SUPPORTING INFORMATION

A unique and stable Polyproline I helix sorted out from conformational equilibrium by solvent polarity

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KEYWORDS "Polyproline I, foldamers, proline mimetic, conformational studies"

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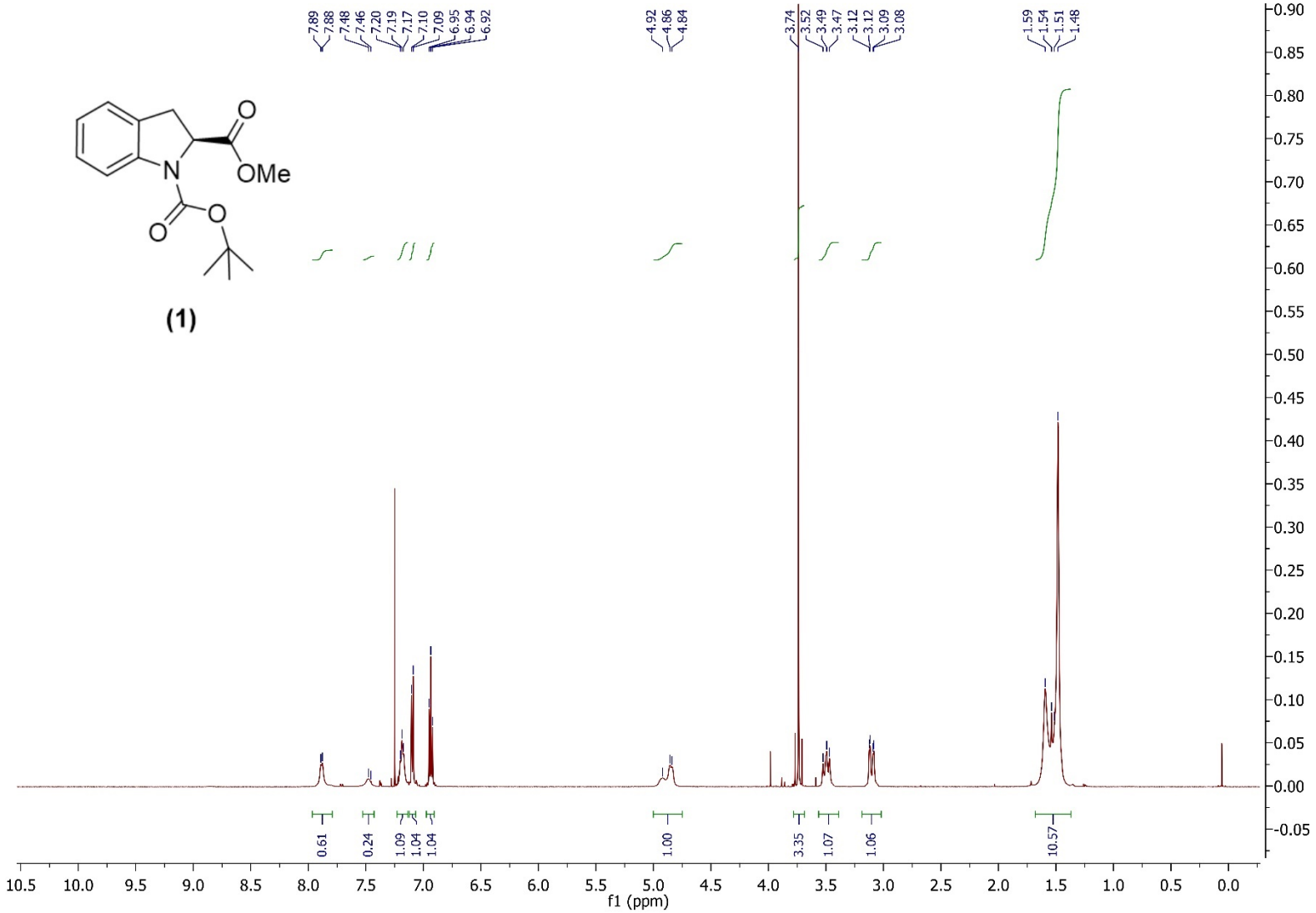
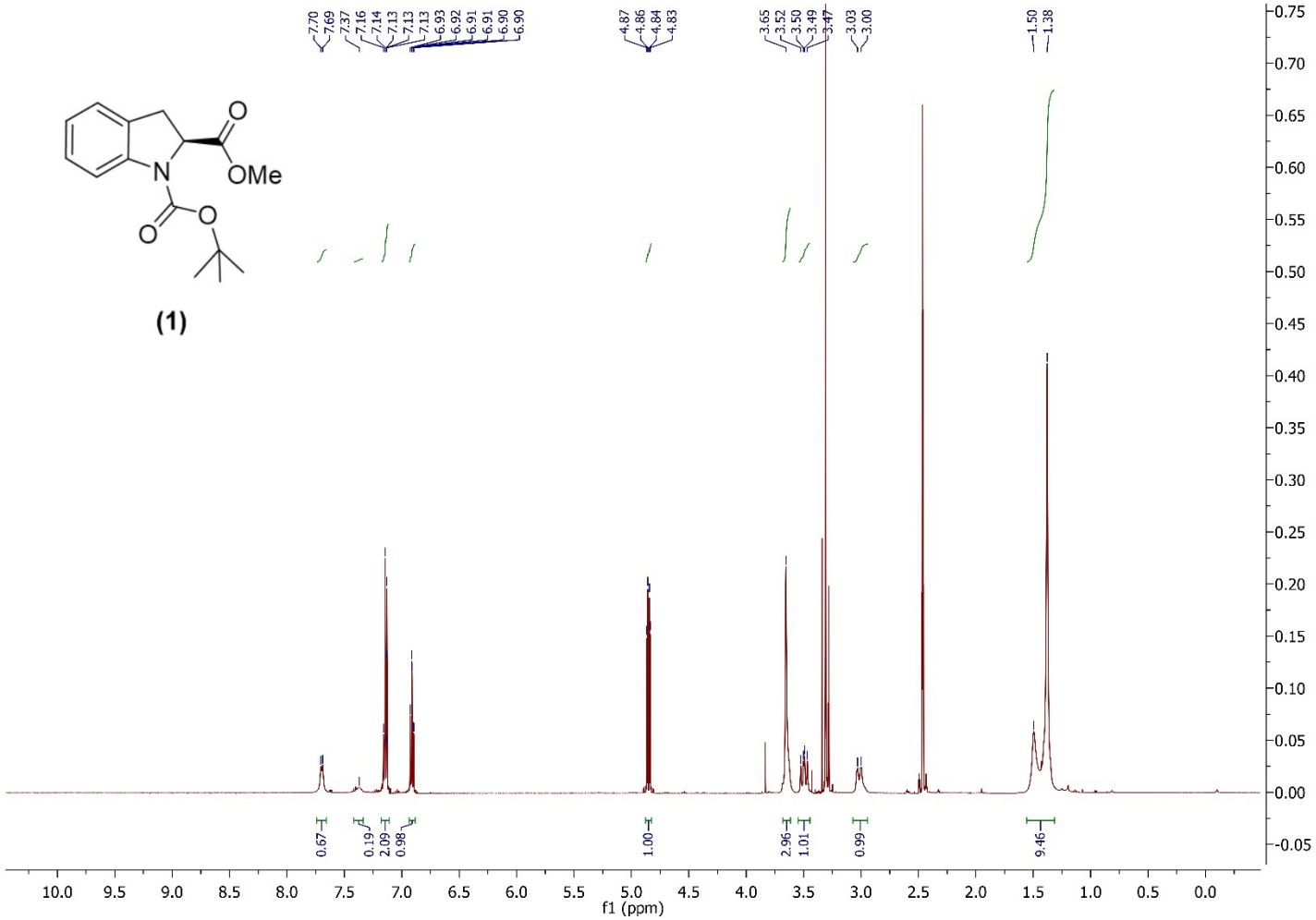
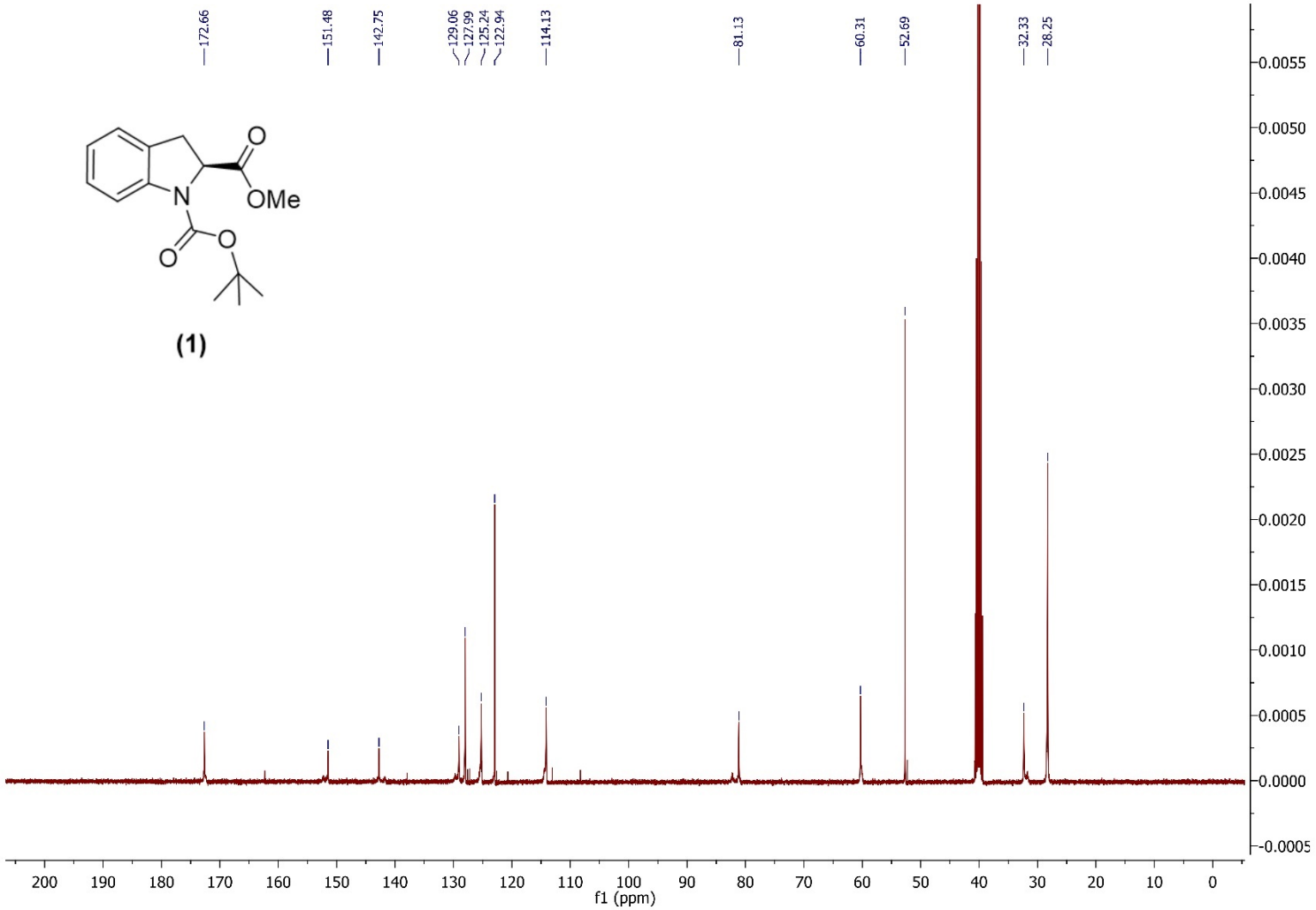
^{1}H NMR spectrum of Boc-(2*S*)-Ind-OMe (**1**) in $CDCl_3$ (0.1 M) at 500 MHz



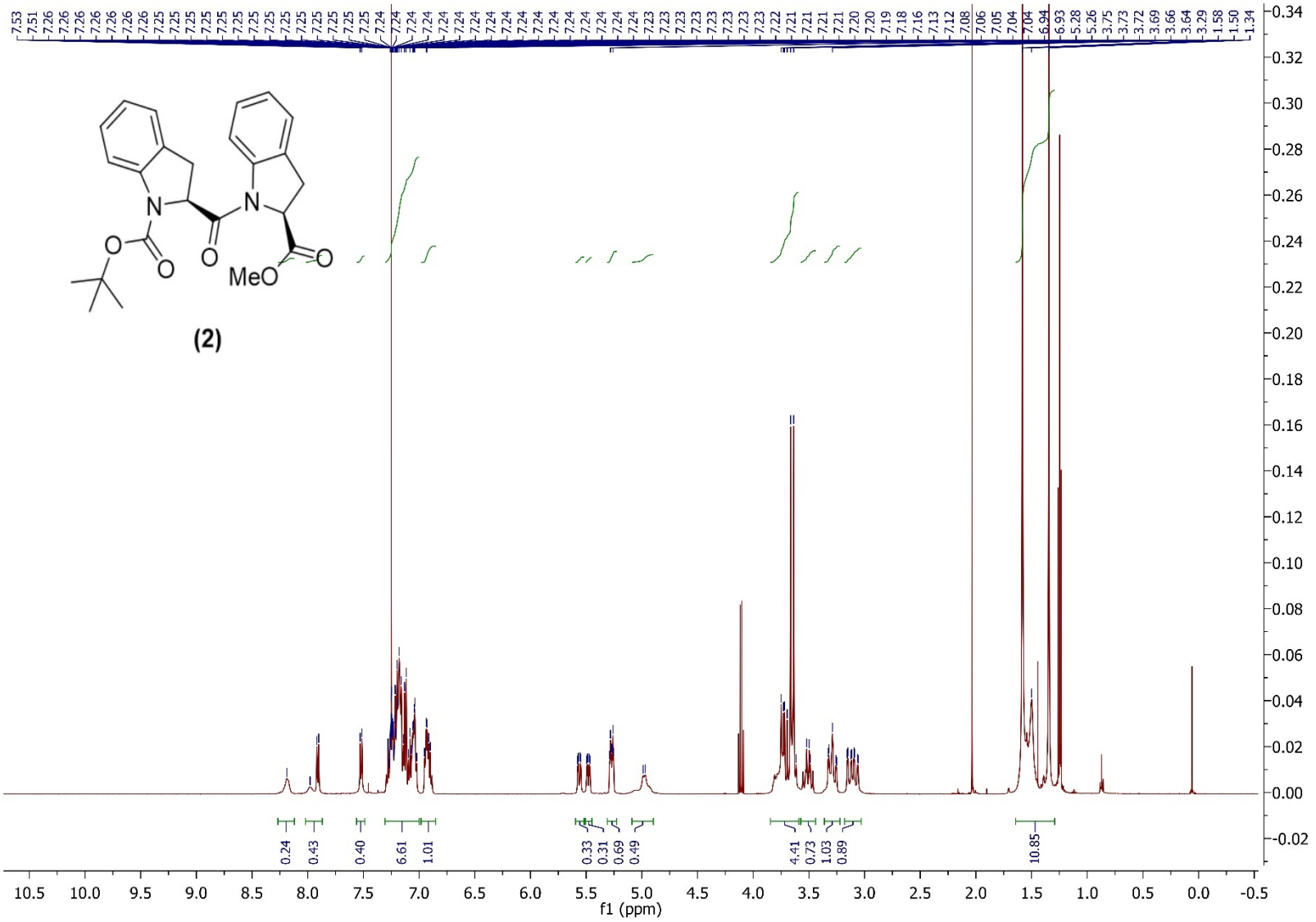
^{1}H NMR spectrum of Boc-(2*S*)-Ind-OMe (**1**) in DMSO-d_6 (0.1 M) at 500 MHz



$^{13}C\{^{1}H\}$NMR spectrum of Boc-(2*S*)-Ind-OMe (**1**) in DMSO-d_6 at 125 MHz



^{1}H NMR spectrum of Boc-((2*S*)-Ind)$_2$-OMe (**2**) in $CDCl_3$ (0.1 M) at 500 MHz



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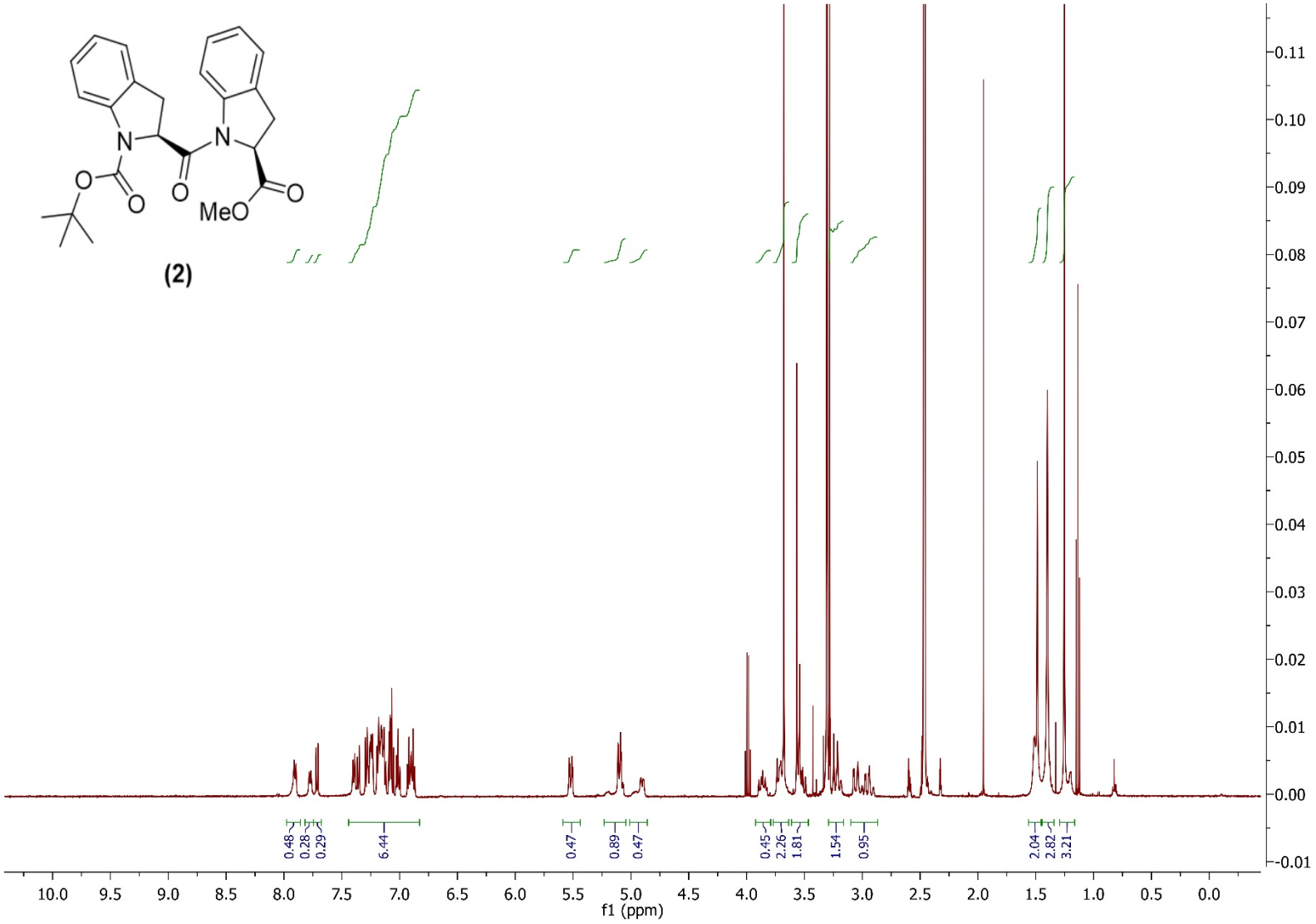

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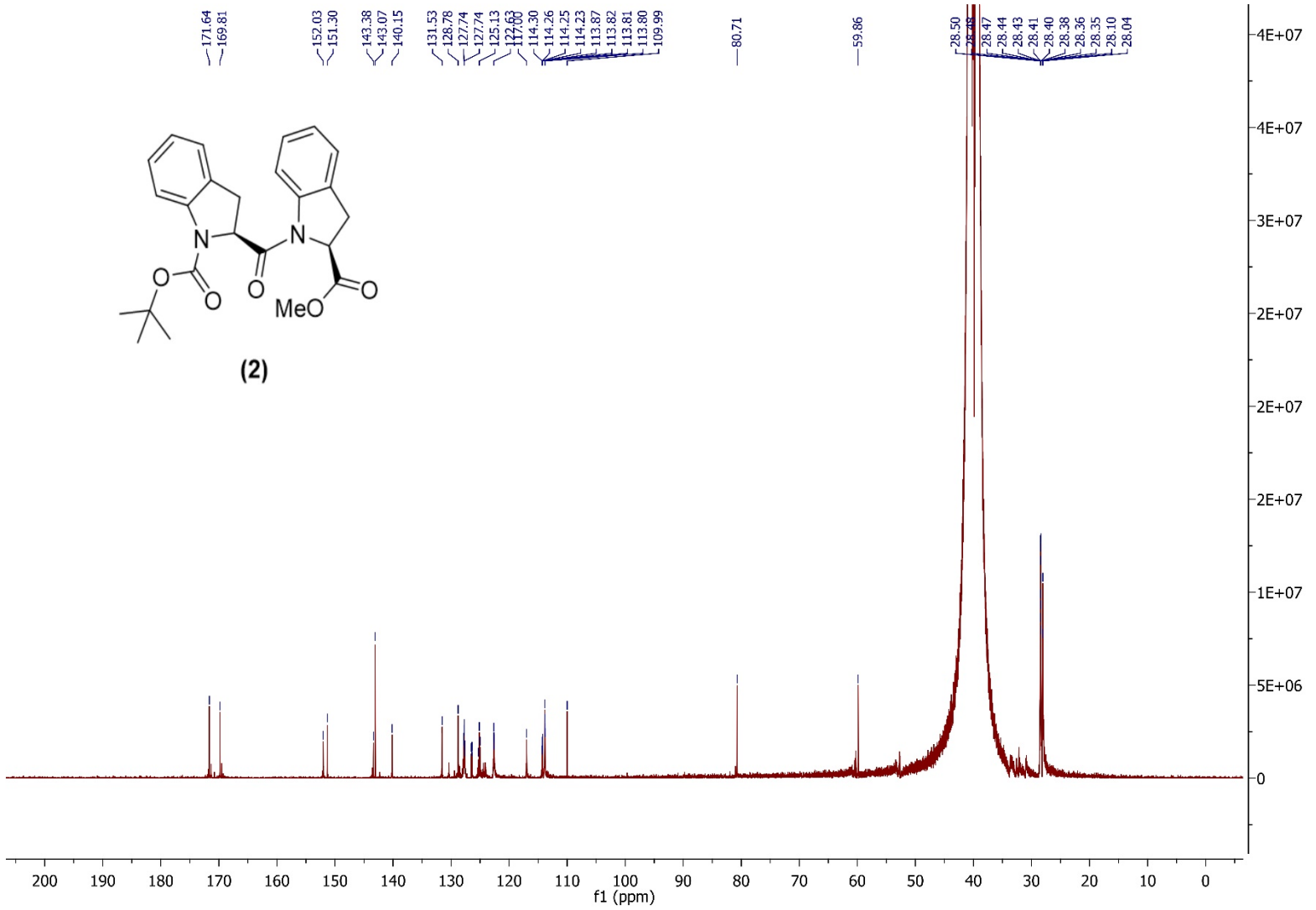
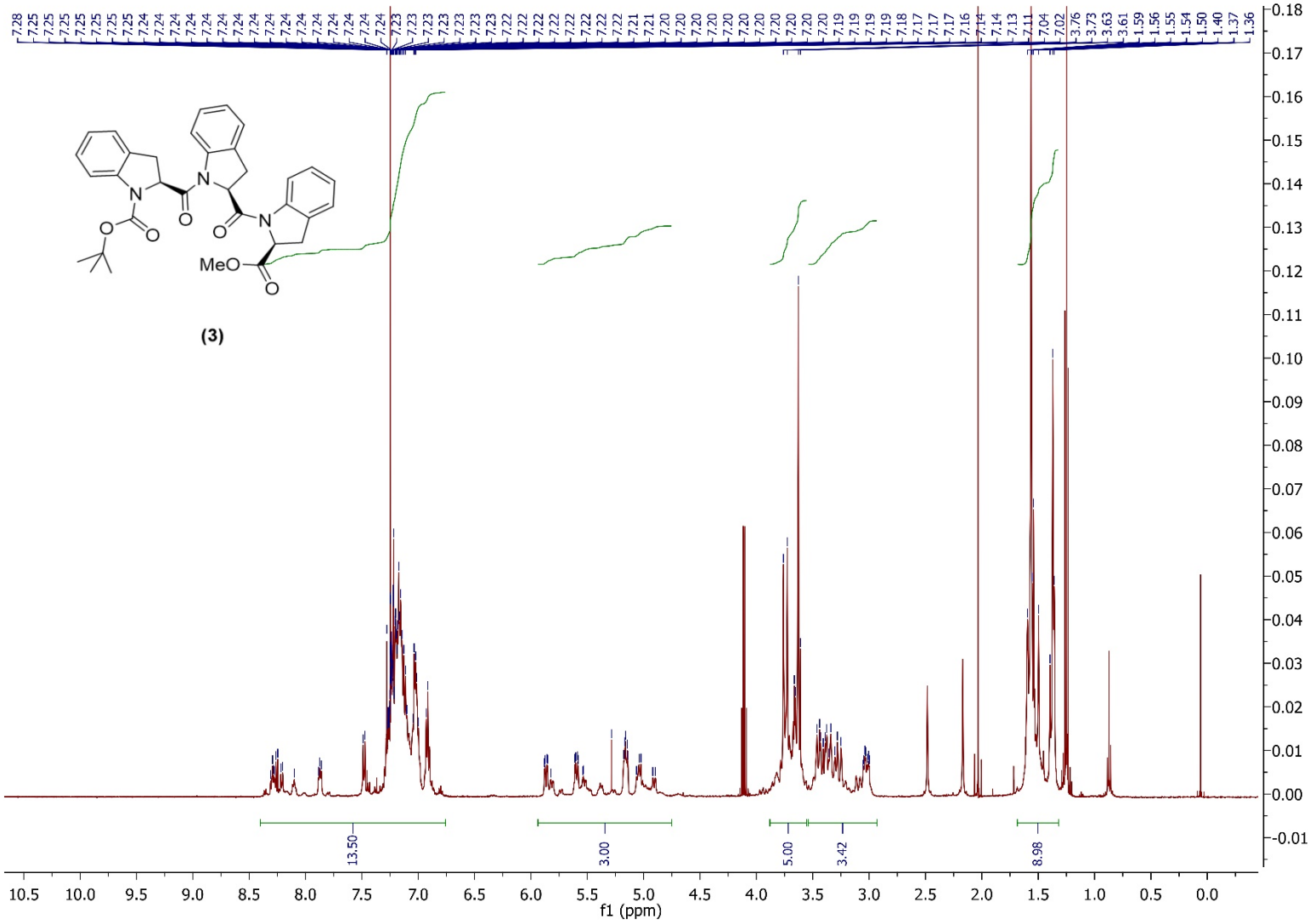
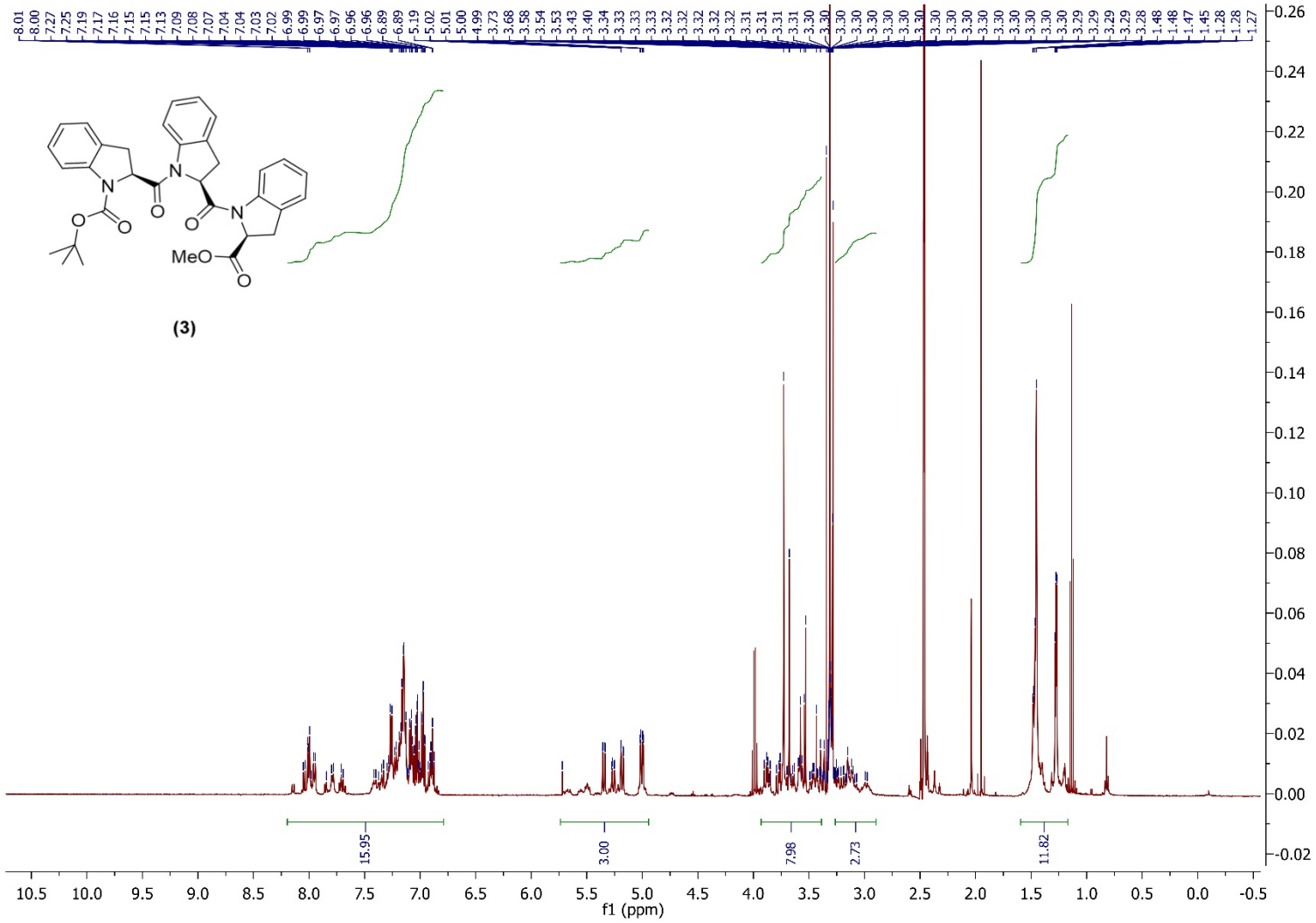


^{1}H NMR spectrum of Boc-((2*S*)-Ind)$_3$-OMe (**3**) in $CDCl_3$ (0.1 M) at 500 MHz



^{1}H NMR spectrum of Boc-((2*S*)-Ind)$_3$-OMe (**3**) in DMSO-d_6 (0.1 M) at 500 MHz



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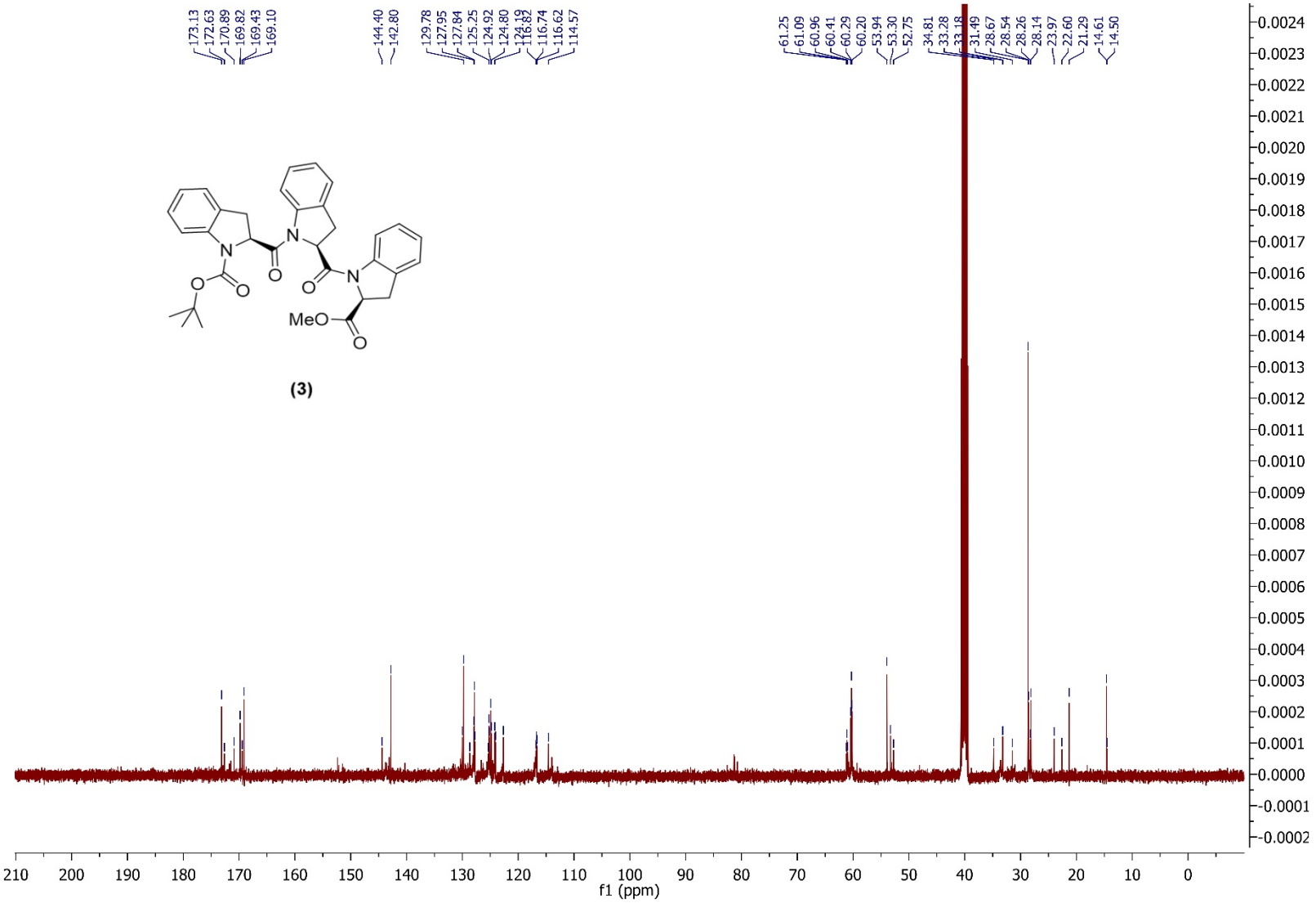
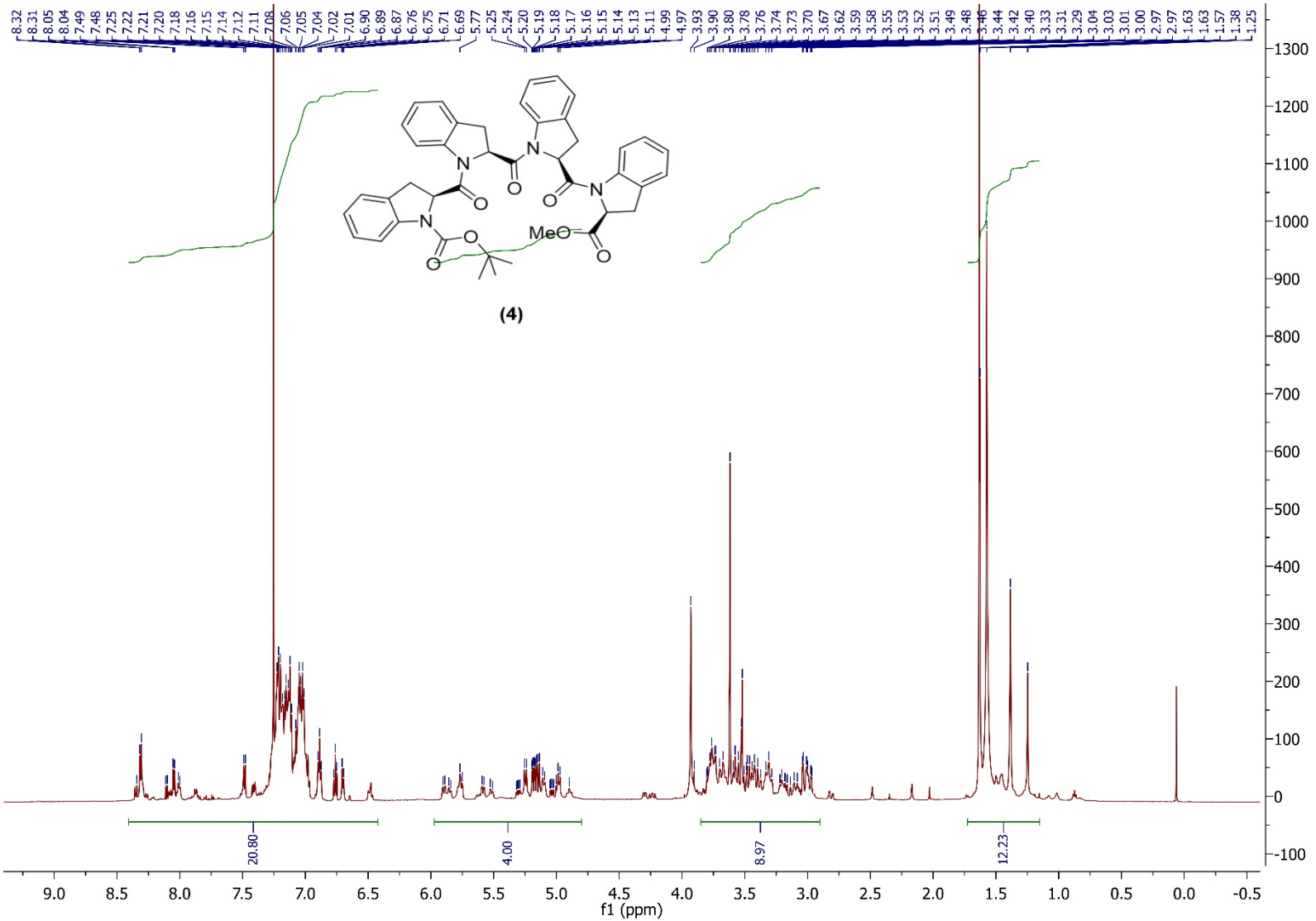


^{1}H NMR spectrum of Boc-((2*S*)-Ind)$_4$-OMe (**4**) in $CDCl_3$ (0.1 M) at 500 MHz



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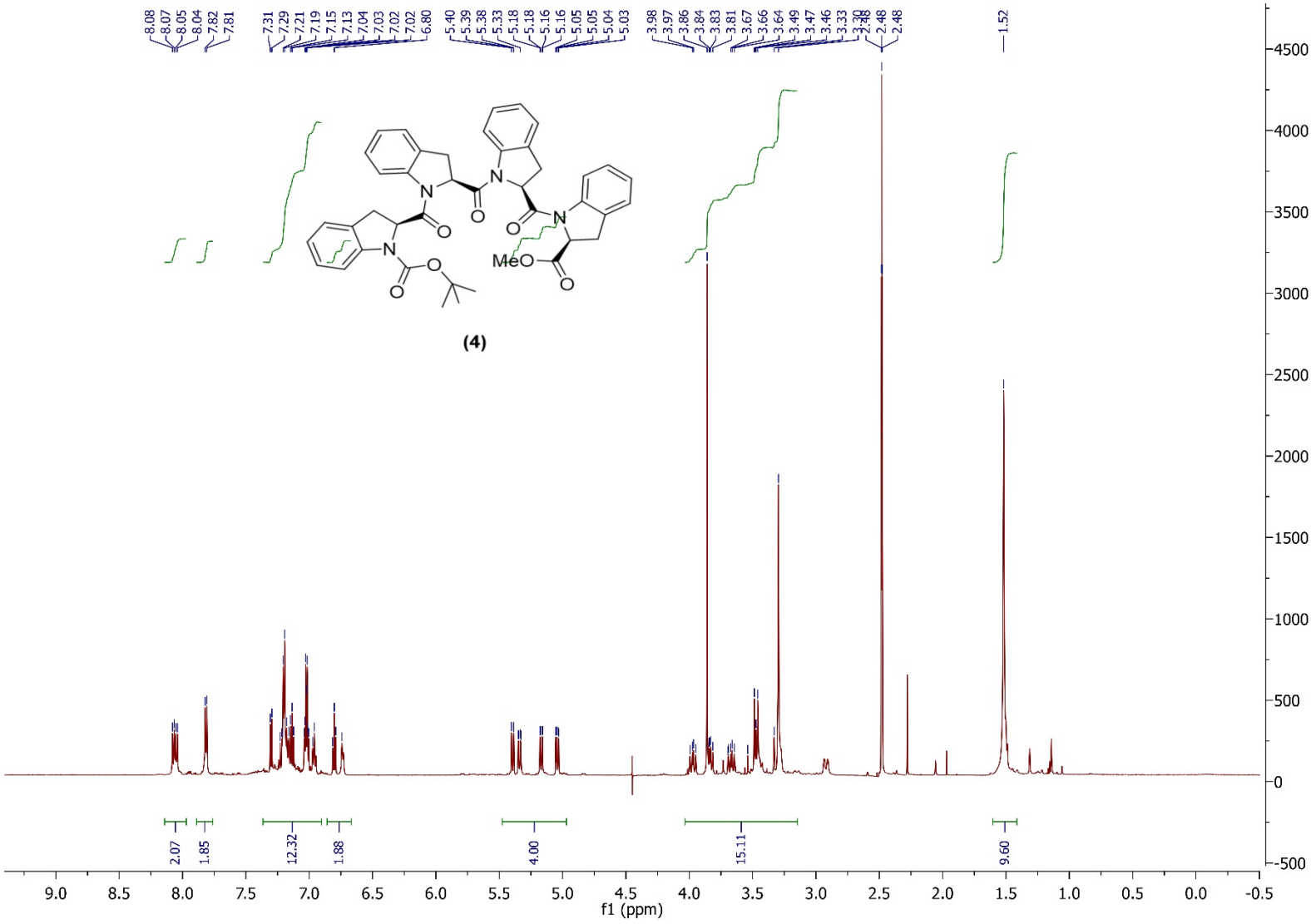

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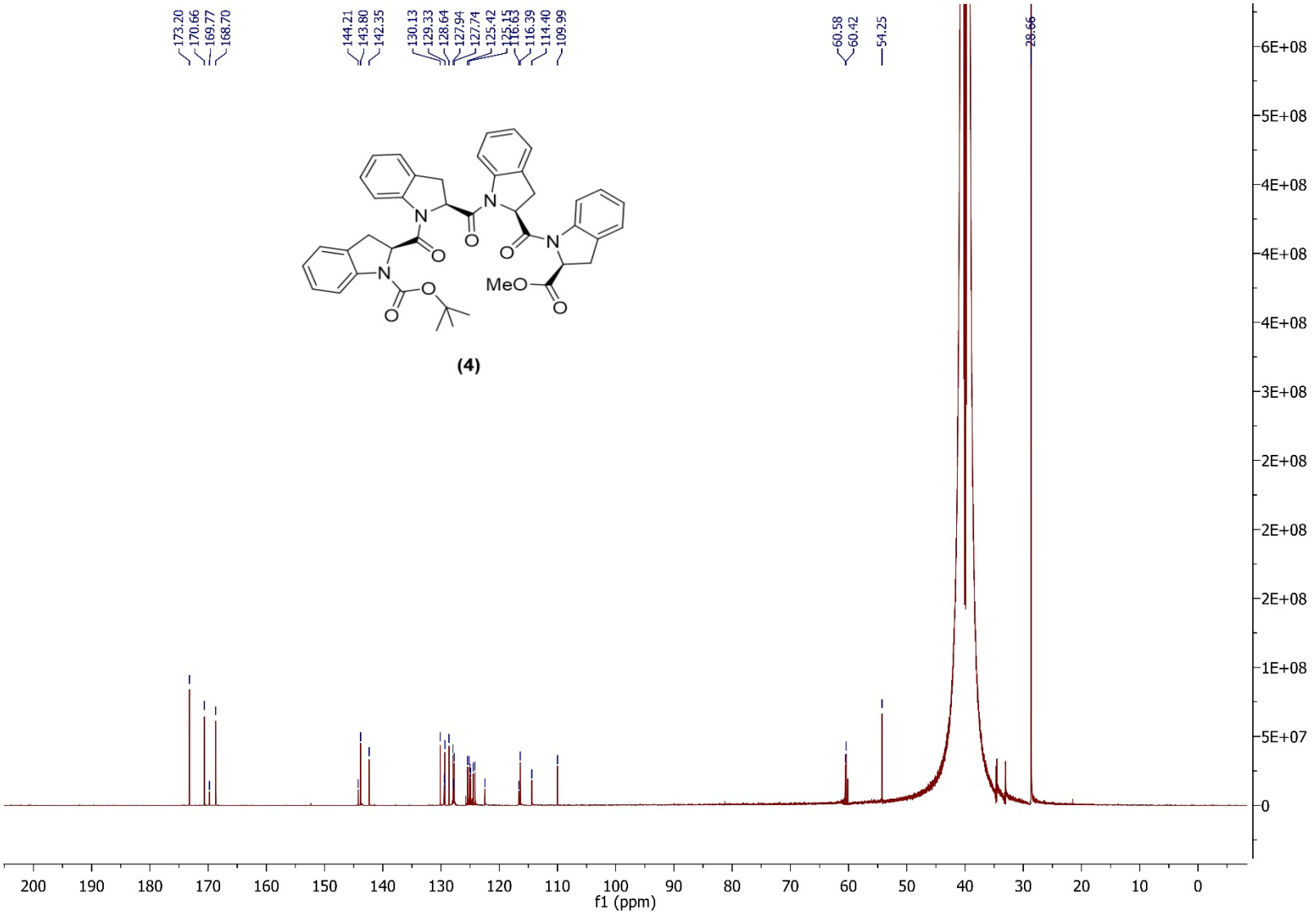
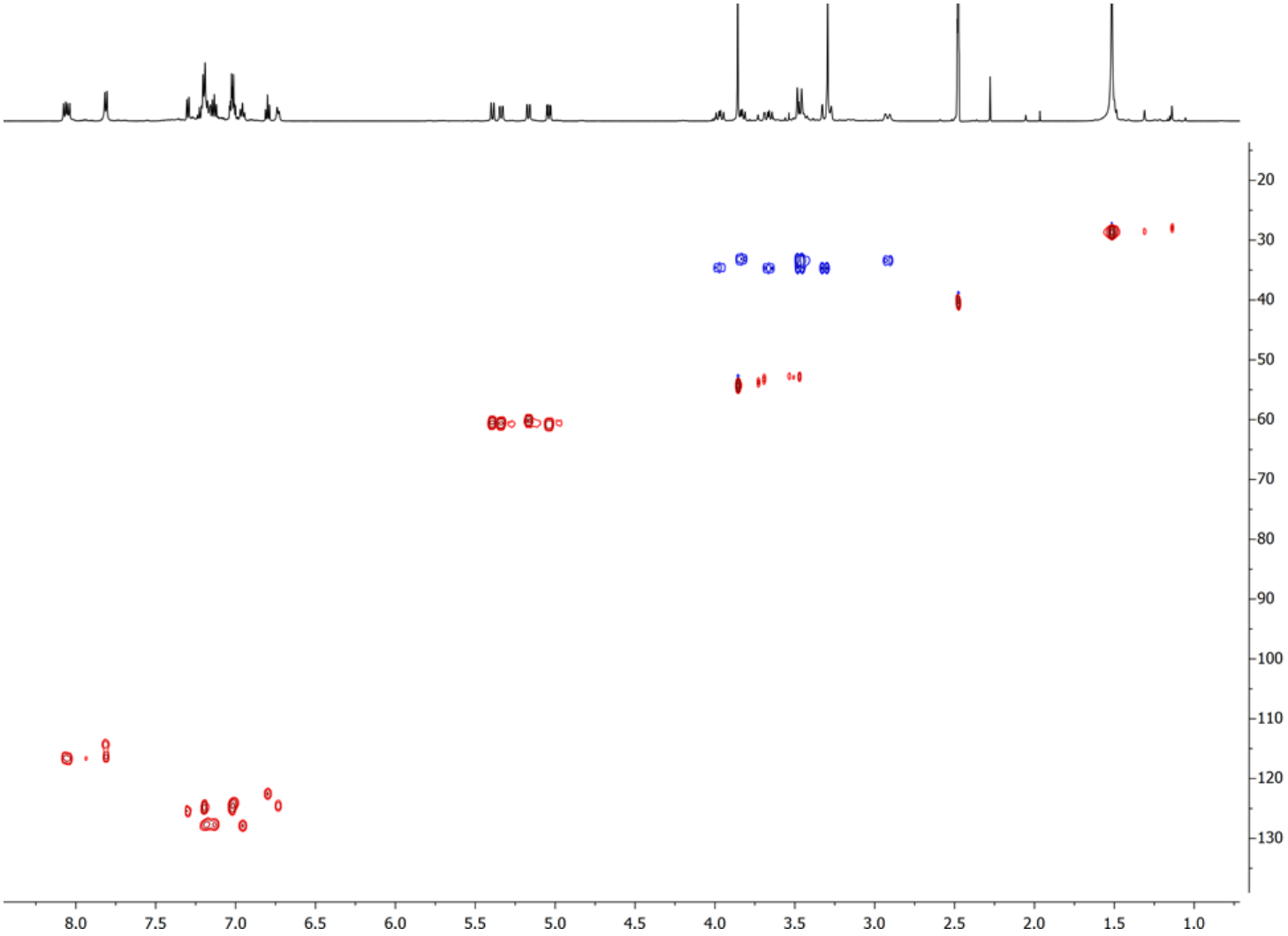
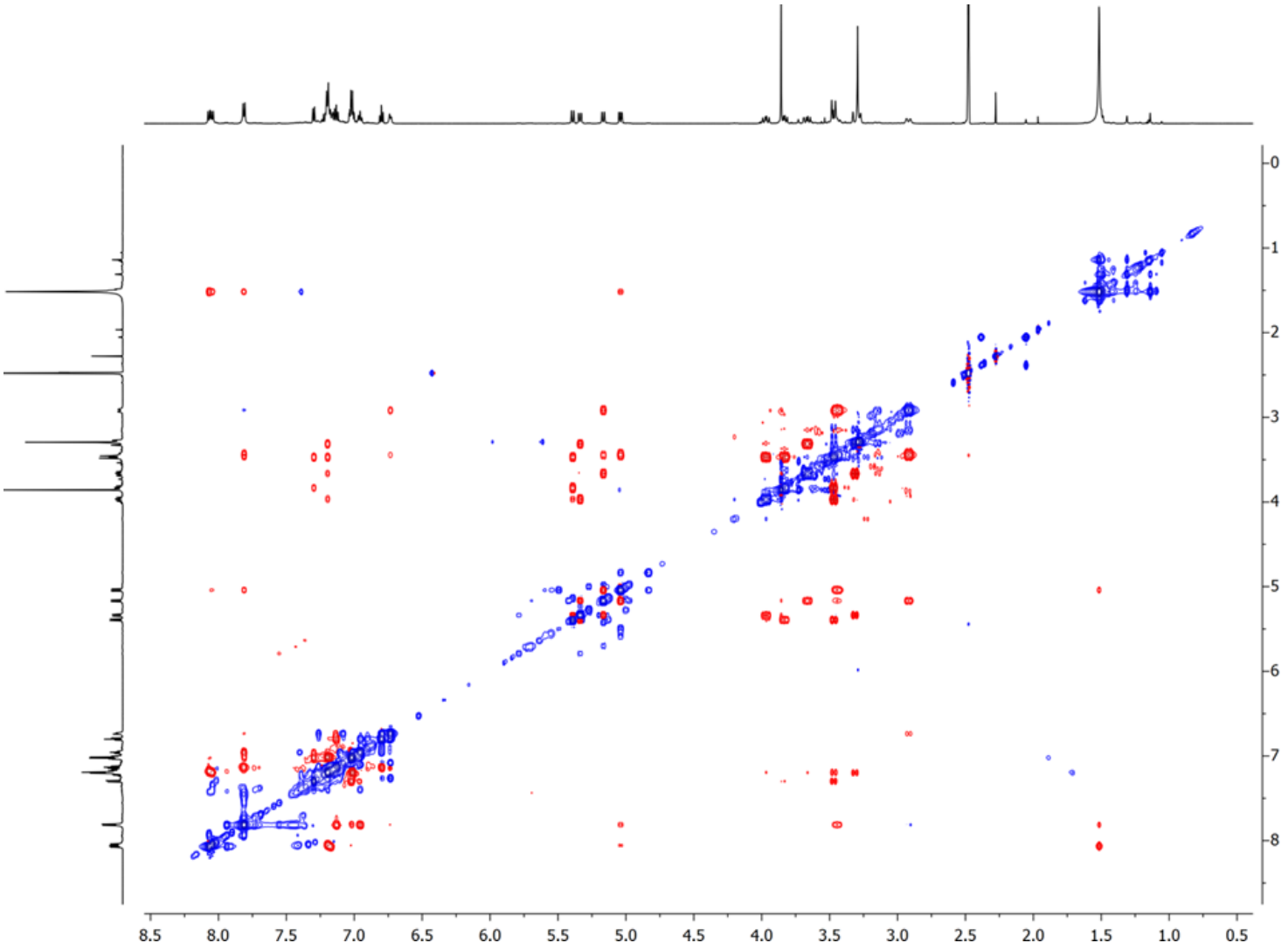


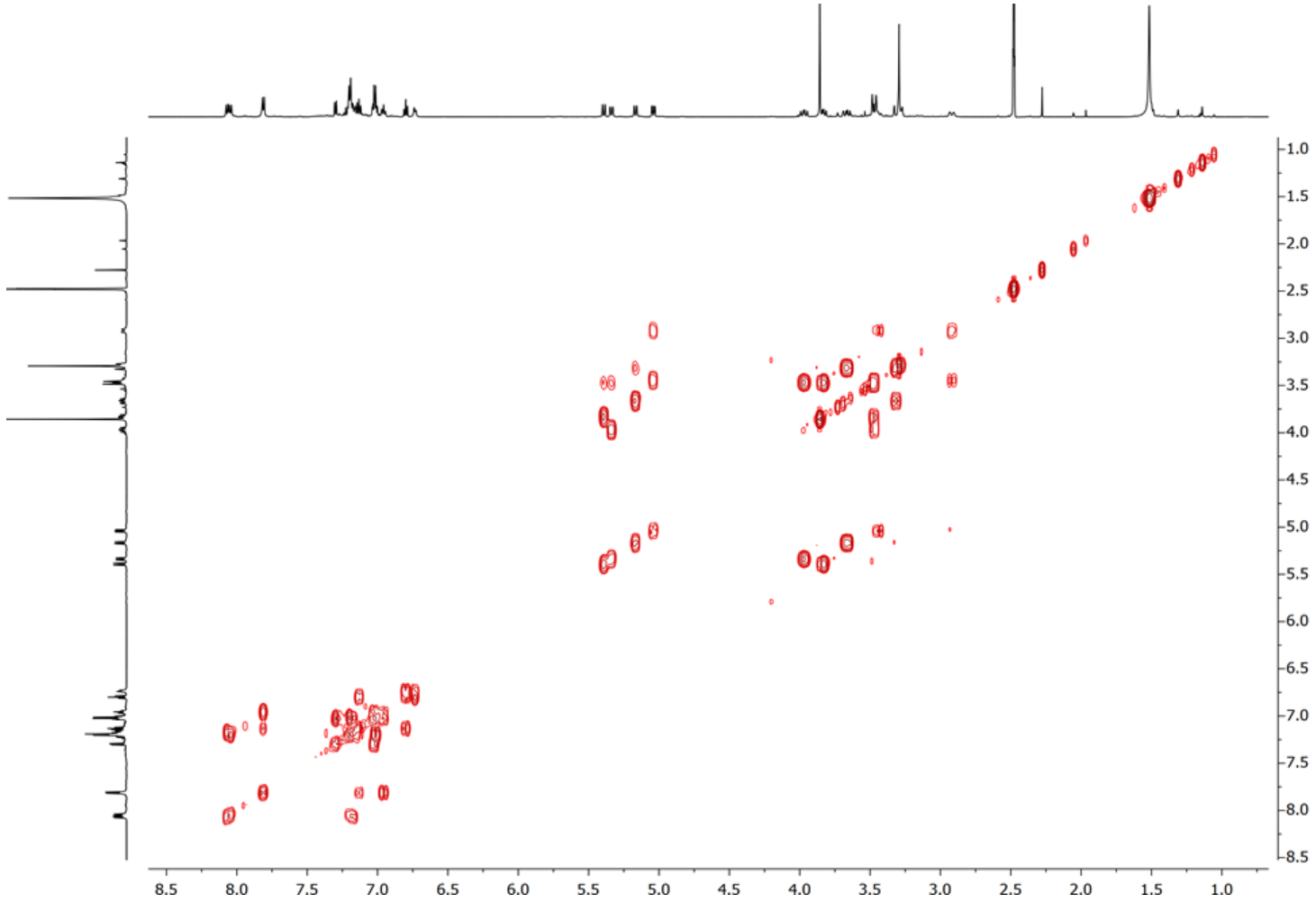
2D HSQC (600 MHz, DMSO-d6, 10 mM, 25 °C) map of Boc-((2*S*)-Ind)$_4$-OMe (**4**)



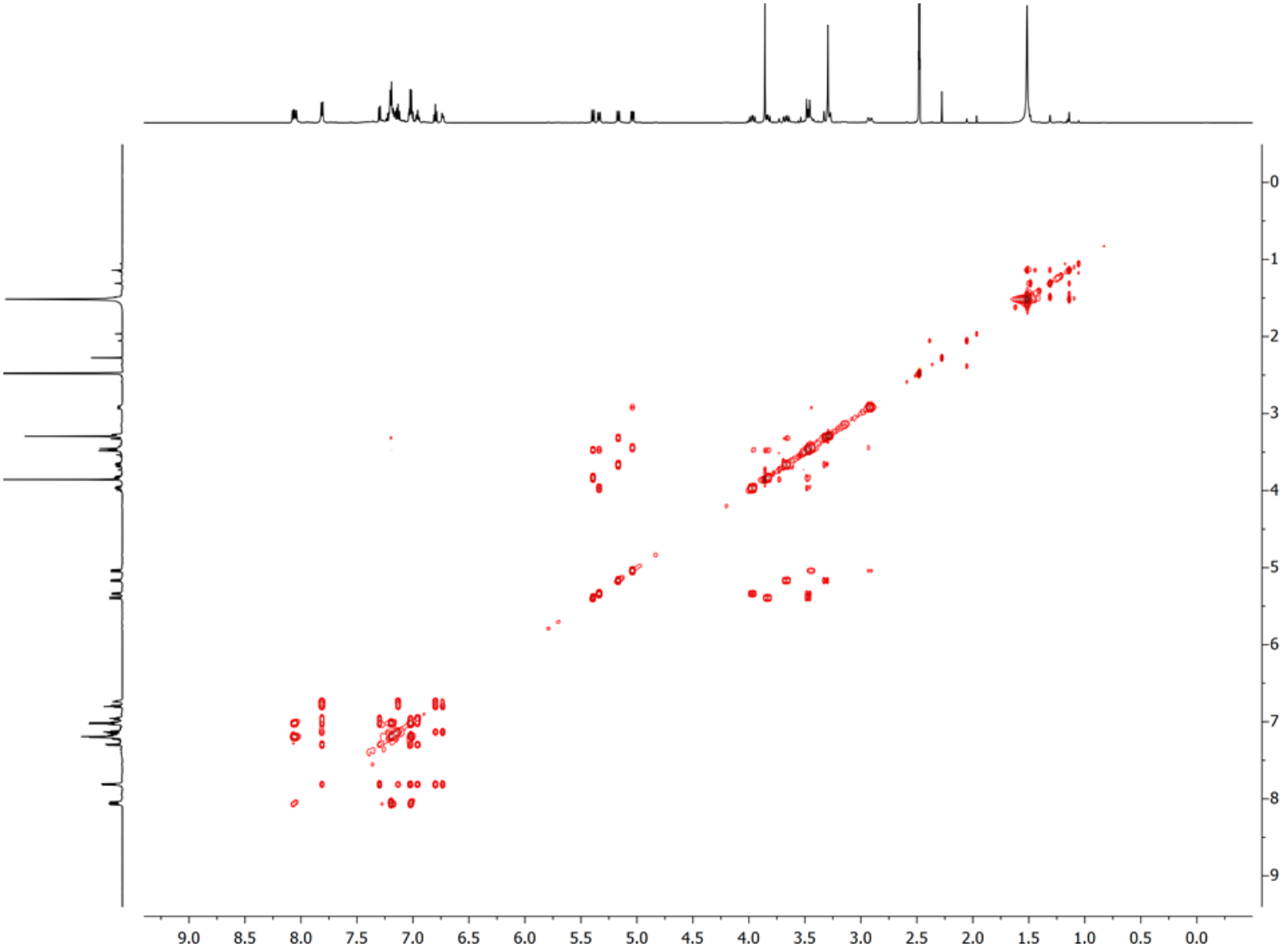
2D ROESY (600 MHz, DMSO-d6, 10 mM, 25 °C, mix 0.6 s) map of Boc-((2*S*)-Ind)$_4$-OMe (**4**)



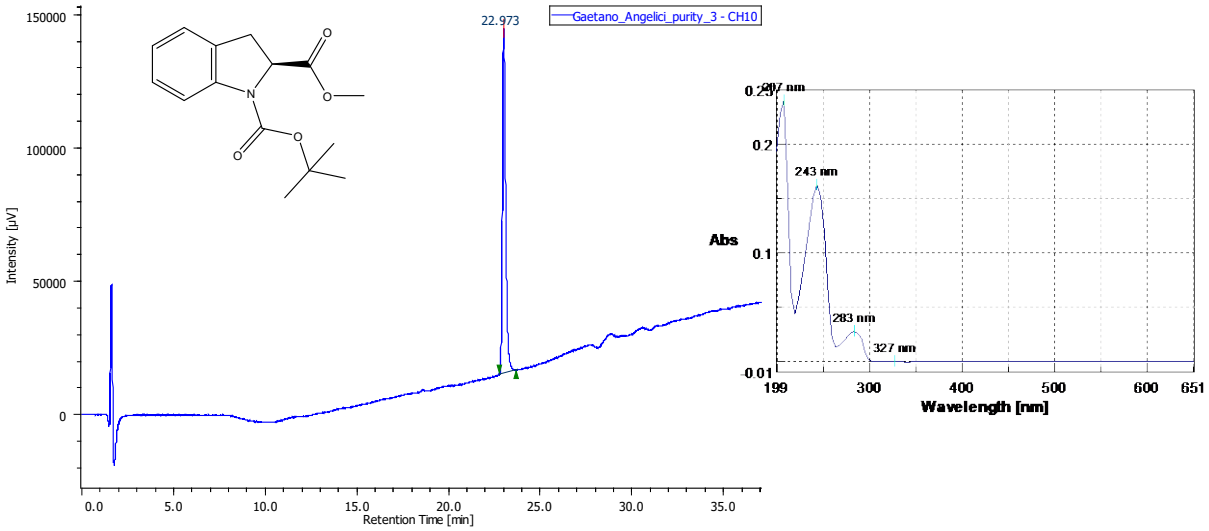
2D COSY (600 MHz, DMSO-d6, 10 mM, 25 °C) map of Boc-((2*S*)-Ind)$_4$-OMe (**4**)

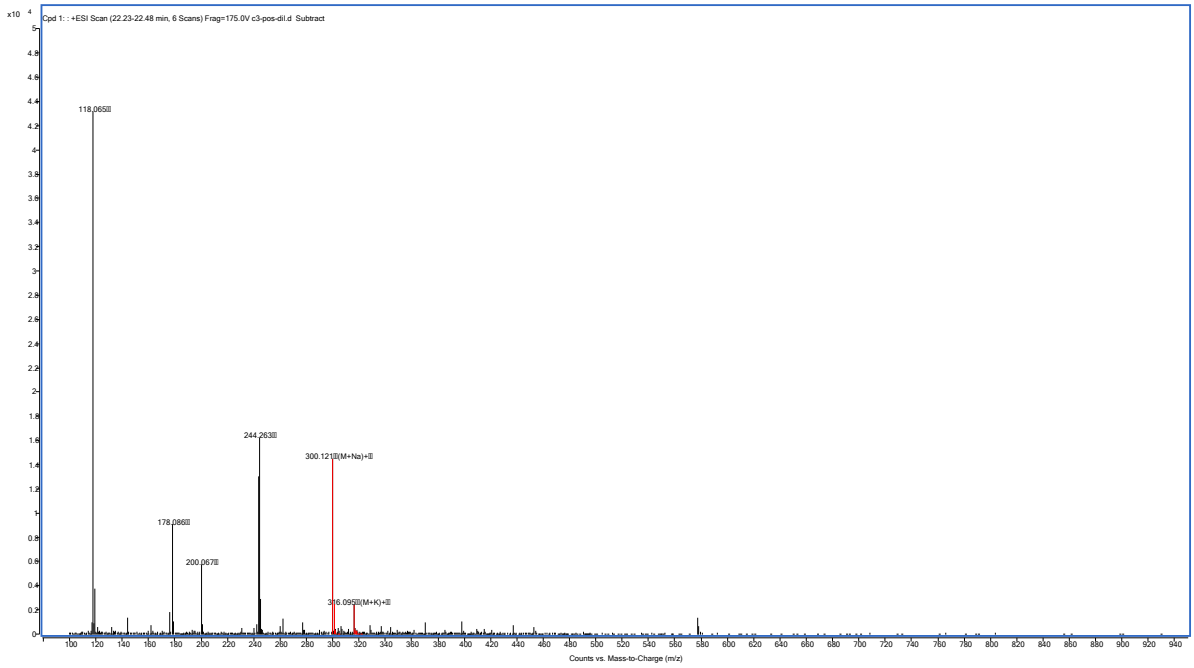


2D TOCSY (600 MHz, DMSO-d6, 10 mM, 25 °C) map of Boc-((2*S*)-Ind)$_4$-OMe (**4**)



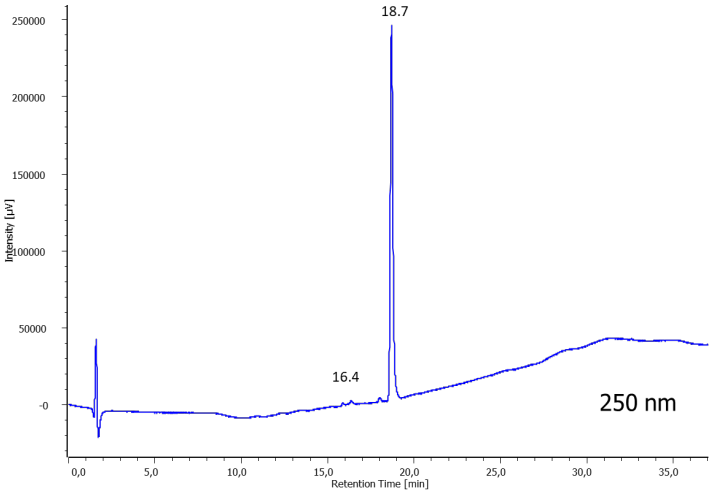
HPLC-MS analysis of (**1**)

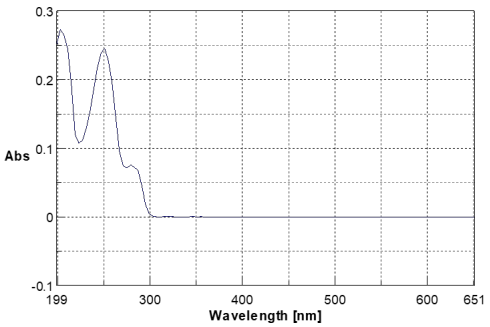


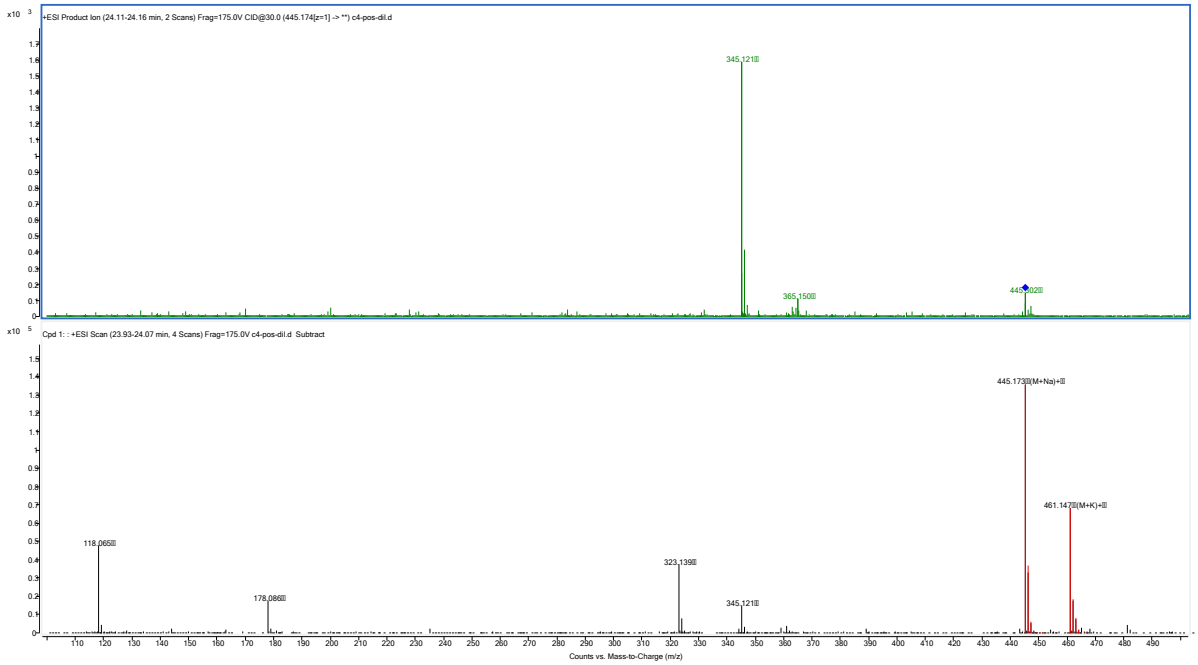


Sample name	Formula	Base peak (ion)	*m/z*		Diff (ppm)
			exact mass	experimental mass	
1	C15H19NO4	**$[M+K]^+$**	316.0946	316.0952	2.0

HPLC-MS analysis of (**2**)

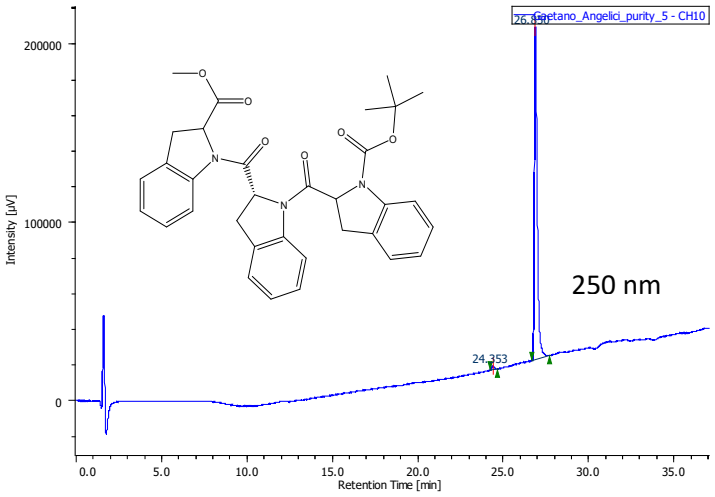


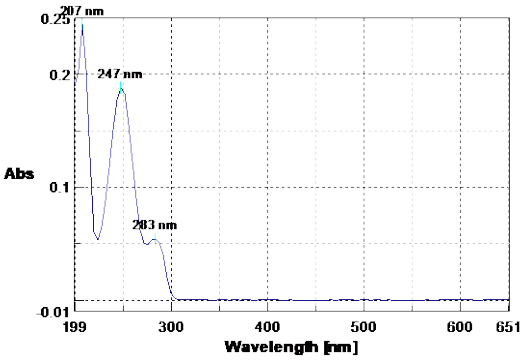


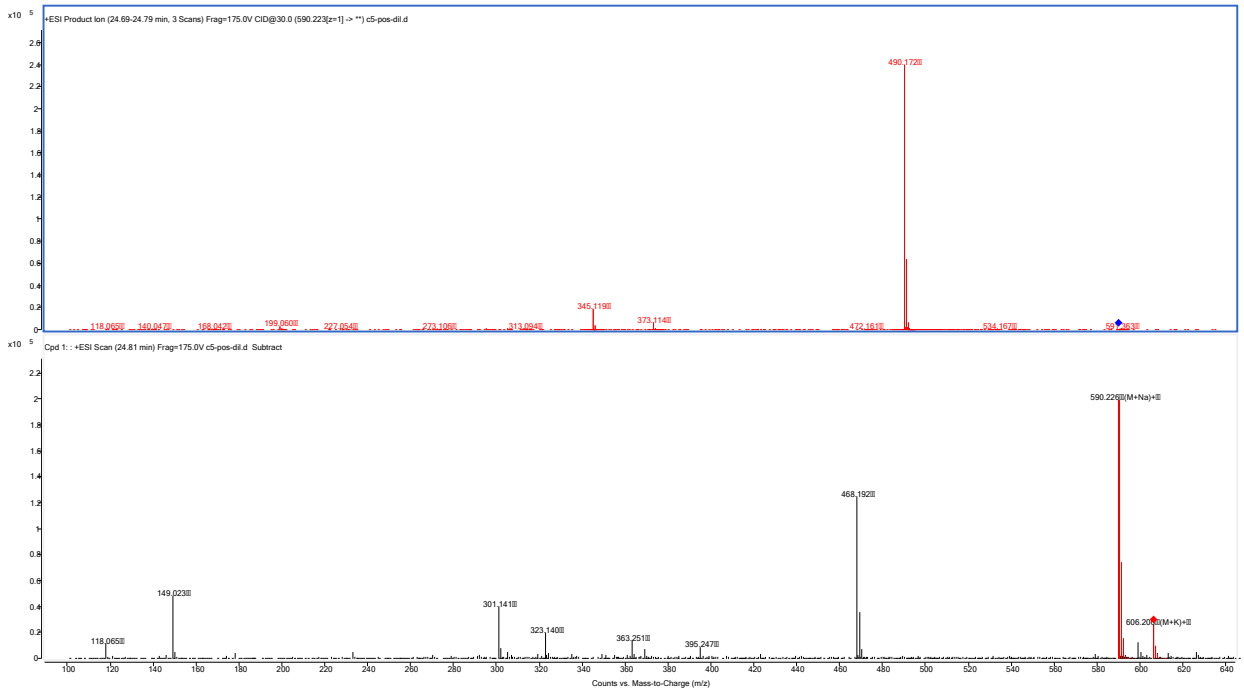


Sample name	Formula	Base peak (ion)	*m/z*		Diff (ppm)
			exact mass	experimental mass	
2	C24H26N2O5	**$[M+Na]^+$**	445.1734	445.1733	0.2

HPLC-MS analysis of (**3**)

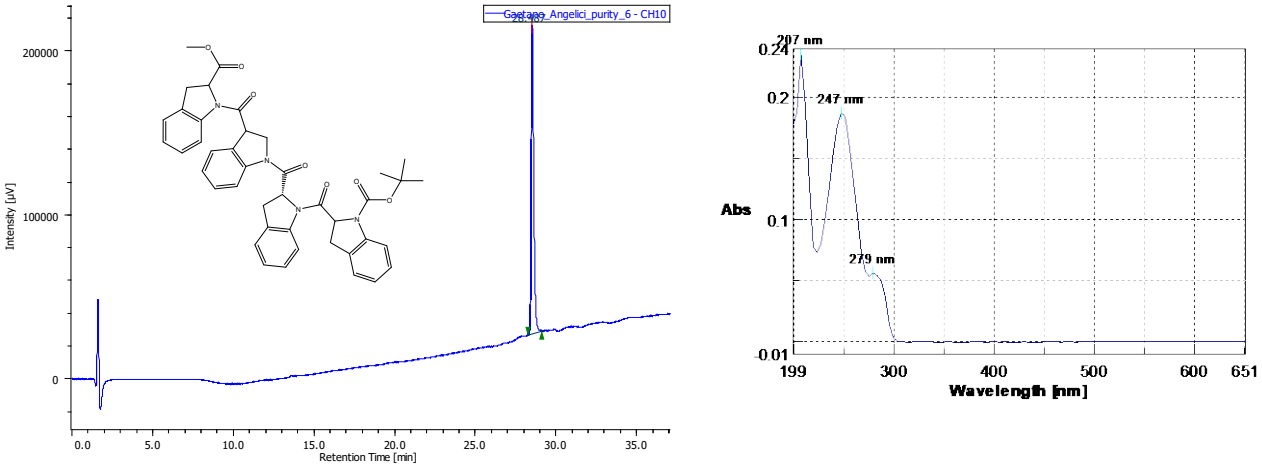


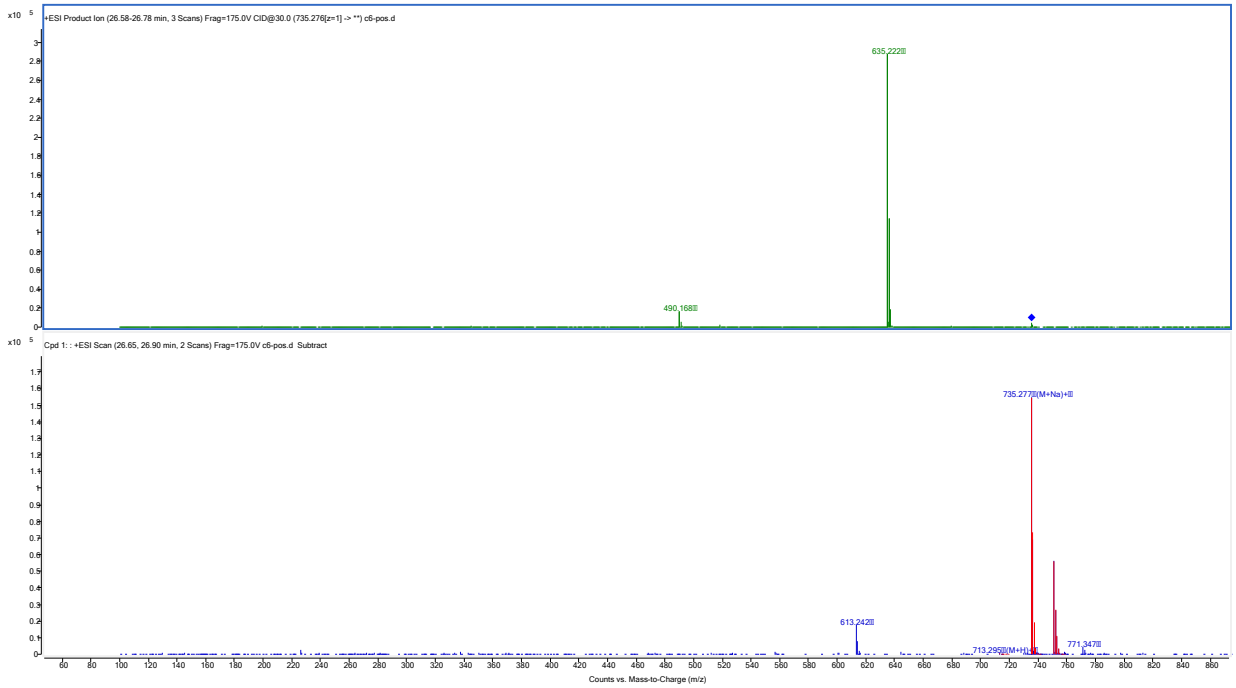




Sample name	Formula	Base peak (ion)	*m/z*		Diff (ppm)
			exact mass	experimental mass	
3	C33H33N3O6	**$[M+K]^+$**	606.2001	606.1999	0.32

HPLC-MS analysis of (**4**)





Sample name	Formula	Base peak (ion)	*m/z*		Diff (ppm)
			exact mass	experimental mass	
4	C42H40N4O7	**$[M+Na]^+$**	735.2789	735.2773	2.2

Table S1. Crystal data and structure refinement of (4)

CCDC number	2173109
Empirical formula	$C_{42}H_{40}N_4O_7$
Formula weight	712.78
Crystal system	Monolinic
Space group	$\boldsymbol{P}\,2_1$
a (Å)	10.4762(8)
b (Å)	9.2900(7)
c (Å)	19.1539(13)
β (°)	100.148(3)
Volume (Å^3)	1835.0(2)
Z	2
ρ_{calc} (g cm^{-1})	1.290
μ (mm^{-1})	0.089
F(000)	752
θ range (°)	3.0 to 26.5
Reflections collected	25312
Independent reflections	7460 (R_{int} = 0.0162)
Goodness-of-fit on F^2	1.041
Final R_1 [$I \geq 2\sigma(I)$]	0.0404
Final wR_2 [$I \geq 2\sigma(I)$]	0.1093
Final R_1 [all data]	0.0432
Final wR_2 [all data]	0.1124

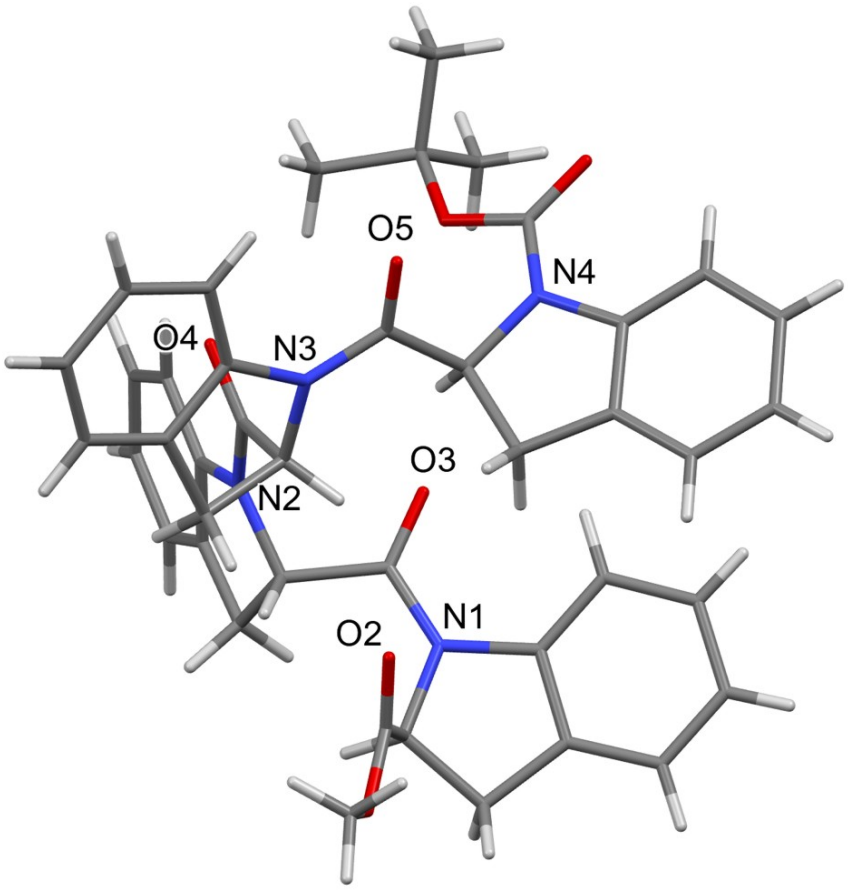


Table S2. Description of main C–H···O interactions

Along the peptide chain, which shows a helical conformation, the peptide groups alternate with the residues of the indoline-2-carboxylic acid which show CO–N–C–CO torsion angles ranging between 70.8 and 85.9 degrees. The peptide groups are essentially planar due both to the resonance effect and to hydrogen interactions with the CH group in position 7 of the indole ring of proline. The strongest C–H···O interactions are listed in the Table and illustrated in the Figure below.

Groups	C···O distance / Å	C–H···O angle / deg
C42–H42B···O6	2.840(8)	120.7
C18–H18···O4	2.853(3)	116.1
C36–H36···O6	2.862(5)	115.2
C27–H27···O5	2.868(4)	115.2
C9–H9···O3	2.903(4)	115.6

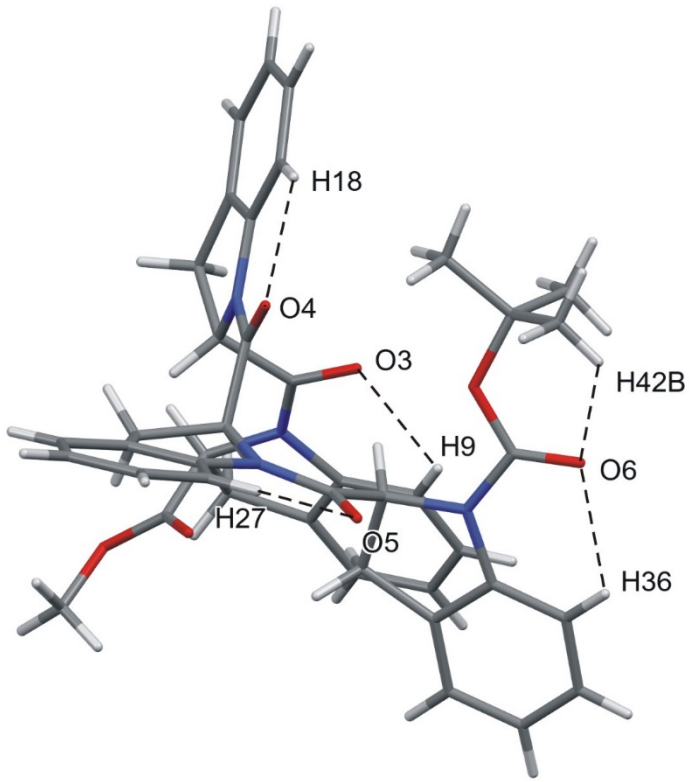


Table S3. Calculated energy differences between conformers

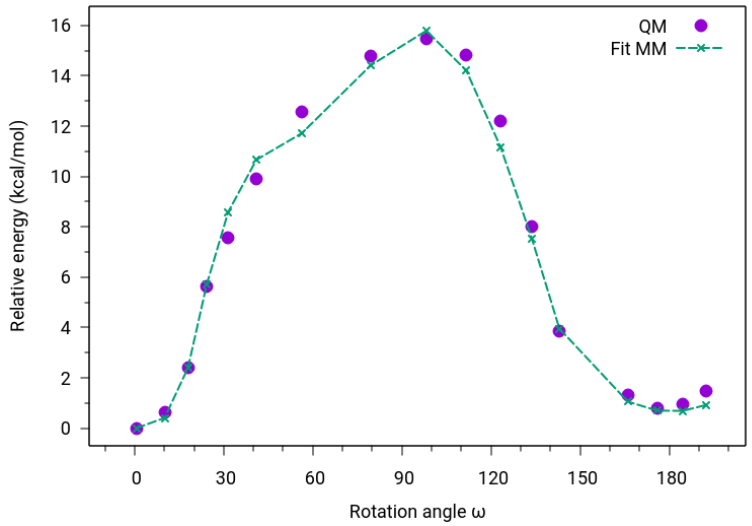
Energies and dihedral angles for the conformations extracted from the PBMetaD simulations in DMSO and chloroform. Some conformations were found in both solvents, while most of them are found only in one of the solvents. The dihedral angles and molecular dipole refer to the DFT-optimized structure (in DMSO where present, otherwise in chloroform). The number of amide bonds in *cis* conformation is also reported.

Conf.	N. cis	ω A	ω B	ω C	ω D	ψ B	ψ C	ψ D	Solv.	G(DMSO)	G(CHCl3)	Dipole (D)
0	3	2	-3	-17	-176	161	145	157	DMSO	3.35		12.4
1	4	3	-11	-13	4	164	160	160	both	0.9	2.78	20.7
2	1	164	-176	-14	176	165	110	174	DMSO	4.85		6.6
3	3	5	-173	-8	-8	145	116	168	both	5.23	5.98	5.1
4	2	-11	179	174	-3	159	172	146	CHCl3		7.05	6.1
5	2	11	2	-176	-172	-31	161	146	CHCl3		1.46	3.0
6	3	0	-14	-28	178	-32	-17	170	DMSO	2.76		8.8
7	2	-13	-172	-17	-178	158	108	174	DMSO	2.81		4.2
8	3	-3	-12	-178	-8	-31	166	144	CHCl3		1.02	3.6
9	2	-164	-7	-4	177	144	140	166	DMSO	4.12		13.3
10	2	-169	0	-178	-15	-31	166	105	CHCl3		5.82	4.7
11	3	178	4	13	11	156	-26	169	CHCl3		8.7	6.8
12	1	-172	2	-177	-172	-30	162	146	CHCl3		2.82	7.8
13	2	-163	34	-4	177	-18	-28	169	DMSO	3.73		5.4
14	3	-6	-10	-173	7	-35	174	-28	CHCl3		2.92	8.8
15	3	-9	-176	-1	11	150	141	-46	DMSO	1.81		6.4
16	3	-178	-7	-15	2	160	163	163	both	1.78	4.21	18.0
17	2	178	7	3	175	151	-36	167	both	0	0	5.6
18	2	-1	-163	-2	180	142	-35	168	DMSO	1.88		15.1

Torsional parameters.

The parameters for the dihedral ω were obtained by fitting a QM torsional profile. QM energies were obtained at the B3LYP/6-311G(d,p) level of theory by optimizing an indoline dimer with frozen ω dihedrals. The initial parameters for the torsion were taken from the Amber ff14SB force field, and fitted to the QM torsional profile. The final fit is reported in the figure below.

Figure: Final torsional profile obtained at the QM level of theory and at the MM level after fitting the dihedral parameters.



The fitted parameters are reported below in the Amber format:

```
CT-C    -N    -CT                1                0.33590000        180.000         -1.0
CT-C    -N    -CT                1                2.78650000        180.000         -2.0
CT-C    -N    -CT                1                0.23450000          0.000         -3.0
CT-C    -N    -CT                1                0.71300000        180.000          6.0
CT-C    -N    -CB                1                0.55290000        180.000         -1.0
CT-C    -N    -CB                1                2.30570000        180.000         -2.0
CT-C    -N    -CB                1                1.18040000          0.000         -3.0
CT-C    -N    -CB                1                0.20880000          0.000          6.0
O    -C    -N    -CB                1                0.44680000          0.000         -1.0
O    -C    -N    -CB                1                2.40780000        180.000         -2.0
O    -C    -N    -CB                1                1.08870000        180.000         -3.0
O    -C    -N    -CB                1                0.00710000        180.000          6.0
O    -C    -N    -CT                1                0.43910000          0.000         -1.0
O    -C    -N    -CT                1                2.55570000        180.000         -2.0
O    -C    -N    -CT                1                0.40840000        180.000         -3.0
O -C -N -CT   1    0.19670000  180.000   6.0
```

Table S4. Calculated ROE distances along the PBMetaD in DMSO

Calculated distances in all the PBMetaD clusters for the inter-unit ROE interactions shown in **Figure 3** and **Figure SI1**. Distances were calculated for the structures belonging to each cluster in the PBMetaD. Each cluster is assigned the same conformation number as its representative in **Table SI3**. Within each cluster, each "average" distance was calculated by averaging $1/R^6$. Distances involving equivalent tBu atoms were averaged in the same way. A NOE violation was detected every time the average distance was above 4 Å.

Cluster	Dist. HAα - HBα	Dist. HBα - HCα	Dist. HCα- HDα	Dist. HAα - HD1	Dist. HAβ'- HBα	Dist. HBβ'- HCα	Dist. HCβ'- HDα	Dist. HC1- tBu	Dist. HB1- tBu	NOE Violations
0	2.52	2.66	4.49	6.07	2.52	2.48	4.69	3.82	3.91	3
1	2.45	2.43	2.51	3.68	2.71	2.54	2.45	3.81	3.83	0
2	4.53	2.09	4.42	7.64	4.51	3.24	4.65	11.42	7.39	7
3	4.39	2.43	2.52	6.81	4.88	2.52	2.43	8.90	5.06	5
6	3.86	3.94	4.48	5.88	3.45	3.70	4.67	8.90	4.55	5
7	4.54	2.07	4.44	7.51	4.60	3.56	4.72	9.78	5.40	7
9	2.32	2.54	4.52	6.16	2.86	2.48	4.76	4.98	6.81	5
13	3.73	3.84	4.41	6.23	3.24	3.96	4.85	8.09	7.14	5
15	4.32	2.52	3.97	7.25	5.02	2.66	3.64	8.81	5.75	5
16	2.36	2.44	2.49	3.64	2.75	2.54	2.48	5.29	6.20	2
17	2.32	3.90	4.46	5.14	3.17	3.73	4.71	6.45	6.01	5
18	4.35	3.91	4.43	4.42	4.92	3.82	4.71	8.71	5.49	7

Figure S1. Intra-unit Ha-Hb(cis) and inter-unit Ha-Hb'(trans) ROE interactions of 4 shown on the DFT-optimized X-ray structure.

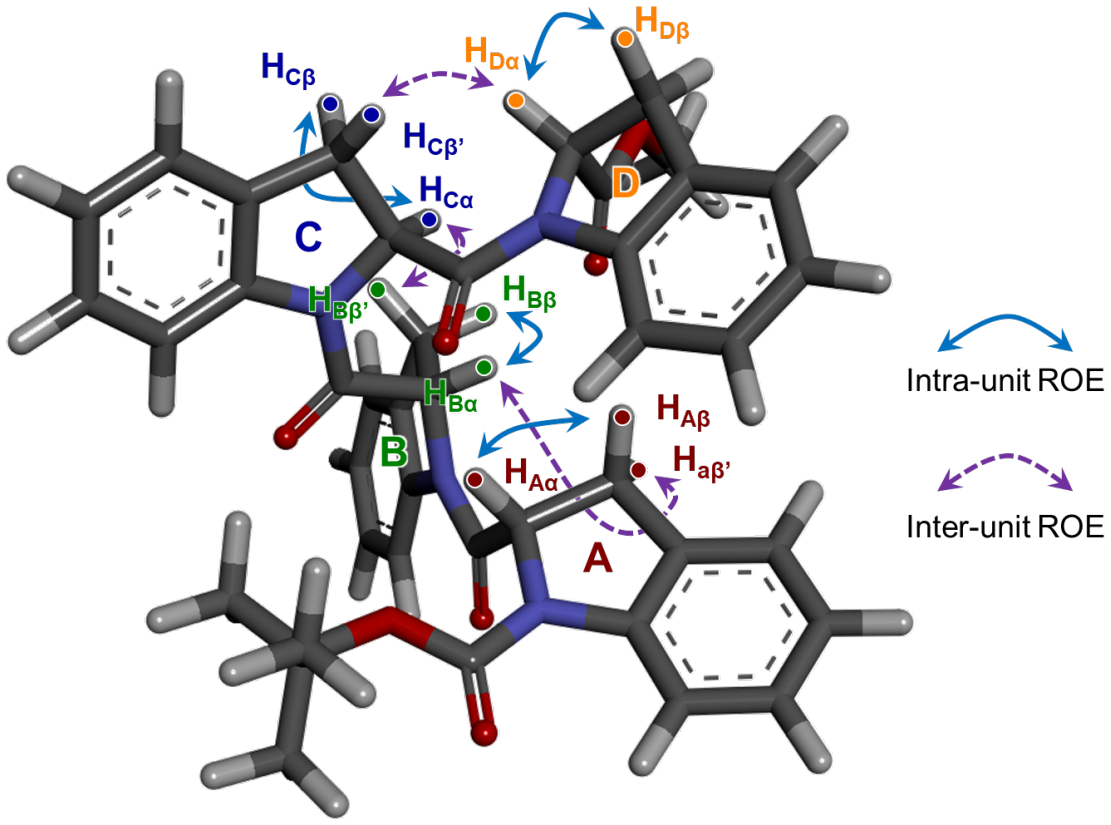
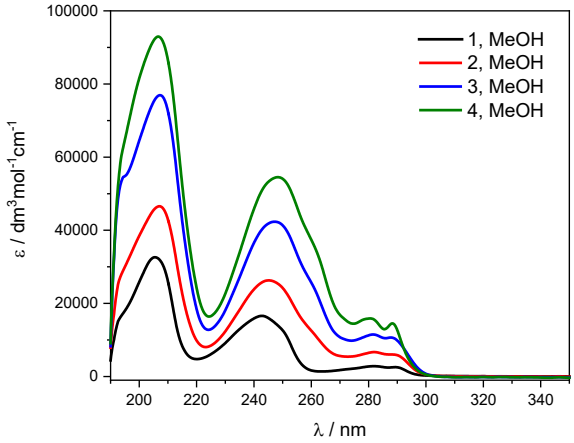
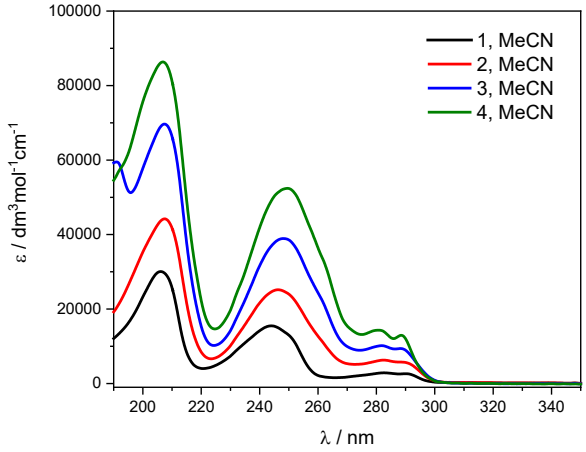


Figure S2. Experimental absorption spectra measured for compounds 1-4 in different solvents.

Cell path length 0.02 cm (MeOH), 0.05 cm (MeCN) and 0.2 cm ($CHCl_3$).





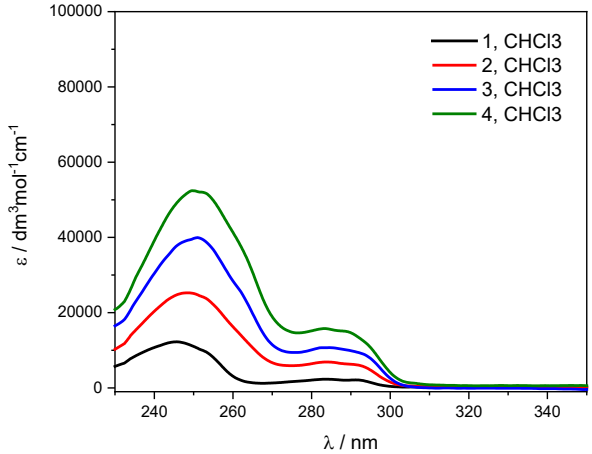


Figure S3. Variable-temperature ECD spectra of **4** measured in MeCN.

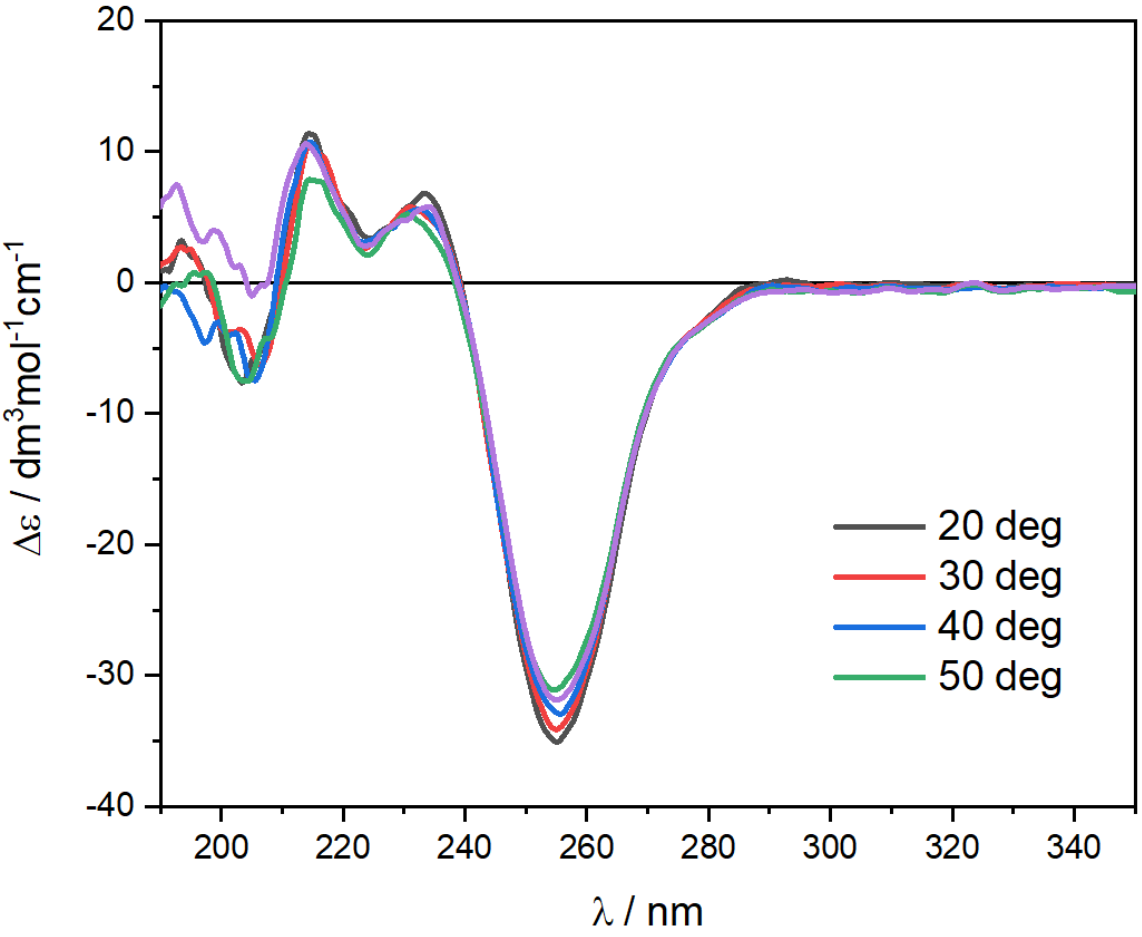


Figure S4. Absorption and ECD spectra of **4** measured in TFE.

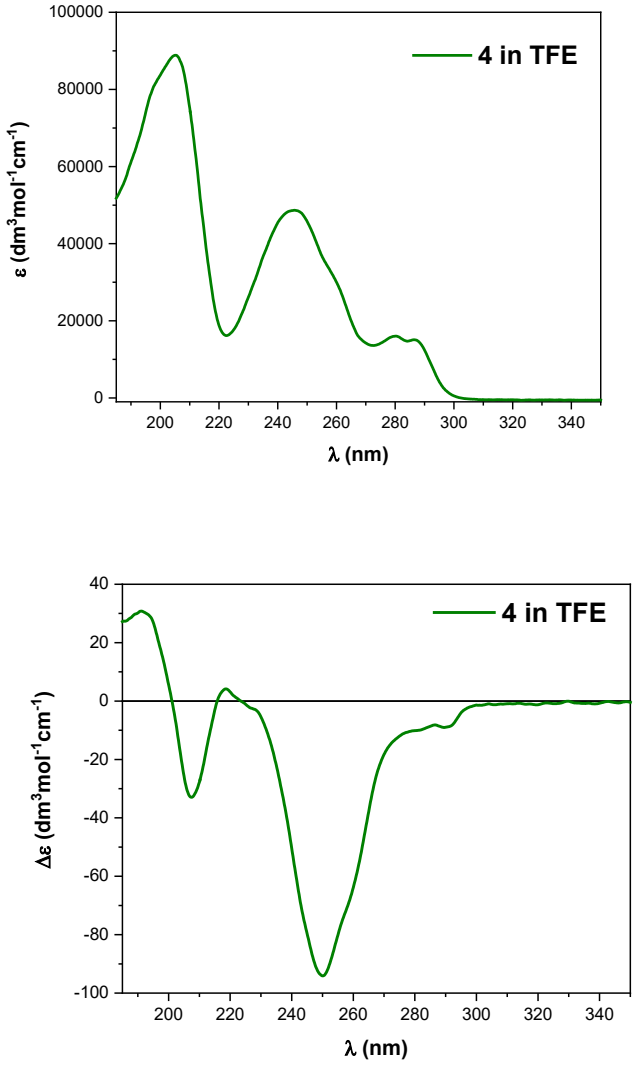


Figure S5. IR (bottom) and VCD (top) spectra of **2** measured in different solvents.

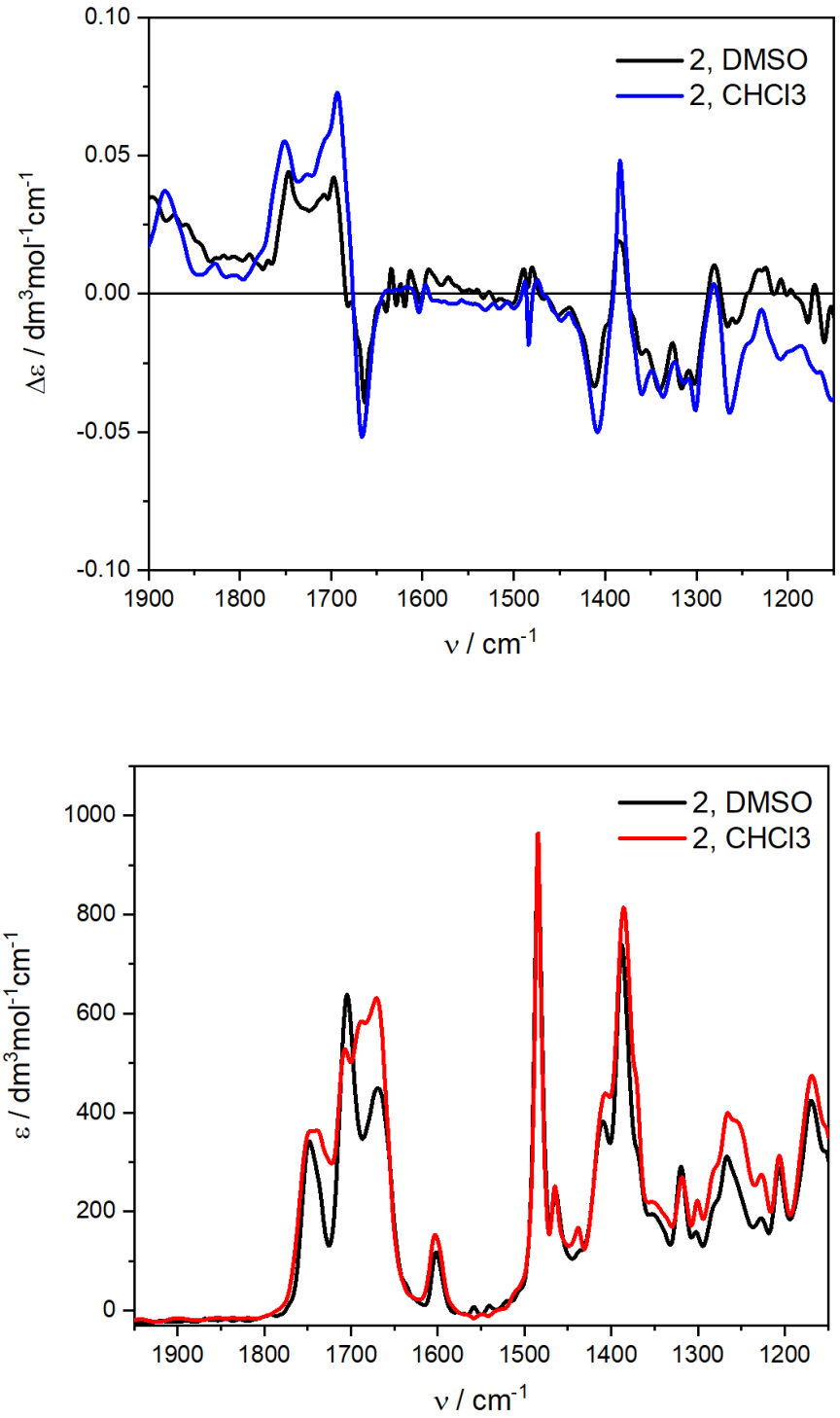


Figure S6. IR (bottom) and VCD (top) spectra of **3** measured in different solvents.

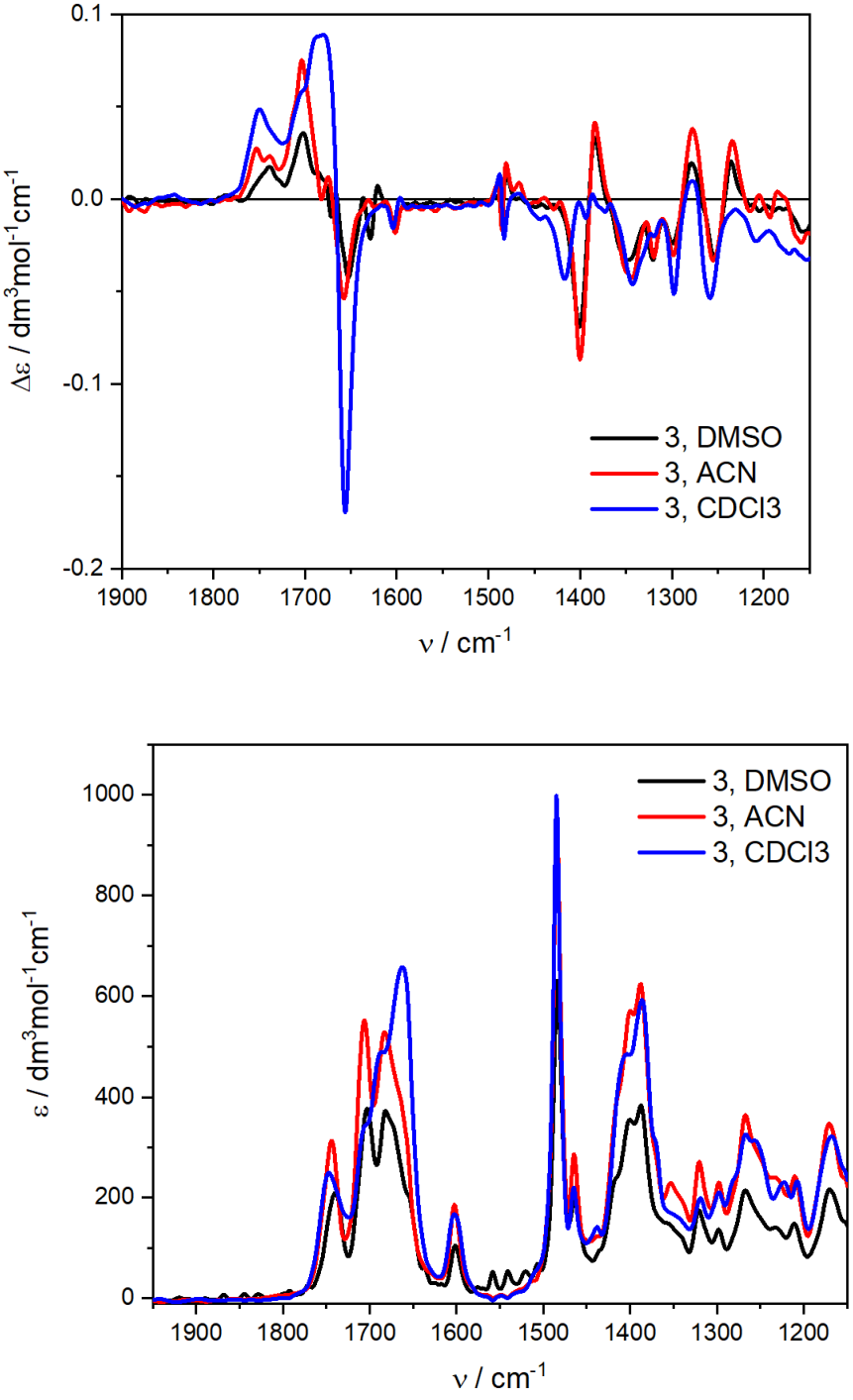


Figure S7. Expansion of the VCD spectrum of (**4**) calculated at B3LYP/6-311+G(d,p)/PCM level using the DFT-optimized X-ray structure.

Plotting parameters: band-width, 8 cm-1, no shift; vertical blue sticks represent the contributing transitions corresponding to the normal modes show below (same order from left to right). Light-blue arrows are the displacement vectors.

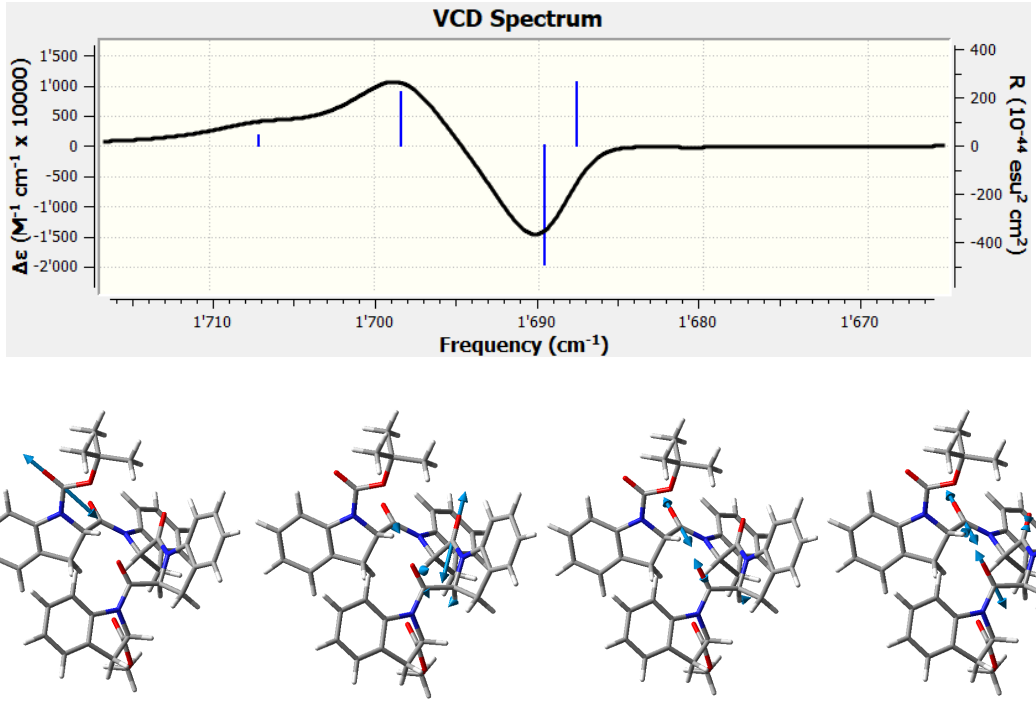


Figure S8. Calculated ECD spectra for **4** at TD-CAM-B3LYP/def2-SVP and at TD-CAM-B3LYP/def2-TZVP level using the structure obtained starting from the X-ray geometry.

Plotting parameters: bandwidth, 0.25 eV; wavelength shift, 20 nm; no scaling.

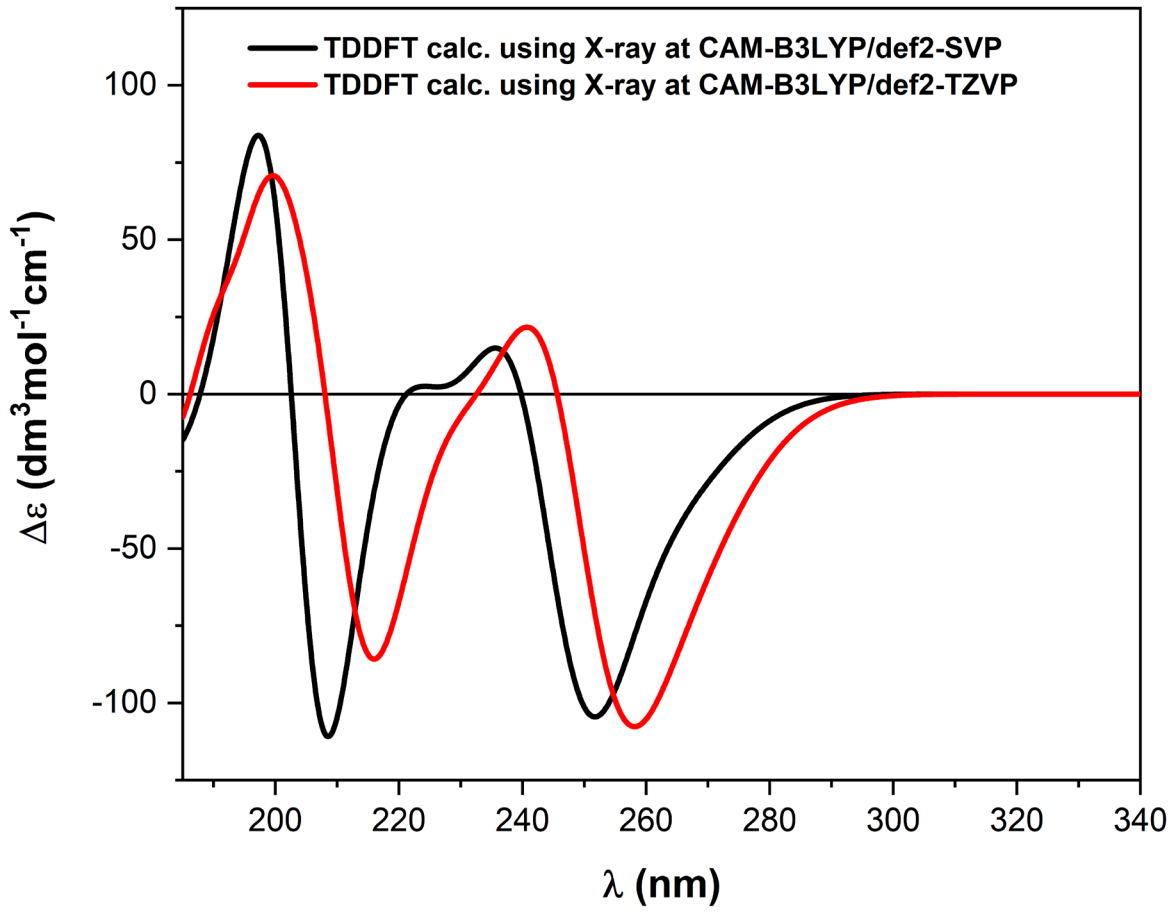


Figure S9. Calculated ECD spectra for 4 at TD-CAM-B3LYP/def2-SVP/PCM for MeOH level using the structures obtained starting from the X-ray geometry and MD simulations.

Plotting parameters: bandwidth, 0.25 eV; wavelength shift, 20 nm; no scaling.

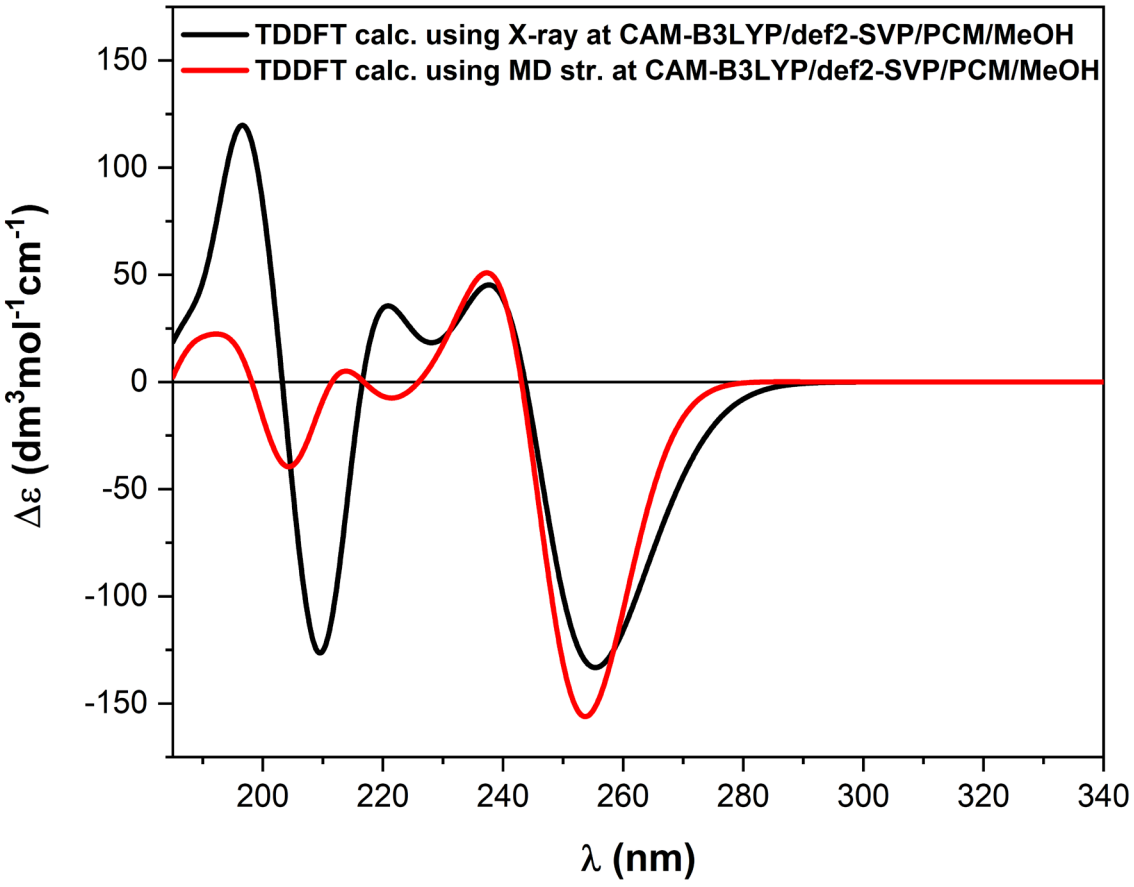


Figure S10. Calculated ECD spectra for **4** at TD-B3LYP/def2-SVP level in vacuum and with PCM solvent model for MeOH using the structures obtained starting from the X-ray geometry and MD simulations.

Plotting parameters: bandwidth, 0.25 eV; wavelength shift, 25 nm; no scaling.

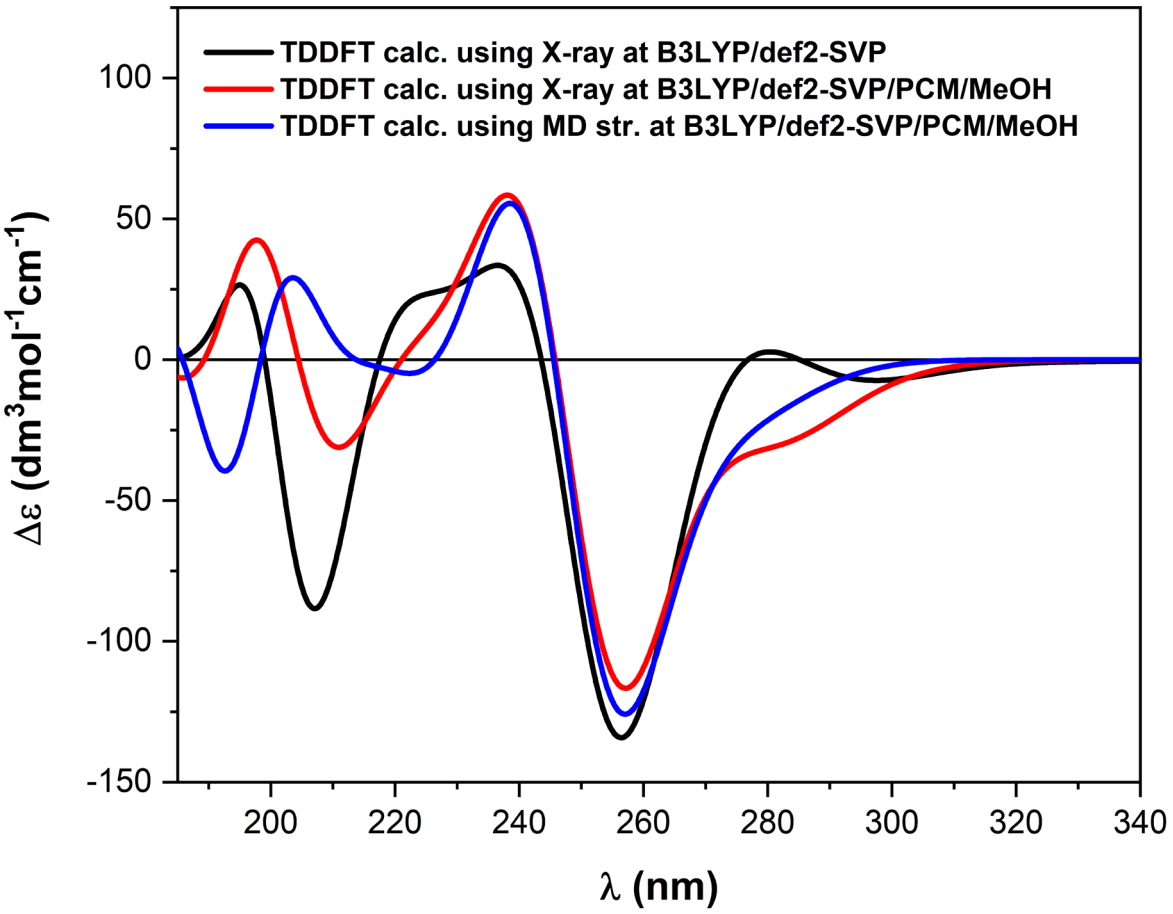
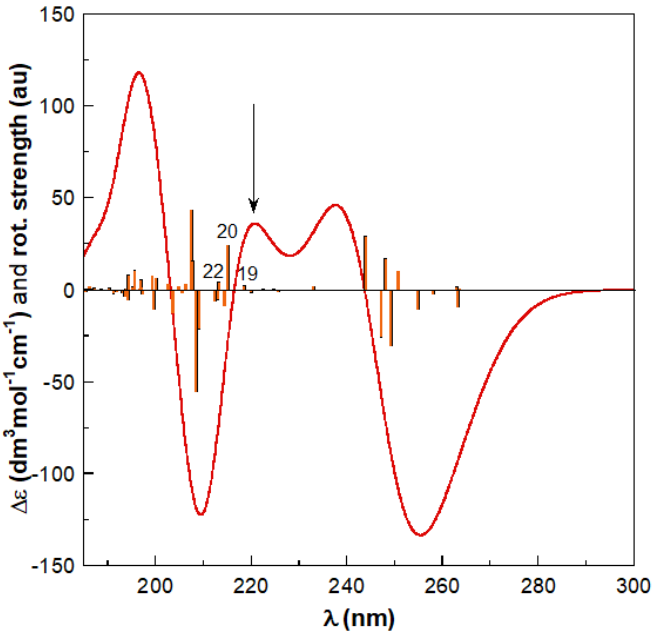


Figure S11. Calculated ECD spectrum (TD-CAM-B3LYP/def2-SVP/PCM for MeCN) using the MD-derived structure with band assignment

Plotting parameters: bandwidth, 0.25 eV; wavelength shift, 20 nm; no scaling.



The positive ECD band indicated by the arrow has main contributions from three excited states, for which the major involved single excitations are listed [(occupied MO -> virtual MO (coefficient)], and the MO displayed below.

Excited State 19: 186 ->189 (-0.32), 187 ->189 (0.55)
Excited State 20: 181 ->189 (-0.27), 181 ->192 (0.29), 185 ->198 (-0.22)
Excited State 22: 188 ->190 (0.55)

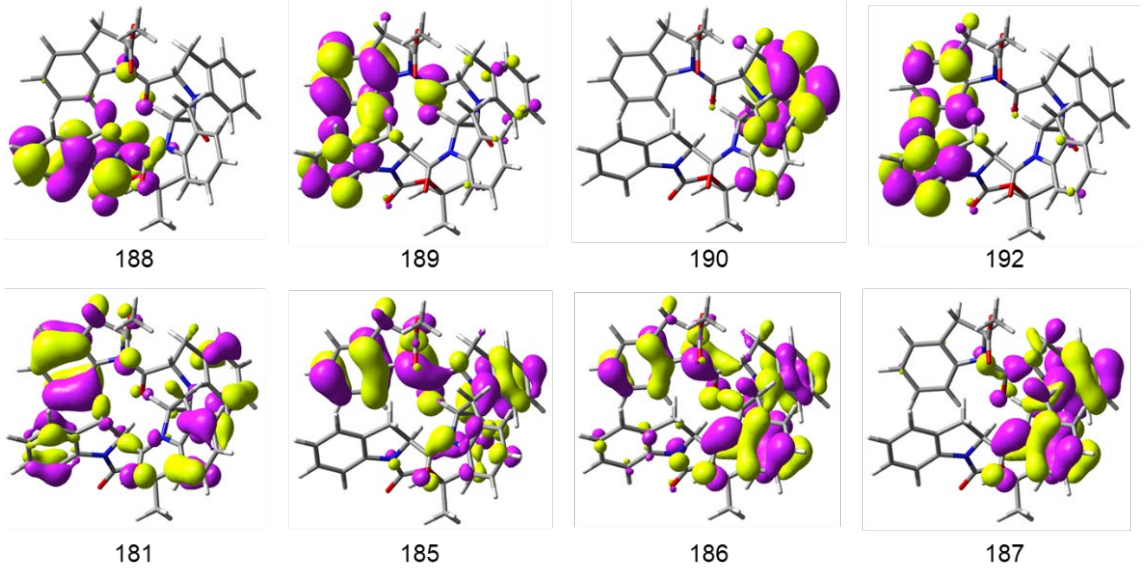
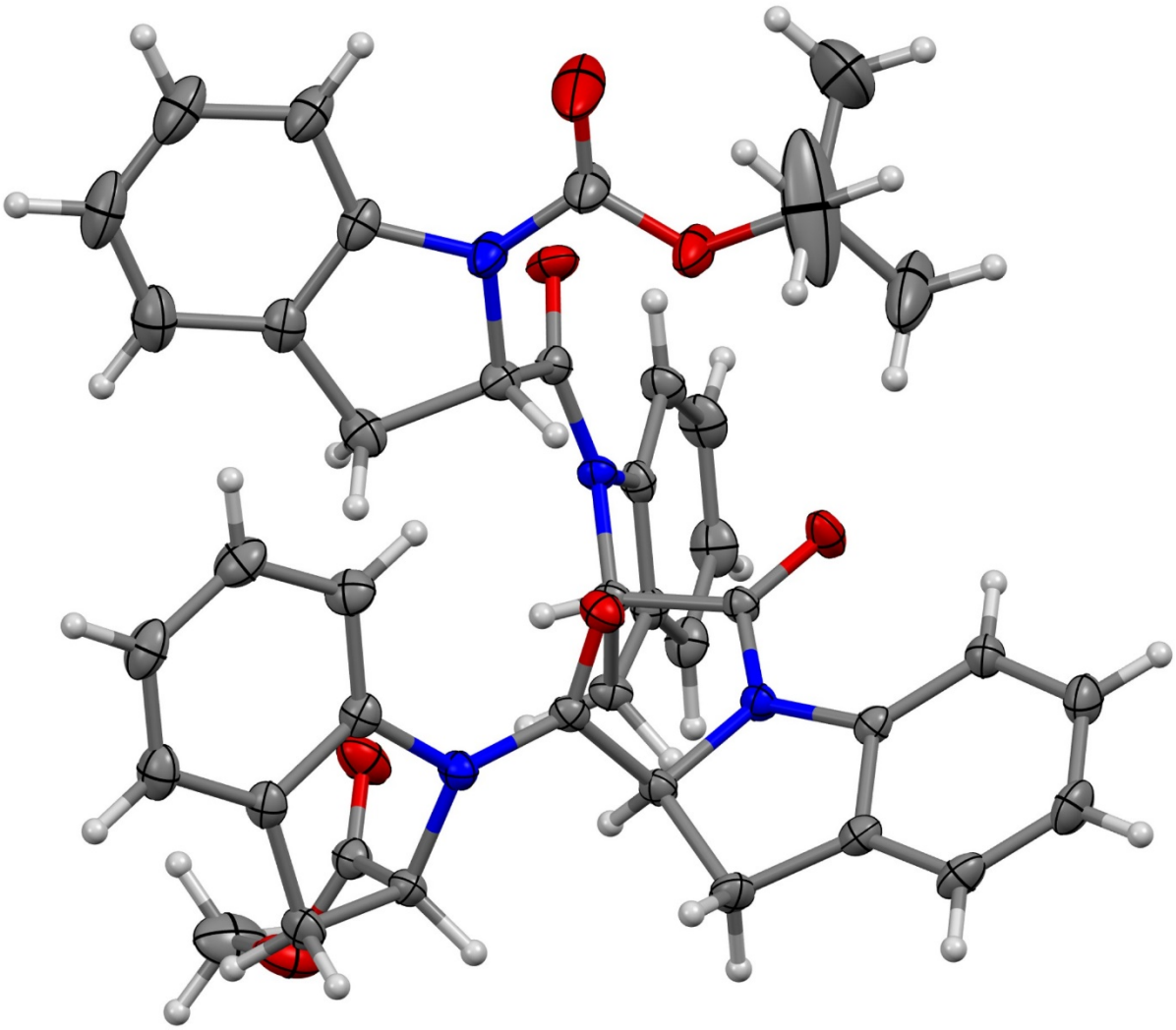


Figure S12. View of the molecular structure of (4). Ellipsoids are represented at 20% probability.



Coordinates of the DFT-optimized geometries

DFT-optimized X-ray structure (**4**)

B3LYP-D3/6-311+G(d,p)/IEFPCM(DMSO)

E=-2370.883667, no imaginary freq

Symbol	X	Y	Z
C	-0.370965	4.483148	3.712077
H	-0.266642	5.496894	4.086986
H	0.520492	3.896067	3.928692
H	-1.249892	4.001053	4.137888
O	-0.532356	4.621826	2.277962
O	-0.662850	2.385398	2.059404
C	-0.676727	3.497688	1.583538
C	-0.861835	3.813001	0.099055
H	-0.047542	4.461995	-0.215654
N	-0.905961	2.579479	-0.709796
C	-2.238280	4.484971	-0.159419
H	-2.631877	4.955418	0.740310
H	-2.134967	5.259778	-0.922961
C	-3.078610	3.340644	-0.662949
C	-4.454195	3.247014	-0.804498
H	-5.092595	4.073058	-0.513449
C	-5.004460	2.069424	-1.321521
H	-6.078697	1.977100	-1.425930
C	-4.175944	1.013226	-1.696036
H	-4.608321	0.098536	-2.082972
C	-2.787927	1.098367	-1.564565
H	-2.151647	0.278404	-1.852756
C	-2.258848	2.271028	-1.032074
C	0.168437	1.813624	-1.046418
O	0.075306	0.821427	-1.758982
C	1.535483	2.240705	-0.482032
H	1.445801	2.568779	0.549222
N	2.469956	1.100414	-0.566598
C	2.187826	3.341517	-1.363765
H	1.451199	3.861658	-1.977419
H	2.684124	4.085432	-0.735929
C	3.183928	2.569507	-2.187856
C	3.916042	2.982013	-3.289253
H	3.791318	3.982733	-3.686689
C	4.816419	2.088297	-3.878497
H	5.394241	2.394351	-4.742216
C	4.968461	0.804549	-3.356460
H	5.665495	0.115652	-3.819132
C	4.233377	0.376890	-2.246581
H	4.344389	-0.618053	-1.849090
C	3.339016	1.278648	-1.674581
C	2.393238	-0.028766	0.200932
O	3.112501	-1.001157	0.022883
C	1.422432	0.014153	1.396303
H	0.524086	0.583852	1.193323
N	1.084510	-1.363281	1.812182
C	2.162744	0.602516	2.628504
H	2.979261	1.263989	2.336535

H	1.463038	1.180284	3.237258
C	2.629306	-0.634115	3.352866
C	3.545875	-0.762600	4.383033
H	4.067407	0.107532	4.765155
C	3.787412	-2.031402	4.922898
H	4.504552	-2.148401	5.726511
C	3.110160	-3.143736	4.425983
H	3.305434	-4.123452	4.846235
C	2.183636	-3.026372	3.383989
H	1.663256	-3.886798	2.995089
C	1.957229	-1.757828	2.859292
C	0.045656	-2.108444	1.326449
O	-0.146974	-3.272518	1.652827
C	-0.940712	-1.348098	0.436652
H	-0.410517	-0.717258	-0.268724
C	-1.926369	-0.533611	1.331007
H	-1.645286	-0.590614	2.384686
H	-1.924240	0.520481	1.060225
C	-3.262230	-1.172798	1.069195
C	-4.496675	-0.867391	1.617434
H	-4.584394	-0.085116	2.362992
C	-5.627242	-1.570474	1.187736
H	-6.599795	-1.339743	1.605728
C	-5.501223	-2.565239	0.219013
H	-6.379704	-3.107100	-0.112116
C	-4.259857	-2.884194	-0.340889
H	-4.162815	-3.650722	-1.093206
C	-3.145773	-2.172820	0.099071
N	-1.802884	-2.267694	-0.321032
C	-1.343398	-3.034739	-1.359510
O	-0.045702	-2.772702	-1.579723
O	-2.033201	-3.824505	-1.983266
C	0.700714	-3.415591	-2.687774
C	2.066489	-2.745796	-2.594429
H	2.507191	-2.895122	-1.608756
H	2.732711	-3.167284	-3.350242
H	1.979885	-1.671869	-2.766219
C	0.804606	-4.915681	-2.425468
H	1.243745	-5.097266	-1.441789
H	-0.172154	-5.394468	-2.474353
H	1.454224	-5.367696	-3.178885
C	0.036826	-3.091678	-4.024859
H	0.692480	-3.422680	-4.833787
H	-0.925550	-3.588634	-4.127734
H	-0.105085	-2.012706	-4.122527

DFT-optimized MD all-cis conformer (**4**)

B3LYP-D3/6-311+G(d,p)/IEFPCM(DMSO)

E=-2370.883667, no imaginary freq

Symbol	X	Y	Z
C	-1.128977	-3.285328	4.403830
C	-3.333840	-1.928323	3.276140
C	-2.419264	-3.493610	4.903839
C	-0.949939	-2.404124	3.348600
C	-2.042373	-1.732894	2.789088

C	-3.502402	-2.818684	4.342321
N	-1.593052	-0.899406	1.725781
C	-0.198990	-1.259872	1.381706
C	0.322017	-1.981497	2.659546
C	-0.182804	-2.236188	0.181881
O	-1.190240	-2.855722	-0.129541
C	-2.335969	0.095536	1.144818
O	-3.510195	0.288730	1.432553
N	1.022374	-2.424088	-0.442349
C	1.262700	-3.369339	-1.479618
C	2.631136	-3.418027	-1.760566
C	3.383541	-2.488472	-0.845237
C	2.252190	-1.641858	-0.188632
C	3.120860	-4.263699	-2.744437
C	2.225465	-5.072956	-3.451317
C	0.862264	-5.022392	-3.162067
C	0.357002	-4.171180	-2.173886
C	2.138156	-0.243265	-0.844015
O	1.228200	0.007222	-1.624460
N	3.118693	0.659072	-0.537395
C	3.257735	1.951512	-1.126470
C	4.473992	2.516070	-0.727468
C	5.234449	1.547371	0.140656
C	4.157450	0.491244	0.501857
C	4.838822	3.780066	-1.166188
C	3.975293	4.480304	-2.014951
C	2.767707	3.907048	-2.411796
C	2.387145	2.633843	-1.975155
C	3.563085	0.702130	1.903642
O	2.384812	0.844795	2.138339
O	4.522787	0.667077	2.825430
C	4.113977	0.821074	4.208421
C	-1.594356	1.032791	0.165134
N	-2.562058	1.883486	-0.552453
C	-2.604830	3.175767	0.023226
C	-1.549617	3.312543	0.932592
C	-0.713876	2.057909	0.943292
C	-1.377310	4.492357	1.639797
C	-2.270631	5.549704	1.430918
C	-3.315644	5.407070	0.518879
C	-3.501388	4.220357	-0.199150
C	-3.376667	1.445167	-1.568484
O	-4.228179	2.139086	-2.099444
O	-3.084889	0.173951	-1.892653
C	-3.813944	-0.539622	-2.978576
C	-3.617276	0.185642	-4.311297
C	-3.121323	-1.900388	-3.004485
C	-5.287815	-0.687691	-2.597986
H	-0.280476	-3.804817	4.835448
H	-4.174792	-1.411285	2.842819
H	-2.575888	-4.181873	5.726245
H	-4.500389	-2.986428	4.731396
H	0.387596	-0.367655	1.183764
H	0.892503	-1.281842	3.276598
H	0.974529	-2.822365	2.419809
H	4.102281	-1.866785	-1.381083
H	3.931351	-3.047588	-0.081458

H	2.414643	-1.543908	0.881684
H	4.183048	-4.297617	-2.960227
H	2.592040	-5.737946	-4.224523
H	0.172170	-5.650307	-3.714234
H	-0.697958	-4.131981	-1.957149
H	6.046824	1.076306	-0.419571
H	5.667044	2.001528	1.030850
H	4.584284	-0.510382	0.481699
H	5.781820	4.216948	-0.857069
H	4.245755	5.470054	-2.363769
H	2.102680	4.455211	-3.069362
H	1.452624	2.194600	-2.284724
H	3.428518	0.020883	4.485158
H	3.635979	1.789845	4.348709
H	5.031958	0.758214	4.785783
H	-1.008414	0.460242	-0.550575
H	-0.476174	1.717832	1.951802
H	0.233200	2.215792	0.420855
H	-0.559021	4.594500	2.344403
H	-2.149726	6.477173	1.978446
H	-4.006420	6.227789	0.360466
H	-4.312904	4.113600	-0.901676
H	-2.553175	0.340485	-4.506984
H	-4.021238	-0.435420	-5.115016
H	-4.125326	1.148063	-4.326133
H	-3.192885	-2.393883	-2.034096
H	-3.593649	-2.535238	-3.757664
H	-2.064915	-1.790952	-3.258377
H	-5.383313	-1.169761	-1.621967
H	-5.792498	0.276894	-2.569535
H	-5.786260	-1.319057	-3.338037

Structures and energies of the optimized clusters

clu_000
B3LYP-D3(BJ)/6-311+G(d,p)/IEFPCM(DMSO)
E= -2371.121968, no imaginary freq

O	0.354227	0.858419	2.517590
C	0.676269	0.048572	3.720222
C	H.092091	0.979713	4.854710
H	0.258476	1.599307	5.182398
H	1.437305	0.381259	5.701255
H	1.913427	1.624879	4.534156
C	-0.512491	-0.840097	4.081003
H	-1.346550	-0.258290	4.468851
H	-0.838976	-1.397053	3.201723
H	-0.196966	-1.552144	4.847498
C	H.846995	-0.796850	3.233130
H	2.203053	-1.431671	4.047428
H	1.533939	-1.427682	2.401503
H	2.669288	-0.163720	2.896567
C	-0.714855	H.659784	2.469142
O	-1.462740	H.931601	3.392083
N	-0.867860	2.142346	H.189336
C	-2.002164	2.823402	0.699232
C	-1.916007	2.939828	-0.691752
C	-0.630267	2.339014	-1.192002
H	0.011542	3.097590	-1.646092
H	-0.808006	1.575125	-1.949211
C	-2.943871	3.522430	-1.414473
H	-2.880176	3.594385	-2.493860
C	-4.070858	3.994282	-0.733986
C	-4.145338	3.879714	0.653998
C	-3.113453	3.294682	H.394626
H	-3.176428	3.195076	2.466452
H	-5.021869	4.244884	1.176263
H	-4.887130	4.444077	-1.285853
C	0.028010	H.748343	0.092752
H	0.072531	0.664731	0.069829
C	H.437491	2.316423	0.272213
O	H.645406	3.318015	0.942289
N	2.411152	H.680828	-0.445246
C	3.723992	2.180191	-0.658927
C	4.277067	H.570740	-1.789196
C	3.276796	0.628176	-2.407994
H	3.704827	-0.335526	-2.684773
H	2.826114	1.064487	-3.303350
C	5.562321	H.887951	-2.195498
H	5.994317	1.415649	-3.070281
C	6.294718	2.826319	-1.458623
C	5.732221	3.428756	-0.334557
C	4.435115	3.114419	0.085853

H	4.000013	3.575919	0.957934
H	C.307653	4.150781	0.232856
H	N.303038	3.081651	-1.761653
C	2.205212	0.483202	-1.291596
H	1.212357	0.493790	-1.718724
C	2.513615	-0.796116	-0.491466
O	3.476256	-0.814307	0.262694
N	H.763184	-1.906619	-0.757400
C	2.053929	-3.219123	-0.293876
C	H.213815	-4.133193	-0.938919
C	0.324603	-3.413413	-1.920585
H	-0.712888	-3.747306	-1.890197
H	0.688888	-3.537516	-2.944153
C	H.297141	-5.485504	-0.653434
H	0.644065	-6.192773	-1.151376
C	2.235590	-5.922638	0.288198
C	3.070022	-5.004305	0.923121
C	2.993190	-3.635595	0.644440
H	3.629593	-2.923643	1.143500
H	3.790365	-5.350024	1.655231
H	2.309816	-6.976815	0.526499
C	0.470125	-1.935551	-1.472539
H	0.487522	-1.259406	-2.317853
C	-0.648084	-1.588866	-0.479186
O	-0.480726	-1.757714	0.723849
N	-1.834063	-1.090966	-0.935816
C	-2.323830	-0.781860	-2.233007
C	-3.527254	-0.076349	-2.113568
C	-3.937171	0.052997	-0.671442
H	-4.913147	-0.403534	-0.495168
H	-3.999003	1.093048	-0.352582
C	-4.187650	0.383788	-3.241077
H	-5.113159	0.938261	-3.140004
C	-3.650171	0.120247	-4.503596
C	-2.474761	-0.618418	-4.617765
C	-1.800318	-1.087685	-3.487389
H	-0.913831	-1.685586	-3.623306
H	-2.072096	-0.846704	-5.597072
H	-4.155479	0.475777	-5.393062
C	-2.813516	-0.691192	0.095672
H	-2.325484	-0.045574	0.820646
C	-3.336492	-1.911643	0.837206
O	-3.436773	-3.020212	0.365951
O	-3.719253	-1.567582	2.068255
C	-4.290611	-2.614308	2.886313
H	-5.182748	-3.018853	2.409097
H	-4.541526	-2.137388	3.829453
H	-3.557749	-3.405967	3.039346

clu_001
B3LYP-D3(BJ)/6-311+G(d,p)/IEFPCM(DMSO)

E= -2371.125946 , no imaginary freq

O	0.463418	2.375947	-1.913068
C	-0.159562	2.633329	-3.234188
C	0.497271	H.748631	-4.292166
H	-0.072574	1.825847	-5.221117
H	1.524808	2.049729	-4.488302
H	0.481656	0.706521	-3.965515
C	-1.602195	2.201220	-3.003868
H	-1.639463	1.145902	-2.734721
H	-2.057008	2.776055	-2.196575
H	-2.181443	2.356260	-3.916758
C	-0.069683	4.120946	-3.561644
H	0.962767	4.430776	-3.714517
H	-0.636536	4.322037	-4.474019
H	-0.504369	4.712434	-2.752360
C	H.787447	2.485575	-1.727960
O	2.582171	2.998972	-2.498618
N	2.134877	H.922618	-0.527616
C	3.450791	H.760083	-0.047307
C	3.441439	0.905875	H.059608
C	2.041727	0.437951	H.351471
H	1.745678	0.637920	2.382992
H	1.936190	-0.633955	1.193335
C	4.625046	0.571039	H.696312
H	4.616313	-0.097799	2.549577
C	5.829976	H.097399	1.217609
C	5.828158	H.949423	0.113905
C	4.639469	2.295786	-0.536661
H	4.638303	2.949190	-1.394619
H	C.763904	2.355157	-0.253110
H	C.763571	0.841986	1.704419
C	H.164597	1.240638	0.341946
H	0.550403	0.596227	-0.276219
C	0.294533	2.242656	H.105625
O	0.654661	3.398846	H.286056
N	-0.842551	H.725216	1.663045
C	-1.631021	2.362717	2.656483
C	-2.451185	H.414138	3.277959
C	-2.182383	0.047519	2.701691
H	-3.090611	-0.519436	2.493527
H	-1.558224	-0.550302	3.370372
C	-3.320771	H.793687	4.286625
H	-3.957276	1.059639	4.767425
C	-3.364160	3.137692	4.676025
C	-2.540082	4.073595	4.053372
C	-1.659548	3.702194	3.031155
H	-1.025968	4.426152	2.544576
H	-2.582153	5.112969	4.357542
H	-4.042234	3.450554	5.460942
C	-1.393670	0.378591	H.405359
H	-0.597037	-0.339580	1.258092

C	-2.383998	0.441128	0.226003
O	-2.961010	H.484971	-0.041778
N	-2.650630	-0.739320	-0.411203
C	-3.586101	-0.909098	-1.464743
C	-3.619944	-2.252622	-1.849024
C	-2.693622	-3.066481	-0.984543
H	-2.052866	-3.730366	-1.566397
H	-3.252340	-3.680420	-0.274240
C	-4.450194	-2.670222	-2.876517
H	-4.471709	-3.712120	-3.174723
C	-5.259068	-1.728133	-3.520415
C	-5.224558	-0.391624	-3.124988
C	-4.388186	0.041519	-2.091823
H	-4.352486	1.076229	-1.794613
H	-5.852019	0.334052	-3.629165
H	-5.911703	-2.038199	-4.327572
C	-1.873747	-1.982505	-0.231732
H	-1.795434	-2.216807	0.825499
C	-0.481622	-1.799049	-0.862072
O	-0.286473	-0.913157	-1.684937
N	0.500237	-2.649361	-0.451053
C	H.873266	-2.538903	-0.812351
C	2.571823	-3.646995	-0.326719
C	H.614978	-4.626251	0.301151
H	1.964837	-5.032861	1.249024
H	1.418334	-5.466265	-0.369262
C	3.947440	-3.725762	-0.476991
H	4.492224	-4.581278	-0.095052
C	4.620504	-2.682889	-1.122174
C	3.910890	-1.589755	-1.616439
C	2.523685	-1.502811	-1.477411
H	1.978152	-0.657590	-1.861434
H	4.437897	-0.780993	-2.107824
H	5.696955	-2.724851	-1.235641
C	0.323198	-3.780575	0.480498
H	-0.560856	-4.362410	0.229381
C	0.192071	-3.301976	H.925604
O	0.356991	-2.162428	2.296905
O	-0.122354	-4.320780	2.719618
C	-0.247797	-4.027317	4.133834
H	-1.035746	-3.291742	4.289931
H	0.698850	-3.650142	4.518390
H	-0.504817	-4.973717	4.600113

clu_002
B3LYP-D3(BJ)/6-311+G(d,p)/IEFPCM(DMSO)
E= -2371.119179, no imaginary freq

O	-3.799416	-1.603324	0.318145
C	-4.527606	-1.601683	H.612705
C	-5.598541	-0.540699	H.377938
H	-5.138884	0.426006	1.164989

H	-6.241188	-0.819911	0.540311
H	-6.217261	-0.440514	2.271808
C	-5.154389	-2.971453	H.854037
H	-5.772465	-3.261856	1.001193
H	-4.391943	-3.730997	2.017267
H	-5.794593	-2.920298	2.738002
C	-3.580656	-1.173977	2.731269
H	-3.090909	-0.232938	2.476070
H	-4.159691	-1.017197	3.644140
H	-2.823480	-1.931573	2.923564
C	-2.699390	-2.335398	0.135205
O	-2.253295	-3.174547	0.900923
N	-2.082457	-2.048696	-1.061308
C	-2.382221	-1.047223	-2.014725
C	-1.331226	-0.960237	-2.937087
C	-0.284664	-1.998920	-2.630613
H	0.729942	-1.598633	-2.640307
H	-0.327543	-2.812706	-3.359768
C	-1.376198	-0.046809	-3.976846
H	-0.552393	0.023291	-4.677921
C	-2.494689	0.782452	-4.107413
C	-3.549512	0.670259	-3.204966
C	-3.512681	-0.244068	-2.147283
H	-4.331469	-0.316177	-1.450886
H	-4.417094	1.311349	-3.310000
H	-2.538536	1.511390	-4.907001
C	-0.694683	-2.508394	-1.223190
H	-0.649307	-3.590144	-1.134861
C	0.168093	-1.851990	-0.140191
O	-0.235836	-0.865704	0.463703
N	H.412010	-2.362939	0.099919
C	H.978506	-3.620907	-0.259403
C	2.868227	-4.026756	0.742446
C	2.925322	-2.992659	H.836564
H	3.945391	-2.753154	2.132357
H	2.382110	-3.329998	2.723466
C	3.551515	-5.225591	0.629277
H	4.238296	-5.538582	1.407290
C	3.353373	-6.020256	-0.505457
C	2.489983	-5.595410	-1.511791
C	H.798470	-4.383610	-1.407944
H	1.170093	-4.064281	-2.223851
H	2.356617	-6.199603	-2.401071
H	3.885338	-6.958189	-0.608804
C	2.206861	-1.775019	H.211773
H	1.519958	-1.307836	1.905846
C	3.233888	-0.783650	0.636391
O	4.216049	-1.218312	0.042182
N	3.052979	0.550945	0.856273
C	4.014704	H.557892	0.561275
C	3.627244	2.754255	H.176477

C	2.352407	2.540619	H.950449
H	1.635751	3.352989	1.835428
H	2.560340	2.420651	3.017797
C	4.400278	3.895356	H.044145
H	4.097143	4.821203	1.519322
C	5.576125	3.833905	0.287840
C	5.956078	2.637541	-0.317862
C	5.181957	H.478720	-0.192783
H	5.472965	0.556357	-0.667645
H	C.865598	2.598604	-0.905915
H	C.189309	4.719276	0.170089
C	H.828414	1.213108	1.346897
H	1.317459	0.589255	2.067050
C	0.908023	H.520476	0.158048
O	H.309444	1.414104	-0.995702
N	-0.339846	2.016316	0.407758
C	-1.111532	2.128217	H.590224
C	-2.416605	2.516657	H.256648
C	-2.565729	2.671884	-0.231105
H	-2.901481	3.675054	-0.501867
H	-3.283728	1.963845	-0.643509
C	-3.376468	2.705215	2.237368
H	-4.381362	3.004474	1.962403
C	-3.037179	2.501875	3.577263
C	-1.740845	2.118097	3.907840
C	-0.763210	H.931135	2.926352
H	0.228120	1.652463	3.240430
H	-1.471142	1.961442	4.945388
H	-3.779189	2.640188	4.353893
C	-1.145222	2.371222	-0.774682
H	-1.152729	1.540323	-1.476430
C	-0.549403	3.589555	-1.464193
O	0.111839	4.443226	-0.918647
O	-0.912782	3.620958	-2.748620
C	-0.489945	4.771663	-3.513565
H	0.598079	4.828911	-3.532316
H	-0.902082	5.682771	-3.080184
H	-0.882118	4.611793	-4.514135

clu_003
B3LYP-D3(BJ)/6-311+G(d,p)/IEFPCM(DMSO)
E= -2371.119916, no imaginary freq

O	-3.551407	0.712708	-0.605382
C	-4.510548	H.361499	-1.529870
C	-5.912340	H.305893	-0.928320
H	-6.289264	0.284849	-0.890594
H	-5.907767	1.723898	0.081071
H	-6.588535	1.904059	-1.543117
C	-3.991989	2.795099	-1.577355
H	-2.973851	2.818922	-1.968469
H	-4.628637	3.395573	-2.230107

H -3.989904 3.240031 -0.580890
C -4.435915 0.708551 -2.907293
H -4.752470 -0.332273 -2.869792
H -5.091247 1.250494 -3.593255
H -3.418398 0.761704 -3.299486
C -3.699576 -0.558081 -0.185064
O -4.458950 -1.388270 -0.654542
N -2.845242 -0.785990 0.858242
C -2.633196 -2.009898 H.523186
C -1.824765 -1.795747 2.645015
C -1.476199 -0.332689 2.768636
H -0.402073 -0.168814 2.870143
H -1.962842 0.119548 3.636231
C -1.479985 -2.854526 3.468138
H -0.851021 -2.691245 4.335916
C -1.947189 -4.136912 3.160733
C -2.744288 -4.339738 2.035857
C -3.101270 -3.279116 H.196693
H -3.722088 -3.432497 0.327534
H -3.094604 -5.337543 1.798497
H -1.679228 -4.975040 3.792474
C -2.026462 0.285139 H.451598
H -2.659046 1.145034 1.629808
C -0.880082 0.628977 0.504366
O -0.334974 -0.258330 -0.140105
N -0.456304 H.926882 0.428730
C -1.133517 3.119684 0.820627
C -0.919568 4.109158 -0.144517
C -0.010009 3.585285 -1.226840
H 0.784978 4.285358 -1.480984
H -0.567965 3.360120 -2.140254
C -1.500613 5.357610 -0.004196
H -1.343724 C.122900 -0.755631
C -2.281932 5.622455 H.126670
C -2.443013 4.648984 2.109899
C -1.854553 3.386495 H.977262
H -1.945213 2.666008 2.777402
H -3.015762 4.871243 3.002190
H -2.741008 C.595877 1.250086
C 0.544958 2.276298 -0.614383
H 0.576996 1.467473 -1.332466
C H.895200 2.536100 0.071972
O 2.007250 3.497379 0.827730
N 2.942849 H.709674 -0.209057
C 4.267576 H.891695 0.275904
C 5.131049 H.024125 -0.401120
C 4.362911 0.231273 -1.424500
H 4.629527 -0.825795 -1.427260
H 4.529747 0.622887 -2.431892
C 6.483718 H.002901 -0.104271
H N.149755 0.327982 -0.629503

C	6.975112	H.863794	0.883096
C	6.108372	2.726941	H.551337
C	4.740488	2.756255	H.260145
H	4.071443	3.421135	1.780660
H	C.494546	3.388603	2.317899
H	O.029937	1.856530	1.130110
C	2.888015	0.460372	-0.993622
H	2.238556	0.575089	-1.852960
C	2.429086	-0.700496	-0.087994
O	2.457048	-0.599496	H.130253
N	2.096712	-1.856427	-0.733206
C	H.755872	-3.083807	-0.106852
C	H.718203	-4.101184	-1.066131
C	2.081295	-3.544857	-2.419433
H	1.419336	-3.883159	-3.215325
H	3.104229	-3.819016	-2.691688
C	H.398967	-5.397401	-0.699108
H	1.366484	-6.186025	-1.442230
C	H.115238	-5.672106	0.643962
C	H.151816	-4.649907	1.589891
C	H.469699	-3.336509	1.230856
H	1.482090	-2.542976	1.959652
H	0.912553	-4.865469	2.623313
H	0.857527	-6.680212	0.946078
C	H.989113	-2.017761	-2.207507
H	2.790716	-1.489356	-2.713816
C	0.670950	-1.405985	-2.690269
O	0.603336	-0.327374	-3.242560
O	-0.370070	-2.183004	-2.421164
C	-1.675788	-1.636517	-2.713032
H	-2.387681	-2.346489	-2.303592
H	-1.804612	-1.535465	-3.790499
H	-1.774506	-0.669890	-2.227076

clu_004
B3LYP-D3(BJ)/6-311+G(d,p)/IEFPCM(Chloroform)
E= -2371.105182, no imaginary freq

O	4.981413	-0.363934	0.366334
C	5.673459	-1.631061	0.053957
C	5.265051	-2.109112	-1.338048
H	5.651427	-3.118660	-1.496945
H	4.176686	-2.134467	-1.422634
H	5.662487	-1.457715	-2.114668
C	N.181899	-1.446837	0.196367
H	N.676221	-2.415030	0.083829
H	N.566091	-0.765903	-0.561148
H	N.423680	-1.052123	1.186087
C	5.127537	-2.567322	H.129095
H	4.041953	-2.652577	1.044197
H	5.567217	-3.560258	1.014796
H	5.370103	-2.191296	2.125202

C	5.064022	0.711795	-0.440297
O	5.873213	0.880971	-1.331840
N	4.097841	H.616582	-0.076419
C	3.768943	2.799418	-0.771095
C	2.631027	3.375200	-0.194333
C	2.187225	2.560321	0.994169
H	1.116919	2.352020	1.001570
H	2.430948	3.076321	1.927309
C	2.103231	4.547923	-0.707857
H	1.224907	4.998196	-0.259270
C	2.721556	5.147586	-1.810678
C	3.857071	4.567442	-2.373593
C	4.401797	3.384811	-1.863292
H	5.275907	2.929990	-2.302401
H	4.330255	5.035306	-3.229126
H	2.316513	C.062128	-2.226735
C	3.021882	H.256759	0.859317
H	3.453785	0.932906	1.801046
C	2.185180	0.127087	0.253653
O	2.183197	-0.082798	-0.952087
N	H.435129	-0.648760	1.092803
C	H.175240	-0.597292	2.486289
C	0.444664	-1.735370	2.854785
C	0.219495	-2.623178	H.660043
H	-0.813377	-2.961448	1.574741
H	0.858575	-3.509069	1.707399
C	0.042883	-1.928222	4.165407
H	-0.526939	-2.809812	4.435708
C	0.374210	-0.971888	5.129414
C	H.091401	0.162212	4.759054
C	H.494659	0.369755	3.436703
H	2.018364	1.278196	3.192357
H	1.335394	0.912849	5.501320
H	0.063550	-1.106740	C.158162
C	0.630685	-1.714460	0.475102
H	1.241347	-2.216758	-0.269362
C	-0.590601	-1.088855	-0.201011
O	-0.891393	0.082807	-0.008692
N	-1.387325	-1.876876	-0.983258
C	-1.313606	-3.229782	-1.397056
C	-2.434655	-3.536580	-2.179265
C	-3.332405	-2.336939	-2.324190
H	-4.338025	-2.542110	-1.950996
H	-3.423486	-2.024291	-3.366308
C	-2.603312	-4.803439	-2.713091
H	-3.476988	-5.027650	-3.314484
C	-1.637748	-5.783731	-2.470834
C	-0.520731	-5.474600	-1.699680
C	-0.342901	-4.200684	-1.154195
H	0.537128	-4.011472	-0.563579
H	0.231794	-6.230985	-1.511322

H	-1.757056	-6.778511	-2.882042
C	-2.625835	-1.243632	-1.482325
H	-2.340666	-0.393265	-2.093043
C	-3.487294	-0.824238	-0.281620
O	-3.538080	-1.532340	0.714539
N	-4.224284	0.315852	-0.424970
C	-5.090370	0.864524	0.555744
C	-5.790086	H.945667	0.012849
C	-5.425388	2.125230	-1.437875
H	-5.189658	3.159018	-1.693630
H	-6.238488	1.800250	-2.092046
C	-6.684161	2.663438	0.789752
H	-7.224758	3.503909	0.369531
C	-6.877236	2.289075	2.123743
C	-6.176109	H.207646	2.654509
C	-5.269981	0.476397	H.880568
H	-4.723173	-0.357583	2.289529
H	-6.327907	0.925104	3.689699
H	-7.570923	2.842754	2.744975
C	-4.195196	H.194481	-1.616865
H	-4.275403	0.609469	-2.529007
C	-2.900386	H.998908	-1.718004
O	-2.271452	2.104147	-2.747300
O	-2.583261	2.583630	-0.568161
C	-1.322458	3.288825	-0.538400
H	-0.517885	2.597708	-0.782269
H	-1.224466	3.654429	0.480138
H	-1.336637	4.116068	-1.247533

clu_005
B3LYP-D3(BJ)/6-311+G(d,p)/IEFPCM(Chloroform)
E= -2371.115279, no imaginary freq

O	4.631238	-0.447941	-0.614569
C	5.878465	-0.172352	0.134629
C	6.406119	H.074779	-0.567470
H	N.333240	1.400828	-0.091612
H	C.607801	0.866742	-1.619914
H	5.677019	1.885112	-0.506989
C	5.539237	0.127084	H.593100
H	5.107727	-0.741690	2.087901
H	C.451835	0.411616	2.121591
H	4.840739	0.964938	1.654168
C	6.844270	-1.344034	-0.017825
H	N.809483	-1.070570	0.415037
H	C.471555	-2.233081	0.487466
H	C.996887	-1.571800	-1.075262
C	3.806338	-1.457608	-0.289137
O	4.009751	-2.315915	0.547712
N	2.653208	-1.344194	-1.030618
C	H.605603	-2.294299	-1.062040
C	0.730475	-1.993065	-2.110569

C	H.183774	-0.758071	-2.843575
H	0.459180	0.049237	-2.729943
H	1.328267	-0.934016	-3.909795
C	-0.387761	-2.781292	-2.332645
H	-1.072710	-2.544321	-3.138347
C	-0.621831	-3.882101	-1.501296
C	0.254813	-4.166291	-0.455407
C	H.379602	-3.373621	-0.212625
H	2.049914	-3.583076	0.605536
H	0.061651	-5.011752	0.194322
H	-1.488096	-4.511219	-1.668880
C	2.538498	-0.397656	-2.163018
H	3.363029	-0.586976	-2.848541
C	2.649804	H.111988	-1.903176
O	3.075245	H.777879	-2.841395
N	2.242091	H.694352	-0.734459
C	2.216738	3.100311	-0.513873
C	H.860768	3.362485	0.812155
C	H.684400	2.076468	1.569072
H	0.765727	2.045864	2.156443
H	2.520441	1.913075	2.254925
C	H.745363	4.664231	1.271221
H	1.464813	4.858261	2.300230
C	H.993183	5.719648	0.388801
C	2.352698	5.451779	-0.930612
C	2.471171	4.141914	-1.404635
H	2.746841	3.939651	-2.425631
H	2.542444	C.272332	-1.612785
H	1.903716	C.743778	0.730633
C	H.682352	1.004408	0.445867
H	2.303394	0.161365	0.706885
C	0.258353	0.533836	0.164899
O	-0.401792	H.020256	-0.747445
N	-0.278158	-0.434494	0.961379
C	0.230187	-1.189802	2.046949
C	-0.676410	-2.208868	2.362622
C	-1.887370	-2.145159	H.474133
H	-2.808434	-2.038582	2.050360
H	-1.974965	-3.047023	0.866060
C	-0.396597	-3.120713	3.365909
H	-1.103119	-3.910280	3.595259
C	0.802791	-3.012431	4.074662
C	H.689367	-1.981627	3.776947
C	H.412569	-1.054017	2.770190
H	2.117915	-0.260524	2.596105
H	2.613686	-1.884991	4.333516
H	1.036742	-3.721246	4.859446
C	-1.625555	-0.906435	0.582656
H	-1.595499	-1.157171	-0.473448
C	-2.636241	0.207686	0.833376
O	-2.502111	0.982053	H.773163

N	-3.696917	0.317369	-0.019312
C	-4.105973	-0.459685	-1.132990
C	-5.004206	0.285266	-1.907900
C	-5.216762	H.644425	-1.291071
H	-6.268592	1.923754	-1.225911
H	-4.701161	2.422495	-1.859668
C	-5.556929	-0.254080	-3.057529
H	-6.248904	0.327591	-3.655785
C	-5.217332	-1.558057	-3.432132
C	-4.351327	-2.305674	-2.637968
C	-3.796019	-1.773240	-1.471556
H	-3.165447	-2.396258	-0.858622
H	-4.110313	-3.325663	-2.913070
H	-5.642646	-1.992480	-4.328549
C	-4.567985	H.493099	0.109994
H	-3.973091	2.359627	0.387531
C	-5.610885	H.263741	1.198128
O	-5.893096	0.195417	H.683560
O	-6.198296	2.423177	H.519656
C	-7.246624	2.359150	2.511942
H	-8.057016	1.720270	2.160966
H	-7.589903	3.382686	2.635348
H	-6.850010	1.970135	3.449419

clu_006
B3LYP-D3(BJ)/6-311+G(d,p)/IEFPCM(DMSO)
E= -2371.122935, no imaginary freq

O	3.826441	-2.294475	0.302806
C	3.936671	-3.639239	-0.315451
C	3.155184	-4.510638	0.662435
H	3.159001	-5.545097	0.313406
H	3.608552	-4.476154	1.655159
H	2.120358	-4.171765	0.736469
C	3.261083	-3.622986	-1.684468
H	3.267964	-4.634486	-2.096450
H	2.220883	-3.303928	-1.591321
H	3.780117	-2.963445	-2.378401
C	5.401247	-4.062086	-0.381076
H	5.959189	-3.450403	-1.087454
H	5.862870	-3.979256	0.605582
H	5.456658	-5.106310	-0.697555
C	4.320674	-1.193217	-0.285965
O	5.068901	-1.160154	-1.246775
N	3.829117	-0.080905	0.350759
C	4.158775	H.263831	0.061804
C	3.498401	2.109508	0.958276
C	2.689569	H.310601	1.946796
H	1.637161	1.591936	1.928861
H	3.044776	1.450373	2.968609
C	3.636190	3.483643	0.853306
H	3.112355	4.139081	1.538846

C	4.449795	4.011270	-0.153996
C	5.108765	3.157918	-1.038014
C	4.972998	H.769158	-0.947271
H	5.473884	1.108063	-1.636770
H	5.736703	3.573020	-1.817792
H	4.563765	5.084306	-0.249839
C	2.908773	-0.164983	H.500772
H	3.394137	-0.726216	2.296625
C	H.606634	-0.946781	1.289241
O	H.153139	-1.529457	2.269403
N	0.967197	-0.989750	0.075644
C	-0.044071	-1.945996	-0.244725
C	-0.371725	-1.847742	-1.599975
C	0.444144	-0.780772	-2.269951
H	-0.174292	-0.057743	-2.800117
H	1.148020	-1.210502	-2.985389
C	-1.316540	-2.694043	-2.158343
H	-1.566805	-2.613818	-3.209865
C	-1.934132	-3.652209	-1.349599
C	-1.597927	-3.746953	-0.001221
C	-0.651623	-2.895988	0.574279
H	-0.413517	-2.959138	1.621512
H	-2.089578	-4.480010	0.626401
H	-2.675577	-4.319520	-1.772083
C	H.210339	-0.110689	-1.095483
H	2.268055	-0.084471	-1.323568
C	0.851045	H.380896	-0.985125
O	H.389132	2.110213	-1.807407
N	0.022521	H.862908	-0.004901
C	-0.201230	3.254205	0.209257
C	-1.203223	3.427155	H.166709
C	-1.684738	2.094324	H.665564
H	-2.771622	2.010269	1.686690
H	-1.319246	1.908625	2.678563
C	-1.579557	4.696848	H.575887
H	-2.358631	4.823588	2.318718
C	-0.934945	5.806350	H.021775
C	0.076241	5.625298	0.078959
C	0.459687	4.349714	-0.343710
H	1.241218	4.216232	-1.071650
H	0.577899	C.488070	-0.343518
H	-1.219471	C.805996	1.327436
C	-1.052141	H.090694	0.663693
H	-0.643419	0.228352	1.172787
C	-2.084205	0.646349	-0.375053
O	-2.074787	H.113365	-1.510633
N	-3.040982	-0.252758	-0.008979
C	-3.287850	-0.981023	H.185634
C	-4.335046	-1.883177	0.963595
C	-4.836084	-1.787910	-0.450906
H	-5.913094	-1.618346	-0.498668

H	-4.620326	-2.700304	-1.009052
C	-4.751955	-2.745195	H.963936
H	-5.557819	-3.445441	1.776642
C	-4.117146	-2.707663	3.208187
C	-3.081488	-1.803546	3.427671
C	-2.656319	-0.928317	2.425441
H	-1.848864	-0.252785	2.646923
H	-2.587441	-1.769435	4.391134
H	-4.431054	-3.377596	3.999209
C	-4.036414	-0.599001	-1.039133
H	-3.524232	-0.869122	-1.959222
C	-4.938647	0.595460	-1.316628
O	-5.163024	H.492769	-0.538308
O	-5.494348	0.481776	-2.525837
C	-6.446293	H.505352	-2.899045
H	-5.960875	2.480742	-2.905597
H	-7.282575	1.510547	-2.200463
H	-6.781245	1.236793	-3.896916

clu_007
B3LYP-D3(BJ)/6-311+G(d,p)/IEFPCM(DMSO)
E= -2371.120577, no imaginary freq

O	3.752352	-0.170518	0.673075
C	4.190899	0.091403	2.063584
C	3.095491	-0.350638	3.031943
H	3.357657	-0.023658	4.040701
H	2.140927	0.100594	2.755642
H	2.981754	-1.433793	3.037540
C	5.528144	-0.594755	2.328115
H	5.422962	-1.677996	2.324970
H	C.259257	-0.304664	1.569779
H	5.904635	-0.279161	3.304222
C	4.345484	H.609018	2.070537
H	5.088932	1.923630	1.335399
H	3.395759	2.090015	1.833001
H	4.667504	1.943793	3.058428
C	3.380374	-1.396781	0.267765
O	3.606932	-2.444688	0.845505
N	2.717334	-1.296705	-0.929594
C	2.121981	-2.365573	-1.628322
C	H.367050	-1.864715	-2.694964
C	H.482783	-0.363069	-2.756916
H	0.510473	0.130474	-2.807319
H	2.056517	-0.053264	-3.633722
C	0.676172	-2.726577	-3.530439
H	0.079784	-2.336080	-4.346854
C	0.754089	-4.104937	-3.302595
C	H.523346	-4.594691	-2.248613
C	2.217692	-3.734601	-1.391449
H	2.799678	-4.112412	-0.565795
H	1.579318	-5.663266	-2.075831

H	0.213319	-4.790030	-3.944068
C	2.245797	-0.000891	-1.449674
H	3.096529	0.647606	-1.635418
C	H.306407	0.638951	-0.426612
O	0.719084	-0.054622	0.394147
N	H.120454	1.992256	-0.471817
C	H.890673	2.989435	-1.140405
C	H.957913	4.134590	-0.339611
C	H.165044	3.928688	0.925253
H	0.510741	4.769873	1.147399
H	1.822205	3.774099	1.785275
C	2.665041	5.245415	-0.768403
H	2.721402	C.131844	-0.147138
C	3.291763	5.213656	-2.019345
C	3.182894	4.084850	-2.828203
C	2.467857	2.959786	-2.404167
H	2.357746	2.116517	-3.068693
H	3.642292	4.075967	-3.809267
H	3.844039	C.077600	-2.368774
C	0.361014	2.639354	0.632830
H	0.355840	1.961717	1.477295
C	-1.059052	2.996378	0.156646
O	-1.218683	3.955812	-0.591549
N	-2.108056	2.270098	0.640899
C	-3.480256	2.588915	0.442175
C	-4.264529	H.763482	1.257223
C	-3.377207	0.856931	2.070650
H	-3.738620	-0.169697	2.123831
H	-3.270992	1.231347	3.093187
C	-5.644460	H.878487	1.253389
H	-6.249834	1.237010	1.883462
C	-6.243205	2.833585	0.424163
C	-5.454320	3.654165	-0.380207
C	-4.059365	3.546062	-0.386292
H	-3.450718	4.175535	-1.014203
H	-5.925210	4.388945	-1.022842
H	-7.321958	2.932276	0.405466
C	-2.030673	0.958951	H.312924
H	-1.170948	0.912980	1.967214
C	-1.942378	-0.142662	0.249503
O	-2.129235	0.108121	-0.936419
N	-1.740226	-1.432211	0.654965
C	-1.224221	-1.965980	H.863469
C	-0.812855	-3.287991	H.648843
C	-1.131937	-3.725970	0.246094
H	-1.908419	-4.495758	0.250572
H	-0.267928	-4.127633	-0.279870
C	-0.220758	-4.021656	2.663887
H	0.103586	-5.039522	2.479645
C	-0.048481	-3.436618	3.921486
C	-0.492813	-2.135921	4.143000

C	-1.091381	-1.388119	3.125110
H	-1.435717	-0.394060	3.355122
H	-0.378043	-1.684414	5.121200
H	0.418822	-3.996071	4.722648
C	-1.627750	-2.424483	-0.431611
H	-0.907585	-2.068071	-1.165381
C	-2.967431	-2.621491	-1.117996
O	-4.046718	-2.513458	-0.582116
O	-2.788970	-2.997546	-2.387528
C	-3.980985	-3.303007	-3.145023
H	-4.620851	-2.422988	-3.206197
H	-4.523571	-4.124197	-2.677013
H	-3.629016	-3.589811	-4.132167

clu_008
B3LYP-D3(BJ)/6-311+G(d,p)/IEFPCM(Chloroform)
E= -2371.118157, no imaginary freq

O	-4.603154	0.415077	0.931328
C	-5.688388	0.973354	0.091917
C	-5.871279	2.367041	0.684122
H	-6.653001	2.898887	0.137883
H	-6.161984	2.302370	1.734503
H	-4.943773	2.938091	0.613681
C	-5.210180	H.059586	-1.356101
H	-5.031667	0.070424	-1.775999
H	-5.974415	1.557522	-1.956847
H	-4.294688	1.651880	-1.415760
C	-6.953968	0.135217	0.248452
H	-6.826925	-0.856977	-0.180260
H	-7.211971	0.036026	1.305330
H	-7.780967	0.637703	-0.259179
C	-4.054691	-0.785450	0.679003
O	-4.505047	-1.645005	-0.057245
N	-2.870092	-0.893063	H.362682
C	-2.035233	-2.034224	H.413096
C	-0.929805	-1.766633	2.227011
C	-1.013697	-0.376472	2.800425
H	-0.133756	0.213296	2.549730
H	-1.097274	-0.395252	3.888161
C	0.051197	-2.728699	2.409555
H	0.912583	-2.510666	3.029443
C	-0.086959	-3.967964	H.775339
C	-1.195069	-4.223626	0.969842
C	-2.187565	-3.260611	0.772700
H	-3.035601	-3.449120	0.134512
H	-1.287653	-5.179557	0.469006
H	0.671168	-4.730580	1.909214
C	-2.311428	0.210416	2.170938
H	-3.026206	0.469842	2.948645
C	-2.075073	H.556998	1.468049
O	-2.184461	2.556298	2.169215

N	-1.756783	H.639516	0.137570
C	-1.575703	2.867647	-0.558860
C	-1.306979	2.608208	-1.906176
C	-1.333809	H.128750	-2.168680
H	-0.476550	0.779899	-2.745603
H	-2.237719	0.846230	-2.715010
C	-1.099102	3.645381	-2.800323
H	-0.887160	3.434535	-3.842293
C	-1.165145	4.963083	-2.338862
C	-1.440420	5.215591	-0.996475
C	-1.649123	4.176647	-0.084572
H	-1.852923	4.376583	0.953464
H	-1.488834	C.238432	-0.641318
H	-0.999845	5.785802	-3.024034
C	-1.346861	0.521998	-0.740345
H	-2.046946	-0.296897	-0.663578
C	0.049408	0.042893	-0.354481
O	0.772114	0.719851	0.370220
N	0.498574	-1.145273	-0.845182
C	-0.090980	-2.154326	-1.646414
C	0.768244	-3.257742	-1.701210
C	2.027816	-2.998163	-0.920317
H	2.914783	-3.077497	-1.552126
H	2.138777	-3.702720	-0.094201
C	0.406225	-4.402807	-2.389232
H	1.075645	-5.255071	-2.416973
C	-0.830217	-4.449667	-3.038715
C	-1.673869	-3.343544	-2.997327
C	-1.315411	-2.182409	-2.308976
H	-2.001884	-1.353405	-2.310581
H	-2.630900	-3.373224	-3.504038
H	-1.128105	-5.340893	-3.577348
C	H.839006	-1.557980	-0.383496
H	1.822545	-1.539535	0.701027
C	2.890752	-0.604907	-0.962096
O	2.793043	-0.213775	-2.117200
N	3.951701	-0.300327	-0.158125
C	5.071497	0.486457	-0.535542
C	6.025981	0.463361	0.485486
C	5.557911	-0.419201	H.613278
H	5.674086	0.042492	2.594562
H	C.105363	-1.365411	1.625699
C	N.209210	H.170905	0.355655
H	N.948068	1.155328	1.148855
C	N.435350	H.906944	-0.812417
C	6.478478	H.921098	-1.825527
C	5.279133	H.212242	-1.705054
H	4.534716	1.226902	-2.484279
H	C.658223	2.496659	-2.726012
H	O.354423	2.468954	-0.927086
C	4.065479	-0.673263	H.271008

H 3.798442 -1.714769 1.424685
C 3.146531 0.166169 2.159677
O 2.451564 -0.313542 3.027873
O 3.255852 H.462365 1.893143
C 2.381453 2.357196 2.618008
H 1.354925 2.184264 2.300438
H 2.702893 3.357497 2.341365
H 2.484699 2.198863 3.690853

clu_009
B3LYP-D3(BJ)/6-311+G(d,p)/IEFPCM(DMSO)
E= -2371.117590, no imaginary freq

O -0.574441 3.523302 -0.042308
C -0.596941 4.265353 H.244209
C -1.867984 5.098800 H.111119
H -2.740872 4.451787 1.002018
H -1.999741 5.712525 2.004325
H -1.807437 5.758387 0.242793
C -0.713938 3.281514 2.406110
H -0.901525 3.842624 3.324705
H -1.547254 2.596721 2.239764
H 0.195546 2.697786 2.530745
C 0.636674 5.157799 H.345206
H 0.546133 5.793283 2.229467
H 1.545639 4.565226 1.431502
H 0.711772 5.803139 0.466769
C 0.354593 2.601795 -0.297955
O H.330097 2.346962 0.385286
N 0.113543 H.932651 -1.480585
C -1.055262 H.925546 -2.279804
C -1.026408 0.818139 -3.138915
C 0.257002 0.052103 -2.956670
H 0.926175 0.216131 -3.805808
H 0.105852 -1.023082 -2.852975
C -2.075255 0.570352 -4.009345
H -2.048076 -0.293475 -4.663840
C -3.169275 H.441560 -4.024229
C -3.185498 2.547890 -3.176891
C -2.131017 2.810909 -2.297167
H -2.161329 3.663063 -1.638931
H -4.034324 3.221641 -3.189399
H -4.002337 1.254681 -4.690921
C 0.849599 0.670364 -1.667089
H 0.612881 0.055457 -0.808251
C 2.356558 0.858656 -1.784812
O 2.834964 H.776521 -2.439511
N 3.113030 -0.122603 -1.207413
C 4.518788 -0.260322 -1.334343
C 4.914821 -1.510533 -0.848554
C 3.712344 -2.294715 -0.392881
H 3.848319 -2.754308 0.586576

H 3.467587 -3.088931 -1.102711
C 6.250545 -1.875646 -0.858420
H C.557010 -2.844086 -0.479758
C N.197388 -0.976627 -1.362989
C 6.792468 0.265919 -1.847496
C 5.446017 0.646124 -1.841021
H 5.132472 1.608664 -2.211427
H N.530919 0.958865 -2.233665
H O.246468 -1.247005 -1.373948
C 2.581020 -1.230561 -0.374576
H 1.682928 -1.631615 -0.826157
C 2.372652 -0.741621 H.070856
O 3.241807 -0.065556 H.603966
N H.256476 -1.159101 1.738882
C H.000055 -0.904844 3.115222
C 0.011898 -1.783323 3.570705
C -0.392078 -2.718423 2.459420
H -1.467715 -2.883772 2.402350
H 0.095859 -3.691335 2.566764
C -0.439984 -1.713687 4.878043
H -1.208695 -2.391552 5.230640
C 0.109120 -0.751408 5.732930
C H.094215 0.119266 5.268596
C H.556974 0.057904 3.950112
H 2.313480 0.734968 3.588267
H 1.508693 0.865960 5.935747
H -0.236616 -0.680048 C.757196
C 0.149114 -1.977821 H.205958
H 0.510369 -2.661678 0.447790
C -0.955592 -1.059675 0.663571
O -0.988058 0.128498 0.967942
N -1.938241 -1.584027 -0.123145
C -2.204482 -2.889896 -0.613901
C -3.346831 -2.851000 -1.423650
C -3.907022 -1.456290 -1.499049
H -4.955379 -1.422445 -1.196643
H -3.841782 -1.047846 -2.508124
C -3.819761 -4.001201 -2.034554
H -4.704976 -3.959923 -2.658682
C -3.146546 -5.209230 -1.834628
C -2.017998 -5.245678 -1.019694
C -1.534368 -4.092388 -0.395874
H -0.670479 -4.178331 0.241571
H -1.500830 -6.182865 -0.853152
H -3.505833 -6.115834 -2.305772
C -3.001905 -0.645266 -0.539292
H -2.557183 0.211611 -1.036331
C -3.760635 -0.148289 0.682993
O -3.954215 -0.794405 H.687064
O -4.227598 H.083742 0.469915
C -5.008630 H.672771 1.534245

H -5.287692 2.659073 1.174239
H -4.404415 1.750900 2.437705
H -5.894355 1.068755 1.729589

clu_010
B3LYP-D3(BJ)/6-311+G(d,p)/IEFPCM(Chloroform)
E= -2371.112403, no imaginary freq

O -4.499704 -0.621487 -0.435124
C -5.514505 -0.571443 -1.518240
C -4.937859 0.156050 -2.730296
H -4.785659 1.213615 -2.523296
H -3.986688 -0.292106 -3.022309
H -5.632845 0.058805 -3.567595
C -5.735214 -2.050390 -1.820418
H -6.464385 -2.155620 -2.626199
H -4.801249 -2.522390 -2.128810
H -6.115894 -2.569292 -0.938205
C -6.794222 0.076027 -0.996120
H -7.131481 -0.430316 -0.088685
H -6.646395 1.132719 -0.781564
H -7.576606 -0.022514 -1.752455
C -4.023649 0.491500 0.124082
O -4.331879 H.635257 -0.163446
N -3.070410 0.225855 H.084915
C -2.770337 -1.004211 H.729785
C -2.045525 -0.750645 2.900817
C -1.792652 0.724496 3.060295
H -0.735673 0.955647 2.918427
H -2.092136 1.102386 4.037711
C -1.660710 -1.794886 3.727119
H -1.105879 -1.593916 4.636636
C -2.003081 -3.104900 3.377338
C -2.705702 -3.347540 2.198549
C -3.091928 -2.305322 H.352890
H -3.620411 -2.505682 0.436539
H -2.951658 -4.364881 1.917989
H -1.715277 -3.929882 4.017944
C -2.658488 H.362287 1.938976
H -3.560171 1.799798 2.368241
C -1.961795 2.572282 H.308194
O -2.127366 3.638612 H.891795
N -1.151227 2.471228 0.211081
C -0.431144 3.568063 -0.340418
C 0.194284 3.172213 -1.525816
C -0.142469 H.744012 -1.841129
H 0.737554 1.152971 -2.095585
H -0.846500 1.687983 -2.675977
C 0.982155 4.056956 -2.242707
H 1.472567 3.735562 -3.154213
C H.145396 5.360387 -1.766029
C 0.515029 5.752064 -0.586337

C	-0.282437	4.866960	0.145248
H	-0.763402	5.172625	1.058569
H	0.645056	C.762889	-0.217642
H	1.763730	C.063344	-2.311245
C	-0.812648	H.239906	-0.532663
H	-1.706120	0.669663	-0.744152
C	0.177442	0.386341	0.258855
O	0.815327	0.859379	H.192651
N	0.364184	-0.903185	-0.155618
C	-0.474311	-1.738296	-0.957697
C	-0.407004	-3.049552	-0.472651
C	0.524288	-3.114667	0.707295
H	1.194928	-3.970919	0.666897
H	-0.043219	-3.154386	1.639655
C	-1.138055	-4.057332	-1.074316
H	-1.089603	-5.070143	-0.691678
C	-1.930744	-3.754762	-2.186290
C	-1.964327	-2.456332	-2.684757
C	-1.229487	-1.430319	-2.081750
H	-1.243763	-0.444743	-2.518485
H	-2.552629	-2.231689	-3.566007
H	-2.503018	-4.535816	-2.672199
C	H.289193	-1.778556	0.614893
H	1.456378	-1.325069	1.584469
C	2.593430	-1.978087	-0.184210
O	2.612079	-2.777501	-1.111771
N	3.712749	-1.300814	0.210486
C	5.013122	-1.499902	-0.335776
C	5.950740	-0.822357	0.453590
C	5.250705	-0.153472	H.608498
H	5.603869	0.854412	1.818056
H	5.354359	-0.746109	2.522507
C	N.297703	-0.862962	0.134137
H	O.022592	-0.337497	0.745413
C	N.706906	-1.590324	-0.988541
C	6.766331	-2.262492	-1.766904
C	5.403299	-2.229164	-1.455537
H	4.675427	-2.743809	-2.060610
H	N.090282	-2.819598	-2.638220
H	O.756343	-1.627102	-1.255281
C	3.778521	-0.157016	H.137344
H	3.081229	-0.257372	1.962951
C	3.430356	H.133583	0.385416
O	3.103269	H.189768	-0.775702
O	3.567905	2.183554	H.194715
C	3.210556	3.472553	0.644680
H	3.794339	3.672878	-0.252647
H	3.441068	4.192600	1.425046
H	2.149850	3.486219	0.408624

clu_011

B3LYP-D3(BJ)/6-311+G(d,p)/IEFPCM(Chloroform)

E= -2371.106804, no imaginary freq

O	3.862856	0.324170	H.410232
C	4.130897	H.377068	2.422629
C	2.932330	H.541371	3.353944
H	2.650823	0.583729	3.794426
H	3.207092	2.222861	4.162793
H	2.074221	1.949052	2.825105
C	5.328077	0.802711	3.173827
H	5.634367	1.494084	3.961294
H	5.070877	-0.153805	3.633979
H	C.170741	0.650868	2.496490
C	4.501882	2.677316	H.714001
H	4.832707	3.407248	2.456425
H	5.322489	2.506784	1.013321
H	3.651728	3.091512	1.174289
C	2.901451	0.471898	0.493649
O	2.052609	H.350415	0.483121
N	2.961107	-0.490391	-0.477917
C	3.909867	-1.516286	-0.701822
C	3.730408	-2.028552	-1.992457
C	2.627922	-1.279621	-2.700281
H	1.926689	-1.944465	-3.207231
H	3.032172	-0.589902	-3.446038
C	4.526037	-3.063387	-2.454195
H	4.383549	-3.460191	-3.453004
C	5.513001	-3.590390	-1.614121
C	5.683834	-3.073759	-0.331361
C	4.884489	-2.030838	0.146945
H	5.017198	-1.640828	1.142915
H	C.446009	-3.488980	0.317778
H	C.140499	-4.402843	-1.959936
C	H.951417	-0.489300	-1.544505
H	1.727394	0.536976	-1.816307
C	0.703067	-1.257179	-1.076857
O	0.802832	-2.131107	-0.230765
N	-0.482925	-0.955741	-1.693640
C	-1.620262	-1.821511	-1.683911
C	-2.491043	-1.470304	-2.715729
C	-1.985892	-0.265023	-3.454570
H	-2.647208	0.586683	-3.293353
H	-1.895534	-0.429036	-4.528567
C	-3.658130	-2.189908	-2.921507
H	-4.335069	-1.915471	-3.722564
C	-3.950284	-3.266532	-2.079667
C	-3.081473	-3.595758	-1.041451
C	-1.903162	-2.877681	-0.823233
H	-1.247544	-3.120823	-0.005612
H	-3.322667	-4.416599	-0.376651
H	-4.860753	-3.835436	-2.226056
C	-0.585354	-0.001742	-2.822470

H	0.183714	-0.240676	-3.555663
C	-0.412751	H.507825	-2.605187
O	-0.107276	2.123014	-3.624520
N	-0.661718	2.147552	-1.424639
C	-0.677134	3.570229	-1.318112
C	-0.780548	3.945540	0.021020
C	-0.811334	2.737898	0.906316
H	-1.673006	2.757620	1.576084
H	0.095380	2.667342	1.509809
C	-0.839816	5.281737	0.384521
H	-0.921417	5.560149	1.429179
C	-0.794787	6.259389	-0.611830
C	-0.695818	5.880140	-1.949244
C	-0.634525	4.535822	-2.325072
H	-0.553092	4.253447	-3.360313
H	-0.664694	C.638964	-2.722427
H	-0.839584	N.308575	-0.345450
C	-0.875787	H.538633	-0.085958
H	-0.061141	0.860687	0.134492
C	-2.222627	0.823246	0.003641
O	-3.084073	0.974931	-0.848143
N	-2.408427	0.027658	H.107630
C	-3.673886	-0.529874	H.454651
C	-3.782496	-0.621347	2.843730
C	-2.541076	-0.056211	3.488322
H	-2.172122	-0.656187	4.320297
H	-2.717467	0.959225	3.855845
C	-4.922453	-1.157962	3.419474
H	-5.012686	-1.234565	4.497002
C	-5.953309	-1.605525	2.585355
C	-5.828863	-1.511170	H.199731
C	-4.682656	-0.970795	0.609758
H	-4.577372	-0.910525	-0.461158
H	-6.628005	-1.871349	0.562490
H	-6.848877	-2.034255	3.019195
C	-1.534849	-0.024842	2.306285
H	-0.876449	0.831878	2.355351
C	-0.684188	-1.296171	2.354676
O	-1.121401	-2.418042	2.275109
O	0.594735	-0.988933	2.593503
C	H.505542	-2.101294	2.766333
H	1.204852	-2.692642	3.631443
H	2.480068	-1.648487	2.925715
H	1.509273	-2.706903	1.864672

clu_012
B3LYP-D3(BJ)/6-311+G(d,p)/IEFPCM(Chloroform)
E= -2371.113844, no imaginary freq

O	-4.309015	-1.379758	0.038530
C	-5.582213	-1.491299	-0.716991
C	-5.424447	-2.839911	-1.412637

H -5.320416 -3.640828 -0.677728
H -6.305544 -3.042829 -2.024648
H -4.543744 -2.838042 -2.057318
C -6.756300 -1.510286 0.257798
H -6.874167 -0.549800 0.756300
H -7.673038 -1.734176 -0.292873
H -6.611223 -2.289131 1.010008
C -5.682336 -0.358828 -1.735951
H -6.557041 -0.526933 -2.368557
H -5.784788 0.607848 -1.246936
H -4.798542 -0.345390 -2.375817
C -4.034935 -0.315491 0.795556
O -4.740273 0.666997 0.947958
N -2.796331 -0.409842 H.391194
C -1.933688 -1.531353 H.503164
C -0.977741 -1.284052 2.495009
C -1.167967 0.084202 3.092218
H -0.312386 0.723995 2.872652
H -1.297959 0.053662 4.174288
C -0.011214 -2.233053 2.789489
H 0.733751 -2.034712 3.551172
C -0.006546 -3.443371 2.089205
C -0.955349 -3.674369 H.095187
C -1.926652 -2.721322 0.779340
H -2.644218 -2.902794 -0.002661
H -0.941672 -4.606895 0.543170
H 0.737309 -4.197968 2.315397
C -2.457606 0.615523 2.400859
H -3.277914 0.667434 3.115606
C -2.284825 2.079669 H.970453
O -2.496948 2.911449 2.846531
N -1.846720 2.441791 0.725876
C -1.508999 3.775882 0.360261
C -1.183808 3.823170 -0.998327
C -1.369127 2.469981 -1.624609
H -0.532372 2.169659 -2.256659
H -2.274719 2.448540 -2.237438
C -0.788481 5.010348 -1.592151
H -0.533666 5.036447 -2.645532
C -0.722056 6.169436 -0.813560
C -1.054660 6.117404 0.538662
C -1.453572 4.924202 H.148340
H -1.709187 4.888987 2.193721
H -1.002229 N.017801 1.139698
H -0.411641 N.105825 -1.261412
C -1.525182 H.534697 -0.395024
H -2.327488 0.826578 -0.538469
C -0.215169 0.800632 -0.121885
O 0.582374 H.216654 0.711590
N 0.067197 -0.326717 -0.836921
C -0.635112 -1.045927 -1.832949

C	0.030765	-2.252019	-2.085449
C	H.271094	-2.366450	-1.243196
H	2.163702	-2.511029	-1.854722
H	1.200057	-3.206517	-0.550438
C	-0.469863	-3.159497	-3.003165
H	0.051356	-4.092481	-3.184791
C	-1.646465	-2.856933	-3.693812
C	-2.289823	-1.644913	-3.461358
C	-1.794124	-0.724072	-2.535294
H	-2.314480	0.209371	-2.406341
H	-3.189447	-1.398231	-4.012182
H	-2.048339	-3.556168	-4.416709
C	H.317682	-1.023770	-0.473301
H	1.312092	-1.162571	0.603431
C	2.505191	-0.161767	-0.891974
O	2.456535	0.528803	-1.902776
N	3.623375	-0.179793	-0.109270
C	3.953568	-0.910956	H.060103
C	5.026726	-0.284073	H.706259
C	5.447586	0.943372	0.938750
H	C.526194	1.007524	0.794011
H	5.125694	1.856673	1.445467
C	5.545892	-0.808932	2.877994
H	C.374148	-0.318513	3.376530
C	4.993857	-1.980996	3.404789
C	3.950148	-2.618153	2.738236
C	3.425827	-2.101098	H.550781
H	2.647809	-2.643899	1.039327
H	3.541888	-3.541222	3.132369
H	5.390543	-2.402935	4.320097
C	4.688932	0.787224	-0.405339
H	4.249468	1.722068	-0.744411
C	5.593782	0.258866	-1.512854
O	5.630642	-0.882609	-1.903106
O	C.372531	H.245012	-1.975231
C	N.320334	0.886375	-3.005138
H	O.011167	0.130110	-2.632469
H	N.848548	1.805474	-3.243755
H	C.794326	0.506048	-3.880441

clu_013
B3LYP-D3(BJ)/6-311+G(d,p)/IEFPCM(DMSO)
E= -2371.122296, no imaginary freq

O	-4.834620	-0.535189	0.403319
C	-5.833265	-0.779369	H.477531
C	-6.523014	0.576883	H.585705
H	-6.964187	0.861553	0.628339
H	-7.317016	0.525718	2.333152
H	-5.810449	1.346991	1.888130
C	-6.810205	-1.858970	H.022129
H	-7.608910	-1.953139	1.761736

H	-7.260666	-1.585714	0.065074
H	-6.312920	-2.822318	0.921110
C	-5.121532	-1.131972	2.781205
H	-4.332615	-0.406372	2.984888
H	-5.847995	-1.103397	3.596673
H	-4.683120	-2.127467	2.739969
C	-3.931337	-1.447523	0.065680
O	-3.871599	-2.599199	0.472090
N	-2.999736	-0.957391	-0.825089
C	-3.000585	0.297888	-1.496038
C	-2.260383	0.198938	-2.676069
C	-1.761204	-1.206116	-2.871507
H	-0.681730	-1.249912	-3.022248
H	-2.219104	-1.679689	-3.741988
C	-2.072290	H.311888	-3.481963
H	-1.494082	1.233405	-4.395742
C	-2.631856	2.533322	-3.096551
C	-3.367981	2.620331	-1.916846
C	-3.561319	H.506798	-1.097538
H	-4.107723	1.587614	-0.173335
H	-3.779579	3.573553	-1.608646
H	-2.483010	3.414025	-3.709302
C	-2.192132	-1.945126	-1.564282
H	-2.822325	-2.801085	-1.797567
C	-0.945332	-2.568277	-0.924058
O	-0.472408	-3.516752	-1.541066
N	-0.301319	-2.027081	0.165071
C	0.969066	-2.526542	0.598192
C	H.166092	-2.241279	1.948401
C	-0.032338	-1.548700	2.525344
H	0.239505	-0.613033	3.014133
H	-0.545385	-2.173291	3.259237
C	2.356371	-2.583788	2.573718
H	2.507753	-2.356320	3.622495
C	3.353207	-3.221653	H.832007
C	3.150624	-3.495762	0.479798
C	H.958219	-3.151634	-0.158151
H	1.814849	-3.358494	-1.205206
H	3.933547	-3.972903	-0.096833
H	4.287314	-3.497060	2.306799
C	-0.954160	-1.296013	H.291899
H	-1.922010	-1.749975	1.468732
C	-1.258779	0.205072	H.200795
O	-2.172435	0.593590	H.924539
N	-0.534999	H.063473	0.431146
C	-0.768369	2.466773	0.357944
C	0.026169	3.014748	-0.651514
C	0.824060	H.934728	-1.327353
H	1.868580	2.203590	-1.484105
H	0.386174	1.689176	-2.297679
C	-0.033049	4.367912	-0.939777

H	0.579596	4.786684	-1.729851
C	-0.897946	5.181121	-0.201319
C	-1.682682	4.627134	0.808782
C	-1.631158	3.262491	H.106222
H	-2.247417	2.834135	1.878270
H	-2.350306	5.262134	1.379572
H	-0.956295	C.241977	-0.413632
C	0.676055	0.742237	-0.345803
H	0.548586	-0.202233	-0.854500
C	H.887376	0.673672	0.585599
O	H.828496	1.092827	1.737239
N	3.058071	0.176617	0.090946
C	3.413104	-0.408630	-1.152615
C	4.723691	-0.895441	-1.072178
C	5.310593	-0.636132	0.287911
H	C.257707	-0.096606	0.232902
H	5.492576	-1.567769	0.825778
C	5.302088	-1.554820	-2.143731
H	C.314016	-1.935234	-2.065271
C	4.565893	-1.730716	-3.318523
C	3.268433	-1.232998	-3.400679
C	2.678258	-0.562717	-2.326370
H	1.677522	-0.186636	-2.448058
H	2.696147	-1.359353	-4.311764
H	5.004867	-2.247396	-4.163104
C	4.214073	0.191054	H.004510
H	3.928217	-0.251112	1.955424
C	4.667850	H.623144	1.250337
O	4.481601	2.550955	0.498072
O	5.353069	H.698874	2.394504
C	5.921636	2.987720	2.723825
H	C.436693	2.842114	3.669128
H	5.129427	3.728560	2.827511
H	C.621139	3.297056	1.947671

clu_014
B3LYP-D3(BJ)/6-311+G(d,p)/IEFPCM(Chloroform)
E= -2371.115503, no imaginary freq

O	-4.799698	0.676010	0.268646
C	-5.513367	H.397192	-0.811000
C	-5.837818	2.732357	-0.148886
H	-4.922639	3.232930	0.172036
H	-6.361416	3.376660	-0.858197
H	-6.476926	2.582485	0.723475
C	-4.566468	H.594767	-1.992835
H	-5.060097	2.209347	-2.748839
H	-3.663581	2.116518	-1.668286
H	-4.292981	0.642844	-2.446487
C	-6.785505	0.644965	-1.190877
H	-7.392141	0.457021	-0.302044
H	-7.370775	1.258673	-1.879988

H -6.556283 -0.304289 -1.671175
C -4.251983 -0.534547 0.075420
O -4.449032 -1.275981 -0.870706
N -3.394957 -0.812150 H.111409
C -2.653766 -2.004890 H.284097
C -1.852725 -1.893997 2.425443
C -2.084006 -0.572107 3.110835
H -1.157091 -0.015078 3.247824
H -2.540315 -0.706599 4.093072
C -1.006288 -2.931646 2.784482
H -0.385022 -2.848478 3.669039
C -0.967392 -4.084417 H.993419
C -1.774930 -4.184146 0.862685
C -2.631050 -3.146309 0.487514
H -3.242269 -3.213222 -0.397951
H -1.728538 -5.072809 0.245368
H -0.304814 -4.899133 2.259347
C -3.067392 0.174712 2.161785
H -3.978949 0.445222 2.688835
C -2.520957 H.535344 1.696863
O -2.833315 2.510606 2.367644
N -1.711171 H.646155 0.596068
C -1.156952 2.874977 0.134282
C -0.484921 2.654010 -1.073208
C -0.646179 H.218143 -1.487492
H 0.254716 0.775290 -1.907445
H -1.438174 1.121212 -2.236647
C 0.172825 3.686969 -1.719400
H 0.696387 3.504522 -2.650991
C 0.149097 4.964280 -1.150362
C -0.533144 5.180266 0.045367
C -1.196877 4.142915 0.708666
H -1.713335 4.312553 1.638325
H -0.546682 C.171461 0.483357
H 0.662268 5.784283 -1.638123
C -1.089569 0.543891 -0.165666
H -1.797003 -0.252369 -0.343018
C 0.110585 -0.001901 0.615171
O 0.522056 0.563876 H.620410
N 0.765285 -1.107679 0.140692
C 0.409016 -2.060194 -0.857967
C H.214061 -3.195574 -0.720915
C 2.193887 -3.031921 0.405044
H 3.218164 -3.020238 0.030116
H 2.112633 -3.830860 1.142366
C H.055666 -4.280658 -1.567040
H 1.682452 -5.156847 -1.447614
C 0.080218 -4.235140 -2.565568
C -0.709774 -3.098080 -2.706819
C -0.552229 -1.996667 -1.863656
H -1.184075 -1.140806 -2.021527

H -1.465820 -3.055729 -3.481439
H -0.057728 -5.079294 -3.230061
C H.807816 -1.669913 1.037332
H 1.336839 -1.825086 2.006180
C 3.060313 -0.856190 H.393592
O 3.604351 -1.185390 2.441920
N 3.598598 0.097572 0.573125
C 4.846261 0.742960 0.813260
C 5.048626 H.749749 -0.134894
C 3.865181 H.849709 -1.055625
H 4.143992 1.852028 -2.110333
H 3.284461 2.755789 -0.867029
C 6.208126 2.508182 -0.124595
H C.358322 3.287210 -0.863426
C N.177387 2.255080 0.849930
C 6.967857 H.251313 1.793619
C 5.802234 0.479996 H.793045
H 5.642876 -0.292728 2.525804
H N.721370 1.057270 2.547981
H O.089787 2.838808 0.870793
C 3.020977 0.597837 -0.686658
H 1.990227 0.889843 -0.546599
C 3.103086 -0.448217 -1.788771
O 3.833328 -1.408454 -1.786765
O 2.261920 -0.135593 -2.782163
C 2.235036 -1.042834 -3.909735
H 1.479130 -0.644114 -4.580384
H 1.961194 -2.041192 -3.572617
H 3.210892 -1.062569 -4.393921

clu_015
B3LYP-D3(BJ)/6-311+G(d,p)/IEFPCM(DMSO)
E= -2371.125605, no imaginary freq

O -3.527304 -0.787546 -0.782996
C -3.829487 -0.940264 -2.225061
C -5.068649 -1.813196 -2.401275
H -5.361068 -1.811112 -3.454038
H -4.874011 -2.839516 -2.094358
H -5.900354 -1.415919 -1.814616
C -4.105084 0.500318 -2.646309
H -4.343700 0.533722 -3.711120
H -4.948036 0.910848 -2.086524
H -3.228027 1.124726 -2.465265
C -2.605701 -1.494240 -2.947336
H -1.725536 -0.882003 -2.744592
H -2.393840 -2.518363 -2.647064
H -2.791363 -1.478596 -4.024181
C -3.147209 -1.818200 -0.010393
O -3.125387 -2.992711 -0.329906
N -2.797782 -1.341192 H.230077
C -2.097521 -2.061469 2.221776

C -1.746169 -1.192588 3.262317
C -2.297912 0.185825 2.988308
H -1.578768 0.982621 3.182304
H -3.183455 0.380646 3.599526
C -1.005285 -1.653691 4.337142
H -0.723269 -0.979689 5.138096
C -0.618970 -2.999585 4.370740
C -0.985202 -3.856919 3.334830
C -1.732890 -3.403120 2.243166
H -1.998973 -4.059922 1.430494
H -0.678468 -4.896115 3.364259
H -0.032488 -3.372572 5.201761
C -2.687827 0.106040 H.488159
H -3.633504 0.584644 1.263597
C -1.563791 0.662845 0.617009
O -0.609203 -0.049275 0.318216
N -1.602858 H.947426 0.173066
C -2.474061 3.036081 0.413694
C -2.118997 4.101166 -0.423775
C -0.930628 3.734684 -1.275853
H -0.127968 4.469538 -1.195886
H -1.201604 3.655655 -2.330897
C -2.823275 5.293312 -0.383055
H -2.543883 C.113851 -1.033906
C -3.889250 5.427778 0.511963
C -4.217870 4.375488 H.363445
C -3.510713 3.170055 H.334074
H -3.769747 2.394167 2.036664
H -5.027271 4.488461 2.074629
H -4.447517 C.354897 0.554880
C -0.502360 2.349301 -0.726910
H -0.429366 1.610287 -1.517012
C 0.789126 2.437754 0.095666
O 0.761444 2.923021 H.220379
N H.942384 1.999418 -0.491059
C 3.245902 2.177305 0.050291
C 4.204225 H.849146 -0.911317
C 3.546153 H.438483 -2.200030
H 3.890761 0.460958 -2.538767
H 3.744234 2.156336 -2.998026
C 5.554980 H.930301 -0.610245
H C.297517 1.673185 -1.356704
C 5.942974 2.340443 0.667899
C 4.978625 2.657237 H.623161
C 3.614073 2.579762 H.332212
H 2.868486 2.819461 2.072044
H 5.286017 2.965363 2.615538
H C.994951 2.402387 0.918958
C 2.028372 H.422010 -1.856223
H 1.486998 2.062248 -2.547172
C H.411571 0.029089 -2.102871

O	0.783693	-0.099670	-3.153491
N	H.627915	-1.016124	-1.260265
C	H.099101	-2.323331	-1.469612
C	H.100994	-3.028754	-0.262425
C	H.599472	-2.147685	0.848565
H	2.309260	-2.640421	1.511863
H	0.765045	-1.775289	1.444633
C	0.658904	-4.341061	-0.216070
H	0.656880	-4.883482	0.721566
C	0.210708	-4.949058	-1.392715
C	0.212373	-4.237422	-2.591506
C	0.657635	-2.913664	-2.650019
H	0.650065	-2.363523	-3.576287
H	-0.137114	-4.713660	-3.500160
H	-0.138994	-5.974395	-1.371902
C	2.254842	-0.971646	0.073999
H	2.055657	-0.031375	0.569621
C	3.761268	-1.192570	-0.027046
O	4.350651	-1.562472	-1.016460
O	4.334726	-0.965958	H.156758
C	5.754440	-1.220855	H.249356
H	5.950610	-2.282815	1.100860
H	C.036787	-0.914097	2.252384
H	C.287156	-0.631606	0.505727

clu_016
B3LYP-D3(BJ)/6-311+G(d,p)/IEFPCM(DMSO)
E= -2371.123231, no imaginary freq

O	-4.090693	-1.654355	-0.954176
C	-4.573802	-2.582617	-2.005611
C	-4.384705	-4.026281	-1.546915
H	-4.850652	-4.177219	-0.570357
H	-4.869051	-4.693958	-2.263357
H	-3.329986	-4.286751	-1.482693
C	-6.055737	-2.229781	-2.092863
H	-6.538854	-2.857660	-2.843980
H	-6.547893	-2.396409	-1.132403
H	-6.186149	-1.183922	-2.378547
C	-3.865703	-2.283108	-3.324616
H	-4.331757	-2.869351	-4.120044
H	-3.966789	-1.224748	-3.576326
H	-2.808897	-2.538350	-3.274943
C	-2.808151	-1.628187	-0.576144
O	-1.916392	-2.344490	-1.003545
N	-2.574492	-0.677605	0.383838
C	-3.423105	0.321444	0.915275
C	-2.677455	H.169107	1.741874
C	-1.235916	0.743432	H.779845
H	-0.916539	0.495240	2.794787
H	-0.568921	1.524939	1.420658
C	-3.276369	2.246406	2.372589

H -2.688278 2.903933 3.002804
C -4.639228 2.484291 2.172220
C -5.375837 H.637244 1.346241
C -4.783338 0.543585 0.707377
H -5.362407 -0.103491 0.069780
H -6.432163 1.823342 1.189679
H -5.119703 3.327535 2.653638
C -1.191850 -0.507859 0.853310
H -0.565252 -0.346485 -0.018159
C -0.707021 -1.722554 H.644444
O -1.486861 -2.463940 2.228786
N 0.651426 -1.850195 H.738688
C H.333482 -2.756855 2.590750
C 2.672226 -2.367953 2.709608
C 2.908163 -1.098266 H.933319
H 3.825392 -1.117445 1.343701
H 2.952606 -0.230708 2.596284
C 3.551004 -3.107493 3.483623
H 4.588619 -2.807126 3.574336
C 3.078734 -4.246085 4.146694
C H.742021 -4.622605 4.025192
C 0.846110 -3.884772 3.244000
H -0.186674 -4.177861 3.145507
H 1.384554 -5.507517 4.538732
H 3.754694 -4.836881 4.753146
C H.642042 -1.007809 1.037255
H 1.298038 0.017897 0.983381
C H.958936 -1.606406 -0.346822
O H.764765 -2.792061 -0.573806
N 2.559044 -0.767051 -1.244601
C 3.007821 -1.137218 -2.539219
C 3.587151 -0.030553 -3.167028
C 3.574320 H.158266 -2.243109
H 3.215138 2.064593 -2.732040
H 4.572701 1.364276 -1.849708
C 4.096780 -0.135972 -4.450741
H 4.542795 0.724750 -4.935585
C 4.027754 -1.368308 -5.108952
C 3.454238 -2.468225 -4.472970
C 2.934036 -2.372802 -3.178353
H 2.484492 -3.221872 -2.690582
H 3.401897 -3.419868 -4.988813
H 4.419377 -1.466546 -6.114197
C 2.628851 0.700622 -1.098597
H 3.039334 0.958232 -0.126966
C H.214577 1.286136 -1.273460
O 0.328775 0.620043 -1.796407
N H.010105 2.553089 -0.820439
C -0.248049 3.221067 -0.809632
C -0.063567 4.550438 -0.421408
C H.404164 4.840323 -0.246755

H 1.633504 5.406313 0.654981
H 1.797609 5.398657 -1.099510
C -1.155048 5.391755 -0.272977
H -1.015053 C.422295 0.031982
C -2.437331 4.888820 -0.517000
C -2.608132 3.562861 -0.909953
C -1.515728 2.707437 -1.069681
H -1.652038 1.681871 -1.369476
H -3.604709 3.172922 -1.076851
H -3.300735 5.531014 -0.392045
C 2.034830 3.420873 -0.209058
H 2.962991 3.393746 -0.775422
C 2.338100 2.993086 H.226834
O H.751638 2.123076 1.829752
O 3.339990 3.714001 H.719497
C 3.728386 3.437653 3.088777
H 4.546152 4.121096 3.296825
H 4.056220 2.402795 3.178202
H 2.888107 3.624046 3.756193

clu_017
B3LYP-D3(BJ)/6-311+G(d,p)/IEFPCM(DMSO)
E= -2371.126363, no imaginary freq

O 3.914149 0.756370 H.813816
C 3.527486 H.439981 3.076823
C 3.088289 2.869791 2.772496
H 2.159819 2.889281 2.204818
H 2.933872 3.401745 3.714052
H 3.863515 3.392774 2.207838
C 2.450454 0.630841 3.794891
H 2.764730 -0.410024 3.899966
H 2.301852 1.045703 4.794321
H 1.504191 0.666010 3.260149
C 4.833860 H.425147 3.863785
H 4.686133 1.915515 4.827810
H 5.163771 0.399738 4.042715
H 5.616666 1.957180 3.319471
C 3.029967 0.549634 0.838551
O H.850487 0.875859 0.853786
N 3.577031 -0.082240 -0.245044
C 4.858408 -0.643540 -0.443905
C 4.910249 -1.231481 -1.713569
C 3.603423 -1.036565 -2.440851
H 3.198830 -1.976496 -2.820971
H 3.716982 -0.359933 -3.290484
C 6.063716 -1.863344 -2.148748
H C.098827 -2.319890 -3.131411
C N.179496 -1.903432 -1.305683
C N.120519 -1.310004 -0.045870
C 5.961675 -0.670981 0.405914
H 5.923774 -0.217066 1.382677

H N.986613 -1.342631 0.604870
H O.087658 -2.395229 -1.632527
C 2.679174 -0.403084 -1.363085
H 2.225305 0.517311 -1.716746
C H.614903 -1.402381 -0.890479
O H.868048 -2.212014 -0.008939
N 0.403474 -1.347337 -1.524684
C -0.654731 -2.278020 -1.323778
C -1.615533 -2.127308 -2.325670
C -1.211916 -1.053820 -3.297303
H -1.969419 -0.272567 -3.363920
H -1.049268 -1.452053 -4.299840
C -2.759768 -2.909791 -2.321946
H -3.507661 -2.788950 -3.097033
C -2.933156 -3.854215 -1.305809
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H -3.822418 -4.472887 -1.290454
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H 0.922172 -0.637948 -3.437258
C 0.048931 H.031493 -2.563632
O 0.440174 H.672903 -3.538196
N -0.469964 H.636983 -1.461563
C -0.600563 3.047937 -1.314018
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H -5.412996 -1.806983 1.910712
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C	-0.789004	-1.658997	3.346354
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C	-4.286614	-0.854204	0.274150
H	-4.425540	-1.207634	-0.744389
C	-5.222043	0.322760	0.514041
O	-4.966645	H.285540	1.199209
O	-6.391904	0.114244	-0.096416
C	-7.416248	H.114639	0.110157
H	-7.652922	1.194013	1.170854
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clu_018
B3LYP-D3(BJ)/6-311+G(d,p)/IEFPCM(DMSO)
E= -2371.122550, no imaginary freq

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C	5.516247	-2.523376	-2.539564
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H	5.139309	-3.314974	-1.887775
H	5.752157	-2.963299	-3.511184
C	3.170050	-2.025955	-3.299217
H	2.418803	-1.245296	-3.427037
H	3.371704	-2.471657	-4.275015
H	2.766672	-2.795073	-2.638057
C	4.947287	-0.269703	-3.571601
H	5.869441	0.149868	-3.173709
H	5.131296	-0.619667	-4.590025
H	4.186442	0.513161	-3.611452
C	4.842089	-0.335496	-0.537975
O	C.021399	-0.088518	-0.718445
N	4.145320	-0.024063	0.599660
C	4.631130	0.671360	H.723109
C	3.621051	0.763130	2.686741
C	2.370229	0.069931	2.206366
H	1.502197	0.729651	2.246037
H	2.140680	-0.809112	2.812286
C	3.856331	H.413624	3.886795
H	3.072913	1.487030	4.632603
C	5.117444	H.973292	4.122736
C	6.118106	H.871219	3.157169
C	5.892889	H.218343	1.940865
H	C.665629	1.138906	1.192147
H	N.092577	2.306621	3.345667
H	5.314909	2.486088	5.056307
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H	2.581566	-1.403747	0.575259
C	H.916782	0.467414	-0.275260

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H -1.437930 2.503672 1.983961
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O	-6.080640	-1.770323	-0.758604
C	-7.460498	-1.335127	-0.762085
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H	-7.518686	-0.284582	-1.045045
H	-7.900574	-1.479846	0.224209