

Supporting Information

Influence of Amino Acid Stereocenters on the Formation of Bicyclic *N,O*-Acetals

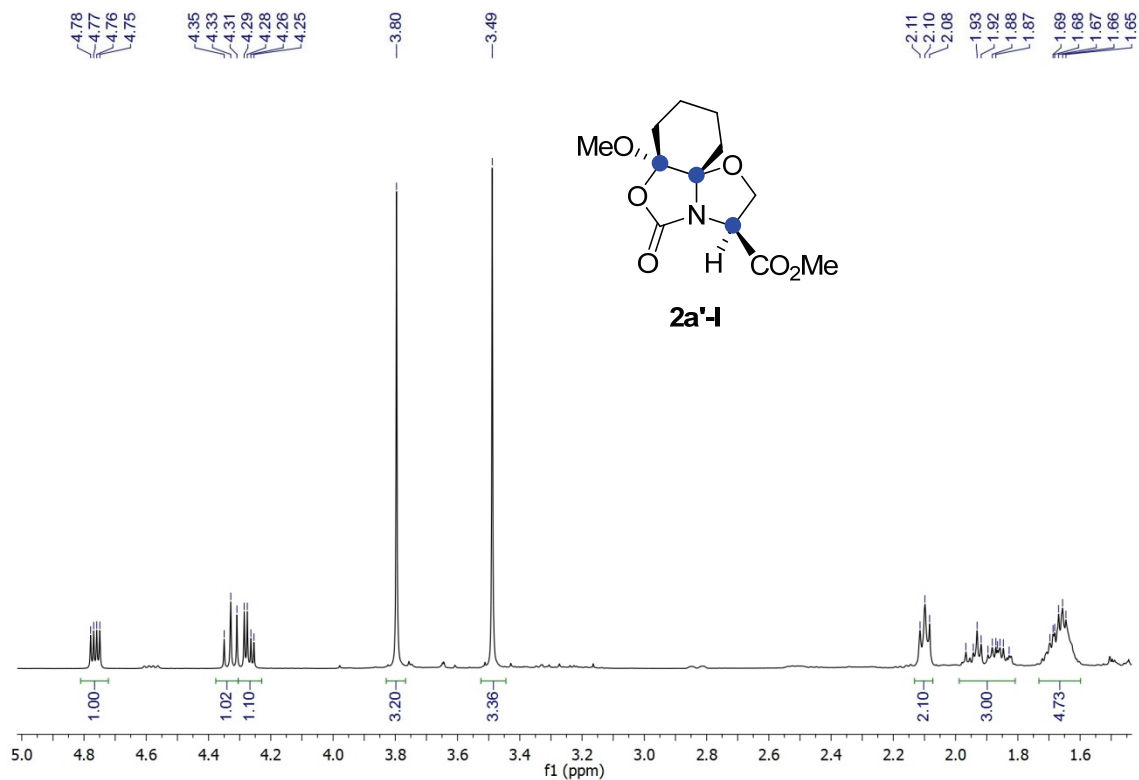
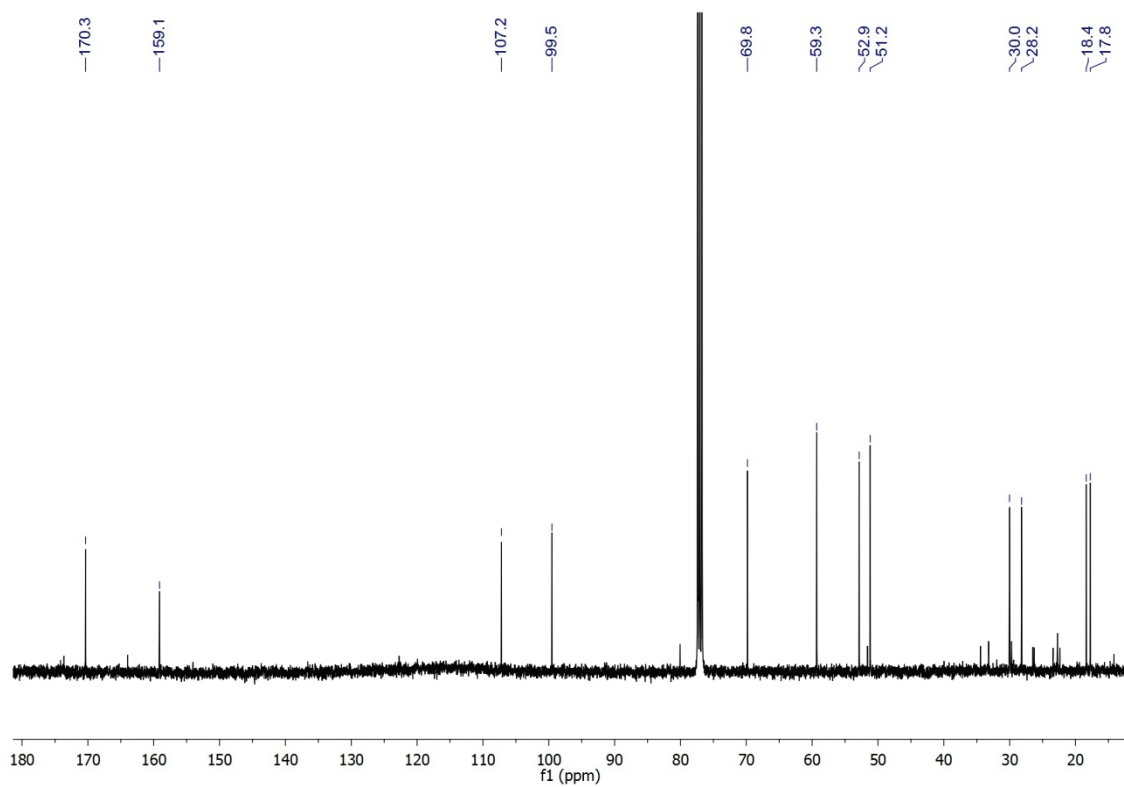
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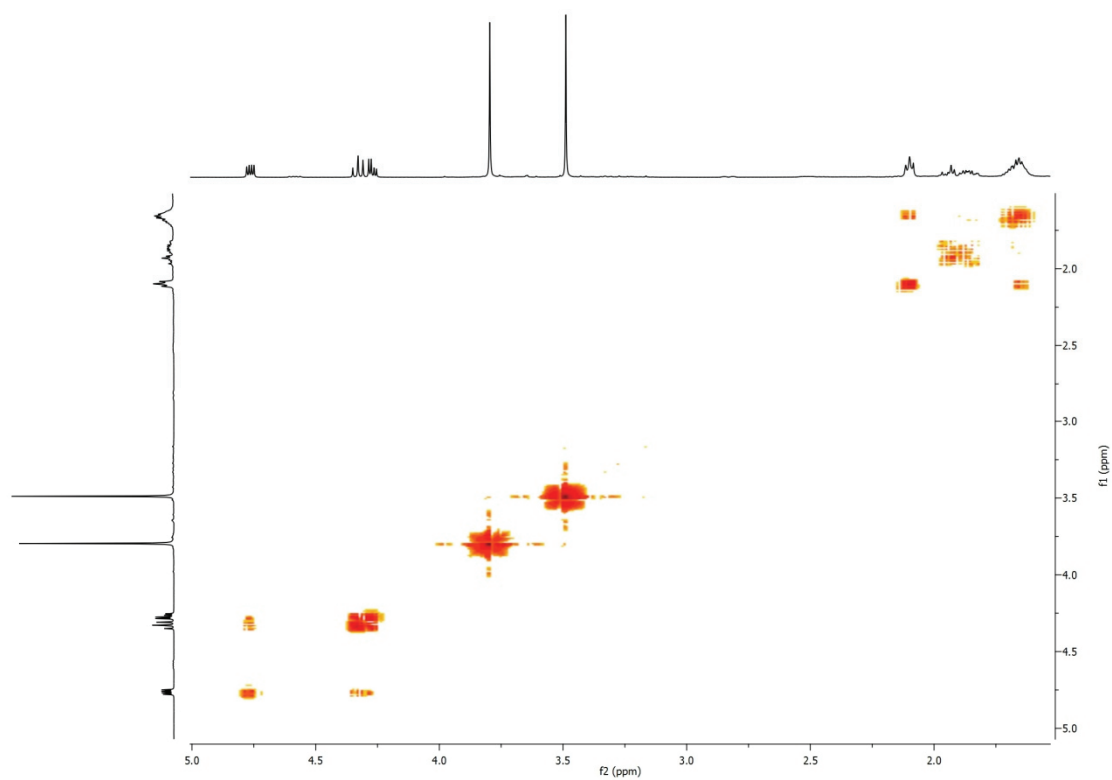
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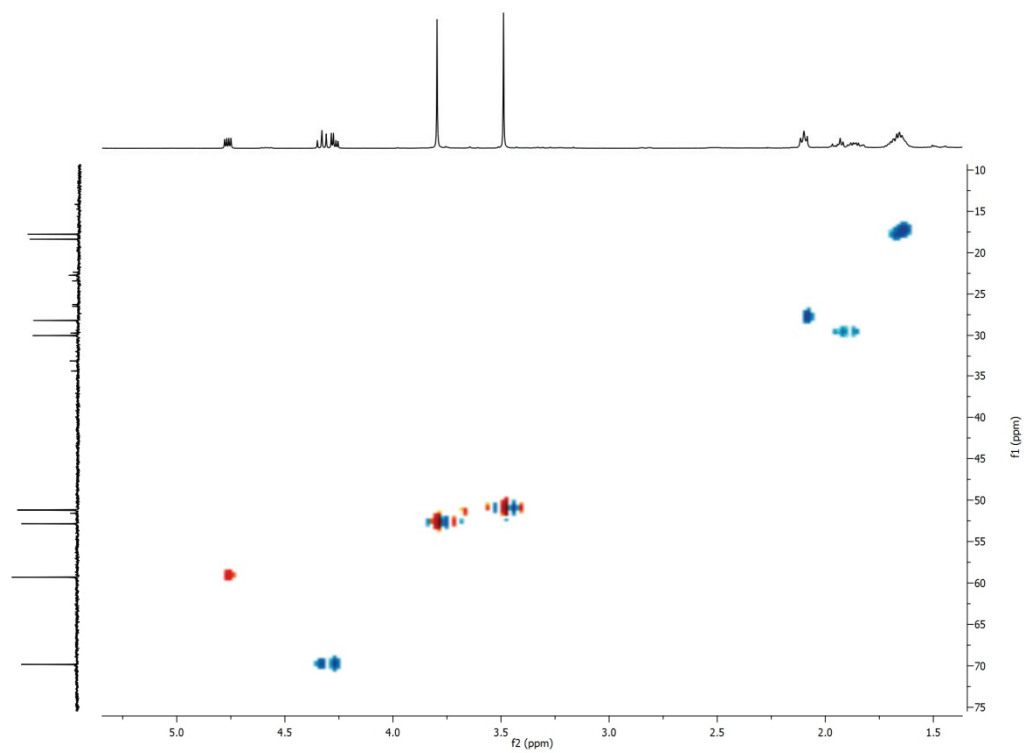
¹ H, ¹³ C, ¹ H- ¹ H and ¹ H- ¹³ C NMR spectra for the most relevant compounds.....	Pages S2-S13
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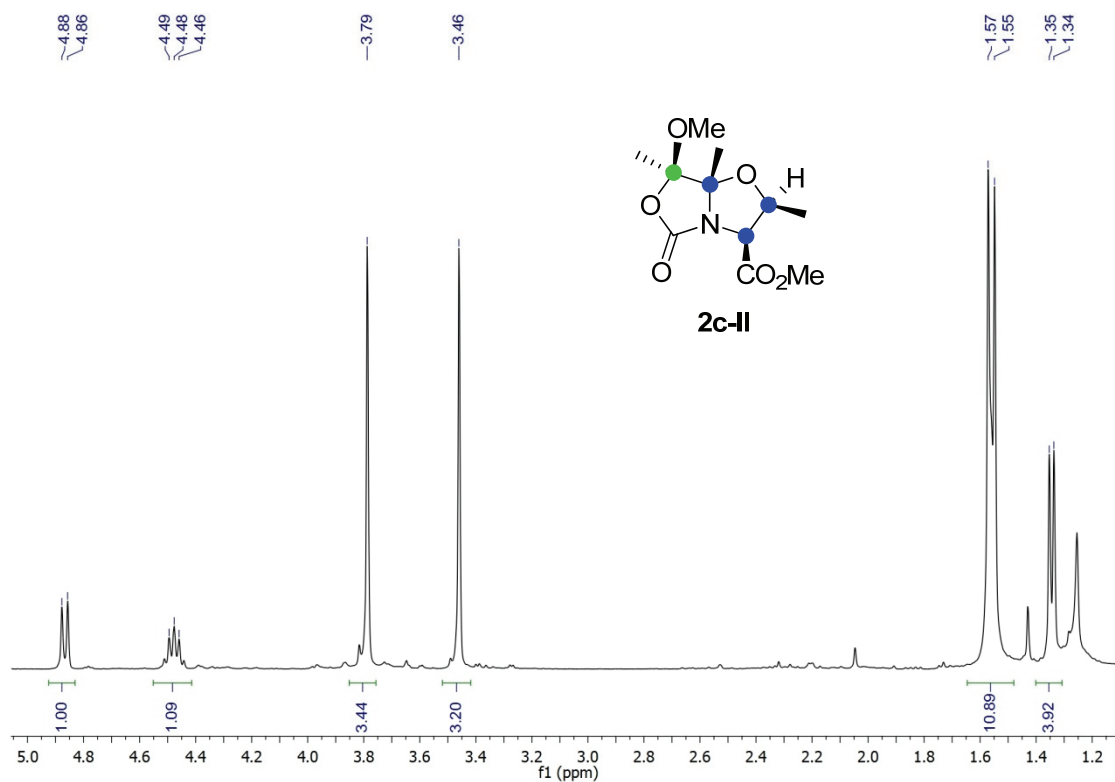
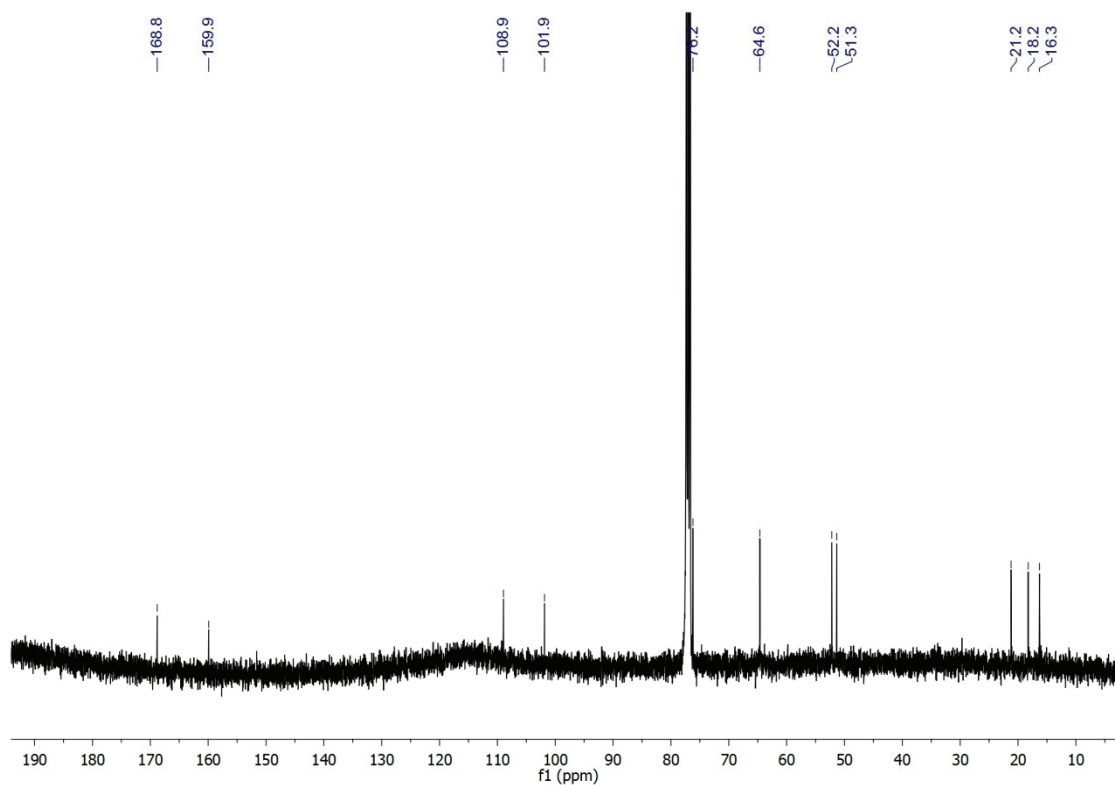
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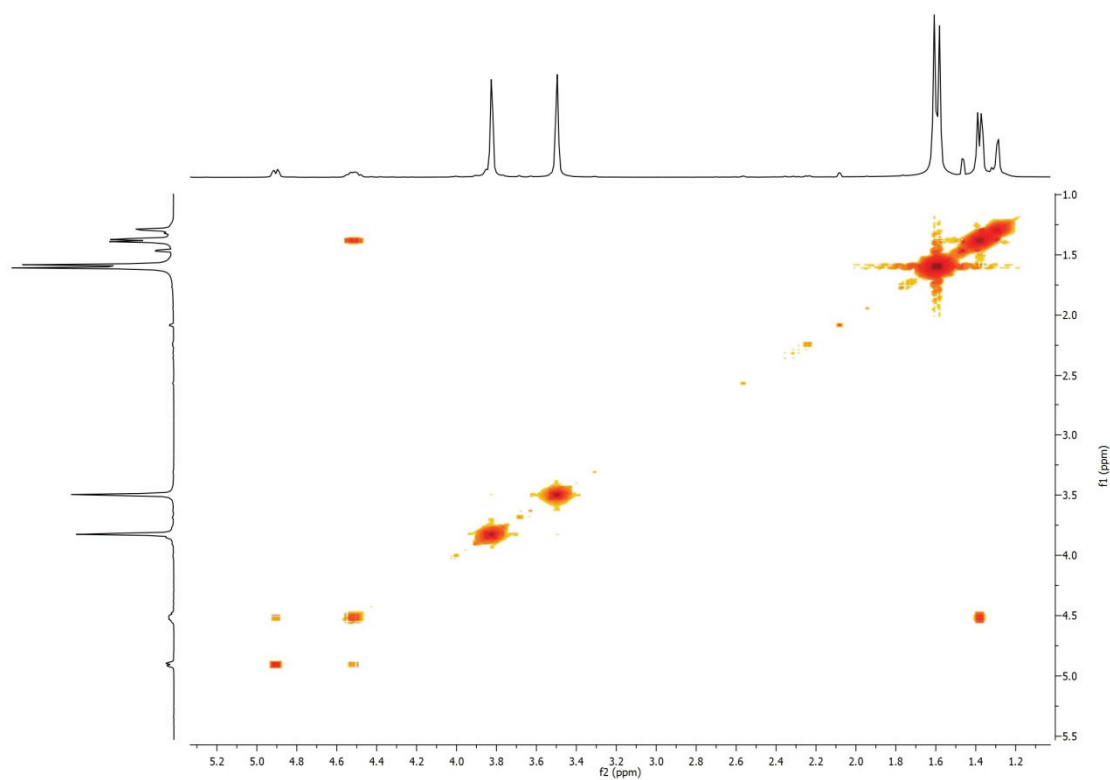
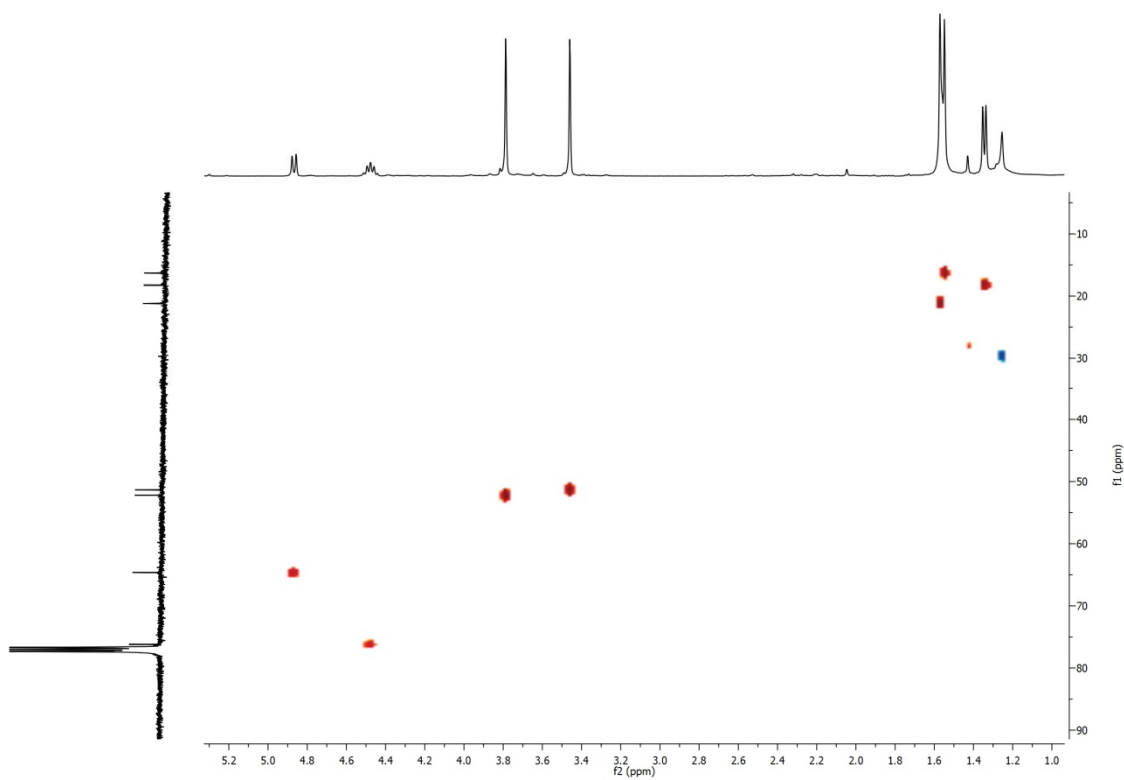
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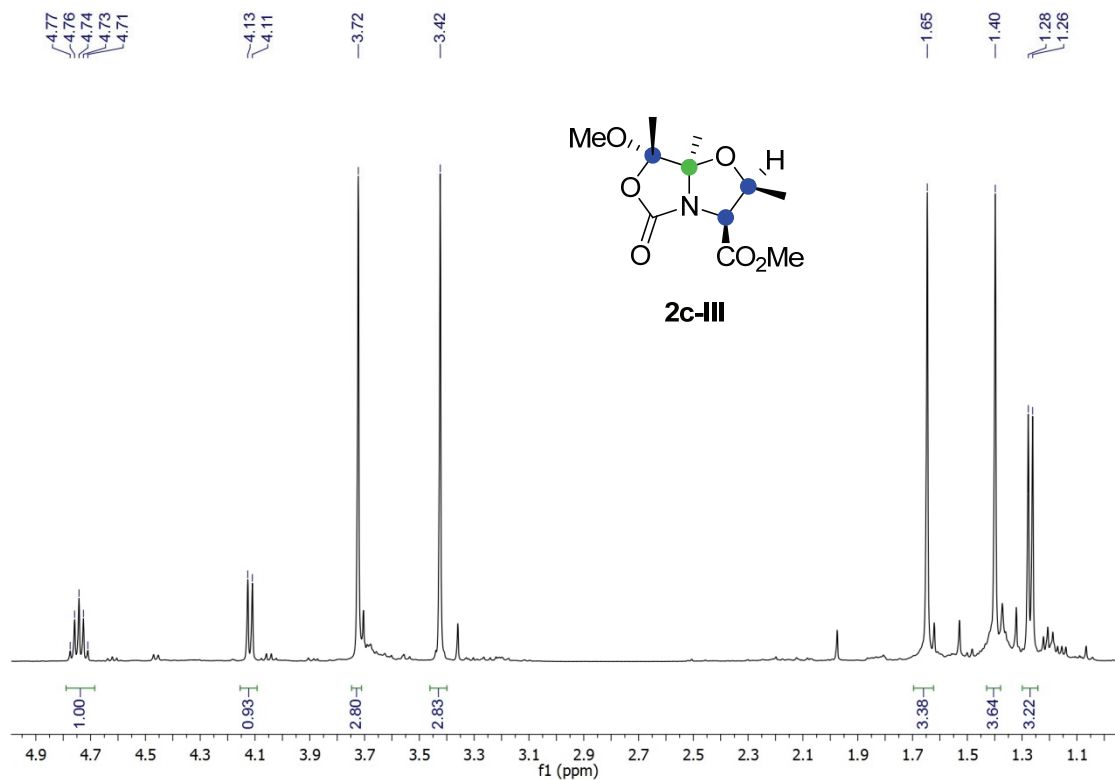
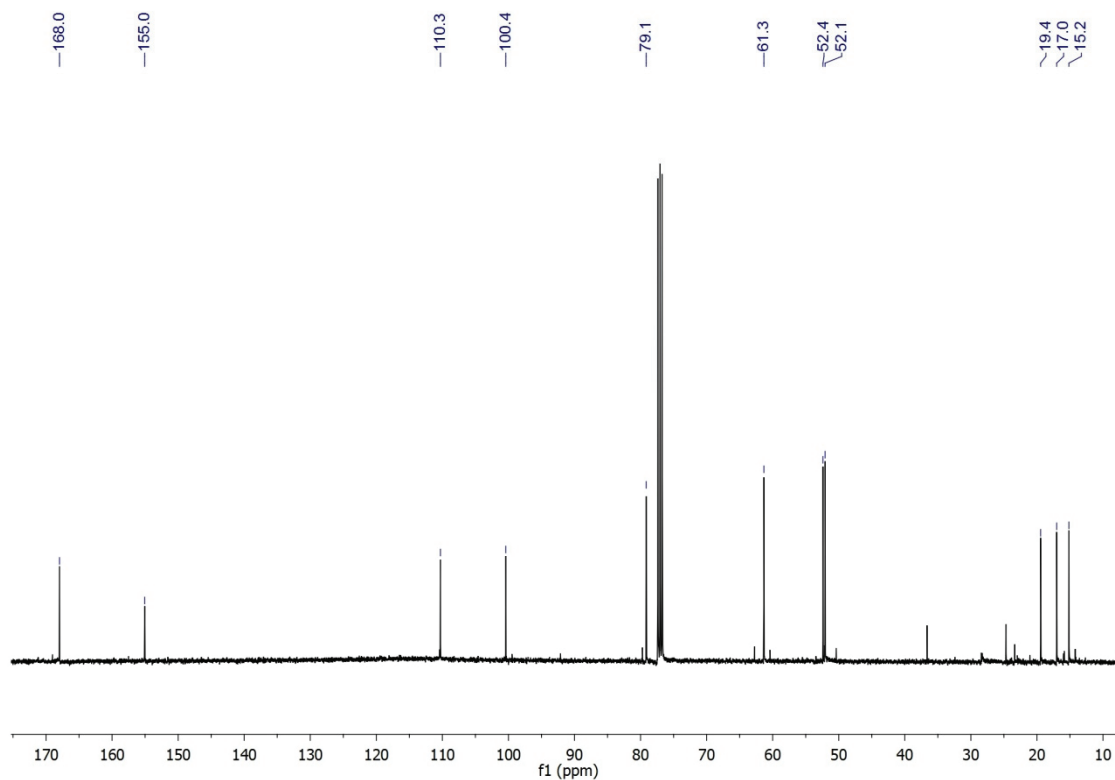


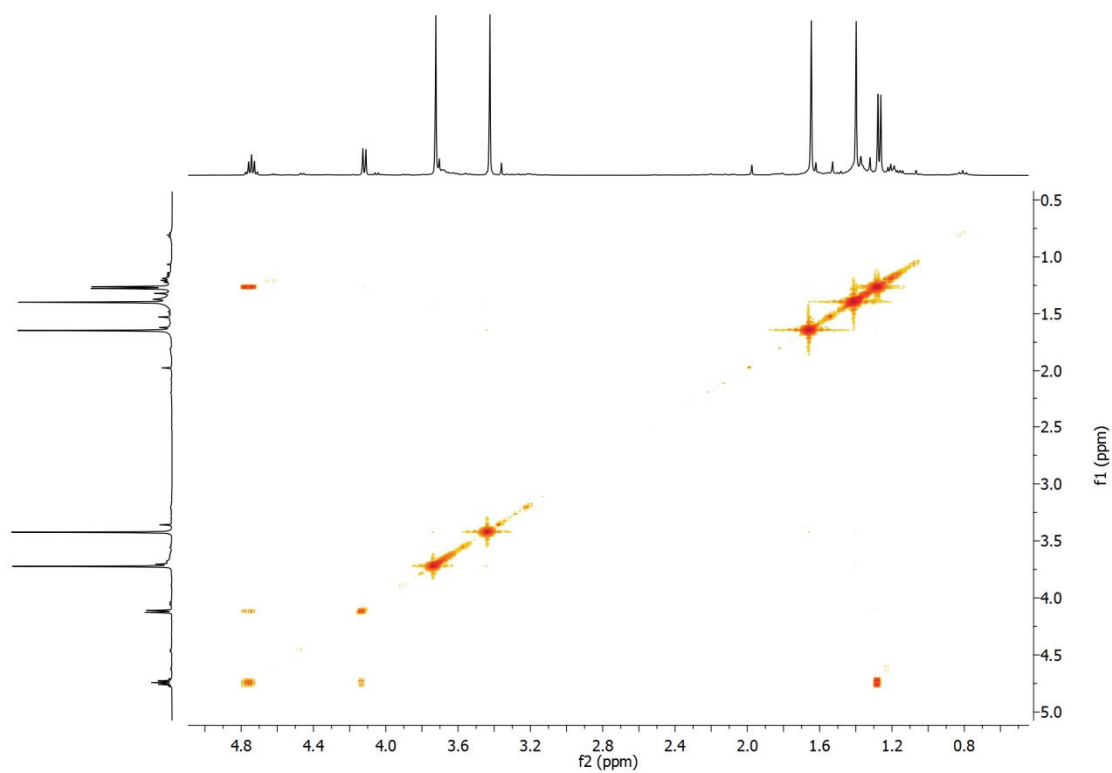
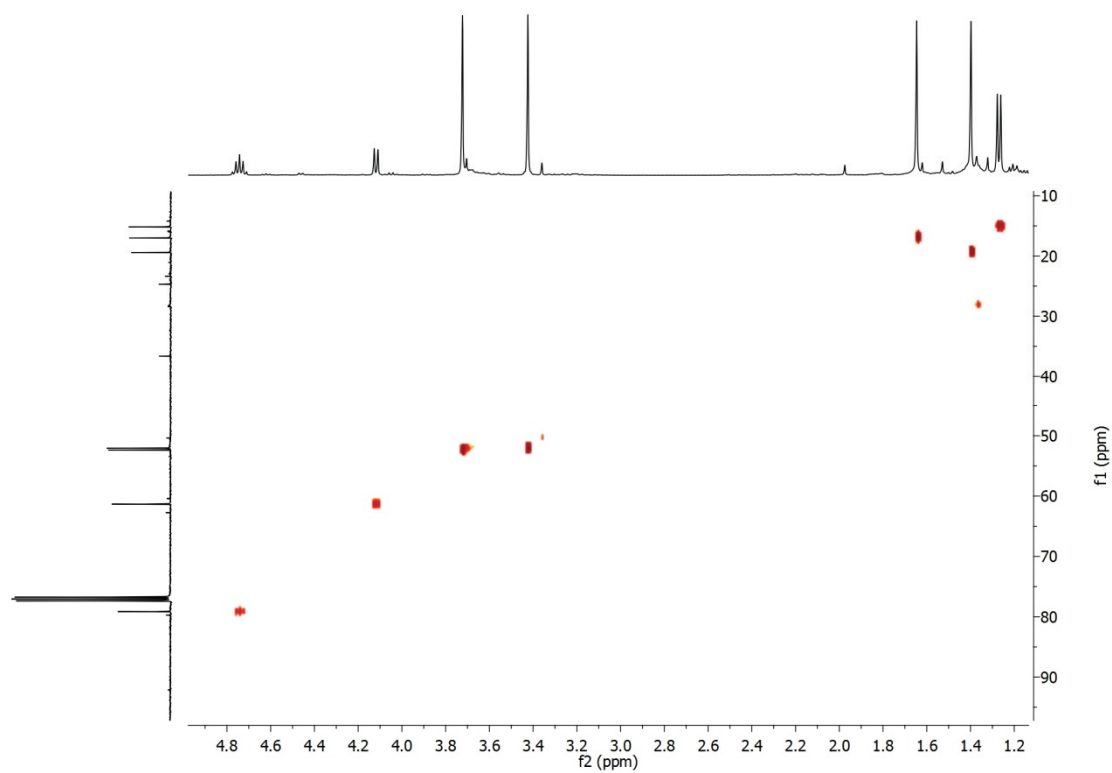
HSQCed (400 MHz, CDCl₃, 298K)

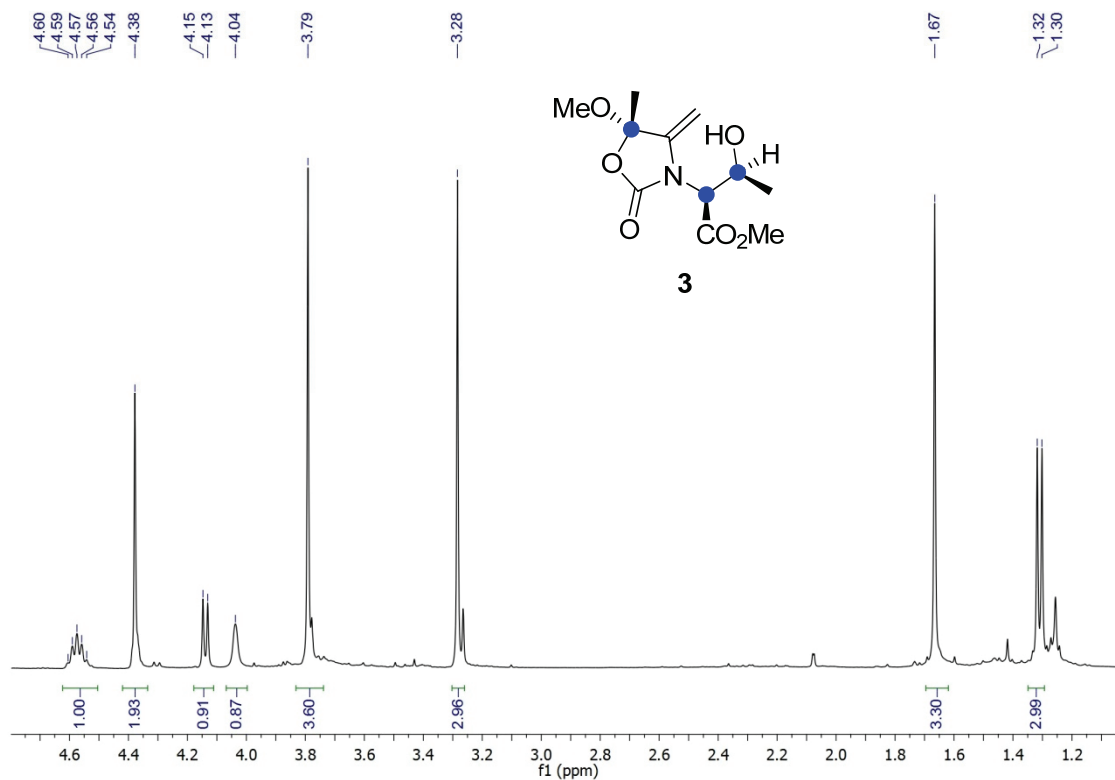
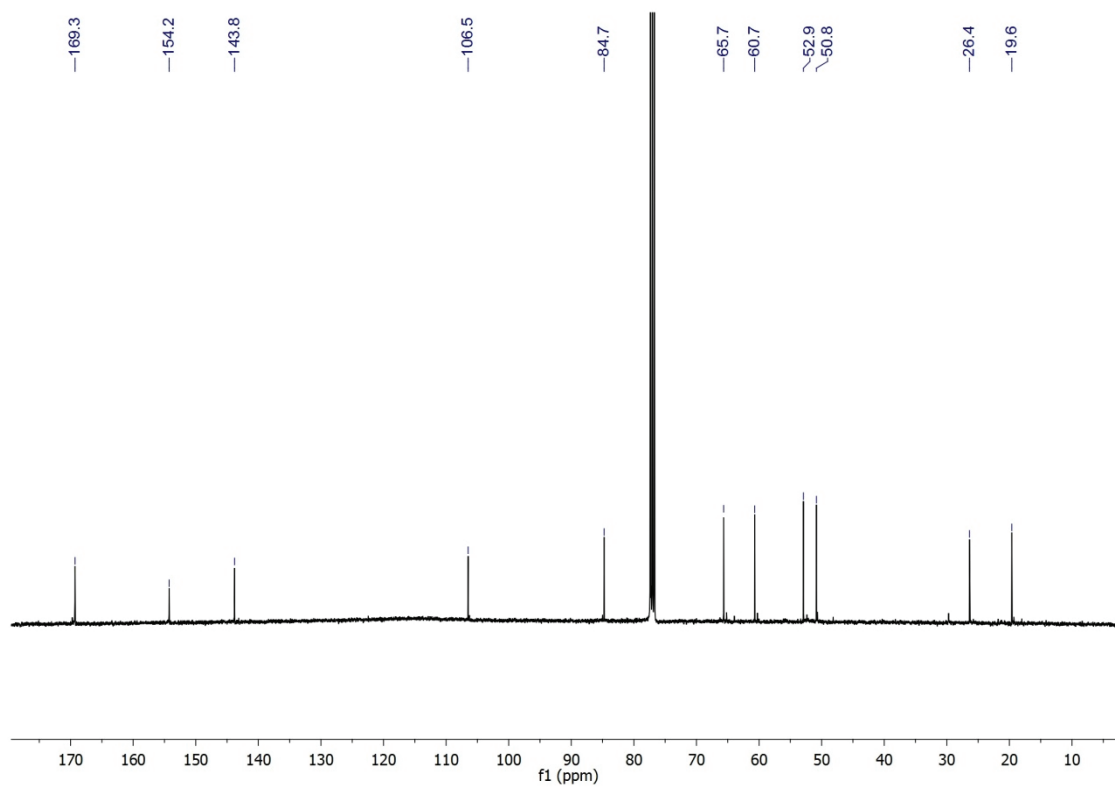


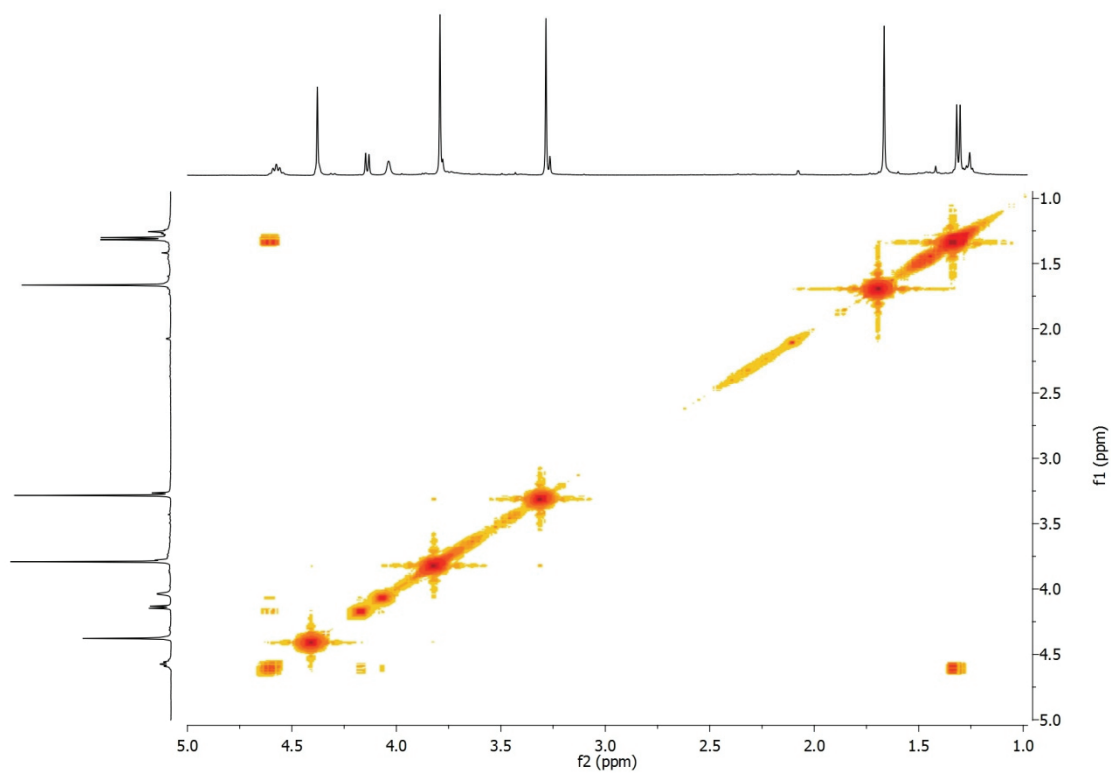
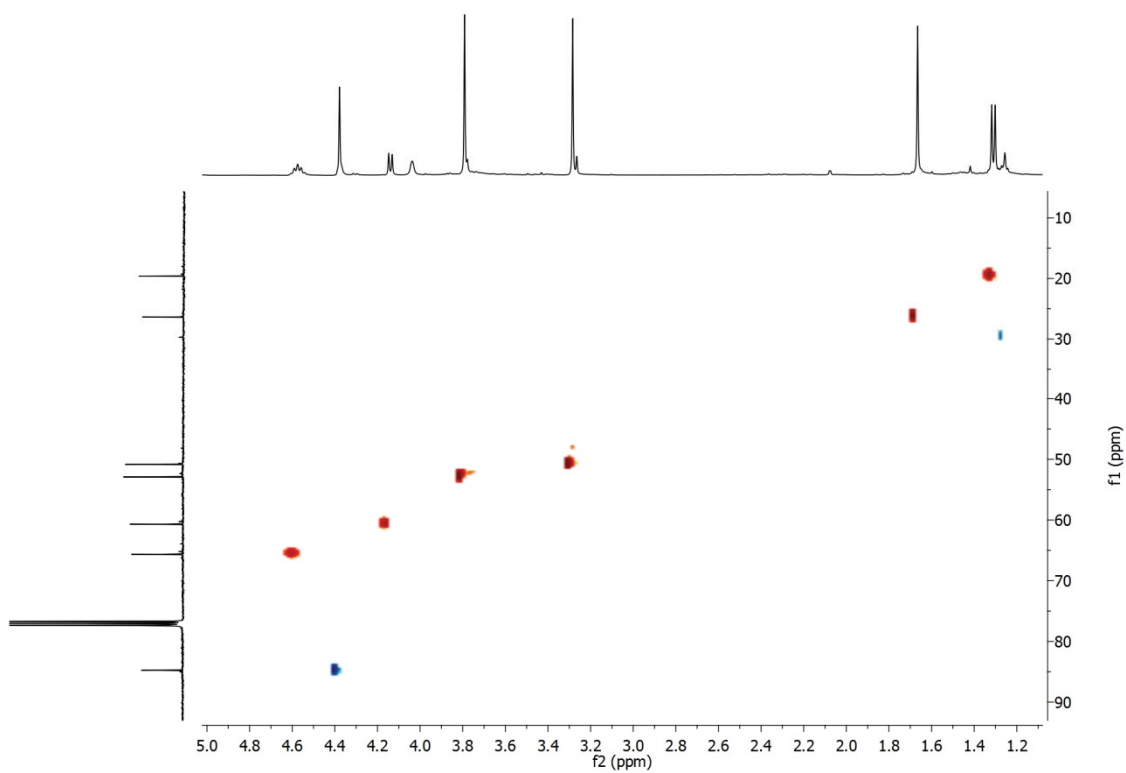
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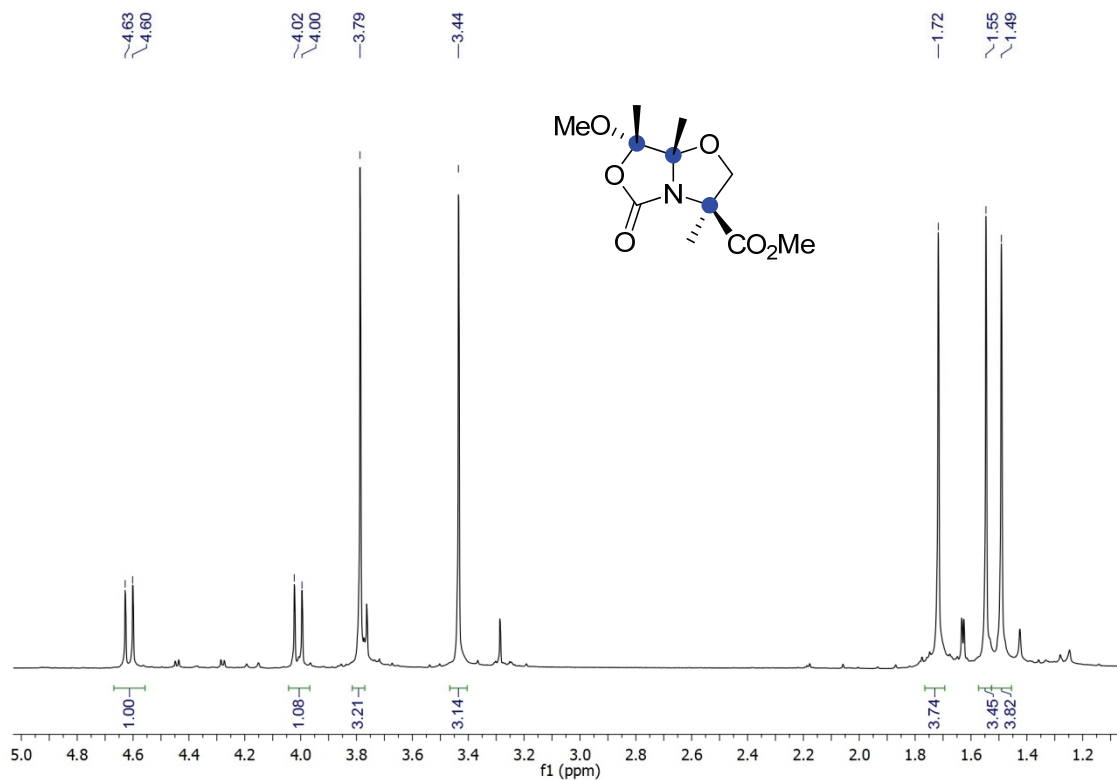
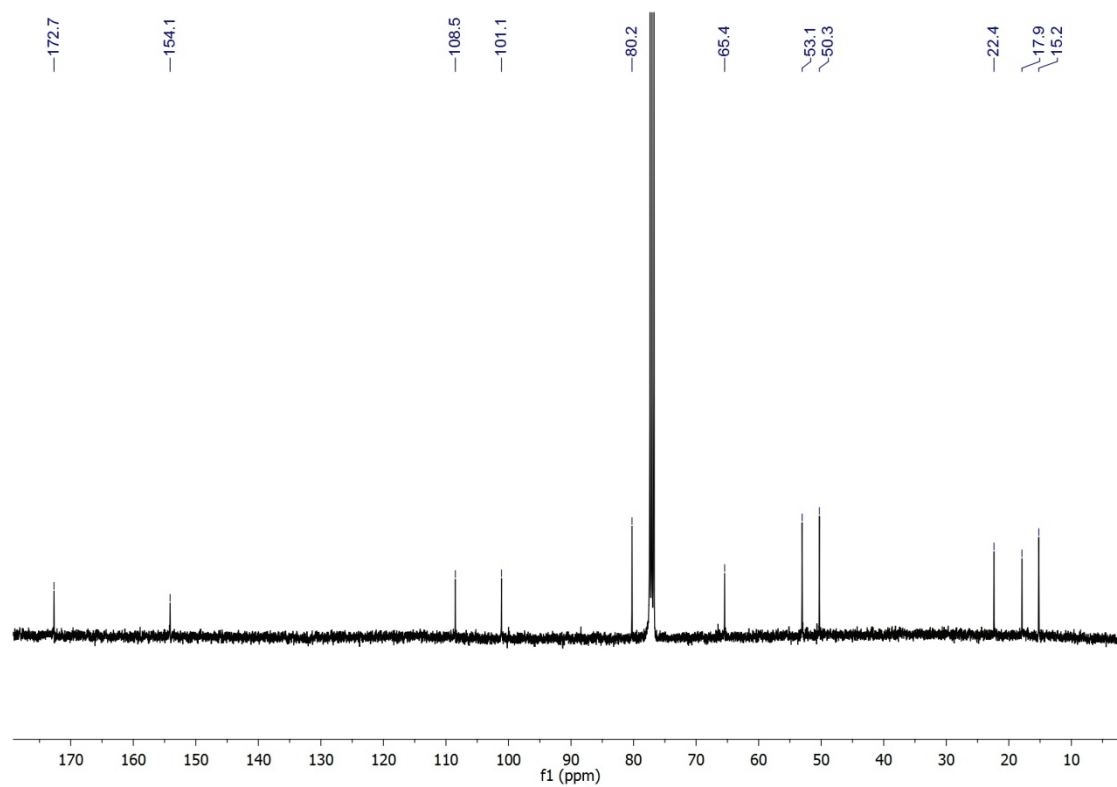
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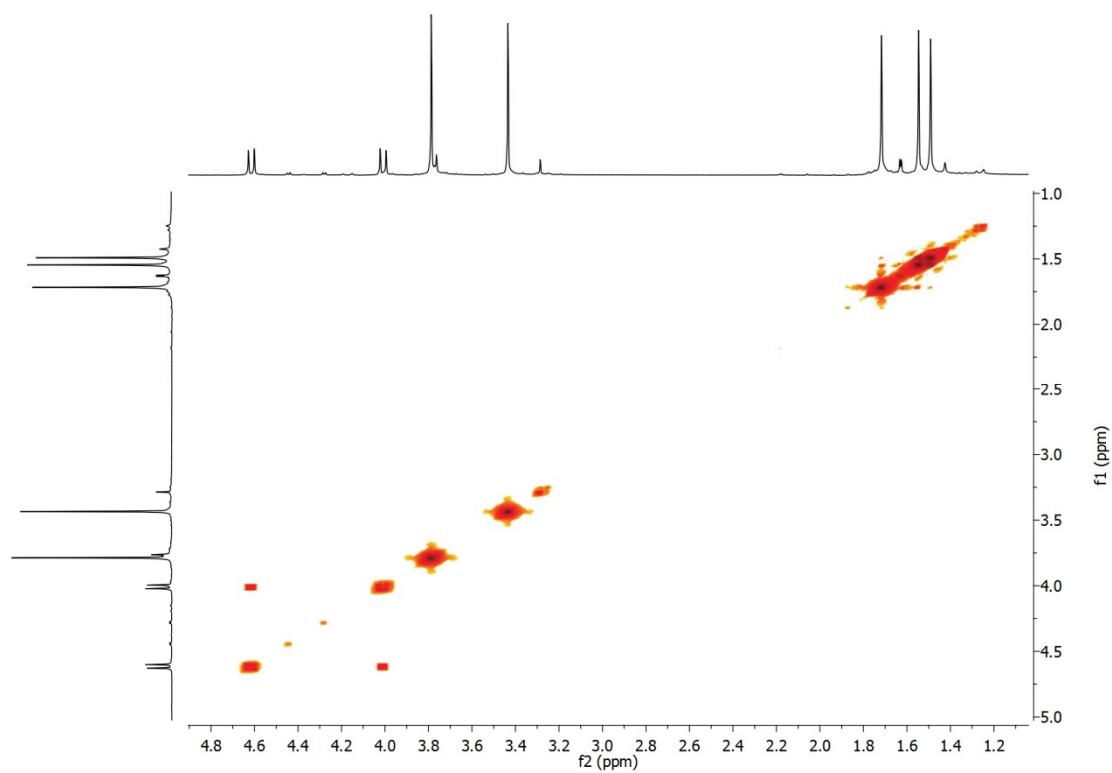
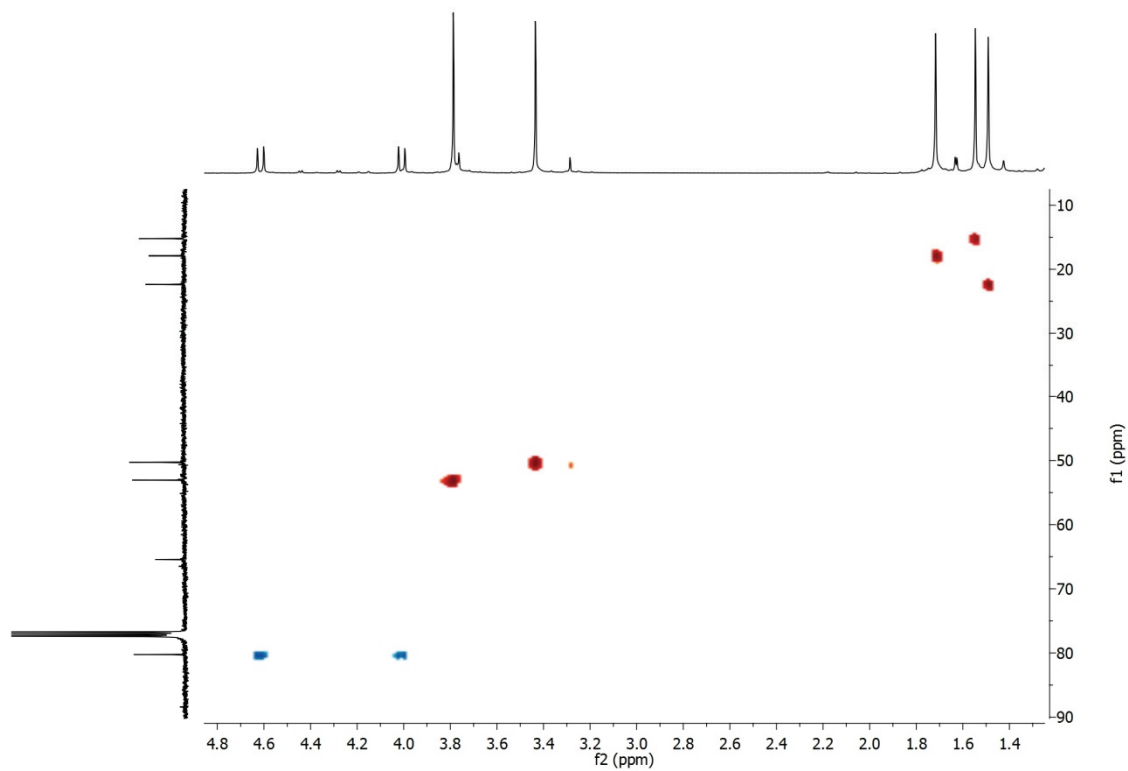
Compound 2c-III¹H NMR (400 MHz, CDCl₃, 298K)¹³C NMR (100 MHz, CDCl₃, 298K)

COSY (400 MHz, CDCl₃, 298K)HSQCed (400 MHz, CDCl₃, 298K)

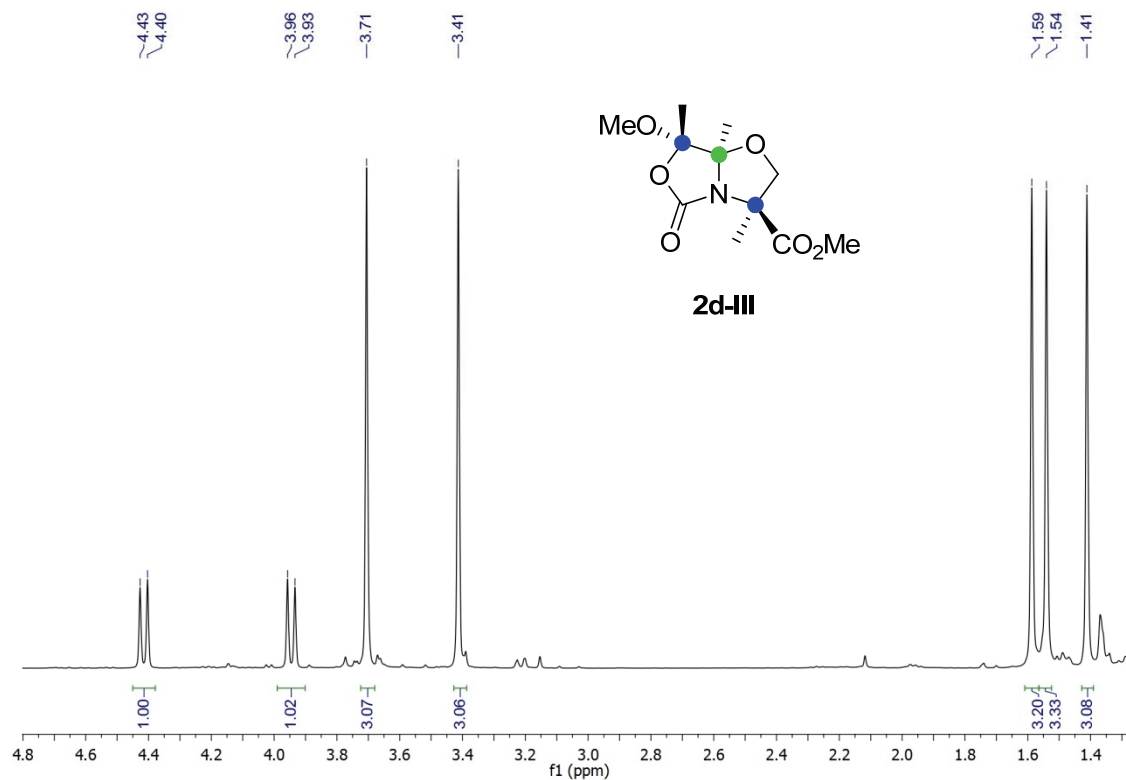
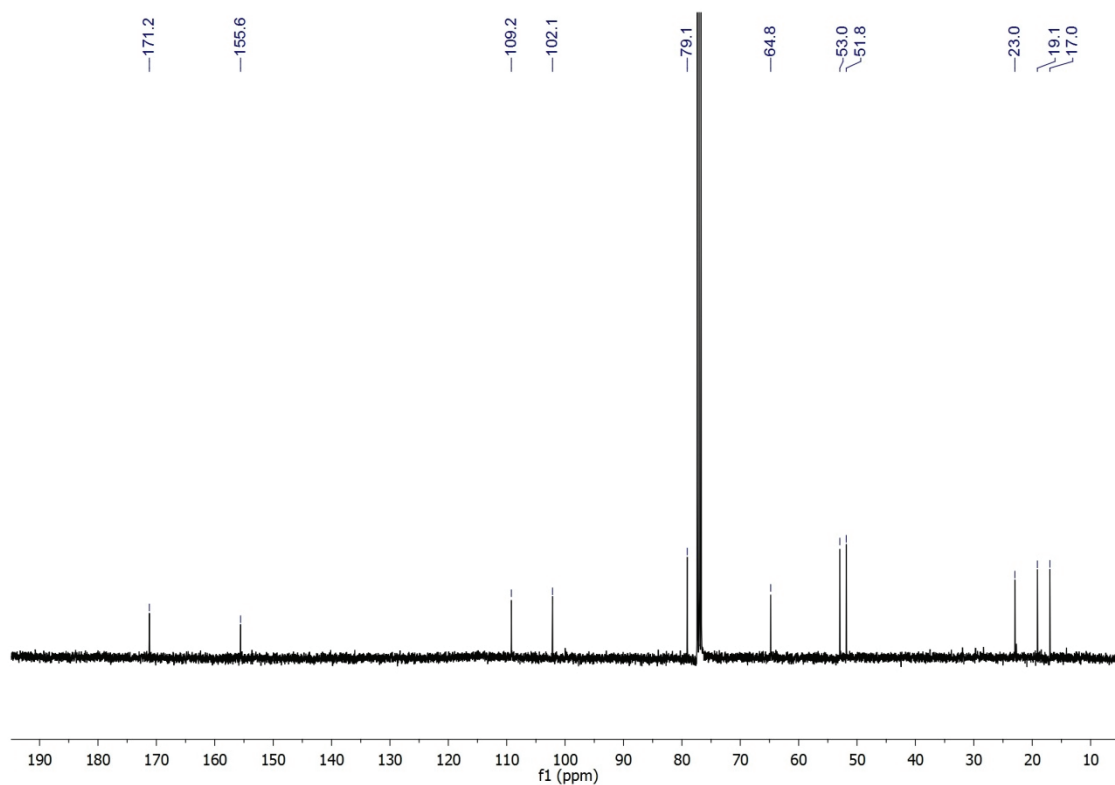
Compound 3¹H NMR (400 MHz, CDCl₃, 298K)¹³C NMR (100 MHz, CDCl₃, 298K)

COSY (400 MHz, CDCl₃, 298K)HSQCed (400 MHz, CDCl₃, 298K)

Compound 2d-I¹H NMR (400 MHz, CDCl₃, 298K)¹³C NMR (100 MHz, CDCl₃, 298K)

COSY (400 MHz, CDCl₃, 298K)HSQCed (400 MHz, CDCl₃, 298K)

Compound 2d-III

 ^1H NMR (400 MHz, CDCl_3 , 298K) ^{13}C NMR (100 MHz, CDCl_3 , 298K)

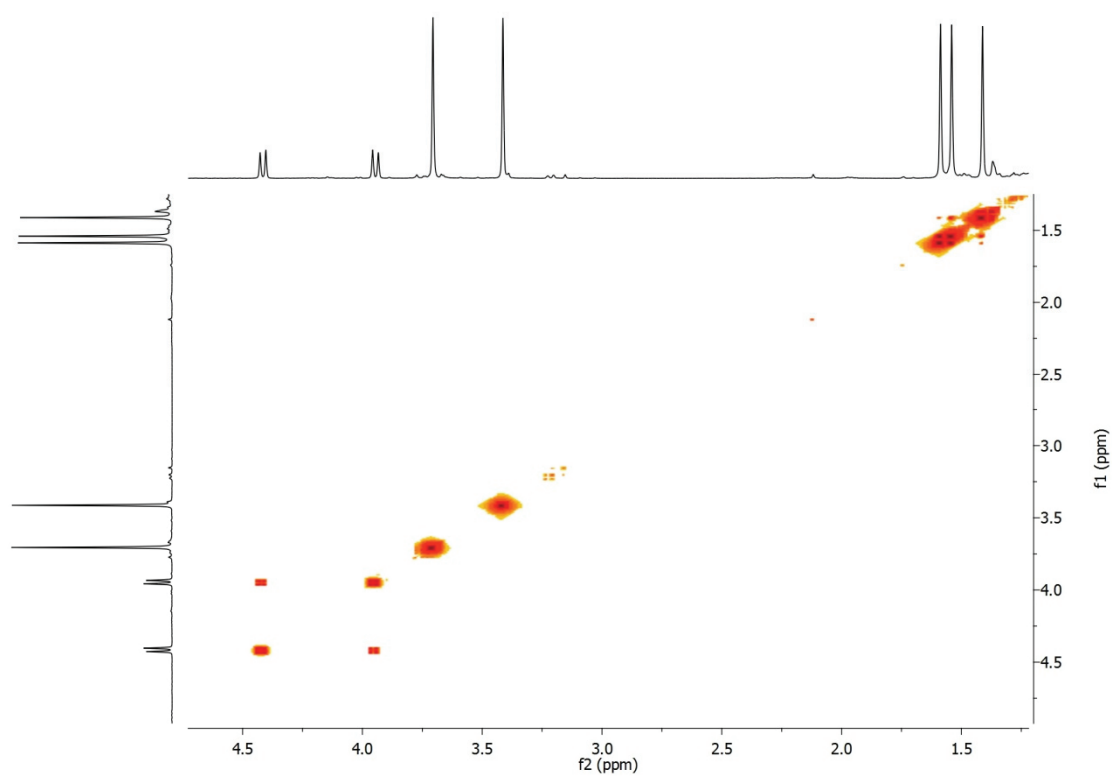
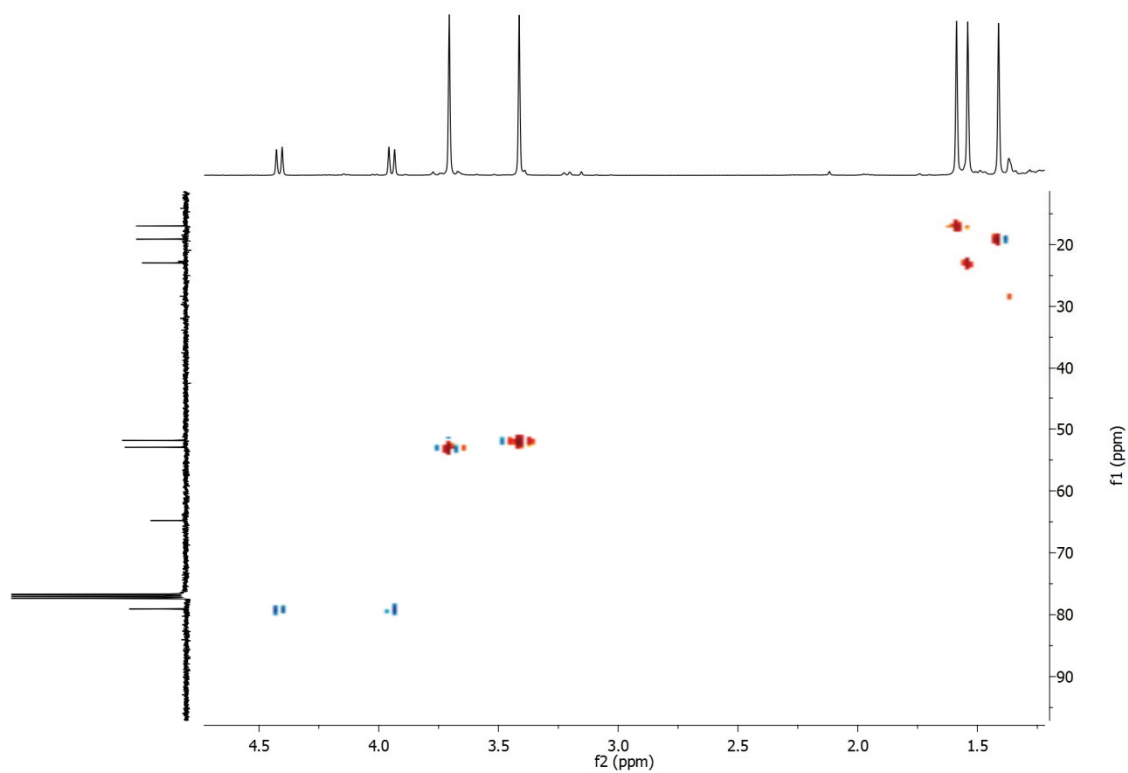
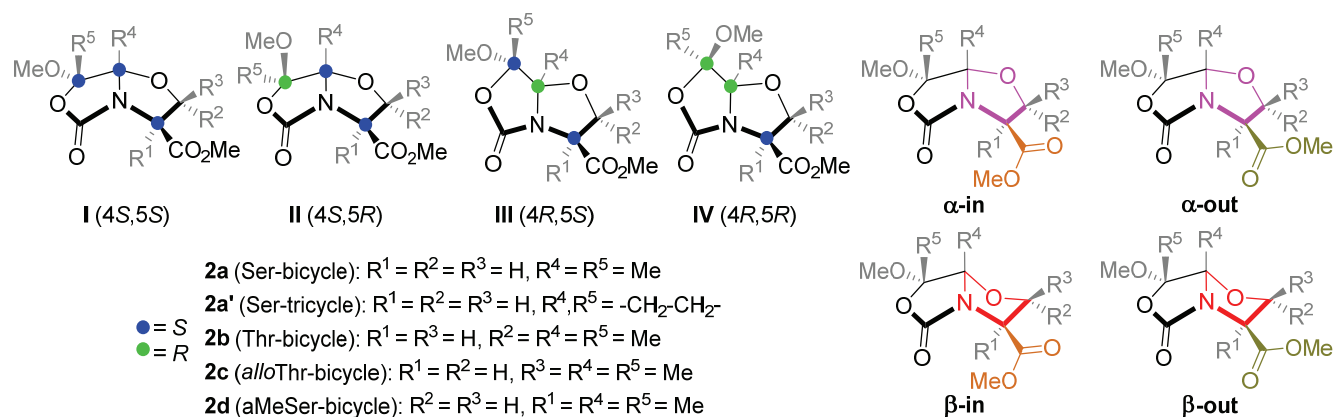
COSY (400 MHz, CDCl₃, 298K)HSQCed (400 MHz, CDCl₃, 298K)

Table S1. B3LYP/6-31+G(d) energies, enthalpies, free energies, and entropies of the structures considered in this work.



All possible conformers and ring isomers were investigated. Some structures converged to the same stationary point upon optimization; redundant isomers were discarded and only the unique structures were included in the Boltzmann distribution of Gibbs free energies, summarized in the following table:

Structure	E_0 (Hartree) ^a	H (Hartree) ^b	S (cal mol ⁻¹ K ⁻¹) ^b	Lowest freq. (cm ⁻¹)	G (Hartree) ^b	ΔG (kcal mol ⁻¹) ^b	mol %	cumulative mol %
2a-I-α-in	-896.224356	-895.937748	152.0	21.0	-896.031740	4.3	0.2	7.1
2a-I-α-out	-896.229189	-895.942551	149.7	38.8	-896.035170	2.2	3.5	
2a-I-β-in	-896.224929	-895.938216	150.8	30.6	-896.031488	4.5	0.2	
2a-I-β-out	-896.228292	-895.941698	151.0	22.4	-896.035100	2.2	3.3	
2a-II-α-in	-896.231337	-895.944623	152.0	20.2	-896.038656	0.0	59.1	90.3
2a-II-β-in	-896.231222	-895.944475	151.0	32.3	-896.037870	0.5	31.2	
2a-III-α-in	-896.226155	-895.939395	149.6	29.8	-896.031922	4.2	0.2	2.5
2a-III-α-out	-896.226773	-895.940212	152.2	29.2	-896.034369	2.7	1.8	
2a-III-β-in	-896.225105	-895.938456	149.8	35.7	-896.031112	4.7	0.1	
2a-III-β-out	-896.224436	-895.937790	152.6	21.5	-896.032188	4.1	0.3	
2a-IV-α-in	-896.220460	-895.934018	150.8	20.7	-896.027323	7.1	0.0	0.1
2a-IV-α-out	-896.224452	-895.937841	149.8	31.4	-896.030528	5.1	0.1	
2a-IV-β-in	-896.220043	-895.933476	150.6	31.0	-896.026661	7.5	0.0	
2a-IV-β-out	-896.223169	-895.936505	149.2	32.4	-896.028810	6.2	0.0	
2b-I-α-in	-935.546860	-935.230006	159.0	30.2	-935.328360	4.2	0.3	0.7
2b-I-α-out	-935.546157	-935.229151	158.6	29.1	-935.327245	4.9	0.1	
2b-I-β-in	-935.545757	-935.228973	160.1	21.0	-935.328020	4.4	0.2	
2b-I-β-out	-935.545422	-935.228552	159.3	25.8	-935.327078	5.0	0.1	
2b-II-α-out	-935.552249	-935.235317	159.6	28.0	-935.334012	0.7	28.8	98.2
2b-II-β-out	-935.552319	-935.235528	161.0	21.1	-935.335091	0.0	69.4	
2b-III-α-in	-935.545328	-935.228588	159.6	27.7	-935.327335	4.9	0.1	0.9
2b-III-α-out	-935.547846	-935.231175	158.8	40.5	-935.329424	3.6	0.7	
2b-III-β-in	-935.544511	-935.227677	160.2	13.5	-935.326793	5.2	0.1	
2b-IV-α-in	-935.545890	-935.229121	158.5	27.0	-935.327142	5.0	0.1	0.1
2b-IV-β-in	-935.544774	-935.227907	157.6	33.3	-935.325373	6.1	0.0	

2c-I-α-in	-935.547639	-935.230820	158.1	35.9	-935.328591	0.8	14.6	57.6
2c-I-β-in	-935.549244	-935.232426	157.6	43.7	-935.329920	0.0	43.0	
2c-II-α-out	-935.548201	-935.231218	158.7	41.8	-935.329375	0.3	27.6	39.7
2c-II-β-out	-935.546917	-935.230029	159.0	35.4	-935.328362	1.0	12.1	
2c-III-α-in	-935.546172	-935.229211	156.2	40.6	-935.325844	2.6	1.6	2.5
2c-III-α-out	-935.542841	-935.226034	157.9	45.9	-935.323701	3.9	0.3	
2c-III-β-in	-935.544882	-935.227948	156.6	45.5	-935.324835	3.2	0.7	
2c-III-β-out	-935.538901	-935.221980	159.0	20.1	-935.320327	6.0	0.0	
2c-IV-α-in	-935.540327	-935.223604	158.1	30.4	-935.321411	5.3	0.0	0.1
2c-IV-α-out	-935.536277	-935.219516	158.1	21.3	-935.317336	7.9	0.0	
2c-IV-β-in	-935.540115	-935.223338	157.6	38.0	-935.320825	5.7	0.0	
2c-IV-β-out	-935.532805	-935.215939	159.5	14.1	-935.314568	9.6	0.0	
2d-I-α-in	-935.542172	-935.225470	156.9	35.0	-935.322500	0.7	7.9	30.0
2d-I-α-out	-935.538899	-935.222025	157.4	26.3	-935.319365	2.7	0.6	
2d-I-β-in	-935.542573	-935.225885	157.8	29.5	-935.323499	0.1	17.7	
2d-I-β-out	-935.534988	-935.218183	159.8	16.2	-935.317024	4.1	0.1	
2d-I-β-out'	-935.539125	-935.222448	160.2	10.9	-935.321568	1.3	3.7	
2d-II-α-in	-935.539820	-935.223228	158.4	31.3	-935.321187	1.5	2.7	41.0
2d-II-α-out	-935.540707	-935.223947	159.1	20.4	-935.322335	0.8	6.9	
2d-II-β-in	-935.541275	-935.224655	159.0	33.1	-935.323002	0.4	11.8	
2d-II-β-out	-935.542514	-935.225667	158.4	29.7	-935.323621	0.0	19.6	
2d-III-α-in	-935.542375	-935.225688	156.9	24.3	-935.322763	0.5	9.8	27.2
2d-III-α-out	-935.542719	-935.226139	157.0	31.9	-935.323230	0.2	14.3	
2d-III-β-in	-935.539495	-935.222899	158.3	22.7	-935.320808	1.8	2.0	
2d-III-β-out	-935.539362	-935.222694	157.6	41.3	-935.320176	2.2	1.2	
2d-IV-α-in	-935.535891	-935.219533	157.8	23.9	-935.317137	4.1	0.1	1.8
2d-IV-α-out	-935.539609	-935.223018	156.5	33.6	-935.319819	2.4	0.9	
2d-IV-β-in	-935.537105	-935.220612	157.5	38.2	-935.318008	3.5	0.2	
2d-IV-β-out	-935.539540	-935.222914	155.8	40.7	-935.319264	2.7	0.6	
2a'-I-α-in	-973.649617	-973.323931	156.4	26.1	-973.420647	0.2	43.4	99.9
2a'-I-β-in	-973.650482	-973.324801	155.5	37.9	-973.420974	0.0	56.6	
2a'-II-α-out	-973.636445	-973.310712	156.4	20.9	-973.407447	8.5	0.0	0.0
2a'-II-β-out	-973.636640	-973.310869	154.8	33.3	-973.406638	9.0	0.0	
2a'-III-α-out	-973.629790	-973.304114	156.1	33.5	-973.400662	12.7	0.0	0.0
2a'-III-β-out	-973.632280	-973.306669	155.7	43.0	-973.402987	11.3	0.0	
2a'-IV-α-in	-973.640411	-973.314714	156.6	31.9	-973.411563	5.9	0.0	0.1
2a'-IV-β-in	-973.640305	-973.314829	156.7	21.7	-973.411732	5.8	0.0	

^a 1 Hartree = 627.5 kcal mol⁻¹. ^b Thermal corrections at 388.15 K.

Cartesian coordinates for the different conformations of the structures considered in this work.

Structure 2a-I-α-in (B3LYP/6-31+G(D))				H	1.56400000	1.44560000	-1.62240000
O	0.57860000	1.42260000	0.98620000	C	-0.66400000	0.70070000	0.00920000
O	1.82410000	-1.31780000	0.20650000	C	4.96240000	0.15090000	0.02820000
O	0.15040000	-2.48620000	1.18630000	H	5.69520000	-0.13130000	-0.72770000
O	-2.90880000	-0.66580000	-0.72410000	H	5.15170000	-0.37450000	0.96750000
N	-0.26260000	-0.48060000	0.06850000	H	4.98140000	1.22970000	0.20400000
C	1.98490000	-0.02110000	-0.45530000	H	1.52520000	-1.45930000	-0.85420000
C	-2.68750000	0.19110000	0.28120000	C	-2.68170000	0.54140000	1.65480000
C	0.10190000	1.53590000	-1.38330000	H	-3.59430000	-0.03060000	1.84180000
H	-0.01970000	0.96150000	-2.30460000	H	-2.91360000	1.60930000	1.70260000
H	0.81170000	2.35170000	-1.55240000	H	-1.96940000	0.29320000	2.44630000
H	-0.86420000	1.98470000	-1.13240000	O	-2.91630000	0.53740000	-0.77990000
C	-1.33110000	-0.01570000	0.95110000	C	-4.27160000	0.08050000	-0.77440000
C	0.53230000	-1.52740000	0.55890000	H	-4.66080000	0.32160000	-1.76530000
O	-3.49450000	1.01180000	0.67260000	H	-4.87170000	0.60070000	-0.01770000
C	-0.73600000	1.30200000	1.54910000	H	-4.32240000	-1.00220000	-0.61640000
H	-0.62170000	1.25240000	2.63390000	Structure 2a-I-β-out (B3LYP/6-31+G(D))			
H	-1.35820000	2.16580000	1.29410000	O	0.15670900	0.90730900	1.50153000
C	0.59490000	0.66790000	-0.22710000	O	1.81840600	-0.41831800	-1.33476700
C	-4.21260000	-0.59620000	-1.33780000	O	2.39806600	-0.34956100	0.91951100
H	-4.20530000	-1.36460000	-2.11060000	O	-2.89287200	0.24510100	-0.71329200
H	-4.37420000	0.39300000	-1.77380000	O	0.32172700	-2.08624300	-1.76271600
H	-4.98990000	-0.79810000	-0.59640000	N	-0.22614700	-0.24474700	-0.44854900
H	-1.48920000	-0.77890000	1.72150000	C	-1.12936200	-0.81465600	0.53823200
C	2.31250000	-0.32830000	-1.91620000	H	-1.11720400	-1.90665400	0.45604400
C	3.18600000	-0.98330000	-1.96770000	O	-3.40374500	-0.66150100	1.29330800
H	2.52360000	0.59150000	-2.46970000	C	0.51937600	0.88501900	0.13401200
H	1.47940000	-0.85170000	-2.39360000	C	0.13038100	2.22513400	-0.48081500
O	2.94900000	0.72800000	0.19530000	H	0.35578700	2.24735300	-1.55123500
C	4.28610000	0.21970000	0.20040000	H	0.66075600	3.04362400	0.01603400
H	4.83120000	0.85010000	0.90520000	H	-0.94429200	2.37293300	-0.35142000
H	4.75440000	0.30000000	-0.78840000	C	0.59407600	-1.03795600	-1.22920100
H	4.31090000	-0.81930000	0.54570000	C	3.00694000	1.51699000	-0.53612600
Structure 2a-I-α-out (B3LYP/6-31+G(D))				H	3.18455600	2.16606300	0.32725700
O	0.09989900	1.19863400	1.18274900	H	2.65027700	2.12076800	-1.37248900
O	2.00246500	-0.72109200	-1.10518800	H	3.95547500	1.06408900	-0.83713700
O	2.27279400	-0.27842000	1.16361600	C	-0.47586300	-0.33144100	1.85693100
O	-3.54043200	-0.58546700	0.57679900	H	0.27248600	-1.05304700	2.19849800
O	0.42859700	-2.33105100	-1.47035300	C	-2.59664900	-0.39546000	0.42486100
N	-0.11992500	-0.24745300	-0.58871600	C	2.00261900	0.43835700	-0.16925600
C	-1.20272300	-0.57099600	0.32246700	C	3.64974200	-1.03634000	0.81543900
H	-1.29451800	-1.65534000	0.42516100	H	3.66040700	-1.75250400	1.63948200
O	-2.72023600	0.84642100	-0.97282400	H	4.49447600	-0.34700100	0.93291000
C	0.64009100	0.91564900	-0.09662400	H	3.73028800	-1.57295500	-0.13580100
C	0.46070000	2.14958100	-0.97211700	C	-4.28055200	0.59945000	-0.89109800
H	0.83423500	1.96806300	-1.98449800	H	-4.32712900	1.09433400	-1.86104300
H	0.99204400	3.00410600	-0.54089700	H	-4.60417700	1.27243500	-0.09298200
H	-0.60479300	2.37920700	-1.03479500	H	-4.90197000	-0.29948200	-0.88347700
C	0.72278900	-1.22456500	-1.08663700	H	-1.19729400	-0.12560900	2.64873500
C	3.24234700	1.24597500	-0.48329000	Structure 2a-II-α-in (B3LYP/6-31+G(D))			
H	3.35998700	2.02948500	0.27206200	O	0.41930000	-1.92600000	-0.20560000
H	3.05721000	1.70868400	-1.45414500	O	1.88680000	0.65000000	-1.09970000
H	4.17749300	0.68433500	-0.55750400	O	0.16050000	1.39800000	-2.36180000
C	-0.69126300	0.09451000	1.63187100	O	-2.77850000	1.15160000	0.25980000
H	-0.07520000	-0.61398200	2.19538100	N	-0.20740000	0.25390000	-0.36410000
C	-2.54844700	-0.00772900	-0.13248500	O	2.39040000	0.75380000	1.16650000
C	2.10265100	0.32192800	-0.09137300	C	2.06540000	-0.11860000	0.11980000
C	3.46377900	-1.04476400	1.36977900	C	-2.66530000	-0.15690000	0.00560000
C	3.29864900	-1.60080000	2.29489100	C	0.25560000	-0.71540000	1.89880000
H	4.33880900	-0.39603400	1.49684300	H	0.32150000	0.27010000	2.36150000
H	3.63204200	-1.74754400	0.54682300	H	0.93260000	-1.39940000	2.41970000
C	-4.87738900	-0.12609100	0.28955800	H	-0.76370000	-1.09890000	2.01250000
H	-5.52697100	-0.70085600	0.94964400	C	-1.39710000	-0.48400000	-0.78480000
H	-5.12281600	-0.31606200	-0.75827800	C	0.56570000	0.83300000	-1.37510000
H	-4.96237600	0.94407400	0.49547200	O	-3.49770000	-0.99020000	0.30690000
H	-1.48422900	0.49164700	2.26956200	C	-0.95070000	-1.97460000	-0.63820000
Structure 2a-I-β-in (B3LYP/6-31+G(D))				H	-0.97310000	-2.51200000	-1.58850000
O	-0.42640000	0.85730000	-1.39640000	H	-1.57530000	-2.50140000	0.08910000
O	-1.93960000	-1.28510000	0.30340000	C	0.62660000	-0.65160000	0.42120000
O	-0.22170000	-2.75560000	0.21930000	C	-3.98770000	1.56770000	0.92700000
O	3.68550000	-0.24570000	-0.51330000	H	-3.89930000	2.64910000	1.02830000
N	0.15740000	-0.45860000	0.36260000	H	-4.06210000	1.09010000	1.90740000
C	-2.11390000	0.16810000	0.28590000	H	-4.86110000	1.30300000	0.32560000
C	2.60730000	0.00080000	0.26060000	C	3.61130000	1.48920000	1.04470000
C	-0.30480000	1.98950000	0.74280000	H	3.58650000	2.23040000	1.84600000
H	-0.34310000	1.86440000	1.82670000	H	3.67080000	1.99910000	0.07750000
H	-0.99710000	2.78060000	0.43720000	H	4.48540000	0.84140000	1.18290000
H	0.70940000	2.30400000	0.48700000	C	3.11510000	-1.18600000	-0.14810000
C	1.35160000	-0.44930000	-0.47510000	H	3.32780000	-1.73920000	0.77230000
C	-0.62700000	-1.61930000	0.28310000	H	4.03820000	-0.72460000	-0.50910000
O	2.65710000	0.52600000	1.35020000	H	2.75470000	-1.88450000	-0.90450000
C	0.94510000	0.53880000	-1.63120000	H	-1.61000000	-0.21620000	-1.82610000
H	1.01510000	0.07290000	-2.61620000				

Structure **2a-II- β -in** (B3LYP/6-31+G(D))

O	-0.26420000	1.01360000	-1.51280000
O	-1.96320000	-1.26940000	-0.24950000
O	-0.24990000	-2.74610000	-0.14700000
O	3.71160000	-0.22260000	-0.25150000
N	0.10230000	-0.46490000	-0.17410000
O	-2.67840000	0.47780000	1.10110000
C	-2.14570000	0.16760000	-0.15610000
C	2.55110000	-0.03420000	0.41330000
C	-0.44600000	1.92090000	0.74250000
H	-0.66130000	1.66830000	1.78080000
H	-1.09290000	2.74690000	0.43090000
H	0.59490000	2.24760000	0.67600000
C	1.38860000	-0.38940000	-0.50700000
C	-0.65800000	-1.61210000	-0.07280000
O	2.47470000	0.38080000	1.54690000
C	1.13110000	0.71800000	-1.59580000
H	1.33860000	0.36120000	-2.60640000
H	1.72960000	1.61780000	-1.40530000
C	-0.68170000	0.72030000	-0.16500000
C	4.91820000	0.09540000	0.47280000
H	5.73340000	-0.12350000	-0.21670000
H	4.99160000	-0.52400000	1.37000000
H	4.92270000	1.15080000	0.75750000
C	-3.96640000	-0.05980000	1.41370000
H	-4.10970000	0.12900000	2.47940000
H	-4.00090000	-1.13810000	1.22610000
H	-4.76020000	0.44570000	0.85030000
C	-3.01700000	0.60780000	-1.32290000
H	-3.23080000	1.67860000	-1.24440000
H	-3.95950000	0.05380000	-1.31860000
H	-2.50590000	0.41810000	-2.26770000
H	1.60540000	-1.35800000	-0.96480000

Structure **2a-III- α -in** (B3LYP/6-31+G(D))

O	-0.37857800	1.69164200	0.86936800
O	-1.30625700	-1.35877400	-0.51899500
O	-3.16212100	-0.06093900	0.00752700
O	3.56726800	0.03774500	-0.26093000
O	0.68245100	-1.83784500	-1.51318700
N	0.11416300	0.32552200	-0.88957300
C	1.39114400	0.93385000	-0.53566500
O	1.97209800	-0.71557500	1.15641300
C	-1.00128500	0.97230900	-0.19066000
C	-1.78378700	1.91877000	-1.09896700
H	-2.22046600	1.37500100	-1.94010400
H	-1.10842600	2.68577300	-1.49282800
H	-2.58805900	2.40249000	-0.53936100
C	-0.08026600	-1.04080800	-1.01925800
C	-1.56220700	-0.63507200	1.77446500
H	-1.98770400	0.12296700	2.43895800
H	-0.48772600	-0.70044100	1.95671700
H	-2.00821800	-1.60892200	1.99446200
C	0.91188800	2.08412200	0.40832800
C	2.31432000	-0.03115600	0.21604800
C	-1.82443200	-0.26422100	0.32143300
C	-4.07728100	-1.11603700	0.31732700
H	-5.01898400	-0.83269200	-0.15692700
H	-4.23295600	-1.20763400	1.39866800
H	-3.73205800	-2.06976600	-0.09552000
C	4.53455800	-0.82145200	0.38033800
H	5.47229400	-0.63816300	-0.14380300
H	4.22763200	-1.86486100	0.27768700
H	4.62340300	-0.56672400	1.43957500
H	1.55064700	2.21743200	1.28371100
H	0.85916400	3.03019900	-0.14649700
H	1.91752800	1.32482800	-1.40963600

Structure **2a-III- α -out** (B3LYP/6-31+G(D))

O	0.65038500	1.90176300	-0.51903700
O	1.24736500	-1.13020000	-0.85868900
O	2.78453300	-0.67938700	0.82212500
O	-3.10471600	-0.53598300	0.90315900
O	-0.91815800	-1.78160600	-0.81684100
N	-0.16557000	0.00640900	0.48610500
C	-1.31870500	0.91805800	0.37864000
H	-1.49538600	1.33779100	1.37415800
O	-3.19267000	0.50354600	-1.10674600
C	1.01795000	0.85684200	0.40205200
C	1.44053300	1.47304200	1.73030200
H	1.67044300	0.70165600	2.46650700
H	0.63986700	2.11509700	2.11144700
H	2.32643200	2.09743200	1.57935700
C	-0.04302100	-1.04304500	-0.43512100
C	2.94870500	0.50614800	-1.31865200
H	3.63904500	1.22810200	-0.87065900
H	2.33146400	1.01965300	-2.05675100
H	3.52546500	-0.27245600	-1.82495100

C	-0.78573000	1.99487200	-0.59438800
C	-2.62870300	0.26114900	-0.06165400
C	2.07070500	-0.10774900	-0.23967600
C	3.71741200	-1.71387100	0.49633800
H	4.02575200	-2.14040400	1.45285400
H	4.59876300	-1.31192500	-0.01797700
H	3.24761200	-2.49104600	-0.11561900
C	-4.28406200	-1.29516100	0.56605300
H	-4.51395600	-1.87768900	1.45804400
H	-4.06558600	-1.95028800	-0.28067200
H	-5.10932000	-0.62400300	0.31488200
H	-1.09758200	3.00453600	-0.30917700
H	-1.10843900	1.79191100	-1.61930200

Structure **2a-III- β -in** (B3LYP/6-31+G(D))

O	-0.23703500	1.48709300	1.17921500
O	-1.17094400	-1.22999400	-0.72044100
O	-3.05534900	-0.07125600	-0.01120200
O	2.13732700	-0.78358900	0.70181700
O	0.75833800	-1.43331600	-1.90172900
N	0.16398100	0.55680300	-0.86029500
C	1.43972400	1.16598400	-0.49278200
O	3.69880000	0.31972200	-0.51033500
C	-0.91466200	1.01901300	0.01480000
C	-1.73697300	2.14169700	-0.61591200
H	-2.21299200	1.80262100	-1.53866800
H	-1.07979400	2.98504800	-0.85263300
H	-2.51316400	2.47846400	0.07575100
C	0.00748700	-0.76761000	-1.22822700
C	-1.47575700	-0.92237400	1.65510900
H	-1.92821200	-0.29972600	2.43277400
H	-0.40420100	-0.99700200	1.84845400
H	-1.90587700	-1.92697100	1.69297800
C	1.01016600	2.02566100	0.74510300
C	2.55519100	0.18067600	-0.13476200
C	-1.71679700	-0.30713800	0.28241600
C	-3.95203400	-1.18272900	0.07515400
H	-4.88828500	-0.83635900	-0.36676500
H	-4.13292100	-1.47211600	1.11721300
H	-3.57387200	-2.03860500	-0.49359600
C	3.11388700	-1.78990400	1.04421600
H	2.59626800	-2.47706200	1.71332400
H	3.97142500	-1.33119200	1.54271400
H	3.44238500	-2.30519900	0.13872900
H	1.71079600	1.95804500	1.57977700
H	0.90191400	3.07862500	0.45503500
H	1.83817200	1.79487100	-1.29230200

Structure **2a-III- β -out** (B3LYP/6-31+G(D))

O	-0.48125700	1.67234200	0.96631900
O	-1.18999800	-1.33112800	0.47591700
O	-2.92333200	-0.36753000	-0.73064700
O	3.07467400	-0.14607400	0.69258800
O	0.89083800	-1.98332700	-0.12550400
N	0.08883100	0.14653400	-0.65190900
C	1.29492700	0.97196000	-0.45467400
H	1.34437100	1.67508800	-1.28982800
O	3.17232100	-0.05167300	-1.56624900
C	-1.02534600	0.94444800	-0.15256900
C	-1.59420800	1.92822400	-1.16834200
H	-1.96345800	1.40940700	-2.05384300
H	-0.82046600	2.64520900	-1.46060600
H	-2.41704100	2.48892000	-0.71453000
C	0.02762600	-1.14026700	-0.10371300
C	-2.70469400	0.11002300	1.66433200
H	-3.39978700	0.95045300	1.56911700
H	-1.95716500	0.35596400	2.41959100
H	-3.25696300	-0.77490100	1.99194500
C	0.95559800	1.70783400	0.86673800
C	2.60855400	0.18359700	-0.52108000
C	-2.02995000	-0.15742900	0.32828200
C	-3.85194000	-1.44728100	-0.59531300
H	-4.31312800	-1.55996800	-1.57841400
H	-4.63101000	-1.21691500	0.14154500
H	-3.34053900	-2.37649900	-0.32335500
C	4.24505100	-0.99009600	0.70488500
H	4.48109700	-1.13762000	1.75865900
H	5.07100600	-0.50027000	0.18334400
H	4.01003600	-1.94094000	0.22104400
H	1.28899700	2.75074400	0.85388100
H	1.38253900	1.19864300	1.73413300

Structure **2a-IV- α -in** (B3LYP/6-31+G(D))

O	0.65290200	0.93372700	-1.59932900
O	1.84878000	-0.57171000	1.31597600
O	2.10004500	-1.19317200	-0.93578600
O	-3.09844700	-0.39046500	-0.31115000
O	-0.09535100	-0.56581100	2.50464700

N	0.20838300	0.79165700	0.63734900	C	2.99039600	1.89549900	-0.57192600
C	-1.11329700	0.89948000	0.01290100	H	2.45311400	2.77848300	-0.91722900
O	-1.15876200	-1.53988500	-0.17965100	H	3.74554000	1.58883700	-1.30017900
C	1.28499200	1.00768500	-0.33530400	H	3.46397600	2.08338100	0.39467700
C	1.98983700	2.35269600	-0.14814400	H	1.40333400	-1.56655200	-2.07660200
H	2.44308400	2.41373200	0.84744900	H	0.67702000	-2.95393000	-1.25571100
H	1.27988900	3.17890900	-0.25188300	H	1.71887700	-2.16758300	0.72557200
H	2.77495900	2.46661000	-0.90391800	Structure 2a-IV-β-out (B3LYP/6-31+G(D))			
C	0.55813200	-0.17148900	1.57081200	O	-0.89736900	-1.46452400	-1.36548100
C	-0.68461900	1.38578400	-1.41422200	O	-1.25144900	0.86970200	1.28263600
C	-1.76405900	-0.49430800	-0.14210200	O	2.36125900	0.74217800	-0.51899300
C	2.24639200	-0.17700400	-0.02351000	O	0.89189400	0.82039600	2.05162300
C	2.95647800	-2.31492800	-0.71251100	N	0.04788700	-0.82824400	0.63411300
H	2.79318900	-2.99080600	-1.55355100	C	1.14842100	-1.29003400	-0.22183800
H	2.70313600	-2.82064200	0.22503700	O	3.46840300	-1.01465900	0.38108800
H	4.01100000	-2.00171900	-0.69120300	C	-1.23476000	-1.06186700	-0.05214400
C	-3.79913800	-2.33902200	-0.52462400	C	-2.03777700	-2.18695100	0.59344700
H	-4.84863400	-1.35767200	-0.62779900	H	-2.29831800	-1.94361900	1.62788100
H	-3.65317400	-2.29766800	0.33091900	H	-1.43135300	-3.09701700	0.59268800
H	-3.43391400	-2.12305400	-1.43137700	H	-2.95439100	-2.37988400	0.02714000
H	-1.29460300	0.96639300	-2.21692800	C	0.01590100	0.33703900	1.37631800
C	-2.01966200	1.90517000	0.73302500	C	0.48347900	-1.17267000	-1.61538800
H	-2.94274600	2.07553500	0.17201700	C	2.45750900	-0.51542000	-0.06249300
H	-2.28139200	1.53846800	1.72963000	C	-1.89347200	0.36352300	0.07715200
H	-1.48682800	2.85501800	0.84393300	C	3.51344800	1.58205500	-0.29768700
H	-0.74115700	2.48340600	-1.45914100	H	3.25361800	2.54634400	-0.73412100
H	3.29484900	0.13532300	0.06978200	H	4.39239100	1.15553500	-0.78734400
Structure 2a-IV-α-out (B3LYP/6-31+G(D))				H	3.69394000	1.67780500	0.77547200
O	-0.95256600	1.63282200	1.14214100	H	0.85098900	-1.91198400	-2.33126200
O	-1.28904500	-1.01381900	-1.19404200	O	-1.45103300	1.09648100	-1.03033300
O	3.34425400	0.40817900	-0.34908400	C	-3.39691700	0.43145800	0.28568100
O	0.92463500	-1.32100700	-1.63498100	H	-3.70584700	1.46293600	0.47601700
N	0.12472200	0.62011800	-0.62237200	H	-3.91031700	0.06977900	-0.61092100
C	1.17053300	1.06769300	0.30961300	H	-3.70584400	-0.16782900	-1.44403000
O	2.32101200	-0.87532000	1.20952200	C	-1.73714100	2.49787100	-1.04933400
C	-1.18833900	1.08517800	-0.13955300	H	-1.12326100	2.91130800	-1.85203500
C	-1.77091200	2.18477500	-1.02210200	H	-2.79340600	2.68808500	-1.27592900
H	-1.94284900	1.82546600	-2.04111300	H	-1.46493400	2.97176400	-0.10032900
H	-1.06192400	3.01655500	-1.06157400	H	0.59375500	-0.16096500	-2.01367900
H	-2.71431300	2.55223600	-0.60609300	H	1.38199900	-2.33116500	0.01700000
C	0.03553600	-0.64335200	-1.17832400	Structure 2a'-I-α-in (B3LYP/6-31+G(D))			
C	0.34650300	1.23509800	1.60329500	O	-2.19184200	-1.35343000	-0.62766500
C	2.32280100	0.06866800	0.44964200	O	0.07575300	-0.55146600	-1.72316400
C	-1.99977100	-0.26677400	-0.16306800	O	3.73402400	-1.09393700	-0.69172500
C	4.44621500	-0.52274000	-0.38907300	O	-0.05891100	-1.06060600	2.64126400
H	5.16189100	-0.08907500	-1.08732000	O	2.97649700	0.71648700	0.42926200
H	4.09161900	-1.49261700	-0.74580700	O	-1.68334500	-0.17525900	1.31383100
H	4.88723900	-0.63075200	0.60511400	C	2.84385100	-0.49967900	-0.11700300
H	0.71929100	2.03038600	2.25365000	N	0.41125700	-0.21292800	0.52476700
O	-1.78229700	-0.86820900	1.08003100	C	-0.39582200	-0.54879000	1.60025200
C	-3.46494300	-0.20391700	-0.55988900	C	1.46045200	-1.12160400	0.08350900
H	-3.87683700	-1.21325500	-0.64348400	C	-3.43142400	-1.91866500	-0.18757200
H	-4.02944400	0.34470100	0.20077000	C	-0.38987300	0.22225900	-0.63279200
H	-3.59276800	0.28603000	-1.52687200	C	-0.21609100	1.70132900	-0.99208900
C	-2.22279800	-2.21998500	1.24565700	C	-0.90088200	2.62488200	0.02213000
H	-1.76854400	-2.56249000	2.17721900	C	0.85349000	-1.65358000	-1.23536600
H	-3.31443900	-2.27616600	1.33744200	C	4.28816000	1.30973000	0.32760200
H	-1.88079100	-2.85188500	0.41955300	C	-2.43254800	2.39400900	0.08692900
H	0.29528900	0.28814900	2.14688800	C	-2.86229000	1.00537200	-0.43582000
H	1.57663700	2.02286100	-0.03764500	C	-1.85126700	-0.09358000	-0.13218100
Structure 2a-IV-β-in (B3LYP/6-31+G(D))				H	1.58582000	-1.91498000	0.82803500
O	-0.51064900	-1.25150700	-1.43529200	H	-3.40217900	-2.96512400	-0.49756600
O	-1.33533000	0.79935100	1.27801000	H	-3.52818400	-1.86282000	0.90181700
O	-1.35039700	1.15729600	-1.02959500	H	-4.28697700	-1.42912600	-0.66800300
O	1.98544500	0.87094200	-0.43200500	H	0.85688700	1.90860100	-1.05121900
O	0.68618700	0.71656500	2.33097500	H	-0.63130300	1.84834500	-1.99770300
N	0.05441000	-0.85350600	0.73562900	H	-0.45389900	2.45378800	1.00885400
C	1.29080200	-1.34652600	0.14476300	H	-0.68635400	3.66915100	-0.23228900
O	3.58267700	-0.61606900	0.16467300	H	0.20762200	-2.51614100	-1.03786900
C	-1.08837800	-1.04923700	-0.16023600	H	1.59952200	-1.90086500	-1.99150600
C	-1.92380200	-2.26593600	0.24654800	H	4.20620500	2.27268700	0.83149300
H	-2.30144600	-2.16528200	1.26858100	H	5.02764400	0.67451700	0.82154800
H	-1.29978100	-3.16453500	0.20767400	H	4.56379900	1.44031200	-0.72198700
H	-2.76592000	-2.40114400	-0.43903600	H	-2.95544800	3.15338900	-0.50701000
C	-0.08996500	0.26824600	1.52168500	H	-2.77528600	2.51732000	1.11953000
C	-3.35091100	0.30315200	0.07104500	H	-2.98305000	1.02088500	-1.52615700
H	-3.73086200	1.29931600	0.31252100	H	-3.83555700	0.73616900	-0.01334500
H	-3.69173300	-0.37607400	0.85433000	Structure 2a'-I-β-in (B3LYP/6-31+G(D))			
H	-3.77296200	-0.01084700	-0.88904600	O	-1.98413700	-1.45714400	-0.87016400
C	0.76520900	-1.85937000	-1.24022900	O	0.17320400	-0.17899200	-1.69411200
C	2.41826400	-0.32258400	-0.01171400	O	2.75264800	1.35994900	0.26060900
C	-1.83182300	0.33387800	-0.01600600	O	-0.10261600	-1.27782200	2.55325300
C	-1.73167000	2.53399500	-0.99405200	O	3.87066400	-0.57522800	-0.09729600
H	-1.09455000	3.03002800	-1.72900200	O	-1.77664000	-0.48138600	1.23146800
H	-1.55678800	2.97010700	-0.00463300	C	2.75868200	0.15760300	0.12073000
H	-2.78089500	2.67100900	-1.28471800				

N	0.33405500	-0.09405600	0.59661800	C	3.34235200	1.17352600	1.63593600
C	-0.46313300	-0.68924000	1.56172000	H	-1.48603400	-0.16581100	-2.63438100
C	1.53840800	-0.76167300	0.13160600	H	-1.77891500	-1.48794400	-1.47437600
C	-3.13798300	-2.25811000	-0.59335600	H	-0.37112600	-2.24737500	0.40390900
C	-0.46576000	0.36711600	-0.55204200	H	0.32673000	-1.36819300	1.76013600
C	-0.51202700	1.88909900	-0.71388700	H	1.63582500	-3.46880800	0.48776300
C	-1.39293400	2.55109200	0.35203900	H	2.45924200	-2.20535500	1.39063800
C	1.09559800	-1.19459600	-1.29281800	H	2.05074500	-2.34664900	-1.63954300
C	5.11116100	0.15789400	-0.16543700	H	3.56550800	-2.53695100	-0.76743700
C	-2.86838500	2.08289800	0.27289600	H	3.89516600	-0.20895800	-0.62007600
C	-3.03843300	0.72437600	-0.44325600	H	2.77021700	-0.17508800	-1.97522800
C	-1.87964300	-0.23487900	-0.20181700	H	-4.87616900	-1.55916500	0.81380200
H	1.75704700	-1.62094300	0.77110000	H	-5.91076700	-0.39811000	-0.08751400
H	-2.92546600	-3.23791300	-1.02587600	H	-5.17908700	0.06567000	1.48647900
H	-3.29934900	-2.36184500	0.48485200	H	3.38239200	1.15675700	2.72685500
H	-4.03510900	-1.84608200	-1.07074700	H	3.20401000	2.20261900	1.28906800
H	0.51510600	2.26013900	-0.66202300	H	4.28412100	0.77406700	1.23793800
H	-0.89294900	2.10152500	-1.72160900	Structure 2a'-III- α -out (B3LYP/6-31+G(D))			
H	-0.97816600	2.32077100	1.34066400	C	-0.80832400	-0.56961300	0.23994100
H	-1.33513800	3.64029800	0.24612400	N	0.39918000	0.14401900	0.62122800
H	0.59890500	-2.17074300	-1.24938000	C	1.47426400	-0.86479400	0.55201500
H	1.90446700	-1.21958500	-2.02609700	C	1.04852600	-1.68531000	-0.69128000
H	5.88054200	0.59419800	-0.33994300	O	-0.36727100	-1.45159300	-0.82671600
H	5.07953100	0.87943200	-0.98595700	C	-1.67268500	0.57147600	-0.32478100
H	5.28904200	0.68410300	0.77570300	O	-0.69554700	1.46274700	-0.88771900
H	-3.47273600	2.82333200	-0.26521100	C	0.50609800	1.24268000	-0.26533600
H	-3.28553200	2.01739300	1.28330900	O	1.48969600	1.90528000	-0.47765400
H	-3.10071900	0.86356700	-1.52977200	H	1.38928400	-1.46879800	1.46034100
H	-3.97615200	0.25464700	-0.12979400	C	-1.60478400	-1.38071600	1.26073600
Structure 2a'-II- α -out (B3LYP/6-31+G(D))				C	-3.06703100	-1.56903900	0.73973700
C	0.44988300	-0.39359000	-0.18821000	C	-3.23895700	-1.34431500	-0.78437800
N	-0.50248000	0.70579200	-0.14310700	C	-2.70263300	0.02778300	-1.30785900
C	-1.67133400	0.29745100	-0.92179100	C	2.88513600	-0.26917900	0.59837400
C	-1.07973500	-0.78755800	-1.88275100	O	3.36964100	0.18023800	1.61238100
O	0.31313700	-0.87712900	-1.54367400	O	3.52768400	-0.37537900	-0.57533300
C	1.78473600	0.34867700	-0.01661700	C	4.83675500	0.22914200	-0.62770600
O	1.52869900	1.61745200	-0.64201200	O	-2.26290500	1.20220100	0.79381500
C	0.17517500	1.83828400	-0.64742100	C	-2.85934000	2.48162400	0.57135900
O	-0.32841800	2.85446900	-1.05490100	H	1.22844200	-2.75770600	-0.56080800
H	-2.04350300	1.17105900	-1.46809100	H	1.55072100	-1.33989000	-1.59805600
C	0.35950500	-1.56301000	0.79087900	H	-1.61104900	-0.86346000	2.22360500
C	1.74957300	-2.27404900	0.86613300	H	-1.11180400	-2.34922300	1.39595000
C	2.68826800	-1.97945700	-0.33215700	H	-3.71884700	-0.87520800	1.27956700
C	2.92562400	-0.46097200	-0.62237000	H	-3.41264000	-2.58073200	0.98083600
C	-2.84613900	-0.22149100	-0.09516600	H	-4.30257100	-1.43484200	-1.03294300
O	-3.63230000	-1.04545900	-0.52108600	H	-2.71864400	-2.14393100	-1.31972700
O	-2.94616800	0.37139900	1.10040100	H	-2.23660300	-0.09845700	-2.28831700
C	-4.08623500	-0.00633200	1.89960500	H	-3.51483900	0.75186200	-1.42245700
O	1.93482900	0.55944200	1.37264300	H	5.20050400	0.03820300	-1.63727800
C	2.96416300	1.46371600	1.77838400	H	5.49432000	-0.22513500	0.11770800
H	-1.14237800	-0.49417400	-2.93275800	H	4.75003600	1.30203500	-0.44084500
H	-1.58245300	-1.75019400	-1.74658900	H	-3.21661000	2.80880700	1.54976000
H	-0.41529400	-2.25442500	0.44142900	H	-3.71029000	2.42338900	-0.11928100
H	0.06627100	-1.19996100	1.77886300	H	-2.12620700	3.19856800	0.18822400
H	1.60243100	-3.35819900	0.93031700	Structure 2a'-III- β -out (B3LYP/6-31+G(D))			
H	2.24500300	-1.96682800	1.79225400	C	-0.79878400	-0.55341300	0.25078500
H	2.26773400	-2.43970400	-1.23105800	N	0.48298000	0.11444300	0.41804200
H	3.65241400	-2.46665900	-0.14713900	C	1.48549600	-0.96353500	0.33421700
H	3.87770100	-0.12154700	-0.20391800	C	0.86112400	-1.90268600	-0.72706400
H	2.96173600	-0.28368100	-1.70023200	O	-0.53501600	-1.54891200	-0.77012500
H	-5.01309800	0.23826500	1.37442400	C	-1.66318300	0.58288000	-0.32130100
H	-3.99550900	0.57419200	2.81746900	O	-0.71586400	1.35045800	-1.08201500
H	-4.06088700	-1.07804300	2.11281800	C	0.53994000	1.10846900	-0.58889500
H	2.84181400	1.57768500	2.85736100	O	1.52504300	1.67635600	-0.98764600
H	2.85107900	2.43750000	1.29113400	H	1.51195900	-1.44580800	1.31768800
H	3.96515200	1.06277500	1.57339000	C	-1.50548000	-1.21542700	1.43263300
Structure 2a'-II- β -out (B3LYP/6-31+G(D))				C	-3.02871700	-1.35351000	1.10883300
C	0.49133200	-0.35872200	-0.13930000	C	-3.37220900	-1.26345800	-0.39959800
N	-0.38809300	0.76652400	0.14475700	C	-2.83432200	0.01692900	-1.11683300
C	-1.66554800	0.51944300	-0.51751300	C	2.91399600	-0.51478300	0.02929100
C	-1.26962100	-0.52753000	-1.62710300	O	3.55660100	-0.90426500	-0.92213800
O	0.14578200	-0.68211600	-1.51126300	O	3.38354300	0.27728200	1.00171800
C	1.87569500	0.30815400	-0.08261500	C	4.69758200	0.82971200	0.78306200
O	1.60780600	1.64846900	-0.52655600	O	-2.07609200	1.35430900	0.78923800
C	0.28255900	1.92388200	-0.31300900	C	-2.63406700	2.63942500	0.50869800
O	-0.21038100	3.00376600	-0.52181200	H	0.96560400	-2.95904500	-0.45821900
H	-2.03096200	1.45183800	-0.95317900	H	1.30136200	-1.73571200	-1.71347000
C	0.47715200	-1.62727000	0.71057300	H	-1.36445600	-0.61509200	2.33518900
C	1.82781800	-2.38999800	0.51606000	H	-1.05310100	-2.19855900	1.60143600
C	2.60967200	-2.60057700	-0.76475900	H	-3.56987900	-0.56873300	1.64642100
C	2.87806700	-0.46886900	-0.92793500	H	-3.39763500	-2.31204600	1.49125300
C	-2.72887200	-0.02352000	0.42758700	H	-4.46136200	-1.31012400	-0.51288700
O	-2.54682400	-0.46056800	1.54111600	H	-2.96234400	-2.14102600	-0.90815100
O	-3.93118600	0.01440000	-0.18672700	H	-2.50029600	-0.22849100	-2.12803900
C	-5.04542100	-0.50801400	0.56602000	H	-3.61567900	0.77755000	-1.20604900
O	2.22538300	0.35464300	1.28501600	H	4.89915800	1.44387600	1.66061500

H	4.69240400	1.43861100	-0.12425400	O	0.34243400	-0.44092300	2.73761700
H	5.43616300	0.02940800	0.68923000	N	-0.10394700	-0.50936000	0.45689200
H	-2.82348100	3.09263600	1.48384200	C	-1.22205800	0.39721800	0.32628100
H	-3.58152200	2.56494400	-0.04035300	H	-1.31748100	1.00119300	1.23254900
H	-1.93172400	3.26105600	-0.05578000	O	-2.68490900	-1.45171900	-0.32789400
Structure 2a'-IV-α-in (B3LYP/6-31+G(D))							
C	-0.84929200	-0.72985600	0.03836400	C	0.68806900	-0.57038200	-0.77339600
N	0.36250700	-0.70008400	0.85645500	H	0.47396900	-1.86792900	-1.54842100
C	1.44423400	-1.45239100	0.23072400	C	0.77715000	-2.73624600	-0.95536000
C	0.73007000	-1.95322900	-1.07023800	H	1.04408200	-1.85208100	-2.48289200
O	-0.40069100	-1.10329500	-1.25196000	H	-0.58913100	-1.96775500	-1.77660200
C	-1.35337900	0.75670200	0.14435300	C	0.68512600	-0.57140300	1.58635100
O	-0.62954200	1.24863600	1.30885400	C	3.25771200	-1.23527400	-0.80287300
C	0.50107300	0.49848800	1.52696200	H	3.44112200	-0.90913000	-1.83160200
O	1.41377700	0.85082300	2.23475900	H	2.99901400	-2.29528900	-0.80326600
H	1.76448500	-2.29408000	0.84969300	H	4.18031600	-1.12120600	-0.22745300
C	-1.90807900	-1.70732300	0.56550000	C	-0.79888600	1.27341600	-0.90466700
C	-3.23735200	-1.58886900	-0.20789600	C	-2.54912100	-0.32041100	0.08200400
C	-3.61567100	-0.11115200	-0.50168300	C	2.14947500	-0.39763800	-0.18669900
C	-2.85807100	0.86006500	0.41712300	C	3.62695700	1.40498500	0.44924700
C	2.71646600	-0.66225100	-0.08582200	H	3.53889400	2.48977600	0.53983100
O	3.82386600	-1.13915500	0.05158300	H	4.50768700	1.17085400	-0.16097400
O	2.46232400	0.54743800	-0.59787200	H	3.73101500	0.96304400	1.44594400
C	3.61260300	1.36403900	-0.89638300	C	-4.89709600	-0.00294700	0.11396400
O	-0.93337800	1.43041000	-0.99959300	H	-5.57605700	0.80464700	0.38745400
C	-1.06292500	2.85381400	-1.00701600	H	-5.07095500	-0.88400300	0.73655000
H	0.41827900	-2.99910600	-0.94571600	H	-5.01637600	-0.27150700	-0.93897200
H	1.35333300	-1.87235300	-1.96313300	C	-0.31343200	2.66457600	-0.51633000
H	-2.06314300	-1.49090500	1.62933600	H	0.47867500	2.60815000	0.23507800
H	-1.51527100	-2.72946500	0.51417900	H	0.08548300	3.17633900	-1.39825200
H	-4.02313600	-2.07312600	0.38436500	H	-1.14944200	3.25351100	-0.11943500
H	-3.16776200	-2.14496500	-1.14890700	H	-1.62179900	1.35991400	-1.62329700
H	-4.69524700	0.03767500	-0.38764100	Structure 2b-I-α-out (B3LYP/6-31+G(D))			
H	-3.37423400	0.13580500	-1.54244300	O	0.44872000	1.17546600	-0.93716700
H	-3.19129000	1.89080700	0.26404700	O	2.01225200	-0.34739400	1.30716700
H	-3.04522100	0.62829900	1.47090200	O	-3.63696700	0.18290400	0.25588900
H	4.18088800	1.55034600	0.01805100	O	0.28256700	-0.25274700	2.76283600
H	3.20788500	2.29324300	-1.29679400	N	-0.07511800	-0.52408700	0.47441400
H	4.24943200	0.86672700	-1.63248800	C	-1.29746300	0.26896300	0.41363500
H	-0.51545500	3.18906700	-1.89023100	H	-1.48573000	0.70612500	1.39775500
H	-0.61992000	3.29652600	-0.10908600	O	-2.52643900	-1.64410300	-0.48704400
H	-2.11007300	3.16901800	-1.09941200	C	0.74102700	-0.20451300	-0.69961700
Structure 2a'-IV-β-in (B3LYP/6-31+G(D))							
C	-0.89034700	-0.71314700	0.12688700	C	0.42290400	-1.02772000	-1.94526300
N	0.29502200	-0.47643600	0.95575900	H	0.50477900	-2.09991300	-1.75673100
C	1.46875200	-1.13425800	0.40408300	H	1.10897100	-0.74061500	-2.74874200
C	0.81334600	-1.95170600	-0.75452100	H	-0.59830700	-0.83376500	-2.27984600
O	-0.38602000	-1.25569800	-1.08023900	C	0.69663000	-0.35873300	1.63249300
C	-1.48898000	0.73433500	-0.00620500	C	-0.94063200	1.38717700	-0.64487900
O	-0.88871300	1.41206900	1.13375300	C	-2.52314900	-0.54011400	0.01027800
C	0.28710200	0.79920900	1.49511000	C	2.19738900	-0.39332100	-0.14360600
O	1.11367100	1.30125100	2.21616500	C	-4.88884700	-0.43551200	-0.10606100
C	1.95061600	-1.79631600	1.12824300	H	-5.65704000	0.28615800	0.17167800
H	-1.90104800	-1.65952300	0.78588700	H	-5.01865800	-1.37096600	0.44371300
C	-3.20576400	-1.76833400	-0.03176100	H	-4.91587700	-0.63774000	-1.18002800
C	-3.62796500	-0.40500300	-0.64004700	C	-1.13627400	2.80928300	-0.14675400
C	-3.01610300	0.77234500	0.13536800	H	-0.80240100	3.52356400	-0.90644100
C	2.51828300	-0.16183500	-0.14397700	H	-2.19629900	2.99228400	0.06201500
O	2.29584800	0.92824300	-0.61594000	H	-0.55942100	2.98097400	0.76836900
O	3.73868000	-0.73425600	-0.08273600	H	-1.52812200	1.23079200	-1.56117200
C	4.82692300	0.04845000	-0.61643600	O	2.95801700	0.68684500	-0.55920700
O	-1.03177700	1.27825900	-1.20259800	C	2.82836600	-1.75268100	-0.44362600
C	-1.05184900	2.70193400	-1.32873100	H	3.07696400	-1.84268100	-1.50511400
H	0.59584800	-2.97384800	-0.41423400	H	3.74002000	-1.87115200	0.14771400
H	1.42906200	-1.99901800	-1.65510100	C	2.14751800	-2.56145100	-0.16489100
H	-2.11107100	-1.27280300	1.79052300	C	4.30789600	0.76075100	-0.09269500
H	-1.43892200	-2.64376900	0.92570300	H	4.94593100	0.01104900	-0.57685500
H	-3.99399500	-2.15170800	0.62774700	H	4.65520900	1.75738000	-0.37139100
H	-3.08192700	-2.50517400	-0.83277500	H	4.35601100	0.64932500	0.99584200
H	-4.72000200	-0.31512000	-0.65579100	Structure 2b-I-β-in (B3LYP/6-31+G(D))			
H	-3.29327300	-0.34231100	-1.68251900	O	0.28243500	0.88385500	-1.44796200
H	-3.39217900	1.72822400	-0.24208300	O	1.74612300	-1.19239500	1.00768500
H	-3.28520600	0.72469300	1.19637300	O	2.52455400	0.70833400	-0.08360700
H	4.65782500	0.25983700	-1.67555700	O	-2.87550600	-0.96181500	0.10246500
H	5.71686500	-0.56609900	-0.48040500	O	0.21550500	-0.75217800	2.64287200
H	4.91524400	0.98848800	-0.06643400	N	-0.23355200	-0.37582400	0.39339400
H	-0.70974700	2.90410100	-2.34529800	C	-1.17950400	0.71808700	0.42813500
H	-0.37073700	3.16784900	-0.61084600	H	-1.17235300	1.16974300	1.42624600
H	-2.06117600	3.11428200	-1.19902700	O	-3.49300700	1.21082500	0.01256800
Structure 2b-I-α-in (B3LYP/6-31+G(D))							
O	0.23128300	0.51111300	-1.56554300	C	0.53507300	-0.37363800	-0.85178600
O	1.97301000	-0.84332700	-1.59266200	C	0.08730800	-1.46801800	-1.81952300
O	2.42055700	0.97392000	-0.18788500	H	0.21368100	-2.46258800	-1.38101500
O	-3.57222300	0.51718900	0.34975400	H	0.65548600	-1.40910400	-2.75311500
Structure 2b-I-β-out (B3LYP/6-31+G(D))							
O	0.23128300	0.51111300	-1.56554300	H	-0.97230400	-1.32652700	-2.04671800
O	1.97301000	-0.84332700	-1.59266200	C	0.52937200	-0.75716600	1.47617100
O	2.42055700	0.97392000	-0.18788500	C	2.93517300	-1.48989400	-1.06203800
O	-3.57222300	0.51718900	0.34975400	H	3.17170100	-1.04626500	-2.03445800
Structure 2b-I-α-in (B3LYP/6-31+G(D))							
O	0.23128300	0.51111300	-1.56554300	H	2.48630100	-2.47277600	-1.21488100

H	3.86558900	-1.63621000	-0.50690600	H	-2.62553700	2.75648200	0.37914400
C	-0.59855600	1.70063800	-0.63999400	H	-1.01501700	2.91620300	1.12277800
C	-2.64010700	0.35598500	0.14918600	H	-1.67487000	1.32828600	-1.42183200
C	2.00317200	-0.57108900	-0.28883800	Structure 2b-II-β-out (B3LYP/6-31+G(D))			
C	3.79023200	0.80390000	0.57716800	O	0.35849700	1.59914000	-0.77827200
H	3.90236000	1.85691600	0.84374500	O	1.96149900	-0.09847800	1.26321200
H	4.61222800	0.51766500	-0.09007000	O	2.56269800	-1.24151000	-0.66722900
H	3.81233200	0.19309700	1.48594200	O	-2.53008600	-1.57301200	0.11627500
C	-4.25293000	-1.34773600	-0.08859800	O	0.24355100	-0.27852000	2.72914100
H	-4.24671800	-2.43759100	-0.08980400	N	-0.12690200	-0.26260000	0.42829600
H	-4.62739800	-0.95799100	-1.03866100	C	-1.37222800	0.49861100	0.43975400
H	-4.86724600	-0.96376500	0.72957600	H	-1.58531200	0.78948800	1.47549000
C	0.13329100	2.89400100	-0.03939700	O	-3.58928800	0.33354000	-0.47785200
O	0.89511500	2.57510000	0.67734500	C	0.67552200	0.20383000	-0.70001300
H	0.62691000	3.46295800	-0.83395300	C	0.36225700	-0.49741200	-2.01747400
H	-0.58561300	3.55195600	0.46388400	H	0.50974000	-1.57431800	-1.92974700
H	-1.39118800	2.05273400	-1.30599800	H	1.01487200	-0.11035000	-2.80604000
Structure 2b-I-β-out (B3LYP/6-31+G(D))				H	-0.67434700	-0.30082200	-2.30944900
O	0.56639500	1.34901600	-0.81766700	C	0.64501500	-0.22658100	1.59140500
O	1.87882900	-0.57777900	1.24784700	C	3.09725500	1.14239000	-0.45575000
O	-2.79702400	-1.27338100	0.14081700	H	4.03307000	0.99026100	0.08867800
O	0.18916000	-0.32701800	2.73391500	H	2.65771100	2.08838600	-0.13702900
N	-0.21329300	-0.37602500	0.43721000	H	3.31127300	1.19463500	-1.52815500
C	-1.31284200	0.58547600	0.43844500	C	-1.03829900	1.75404800	-0.44608700
H	-1.46515000	0.92611400	1.46940600	C	-2.61250000	-0.24741100	-0.04419700
O	-3.53844100	0.77803800	-0.45128400	C	2.13471600	-0.00133900	-0.17449900
C	0.63802800	-0.07149400	-0.71456600	C	3.82632900	-1.72364400	-0.20197300
C	0.17509300	-0.71446200	-2.02150200	H	3.88697100	-2.75916400	-0.54256000
H	0.09562500	-1.80081600	-1.93907400	H	3.88252700	-1.69518000	0.89128800
H	0.87852600	-0.45917800	-2.82038600	H	4.65733800	-1.15444400	-0.63605800
H	-0.80643600	-0.32464600	-2.30725900	C	-3.70867000	-2.32692100	-0.23583600
C	0.57783700	-0.41239600	1.59307200	H	-3.45450700	-3.36613400	-0.02819100
C	-0.77513100	1.74990400	-0.47079900	H	-3.94539000	-2.18764500	-1.29379800
C	-2.66320000	0.04927100	-0.02492600	H	-4.55773800	-2.00499700	0.37248200
C	2.04567500	-0.54163600	-0.20626100	H	-1.63339000	1.72089900	-1.36558700
C	-4.08972400	-1.82210700	-0.18967400	C	-1.24031800	3.09061800	0.24756000
H	-4.00743800	-2.88938400	0.01535300	H	-0.90221500	3.90705400	-0.39918000
H	-4.31955400	-1.64420200	-1.24338600	H	-2.30404300	3.23998300	0.46332900
H	-4.86335200	-1.36557100	0.43292700	H	-0.67768000	3.13412800	1.18691700
C	-0.72561900	3.10944200	0.20600300	Structure 2b-III-α-in (B3LYP/6-31+G(D))			
H	-0.25707600	3.84311900	-0.45801100	O	-0.48668800	1.81169700	0.47847900
H	-1.74212100	3.44852900	0.43500300	O	-1.40731700	-1.50535400	-0.14102800
H	-0.14667200	3.06308700	1.13504100	O	-3.25869700	-0.10064900	-0.17594000
H	-1.38372800	1.81234000	-1.38050000	O	2.48980300	-0.81301400	0.78957500
O	2.97326000	0.42472300	-0.55498800	O	0.59634400	-2.25321400	-0.89812700
C	2.43587300	-1.95943000	-0.62263700	N	0.07203200	0.01474500	-0.84279700
H	2.65557200	-2.00480600	-1.69351700	C	1.32278800	0.73423300	-0.59985000
H	3.32029700	-2.27596200	-0.06369000	H	1.55816900	1.36272900	-1.46455900
H	1.63069600	-2.66206300	-0.39072600	O	3.46106500	-0.23081600	-1.17091900
C	4.31660900	0.24439100	-0.09851100	C	-1.05206300	0.83865400	-0.40067000
H	4.82109200	-0.57069300	-0.63234000	C	-1.73216000	1.57478500	-1.55096900
H	4.82528800	1.18416700	-0.32127800	H	-2.18122900	0.87085300	-2.25524500
H	4.34446200	0.06158800	0.98098500	H	-0.98252000	2.17899700	-2.07162200
Structure 2b-II-α-out (B3LYP/6-31+G(D))				H	-2.51489700	2.23455500	-1.16774000
O	0.27996900	1.49969500	-0.75640600	C	-0.15113400	-1.33717500	-0.64707100
O	2.04223700	-0.04865500	1.29395200	C	-1.87692300	-0.20454500	1.83815200
O	2.83632900	-1.02868800	-0.65438000	H	-2.33092300	0.71019500	2.22939500
O	-3.62374800	-0.19908900	0.25252600	H	-0.83361600	-0.24143000	2.16126200
O	0.33364200	-0.50203300	2.70881800	H	-2.38603000	-1.07705700	2.25638200
N	0.00474700	-0.43305800	0.40292500	C	0.93400600	1.60947500	0.62510200
C	-1.31556700	0.18410700	0.43197300	C	2.54194200	-0.16519200	-0.38514200
H	-1.55438400	0.46676800	1.46103100	C	-1.96558100	-0.22824300	0.31700000
O	-2.28453700	-1.75054800	-0.70928000	C	-4.23227400	-1.04806200	0.27366100
C	0.77212200	0.15049000	-0.69640100	H	-5.10930700	-0.88453700	-0.35550300
C	0.59444500	-0.55041700	-2.03787400	H	-4.50650600	-0.87646700	1.32144900
H	0.87631100	-1.60081700	-1.96517700	H	-3.87300300	-2.07394500	0.14106300
H	1.22042400	-0.06109100	-2.79071900	C	3.52317300	-1.79560700	1.01370200
H	-0.44837800	-0.49500800	-2.35941800	H	3.32429800	-2.19989100	2.00608900
C	0.74697400	-0.35304900	1.58376800	H	4.50839700	-1.32482100	0.97306500
C	3.04086800	1.39453300	-0.35165900	H	3.44959500	-2.57735600	0.25429500
H	3.98075500	1.34378300	0.20467600	C	1.63327300	2.95588800	0.69991500
H	2.47815100	2.26263600	-0.00596100	H	1.46500700	3.53557700	-0.21421800
H	3.26221100	1.51724000	-1.41677500	H	1.25415900	3.53284500	1.54940900
C	-1.12908100	1.46276600	-0.47743000	H	2.71271600	2.81741800	0.83526900
C	-2.42511200	-0.72838000	-0.07749200	H	1.11512400	1.03464600	1.54149600
C	2.23353200	0.12336700	-0.13422300	Structure 2b-III-α-out (B3LYP/6-31+G(D))			
C	4.13822900	-1.36104900	-0.16488100	O	0.59662500	1.81260200	-0.29092800
H	4.34184600	-2.36648200	-0.53844800	O	1.41879100	-1.14265200	-0.94579900
H	4.15997600	-1.36725000	0.92995100	O	2.93214300	-0.73409400	0.76440700
H	4.90036000	-0.67396000	-0.55241200	O	-2.91844600	-1.05501900	0.88985900
C	-4.78461100	-0.93403900	-0.18741500	O	-0.69044100	-1.95587100	-0.97566300
H	-5.64023000	-0.36208900	0.17160700	N	-0.07513200	-0.24496000	-0.49223000
H	-4.77987700	-1.93750000	0.24527700	C	-1.28700200	0.59004000	0.42536500
H	-4.79641000	-1.00812000	-1.27798700	H	-1.47709600	0.97227300	1.43548300
C	-1.54869500	2.76753500	0.17765000	O	-3.18748100	0.14476400	-1.01178300
H	-1.32832900	3.61168600	-0.48415200				

C	1.04398400	0.69521800	0.50044300	H	-1.82804800	-1.13256500	3.16216000
C	1.43232700	1.19200900	1.88811200	H	-2.09516500	-2.27521600	1.81774200
H	1.73786300	0.36594700	2.53137500	H	-3.41622800	-1.18143300	2.35449600
H	0.58530800	1.71606600	2.34130100	C	4.33161400	-1.12325500	-0.17379000
H	2.25982800	1.90340600	1.80380900	H	5.03646300	-1.16372000	-1.00407700
C	0.12744400	-1.19320900	-0.52037600	H	3.92184800	-2.11348600	0.03884300
C	2.98037000	0.65996900	-1.25200100	H	4.80775900	-0.71804500	0.72275500
H	3.60951900	1.39538800	-0.74016900	C	1.03199100	3.04247200	0.90253500
H	2.31799400	1.18457800	-1.94168700	H	1.14831800	3.60153900	-0.03296200
H	3.61776800	-0.01889800	-1.82498200	H	0.39555300	3.62478700	1.57648100
C	-0.83619000	1.73427100	-0.50892100	H	2.01486500	2.93288100	1.37577200
C	-2.55540600	-0.13870400	-0.01661800	H	0.31448600	1.11609000	1.58671000
C	2.16384400	-0.12048000	-0.23396900	Structure 2b-IV-β-in (B3LYP/6-31+G(D))			
C	3.94573400	-1.64833400	0.33682500	O	-0.77605900	1.80070100	0.55130900
H	4.28101800	-2.15734900	1.24263200	O	-1.47485800	-1.38615400	-0.84240600
H	4.79581900	-1.12170400	-0.11364200	O	-1.52692100	-0.60704200	1.35594000
H	3.54394500	-2.38432000	-0.36759300	O	2.22894100	-0.87127400	0.61317400
C	-4.04700100	-1.87934500	0.53384800	O	0.60380300	-1.86102600	-1.64414000
H	-4.18295700	-2.55727500	1.37635500	N	-0.01602100	0.29680300	-0.01259400
H	-3.81904400	-2.43504400	-0.37896400	C	1.16873000	0.96920200	-0.47127900
H	-4.93651900	-1.26254800	0.38217600	H	1.46576200	1.78526900	-1.13756100
H	-1.01142500	1.43338700	-1.54883200	O	3.42574400	0.25602000	-0.94188300
C	-1.48061700	3.08369500	-0.24240000	C	-1.22912900	0.91538000	-0.45009600
H	-1.04220300	3.84837200	-0.89158200	C	-1.99432900	1.72824300	-1.49059800
H	-2.55473900	3.03085500	-0.45295800	H	-2.34569400	1.09328900	-2.30948100
H	-1.33361800	3.39296500	0.79908000	H	-1.32574400	2.48895400	-1.90309100
Structure 2b-III-β-in (B3LYP/6-31+G(D))				H	-2.85165800	2.23105100	-1.03185300
O	0.45559700	1.71161000	-0.54946400	C	-0.18353500	-1.06100300	-1.19936500
O	1.39354300	-1.29709100	-0.70376100	C	-3.50891500	-0.37367800	-0.05134500
O	3.08349600	-0.45789500	0.64589500	H	-3.90260900	-1.35701400	0.22025600
O	-3.01414100	-0.43822800	-0.62472900	H	-3.83332200	-0.15980800	-1.07135600
O	-0.62481200	-2.20956900	-0.24738700	H	-3.93241300	0.37466100	0.62616000
N	0.02390200	-0.17505700	0.69833800	C	0.60567200	1.53037800	0.86543400
C	-1.24276500	0.57626900	0.62443800	C	2.40100400	0.07730600	-0.32000500
H	-1.32462900	1.16307600	1.54495600	C	-1.99323900	-0.36540500	0.05845600
O	-2.97061700	-0.78398200	1.61103000	C	-1.91658900	-1.83558600	1.97601600
C	1.07083300	0.79061700	0.37263600	H	-1.27754900	-1.93579400	2.85563400
C	1.59259200	1.57030800	1.57383600	H	-1.75349700	-2.68744200	1.30727900
H	2.03614300	0.90280200	2.31342400	H	-2.96448200	-1.80584700	2.29900600
H	0.77136600	2.12970700	2.03200700	C	3.29534200	-1.83490400	0.73693000
H	2.34804400	2.29074500	1.24484400	H	2.98394000	-2.50622800	1.53710900
C	0.17522500	-1.31835800	-0.09610800	H	4.23250900	-1.33315000	0.99039600
C	2.75560800	0.47207100	-1.59773500	H	3.40600400	-2.37876700	-0.20407600
H	3.37663200	1.33763700	-1.34538500	H	0.64621900	0.74411400	1.62542700
H	1.97040300	0.79312100	-2.28340700	C	1.26121400	2.80650400	1.35920400
H	3.37399800	-0.27766800	-2.09878500	H	0.75345800	3.16686300	2.25961700
C	-0.97971000	1.50835900	-0.58214300	H	2.31209400	2.62109500	1.61113700
C	-2.49081300	-0.31213400	0.60479300	H	1.21658000	3.59270700	0.59750200
C	2.14370300	-0.11122000	-0.33382200	Structure 2c-I-α-in (B3LYP/6-31+G(D))			
C	4.09277800	-1.40221800	0.27720900	O	-0.09521500	1.18246000	1.05804400
H	4.58414900	-1.68340800	1.21071300	O	-2.04480800	-1.29616000	-0.55975600
H	4.83346900	-0.95492600	-0.39688600	O	2.68947600	-0.85634800	0.48796800
H	3.65250100	-2.29160400	-0.18559400	O	-0.61861800	-1.67705800	-2.29832800
C	-4.13910900	-1.33499100	-0.73598500	N	0.07858400	-0.62842000	-0.33951900
H	-4.42881900	-1.30274000	-1.78624600	C	1.05686400	0.33281600	-0.82692000
H	-4.95703000	-0.99868900	-0.09386700	H	0.98580600	0.41142500	-1.91466700
H	-3.83070300	-2.34252900	-0.44747900	O	3.42917000	0.48885900	-1.16947100
H	-1.22914900	0.98086500	-1.51002900	C	-0.59350800	-0.12460700	0.87348100
C	-1.69460100	2.84820200	-0.53348500	C	-0.26084800	-0.94327600	2.11622500
H	-1.38152500	3.47669000	-1.37332800	H	-0.58911000	-1.98094700	2.00167400
H	-2.77863000	2.69991600	-0.60479100	H	-0.74168300	-0.51027000	2.99914500
H	-1.47051600	3.38221300	0.39700900	H	0.82104400	-0.93400900	2.25884900
Structure 2b-IV-α-in (B3LYP/6-31+G(D))				C	-0.82345400	-1.23752400	-1.19263500
O	-0.88578300	1.85014700	0.05684200	C	0.54679800	1.64875200	-0.14531100
O	-1.46180300	-1.60076100	-0.52124100	H	-0.21905700	2.07184900	-0.80509100
O	-1.83164000	-0.25290300	1.34477000	C	2.51796300	-0.00294100	-0.53450900
O	3.27352700	-0.24804800	-0.61736400	C	-2.10421700	-0.22492300	0.42671700
O	0.71036900	-2.24163900	-0.76864300	C	1.57017200	2.70692300	0.22122800
N	0.05645400	-0.00921400	-0.91632200	H	2.08803700	3.06426500	-0.67464700
C	1.16181000	0.79123400	-0.37476200	H	2.31623600	2.31865800	0.92203500
H	1.59688800	1.39753500	-1.17680200	H	1.06353400	3.55445400	0.69398200
O	2.26041900	-0.46216700	1.39490700	C	4.05611100	-1.20722300	0.79031600
C	-1.20913000	0.72648600	-0.73245500	H	3.99453100	-1.91511900	1.61695500
C	-1.78146900	1.22452600	-2.05622400	H	4.62096400	-0.31770400	1.08074700
H	-2.01890800	0.39107500	-2.72413900	H	4.52679400	-1.66858600	-0.08121600
H	-1.03690800	1.85973700	-2.54418400	O	-2.39960900	0.98075700	-0.22407000
H	-2.68545700	1.81778200	-1.88558000	C	-3.13123900	-0.61403500	1.47598900
C	-0.12104900	-1.36669500	-0.72346300	H	-3.21306700	0.17862200	2.22654900
C	-3.56290100	-0.43734200	-0.36681400	H	-4.10980000	-0.76029400	1.01054000
H	-4.02537900	-1.30835700	0.10563900	H	-2.85783700	-1.54863600	-1.96871100
H	-3.71831000	-0.52524200	-1.44367600	C	-3.66519200	1.07849700	-0.88575900
H	-4.06160900	0.46637200	-0.00232800	H	-4.48168800	1.21457900	-0.16638100
C	0.41760200	1.67787600	0.65348200	H	-3.59866400	1.96637600	-1.51781000
C	2.27112200	-0.05723100	0.25249700	H	-3.85600000	0.19971500	-1.51077300
C	-2.08347800	-0.37878300	-0.02482000				
C	-2.33379000	-1.27966600	2.20601900				

Structure **2c-I- β -in** (B3LYP/6-31+G(D))

O	0.18982800	-1.55212600	0.34200200
O	2.13942300	1.38989300	0.07142600
O	2.35405700	-0.71262100	-0.90359700
O	-3.45747200	0.39225600	-0.68118100
O	0.56208300	0.65807000	-0.98066300
N	0.00825200	0.73040700	0.20145600
C	-1.10891500	0.20318200	-0.56390200
H	-1.20189600	0.74610200	-1.50727200
O	-2.56689600	0.30060900	1.39589400
C	0.76446500	-0.36158000	0.84151000
C	0.62429500	-0.36228900	2.35902000
H	1.02601600	0.56031900	2.78933900
H	1.15180200	-1.21906800	2.79063600
H	-0.43685000	-0.42697900	2.60707900
C	0.85438000	1.69217400	-0.31701600
C	3.37941100	-0.28715400	1.27325700
H	3.48048100	-1.36009300	1.46515200
H	3.22691200	0.23377100	2.21992600
H	4.31180100	0.08265000	0.83812500
C	-0.63378400	-1.27056800	-0.80310900
H	-0.00008700	-1.26054900	-1.69800000
C	-2.43247400	0.31194800	0.19171800
C	2.22119400	-0.04352200	0.32145700
C	-1.69609200	-2.34859400	-0.92139100
H	-2.33541400	-2.16086400	-1.79079400
H	-2.32012400	-2.39367600	-0.02269400
H	-1.21438500	-3.32295000	-1.05146500
C	3.52853600	-0.44233600	-1.67522300
H	3.33364300	-0.86259500	-2.66405800
H	4.41002700	-0.93512400	-1.24738600
H	3.70588700	0.63464500	-1.76517000
C	-4.77778800	0.46227200	-0.10482700
H	-5.45942000	0.51960200	-0.95344200
H	-4.86601000	1.35138400	0.52445600
H	-4.97770800	-0.42926400	0.49535000

Structure **2c-II- α -out** (B3LYP/6-31+G(D))

O	-0.27131200	1.52738100	-0.71779700
O	-2.11786200	-1.01175200	-0.83091400
O	-2.84107300	-0.12753700	1.18611700
O	3.56640800	-0.60371000	-0.18723800
O	-0.47218000	-2.45149300	-1.41288600
N	-0.04573000	-0.63391700	-0.01605300
C	1.26510400	-0.31200200	-0.56746700
H	1.48782000	-1.02336500	-1.36571700
O	2.28608500	-0.36320100	1.66074500
C	-0.76592000	0.60419200	0.26775500
C	-0.55584200	1.17245900	1.66606500
H	-0.86895100	0.45885600	2.42849400
H	-1.14233200	2.09071500	1.77248300
H	0.49879200	1.40549300	1.81924600
C	-0.83961900	-1.47285200	-0.80751400
C	-3.04656100	1.20658300	-0.85885500
H	-4.00354300	0.77404900	-1.16290600
H	-2.48964000	1.48774500	-1.75353000
H	-3.23321900	2.10563300	-0.26277200
C	1.04128400	1.13209600	-1.16946100
H	0.97622000	1.03600200	-2.25937500
C	2.39341700	-0.42521200	0.45655600
C	-2.25209700	0.19981800	-0.04104500
C	2.07679700	2.19553900	-0.82342400
H	3.05111100	1.93369100	-1.25084000
H	2.18778800	2.31910100	0.25900900
H	1.76365000	3.15564400	-1.24550900
C	-4.16770800	-0.66019800	1.15155600
H	-4.36205400	-1.02380500	2.16248700
H	-4.24263000	-1.49282600	0.44403400
H	-4.90432400	0.11309500	0.90140900
C	4.73768300	-0.71298100	0.64726700
H	5.56967800	-0.85552600	-0.04230900
H	4.64071700	-1.56833400	1.32039700
H	4.87126900	0.19910400	1.23493700

Structure **2c-II- β -out** (B3LYP/6-31+G(D))

O	0.23904100	1.71674500	-0.38296900
O	2.10564100	-0.22916900	1.22139000
O	2.60962600	-0.93540500	-0.92954500
O	-2.33989300	-1.38763100	-0.52472600
O	0.53650800	-0.82324000	2.74104700
N	-0.04012300	-0.35482100	0.53166900
C	-1.29955400	0.32098200	0.82333800
H	-1.43733300	0.33212200	1.90805900
O	-3.67108200	0.04468800	0.60532300
C	0.63784000	0.34907900	-0.55193700
C	0.28068300	-0.12812400	-1.95589600
H	0.49879800	-1.18952400	-2.07669200
H	0.85938100	0.44172200	-2.68966000

H	-0.78065700	0.04205100	-2.14799900
C	0.83362000	-0.51047900	1.61298500
C	3.01755900	1.39736100	-0.29710200
H	4.00524800	1.21100900	0.13317900
H	2.55603700	2.23013200	0.23503100
H	3.13213200	1.67224500	-1.35060700
C	-1.03230200	1.79054600	0.30459800
H	-0.86809900	2.43146300	1.17787600
C	-2.56506100	-0.34525900	0.28703600
C	2.14981500	0.15377900	-0.17771800
C	-2.09251100	2.42639300	-0.58461300
H	-3.03087400	2.54970100	-0.03533900
H	-2.29219200	1.82428400	-1.47734500
H	-1.74209000	3.41118500	-0.90972600
C	3.93458800	-1.40052600	-0.65814700
H	4.02682800	-2.34743300	-1.19376400
H	4.08224100	-1.57152700	-0.41337100
H	4.69074000	-0.70099200	-1.03490200
C	-3.51364500	-2.08163400	-0.99722800
H	-3.13513000	-2.88588900	-1.62789600
H	-4.15184900	-1.40360900	-1.56961500
H	-4.07724600	-2.48380900	-0.15171000

Structure **2c-III- α -in** (B3LYP/6-31+G(D))

O	-0.30171400	1.71589300	0.39247500
O	-1.57155400	-1.46917900	-0.24036700
O	-3.26639400	0.08473900	0.10084200
O	3.42881200	-0.44550900	-0.33571400
O	0.28714400	-2.34479700	-1.21581300
N	-0.03032700	-0.05138900	-1.02187400
C	1.31215900	0.48452300	-0.83984500
H	1.84583500	0.59284300	-1.78752900
O	1.76571400	-0.86815700	1.13778800
C	-1.04683600	0.83352300	-0.43781100
C	-1.81844700	1.61042200	-1.50458500
H	-2.34846400	0.92665500	-2.17213100
H	-1.11973500	2.20600500	-2.10075200
H	-2.54784300	2.27472100	-1.03489800
C	-0.35899000	-1.38825500	-0.85780300
C	-1.59427400	-0.26106400	1.85783000
H	-1.90185600	0.65936400	2.36338800
H	-0.51980000	-0.39778500	1.99180100
H	-2.10748300	-1.11583400	2.30708900
C	0.97798300	1.89462100	-0.22916700
H	0.87405900	2.59152600	-1.07353700
C	2.16168400	-0.37034900	0.10556000
C	-1.92975900	-0.17893600	0.37534400
C	1.95565300	2.47282100	0.77829700
H	2.94233700	2.60368600	0.31959800
H	2.05035400	1.52565800	1.65505300
H	1.60002300	3.45366400	1.10928900
C	-4.24031800	-0.78964600	0.67807300
H	-5.18684400	-0.52542300	0.20221200
H	-4.32723100	-0.63555400	1.76012400
H	-4.00389900	-1.83750000	0.46496300
C	4.33709400	-1.21595800	0.48012800
H	5.29343300	-1.17736600	-0.04120600
H	3.97911600	-2.24478800	0.56315600
H	4.41853200	-0.77427500	1.47669200

Structure **2c-III- α -out** (B3LYP/6-31+G(D))

O	0.66591300	1.86039600	0.37714100
O	1.35051900	-0.76878900	-1.18079900
O	2.84872500	-1.01600300	0.57405000
O	-2.84809500	-1.17651200	0.73823500
O	-0.80021400	-1.40661500	-1.46903700
N	-0.11477900	-0.29753400	0.47096600
C	-1.27741600	0.57578300	0.69063900
H	-1.39634800	0.66014400	1.77766600
O	-3.40221700	0.63545900	-0.49546200
C	1.04730400	0.52954400	0.77659100
C	1.43960900	0.54360400	2.24962400
H	1.68941400	-0.45824100	2.60086700
H	0.61645300	0.94769600	2.84714600
H	2.30582000	1.19759800	2.39046500
C	0.05036500	-0.88057000	-0.79221600
C	3.01747600	0.94181700	-0.89117600
H	3.68563600	1.42522400	-0.17106000
H	2.40190200	1.70609200	-1.36650000
H	3.61800100	0.44662300	-1.65887900
C	-0.76889300	1.94378400	0.14742900
C	-2.61416400	0.02603300	0.19511000
C	2.13650500	-0.07203700	-0.17853800
C	3.81644300	-1.80626100	-0.12241500
H	4.11670700	-2.58603400	0.58028500
H	4.69686100	-1.21247300	-0.39664600
H	3.38199600	-2.26765400	-1.01557300
C	-4.05519400	-1.83792400	0.31012400

H	-4.06828500	-2.78499600	0.84936300	O	0.15201600	-1.95081500	-1.84572900
H	-4.01798300	-2.00753200	-0.76872900	N	-0.13910400	0.22862800	-1.08526900
H	-4.93101100	-1.23397400	0.56130600	C	1.18748700	0.71339100	-0.74326000
C	-1.02716500	2.26853200	-1.31930500	H	1.73887800	1.04873400	-1.62596400
H	-2.08849800	2.46212800	-1.49006900	O	1.65069000	-1.14133400	0.78566600
H	-0.45094300	3.16203500	-1.58366100	C	-1.18964400	0.95976100	-0.36512500
H	-0.71827800	1.45204700	-1.97949900	C	-1.94430200	1.91532100	-1.29342100
H	-1.14425600	2.75674400	0.77852600	H	-2.41334900	1.37404600	-2.12086500
Structure 2c-III-β-in (B3LYP/6-31+G(D))							
O	-0.14317600	1.64166400	0.67008200	H	-1.24254300	2.63839000	-1.72064600
O	-1.47713400	-1.35039600	-0.46808800	H	-2.71273500	2.46400600	-0.73993200
O	-3.15887500	0.13324300	0.13920700	C	-0.48637900	-1.09248400	-1.28627700
O	1.87567700	-1.03602800	0.69262100	C	-3.57563300	-0.04895700	0.18424800
O	0.31637900	-2.04161100	-1.68038300	H	-4.06050600	-0.98361300	0.47871900
N	0.03333000	0.18277100	-1.06783500	H	-3.94917700	0.21872500	-0.80595400
C	1.38659000	0.70008400	-0.89297100	H	-3.85424300	0.73080400	0.90036100
H	1.82633600	1.02559400	-1.83924600	C	0.82093600	1.94838800	0.16245400
O	3.55091900	-0.32822900	-0.65205000	C	0.79259600	2.83032200	-0.49528700
C	-0.93983000	0.95477200	-0.28827400	C	2.04560900	-0.33263400	-0.02151600
C	-1.72647000	1.94010300	-1.15281400	C	-2.06466700	-0.22955200	0.18352200
H	-2.29555400	1.41068600	-1.92055600	C	1.72378900	2.23454300	1.34940500
H	-1.03771100	2.62843100	-1.64720900	H	2.74400600	2.44935800	1.01214200
H	-2.42220400	2.51397000	-0.53574500	H	1.74082000	1.38606900	2.03974300
C	-0.29770900	-1.15833300	-1.12932700	H	1.34876800	3.11055700	1.88798500
C	-1.47762400	-0.50504100	1.79818500	C	-1.97316500	-1.79673400	2.01462000
H	-1.78687000	0.31578900	2.45226600	H	-1.29687600	-1.96511400	2.85450200
H	-0.40127400	-0.64963200	1.90362000	H	-1.88292600	-2.62448200	1.30403600
H	-1.98316500	-1.42632200	2.10069800	H	-3.00312300	-1.73223500	2.38905800
C	1.10705800	1.94377700	0.03291100	C	4.26721700	-1.10431200	0.22911500
H	0.97097900	2.81177400	-0.62772400	H	5.24131000	-0.84763500	-0.18748300
C	2.39306200	-0.28673100	-0.29501600	H	3.99721400	-2.13385200	-0.01833600
C	-1.82062300	-0.17921600	0.35062200	H	4.26269400	-0.97697000	1.31485900
C	2.14856500	2.28050600	1.08456500	Structure 2c-IV-α-out (B3LYP/6-31+G(D))			
H	3.11211200	2.49602600	0.61016600	O	0.84036500	1.55183400	0.81878100
H	2.27929100	1.45752000	1.79334300	O	1.28337700	-1.10789000	-1.01399000
H	1.83171800	3.16841100	1.64081100	O	-3.08894000	-0.92115600	0.49224800
C	-4.13226700	-0.82669000	0.56087400	O	-0.90531400	-1.31792500	-1.53660200
H	-5.08034000	-0.48265300	0.14281800	N	-0.22534500	-0.46837100	0.53030600
H	-4.21423800	-0.86178400	1.65381500	C	-1.26728200	0.55110300	0.73597500
H	-3.89923400	-1.82207500	0.16838300	H	-1.47938300	0.56278300	1.81231200
C	2.74642300	-2.04997000	1.23841900	O	-3.21387500	1.03183000	-0.64147500
H	2.15729000	-2.55272000	2.00531400	C	1.01378700	0.14291800	1.00975500
H	3.63954000	-1.59095800	1.66963700	C	1.28270000	-0.08691900	2.49589100
H	3.03269800	-2.75015900	0.45031300	H	1.37313100	-1.14710300	2.74267200
Structure 2c-III-β-out (B3LYP/6-31+G(D))							
O	0.55422200	1.85941100	-0.00727100	H	0.46412600	0.33758300	3.08415900
O	1.34385700	-1.01208900	-0.99351800	H	2.20138200	0.43361100	2.78449200
O	3.02705300	-0.71023000	0.57661500	C	-0.04211900	-0.98695500	-0.75815800
O	-3.24568600	-0.01199900	-0.37210700	C	-0.50823200	1.85751700	0.37679900
O	-0.75133300	-1.85816700	-0.86949600	C	-2.61107100	0.25938200	0.07168800
N	0.00405000	-0.26538200	0.66181100	C	2.09174200	-0.49293700	0.04006200
C	-1.21608500	0.54441300	0.81199300	C	-4.32531200	-1.35015800	-0.11167300
H	-1.22555500	0.88490700	1.85520500	H	-4.55023400	-2.31194600	0.34924900
O	-2.80848400	-1.08213400	1.56703600	H	-4.18703900	-1.46078400	-1.19003300
C	1.10218400	0.69156000	0.63589200	H	-5.11962800	-0.62652800	0.08897400
C	1.63148000	1.08166000	2.01090300	C	-0.49831400	2.29664600	-1.08324100
H	2.00907700	0.21154200	2.54902700	H	-1.48606200	2.65533600	-1.38255800
H	0.83425100	1.55459500	2.59254800	H	0.23215400	3.10484000	-1.19437900
H	2.44038700	1.81032000	1.89843200	H	-0.20902000	1.48477600	-1.75707900
C	0.10473700	-1.12249600	-0.44027000	H	-0.85829700	2.68099400	1.00824200
C	2.84092200	0.84485800	-1.30856000	O	2.84274800	0.54235900	-0.49220700
H	3.50396200	1.55440900	-0.80311300	C	2.92718000	-1.62397400	0.63670800
H	2.10178400	1.40373500	-1.88342400	H	3.51334200	-2.10394300	-0.15134600
H	3.43026000	0.23245700	-1.99621200	H	3.60789800	-1.24336800	1.40398000
C	-0.89684200	1.78059700	-0.08823000	H	2.28262400	-2.38990800	1.07562500
C	-2.49756900	-0.29335700	0.70263000	C	3.84177900	0.20489400	-1.45872300
C	2.14812500	-0.03558600	-0.28076800	H	4.16162500	1.15664200	-1.88715000
C	3.99217400	-1.57614000	-0.02756400	H	4.70577500	-0.28571200	-0.99384800
H	4.44242000	-2.13122000	0.79772700	H	3.42898200	-0.43018800	-2.24997800
H	4.77370300	-1.00682000	-0.54528900	Structure 2c-IV-β-in (B3LYP/6-31+G(D))			
H	3.51534900	-2.27646800	-0.72131100	O	0.35754100	1.56213200	-0.92223000
C	-4.43284500	-0.81792900	-0.53133800	O	1.65654400	-1.06935900	0.99797500
H	-4.90407300	-0.45503200	-1.44481600	O	1.39586700	-0.78668900	-1.30786900
H	-5.09599700	-0.69039600	0.32795500	O	-1.75309600	-1.11876800	-0.37726400
H	-4.15139100	-1.86894300	-0.62837600	O	-0.21698800	-1.51024100	2.22222500
C	-1.30453200	1.76182900	-1.55826600	N	0.06563700	0.48808900	1.06375800
H	-2.38219600	1.90346300	-1.66781900	C	-1.26857300	0.96119700	0.72410500
H	-0.78826900	2.58477000	-2.06492200	H	-1.73299100	1.49742700	1.55621600
H	-1.03147000	0.82453300	-2.05203200	O	-3.46177600	-0.01372800	0.60745000
H	-1.28812300	2.68703200	0.38814800	C	1.08617600	1.05596400	0.17536600
Structure 2c-IV-α-in (B3LYP/6-31+G(D))							
O	-0.50388100	1.67618900	0.63843100	C	1.87361100	2.17451500	0.86521000
O	-1.75533900	-1.27816600	-0.79006000	H	2.36978300	1.81011600	1.76989800
O	-1.54849000	-0.56372500	1.42975800	H	1.18875800	2.97545300	1.16001700
O	3.33693200	-0.19063500	-0.38714500	H	2.62269400	2.59375200	0.18629300
				C	0.40717100	-0.77358300	1.49671400
				C	3.45447300	-0.05327100	-0.22800800
				H	3.93513100	-1.03036500	-0.32426700
				H	3.84541200	0.41629000	0.67628500

H	3.72088200	0.55715900	-1.09689000	H	2.11858600	2.29228400	1.11682000
C	-0.93088300	1.97147100	-0.43825500	H	1.65273100	2.52048300	-0.58640700
H	-0.84082100	2.96766400	0.01945800	H	0.41865800	2.58185900	0.67884200
C	-2.28380100	-0.11647900	0.33119000	Structure 2d-I-β-in (B3LYP/6-31+G(D))			
C	1.94362000	-0.22211500	-0.15881100	O	-0.25232800	0.78659900	-1.64214500
C	-1.90277800	2.04223800	-1.60165600	O	-1.87446300	-0.08390400	1.39732600
H	-2.89703300	2.34008300	-1.25184900	O	-2.44726100	-0.47768300	-0.82734500
H	-1.97641400	1.07612500	-2.10949500	O	2.77505400	0.45686000	0.77287300
H	-1.55240300	2.78597500	-2.32429500	O	-0.32395300	-1.53071000	2.22291900
C	1.88024000	-2.07128700	-1.70274600	N	0.14872100	-0.08824200	0.44626200
H	1.19061200	-2.41686600	-2.47562300	C	1.09385400	-0.76018700	-0.45324100
H	1.87220800	-2.77575900	-0.86394300	O	3.29632500	-0.22473700	-1.31546800
H	2.88887100	-2.00948100	-2.13059700	C	-0.61258600	0.93919900	-0.28483900
C	-2.65126400	-2.19207300	-0.72398600	C	-0.24746900	2.35783800	0.14509700
H	-2.04504200	-2.90315000	-1.28478100	H	-0.47792600	2.52138700	1.20216200
H	-3.47561100	-1.81500200	-1.33472000	H	-0.78892200	3.09207600	-0.45976500
H	-3.04617400	-2.65228100	0.18494500	H	0.82477400	2.50689500	-0.00268600
Structure 2c-IV-β-out (B3LYP/6-31+G(D))				C	-0.62646100	-0.67777000	1.42332900
O	-0.73488100	0.57825900	1.63443600	C	-3.11822900	1.61875100	0.23506300
O	-1.32405500	-0.88754100	-1.19846900	H	-3.29642900	2.08894100	-0.73735300
O	3.16404800	-0.54673800	0.32623600	H	-2.79060300	2.37776600	0.94751100
O	0.86235900	-1.11542100	-1.72929600	H	-4.06040500	1.20489600	0.60453600
N	0.09493200	0.71777100	-0.50517300	C	0.42132400	-0.46535700	-1.81933400
C	1.23324800	0.89593500	0.41317500	C	2.50274400	-0.13254000	-0.39990300
H	1.32225800	1.97453400	0.57936100	C	-2.08100600	0.51877500	0.08975700
O	3.06941100	1.20109000	-1.10023500	C	-3.68204800	-1.16144700	-0.59418200
C	-1.09702200	0.96260600	0.30218300	H	-3.66865200	-2.02804200	-1.25846500
C	-1.52879300	2.42715100	0.34779300	H	-4.54262200	-0.53151100	-0.85026500
H	-1.76479800	2.82150800	-0.64310500	H	-3.75953900	-1.49917500	0.44491100
H	-0.72593100	3.03208800	0.77858800	C	4.11229000	0.97686700	0.92124500
H	-2.40396500	2.52785200	0.99755100	H	4.14326600	1.40357500	1.92370400
C	-0.02576200	-0.49812800	-1.19024800	H	4.30740900	1.74196000	0.16536600
C	0.67967200	0.26197800	1.72436300	H	4.84394300	0.17125300	0.81902100
C	2.57667200	0.52294900	-0.22604700	H	1.14014800	-0.34812100	-2.63115900
C	-2.14945400	-0.01269100	-0.36368200	H	-0.30129800	-1.25413400	-2.05385600
C	4.40813800	-0.95502600	-0.28102700	C	1.25635200	-2.26821400	-0.20401100
H	4.73362200	-1.82439400	0.29034200	H	1.91346700	-2.67969400	-0.97640500
H	5.14324100	-0.14866700	-0.21891800	H	1.68662900	-2.46796500	0.77962900
H	4.23533000	-1.21801100	-1.32716000	H	0.28613700	-2.76930000	-0.25988000
C	0.85124900	-1.23541200	1.96134400	Structure 2d-I-β-out (B3LYP/6-31+G(D))			
H	1.88148600	-1.47061700	2.23909300	O	-0.65235400	-0.65575900	1.62654200
H	0.18489800	-1.52478800	2.78074800	O	-1.87841900	1.04652600	-0.82036500
H	0.58841400	-1.83065600	1.08214500	O	2.74705600	-0.09357900	-1.07995800
H	1.06084100	0.81579900	2.58983300	O	-0.18166100	2.52138600	-1.01097200
O	-2.74038800	-0.75311500	0.64715700	N	0.17626400	0.34132800	-0.24257600
C	-3.14395800	0.65219600	-1.31348000	C	1.27827500	0.47326500	0.72989600
H	-3.70526600	-0.11349500	-1.85521000	O	3.32647500	-0.81261000	0.98026000
H	-3.84559000	1.28572200	-0.76274600	C	-0.69283300	-0.74699900	0.20579900
H	-2.61860200	1.25846800	-2.05576400	C	-0.21524500	-2.13564600	-0.22682500
C	-3.69127300	-1.75116500	0.26528900	H	-0.11059700	-2.21562700	-1.31138900
H	-3.88610900	-2.32608500	1.17259400	H	-0.92331600	-2.89148500	0.12700500
H	-4.63069800	-1.30444900	-0.08276300	H	0.75556000	-2.35790400	0.22585900
H	-3.28192000	-2.41384900	-0.50498400	C	-0.57346700	1.42128600	-0.70185400
Structure 2d-I-α-in (B3LYP/6-31+G(D))				C	0.67397200	-0.25475300	1.98506600
O	-0.10713800	-1.19242200	1.25093000	C	2.55147100	-0.24144200	0.23760700
O	-2.12223800	0.46380800	-1.16110300	C	-2.09724800	-0.32030500	-0.36826400
O	-2.30752400	0.29621700	1.15568700	C	3.97392300	-0.64107000	-1.60397300
O	3.45024900	0.15935300	0.63132800	H	3.95724000	-0.41065700	-2.66912600
O	-0.62406000	2.02725000	-1.85925800	H	4.00732100	-1.72139200	-1.44037200
N	0.02116100	0.16985200	-0.59662900	H	4.83444400	-0.17368800	-1.11836400
C	1.13430600	0.57416400	0.26618400	H	1.28505900	-1.11521300	2.27493100
O	2.55119100	-0.78832800	-1.21065800	O	-3.00454800	-0.33762500	0.68089200
C	-0.68578100	-0.98959800	-0.02480900	C	-2.56511300	-1.09888600	-1.59770900
C	-0.49486100	-2.26335900	-0.84219600	H	-2.80757400	-2.13324200	-1.33676500
H	-0.91156200	-2.14967800	-1.84757300	H	-3.45408100	-0.62077100	-2.01722600
H	-0.98100200	-3.10930100	-0.34548600	H	-1.79621700	-1.09395800	-2.37460000
H	0.57354700	-2.46562100	-0.93591800	C	-4.32864500	0.13120600	0.41459500
C	-0.85522400	1.00809400	-1.25406900	H	-4.89493100	-0.57808100	-0.20190100
C	-3.28388600	-1.44165700	-0.25885100	H	-4.80728100	0.21274000	1.39235200
H	-3.34310300	-2.13426600	0.58685500	H	-4.31035000	1.11540600	-0.06574100
H	-3.12326000	-2.00866400	-1.17724800	H	0.58653500	0.42372900	2.83710000
H	-4.24003500	-0.92016600	-0.35572100	C	1.69463500	1.91766000	1.06968400
C	0.65506400	-0.03954600	1.61499900	H	2.07853600	2.44727600	0.19663400
C	2.43407100	-0.10663700	-0.21774700	H	0.84323700	2.47835300	1.46414800
C	-2.16136700	-0.44527800	-0.02744300	H	2.47181200	1.87260800	1.84016100
C	-3.51650100	1.04411400	1.31494900	Structure 2d-I-α-out (B3LYP/6-31+G(D))			
H	-3.33869900	1.71635500	2.15702500	O	0.69619600	1.30881400	1.34394200
H	-4.36262500	0.38928300	1.55643200	O	1.76274100	-0.78461700	-1.26861000
H	-3.74154300	1.63329000	0.41927800	O	-3.42228500	-0.67451300	0.14743000
C	4.72684200	-0.41885700	0.29102300	O	-0.14651100	-2.01247800	-1.49017700
H	5.40843900	-0.09425600	1.07742900	N	-0.10462200	0.02477900	-0.36014600
H	5.05837700	-0.05488500	-0.68474600	C	-1.15719900	-0.04247400	0.66765000
H	4.65383800	-1.50920600	0.26630200	O	-2.72041200	1.33977700	-0.58515400
H	1.47034600	-0.36860100	2.26187200	C	0.92997700	1.01000900	-0.01685600
H	0.02489200	0.68637600	2.14075100	C	0.82427200	2.26671600	-0.88170400
C	1.34574200	2.09168400	0.37004200				

H	0.95843300	2.02715800	-1.94129200	H	2.64613800	1.91849700	1.36415900
H	1.57524900	3.00366000	-0.57943400	H	2.00910300	2.52987800	-0.18470200
H	-0.17173800	2.70179600	-0.76461300	H	0.97463800	2.51593400	1.24728000
C	0.42115800	-1.03436900	-1.06347800	C	-2.55215100	0.13015400	1.64655100
C	-0.70561400	1.15475200	1.57229100	H	-3.49217900	0.68839000	1.66313100
C	-2.51006200	0.29751200	0.00146300	H	-2.66224200	-0.79535600	2.21850800
C	2.23052400	0.16054400	-0.25730300	H	-1.79275900	0.74931800	2.13110900
C	-4.69702300	-0.44672200	-0.48865400	O	-3.03921900	-1.03811500	-0.44011100
H	-5.29277500	-1.33040400	-0.26055300	C	-4.40974800	-0.63489000	-0.51451600
H	-4.56136900	-0.33717800	-1.56736300	H	-4.87970200	-1.32971100	-1.21329400
H	-5.16492100	0.45513600	-0.08573200	H	-4.90715500	-0.71689700	0.45953400
H	-1.24468200	2.07022500	1.30386500	H	-4.49973800	0.38656700	-0.89865000
O	2.48766900	-0.52773700	0.93049500	Structure 2d-II-α-out (B3LYP/6-31+G(D))			
C	3.44397300	0.87893300	-0.82405500	O	-0.31911900	-0.73102500	1.68843000
H	3.84334500	1.57583000	-0.08011100	O	-2.07608800	1.20060300	-0.18221800
H	4.22199800	0.15632900	-1.08425100	O	-2.82275900	-0.88835700	-0.84949700
H	3.18839600	1.42927300	-1.73096000	O	3.57834300	-0.28115500	0.16732200
C	3.53676100	-1.49960200	0.90875700	O	-0.43844800	2.60249600	-0.85613900
H	4.52473400	-1.02297800	0.89992300	N	0.02280400	0.39189100	-0.25551500
H	3.42729800	-2.06832800	1.83443600	C	1.33536700	0.45578600	0.40619800
H	3.43796700	-2.17524300	0.05208800	O	2.27004300	-0.47703400	-1.66553000
H	-0.84418000	0.93871600	2.63368200	C	-0.75301600	-0.70302100	0.31984100
C	-1.14914300	-1.36687400	1.44076200	C	-0.50848100	-2.05793600	-0.34104000
H	-1.34252500	-2.21614100	0.78329400	H	-0.72883300	-2.01464300	-1.40778000
H	-0.16952600	-1.49464800	1.91222800	H	-1.14570000	-2.81454400	0.12603100
H	-1.91826200	-1.35116800	2.21916100	H	0.53539500	-2.35784400	-0.21541000
Structure 2d-I-β-out' (B3LYP/6-31+G(D))				C	-0.77468800	1.50852300	-0.47148400
O	-0.55967500	0.47089600	-1.82162800	C	-3.03289200	-0.22851700	1.49900200
O	-1.74152700	0.03927300	1.46408200	H	-3.98393600	0.29397200	1.36540400
O	2.73900300	0.73602800	0.60685200	H	-2.48084200	0.25532100	2.30594000
O	0.01318200	-1.17168500	2.27568300	H	-3.23007100	-1.26749100	1.78163200
N	0.16207800	0.05759400	0.30256300	C	1.08102900	-0.45987000	1.67042900
C	1.13234900	-0.63758100	-0.54873700	C	2.41364700	-0.15418700	-0.50946300
O	3.52486100	-0.96995500	-0.64535700	C	-2.22867300	-0.18395900	0.20698300
C	-0.76209900	0.88304400	-0.48379300	C	-4.13325000	-0.47922600	-1.24902100
C	-0.46930300	2.37672400	-0.32722600	H	-4.33008400	-1.00574600	-2.18506000
H	-0.55646600	2.68798200	0.71834400	H	-4.17446700	0.60109500	-1.42222200
H	-1.15597000	2.96897900	-0.94018500	H	-4.88867200	-0.77099300	-0.50905000
H	0.55492200	2.58086600	-0.65142800	C	4.68867700	-0.81938100	-0.57927700
C	-0.45059100	-0.45170600	1.42323100	H	5.52435400	-0.83764000	0.12051000
C	0.79414000	0.03433900	-1.92657200	H	4.91319600	-0.17838700	-1.43549500
C	2.59536500	-0.33098900	-0.19327600	H	4.45561100	-1.82737300	-0.93208600
C	-2.14199700	0.42924400	0.11573600	H	1.65675500	-1.39145300	1.61890900
C	4.09568100	1.07797800	0.95811800	H	1.33111000	0.05823900	2.59882300
H	4.01107400	1.94191200	1.61729000	C	1.77738500	1.86839500	0.83318400
H	4.66977900	1.32546600	0.06128200	H	1.92249600	2.52672800	-0.02485800
H	4.57129100	0.24111700	1.47522700	H	1.02242100	2.31965100	1.48399500
H	1.45914700	0.88509700	-2.13114000	H	2.71523400	1.78400700	1.38826300
O	-2.53414400	-0.70568500	-0.59819600	Structure 2d-II-β-in (B3LYP/6-31+G(D))			
C	-3.23406100	1.47838500	0.24352400	O	-0.25807100	-0.55067700	1.77697100
H	-3.75653800	1.78085600	-0.75135900	O	-1.90587700	0.84157400	-0.97875300
H	-4.08273800	1.07131200	0.79956200	O	2.62927200	-0.57963100	-1.05900000
H	-2.87705600	2.35668200	0.78415900	O	-0.20492100	2.09881600	-1.78797600
C	-3.67534300	-1.42055200	-0.11548200	N	0.16537400	0.33685300	-0.30246900
H	-4.60692000	-0.88418500	-0.33430500	C	1.33256100	0.69421600	0.51001300
H	-3.67681100	-2.36789900	-0.65830200	O	3.34491100	-0.54723700	1.08285500
H	-3.59724400	-1.61596200	0.95941700	C	-0.66158900	-0.63918900	0.40785400
H	0.85741300	-0.67609000	-2.75235200	C	-0.44201000	-2.07597100	-0.05687700
C	0.91082200	-2.15791600	-0.59890900	H	-0.71342300	-2.19294600	-1.10858700
H	1.02004500	-2.60338400	0.39294500	H	-1.05101400	-2.75909000	0.54052800
H	-0.09814400	-2.36090100	-0.97073700	H	0.61188000	-2.33570700	0.07583500
H	1.64629000	-2.61180500	-1.26753900	C	-0.58870500	1.19237500	-1.08648200
Structure 2d-II-α-in (B3LYP/6-31+G(D))				C	0.76080300	0.44408800	1.92831000
O	-0.09094700	-1.17869600	1.27824900	C	2.53684400	-0.23325900	0.23166200
O	-2.08947400	1.07959900	-0.52816000	C	-2.11308900	-0.09217300	0.12960100
O	3.50993300	-0.37057500	0.38334600	C	3.78160700	-1.36688100	-1.42361900
O	-0.49592200	2.60406800	-1.04537800	H	3.68751500	-1.53017700	-2.49702000
N	0.04699100	0.44517100	-0.34364000	H	3.77602000	-2.31722400	-0.88357300
C	1.30733300	0.53973400	0.39357000	H	4.70037700	-0.82231800	-1.19119200
O	2.39734600	-0.43170800	-1.58192100	H	1.51032500	0.06828900	2.62656000
C	-0.69483400	-0.75493500	0.05032500	H	0.32502100	1.37513800	2.31657500
C	-0.59035900	-1.90152700	-0.94974000	C	1.83237800	2.13806600	0.33531600
H	-1.03070700	-1.61977900	-1.90891500	H	2.64503100	2.31072800	1.04867200
H	-1.11964400	-2.77776600	-0.56641700	H	2.19644400	2.31526700	-0.67823800
H	0.46198100	-2.14853600	-1.10245300	H	1.02970800	2.85231300	0.53621300
C	-0.79369600	1.49388600	-0.67183400	C	-2.71752100	0.68843200	1.29092100
C	0.91868600	-0.24882600	1.67608800	H	-3.63403100	1.19017500	0.96891800
C	2.43573800	-0.15256000	-0.40605200	H	-2.93673000	0.01637800	2.12520900
C	-2.15508200	-0.18432200	0.20834200	H	-2.02307000	1.45696300	1.64022100
C	4.95664000	-0.95640800	-0.26196700	O	-2.90481100	-1.14615700	-0.31218200
H	5.41584100	-1.04076100	0.51860400	C	-4.24309200	-0.84140500	-0.71580200
H	5.00726200	-0.31062000	-1.07225500	H	-4.61666500	-1.74916000	-1.19368700
H	4.40611500	-1.94030200	-0.66464600	H	-4.87867700	-0.60367300	0.14564100
H	1.74622200	-0.80954600	2.11370800	H	-4.25948400	-0.01622700	-1.43548700
O	0.52236700	0.45371900	2.42311200				
C	1.76308200	1.97165800	0.72081700				

Structure **2d-II- β -out** (B3LYP/6-31+G(D))

O	-0.46975200	-1.13669200	-1.57781300
O	-1.95371600	-0.51984300	1.13795500
O	-2.57226400	1.34950600	-0.08415200
O	2.53900600	1.14362400	0.67369700
O	-0.23735600	-0.91313600	2.55269000
N	0.13153100	-0.14130900	0.37518100
C	1.37043800	-0.81700200	-0.05734100
O	3.34944200	0.08221400	-1.14682400
C	-0.71795200	0.03968100	-0.79952100
C	-0.39355800	1.29098500	-1.61328000
H	-0.47967500	2.18935200	-1.00091700
H	-1.08529700	1.36967200	-2.45724400
H	0.62230200	1.22551800	-2.01551200
C	-0.62534100	-0.56323400	1.46448000
C	-3.15477400	-0.88222700	-0.91335200
H	-4.07738500	-0.96317600	-0.33229600
H	-2.73685800	-1.88115000	-1.04504500
H	-3.38665900	-0.46432800	-1.89820300
C	0.92168800	-1.44540200	-1.42816700
C	2.51786300	0.19045100	-0.26602400
C	-2.15901500	0.01221900	-0.19001200
C	-3.80575700	1.59549700	0.59626800
H	-3.85159700	2.67751400	0.73528900
H	-3.82389000	1.10068500	1.57286800
H	-4.66646800	1.27534500	-0.00363600
C	3.64009800	2.07275400	0.61133900
H	3.48721400	2.75252300	1.44935400
H	3.62411900	2.61541700	-0.33735300
H	4.58986100	1.54064100	0.70970600
H	1.50778200	-1.04049200	-2.25824600
H	1.01358300	-2.53395600	-1.42079700
C	1.90389400	-1.89615000	0.90383200
H	2.17547500	-1.47822300	1.87426300
H	1.15189500	-2.67354300	1.06397000
H	2.78649600	-2.35344800	0.44378000

Structure **2d-III- α -in** (B3LYP/6-31+G(D))

O	0.43815800	1.27792000	-1.37481700
O	1.44076700	-1.20281200	0.82629600
O	3.27003200	0.00443600	0.05615900
O	-3.43064400	-0.28706500	-0.00025000
O	-0.55060500	-1.45980700	1.89078900
N	-0.04120300	0.46795800	0.70264400
C	-1.34613200	0.90117100	0.18389900
O	-1.64259800	-1.18176200	-1.04325200
C	1.06285400	0.93592500	-0.14035300
C	1.77724900	2.15007600	0.45258800
H	2.20465800	1.91043600	1.42911700
H	1.06186600	2.96966100	0.57633700
H	2.58203000	2.47664600	-0.21062300
C	0.19689400	-0.80089300	1.20475400
C	1.80686400	-1.11391300	-1.56166600
H	2.23954300	-0.53970300	-2.38667800
H	0.74958100	-1.28795400	-1.76814500
H	2.30900800	-2.08246400	-1.48649000
C	-0.87239200	1.73490400	-1.06085200
C	-2.13426700	-0.32217600	-0.34221300
C	1.96159400	-0.34988900	-0.25438800
C	4.24237700	-1.04398600	0.09321300
H	5.13907500	-0.59436100	0.52439900
H	4.47383400	-1.41244600	-0.91308900
H	3.90623000	-1.87046500	0.72823600
C	-4.23241400	-1.39535300	-0.46263700
H	-5.23601200	-1.19865200	-0.08572000
H	-3.83937600	-2.33073200	-0.05769500
H	-4.22653300	-1.43690600	-1.55476800
H	-1.49735800	1.58548200	-1.94385200
H	-0.86580800	2.80329200	-0.80370000
C	-2.12507300	1.74610800	1.19539200
H	-3.03147100	2.16451400	0.74618700
H	-2.41621400	1.14150400	2.05801700
H	-1.49084200	2.56731800	1.54413200

Structure **2d-III- β -in** (B3LYP/6-31+G(D))

O	0.26314100	1.02159400	-1.56314000
O	1.33581000	-1.04177800	0.95385000
O	3.15243900	0.12503200	0.09996700
O	-1.79889900	-1.24628000	-0.66334200
O	-0.61915400	-1.12610100	2.10431400
N	-0.13943300	0.61146700	0.64048100
C	-1.45954200	0.99702600	0.11547700
O	-3.57773000	-0.19752700	0.25220000
C	0.92863700	0.94095800	-0.30321900
C	1.61740300	2.26646300	0.02116200
H	2.07065000	2.23633100	1.01431900
H	0.88119100	3.07598100	-0.00287300
H	2.39819600	2.47616800	-0.71417000

C	0.10661100	-0.57223000	1.31111800
C	1.80166100	-1.25411200	-1.40462100
H	2.25464600	-0.77774200	-2.27939800
H	0.76217700	-1.49156300	-1.63590700
H	2.33021600	-2.18464000	-1.17980100
C	-1.04299900	1.52940400	-1.30577400
C	-2.40634200	-0.21157000	-0.05506100
C	1.86818800	-0.31893000	-0.20423700
C	4.15011000	-0.87039500	0.34422000
H	5.01179400	-0.32820100	0.73857600
H	4.44184000	-1.38232800	-0.58061900
H	3.80624200	-1.59901200	1.08577400
C	-2.59401800	-2.44110700	-0.81413400
H	-1.94527800	-3.15712200	-1.31870100
H	-3.48339900	-2.23136000	-1.41362500
H	-2.88922500	-2.81270900	0.16988100
H	-1.69849800	-1.17993600	-2.10623400
H	-1.04267800	2.62783900	-1.30077500
C	-2.14239200	2.06915600	0.96702000
H	-3.05966700	2.42089200	0.48463800
H	-2.40847700	1.66465500	1.94683900
H	-1.46244900	2.91510100	1.10620600

Structure **2d-III- α -out** (B3LYP/6-31+G(D))

O	-0.74320800	1.73864800	0.99060800
O	-1.36546500	-1.35363100	-0.62475700
O	3.38296300	-0.22581500	-0.30052800
O	0.75199300	-1.78822800	-1.32268000
N	0.10443800	0.33181900	-0.61626000
C	1.29591600	0.92620200	0.02002100
O	2.05077600	-0.95463700	1.36760700
C	-1.13143400	0.95066500	-0.12643700
C	-1.79470000	1.86524400	-1.15322100
H	-2.09937300	1.30139000	-2.03857600
H	-1.08373800	2.64194800	-1.44735600
H	-2.68073400	2.33590700	-0.71993600
C	-0.07247300	-1.01533000	-0.89135400
C	0.64293000	1.54153400	1.29695600
C	2.27349300	-0.20003000	0.44298800
C	-1.99196100	-0.32069300	0.22034000
C	4.28789100	-1.32018800	-0.03955600
H	5.11343300	-1.18021900	-0.73718000
H	3.77549400	-2.26706500	-0.22396900
H	4.63921000	-1.28220700	0.99458300
H	1.06762300	2.51808900	1.54723700
H	0.74989500	0.86218900	2.14697600
C	1.94397400	1.98519000	-0.88019100
H	2.25638800	1.54697700	-1.83072300
H	1.22744700	2.78788100	-1.08071900
H	2.82250300	2.42195700	-0.39318700
O	-3.29245600	-0.11623300	-0.21465400
C	-4.21720900	-1.19781500	-0.06498700
H	-4.49771100	-1.34366200	0.98485300
H	-5.10215200	-0.90477400	-0.63323600
H	-3.80805200	-2.12575800	-0.47817900
C	-1.87826200	-0.77458400	1.67061100
H	-2.35699300	-0.04585300	2.33113700
H	-2.35102400	-1.75229900	1.79750800
H	-0.82909100	-0.87923500	1.95880500

Structure **2d-III- β -out** (B3LYP/6-31+G(D))

O	-0.54525300	1.48027200	1.35821700
O	-1.32248100	-1.13298200	-0.89135100
O	2.05816000	-1.18842600	0.69798400
O	0.70965100	-1.33644900	-1.88484400
N	0.14466300	0.52899500	-0.61372200
C	1.39087000	1.00793000	0.00599700
O	3.58319300	0.03769400	-0.43177500
C	-1.03589400	0.99536800	0.11375700
C	-1.77436100	2.13038600	-0.59181400
H	-2.15460200	1.80387100	-1.56298800
H	-1.08532400	2.96641700	-0.73709600
H	-2.61803900	2.46473300	0.01699400
C	-0.06091100	-0.70932600	-1.19532900
C	0.87527300	1.31796500	1.45182100
C	2.47572200	-0.09364200	0.03726800
C	-1.87943000	-0.33074700	0.20981100
C	2.94980300	-2.32317500	0.66209200
H	2.45319600	-3.09765900	1.24654600
H	3.91470500	-2.05997500	1.10207400
H	3.08551700	-2.64562400	-0.37271200
H	1.29641200	2.25045200	1.83944100
H	1.10614200	0.50077000	2.14163100
C	1.94186400	2.24886200	-0.70385000
H	2.17866700	2.01656800	-1.74522900
H	1.20274500	3.05497700	-0.67775200
H	2.85716700	2.59448500	-0.21400800
O	-3.20602500	-0.04084600	-0.07489300

C	-4.12237000	-1.13779900	-0.14290600	H	3.04307900	-2.14822300	0.30863900
H	-4.32837400	-1.55157900	0.85141400	H	2.29750700	-1.62093400	1.83364500
H	-5.04425500	-0.72177500	-0.55387800	H	1.54444000	-2.92087700	0.89093500
H	-3.74708600	-1.92284000	-0.80771600	H	0.89148300	-2.52039400	-1.43232100
C	-1.67506900	-1.10651900	1.50517800	Structure 2d-IV-β-in (B3LYP/6-31+G(D))			
H	-2.11890800	-0.56202100	2.34347200	O	0.83856100	1.39730400	-1.40593900
H	-2.13228300	-2.09662000	1.42586100	O	1.39428500	-0.82198700	1.30999600
H	-0.60926500	-1.24707100	1.70116600	O	-1.96424700	-1.19830100	-0.49420600
Structure 2d-IV-α-in (B3LYP/6-31+G(D))				O	-0.72302100	-0.87958700	2.14397900
O	-0.98095000	1.53036600	1.21035900	N	-0.04482600	0.74256400	0.61149100
O	-1.42135100	-0.99427600	-1.24475500	C	-1.20494900	1.06393500	-0.24913500
O	3.23876900	-0.03537200	-0.28851100	O	-3.46032700	0.31179200	0.26692400
O	0.76789900	-1.31301100	-1.77753700	C	1.21427700	1.04829600	-0.09132300
N	0.04690800	0.57267600	-0.60982700	C	1.95558600	2.23435200	0.52104800
C	1.13367400	0.92463700	0.33697100	H	2.23197800	2.03303800	1.56039500
O	1.97573900	-1.20752300	1.16763900	H	1.30441300	3.11116200	0.49938000
C	-1.25187900	1.03732000	-0.08321700	H	2.85993400	2.45820700	-0.05354400
C	-1.84833100	2.17311600	-0.91094300	C	0.09581000	-0.37227300	1.41548100
H	-2.03717000	1.85401800	-1.94039600	C	-0.51278900	0.98279300	-1.64505000
H	-1.14510200	3.00910000	-0.93053900	C	-2.34350900	0.03014200	-0.10750600
H	-2.78653800	2.51833700	-0.46521900	C	1.97509700	-0.32161600	0.07098500
C	-0.09021500	-0.64762900	-1.24796400	C	-2.92382600	-2.25110300	-0.26710100
C	0.30191500	1.05555200	1.64339500	H	-2.44756100	-3.15844300	-0.63857700
C	2.14644300	-0.23857600	0.45817400	H	-3.84892900	-2.04502800	-0.81112900
C	-2.08687600	-0.29849900	-0.15002600	H	-3.13017100	-2.33164000	0.80266600
C	4.17785800	-1.12929100	-0.33578200	H	-0.94280600	1.68045800	-2.36831400
H	4.98101300	-0.78845900	-0.98914100	O	1.56529200	-1.12353800	-1.00037600
H	3.68617300	-2.01272300	-0.74964300	C	3.48387900	-0.27970100	-0.24871500
H	4.55613000	-1.34880800	0.66585200	H	3.86601300	-1.28126300	0.46434600
H	0.70623000	1.80341300	2.33065600	H	3.95399400	0.08572600	-0.66992300
O	-1.83968200	-0.96883900	1.05127400	H	3.76797900	0.36698000	1.08068300
C	-3.56380000	-0.19763900	-0.49274800	C	1.93941500	-2.50330500	-0.97074100
H	-3.99207400	-1.19717600	-0.60679200	H	1.34824300	-2.98422300	-1.75263900
H	-4.09391600	0.32193500	0.31178000	H	3.00436400	-2.63553000	-1.19843000
H	-3.71873900	0.33723300	-1.43149900	H	1.70347100	-2.95759900	-0.00257800
C	-2.27921400	-2.32674800	1.15579300	H	-0.53022300	-0.03714500	-2.03416500
H	-1.80164300	-2.71898800	2.05549000	C	-1.74459000	2.46489000	0.05610500
H	-3.36841700	-2.38674400	1.27207800	H	-2.08490200	2.52494600	1.09283200
H	-1.95974400	-2.91372300	0.28860600	H	-0.96065200	3.21019900	-0.10782300
H	0.20910000	0.08706700	2.13765800	H	-2.59210500	2.69827800	-0.59550700
C	1.79873100	2.24766900	-0.06522900	Structure 2d-IV-β-out (B3LYP/6-31+G(D))			
H	2.21317200	2.18416000	-1.07357500	O	-0.45287900	-0.96807700	-1.61396600
H	1.06098000	3.05551600	-0.03364400	O	-1.49858000	0.50579000	1.37535200
H	2.60895900	2.49687600	0.62882700	O	-1.73424700	1.14265600	-0.85965000
Structure 2d-IV-α-out (B3LYP/6-31+G(D))				O	1.54571600	1.37370500	-0.45324800
O	-0.43556500	-0.92136100	-1.64810700	O	0.55778500	0.64830700	2.34989800
O	-1.76580100	0.51603600	1.27819200	N	0.12553600	-0.79530100	0.58089000
O	-1.49960200	1.33857700	-0.90299900	C	1.41689800	-0.99172600	-0.08574400
O	3.23091100	0.26452600	-0.40011700	O	3.47589700	0.29853200	0.01101300
O	0.06774400	0.34175000	2.62096300	C	-1.00111900	-1.06590800	-0.31325200
N	-0.11148900	-0.82833700	0.61269900	C	-1.58901000	-2.46232100	-0.08800400
C	1.23601000	-0.95145600	0.05868100	H	-1.92279400	-2.59188300	0.94597000
O	1.42335000	1.49791100	0.15851800	H	-0.82331800	-3.21749600	-0.28989300
C	-1.14397800	-0.96679500	-0.42337400	H	-2.43085500	-2.63873900	-0.76453900
C	-1.89661200	-2.29384800	-0.29281200	C	-0.17140800	0.17433900	1.51039700
H	-2.37701400	-2.38141500	0.68671200	C	-3.45806800	-0.21766700	0.19583500
H	-1.19158800	-3.12433200	-0.39664000	H	-3.99878900	0.64749700	0.58831300
H	-2.65590100	-2.38396000	-1.07583400	H	-3.61301100	-1.04362900	0.89209900
C	-0.50863200	0.05549500	1.60064100	H	-3.87900200	-0.48254400	-0.77938600
C	-3.53808000	0.15609600	-0.30186900	C	0.91699700	-1.35420400	-1.53434100
H	-4.03539600	1.07093400	0.03141500	C	2.27240300	0.29338900	-0.14042700
H	-3.92828000	-0.66855300	0.29772800	C	-1.98035100	0.11885400	0.05042000
H	-3.78394200	-0.01181400	-1.35529100	C	-2.37529000	2.39770900	-0.62439800
C	0.87343800	-1.42129100	-1.38859900	H	-1.89373900	3.10178000	-1.30612100
C	1.94020200	0.42282500	-0.03015600	H	-2.23046500	2.73150100	0.40879100
C	-2.03111400	0.30183500	-0.14330200	H	-3.44658100	2.35578700	-0.85835800
C	-1.90226500	2.67108400	-0.58022100	C	2.26107700	2.62361100	-0.50497000
H	-1.23891800	3.31953500	-1.15518100	H	1.51347700	3.37024900	-0.77221100
H	-1.77430700	2.87565800	0.48719400	H	3.05186400	2.57761500	-1.25831200
H	-2.94110700	2.86346500	-0.87872600	H	2.69596500	2.84279200	0.47324300
C	3.99027100	1.48076000	-0.55752600	H	1.45557000	-0.82137400	-2.32111900
H	4.99272800	1.15912400	-0.84067500	C	2.23449800	-2.12184900	0.54757400
H	4.01135700	2.03606400	0.38344500	H	3.13737000	-2.32197300	-0.03705100
H	3.54739900	2.10503900	-1.33804300	H	2.54037000	-1.84795200	1.56071800
H	1.54437400	-1.02487600	-2.15257600	H	1.62810400	-3.03178700	0.59568800
C	2.09179500	-1.97563500	0.81938400	H	1.02777400	-2.43540600	-1.69779100