	3.040029	1.393142
C	-2.103560	1.925125	1.289255

C	-3.351406	2.024375	0.848582	H	-3.808788	2.973990	0.592531
C	0.832691	-0.435728	-0.989276	H	1.035982	-0.746529	-2.016499
C	0.646561	1.086401	-1.036335	H	-5.051527	-1.352693	-0.209815
O	0.282232	1.562134	0.151673	H	-3.461462	-0.774150	-2.654494
C	-4.253113	-1.554647	0.503558	H	-5.348127	-2.998574	1.654740
C	-4.216134	0.839795	0.651947	H	-4.025903	-2.220953	2.542431
O	-3.537620	-0.314692	0.724633	H	-5.531896	-1.334919	2.224437
O	0.845536	1.763277	-2.013770	H	1.643400	3.512908	1.376960
O	-1.796261	0.097984	-1.961017	H	0.813330	4.866542	0.591673
O	-3.698868	-1.652652	-2.323456	H	1.800494	3.761213	-0.375984
C	-4.822996	-2.055267	1.814516	H	1.735732	-1.039729	0.827005
O	-5.402476	0.906199	0.420612	H	2.898763	0.181783	-2.417885
C	1.118454	3.825318	0.471946	H	5.241069	0.516874	-2.957092
N	1.937030	-0.800470	-0.134260	H	7.020785	0.018137	-1.289458
C	3.253324	-0.562513	-0.420045	H	6.369942	-0.830657	0.934815
C	3.647414	-0.064409	-1.676888	H	4.687210	-1.857857	3.512599
C	4.977782	0.132843	-1.977686	ωB97X Energy = -1472.05165692 a.u.			
C	5.978100	-0.143163	-1.047360				
C	5.611847	-0.616947	0.192585	(2*R*,8*R*,10*R*,13*S*)-**15**, Conf C			
C	4.270315	-0.831637	0.532246				
C	3.938131	-1.322150	1.880055	C	-0.087686	2.514505	-1.831820
O	2.813437	-1.516292	2.306803	C	0.797422	1.269850	-1.775853
O	5.008893	-1.549731	2.654671	C	0.308346	0.029133	-2.495052
H	-2.116126	-2.883775	-1.880890	C	-1.378435	2.373021	-0.998686
H	-0.197732	-2.239038	-0.449031	C	3.551153	-1.476401	0.440746
H	-0.649463	-0.854521	0.534515	C	3.478457	-0.756205	1.789293
H	-3.768118	-3.463290	-0.286090	C	2.833874	0.582812	1.627415
H	-2.445616	-2.724146	0.599445	C	1.566869	0.814257	1.945718
H	-0.593318	3.220676	-0.691068	C	0.483776	-1.278625	-1.698826
H	-1.604115	4.014527	1.344383	C	1.960476	-1.475126	-1.349400
H	-0.582473	2.973726	2.346642	O	2.182419	-1.553872	-0.043858
H	-1.730964	0.940504	1.547108	C	-1.256069	2.669176	0.490782

C	0.873492	2.004779	1.423170
O	-0.392207	1.689960	1.121751
O	2.810460	-1.555501	-2.200783
O	1.882264	1.294118	-1.241342
O	0.630691	3.683640	-1.532883
C	-2.595646	2.571934	1.191223
O	1.368959	3.093070	1.208974
C	4.137212	-2.867171	0.544752
N	-0.358826	-1.348659	-0.530848
C	-1.713762	-1.488450	-0.565769
C	-2.397475	-1.682241	-1.783568
C	-3.771398	-1.785952	-1.826124
C	-4.538733	-1.699081	-0.666732
C	-3.891146	-1.524665	0.536630
C	-2.497138	-1.428366	0.617690
C	-1.865968	-1.304258	1.941481
O	-0.684753	-1.476269	2.178969
O	-2.724476	-0.991690	2.923806
H	-0.395659	2.602779	-2.878890
H	0.893498	-0.037006	-3.417191
H	-0.734803	0.140169	-2.790137
H	-2.102598	3.085806	-1.398770
H	-1.810431	1.375551	-1.130570
H	4.112580	-0.875388	-0.277333
H	4.500263	-0.659712	2.164358
H	2.913550	-1.373336	2.492810
H	3.394970	1.347135	1.095766
H	0.943948	0.049200	2.394971
H	0.250744	-2.103139	-2.380438
H	-0.818277	3.655865	0.643866
H	1.045045	3.580050	-0.661252
H	-3.024948	1.575016	1.061023
H	-2.481682	2.767953	2.257778
H	-3.288615	3.305548	0.776980
H	3.541040	-3.482257	1.221671
H	5.155047	-2.808534	0.933994
H	4.169029	-3.345695	-0.434287
H	0.078612	-1.281229	0.375961
H	-1.842729	-1.764623	-2.708423
H	-4.254304	-1.939582	-2.784823
H	-5.617528	-1.777888	-0.707449
H	-4.461768	-1.470231	1.455025
H	-2.225789	-0.971047	3.751804

ωB97X Energy = -1472.05138767 a.u.

(2*R*,8*R*,10*R*,13*S*)-**15**, Conf D

C	-2.190441	-2.451531	-0.991473
C	-1.522250	-1.084711	-1.094984
C	-0.218534	-0.844272	-0.381983
C	-2.566190	-2.872160	0.432847
C	-0.586203	3.430538	-0.606431
C	-1.540912	3.647361	0.565649
C	-2.636870	2.630851	0.550614
C	-2.617370	1.540634	1.305109
C	0.776269	0.006222	-1.190908
C	0.259049	1.398764	-1.547517
O	-0.060849	2.084112	-0.453043
C	-3.616710	-1.987977	1.081328
C	-3.562800	0.428293	1.075173
O	-2.956029	-0.730933	1.375286
O	0.208849	1.832622	-2.670047
O	-2.032669	-0.230461	-1.791149
O	-3.325305	-2.490437	-1.823100

C	-4.165694	-2.560616	2.370684
O	-4.682318	0.515663	0.629265
C	0.561180	4.417260	-0.625781
N	2.014920	0.202705	-0.468860
C	2.995244	-0.744513	-0.347369
C	2.993948	-1.907367	-1.141106
C	4.005636	-2.838010	-1.043458
C	5.062811	-2.664674	-0.152142
C	5.079044	-1.537528	0.638574
C	4.067676	-0.571818	0.565739
C	4.130045	0.602874	1.452218
O	3.289628	1.481774	1.526768
O	5.228687	0.644244	2.220057
H	-1.441263	-3.165403	-1.361325
H	0.256281	-1.793514	-0.124737
H	-0.450657	-0.334555	0.557538
H	-2.961796	-3.887952	0.369900
H	-1.675269	-2.911830	1.066069
H	-1.132912	3.460703	-1.550731
H	-1.947326	4.657539	0.477870
H	-0.976017	3.588784	1.499564
H	-3.425583	2.749827	-0.189064
H	-1.817107	1.359602	2.014824
H	0.979351	-0.469604	-2.150005
H	-4.424243	-1.788693	0.376579
H	-3.392830	-1.620156	-2.242145
H	-4.677109	-3.503622	2.171226
H	-3.360340	-2.745899	3.084637
H	-4.881596	-1.870645	2.819718
H	1.127367	4.361057	0.306230
H	0.173914	5.431230	-0.737873
H	1.231512	4.210983	-1.460809
H	2.017764	0.921216	0.243847
H	2.192080	-2.081973	-1.846116
H	3.968956	-3.719292	-1.674292
H	5.852686	-3.401259	-0.079780
H	5.886222	-1.383092	1.342785
H	5.171981	1.439216	2.767115

ωB97X Energy = -1472.05065247 a.u.

(2*R*,8*R*,10*R*,13*S*)-**15**, Conf E

C	-1.996468	-2.531203	-0.835687
C	-1.326618	-1.190119	-1.111571
C	-0.046288	-0.861631	-0.390167
C	-2.355374	-2.773153	0.633694
C	-0.820619	3.275807	-0.564604
C	-1.743992	3.348052	0.653479
C	-2.391715	2.022879	0.894684
C	-3.638896	1.694323	0.582003
C	0.908725	0.037306	-1.193687
C	0.312227	1.400311	-1.536197
O	-0.081382	2.029969	-0.430723
C	-3.550011	-1.973217	1.118493
C	-4.157794	0.317097	0.738768
O	-3.187552	-0.578111	0.972965
O	0.244796	1.857322	-2.647393
O	-1.798985	-0.451621	-1.950625
O	-3.129539	-2.677318	-1.656045
C	-3.899787	-2.259906	2.564048
O	-5.328432	0.025947	0.638227
C	0.136581	4.442171	-0.660454
N	2.136238	0.290608	-0.469103
C	3.147194	-0.622907	-0.332262

C	3.192708	-1.787173	-1.122054
C	4.233101	-2.684025	-1.010464
C	5.274066	-2.473320	-0.108319
C	5.244923	-1.343825	0.678856
C	4.203058	-0.412161	0.591758
C	4.215879	0.766206	1.475785
O	3.345481	1.616322	1.538053
O	5.303441	0.846173	2.256034
H	-1.241396	-3.279167	-1.117072
H	0.475519	-1.782923	-0.120420
H	-0.310440	-0.365823	0.548758
H	-2.595498	-3.832006	0.749666
H	-1.486962	-2.573915	1.268442
H	-1.419663	3.191194	-1.473432
H	-2.486584	4.127019	0.469441
H	-1.158068	3.637664	1.530414
H	-1.750752	1.254813	1.311898
H	-4.350163	2.409991	0.183719
H	1.133542	-0.422266	-2.155923
H	-4.406284	-2.162627	0.471629
H	-3.171641	-1.884257	-2.210271
H	-4.755075	-1.660600	2.878162
H	-4.159052	-3.313445	2.681851
H	-3.052627	-2.036017	3.215907
H	0.787963	4.470369	0.215482
H	-0.426453	5.376279	-0.703426
H	0.749629	4.367757	-1.558730
H	2.105802	1.007746	0.244300
H	2.405013	-1.990235	-1.835317
H	4.232085	-3.568033	-1.638499
H	6.086579	-3.183649	-0.024561
H	6.038947	-1.160958	1.391182
H	5.213892	1.640294	2.799962

ωB97X Energy = -1472.05048145 a.u.

(2*R*,8*R*,10*R*,13*S*)-**15**, Conf F

C	-2.838189	-1.682055	-1.348754
C	-1.474059	-1.123740	-0.902467
C	-0.587665	-0.610983	-2.014506
C	-3.765953	-2.101221	-0.204489
C	0.882948	3.085164	0.643392
C	-0.300425	3.169349	1.611622
C	-1.547454	2.640812	0.986666
C	-2.215464	1.589355	1.444390
C	0.725989	0.061134	-1.600703
C	0.461402	1.482178	-1.081262
O	0.986016	1.732661	0.112181
C	-4.609605	-1.024140	0.468354
C	-3.259586	0.947501	0.626388
O	-3.761952	-0.123074	1.229394
O	-0.140131	2.288351	-1.752134
O	-1.108659	-1.173274	0.250880
O	-3.458849	-0.850587	-2.309348
C	-5.586576	-1.617474	1.461326
O	-3.573087	1.296745	-0.499861
C	2.203504	3.383764	1.315762
N	1.537968	-0.774434	-0.761219
C	2.886060	-0.605882	-0.604973
C	3.608396	0.309028	-1.397776
C	4.972970	0.448719	-1.269897
C	5.692861	-0.305280	-0.344974
C	5.007112	-1.197810	0.447699
C	3.620344	-1.365232	0.343711

C	2.948519	-2.327341	1.233148
O	1.747439	-2.507818	1.306091
O	3.791758	-3.031118	2.006807
H	-2.574993	-2.599619	-1.887899
H	-1.160609	0.076106	-2.637798
H	-0.360672	-1.471978	-2.651567
H	-4.471597	-2.825629	-0.618007
H	-3.177993	-2.620017	0.556110
H	0.714149	3.755225	-0.199938
H	-0.420421	4.224284	1.875301
H	-0.068247	2.617687	2.526220
H	-1.862011	3.089247	0.048308
H	-1.940946	1.084482	2.363364
H	1.250969	0.232071	-2.544110
H	-5.147786	-0.434876	-0.275508
H	-3.658424	-0.003836	-1.877956
H	-5.059222	-2.198885	2.220223
H	-6.154376	-0.828198	1.954523
H	-6.286354	-2.274899	0.944078
H	3.019820	3.338190	0.593897
H	2.398321	2.664265	2.113394
H	2.178231	4.384728	1.749397
H	1.063371	-1.276500	-0.023174
H	3.093317	0.928056	-2.119973
H	5.486784	1.165875	-1.900667
H	6.764312	-0.187669	-0.245605
H	5.541192	-1.791129	1.178516
H	3.256353	-3.616106	2.559362

ωB97X Energy = -1472.04973668 a.u.

(2*R*,8*R*,10*R*,13*S*)-**15**, Conf G

C	-2.587172	-2.503680	-0.681334
C	-1.621083	-1.365973	-1.007300
C	-0.442080	-1.159877	-0.094167
C	-3.228004	-2.425301	0.706527
C	0.198412	3.019779	0.675690
C	-1.210887	3.443240	0.235097
C	-2.207275	2.352663	0.469356
C	-3.126441	1.989160	-0.416023
C	0.720117	-0.403331	-0.745855
C	0.497208	1.116317	-0.758452
O	0.387336	1.591068	0.478521
C	-4.246535	-1.308575	0.845720
C	-4.042119	0.845510	-0.214564
O	-3.526440	-0.070756	0.617848
O	0.471092	1.795173	-1.754879
O	-1.782827	-0.723916	-2.023226
O	-3.579462	-2.585533	-1.675596
C	-4.891213	-1.255666	2.213928
O	-5.109287	0.729812	-0.772126
C	0.461019	3.257711	2.146173
N	1.935100	-0.739347	-0.041762
C	3.192970	-0.458756	-0.499727
C	3.395835	0.068841	-1.789647
C	4.666046	0.302966	-2.270505
C	5.792814	0.035202	-1.495496
C	5.614750	-0.466730	-0.225497
C	4.339464	-0.717494	0.295650
C	4.209472	-1.241010	1.665645
O	3.159804	-1.448236	2.248443
O	5.382926	-1.484215	2.267627
H	-1.966582	-3.410641	-0.707636
H	-0.082625	-2.138601	0.233928

H	-0.792342	-0.638867	0.802491
H	-3.738990	-3.372811	0.890314
H	-2.452848	-2.328361	1.472193
H	0.940624	3.536454	0.065405
H	-1.214339	3.719712	-0.819377
H	-1.482431	4.333444	0.810433
H	-2.138291	1.806750	1.406705
H	-3.258806	2.517148	-1.354657
H	0.798480	-0.706199	-1.791230
H	-5.002386	-1.401461	0.067251
H	-3.355212	-1.925552	-2.347524
H	-5.425258	-2.187292	2.408457
H	-4.136683	-1.118945	2.991421
H	-5.606378	-0.433598	2.268434
H	-0.289519	2.759757	2.764115
H	0.424146	4.327814	2.353798
H	1.446139	2.882944	2.425088
H	1.869792	-0.973796	0.939211
H	2.546172	0.305931	-2.415847
H	4.781035	0.709126	-3.269398
H	6.787188	0.223264	-1.879761
H	6.474626	-0.674984	0.397917
H	5.191874	-1.812974	3.156394

ωB97X Energy = -1472.04896133 a.u.

Table S5. Cartesian coordinates and energies of the low-energy conformers calculated at the SOGGA11-X/TZVP SMD/MeCN level.

(1*S*,5*S*,9*S*,17*S*)-**13**, Conf A

C	3.224834	0.781690	-1.581469
C	4.323994	0.081780	-0.781038
C	3.950464	-1.330720	-0.285131
C	2.578173	-1.198828	0.402134
C	1.421040	-0.536676	-0.399110
C	1.878845	0.857562	-0.852975
C	1.917585	-2.405176	1.057162
C	0.600786	-1.800253	1.561544
C	0.267313	-0.655714	0.609131
C	4.979395	-1.758276	0.769898
C	4.011570	-2.352695	-1.428723
C	0.950847	-1.320344	-1.645399
O	2.006388	1.680875	0.331815
C	1.965690	3.010996	0.187104
O	1.789898	3.564909	-0.872790
C	2.168542	3.708027	1.499417
C	-0.896796	0.012730	0.623592
C	-1.940431	-0.376588	1.633967
N	-3.189316	-0.605736	1.145883
C	-3.629334	-0.267391	-0.203403
C	-3.639471	1.260824	-0.226686
O	-2.441036	1.848921	-0.071439
C	-1.225357	1.129227	-0.353087
O	-4.625105	1.948946	-0.239334
O	-1.698560	-0.516099	2.825293
C	-4.987571	-0.888388	-0.537589
C	-5.353084	-0.596402	-1.992270
C	-4.976653	-2.395296	-0.286381
H	2.761328	-0.491081	1.222212
H	3.536684	1.798315	-1.831600
H	3.060635	0.271125	-2.533509
H	4.569361	0.695640	0.092643
H	5.233038	0.028508	-1.389154
H	1.147939	1.323683	-1.513058
H	1.739786	-3.207669	0.336680
H	2.510107	-2.819030	1.874274
H	0.744074	-1.390180	2.563334
H	-0.215941	-2.520906	1.634579
H	4.808509	-2.786152	1.102269
H	5.991325	-1.708074	0.356195
H	4.940574	-1.106994	1.648397
H	3.572972	-3.309769	-1.132377
H	5.056669	-2.538637	-1.694590
H	3.504003	-2.017680	-2.332980
H	0.022601	-0.886522	-2.024574
H	0.752841	-2.365720	-1.405201
H	1.677993	-1.292728	-2.453836
H	1.495703	3.298393	2.254061
H	1.995654	4.775326	1.380089
H	3.193492	3.539730	1.838478
H	-3.912970	-0.699049	1.845515
H	-2.895861	-0.647539	-0.918332
H	-0.472853	1.911263	-0.295578
H	-1.261916	0.773094	-1.385432
H	-5.734668	-0.423566	0.113866
H	-5.380454	0.474235	-2.200685
H	-4.630369	-1.061230	-2.670288

H	-6.338316	-1.009022	-2.221090
H	-4.792666	-2.640350	0.761251
H	-4.206343	-2.885276	-0.890166
H	-5.942707	-2.822933	-0.565052

SOGGA11-X Energy = -1289.22376588 a.u.

(1*S*,5*S*,9*S*,17*S*)-**13**, Conf B

C	3.331699	0.808621	-1.476555
C	4.385614	0.087928	-0.634575
C	3.985088	-1.335023	-0.192786
C	2.578791	-1.215200	0.424207
C	1.466137	-0.531201	-0.421299
C	1.949405	0.871982	-0.818320
C	1.881824	-2.433190	1.017021
C	0.544163	-1.832747	1.468777
C	0.263403	-0.666812	0.525447
C	4.956681	-1.789594	0.904477
C	4.105462	-2.329877	-1.355067
C	1.059759	-1.284819	-1.707794
O	2.016747	1.666557	0.390725
C	1.992591	2.999966	0.276097
O	1.882497	3.580398	-0.778415
C	2.113743	3.663109	1.615881
C	-0.895312	0.010210	0.499768
C	-1.984556	-0.382517	1.456329
N	-3.214313	-0.584574	0.914259
C	-3.602205	-0.250627	-0.449387
C	-3.584410	1.272690	-0.561637
O	-2.410530	1.854592	-0.251729
C	-1.172601	1.147456	-0.466762
O	-4.529761	1.968506	-0.817846
O	-1.795908	-0.543282	2.655045
C	-4.945920	-0.882526	-0.838219
C	-4.776237	-2.385248	-1.054825
C	-6.073796	-0.600334	0.155353
H	2.719644	-0.526687	1.268513
H	3.658263	1.829566	-1.686817
H	3.217774	0.320222	-2.447358
H	4.583133	0.680481	0.265480
H	5.326360	0.047880	-1.193445
H	1.254093	1.355391	-1.504167
H	1.736644	-3.218491	0.270586
H	2.431005	-2.868794	1.852955
H	0.639054	-1.444901	2.485029
H	-0.278237	-2.550435	1.485088
H	4.768628	-2.825235	1.201392
H	5.989208	-1.730110	0.546665
H	4.870703	-1.160308	1.795442
H	3.657565	-3.294933	-1.101487
H	5.162937	-2.506096	-1.574683
H	3.639987	-1.975691	-2.274376
H	0.146083	-0.848106	-2.117840
H	0.859682	-2.337577	-1.504448
H	1.822135	-1.231486	-2.481921
H	3.075581	3.405012	2.064038
H	1.328134	3.302159	2.282066
H	2.038882	4.742078	1.500852
H	-3.959946	-0.686698	1.587798
H	-2.844932	-0.644248	-1.132565
H	-0.430174	1.932187	-0.345930
H	-1.143930	0.813650	-1.507153
H	-5.213187	-0.423339	-1.793715
H	-4.029641	-2.595663	-1.825096

H	-4.462635	-2.883288	-0.132750
H	-5.722552	-2.831847	-1.369230
H	-6.172908	0.464774	0.369206
H	-5.926010	-1.134379	1.099379
H	-7.021455	-0.950730	-0.260346

SOGGA11-X Energy = -1289.22244261 a.u.

(1*S*,5*S*,9*S*,17*S*)-**13**, Conf C

C	3.276205	1.547496	-0.879371
C	4.195838	1.103817	0.255086
C	4.266184	-0.424491	0.433365
C	2.810345	-0.923949	0.503641
C	1.831255	-0.528831	-0.643900
C	1.846562	1.005199	-0.777845
C	2.532099	-2.401365	0.722604
C	1.002917	-2.459644	0.646342
C	0.553181	-1.259011	-0.176348
C	4.943838	-0.724073	1.777032
C	5.119693	-1.066258	-0.668587
C	2.152373	-1.137051	-2.027743
O	1.189451	1.551371	0.386329
C	0.657885	2.776288	0.291720
O	0.710195	3.455471	-0.706148
C	0.034943	3.201197	1.587487
C	-0.737621	-0.973774	-0.457994
C	-1.848847	-1.808308	0.092459
N	-3.125243	-1.318298	0.063382
C	-3.772891	-0.127586	-0.481978
C	-3.009778	1.161476	-0.170136
O	-1.753252	1.247828	-0.615417
C	-1.165419	0.150256	-1.350617
O	-3.488540	2.110144	0.395343
O	-1.678446	-2.915226	0.596973
C	-5.229863	-0.054842	0.013511
C	-6.079903	-1.135206	-0.656045
C	-5.364567	-0.112712	1.534908
H	2.393641	-0.411853	1.382235
H	3.218402	2.637782	-0.911587
H	3.683781	1.236444	-1.844505
H	3.842009	1.544030	1.193887
H	5.201505	1.501688	0.083251
H	1.306873	1.340786	-1.661112
H	2.990291	-3.013569	-0.058407
H	2.902155	-2.762400	1.683206
H	0.561478	-2.392762	1.643964
H	0.620581	-3.385077	0.219808
H	5.094181	-1.797652	1.920874
H	5.925796	-0.243076	1.820475
H	4.346655	-0.349743	2.613993
H	4.856885	-0.722295	-1.668613
H	5.036307	-2.156466	-0.655979
H	6.172261	-0.815442	-0.505356
H	2.282834	-2.218808	-1.969992
H	3.052344	-0.714550	-2.470185
H	1.321451	-0.939624	-2.709521
H	-0.506562	2.375430	2.047583
H	-0.630273	4.044839	1.416220
H	0.831265	3.508047	2.271341
H	-3.771418	-1.994386	0.441871
H	-3.820292	-0.186284	-1.576522
H	-0.335309	0.593457	-1.881324
H	-1.871199	-0.197428	-2.106316
H	-5.594416	0.917720	-0.324371

H	-6.008828	-1.080065	-1.745604
H	-5.780825	-2.142193	-0.347804
H	-7.129128	-1.010832	-0.378054
H	-4.755875	0.649517	2.022905
H	-5.074687	-1.090163	1.930934
H	-6.407015	0.054528	1.816858

SOGGA11-X Energy = -1289.22196301 a.u.

(1*S*,5*S*,9*S*,17*S*)-**13**, Conf D

C	-3.229130	1.598097	0.951777
C	-4.232062	1.144927	-0.104916
C	-4.333831	-0.385648	-0.239639
C	-2.892798	-0.904253	-0.406789
C	-1.823220	-0.501230	0.654403
C	-1.816069	1.035658	0.764411
C	-2.648050	-2.387771	-0.619373
C	-1.119143	-2.455707	-0.674155
C	-0.591705	-1.252898	0.098119
C	-5.113789	-0.708119	-1.521332
C	-5.109873	-0.990375	0.938039
C	-2.041663	-1.081293	2.069802
O	-1.228784	1.559272	-0.446758
C	-0.663811	2.771962	-0.398706
O	-0.622359	3.454140	0.597851
C	-0.137656	3.185242	-1.740293
C	0.721412	-0.980797	0.278148
C	1.774290	-1.828020	-0.369000
N	3.077313	-1.408343	-0.358124
C	3.773527	-0.281867	0.260883
C	3.060213	1.003716	-0.162426
O	1.837768	1.195365	0.346290
C	1.213917	0.151905	1.130347
O	3.510618	1.821610	-0.921202
O	1.527304	-2.880158	-0.952110
C	5.258239	-0.273595	-0.134435
C	5.996142	0.818478	0.641248
C	5.923573	-1.623700	0.142643
H	-2.538475	-0.413648	-1.324364
H	-3.155722	2.688077	0.958498
H	-3.571605	1.311623	1.949496
H	-3.938211	1.557395	-1.076397
H	-5.217360	1.562345	0.127434
H	-1.220051	1.379159	1.607175
H	-3.043286	-2.981319	0.209005
H	-3.101355	-2.762243	-1.538124
H	-0.767861	-2.393227	-1.706819
H	-0.704825	-3.382898	-0.281912
H	-5.290872	-1.782309	-1.624800
H	-6.088872	-0.211691	-1.504947
H	-4.575417	-0.365540	-2.410291
H	-5.038806	-2.081526	0.945685
H	-6.169019	-0.730928	0.846891
H	-4.771096	-0.625869	1.907641
H	-1.159244	-0.878405	2.681784
H	-2.185212	-2.162471	2.043897
H	-2.901605	-0.640453	2.570223
H	-0.966089	3.603801	-2.319002
H	0.263084	2.333058	-2.287147
H	0.624341	3.951846	-1.614435
H	3.670071	-2.048604	-0.862614
H	3.738593	-0.361580	1.351654
H	0.411891	0.649820	1.653282
H	1.908901	-0.200648	1.892350

H	5.321600	-0.054872	-1.204636
H	5.567395	1.806412	0.471738
H	5.970333	0.609360	1.715382
H	7.043778	0.849346	0.333576
H	5.544191	-2.434761	-0.482820
H	5.797113	-1.914438	1.190078
H	6.995039	-1.546500	-0.055713

SOGGA11-X Energy = -1289.22128336 a.u.

(1*S*,5*S*,9*S*,17*S*)-**13**, Conf E

C	3.178084	1.697601	-0.848690
C	4.137737	1.280709	0.262315
C	4.305207	-0.244604	0.393791
C	2.883519	-0.834401	0.467140
C	1.864545	-0.468428	-0.655266
C	1.785103	1.067028	-0.747344
C	2.699835	-2.331508	0.647562
C	1.176371	-2.481256	0.591603
C	0.640709	-1.289869	-0.192367
C	5.018975	-0.539710	1.719943
C	5.181172	-0.801844	-0.736089
C	2.199936	-1.017100	-2.060355
O	1.107629	1.541660	0.435997
C	0.496585	2.731268	0.377363
O	0.491473	3.435600	-0.604364
C	-0.135149	3.083838	1.690425
C	-0.669135	-1.081275	-0.453881
C	-1.717185	-2.005748	0.079525
N	-3.026775	-1.612729	0.054787
C	-3.751510	-0.461050	-0.481544
C	-3.084951	0.855893	-0.079010
O	-1.845661	1.062296	-0.538628
C	-1.173907	0.040685	-1.309902
O	-3.603566	1.718656	0.580556
O	-1.465511	-3.105705	0.564855
C	-5.229976	-0.575985	-0.062314
C	-5.466721	-0.547274	1.447858
C	-6.094806	0.450350	-0.790898
H	2.450129	-0.373415	1.365945
H	3.054589	2.782932	-0.851388
H	3.590926	1.436577	-1.826229
H	3.767874	1.669371	1.217675
H	5.114178	1.746322	0.092272
H	1.217837	1.392635	-1.617011
H	3.181838	-2.892822	-0.156939
H	3.106829	-2.695095	1.592033
H	0.748030	-2.465382	1.596988
H	0.844150	-3.417740	0.147794
H	5.239644	-1.605139	1.830059
H	5.968756	0.001859	1.766042
H	4.411014	-0.229040	2.575059
H	6.217428	-0.485470	-0.582371
H	5.170306	-1.895236	-0.748090
H	4.880201	-0.454048	-1.723967
H	2.394375	-2.090390	-2.035637
H	3.065998	-0.528652	-2.502838
H	1.348173	-0.850184	-2.724346
H	-0.852434	3.889396	1.548807
H	0.649423	3.420591	2.373818
H	-0.619977	2.214867	2.134082
H	-3.628871	-2.338191	0.414284
H	-3.746179	-0.486459	-1.577120
H	-0.374578	0.563635	-1.814087

H	-1.844292	-0.328248	-2.087067
H	-5.528902	-1.566232	-0.426462
H	-6.511605	-0.789880	1.657369
H	-4.848862	-1.279963	1.973578
H	-5.253886	0.438623	1.861913
H	-5.885473	1.463939	-0.444689
H	-7.151635	0.241769	-0.608135
H	-5.929124	0.414209	-1.871362

SOGGA11-X Energy = -1289.22057352 a.u.

(1*S*,5*S*,9*S*,17*S*)-**13**, Conf F

C	3.357431	0.702476	-1.412197
C	4.333418	-0.181051	-0.634991
C	3.773036	-1.569966	-0.264945
C	2.405624	-1.319040	0.397525
C	1.362874	-0.464147	-0.379939
C	2.000480	0.889187	-0.725946
C	1.582929	-2.476773	0.948601
C	0.340914	-1.744556	1.471440
C	0.176118	-0.510132	0.592982
C	4.704432	-2.204788	0.776299
C	3.745357	-2.498560	-1.486607
C	0.830196	-1.090737	-1.688104
O	2.170596	1.621887	0.510210
C	2.216155	2.958233	0.452996
O	2.089717	3.590244	-0.569523
C	2.452392	3.554806	1.808473
C	-0.904552	0.281726	0.660745
C	-2.009560	0.007532	1.632576
N	-3.244740	0.051934	1.056909
C	-3.508545	-0.375865	-0.314666
C	-3.113808	0.622823	-1.413787
O	-2.009541	1.366581	-1.316002
C	-1.182780	1.524982	-0.133811
O	-3.725133	0.679963	-2.452745
O	-1.861066	-0.130972	2.837632
C	-4.981622	-0.801127	-0.461622
C	-5.266257	-2.068662	0.342738
C	-5.959580	0.319233	-0.107566
H	2.647013	-0.697763	1.271442
H	3.795808	1.690345	-1.574196
H	3.172894	0.285402	-2.405382
H	4.613367	0.331521	0.291872
H	5.253373	-0.299329	-1.216786
H	1.360175	1.473252	-1.385335
H	1.321396	-3.193316	0.165596
H	2.095619	-3.022004	1.742137
H	0.512816	-1.415583	2.499450
H	-0.563063	-2.356541	1.485102
H	4.396759	-3.225940	1.018535
H	5.728274	-2.249342	0.392422
H	4.716337	-1.625001	1.704244
H	3.175893	-3.409772	-1.282513
H	4.767071	-2.799311	-1.737729
H	3.320733	-2.028894	-2.373632
H	-0.009504	-0.495116	-2.053973
H	0.470289	-2.107997	-1.526775
H	1.583879	-1.119828	-2.471871
H	3.486364	3.359998	2.104247
H	1.799455	3.093472	2.549970
H	2.285011	4.629047	1.771936
H	-4.002829	-0.094596	1.707126
H	-2.893928	-1.256547	-0.543674

H	-1.671264	2.268584	0.498536
H	-0.278108	1.969935	-0.530629
H	-5.106810	-1.036742	-1.518828
H	-4.583125	-2.875848	0.065358
H	-5.175286	-1.904818	1.420624
H	-6.286749	-2.408911	0.151434
H	-5.756040	1.227912	-0.678700
H	-5.925968	0.571135	0.956748
H	-6.981156	0.003870	-0.332878

SOGGA11-X Energy = -1289.22051659 a.u.

(1*S*,5*S*,9*S*,17*S*)-**13**, Conf G

C	3.059055	1.580732	-0.669142
C	3.785054	1.103352	0.587935
C	3.828725	-0.429280	0.745992
C	2.383134	-0.930895	0.557985
C	1.613848	-0.492756	-0.724118
C	1.629029	1.042654	-0.797627
C	2.069207	-2.415386	0.679165
C	0.574941	-2.462320	0.337687
C	0.287567	-1.242948	-0.529060
C	4.268218	-0.755434	2.179703
C	4.861587	-1.049439	-0.204746
C	2.173845	-1.049094	-2.053992
O	0.818163	1.545883	0.288772
C	0.367456	2.802918	0.198857
O	0.599353	3.534591	-0.734692
C	-0.465735	3.186314	1.385319
C	-0.926640	-0.977463	-1.044040
C	-2.085058	-1.900701	-0.840551
N	-3.311810	-1.294936	-0.811271
C	-3.698098	-0.035691	-0.185937
C	-2.952112	1.251025	-0.552278
O	-1.866446	1.306435	-1.315395
C	-1.263205	0.158679	-1.962327
O	-3.382366	2.294166	-0.116641
O	-2.002269	-3.122317	-0.843653
C	-3.822671	-0.128681	1.360859
C	-4.805180	-1.228923	1.753046
C	-2.478453	-0.313826	2.057665
H	1.824740	-0.446076	1.370792
H	3.013952	2.671301	-0.682625
H	3.611507	1.287735	-1.565023
H	3.284292	1.524279	1.466673
H	4.804938	1.501732	0.589542
H	1.204538	1.406767	-1.731729
H	2.651321	-3.006387	-0.032608
H	2.269498	-2.809110	1.676452
H	-0.028106	-2.392244	1.249875
H	0.266856	-3.376852	-0.164236
H	4.391438	-1.832197	2.326105
H	5.228645	-0.279325	2.399943
H	3.537302	-0.395250	2.910050
H	4.773705	-0.686896	-1.228607
H	5.869157	-0.800006	0.141811
H	4.782596	-2.139939	-0.225811
H	2.293253	-2.132857	-2.012045
H	3.136635	-0.615625	-2.314814
H	1.475060	-0.822917	-2.863109
H	-0.259993	2.552910	2.246356
H	-1.518170	3.080745	1.105288
H	-0.281293	4.232233	1.630058
H	-4.058821	-1.974062	-0.775461

H	-4.704405	0.164367	-0.562658
H	-0.383109	0.572539	-2.440701
H	-1.942649	-0.176913	-2.746736
H	-4.243010	0.830822	1.669851
H	-5.767765	-1.103863	1.248912
H	-4.417808	-2.222223	1.508609
H	-4.983204	-1.203210	2.830772
H	-1.778009	0.492260	1.818455
H	-2.010321	-1.264653	1.784592
H	-2.618661	-0.319623	3.141420

SOGGA11-X Energy = -1289.22019998 a.u.

(1*R*,5*R*,9*R*,17*S*)-**13**, Conf A

C	-3.182193	1.576059	-0.968434
C	-4.122391	1.221241	0.183660
C	-4.224498	-0.289750	0.474602
C	-2.779673	-0.814812	0.577966
C	-1.806606	-0.516830	-0.600148
C	-1.768373	1.007232	-0.808409
C	-2.522074	-2.278116	0.902288
C	-0.992959	-2.372548	0.813284
C	-0.542893	-1.250104	-0.117194
C	-5.097875	-0.992086	-0.573617
C	-4.903936	-0.472286	1.838558
C	-2.169007	-1.190734	-1.943169
O	-1.144838	1.591533	0.362782
C	-0.641116	2.827099	0.261469
O	-0.603847	3.455178	-0.770700
C	-0.157900	3.333378	1.587954
C	0.737013	-1.006717	-0.454800
C	1.830821	-1.849131	0.135125
N	2.994897	-1.227545	0.470243
C	3.406512	0.131890	0.147252
C	3.527302	0.222292	-1.373218
O	2.407652	-0.082961	-2.053734
C	1.122293	0.093703	-1.424680
O	4.532238	0.467551	-1.984638
O	1.710870	-3.051444	0.340088
C	4.691322	0.527357	0.890202
C	4.392962	0.750383	2.372108
C	5.846729	-0.459049	0.711265
H	-2.348535	-0.250531	1.415907
H	-3.585629	1.217656	-1.918330
H	-3.103695	2.661410	-1.063568
H	-5.118914	1.622891	-0.027345
H	-3.770865	1.721652	1.092488
H	-1.177057	1.283112	-1.679947
H	-2.889461	-2.560461	1.889843
H	-2.997672	-2.938522	0.172643
H	-0.639528	-3.336584	0.455611
H	-0.540985	-2.227193	1.799391
H	-6.143341	-0.704379	-0.426473
H	-4.831743	-0.730803	-1.597365
H	-5.040758	-2.079995	-0.478499
H	-5.875724	0.030803	1.848187
H	-5.075968	-1.528737	2.063146
H	-4.296236	-0.048649	2.643893
H	-3.037080	-0.739187	-2.418568
H	-2.374636	-2.253752	-1.808711
H	-1.331098	-1.103478	-2.639028
H	0.550790	4.145192	1.436550
H	-1.020497	3.716239	2.140484

H	0.292289	2.534666	2.175781
H	3.734661	-1.868923	0.716292
H	2.625498	0.825824	0.465579
H	0.438726	0.100579	-2.269308
H	1.098055	1.084655	-0.967238
H	4.991441	1.482725	0.451227
H	3.617881	1.507988	2.513361
H	4.055753	-0.173705	2.850723
H	5.293173	1.085020	2.893107
H	6.755854	-0.034794	1.143837
H	5.661866	-1.404142	1.232050
H	6.041785	-0.673448	-0.340189

SOGGA11-X Energy = -1289.22244705 a.u.

(1*R*,5*R*,9*R*,17*S*)-**13**, Conf B

C	3.440100	1.088938	1.250432
C	4.492642	0.401494	0.383812
C	4.178907	-1.076168	0.078114
C	2.732196	-1.107623	-0.449319
C	1.609303	-0.465459	0.420357
C	2.010318	0.992240	0.708054
C	2.114718	-2.411711	-0.926216
C	0.717501	-1.946369	-1.345064
C	0.367634	-0.767133	-0.449020
C	4.447112	-1.964309	1.300368
C	5.111956	-1.544511	-1.046485
C	1.330250	-1.162111	1.770798
O	1.900963	1.729845	-0.531454
C	1.647112	3.042625	-0.468817
O	1.490664	3.647429	0.565715
C	1.579394	3.647878	-1.839301
C	-0.855595	-0.197703	-0.395472
C	-1.957524	-0.670854	-1.288208
N	-3.252533	-0.428190	-0.928198
C	-3.904025	0.317409	0.146698
C	-3.276257	0.069683	1.520593
O	-1.990792	0.400932	1.672052
C	-1.230679	0.904694	0.547641
O	-3.881787	-0.338360	2.477477
O	-1.756619	-1.277549	-2.336779
C	-5.413355	0.008966	0.151766
C	-6.096816	0.653116	-1.054996
C	-5.734387	-1.483059	0.234964
H	2.763852	-0.464001	-1.339905
H	3.440856	0.664950	2.257708
H	3.683496	2.148054	1.367551
H	5.469302	0.478834	0.872778
H	4.575482	0.937714	-0.567964
H	1.354390	1.456199	1.441036
H	2.656870	-2.858445	-1.760718
H	2.067493	-3.153287	-0.124256
H	-0.046914	-2.721768	-1.305134
H	0.738315	-1.599340	-2.380722
H	5.526574	-2.049010	1.458457
H	4.016836	-1.570305	2.220647
H	4.056631	-2.975250	1.152869
H	6.156588	-1.380529	-0.764734
H	4.987893	-2.611364	-1.252095
H	4.922125	-0.995754	-1.973999
H	2.138100	-1.022668	2.486172
H	1.173257	-2.234207	1.642917
H	0.420939	-0.745570	2.210463
H	0.821665	3.134372	-2.434001

H	1.339293	4.705987	-1.763611
H	2.540081	3.521226	-2.342733
H	-3.889826	-0.754889	-1.639196
H	-3.805152	1.396664	-0.027915
H	-0.372093	1.368250	1.009599
H	-1.799275	1.690521	0.049053
H	-5.798582	0.491764	1.052486
H	-5.909369	1.729501	-1.090663
H	-5.756881	0.219619	-2.000965
H	-7.176962	0.499042	-0.998968
H	-6.811506	-1.619234	0.359318
H	-5.443696	-2.011533	-0.677240
H	-5.234504	-1.956798	1.080868

SOGGA11-X Energy = -1289.22170048 a.u.

(1*R*,5*R*,9*R*,17*S*)-**13**, Conf C

C	3.103232	1.639572	1.019135
C	4.097168	1.337331	-0.101965
C	4.275112	-0.164372	-0.403619
C	2.858453	-0.750434	-0.562346
C	1.833140	-0.505787	0.583865
C	1.721602	1.012865	0.802477
C	2.670668	-2.219385	-0.909169
C	1.143701	-2.371323	-0.881037
C	0.617864	-1.283210	0.050016
C	5.141715	-0.841180	0.666395
C	5.008128	-0.301701	-1.744910
C	2.176514	-1.176592	1.933364
O	1.115960	1.579060	-0.386706
C	0.558803	2.792350	-0.298229
O	0.461277	3.413409	0.734227
C	0.098523	3.282511	-1.638924
C	-0.680658	-1.096191	0.351028
C	-1.721336	-1.966575	-0.293256
N	-2.894354	-1.378161	-0.659655
C	-3.359660	-0.041151	-0.312187
C	-3.549885	-0.037292	1.204826
O	-2.432448	-0.275334	1.915618
C	-1.137668	-0.032300	1.331805
O	-4.594763	0.063756	1.790230
O	-1.549913	-3.158413	-0.519703
C	-4.594391	0.345152	-1.140664
C	-5.790047	-0.597316	-0.995913
C	-4.995235	1.793272	-0.862203
H	2.433792	-0.195776	-1.409910
H	3.487053	1.287881	1.979603
H	2.975448	2.719515	1.121687
H	5.067300	1.779355	0.147275
H	3.755406	1.831828	-1.017709
H	1.087668	1.255717	1.653370
H	3.085501	-2.478598	-1.884217
H	3.142315	-2.868663	-0.167049
H	0.812736	-3.353853	-0.553764
H	0.725784	-2.224114	-1.881836
H	4.817907	-0.620457	1.682893
H	5.149904	-1.927992	0.544592
H	6.174622	-0.492448	0.571159
H	5.957756	0.241652	-1.716263
H	5.232129	-1.347347	-1.973986
H	4.410793	0.105310	-2.566428
H	1.308932	-1.141002	2.596472
H	3.000417	-0.686170	2.447393
H	2.442446	-2.225707	1.796411

H	-0.618858	4.090295	-1.509706
H	-0.335689	2.473620	-2.225584
H	0.968520	3.663400	-2.180915
H	-3.605159	-2.037351	-0.942302
H	-2.579557	0.678854	-0.564289
H	-0.481376	-0.020064	2.197964
H	-1.137582	0.969265	0.898105
H	-4.249043	0.288732	-2.178596
H	-6.186754	-0.584128	0.019788
H	-6.582548	-0.278354	-1.677387
H	-5.547393	-1.631303	-1.256802
H	-5.773869	2.105336	-1.562063
H	-5.387395	1.908835	0.150532
H	-4.146076	2.471561	-0.981102

SOGGA11-X Energy = -1289.22118003 a.u.

(1*R*,5*R*,9*R*,17*S*)-**13**, Conf D

C	-3.121496	1.666449	-0.630583
C	-3.866174	1.232502	0.631258
C	-3.992091	-0.295288	0.796879
C	-2.576054	-0.872160	0.607831
C	-1.791481	-0.483538	-0.681075
C	-1.725620	1.049426	-0.770093
C	-2.334822	-2.369953	0.740466
C	-0.841855	-2.488419	0.405365
C	-0.501887	-1.286531	-0.469947
C	-5.056704	-0.866008	-0.149314
C	-4.445928	-0.589237	2.232878
C	-2.379025	-1.020539	-2.005960
O	-0.867472	1.513176	0.297141
C	-0.336959	2.737271	0.188898
O	-0.533840	3.476099	-0.746194
C	0.489903	3.079598	1.392957
C	0.726905	-1.074756	-0.964523
C	1.854358	-2.024176	-0.697260
N	3.016605	-1.393207	-0.369867
C	3.071059	-0.134989	0.368812
C	2.825782	1.122466	-0.476698
O	1.844742	1.152164	-1.382038
C	1.137383	0.006716	-1.922257
O	3.420792	2.151858	-0.270648
O	1.802920	-3.235149	-0.857835
C	4.392274	-0.032528	1.152160
C	4.440806	-1.065744	2.277221
C	5.627231	-0.129153	0.255908
H	-1.989676	-0.409285	1.413767
H	-3.695103	1.402896	-1.522725
H	-3.016294	2.753059	-0.647221
H	-4.862728	1.686137	0.635876
H	-3.339511	1.628690	1.506400
H	-1.294580	1.378045	-1.714579
H	-2.557002	-2.747005	1.739593
H	-2.942699	-2.936222	0.030344
H	-0.577311	-3.419659	-0.093518
H	-0.242996	-2.442362	1.320528
H	-4.940840	-0.528290	-1.178722
H	-5.044807	-1.959594	-0.150908
H	-6.048791	-0.549128	0.186723
H	-5.381619	-0.064949	2.450522
H	-4.621694	-1.657705	2.386364
H	-3.697406	-0.260439	2.960185
H	-1.660933	-0.852802	-2.812469
H	-3.307880	-0.525235	-2.280637

H	-2.572420	-2.092987	-1.951382
H	1.125875	3.934113	1.173571
H	-0.185848	3.337790	2.213119
H	1.091113	2.227812	1.712055
H	3.794454	-2.018362	-0.220531
H	2.253876	-0.113616	1.102041
H	1.779792	-0.419613	-2.696180
H	0.280299	0.452136	-2.415500
H	4.380695	0.960183	1.603723
H	3.572034	-0.978733	2.935161
H	4.474380	-2.090411	1.894716
H	5.338603	-0.915103	2.881391
H	5.590156	0.592260	-0.562922
H	6.525621	0.075808	0.843150
H	5.746241	-1.128609	-0.173812

SOGGA11-X Energy = -1289.22086997 a.u.

(1*R*,5*R*,9*R*,17*S*)-**13**, Conf E

C	-3.278089	0.563061	-1.402146
C	-4.190878	-0.352778	-0.587239
C	-3.541148	-1.690068	-0.176626
C	-2.186372	-1.331822	0.462457
C	-1.203885	-0.440947	-0.351723
C	-1.929796	0.856370	-0.736611
C	-1.289630	-2.417779	1.040246
C	-0.093623	-1.593427	1.529210
C	-0.005177	-0.383561	0.609373
C	-3.466669	-2.656817	-1.366524
C	-4.422684	-2.345174	0.895081
C	-0.639590	-1.078300	-1.641924
O	-2.135883	1.616515	0.477501
C	-2.268139	2.944850	0.380528
O	-2.189885	3.552458	-0.661353
C	-2.525522	3.564992	1.721523
C	1.030482	0.474270	0.624188
C	2.155974	0.314223	1.592255
N	3.385710	0.672953	1.111800
C	3.959750	0.456328	-0.212824
C	3.189669	0.898702	-1.464358
O	1.969580	1.428767	-1.454594
C	1.207136	1.680477	-0.249300
O	3.732838	0.773301	-2.535713
O	2.009851	0.019910	2.771593
C	4.477436	-0.993400	-0.424751
C	5.483022	-1.371242	0.659602
C	3.353384	-2.020028	-0.517021
H	-2.458563	-0.698391	1.318283
H	-3.076677	0.127767	-2.384123
H	-3.777940	1.516487	-1.590240
H	-5.105972	-0.547741	-1.156092
H	-4.496028	0.172261	0.324525
H	-1.336962	1.458442	-1.422793
H	-1.760693	-2.968552	1.855342
H	-0.991835	-3.140444	0.276317
H	0.847584	-2.145697	1.565096
H	-0.280860	-1.237341	2.545020
H	-3.086497	-2.190468	-2.275148
H	-2.834302	-3.520578	-1.141953
H	-4.468958	-3.033458	-1.592107
H	-5.446080	-2.460195	0.524837
H	-4.054908	-3.339332	1.164275
H	-4.458751	-1.738863	1.805311
H	0.151412	-0.438653	-2.040497

H	-1.395868	-1.194802	-2.415248
H	-0.206133	-2.060006	-1.444927
H	-3.499784	3.233819	2.088585
H	-1.770602	3.239974	2.438952
H	-2.518161	4.649122	1.633621
H	4.091693	0.644124	1.833823
H	4.839728	1.104636	-0.244211
H	0.269201	2.064538	-0.630078
H	1.699123	2.482970	0.300812
H	5.001801	-0.969476	-1.382276
H	6.288497	-0.634871	0.733480
H	5.007408	-1.456771	1.641002
H	5.932749	-2.339946	0.429074
H	3.769021	-3.010404	-0.718580
H	2.791057	-2.087725	0.419303
H	2.650411	-1.786298	-1.321944

SOGGA11-X Energy = -1289.22045859 a.u.

(1*R*,5*R*,9*R*,17*S*)-**13**, Conf F

C	-2.995922	0.785741	-1.619340
C	-4.134919	0.166386	-0.808668
C	-3.813566	-1.222196	-0.217963
C	-2.458322	-1.082956	0.500223
C	-1.260624	-0.506240	-0.307842
C	-1.666132	0.867984	-0.862132
C	-1.850448	-2.262078	1.248221
C	-0.534072	-1.659381	1.754830
C	-0.138077	-0.590901	0.740157
C	-3.868873	-2.309087	-1.300244
C	-4.882956	-1.559919	0.829307
C	-0.781157	-1.383247	-1.486037
O	-1.799461	1.768228	0.264929
C	-1.706894	3.084472	0.040507
O	-1.477026	3.564906	-1.044620
C	-1.927884	3.868331	1.299821
C	1.045989	0.043753	0.741046
C	2.045356	-0.304094	1.806121
N	3.321819	-0.557928	1.413166
C	3.927841	-0.331159	0.108617
C	3.843870	1.161365	-0.210570
O	2.658566	1.777156	-0.071915
C	1.421274	1.078723	-0.301652
O	4.813948	1.826549	-0.463818
O	1.740387	-0.396902	2.988902
C	3.465303	-1.294262	-1.006203
C	4.036830	-0.866234	-2.355651
C	3.893892	-2.715995	-0.653144
H	-2.642727	-0.319631	1.268591
H	-2.824396	0.214821	-2.534888
H	-3.270610	1.794140	-1.937442
H	-5.028563	0.099649	-1.437938
H	-4.386181	0.839135	0.018660
H	-0.906214	1.270940	-1.530962
H	-2.476821	-2.610598	2.070665
H	-1.672596	-3.111371	0.583477
H	0.258934	-2.394294	1.904769
H	-0.697189	-1.178855	2.721487
H	-3.323580	-2.043206	-2.205440
H	-3.468607	-3.258565	-0.933330
H	-4.910238	-2.481795	-1.588799
H	-5.881031	-1.507772	0.383472
H	-4.750176	-2.570511	1.225829
H	-4.850593	-0.859214	1.669112

H	0.187307	-1.025297	-1.843526
H	-1.466443	-1.360933	-2.330721
H	-0.655436	-2.422666	-1.180881
H	-2.971921	3.765038	1.605208
H	-1.304464	3.477027	2.104894
H	-1.702982	4.918157	1.124910
H	3.963388	-0.699941	2.178400
H	4.994743	-0.505907	0.247878
H	1.445673	0.659452	-1.310085
H	0.695226	1.887452	-0.297869
H	2.375022	-1.274805	-1.066808
H	3.677955	0.120985	-2.661237
H	5.130379	-0.833620	-2.326637
H	3.742452	-1.578055	-3.129932
H	3.524484	-3.419347	-1.403162
H	4.985259	-2.794503	-0.623307
H	3.502843	-3.023958	0.319194

SOGGA11-X Energy = -1289.21984761 a.u.

(1*R*,5*R*,9*R*,17*S*)-**13**, Conf G

C	-3.166059	0.507277	-1.520119
C	-4.113920	-0.374004	-0.707484
C	-3.484161	-1.693930	-0.217443
C	-2.158072	-1.310678	0.466018
C	-1.140313	-0.448232	-0.336602
C	-1.848656	0.830042	-0.808300
C	-1.287880	-2.374202	1.122028
C	-0.113319	-1.531510	1.632360
C	0.006190	-0.346714	0.681466
C	-3.359208	-2.705372	-1.364738
C	-4.412597	-2.307270	0.839316
C	-0.515225	-1.133020	-1.572652
O	-2.108698	1.642613	0.360313
C	-2.241719	2.964387	0.197225
O	-2.126389	3.523764	-0.868013
C	-2.551470	3.644167	1.497556
C	1.030193	0.520068	0.733357
C	2.087591	0.398723	1.788025
N	3.363644	0.571941	1.335232
C	3.861096	0.187744	0.016735
C	3.422699	1.086248	-1.141026
O	2.161630	1.510899	-1.271138
C	1.253216	1.707728	-0.155373
O	4.200118	1.348956	-2.025520
O	1.852584	0.268966	2.981500
C	3.621583	-1.313926	-0.308037
C	4.120834	-1.704818	-1.696794
C	4.296903	-2.175114	0.758436
H	-2.466329	-0.646959	1.285932
H	-2.922362	0.030003	-2.472423
H	-3.656138	1.451264	-1.770581
H	-5.005315	-0.591300	-1.305152
H	-4.455215	0.187424	0.169072
H	-1.223653	1.401565	-1.492412
H	-1.794525	-2.895034	1.935604
H	-0.957768	-3.125055	0.399662
H	0.827629	-2.080491	1.710083
H	-0.336269	-1.152146	2.632181
H	-2.924910	-2.278660	-2.268536
H	-2.751177	-3.566811	-1.073646
H	-4.353002	-3.079399	-1.628970
H	-5.418514	-2.439369	0.428966
H	-4.056929	-3.288774	1.165285

H	-4.489341	-1.664013	1.721133
H	0.292335	-0.506257	-1.958484
H	-1.233599	-1.282058	-2.375955
H	-0.089365	-2.105056	-1.319524
H	-3.536342	3.323162	1.844764
H	-1.821049	3.358250	2.255878
H	-2.546979	4.723094	1.359213
H	4.057672	0.521645	2.065956
H	4.939153	0.342375	0.060818
H	0.343577	2.036186	-0.641728
H	1.641071	2.544870	0.428437
H	2.542319	-1.491461	-0.267629
H	3.584066	-1.187844	-2.494431
H	5.186574	-1.484861	-1.808861
H	3.981470	-2.778482	-1.844047
H	4.098221	-3.231985	0.565722
H	5.381632	-2.027513	0.742356
H	3.937350	-1.947042	1.763841

SOGGA11-X Energy = -1289.21975669 a.u.

Table S6. Cartesian coordinates and energies of the low-energy conformers calculated at the B3LYP/TZVP PCM/$CHCl_3$ level.

(2*R*,8*R*,10*R*,13*R*)-**15**, Conf A

C	0.901525	-2.457579	0.469443
C	0.592813	-0.960994	0.387973
C	0.076265	-0.395942	-0.918625
C	1.952547	-2.970631	-0.533577
C	1.760143	3.383160	-0.114846
C	3.185801	3.062770	-0.599070
C	3.474102	1.598817	-0.511082
C	4.221679	0.990949	0.409104
C	-0.882411	0.808672	-0.750389
C	-0.223019	2.008815	-0.058019
O	0.886324	2.370151	-0.717867
C	3.391526	-2.584063	-0.215546
C	4.335322	-0.478609	0.513741
O	3.452955	-1.127990	-0.280492
O	-0.664085	2.568114	0.913521
O	0.706833	-0.276642	1.385246
O	1.266444	-2.805867	1.788496
C	4.390214	-3.186879	-1.191255
O	5.111056	-1.041804	1.257783
C	1.298665	4.775777	-0.500805
N	-2.094641	0.474259	-0.045417
C	-3.202787	-0.088420	-0.605942
C	-3.232479	-0.458559	-1.970366
C	-4.357044	-1.023733	-2.539913
C	-5.508002	-1.260210	-1.784894
C	-5.504014	-0.913410	-0.448315
C	-4.382400	-0.332450	0.165902
C	-4.437794	0.021134	1.588915
O	-3.540337	0.549330	2.228703
O	-5.612644	-0.291443	2.188490
H	-0.049543	-2.948693	0.214795
H	-0.435732	-1.179837	-1.478792
H	0.939915	-0.098997	-1.518261
H	1.898764	-4.061287	-0.528259
H	1.690916	-2.647920	-1.544689
H	1.701767	3.245341	0.964671
H	3.881680	3.643969	0.009239
H	3.289654	3.395645	-1.636332
H	2.972728	0.981065	-1.244139
H	4.775176	1.538975	1.162581
H	-1.120956	1.162076	-1.758324
H	3.635032	-2.877503	0.803633
H	1.210614	-1.989666	2.313687
H	4.171028	-2.878057	-2.215591
H	5.405025	-2.878562	-0.940437
H	4.346710	-4.276586	-1.142643
H	0.301558	4.976148	-0.110687
H	1.287204	4.889683	-1.586550
H	1.983181	5.517824	-0.084853
H	-2.172430	0.774903	0.920060
H	-2.362456	-0.298085	-2.590565
H	-4.335639	-1.287375	-3.590743
H	-6.384346	-1.706136	-2.235602
H	-6.383381	-1.086378	0.155406
H	-5.540259	-0.012836	3.114665

B3LYP Energy = -1472.40856875 a.u.

(2*R*,8*R*,10*R*,13*R*)-**15**, Conf B

C	-0.789356	2.480447	0.647549
C	-0.658669	0.964030	0.482009
C	-0.203874	0.394007	-0.844211
C	-1.776976	3.179477	-0.305249
C	-1.785908	-3.506010	-0.034721
C	-3.254196	-3.238429	-0.397536
C	-3.738162	-1.940175	0.165449
C	-3.834612	-0.823978	-0.553289
C	0.746907	-0.819796	-0.702615
C	0.109926	-2.019068	0.015142
O	-1.014474	-2.397159	-0.605399
C	-3.238281	2.787149	-0.118252
C	-4.039981	0.494796	0.079331
O	-3.365070	1.427650	-0.636067
O	0.594092	-2.573816	0.970129
O	-0.870992	0.248808	1.442121
O	-1.116320	2.791242	1.986628
C	-4.199968	3.690607	-0.872516
O	-4.647193	0.724803	1.100643
C	-1.273164	-4.823655	-0.589636
N	1.984413	-0.490620	-0.037673
C	3.078943	0.058499	-0.637480
C	3.064640	0.429746	-2.001854
C	4.174260	0.984224	-2.609980
C	5.353315	1.208241	-1.895671
C	5.392846	0.859407	-0.560178
C	4.287797	0.288516	0.092314
C	4.390334	-0.069605	1.511607
O	3.514286	-0.599353	2.179255
O	5.584714	0.240196	2.072835
H	0.212348	2.872479	0.416617
H	0.292775	1.165959	-1.432819
H	-1.098222	0.097783	-1.396289
H	-1.685123	4.250461	-0.113442
H	-1.481213	3.016301	-1.344676
H	-1.649513	-3.471357	1.046034
H	-3.840099	-4.070872	0.001242
H	-3.357196	-3.248457	-1.485170
H	-3.919831	-1.894927	1.235545
H	-3.604498	-0.820241	-1.612238
H	0.950457	-1.178558	-1.716332
H	-3.489305	2.766577	0.940690
H	-1.159002	1.945217	2.463629
H	-5.227000	3.347075	-0.744565
H	-4.132835	4.709913	-0.488156
H	-3.966931	3.706811	-1.939305
H	-1.851288	-5.649554	-0.171202
H	-0.226916	-4.973325	-0.324442
H	-1.370821	-4.849859	-1.676621
H	2.099574	-0.809949	0.918153
H	2.172098	0.278708	-2.591658
H	4.118722	1.248970	-3.659278
H	6.217778	1.645809	-2.376513
H	6.294695	1.022271	0.012372
H	5.543172	-0.042442	2.999695

B3LYP Energy = -1472.40840575 a.u.

(2*R*,8*R*,10*R*,13*R*)-**15**, Conf C

C	1.564934	-2.574625	-0.258431
C	0.881162	-1.233544	0.018182
C	0.310706	-0.455426	-1.149836

C	2.753235	-2.530858	-1.236580
C	1.019715	3.345651	0.588428
C	2.496578	3.474996	0.175243
C	3.118628	2.131406	-0.030551
C	3.937181	1.499322	0.809562
C	-0.899027	0.441775	-0.814450
C	-0.565637	1.568482	0.187649
O	0.433377	2.331044	-0.293032
C	4.028993	-1.911493	-0.680189
C	4.394211	0.110264	0.597621
O	3.721530	-0.513599	-0.397383
O	-1.140037	1.765511	1.226218
O	0.749159	-0.860486	1.167107
O	1.952686	-3.180505	0.956455
C	5.192962	-1.996524	-1.655296
O	5.255806	-0.424054	1.264275
C	0.251668	4.649300	0.476906
N	-2.021802	-0.354360	-0.392702
C	-3.335517	0.011719	-0.510233
C	-3.724628	1.159183	-1.234761
C	-5.055918	1.491044	-1.395090
C	-6.068507	0.706999	-0.837365
C	-5.714244	-0.411586	-0.110164
C	-4.371339	-0.782314	0.072534
C	-4.051422	-1.973532	0.867046
O	-2.926750	-2.387709	1.115042
O	-5.137628	-2.628654	1.340852
H	0.781550	-3.183647	-0.735015
H	0.020872	-1.142113	-1.946928
H	1.117227	0.163672	-1.548153
H	2.983838	-3.563258	-1.507690
H	2.458980	-2.022926	-2.158554
H	0.959259	2.952644	1.603107
H	3.012012	4.038621	0.955440
H	2.556369	4.053841	-0.751343
H	2.818028	1.612253	-0.930845
H	4.304941	1.959951	1.718983
H	-1.145617	0.943744	-1.751839
H	4.289317	-2.387866	0.262954
H	1.631115	-2.602808	1.668934
H	6.081143	-1.525861	-1.234368
H	5.430080	-3.041971	-1.861417
H	4.947311	-1.505667	-2.599352
H	-0.777170	4.523026	0.812254
H	0.249387	5.007529	-0.554503
H	0.723640	5.409251	1.103097
H	-1.851959	-1.092172	0.281261
H	-2.974566	1.804788	-1.667923
H	-5.309517	2.381138	-1.958592
H	-7.108923	0.974675	-0.963640
H	-6.480290	-1.026803	0.339676
H	-4.811955	-3.383346	1.855749

B3LYP Energy = -1472.40758299 a.u.

(2*R*,8*R*,10*R*,13*R*)-**15**, Conf D

C	1.536197	-2.599798	0.029666
C	0.994576	-1.175507	0.179178
C	0.429013	-0.463855	-1.032540
C	2.686807	-2.785802	-0.976628
C	0.928655	3.473636	0.645734
C	2.420375	3.677204	0.341286
C	3.222272	2.455988	0.662067
C	3.603707	1.572178	-0.257437

C	-0.793331	0.433986	-0.747648
C	-0.509433	1.575936	0.255782
O	0.487858	2.356417	-0.193270
C	3.985998	-2.077480	-0.608826
C	4.142607	0.246824	0.108769
O	3.748284	-0.653162	-0.825230
O	-1.136467	1.774699	1.264281
O	0.979536	-0.664754	1.282572
O	1.921897	-3.102128	1.292262
C	5.165156	-2.512254	-1.463497
O	4.776519	-0.032160	1.101299
C	0.092052	4.704699	0.341317
N	-1.925938	-0.366178	-0.359827
C	-3.237828	-0.016332	-0.524757
C	-3.613075	1.137033	-1.247326
C	-4.941197	1.454154	-1.455192
C	-5.964609	0.648991	-0.949085
C	-5.624672	-0.476039	-0.225206
C	-4.285060	-0.833036	0.004283
C	-3.979976	-2.033378	0.789910
O	-2.859519	-2.439833	1.070295
O	-5.073908	-2.708370	1.214830
H	0.681628	-3.180358	-0.349835
H	0.155894	-1.184499	-1.804236
H	1.235199	0.150151	-1.438430
H	2.885411	-3.858434	-1.022970
H	2.368737	-2.477982	-1.975839
H	0.791760	3.172057	1.684242
H	2.759289	4.526465	0.940444
H	2.532750	3.945521	-0.711889
H	3.408039	2.239500	1.710322
H	3.384793	1.729814	-1.306923
H	-1.010670	0.926758	-1.697465
H	4.208579	-2.224147	0.446466
H	1.704351	-2.413891	1.943228
H	6.059754	-1.949789	-1.194043
H	5.370170	-3.572386	-1.304464
H	4.958896	-2.354414	-2.524173
H	0.427364	5.541068	0.957444
H	-0.958771	4.520514	0.562946
H	0.189219	4.988633	-0.708415
H	-1.774992	-1.126404	0.293228
H	-2.854442	1.797626	-1.641253
H	-5.184452	2.349232	-2.015351
H	-7.002668	0.905633	-1.112257
H	-6.399720	-1.107677	0.184759
H	-4.757559	-3.468317	1.727841

B3LYP Energy = -1472.40715624 a.u.

(2*R*,8*R*,10*R*,13*R*)-**15**, Conf E

C	1.883052	-2.868482	0.021468
C	0.947367	-1.752602	-0.484558
C	0.468654	-0.712201	0.514607
C	3.211460	-2.929900	-0.749005
C	0.705589	3.594675	0.619424
C	2.122285	3.818783	0.066100
C	3.050933	2.697975	0.420388
C	3.299715	1.667066	-0.386666
C	-0.668916	0.175767	-0.014379
C	-0.572940	1.538253	0.693950
O	0.238399	2.353724	0.003056
C	4.257901	-1.897700	-0.345100
C	4.059696	0.481485	0.062130

O	3.711919	-0.587744	-0.690662
O	-1.100412	1.813847	1.743651
O	0.612015	-1.743996	-1.648503
O	2.162488	-2.786432	1.416891
C	5.581743	-2.100569	-1.066360
O	4.839443	0.435781	0.989153
C	-0.248285	4.727924	0.284527
N	-1.933727	-0.482352	0.193088
C	-3.109610	-0.127055	-0.402709
C	-3.154527	0.867467	-1.404137
C	-4.339750	1.201210	-2.029923
C	-5.539799	0.571928	-1.688596
C	-5.524052	-0.396704	-0.705186
C	-4.338274	-0.765754	-0.047604
C	-4.377773	-1.793579	0.997158
O	-3.420431	-2.188991	1.650895
O	-5.609464	-2.312933	1.214128
H	1.340812	-3.793876	-0.203044
H	1.342689	-0.108739	0.770167
H	0.176520	-1.191072	1.450772
H	3.647045	-3.915686	-0.573675
H	2.999129	-2.851347	-1.816841
H	0.736037	3.433786	1.697693
H	2.490498	4.761691	0.477971
H	2.054705	3.932447	-1.018297
H	3.477535	2.695195	1.419680
H	2.856341	1.608152	-1.373295
H	-0.498220	0.334682	-1.079260
H	4.410185	-1.916265	0.732432
H	1.479459	-3.252275	1.911076
H	5.444142	-2.062340	-2.148829
H	6.298464	-1.332989	-0.774790
H	6.002725	-3.073211	-0.805164
H	-1.244607	4.518534	0.673065
H	-0.312842	4.872038	-0.795624
H	0.106288	5.655970	0.736758
H	-2.023891	-1.118778	0.975063
H	-2.248203	1.379749	-1.693077
H	-4.330282	1.968039	-2.795396
H	-6.464659	0.840577	-2.181099
H	-6.441879	-0.891608	-0.421595
H	-5.520365	-2.970186	1.921661

B3LYP Energy = -1472.40648103 a.u.

(2*R*,8*R*,10*R*,13*R*)-**15**, Conf F

C	1.597978	-2.415818	0.747574
C	0.891745	-1.323729	-0.087904
C	0.116964	-0.270016	0.685223
C	2.819180	-3.047466	0.053926
C	1.172843	3.756797	-0.391330
C	2.678550	3.562683	-0.627490
C	3.181423	2.384586	0.138730
C	3.664598	1.272218	-0.414797
C	-0.838549	0.611763	-0.177060
C	-0.507772	2.083754	0.062330
O	0.552645	2.455894	-0.664836
C	4.165176	-2.338071	0.209735
C	3.860677	0.056341	0.389436
O	4.101926	-1.004658	-0.392507
O	-1.095307	2.795832	0.841711
O	0.902253	-1.370709	-1.299769
O	1.818528	-2.049274	2.099088
C	5.287227	-3.075235	-0.500655

O	3.732180	-0.013983	1.604453
C	0.557090	4.819483	-1.281809
N	-2.236685	0.416367	0.133457
C	-3.048742	-0.544325	-0.388543
C	-2.580189	-1.459625	-1.359809
C	-3.412798	-2.417698	-1.903111
C	-4.749607	-2.525780	-1.508700
C	-5.229531	-1.650376	-0.555974
C	-4.415884	-0.659577	0.020455
C	-4.978086	0.237984	1.033298
O	-4.373908	1.127382	1.617258
O	-6.287193	0.011884	1.306715
H	0.831801	-3.199794	0.791472
H	0.852814	0.336848	1.219779
H	-0.454784	-0.763301	1.473535
H	2.950456	-4.048800	0.469700
H	2.590048	-3.161732	-1.006865
H	0.985831	3.987451	0.657772
H	3.176357	4.479687	-0.297012
H	2.873272	3.441875	-1.695062
H	3.050370	2.406548	1.217594
H	3.795880	1.173933	-1.484916
H	-0.643741	0.399553	-1.228249
H	4.410691	-2.213457	1.263271
H	2.514257	-1.368079	2.134069
H	5.077714	-3.169460	-1.567529
H	6.231747	-2.545122	-0.375290
H	5.397935	-4.075753	-0.079979
H	-0.505765	4.931527	-1.068856
H	0.681963	4.560417	-2.334588
H	1.044520	5.779517	-1.101621
H	-2.641988	1.021063	0.839738
H	-1.551688	-1.413734	-1.686634
H	-3.012208	-3.096552	-2.646845
H	-5.394493	-3.281030	-1.937529
H	-6.258453	-1.717081	-0.232499
H	-6.548482	0.654598	1.984279

B3LYP Energy = -1472.40639138 a.u.

(2*R*,8*R*,10*R*,13*R*)-**15**, Conf G

C	0.930103	-2.471571	0.477702
C	0.598983	-0.979892	0.394307
C	0.077554	-0.423377	-0.913898
C	1.991120	-2.970394	-0.522032
C	1.722870	3.388614	-0.148171
C	3.150240	3.081165	-0.635194
C	3.455715	1.621382	-0.533887
C	4.202590	1.030675	0.397933
C	-0.890834	0.773986	-0.750132
C	-0.237908	1.983708	-0.067741
O	0.858965	2.358110	-0.737624
C	3.423046	-2.559994	-0.202362
C	4.333759	-0.436407	0.516385
O	3.462287	-1.103331	-0.275191
O	-0.676917	2.537973	0.908806
O	0.700054	-0.293597	1.391972
O	1.296567	-2.813068	1.798253
C	4.433669	-3.152342	-1.172109
O	5.113314	-0.983249	1.268505
C	1.240428	4.770409	-0.546505
N	-2.094969	0.437364	-0.030892
C	-3.214987	-0.123478	-0.579223
C	-3.226023	-0.516607	-1.938301

C	-4.339909	-1.085383	-2.524652
C	-5.505695	-1.303786	-1.789183
C	-5.520418	-0.933570	-0.459924
C	-4.411130	-0.348593	0.172614
C	-4.614985	-0.013756	1.597489
O	-5.639048	-0.213844	2.218923
O	-3.542193	0.559141	2.207212
H	-0.012687	-2.977385	0.221548
H	-0.427536	-1.213966	-1.470798
H	0.938495	-0.121946	-1.515232
H	1.954590	-4.061708	-0.513082
H	1.726120	-2.655454	-1.534707
H	1.670618	3.260622	0.932810
H	3.840978	3.676297	-0.034535
H	3.246675	3.405675	-1.675689
H	2.967947	0.991645	-1.266012
H	4.743391	1.592280	1.150640
H	-1.137191	1.118961	-1.759063
H	3.668282	-2.844117	0.819054
H	1.233735	-1.995880	2.320954
H	5.442935	-2.827398	-0.919867
H	4.406540	-4.242313	-1.118157
H	4.212909	-2.851932	-2.198596
H	1.916799	5.525939	-0.141751
H	0.242489	4.961615	-0.153715
H	1.222166	4.872732	-1.633260
H	-2.154857	0.786930	0.914319
H	-2.343898	-0.371327	-2.544571
H	-4.296299	-1.364801	-3.570688
H	-6.376837	-1.752395	-2.247239
H	-6.407062	-1.086352	0.140283
H	-3.786892	0.742909	3.128058

B3LYP Energy = -1472.40562280 a.u.

(2*R*,8*R*,10*R*,13*R*)-**15**, Conf H

C	0.816331	-2.485622	0.660829
C	0.665980	-0.972144	0.487121
C	0.203543	-0.414819	-0.841729
C	1.814462	-3.176638	-0.287001
C	1.745173	3.513264	-0.066615
C	3.215032	3.259506	-0.432109
C	3.715523	1.972253	0.141662
C	3.822699	0.850635	-0.566963
C	-0.758670	0.790281	-0.704710
C	-0.129092	1.999753	0.003029
O	0.984432	2.390074	-0.625653
C	3.270075	-2.763647	-0.100358
C	4.043983	-0.460033	0.077338
O	3.379267	-1.406655	-0.629036
O	-0.613643	2.550459	0.961432
O	0.869151	-0.249100	1.443667
O	1.145015	-2.784636	2.002369
C	4.245465	-3.660128	-0.845200
O	4.654310	-0.673680	1.100378
C	1.214282	4.819205	-0.631608
N	-1.987367	0.456215	-0.023826
C	-3.091617	-0.097090	-0.611600
C	-3.056335	-0.495274	-1.968714
C	-4.151198	-1.061877	-2.592068
C	-5.343215	-1.272566	-1.897714
C	-5.403749	-0.895916	-0.571538
C	-4.315459	-0.311981	0.097295
C	-4.569699	0.031765	1.512018

O	-5.611577	-0.174801	2.100880
O	-3.524674	0.623307	2.151378
H	-0.179673	-2.892243	0.431024
H	-0.286020	-1.195652	-1.424359
H	1.093652	-0.113174	-1.397773
H	1.736364	-4.247591	-0.089174
H	1.517950	-3.023262	-1.327684
H	1.612563	3.485692	1.014752
H	3.792328	4.102563	-0.043280
H	3.314307	3.260426	-1.520103
H	3.900727	1.939148	1.211604
H	3.590482	0.834582	-1.625343
H	-0.971224	1.140767	-1.719516
H	3.518740	-2.731011	0.958825
H	1.185190	-1.934702	2.472437
H	4.191090	-4.677081	-0.452710
H	4.015172	-3.688064	-1.912315
H	5.267487	-3.301824	-0.717668
H	1.784154	5.655693	-0.223065
H	0.167252	4.958951	-0.363947
H	1.307621	4.836543	-1.719108
H	-2.087926	0.833643	0.907381
H	-2.153219	-0.355605	-2.544608
H	-4.071668	-1.345157	-3.634946
H	-6.199468	-1.719489	-2.384592
H	-6.311881	-1.041828	-0.002595
H	-3.801762	0.811850	3.062035

B3LYP Energy = -1472.40545694 a.u.

(2*R*,8*R*,10*R*,13*R*)-**15**, Conf I

C	-2.675076	-2.429059	0.256386
C	-1.559491	-1.444308	0.683267
C	-0.301354	-1.452719	-0.171899
C	-4.017629	-2.231613	0.983419
C	0.133756	3.290295	-0.670666
C	-1.351135	3.669062	-0.515005
C	-2.252325	2.552901	-0.927091
C	-3.085899	1.923935	-0.098219
C	0.710588	-0.348626	0.169154
C	0.450584	0.897758	-0.700213
O	0.378777	2.023561	0.028182
C	-4.991581	-1.195918	0.419225
C	-3.750660	0.669855	-0.486668
O	-4.427783	0.147754	0.543971
O	0.359567	0.851397	-1.904817
O	-1.642081	-0.798326	1.705716
O	-2.794700	-2.552659	-1.152687
C	-6.307792	-1.175767	1.177493
O	-3.643032	0.120507	-1.574437
C	1.067890	4.321434	-0.068276
N	2.057282	-0.834704	-0.079484
C	3.201706	-0.365551	0.503403
C	3.167292	0.594049	1.539361
C	4.324910	1.020366	2.159887
C	5.575871	0.527959	1.777602
C	5.638242	-0.396569	0.755035
C	4.482861	-0.858179	0.100975
C	4.608877	-1.834974	-0.985583
O	3.685489	-2.302174	-1.639670
O	5.883812	-2.213148	-1.242838
H	-2.285411	-3.398338	0.591008
H	-0.558866	-1.445014	-1.230275
H	0.167584	-2.426176	0.012608

H	-4.541476	-3.189569	0.951940
H	-3.817926	-2.004308	2.031974
H	0.361506	3.127186	-1.722456
H	-1.518117	4.547297	-1.147374
H	-1.548833	3.960307	0.518996
H	-2.149356	2.179691	-1.941532
H	-3.214377	2.237213	0.930191
H	0.599525	-0.081637	1.217375
H	-5.175412	-1.382813	-0.637859
H	-3.118908	-1.704683	-1.508349
H	-6.145893	-0.958157	2.234720
H	-6.974902	-0.419156	0.763453
H	-6.798469	-2.146667	1.095093
H	2.107957	4.027642	-0.211268
H	0.881009	4.439379	1.000526
H	0.913912	5.286668	-0.553993
H	2.200002	-1.432132	-0.885911
H	2.222179	1.015033	1.847950
H	4.252873	1.755025	2.953176
H	6.478199	0.868909	2.267165
H	6.595086	-0.784694	0.436435
H	5.848924	-2.849351	-1.974084

B3LYP Energy = -1472.40530042 a.u.

(2*R*,8*R*,10*R*,13*S*)-**15**, Conf A

C	-2.520835	-2.287110	-1.239979
C	-1.554598	-1.099468	-1.267993
C	-0.339845	-1.138923	-0.368883
C	-3.168063	-2.584961	0.126170
C	-0.246309	3.092499	0.132194
C	-1.323954	3.198647	1.227033
C	-2.265901	2.039330	1.169444
C	-3.496563	2.041649	0.658733
C	0.867645	-0.348882	-0.904822
C	0.605123	1.163610	-1.041725
O	0.182933	1.691029	0.115813
C	-4.249254	-1.602708	0.557446
C	-4.306858	0.815920	0.506400
O	-3.591736	-0.311882	0.726720
O	0.801457	1.791541	-2.053690
O	-1.744877	-0.199380	-2.062249
O	-3.511660	-2.125385	-2.233287
C	-4.926936	-2.009828	1.856716
O	-5.477135	0.817759	0.185150
C	0.940783	4.006388	0.370795
N	1.997252	-0.606675	-0.033803
C	3.315865	-0.490491	-0.375480
C	3.710757	-0.101986	-1.674033
C	5.045256	-0.029252	-2.022778
C	6.052547	-0.325484	-1.100280
C	5.691742	-0.689398	0.181061
C	4.345127	-0.778054	0.574470
C	4.015031	-1.162356	1.949995
O	2.885706	-1.255358	2.416248
O	5.093593	-1.421730	2.725319
H	-1.896944	-3.157301	-1.491954
H	-0.031393	-2.175629	-0.218255
H	-0.634675	-0.755840	0.612256
H	-3.632673	-3.570449	0.053155
H	-2.395814	-2.658094	0.896381
H	-0.694807	3.294498	-0.840386
H	-1.847125	4.146988	1.088548

H	-0.834468	3.225294	2.205082
H	-1.869346	1.100124	1.531454
H	-3.974725	2.945166	0.298890
H	1.094049	-0.698783	-1.912261
H	-4.986737	-1.494627	-0.235572
H	-3.320943	-1.282515	-2.678752
H	-5.418186	-2.976788	1.733155
H	-4.199602	-2.092671	2.667067
H	-5.685421	-1.279599	2.138271
H	1.437083	3.754894	1.309985
H	0.600657	5.042489	0.428227
H	1.660673	3.929066	-0.443288
H	1.818743	-0.801809	0.944269
H	2.961605	0.163575	-2.405378
H	5.306456	0.272840	-3.029974
H	7.095304	-0.262551	-1.380900
H	6.454384	-0.913336	0.913171
H	4.762350	-1.655822	3.606333

B3LYP Energy = -1472.40762461 a.u.

(2*R*,8*R*,10*R*,13*S*)-**15**, Conf B

C	2.655522	-2.191704	1.337998
C	1.704727	-0.994122	1.239614
C	0.491644	-1.086814	0.343884
C	3.342499	-2.612070	0.024621
C	0.038090	3.214346	0.035386
C	1.108676	3.515641	-1.024430
C	2.382239	2.781441	-0.746476
C	2.705925	1.640041	-1.350150
C	-0.749031	-0.367963	0.906628
C	-0.566178	1.148511	1.121013
O	-0.172941	1.765593	0.000476
C	4.305491	-1.582345	-0.555221
C	3.806894	0.782057	-0.869602
O	3.474725	-0.512338	-1.098256
O	-0.818257	1.705116	2.163416
O	1.915635	-0.019277	1.935994
O	3.627780	-1.948866	2.334348
C	5.178239	-2.140807	-1.667404
O	4.817015	1.138071	-0.305550
C	-1.274710	3.929673	-0.234587
N	-1.864965	-0.631914	0.020359
C	-3.187396	-0.613841	0.367042
C	-3.601486	-0.335398	1.687943
C	-4.937159	-0.361709	2.038580
C	-5.928148	-0.651889	1.096742
C	-5.549812	-0.908181	-0.205391
C	-4.201127	-0.894963	-0.601445
C	-3.853656	-1.167819	-1.999155
O	-2.722041	-1.168987	-2.468816
O	-4.918608	-1.431855	-2.791802
H	2.020448	-3.033354	1.650586
H	0.232211	-2.132847	0.172301
H	0.764574	-0.662446	-0.626225
H	3.906963	-3.519384	0.248875
H	2.594068	-2.879761	-0.725541
H	0.408090	3.463779	1.029975
H	1.276628	4.595729	-1.016597
H	0.716864	3.244877	-2.007645
H	3.009761	3.149560	0.060322
H	2.070209	1.217604	-2.119175
H	-0.966319	-0.773994	1.894778
H	4.924118	-1.159288	0.234234

H	3.445029	-1.062335	2.689258
H	5.817287	-2.934728	-1.276769
H	4.568354	-2.552295	-2.474335
H	5.819792	-1.360275	-2.077736
H	-1.675663	3.644232	-1.208855
H	-1.114821	5.009462	-0.228814
H	-2.009675	3.690907	0.533501
H	-1.677297	-0.755367	-0.967702
H	-2.867791	-0.076292	2.436884
H	-5.212767	-0.142720	3.063300
H	-6.972244	-0.666303	1.379094
H	-6.299961	-1.125143	-0.952295
H	-4.577021	-1.588379	-3.685974

B3LYP Energy = -1472.40742332 a.u.

(2*R*,8*R*,10*R*,13*S*)-**15**, Conf C

C	-2.068978	-2.630310	-0.606862
C	-1.338542	-1.342567	-0.999629
C	-0.098745	-0.946013	-0.231649
C	-2.587245	-2.685183	0.843027
C	-0.735928	3.244405	-0.691285
C	-1.745564	3.421130	0.457024
C	-2.465309	2.142116	0.742946
C	-3.703410	1.827441	0.364300
C	0.916793	-0.106282	-1.042890
C	0.381428	1.258732	-1.493679
O	-0.053802	1.969694	-0.442751
C	-3.803185	-1.814252	1.132440
C	-4.289568	0.485208	0.558282
O	-3.375390	-0.431130	0.952837
O	0.388750	1.647408	-2.634341
O	-1.729083	-0.713160	-1.964386
O	-3.117146	-2.885545	-1.518663
C	-4.339605	-2.008495	2.542477
O	-5.457079	0.224974	0.353362
C	0.271692	4.374226	-0.783269
N	2.129165	0.133956	-0.280887
C	3.221931	-0.685410	-0.240026
C	3.312282	-1.844270	-1.042188
C	4.433378	-2.650488	-1.015267
C	5.518977	-2.353344	-0.187325
C	5.452210	-1.231453	0.613593
C	4.329310	-0.386334	0.614594
C	4.305818	0.784353	1.497070
O	3.374198	1.569953	1.618968
O	5.439246	0.955855	2.216851
H	-1.309281	-3.420097	-0.702214
H	0.407608	-1.840776	0.137056
H	-0.411373	-0.384127	0.652072
H	-2.873463	-3.720238	1.041056
H	-1.778063	-2.445054	1.537449
H	-1.272140	3.131410	-1.633261
H	-2.438090	4.214829	0.169782
H	-1.210697	3.750034	1.352805
H	-1.886099	1.387552	1.258433
H	-4.355595	2.534950	-0.134269
H	1.162569	-0.622019	-1.967970
H	-4.583228	-2.015035	0.400500
H	-3.104918	-2.155260	-2.160574
H	-5.197640	-1.360058	2.718392
H	-4.663630	-3.042020	2.678435
H	-3.571522	-1.786455	3.286304
H	0.865202	4.435870	0.130630

H	-0.253229	5.322220	-0.917719
H	0.939665	4.231346	-1.632015
H	2.124009	0.889576	0.395359
H	2.494989	-2.113689	-1.695141
H	4.461629	-3.528524	-1.649486
H	6.393303	-2.989902	-0.171527
H	6.278049	-0.984152	1.265110
H	5.313796	1.748277	2.761876

B3LYP Energy = -1472.40651713 a.u.

(2*R*,8*R*,10*R*,13*S*)-**15**, Conf D

C	-2.202873	-2.564643	-0.820125
C	-1.504228	-1.219206	-1.041470
C	-0.245188	-0.898539	-0.271642
C	-2.718580	-2.823921	0.608495
C	-0.548825	3.402622	-0.721034
C	-1.573417	3.689171	0.386828
C	-2.702576	2.708167	0.361723
C	-2.774668	1.659993	1.179117
C	0.800108	-0.088636	-1.077564
C	0.329249	1.302452	-1.525764
O	-0.056502	2.043358	-0.478165
C	-3.814132	-1.874330	1.079328
C	-3.730501	0.556968	0.954234
O	-3.154022	-0.602067	1.356057
O	0.361732	1.685211	-2.669143
O	-1.950416	-0.459411	-1.881177
O	-3.260098	-2.712265	-1.746813
C	-4.516872	-2.350247	2.340288
O	-4.823713	0.633300	0.439998
C	0.616614	4.376258	-0.715986
N	2.020480	0.098594	-0.313283
C	3.072023	-0.773088	-0.264804
C	3.120951	-1.924961	-1.080803
C	4.201983	-2.783947	-1.047026
C	5.286749	-2.549177	-0.198345
C	5.259704	-1.435656	0.616376
C	4.178235	-0.538207	0.611029
C	4.195804	0.619291	1.510967
O	3.302669	1.448961	1.627436
O	5.322065	0.722656	2.254848
H	-1.434489	-3.323629	-1.025965
H	0.226447	-1.817779	0.080234
H	-0.534917	-0.332283	0.616547
H	-3.121895	-3.838481	0.608781
H	-1.888815	-2.810575	1.319756
H	-1.035296	3.397749	-1.696349
H	-1.943718	4.705638	0.229100
H	-1.064059	3.664939	1.352886
H	-3.437619	2.809489	-0.431938
H	-2.025754	1.497150	1.945097
H	1.028979	-0.608123	-2.004971
H	-4.538001	-1.709399	0.283086
H	-3.284364	-1.893312	-2.270457
H	-5.030932	-3.293377	2.146725
H	-3.802518	-2.505093	3.151578
H	-5.259195	-1.619528	2.662996
H	1.135709	4.353767	0.243814
H	0.250080	5.389867	-0.888442
H	1.326001	4.132396	-1.506415
H	2.037404	0.842632	0.375570
H	2.303080	-2.147198	-1.750541
H	4.198904	-3.654199	-1.692512

H	6.129642	-3.226670	-0.177242
H	6.085198	-1.236417	1.284510
H	5.225689	1.512162	2.809885

B3LYP Energy = -1472.40636838 a.u.

(2*R*,8*R*,10*R*,13*S*)-**15**, Conf E

C	-2.294506	-2.250865	-0.719087
C	-1.165896	-1.676386	-1.574009
C	-0.843310	-0.208861	-1.378845
C	-3.635355	-1.487447	-0.879322
C	0.446525	3.586324	0.029055
C	-0.577792	3.703958	1.168983
C	-1.876934	3.051686	0.816481
C	-2.310897	1.906554	1.343737
C	0.652720	0.137020	-1.453092
C	0.739516	1.677728	-1.431001
O	0.648065	2.151393	-0.183628
C	-4.305581	-1.057683	0.430182
C	-3.475359	1.191833	0.778172
O	-3.420050	-0.117929	1.119513
O	0.800033	2.354327	-2.430806
O	-0.564639	-2.390192	-2.349112
O	-2.465734	-3.627154	-0.998201
C	-4.595991	-2.182963	1.404365
O	-4.324593	1.667028	0.054806
C	1.778437	4.239418	0.349733
N	1.359299	-0.521039	-0.381426
C	2.718516	-0.660925	-0.313076
C	3.550109	-0.295579	-1.393228
C	4.918276	-0.480452	-1.337976
C	5.528394	-1.028533	-0.207079
C	4.737507	-1.380717	0.868270
C	3.343228	-1.207273	0.850073
C	2.550659	-1.577673	2.027216
O	1.340998	-1.430930	2.150645
O	3.276474	-2.117959	3.033512
H	-1.939621	-2.131337	0.314861
H	-1.246376	0.129282	-0.425378
H	-1.373056	0.344368	-2.160566
H	-3.520153	-0.600670	-1.504160
H	-4.312514	-2.154094	-1.415004
H	0.035737	3.997709	-0.893116
H	-0.730586	4.771282	1.355033
H	-0.156541	3.263562	2.075210
H	-2.457973	3.507077	0.018558
H	-1.749601	1.389012	2.112562
H	1.039658	-0.186690	-2.418414
H	-5.223541	-0.525465	0.183615
H	-1.755755	-3.871626	-1.615124
H	-5.270811	-2.904193	0.940727
H	-3.687178	-2.708406	1.701127
H	-5.074535	-1.790764	2.302270
H	2.475683	4.116450	-0.479223
H	2.219090	3.802154	1.247303
H	1.635493	5.308294	0.518686
H	0.871550	-0.674495	0.493303
H	3.117722	0.137380	-2.283555
H	5.520706	-0.189008	-2.190050
H	6.600213	-1.169696	-0.170851
H	5.189661	-1.799244	1.756015
H	2.659613	-2.317273	3.754998

B3LYP Energy = -1472.40501401 a.u.

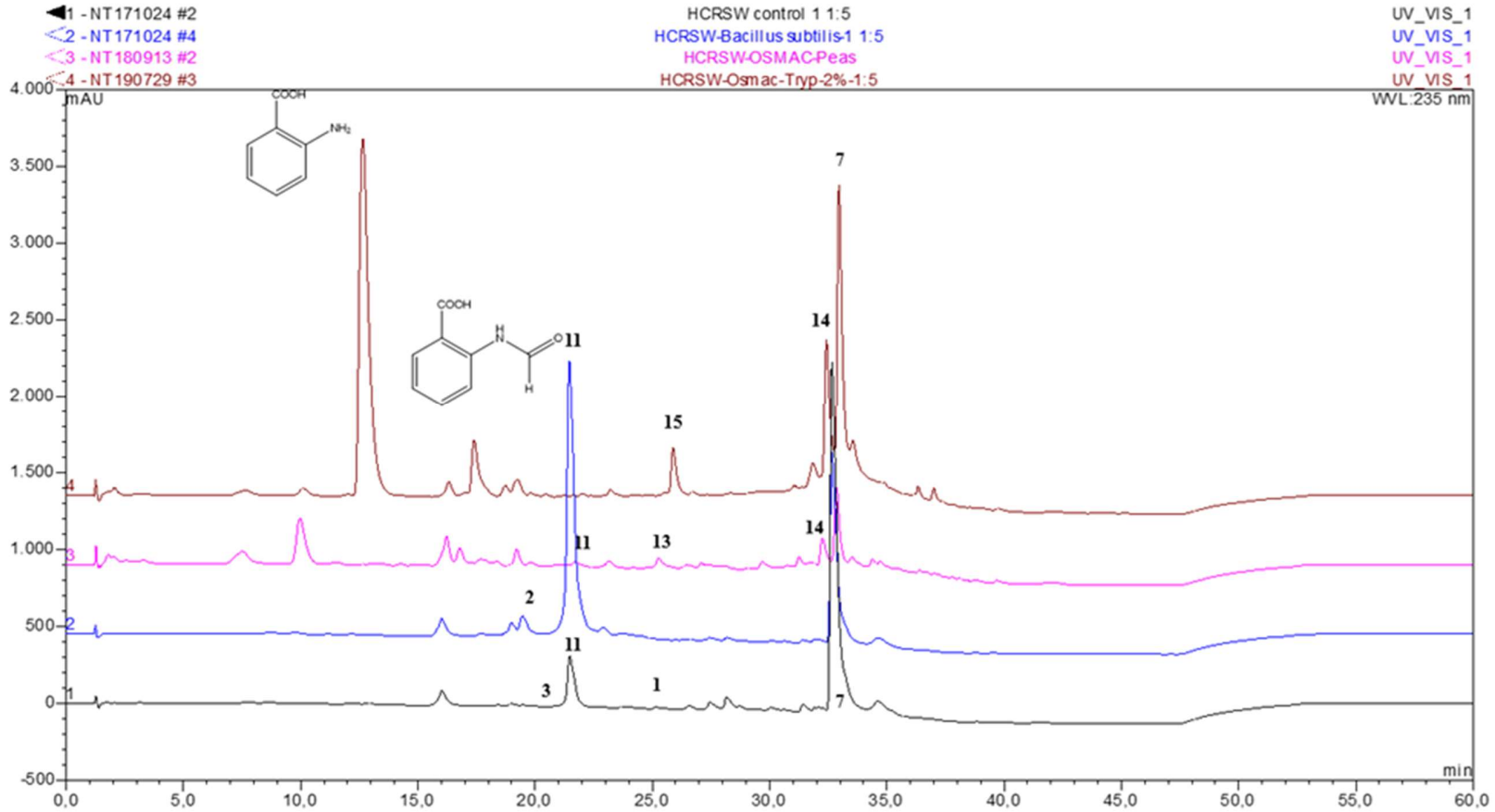


Figure S55. HPLC overlays of the crude extracts.

Table S7. Yield (mg/flask) of compound **11** in axenic fungal control and in coculture with *Bacillus subtilis*.

flask number	Control	Coculture
1	13.4	72.3
2	1.8	65.1
3	1.9	51.5
4	14.0	74.7
5	2.3	76.8
$\bar{x}$	6.7 ± 5.8	68.1 ± 9.2

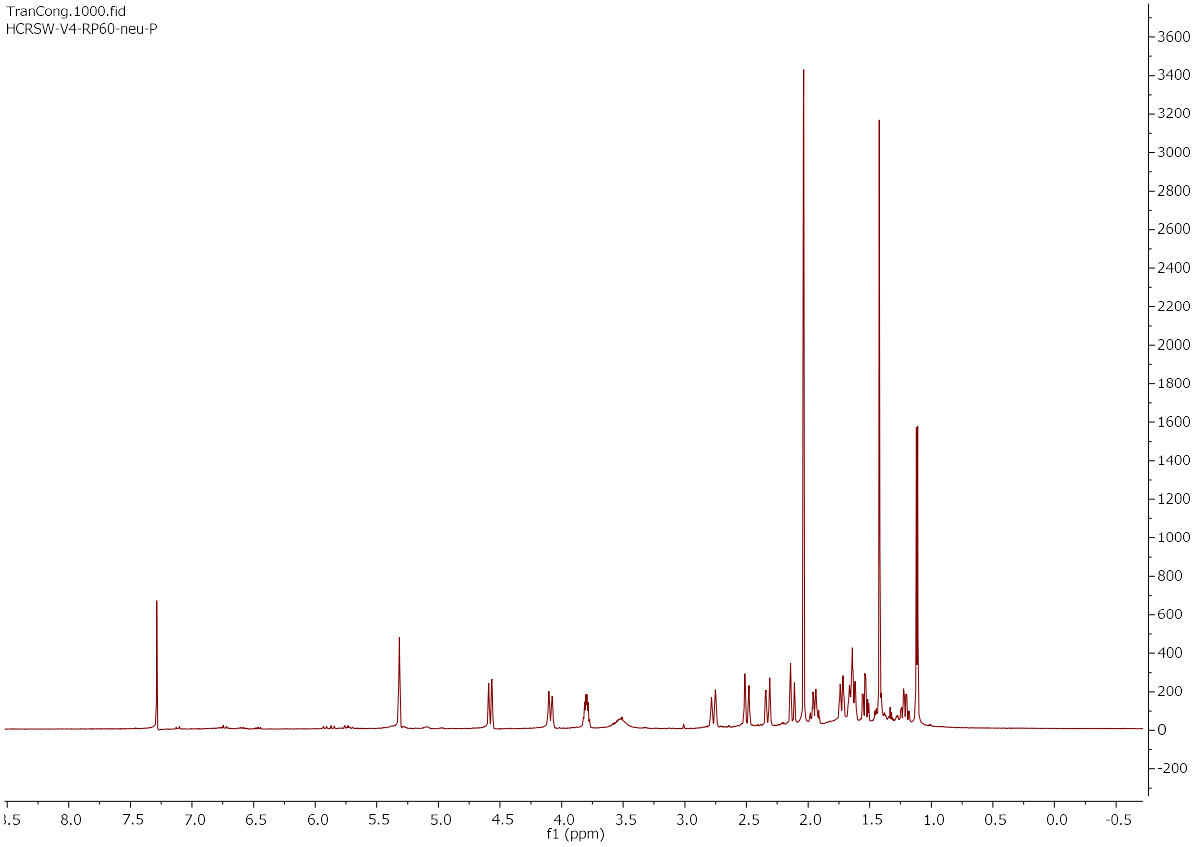


Figure S56. The ^{1}H NMR (600 MHz, CD_3Cl) spectrum of compound **2** after storage in EtOAc.

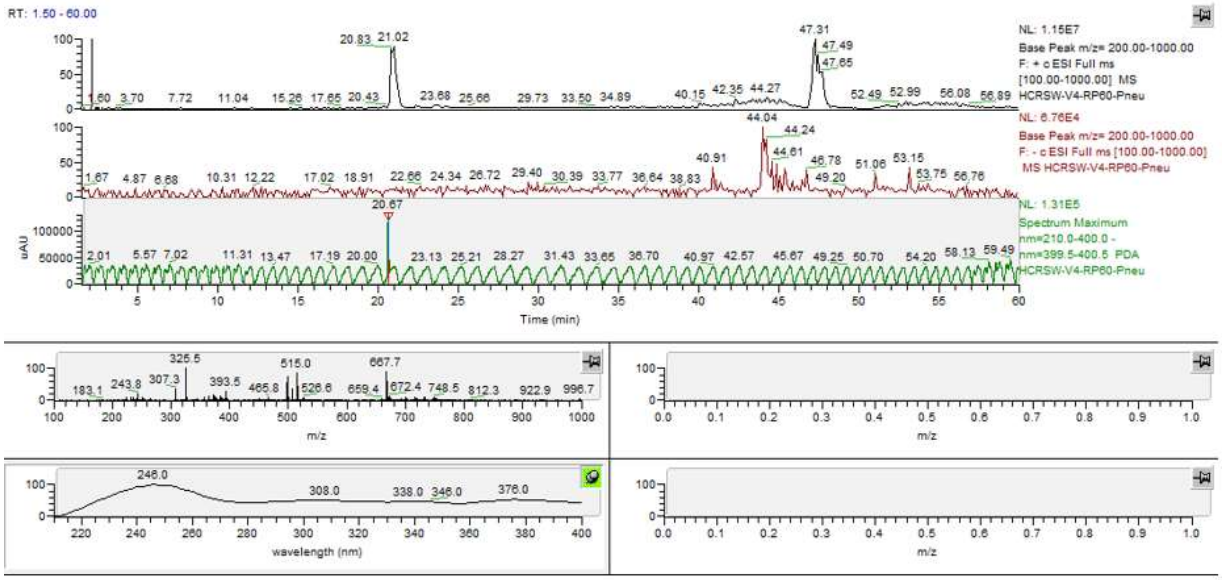


Figure S57. LCMS of compound **2** after storage in EtOAc.

Table S8. Raw data of compound **7** against the L51178Y mouse lymphoma cell line.

Blank						Mean	Mean-Blank	Growth in %	Growth Inhibition in %	Cons. (µg/ml)	SD
0.039	0.039	0.039	0.024	0.039	0.015						
0.197	0.483	0.498	0.391	0.451	0.406	0.446	0.249	100.0	0.0	0	0.05
0.204	0.358	0.351	0.328	0.418	0.379	0.367	0.163	65.4	34.6	0.1	0.03
0.205	0.203	0.206	0.196	0.207	0.187	0.200	-0.005	-2.1	102.1	0.3	0.01
0.2	0.209	0.187	0.197	0.187	0.201	0.196	-0.004	-1.5	101.5	1	0.01
0.23	0.238	0.211	0.228	0.204	0.23	0.222	-0.008	-3.1	103.1	3	0.01
0.367	0.358	0.343	0.36	0.352	0.351	0.353	-0.014	-5.7	105.7	10	0.01
0.039	0.039	0.026	0.039	0.011	0.037			IC_{50} 0.14 µg/mL			

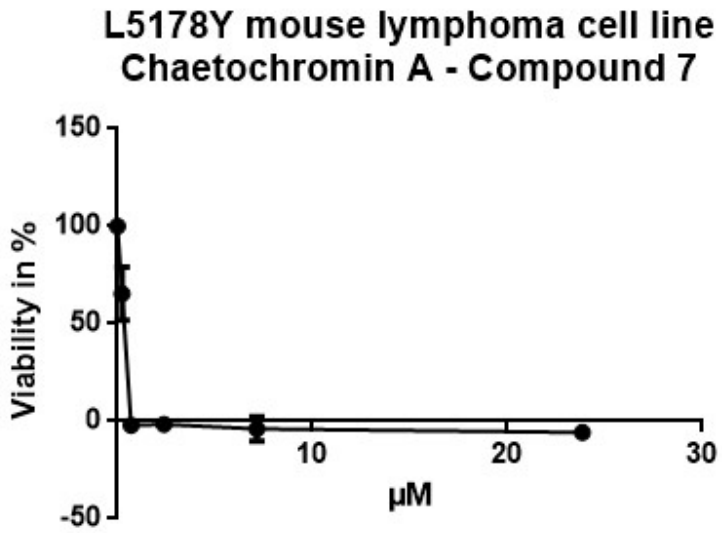


Figure S58. Dose-dependence curve of compound **7** against the L5178Y mouse lymphoma cell line.

Table S9. Raw data of compound **11** against the L51178Y mouse lymphoma cell line.

Blank						Mean	Mean-Blank	Growth in %	Growth Inhibition in %	Cons. (µg/ml)	SD
0.038	0.012	0.006	0.034	0.034	0.068						
0.153	0.709	0.65	0.749	0.637	0.831	0.715	0.563	100.0	0.0	0	0.08
0.164	0.342	0.357	0.563	0.559	0.63	0.490	0.326	58.0	42.0	0.1	0.13
0.15	0.153	0.176	0.24	0.278	0.31	0.231	0.081	14.5	85.5	0.3	0.07
0.146	0.112	0.149	0.169	0.264	0.272	0.193	0.047	8.4	91.6	1	0.07
0.14	0.149	0.157	0.168	0.294	0.276	0.209	0.069	12.2	87.8	3	0.07
0.153	0.236		0.177	0.309	0.279	0.250	0.098	17.3	82.7	10	0.06
0.03	0.035	0.005	0.001	0.073	0.062			IC_{50} 0.14 µg/mL			

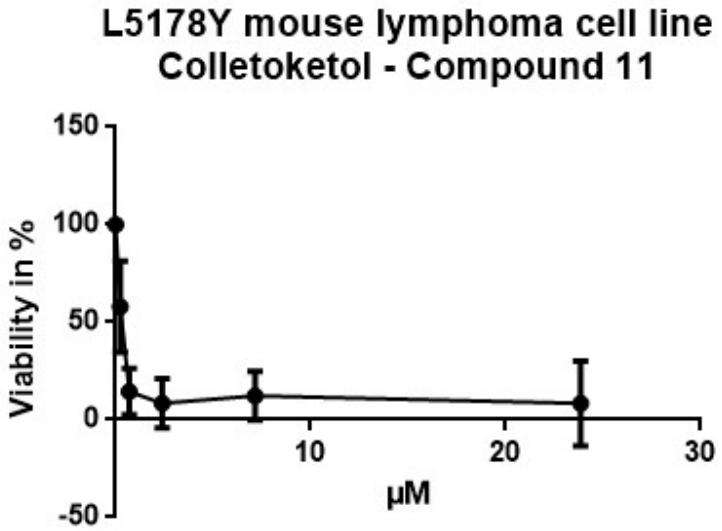


Figure S59. Dose-dependence curve of compound **11** against the L5178Y mouse lymphoma cell line.

Table S10. Raw data of compound **15** against the L51178Y mouse lymphoma cell line.

Blank						Mean	Mean-Blank	Growth in %	Growth Inhibition in %	Cons. (µg/ml)	SD
0.206	0.075	0.204	0.181	0.283	0.264						
0.521	0.695	0.925	0.933	1.043	1.045	0.928	0.407	100.0	0.0	0	0.14
0.5		0.539	0.578	0.639	0.659	0.604	0.104	25.5	74.5	0.1	0.06
0.539	0.312	0.427	0.463	0.542	0.57	0.463	-0.076	-18.7	118.7	0.3	0.10
0.513	0.338	0.414	0.505	0.534	0.611	0.480	-0.033	-8.0	108.0	1	0.11
0.488	0.365	0.38	0.481	0.497	0.589	0.462	-0.026	-6.3	106.3	3	0.09
0.526	0.444	0.391	0.912	0.527	0.604	0.576	0.050	12.2	87.8	10	0.20
0.266	0.15	0.134	0.252	0.232	0.292			IC_{50} 0.065 µg/mL			

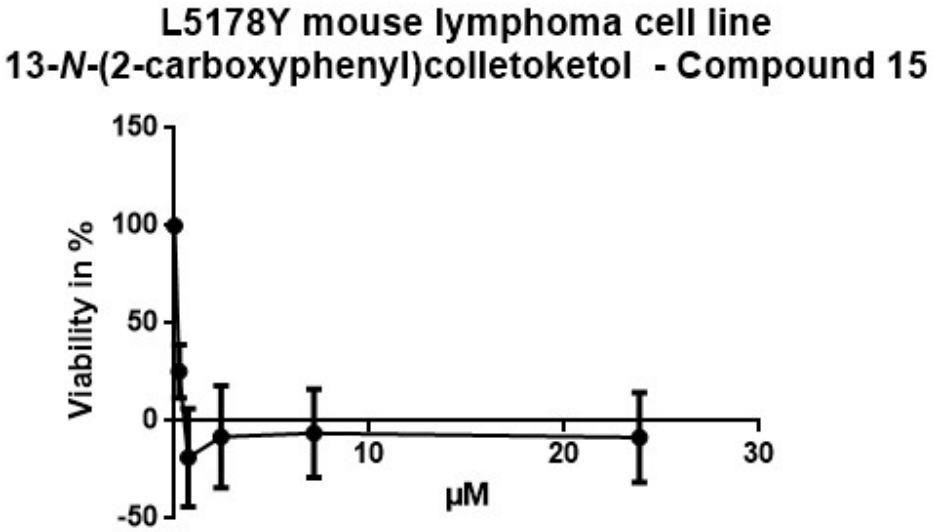


Figure S60. Dose-dependence curve of compound **15** against the L5178Y mouse lymphoma cell line.