

# Supplementary information for

## Theoretical Design, Synthesis, and in vitro Neurobiological Application of a Highly Efficient Two-photon Caged GABA Validated on an Epileptic Case

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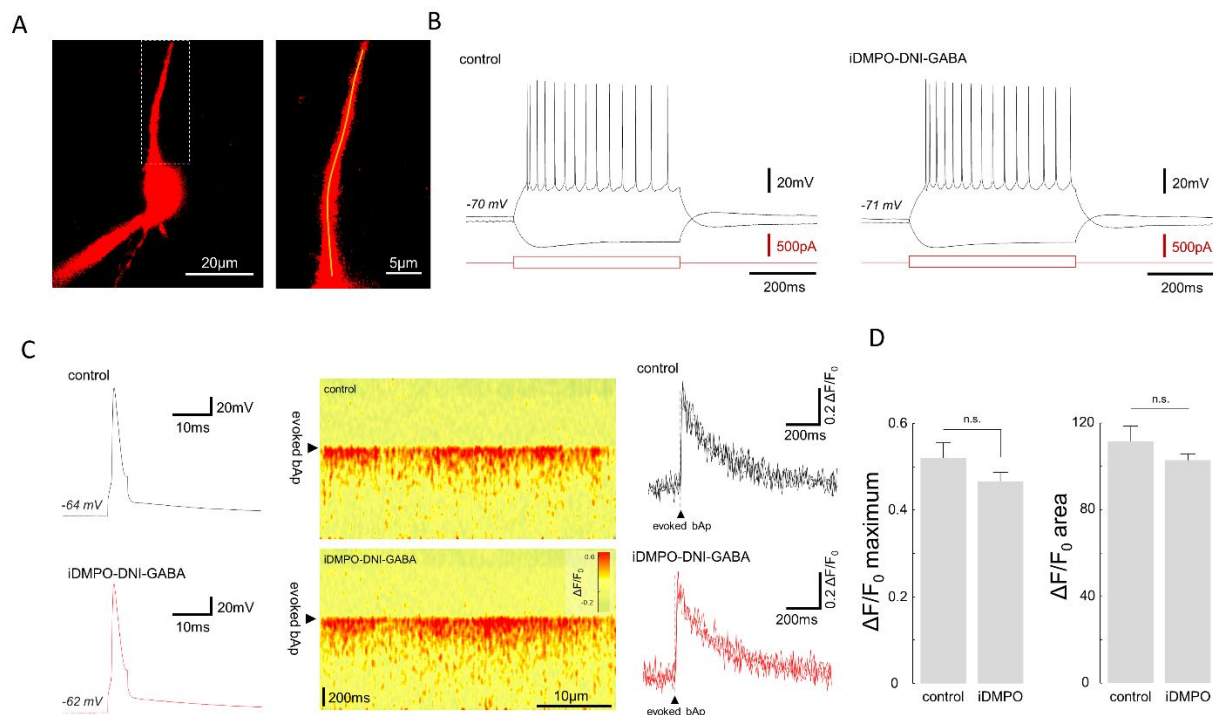
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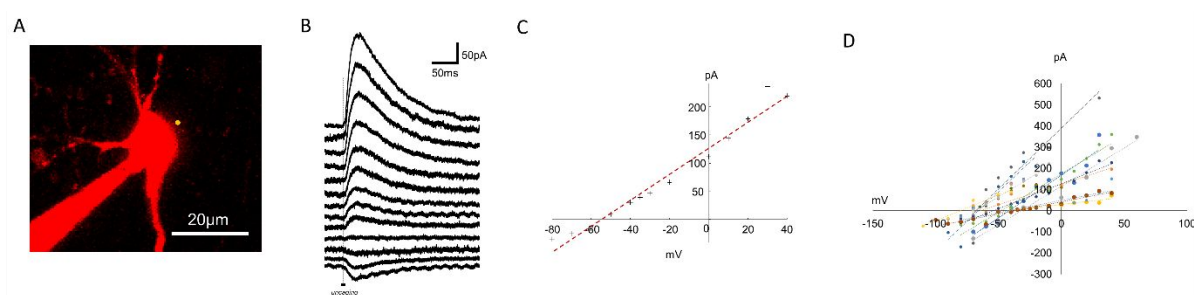
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## Supplementary figures (Figures S1–S8) for the neurobiological investigations



**Figure S1.** Bath application of iDMPO-DNI-GABA did not affect the basic physiological properties of pyramidal neurons. **A:** Maximal intensity z projection image of a cortical pyramidal neuron filled with Fluo-4 and Alexa 594. Left: White box indicates the measured dendritic segment. Right: enlarged view of the measured dendrite on left panel. Yellow line indicates the location of two-photon imaging before (control) and after the bath application of iDMPO-DNI-GABA (2.5mM). **B:** Ramp test of the previously patched pyramidal neuron before (left) and after (right) iDMPO-DNI-GABA application. **C:** Somatically evoked single action potential (left) and the corresponding backpropagating dendritic Ca<sup>2+</sup> transients (right) in control (top) and in the presence of iDMPO-DNI-GABA (bottom). **D:** Bar graphs of Ca<sup>2+</sup> transient amplitude (left) and area (right) (data for C).



**Figure S2.** The reversal of the uncaging evoked currents is close to the reported chloride reversal potential. **A:** Maximal intensity z projection image of a cortical pyramidal neuron filled with Fluo-4 and Alexa 594. Yellow dot indicates the uncaging site. **B:** Representative currents induced by iDMPO-DNI-GABA uncaging at different holding potentials (10 mV intervals from -80 to +40 mV). At -60 mV (near reversal potential) GABA uncaging induced no obvious change in baseline current. **C:** I-V curve of the GABA uncaging induced responses shown on B. **D:** Same as in C for 12 neurons (reversal potential:  $-60.77 \pm 4.87$  mean  $\pm$  s.e.m.).

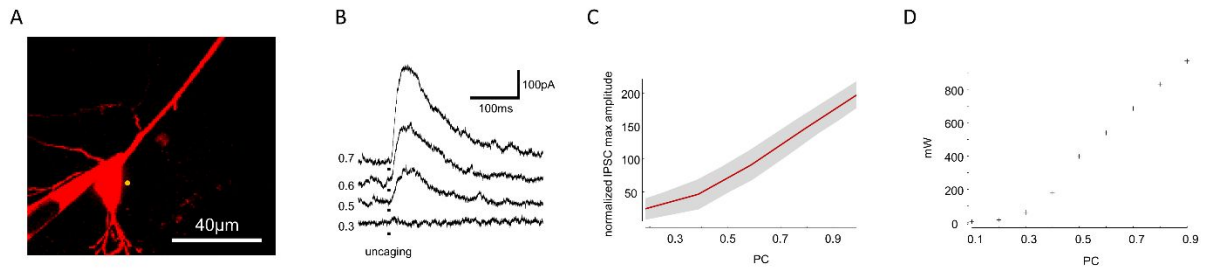


Figure S3. Laser power dependence of photolysis evoked IPSCs. A: Maximal intensity z projection image of a cortical pyramidal neuron filled with Fluo-4 and Alexa 594. Yellow dot indicates the uncaging site. B: Representative IPSCs evoked by iDMPO-DNI-GABA uncaging with different laser powers at 740 nm. C: Normalized IPSC amplitude as a function of laser power (PC: Pockels cell driver voltage in volts, used for intensity control). D: Laser power as a function of PC (measured before the objective).

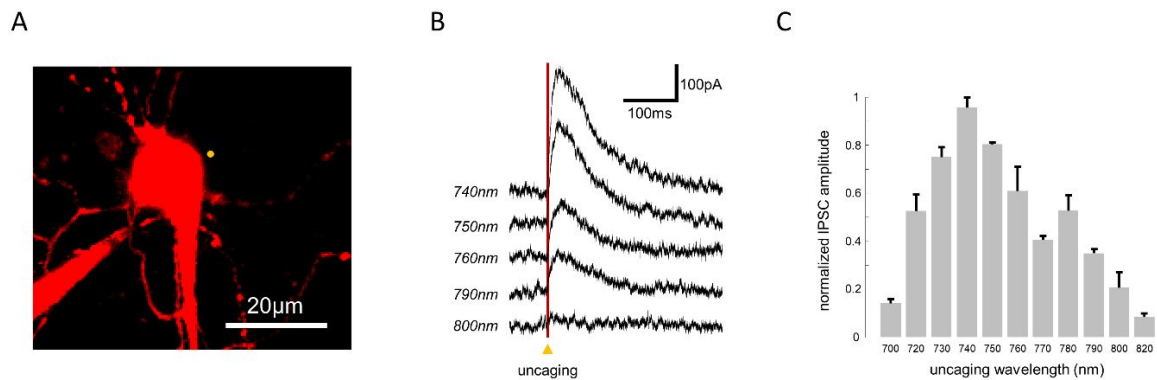


Figure S4. Wavelength dependence of photolysis evoked IPSCs. A: Maximal intensity z projection image of a cortical pyramidal neuron filled with Fluo-4 and Alexa 594. Yellow dot indicates the uncaging site. B: Representative IPSCs evoked by iDMPO-DNI-GABA uncaging with different two-photon excitation wavelengths. C: Bar graphs of the wavelength profile show that the amplitude of IPSCs were the largest at 740 nm ( $n=6$  cells).

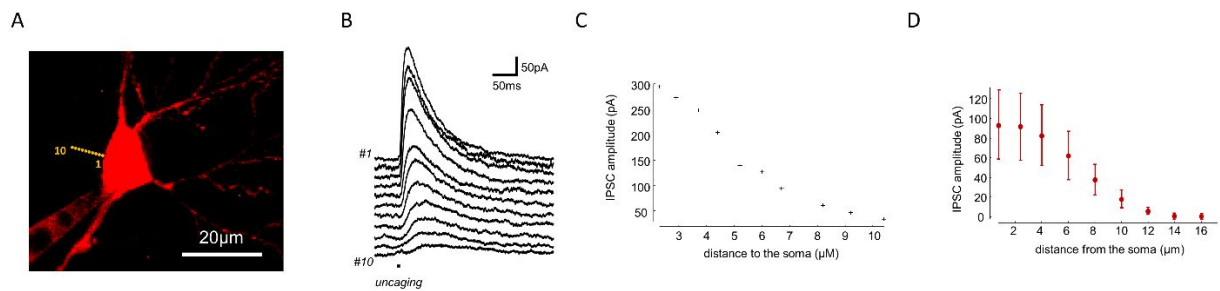


Figure S5. Spatial precision of two-photon uncaging of iDMPO-DNI-GABA (measured at 740 nm). A: Maximal intensity z projection image of a cortical pyramidal neuron filled with Fluo-4 and Alexa 594. Yellow dots indicate the uncaging sites. We denoted a series of points in a straight line at different distances from the soma of pyramidal neurons. B: Example traces of the evoked current corresponding to each point in A. C: Uncaging evoked IPSC amplitude as a function of distance to the soma. D: Same as in C for four cells (mean  $\pm$  s.e.m.).

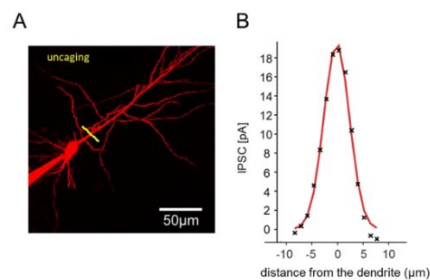


Figure S6. Spatial dependence of IPSC amplitudes at proximal dendritic segment to two-photon uncaging of iDMPO-DNI-GABA. A: Maximal intensity z projection image of a cortical pyramidal neuron filled with Fluo-4 and Alexa 594. Yellow dots

indicate the uncaging sites at both sides of the measured dendrite. B: Plot of IPSC amplitudes measured in a single cell as a function of the distance to the dendrite. Red curve indicates Gaussian fit.

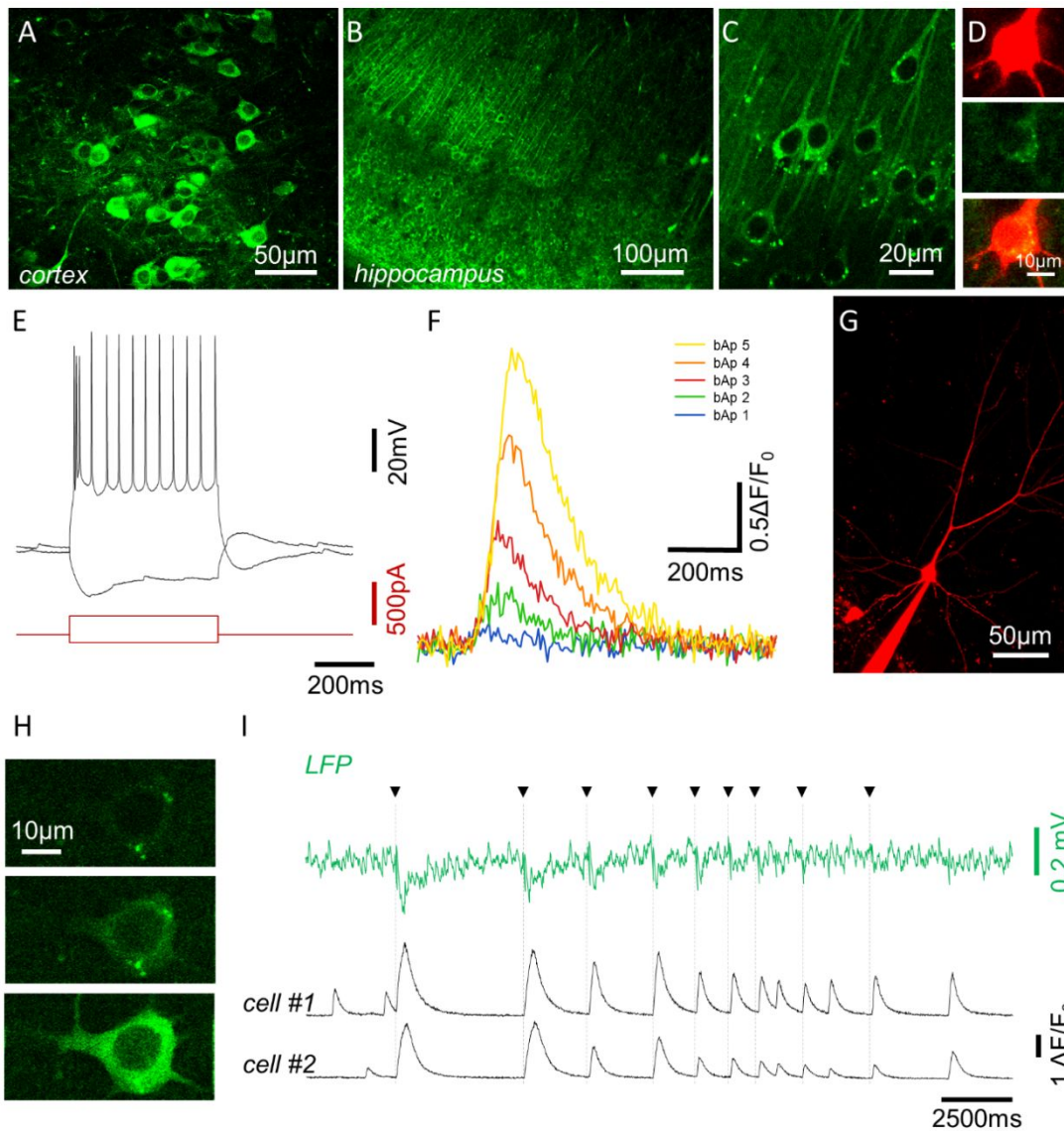
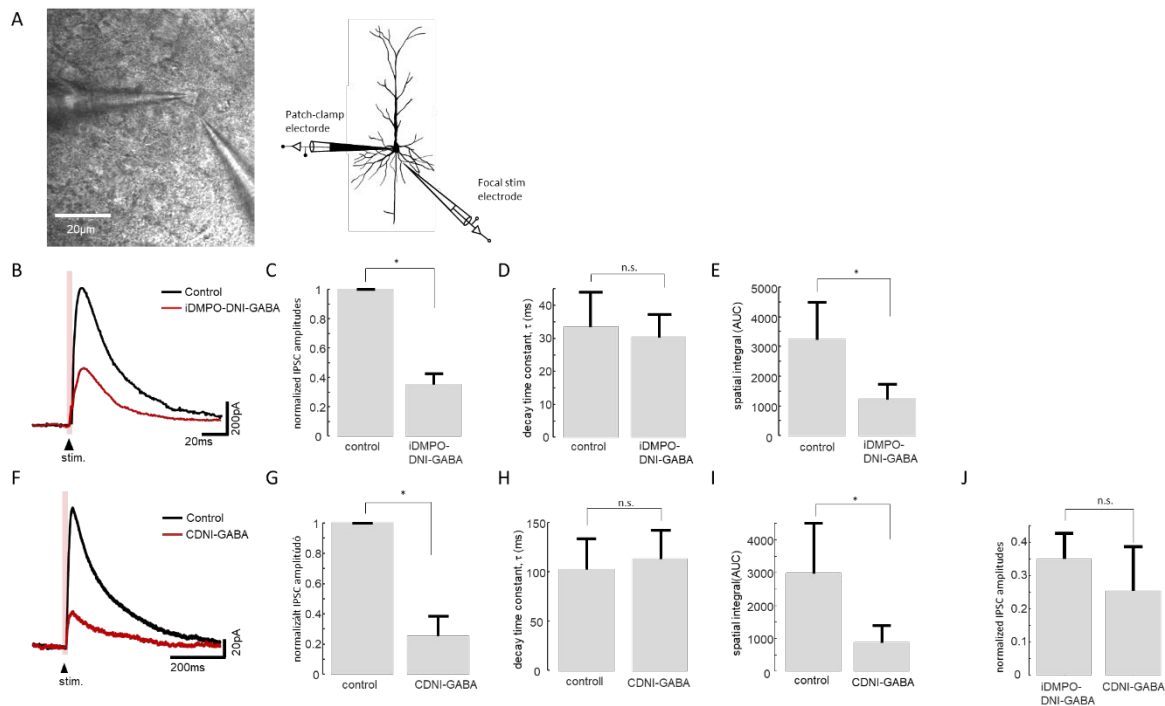


Figure S7. Two-photon calcium imaging of transgenic Thy1-GCaMP6f neurons in vitro. A-C: Neurons expressing GCaMP6f in cortical (A) and hippocampal (B-C) region. D: GCaMP6f neuron filled with Alexa594 via patch clamp pipette. E: Example ramp test of a patched neuron expressing GCaMP6f. F: Calcium transients of 1 to 5 somatically evoked backpropagating action potentials. G: Two-photon z projection image of an Alexa594 filled neuron after patch clamp. H: Two-photon image of an example cell expressing GCaMP6f before, at the beginning and during epileptic activity evoked by the bath application of 4-AP. I: LFP (top) and calcium transients (bottom) of two GCaMP6f expressing neuron during 4-AP evoked activity in vitro.



**Figure S8.** Comparison study of iDMPO-DNI-GABA and CDNI-GABA on antagonist effect evoked by focal stimulation of pyramidal neurons. **A:** Camera image of a whole cell patched clamped pyramidal cell (left). Pipette on the left indicates the patch pipette while on the right visualized the focal stim pipette located close to the somatic area. Left panel shows the experimental design. **B:** Voltage clamp recorded evoked event before (black) and after the bath application of 350  $\mu$ M iDMPO-DNI-GABA (red). **C-E:** Bar graphs show the focal stimulation evoked IPSC changes after applied iDMPO-DNI-GABA in different parameters: IPSCs amplitude, decay time constant and spatial integral (n=8 cells). **F-I:** Same as in B-E with the effect of bath applied CDNI-GABA 350  $\mu$ M, n=3 cells. **J:** Normalised IPSC amplitudes of iDMPO-DNI-GABA and CDNI-GABA plotted in the same diagram.

	Before	After	p-value
<b>Frequency (Hz)</b>	57.5 $\pm$ 7.5	50 $\pm$ 4.082	0.41
<b>Frequency (Hz) during the first and last 100ms</b>	35 $\pm$ 5	30 $\pm$ 7	0.58
<b>Adaptation</b>	0.62 $\pm$ 0.07	0.58 $\pm$ 0.09	0.74
<b>Resistance (M<math>\Omega</math>)</b>	126.1 $\pm$ 9.7	173 $\pm$ 59.6	0.46
<b>Ap half width (ms)</b>	1.4 $\pm$ 0.3	2.1 $\pm$ 0.5	0.27
<b>Resting membrane potential (mV)</b>	-65.42 $\pm$ 2.01	-68 $\pm$ 1.8	0.37

**Table S1. Pyramidal neuron average electrophysiological parameters before and after the application of iDMPO-DNI-GABA.** The intrinsic membrane properties (Table S1) of pyramidal cells were measured in a whole-cell current-clamp configuration. The resting membrane potential was estimated when there was no holding current. Input resistance was calculated from voltage responses to current injections (500 ms, 50 pA). The action potential (Ap) properties (e.g. half width) were measured at the first Ap, evoked by an increased depolarizing current injection. Aps were induced with somatic current injections (500-700 pA for 5 ms, five current steps at 40 Hz).

# Determination of free GABA content of the caged compounds<sup>1</sup>

## *Materials*

Ortho-phthalaldehyde (OPA), mercapto propionic acid (MPA), and GABA were obtained from Sigma. Cage GABA-trifluoroacetic acetate were the products of Femtonics (Budapest, Hungary). HPLC-grade methanol and acetonitrile, solvents were purchased from Sigma–Aldrich. Reagents were of the highest purity available.

## *Standard solutions*

Standard solutions of GABA have been prepared with distilled water in the concentrations of  $\sim 2\text{--}5 \times 10^{-3}$  M (weighed with analytical precision) and further diluted before use. Stock solution of OPA contained 0.20 g OPA (weighed with analytical precision) in 10 mL methanol (further on: methanolic OPA solution).

## *Cage-GABA samples*

Cage-GABA (**1a** – 10 mg, **2a** and **2b** – 14 mg) were weighed with analytical precision and dissolved in 50 mL distilled water.

## *Buffer solution*

Borate buffer was mixed in 50/50 (V/V) ratios from 0.4 M boric acid (dissolved in 0.4 M potassium chloride) and from 0.4 M sodium hydroxide.

## *Reagent solutions*

OPA–MPA reagents were obtained by mixing, in order of listing, 0.5–1 mL or 1 mL methanolic OPA and 4 mL buffer solution and various amounts of MPA (20–40  $\mu$ L), solutions. The molar ratio of OPA to MPA was  $[\text{OPA}] - [\text{MPA}] = 1:3$ . The final pH of the reagent solutions were adjusted by 2.5 M sodium hydroxide to  $\text{pH } 9.30 \pm 0.05$ .

## *Derivatization procedure*

Derivatizations of blank, standard and sample solutions were performed with reagent solutions (reagent's age 90 min), saved in the refrigerator no longer than < 9 days, at  $\sim 4^\circ\text{C}$ . 400  $\mu$ L of reagent solutions were mixed with 60  $\mu$ L of GABA or cage-GABA solutions and let react for 5 min before injection. The molar ratios of  $[\text{OPA}]/[\text{cage-GABA}]$  were 10/1–100/1. Note: to protect the cage-GABA from direct light, stability studies were performed in amber glass vials.

## *Chromatography HPLC-DAD/FI*

The system was a Waters HPLC instrument (Waters, Milford, MA, USA), consisting of a Waters 996 (DAD and a Waters 474 FI detectors, a Waters 616 Controller quaternary pump with a thermostat able column area and a Waters 717 Autosampler, operating with the Millennium Software. The analytical columns were a BST Hypersil ODS, 15 cm  $\times$  4.0 mm, 5  $\mu$ m with guard columns (BST Hypersil ODS 20 mm  $\times$  4 mm, 5  $\mu$ m). Detections have been performed simultaneously: DAD and FI detectors were connected in order of listing. DAD data have been recorded between 190 and 400 nm (DAD). The fluorescence intensities of OPA–GABA derivative was evaluated at the optimum fluorescence conditions of isoindoles (EEx/EEm= 337/454 nm). The eluent consisted of two components: eluent A was 0.05 M sodium acetate ( $\text{pH } 7.20 \pm 0.05$ ), while eluent B was prepared from 0.1 M sodium acetate/acetonitrile/methanol (46/44/10), mixed in volume ratios and titrated with glacial acetic acid or 1.0 M sodium hydroxide to  $\text{pH } 7.20 \pm 0.05$ . Elutions were performed in the gradient mode (at  $40^\circ\text{C}$ ): starting with 1% B holding for 1 min (flow rate: 1.3 mL/min), reaching the 100% B and 2.0 mL/min flow

rate within 7 min, afterward 3 min isocratic elution with 100% B was performed; finally returning to the initial concentration (1% B) in 1 min then equilibrating for 4 min.

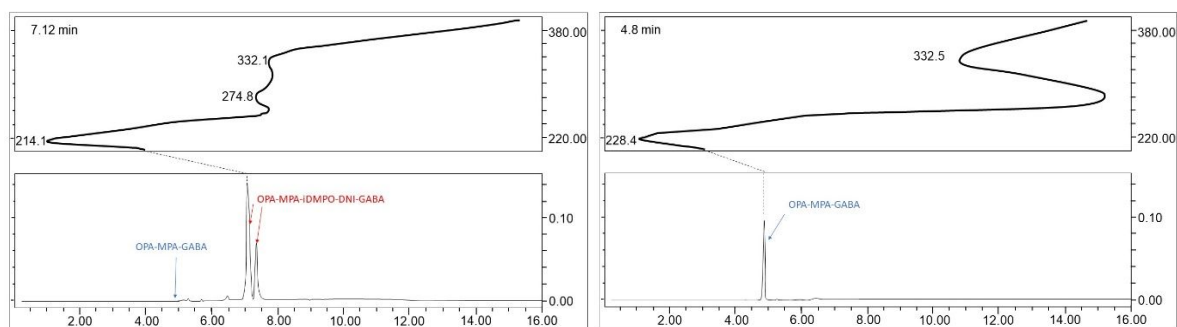


Figure S9. UV chromatogram and DAD spectrum of the OPA-MPA derivatised iDMPO-DNI-GABA (2a, left) and GABA (right). Red arrows show the iDMPO-DNI-GABA-OPA-MPA isomers, blue arrow shows the GABA-OPA-MPA derivative. Chromatogram was extracted at 332 nm. According to results 1.3 nmol ( $\pm 0.4$  nm) GABA were detected in 22.8  $\mu$ mol iDMPO-DNI-GABA (14.2 mg), which correspond to 9 ppm GABA content.





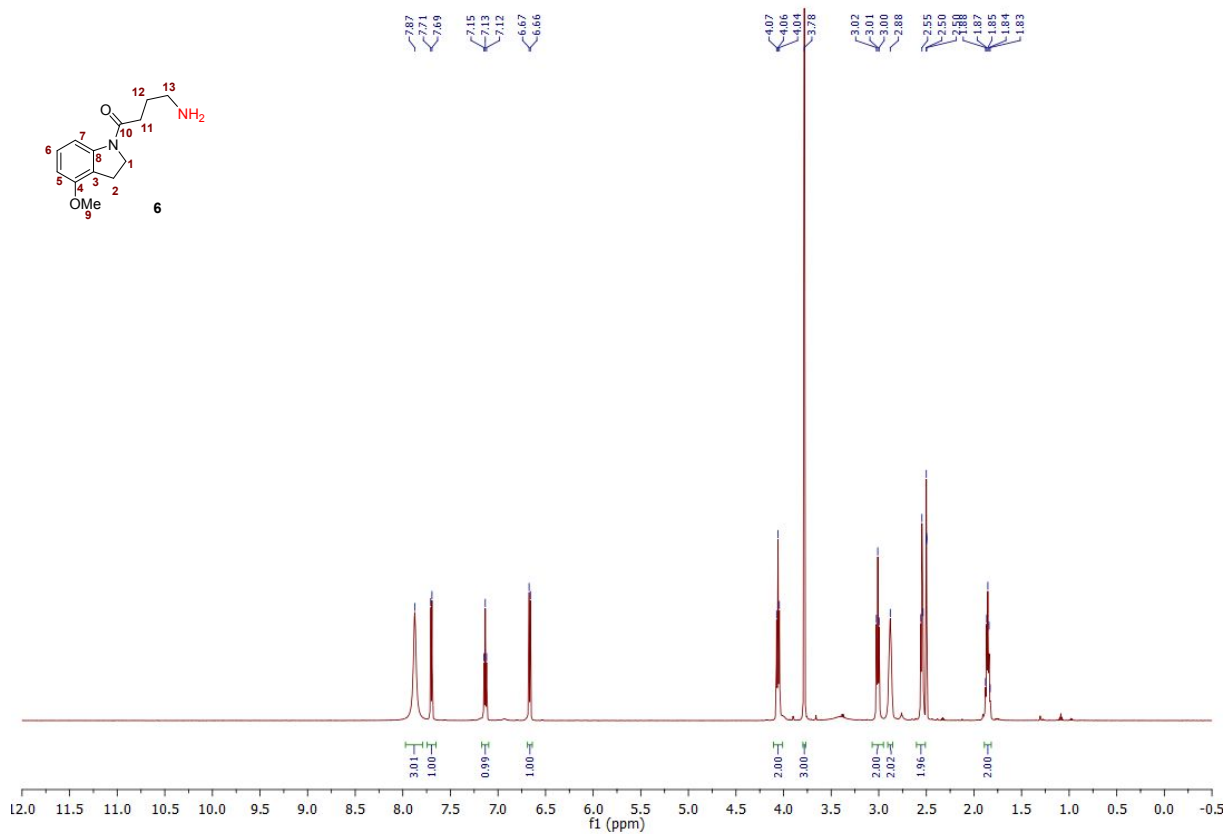


Figure S12. <sup>1</sup>H NMR spectrum of 6 in DMSO-d<sub>6</sub>.

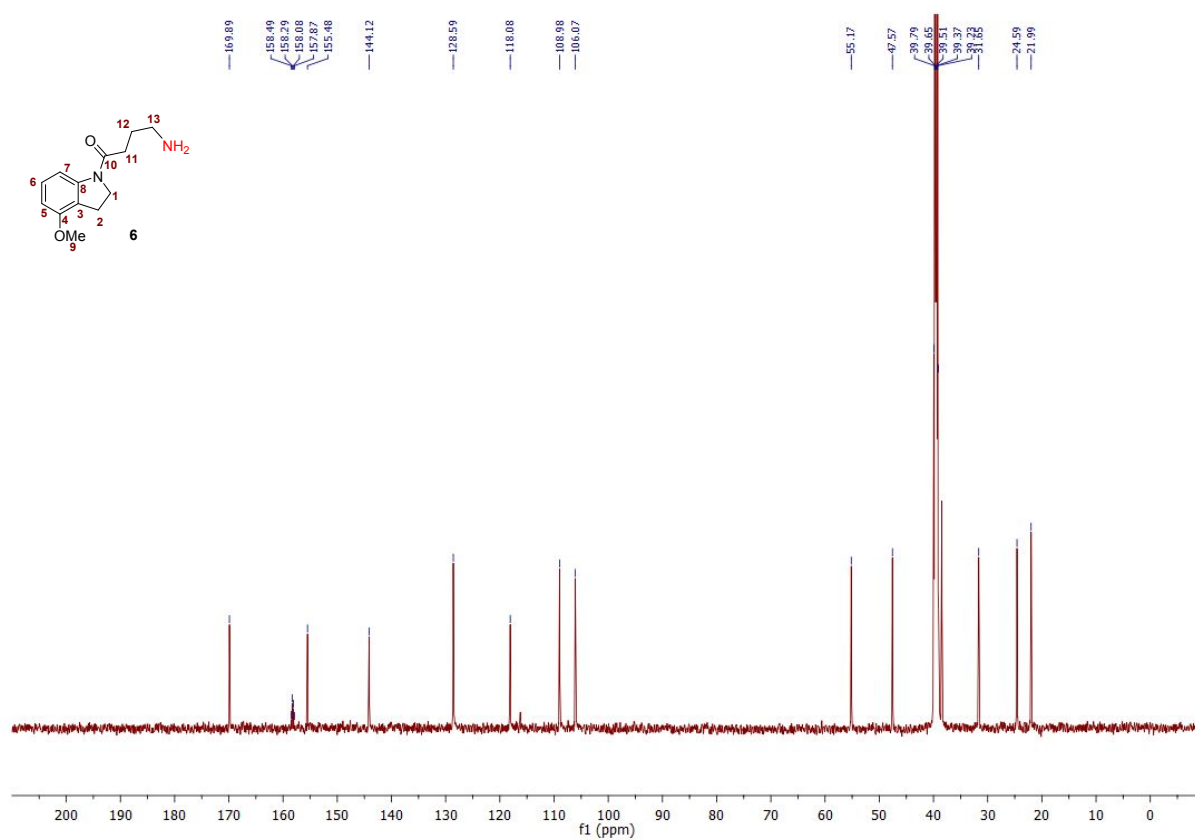


Figure S13. <sup>13</sup>C NMR spectrum of 6 in DMSO-d<sub>6</sub>.

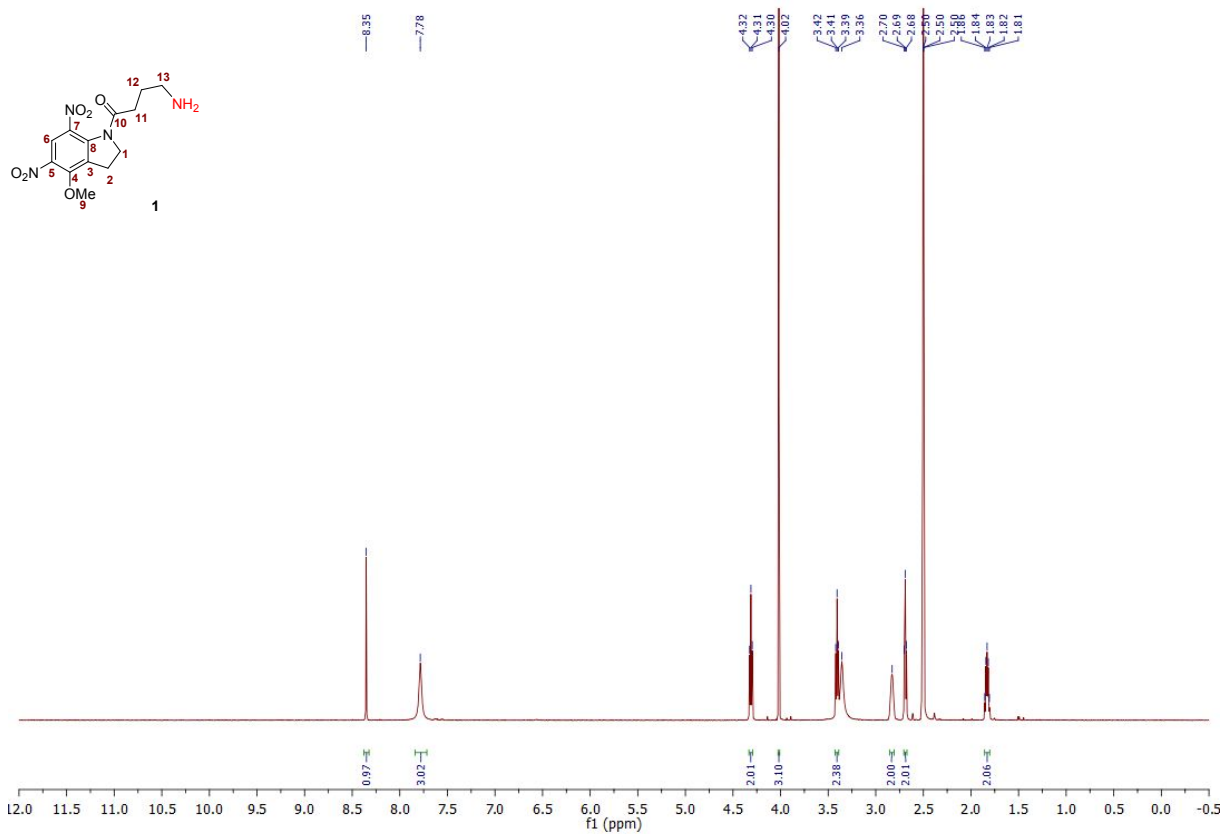


Figure S14. <sup>1</sup>H NMR spectrum of 1 in DMSO-d<sub>6</sub>.

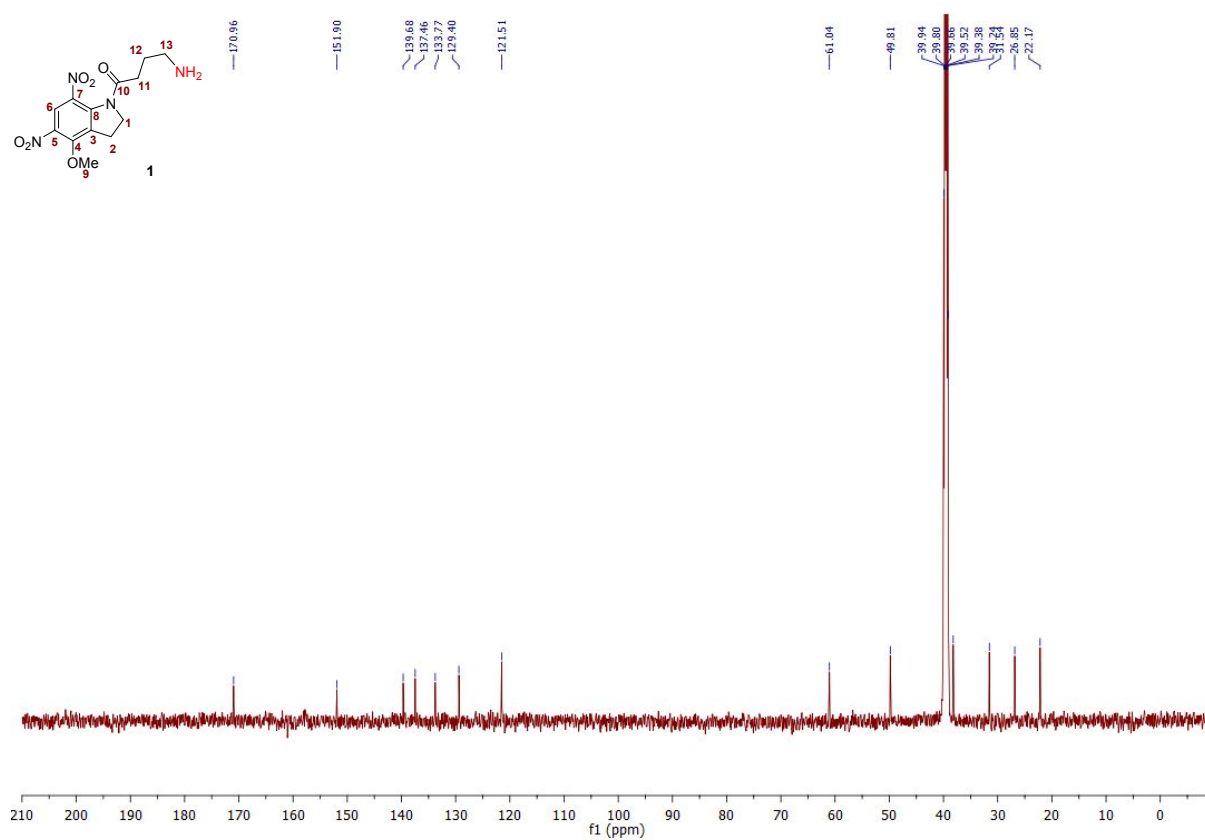


Figure S15. <sup>13</sup>C NMR spectrum of 1 in DMSO-d<sub>6</sub>.

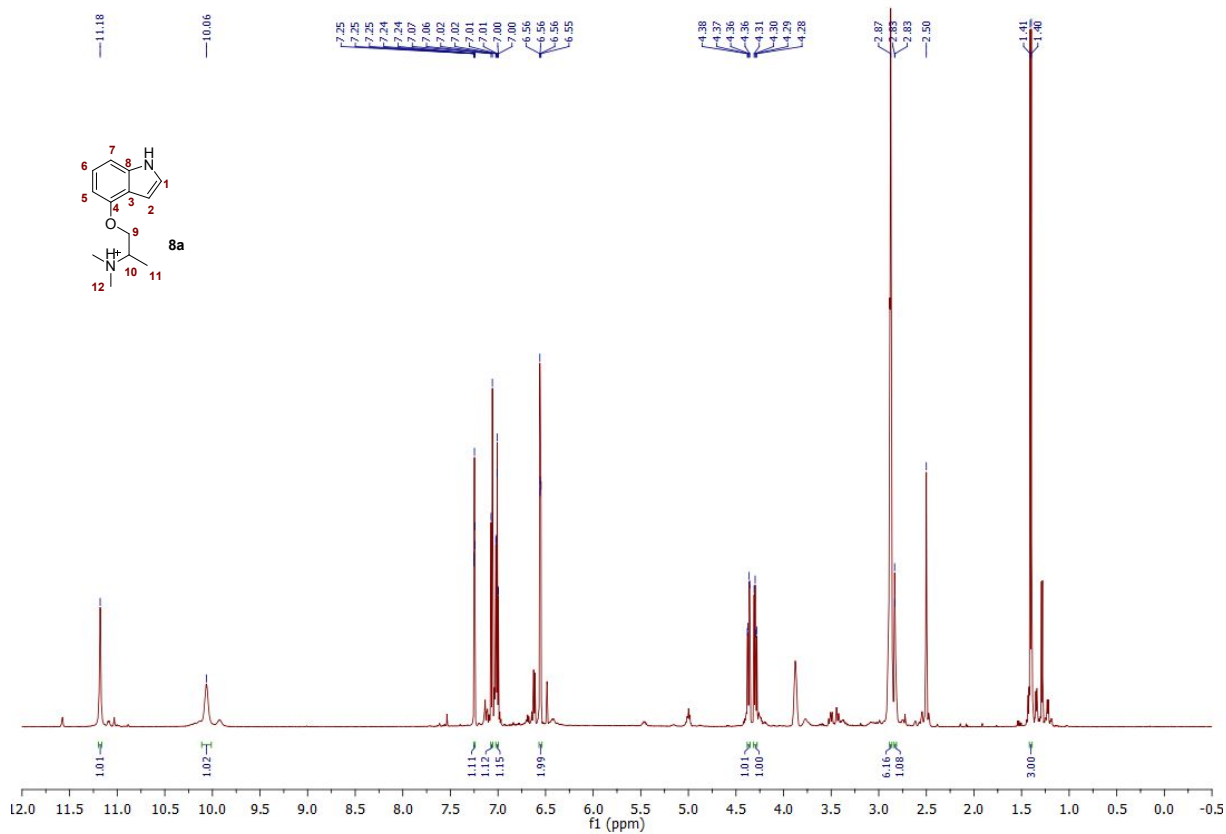


Figure S16. <sup>1</sup>H NMR spectrum of **8a** in DMSO-d<sub>6</sub>.

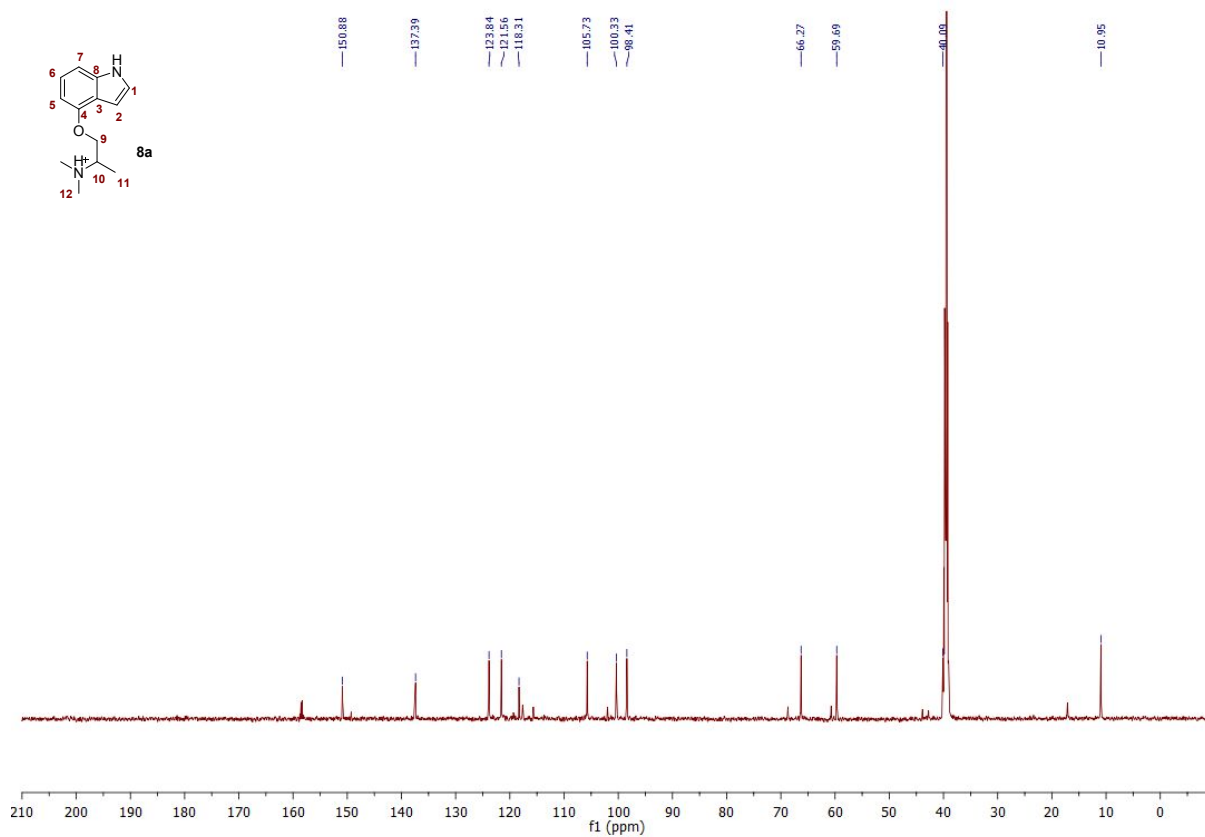


Figure S17. <sup>13</sup>C NMR spectrum of **8a** in DMSO-d<sub>6</sub>.

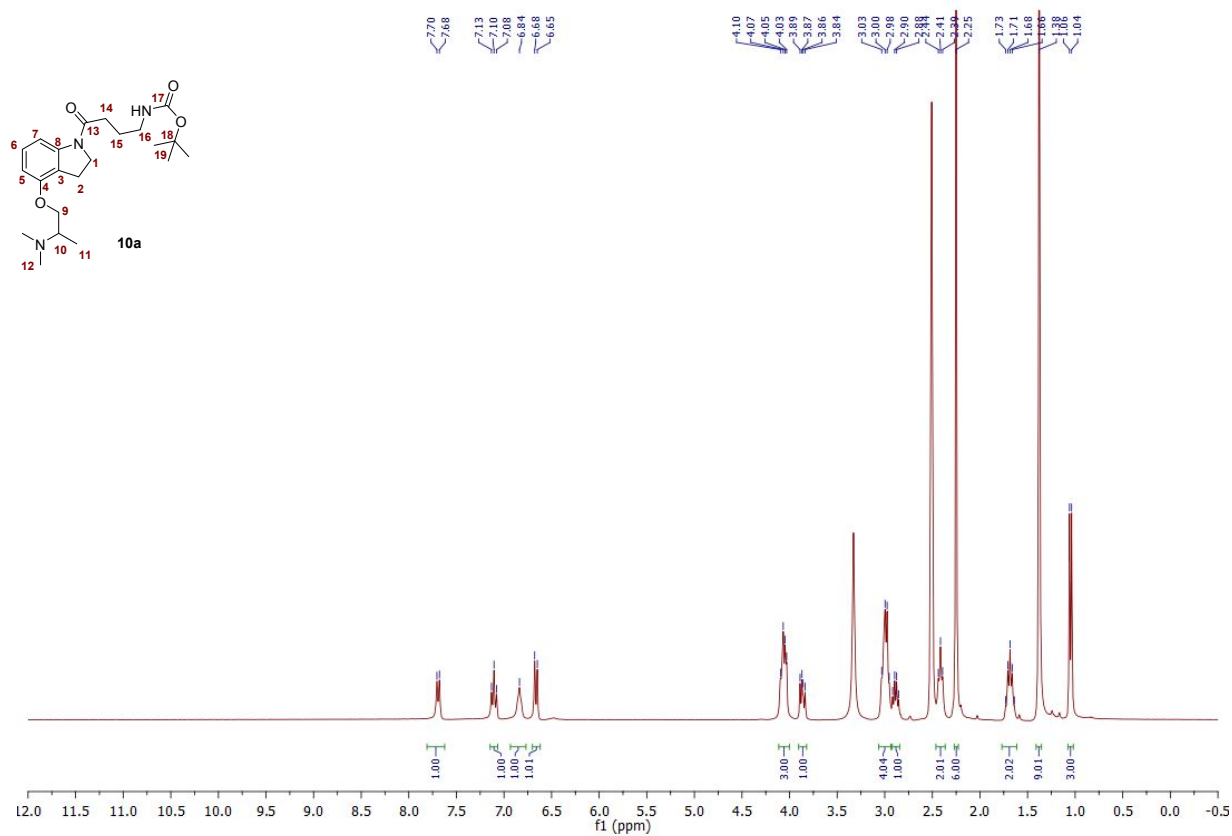


Figure S18.  $^1\text{H}$  NMR spectrum of **10a** in  $\text{DMSO-d}_6$ .

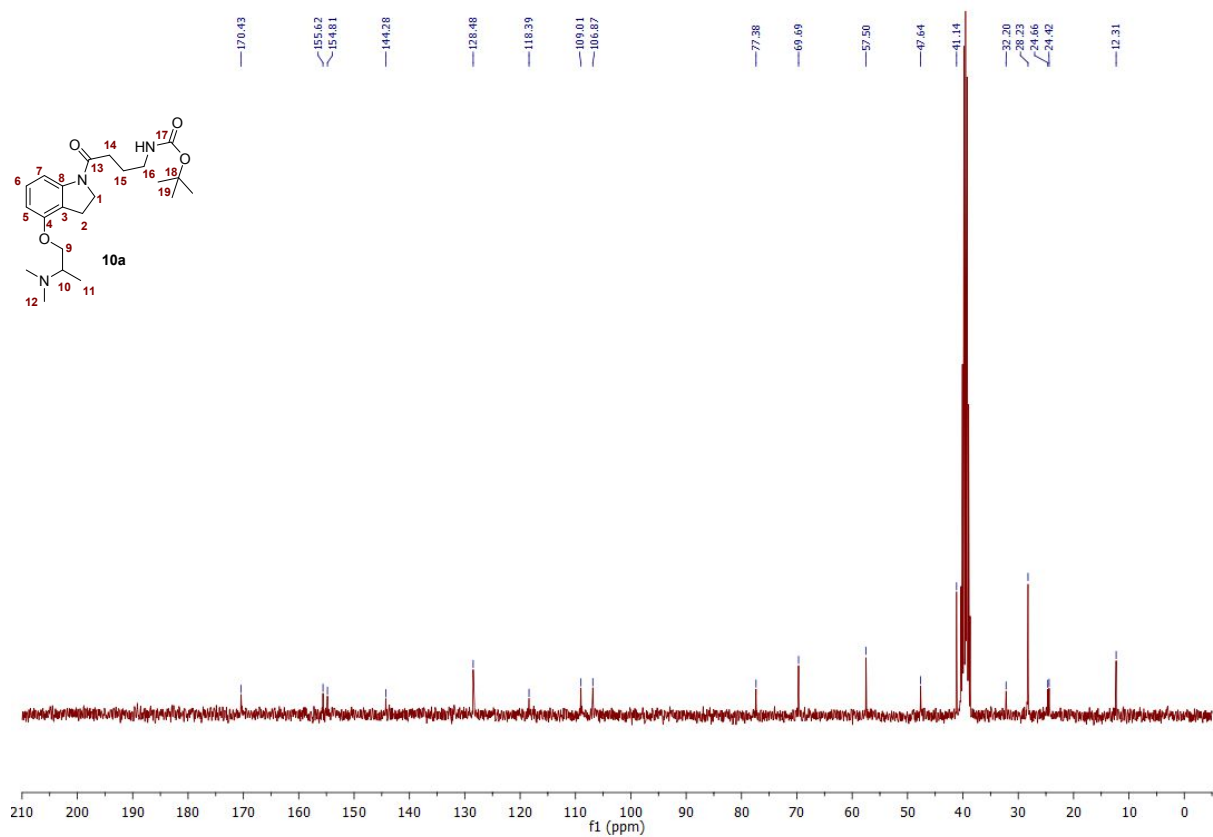


Figure S19.  $^{13}\text{C}$  NMR spectrum of **10a** in  $\text{DMSO-d}_6$ .

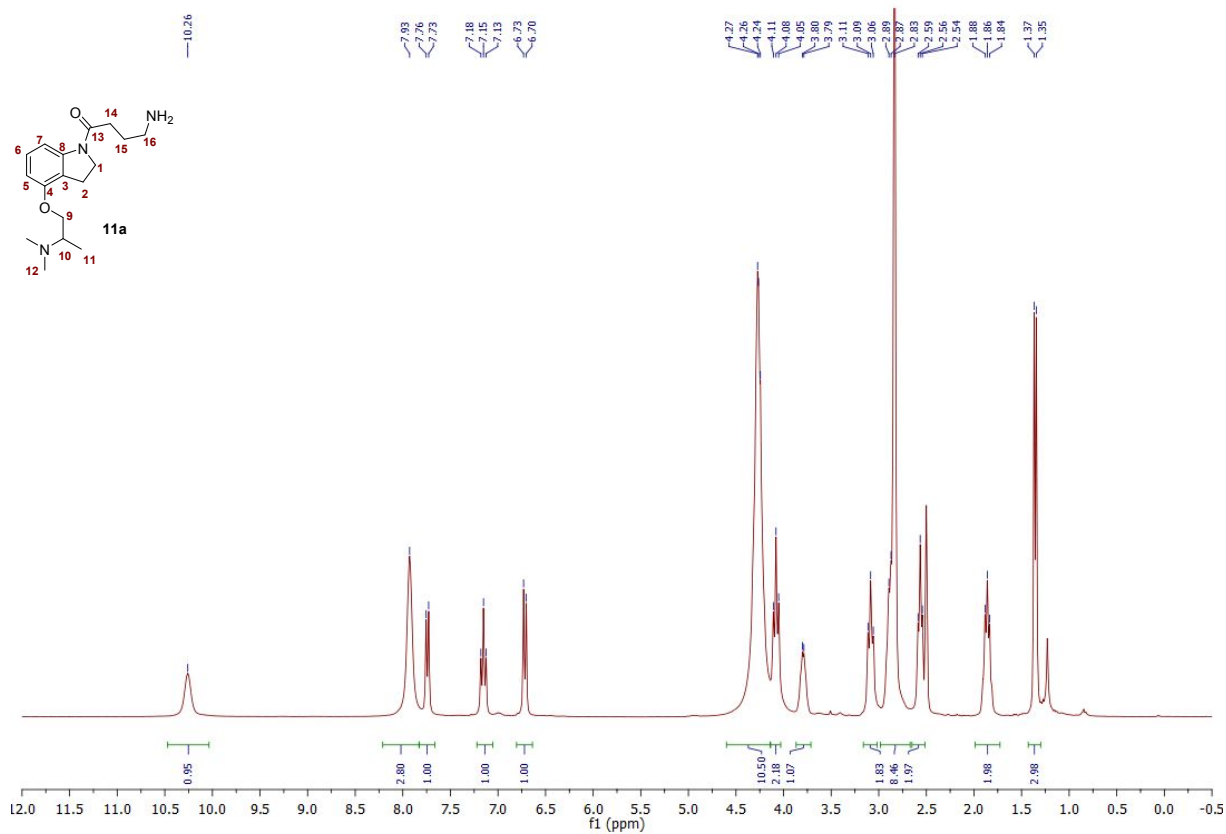


Figure S20.  $^1\text{H}$  NMR spectrum of **11a** in  $\text{DMSO-d}_6$ .

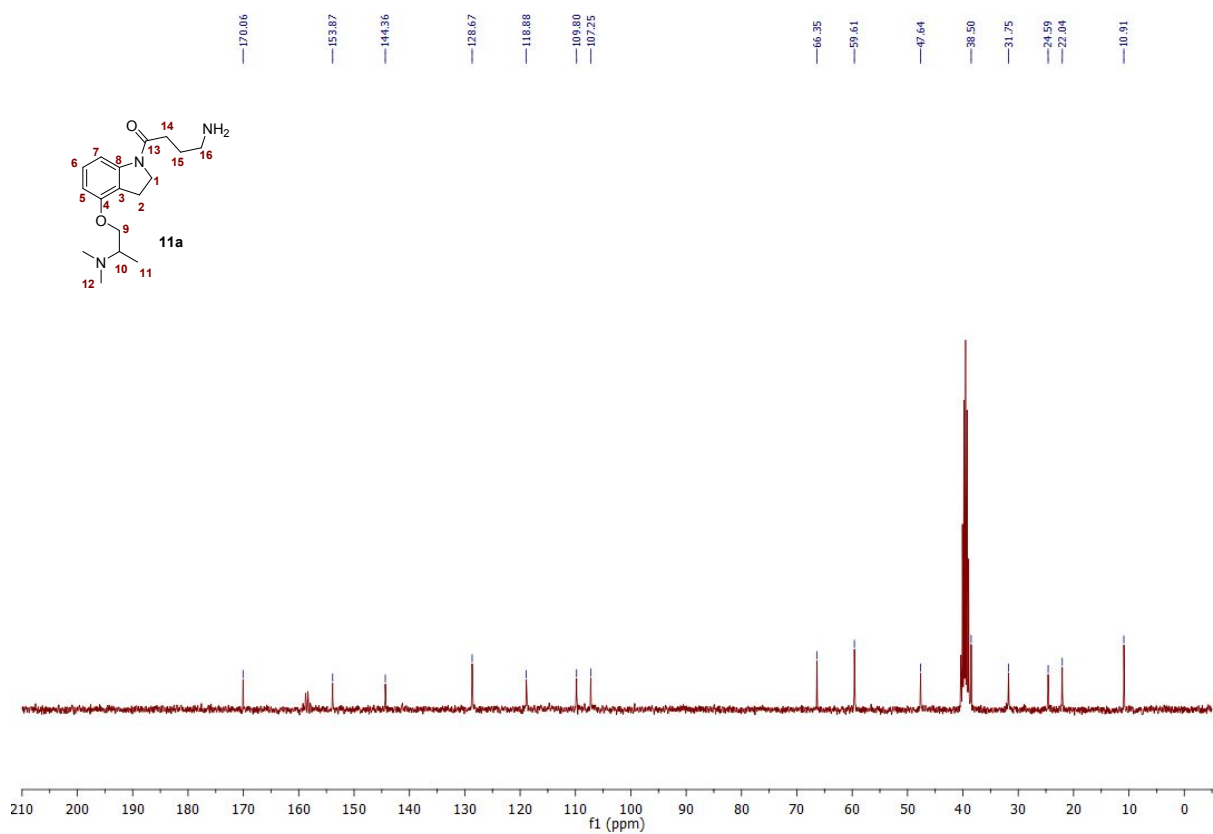


Figure S21.  $^{13}\text{C}$  NMR spectrum of **11a** in  $\text{DMSO-d}_6$ .

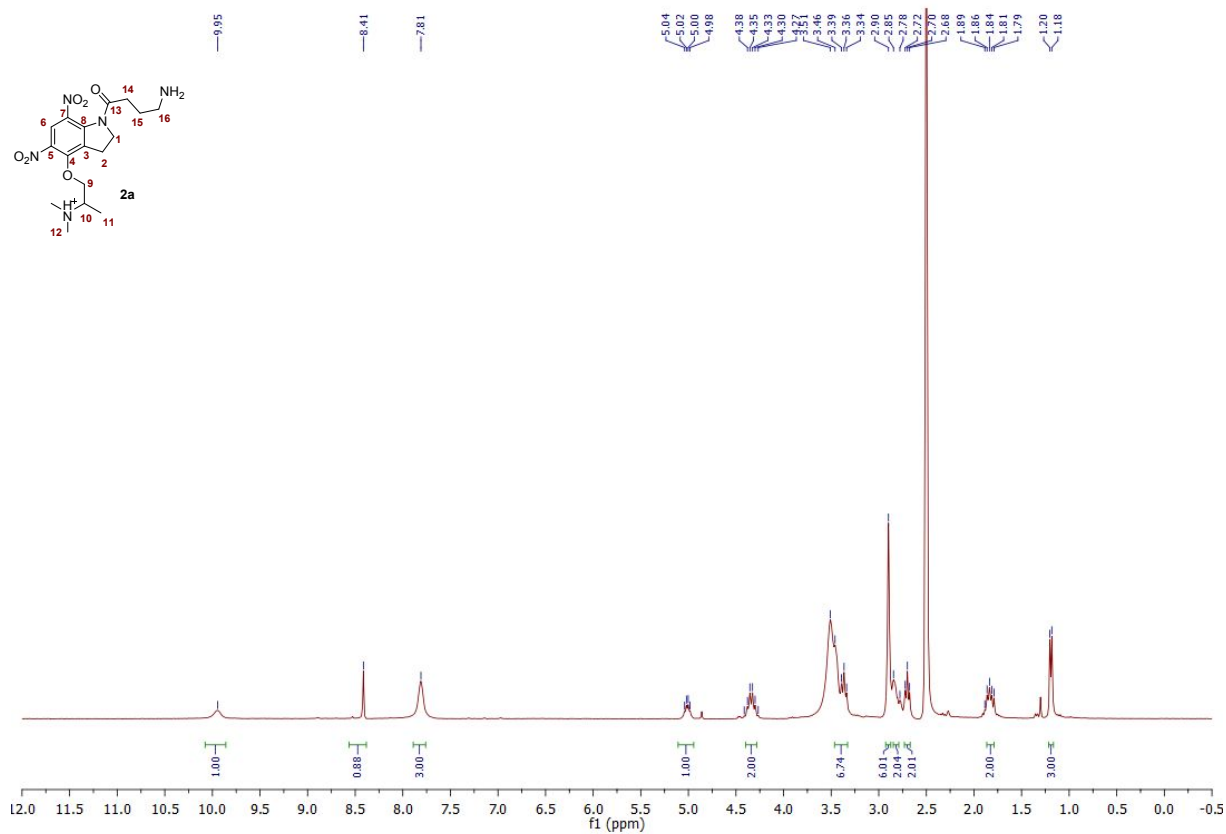


Figure S22. <sup>1</sup>H NMR spectrum of **2a** in DMSO-d<sub>6</sub>.

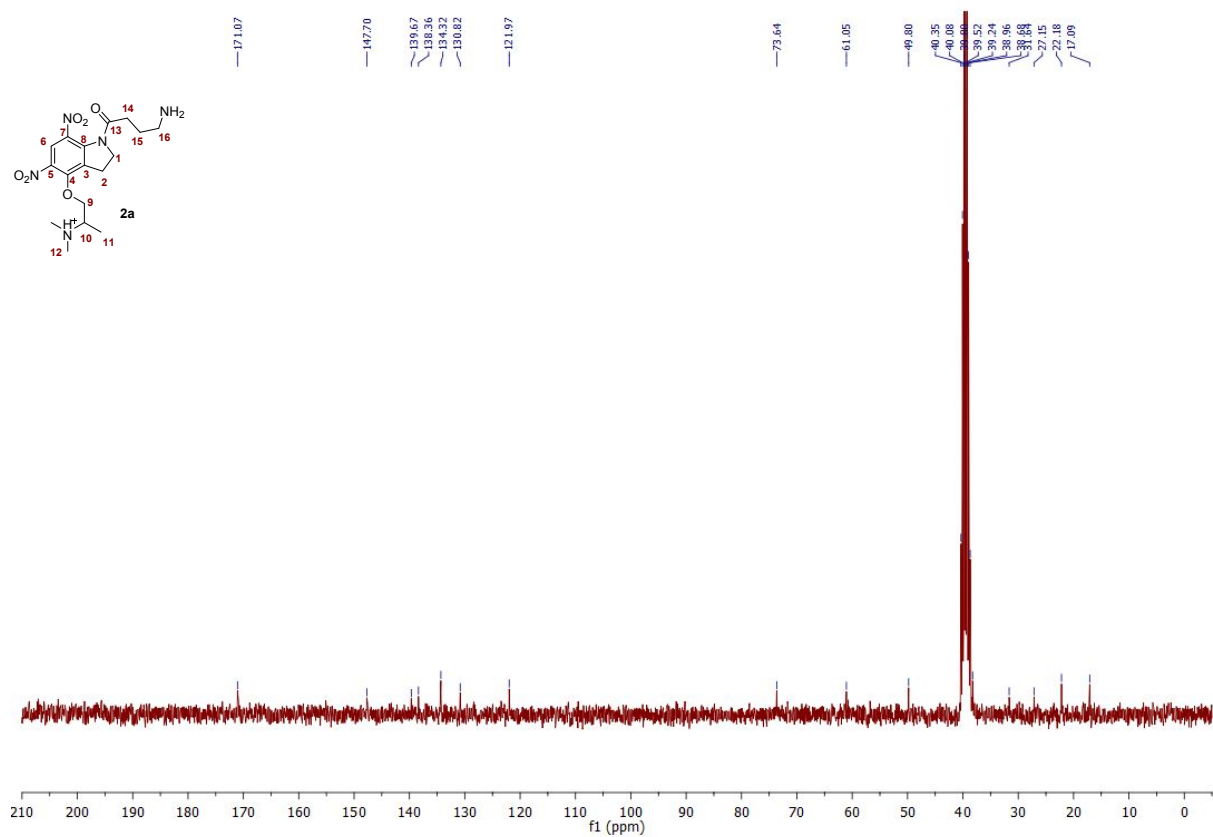


Figure S23. <sup>13</sup>C NMR spectrum of **2a** in DMSO-d<sub>6</sub>.

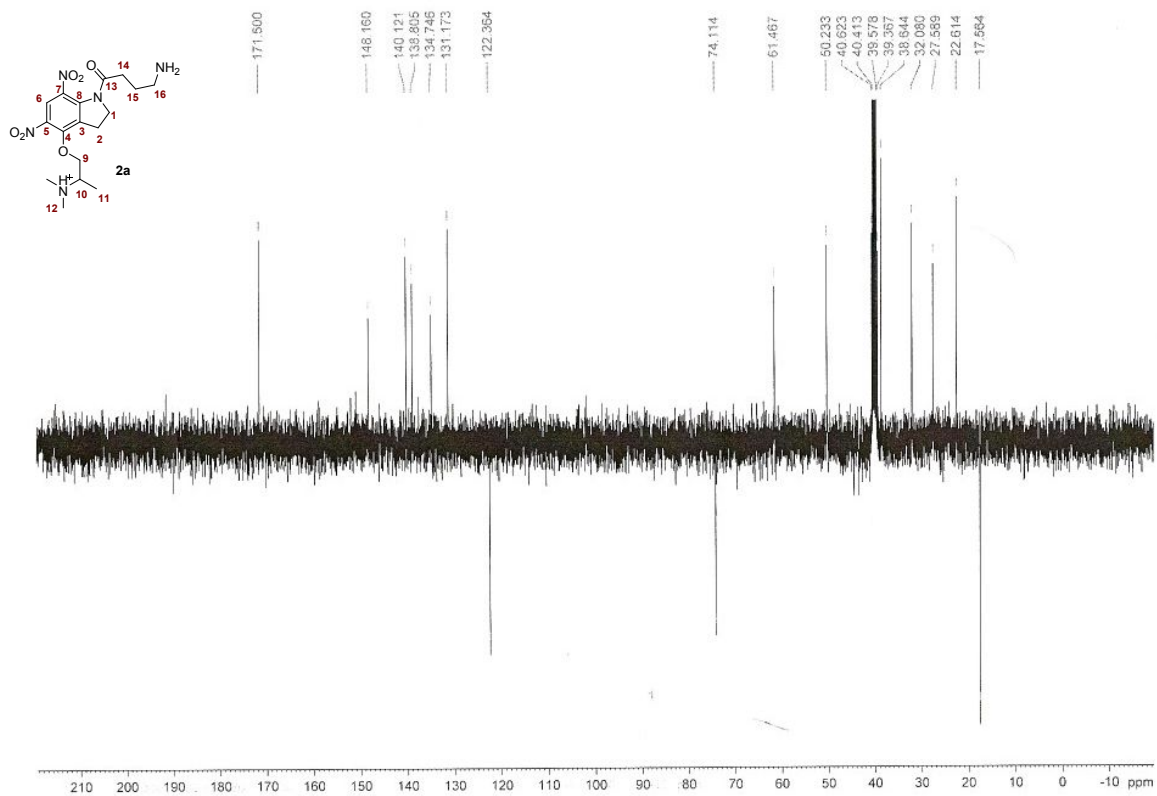


Figure S24. APT spectrum of **2a** in DMSO-d<sub>6</sub>.

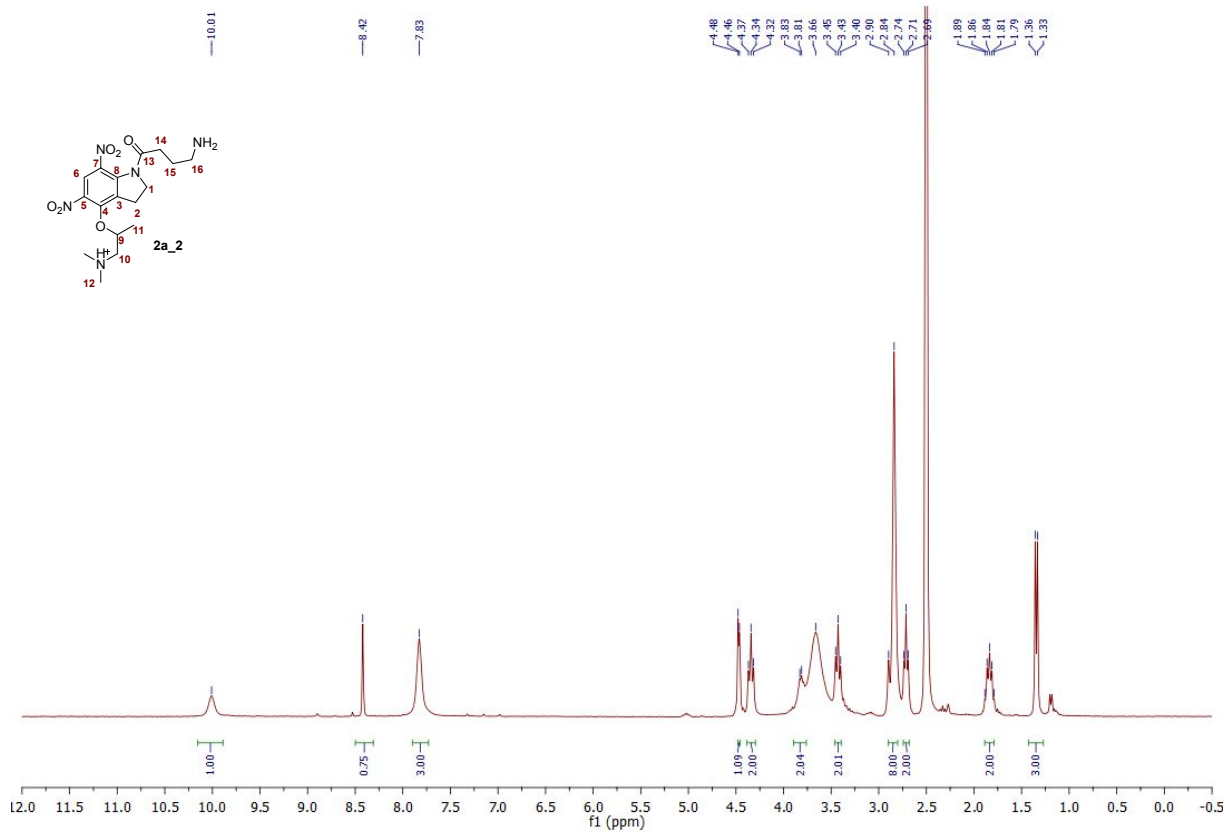


Figure S25. <sup>1</sup>H NMR spectrum of **2a<sub>a</sub>** in DMSO-d<sub>6</sub>.

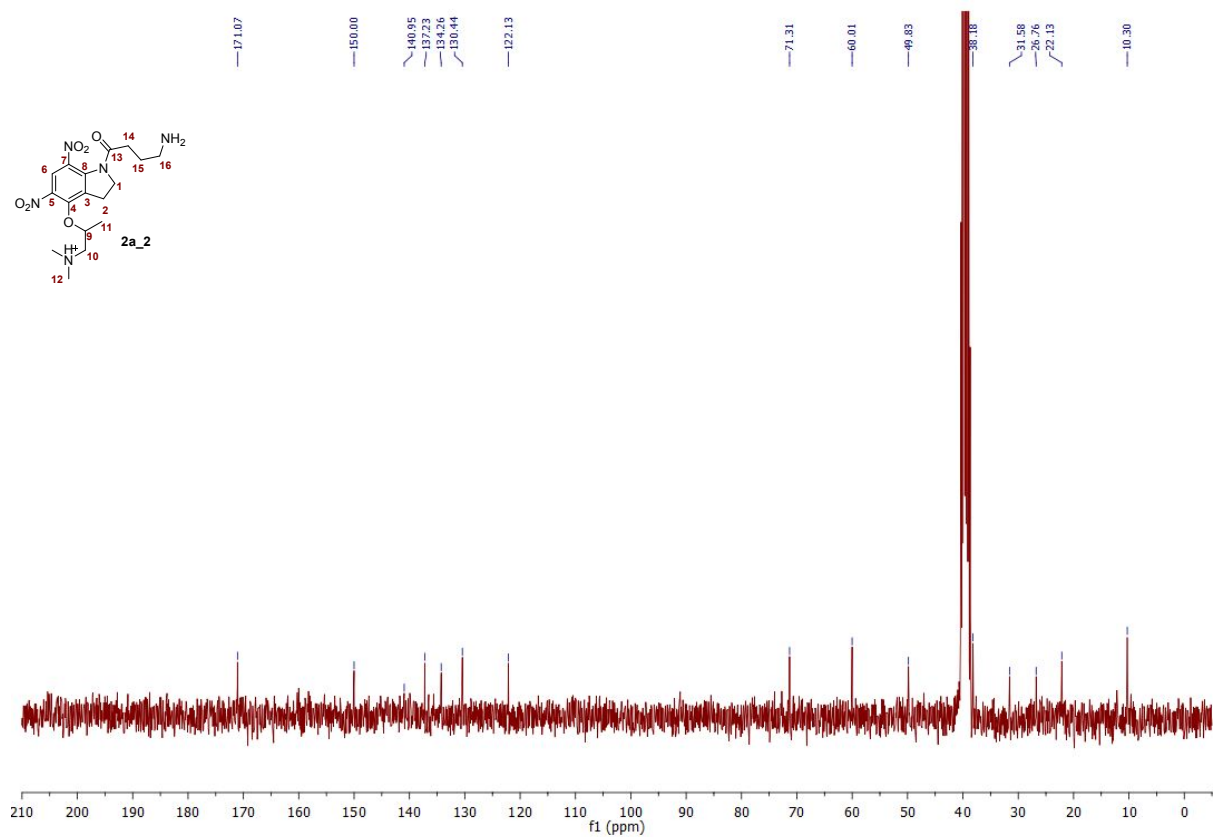


Figure S26. <sup>13</sup>C NMR spectrum of **2a<sub>a</sub>** in DMSO-d<sub>6</sub>.



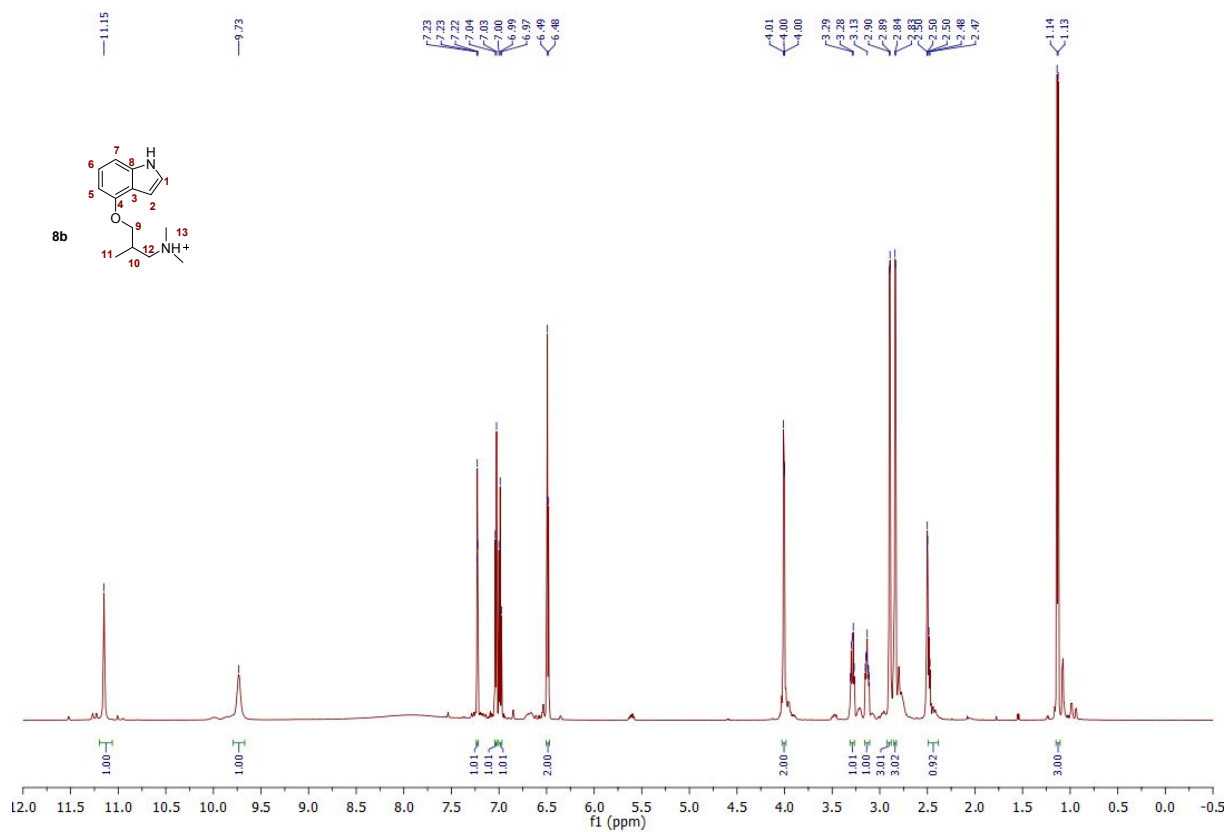


Figure S27.  $^1\text{H}$  NMR spectrum of **8b** in DMSO- $d_6$ .

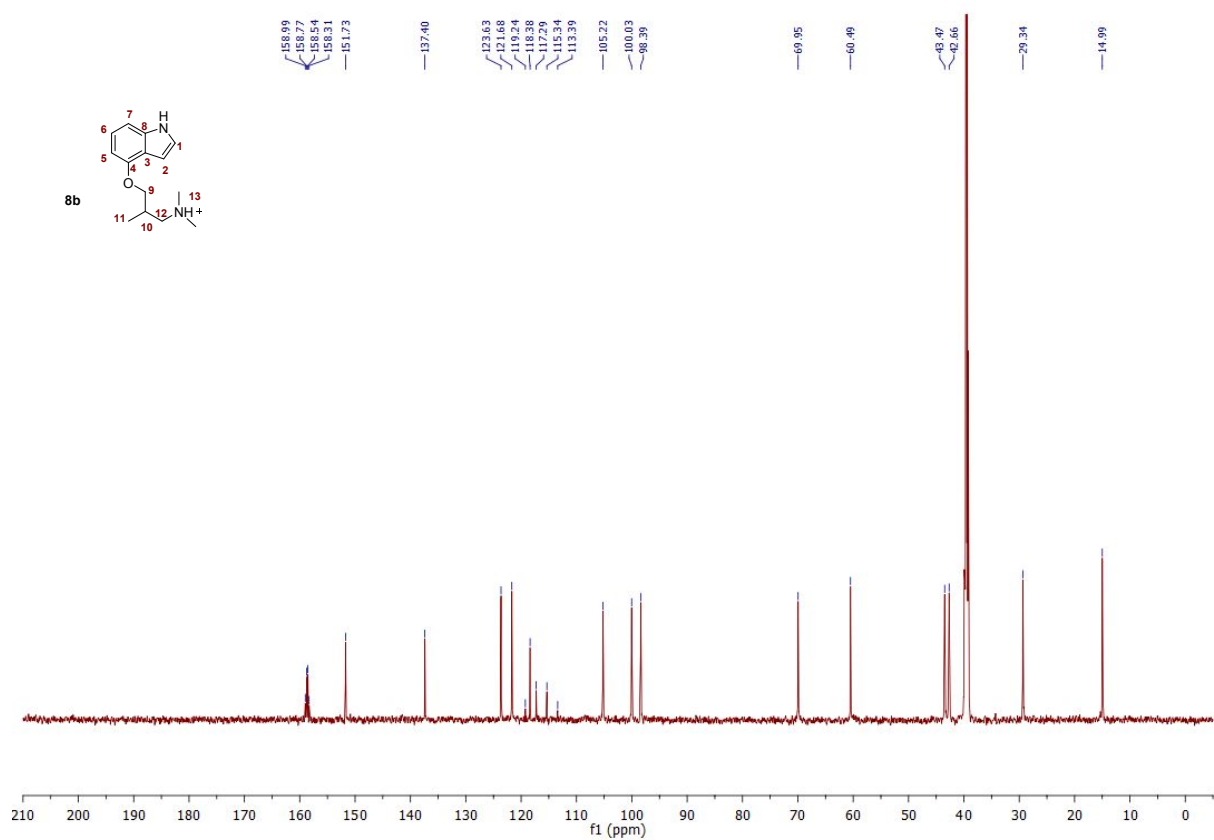


Figure S28.  $^{13}\text{C}$  NMR spectrum of **8b** in DMSO- $d_6$ .

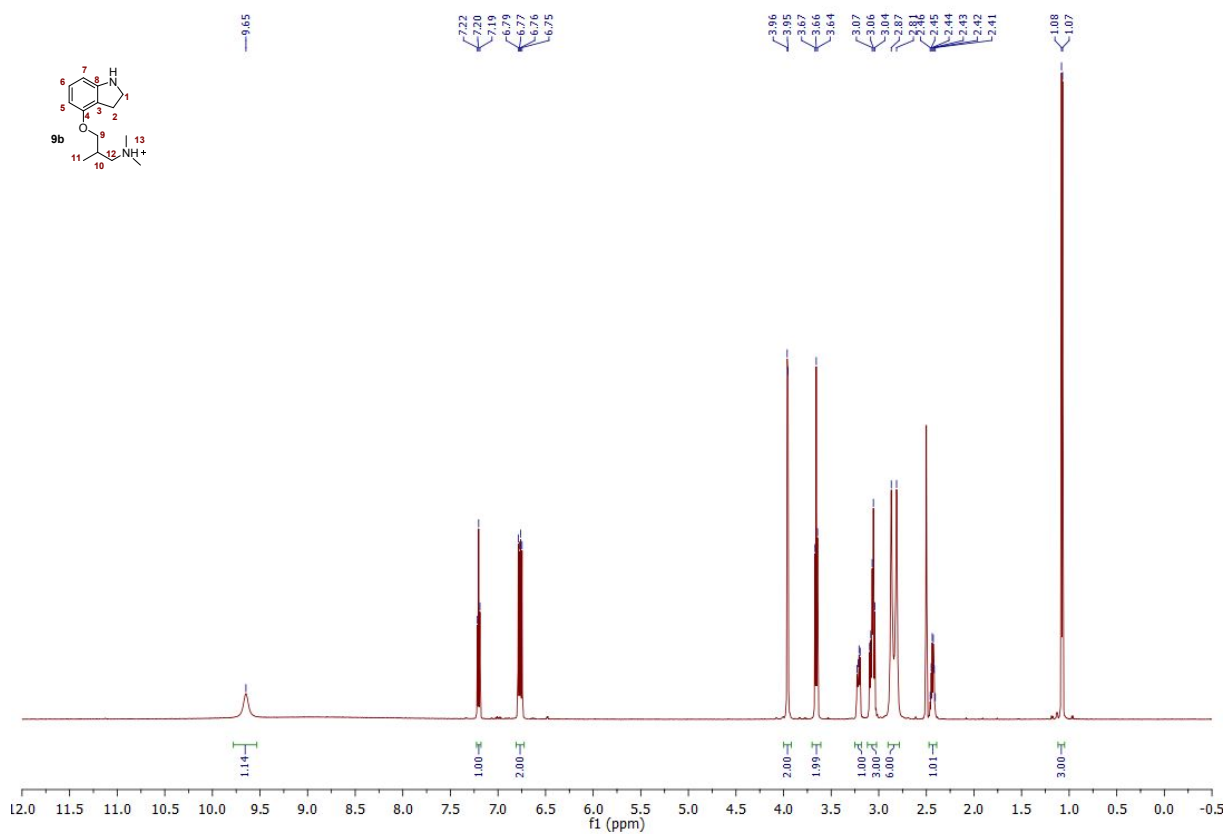


Figure S29. <sup>1</sup>H NMR spectrum of 9b in DMSO-d<sub>6</sub>.

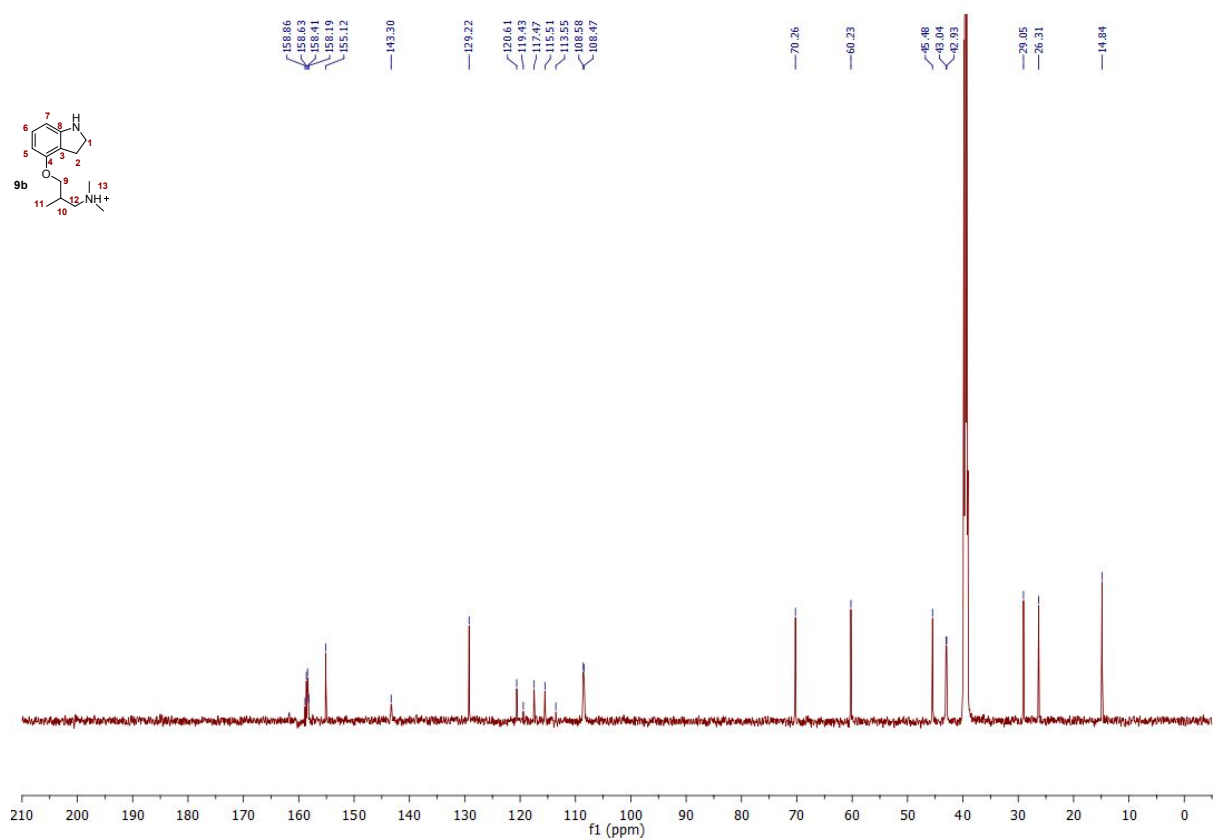


Figure S30. <sup>13</sup>C NMR spectrum of 9b in DMSO-d<sub>6</sub>.

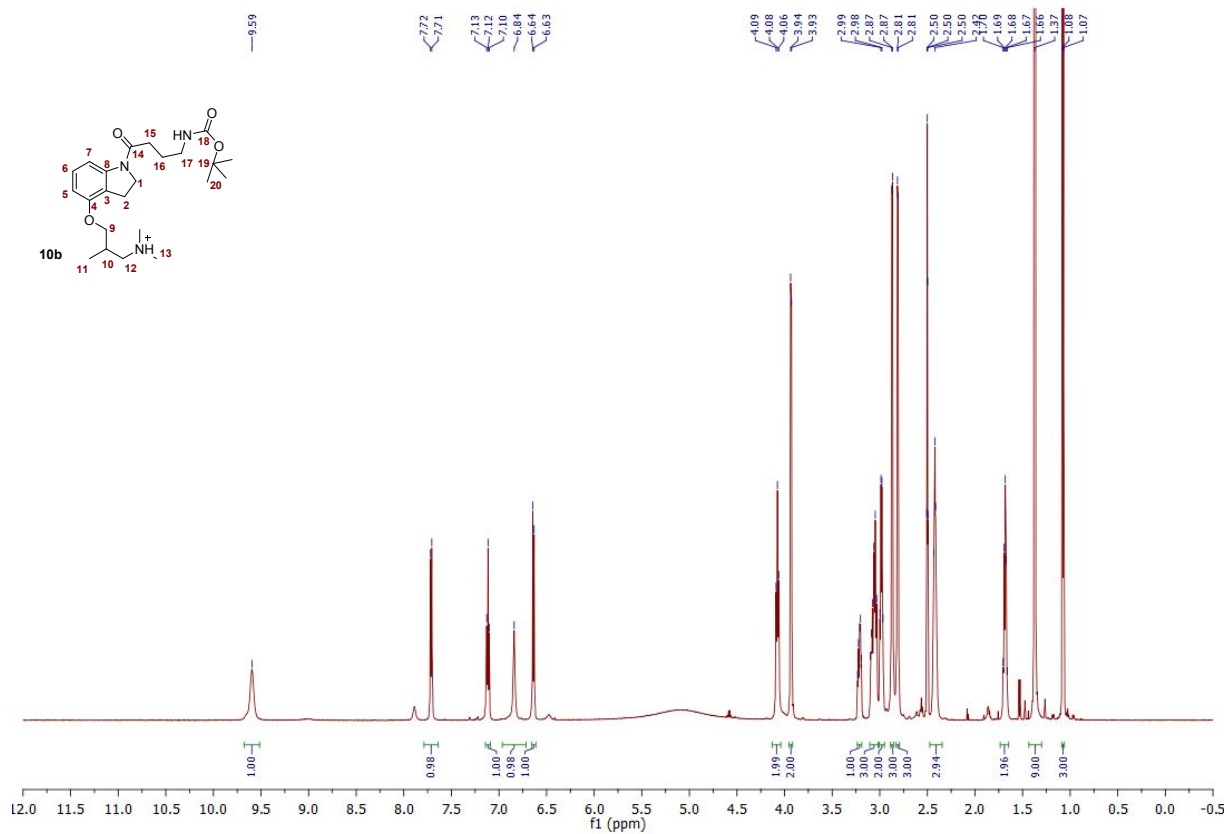


Figure S31. <sup>1</sup>H NMR spectrum of 10b in DMSO-d<sub>6</sub>.

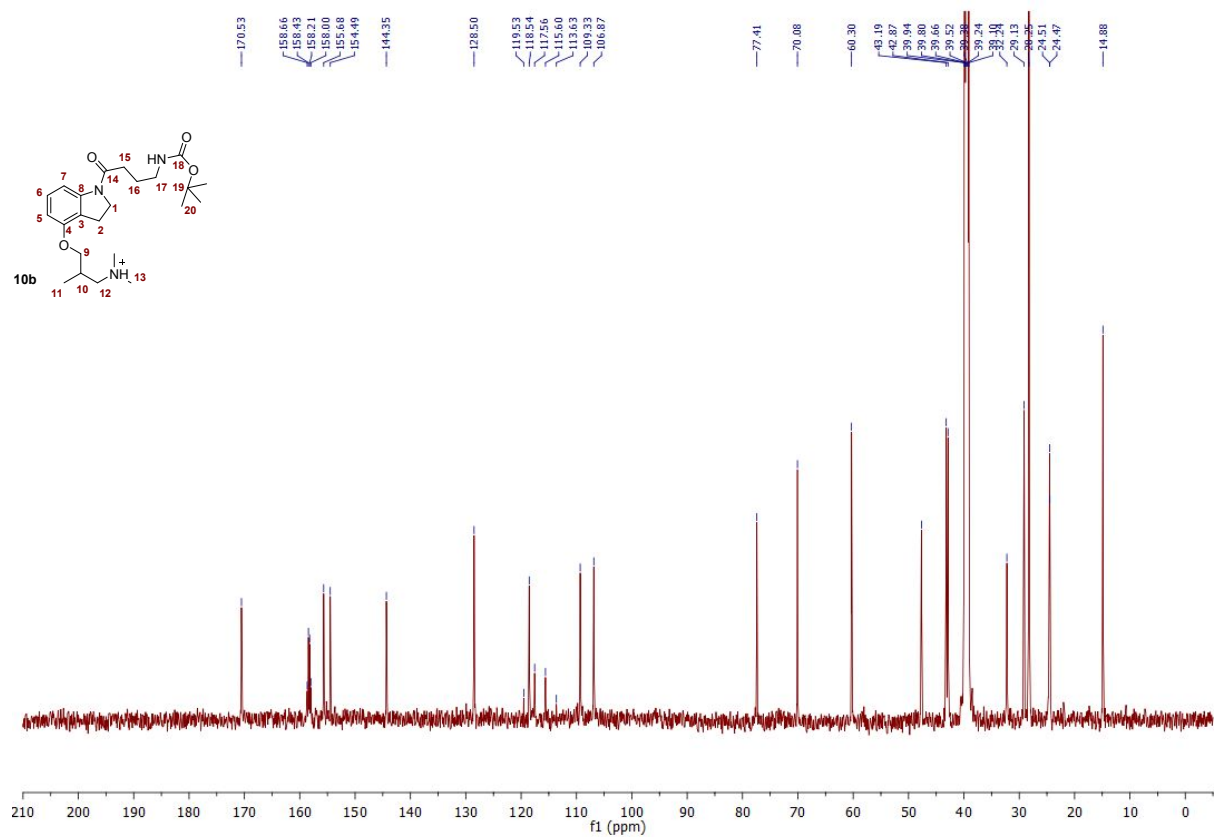


Figure S32. <sup>13</sup>C NMR spectrum of 10b in DMSO-d<sub>6</sub>.



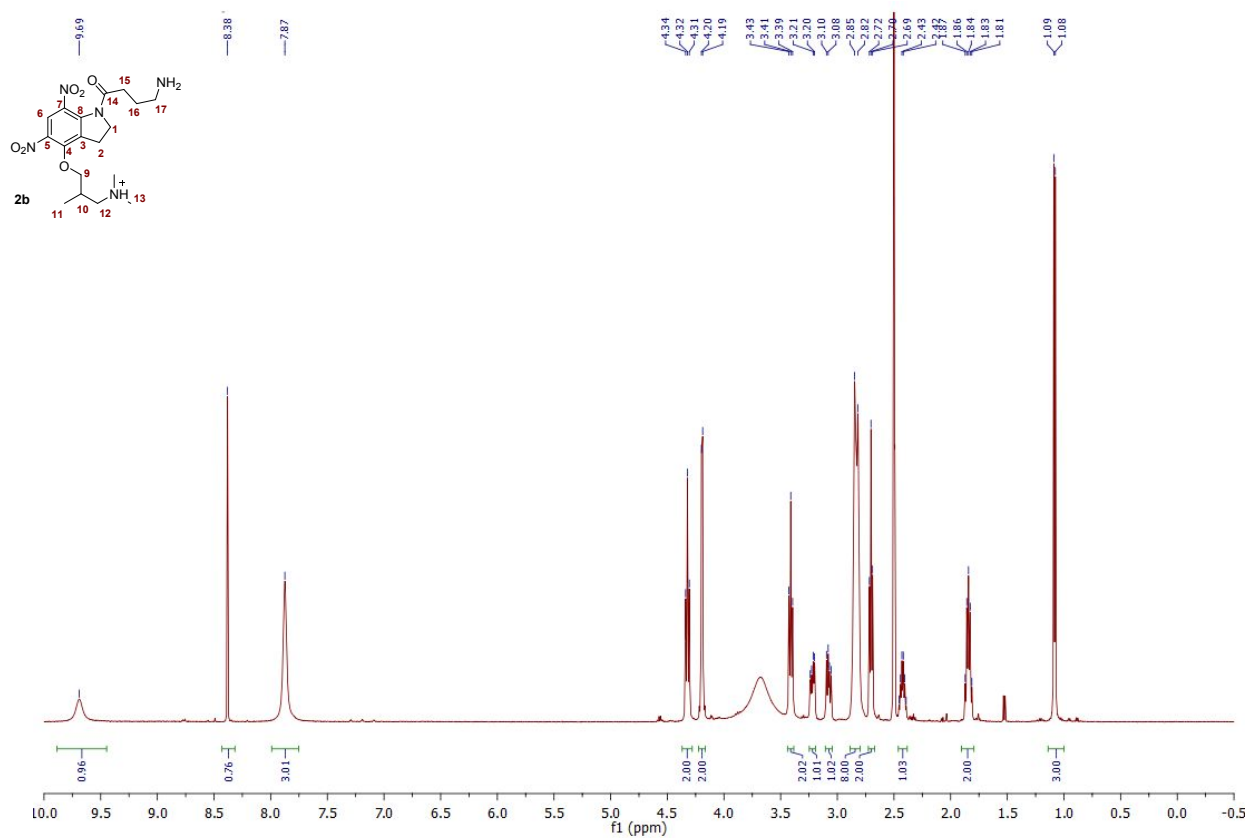


Figure S35. <sup>1</sup>H NMR spectrum of 2b in DMSO-d<sub>6</sub>.

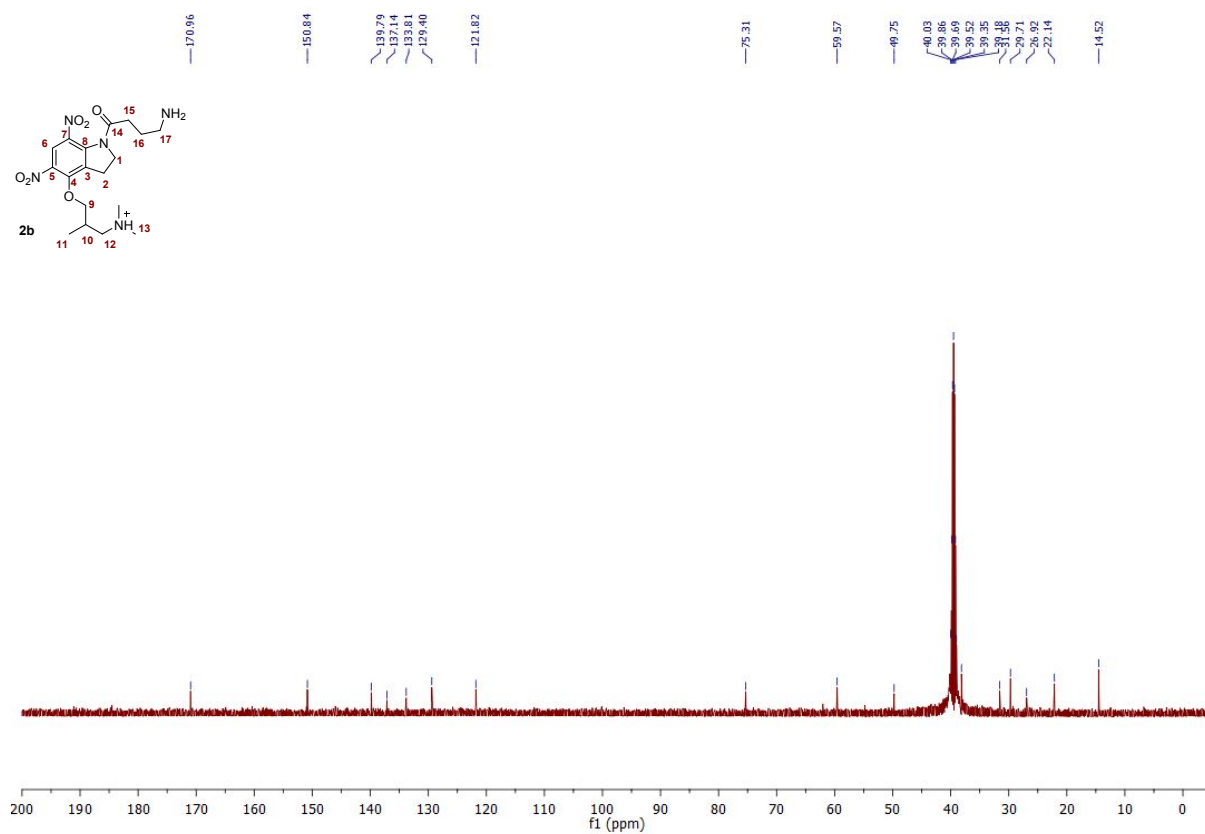


Figure S36. <sup>13</sup>C NMR spectrum of 2b in DMSO-d<sub>6</sub>.

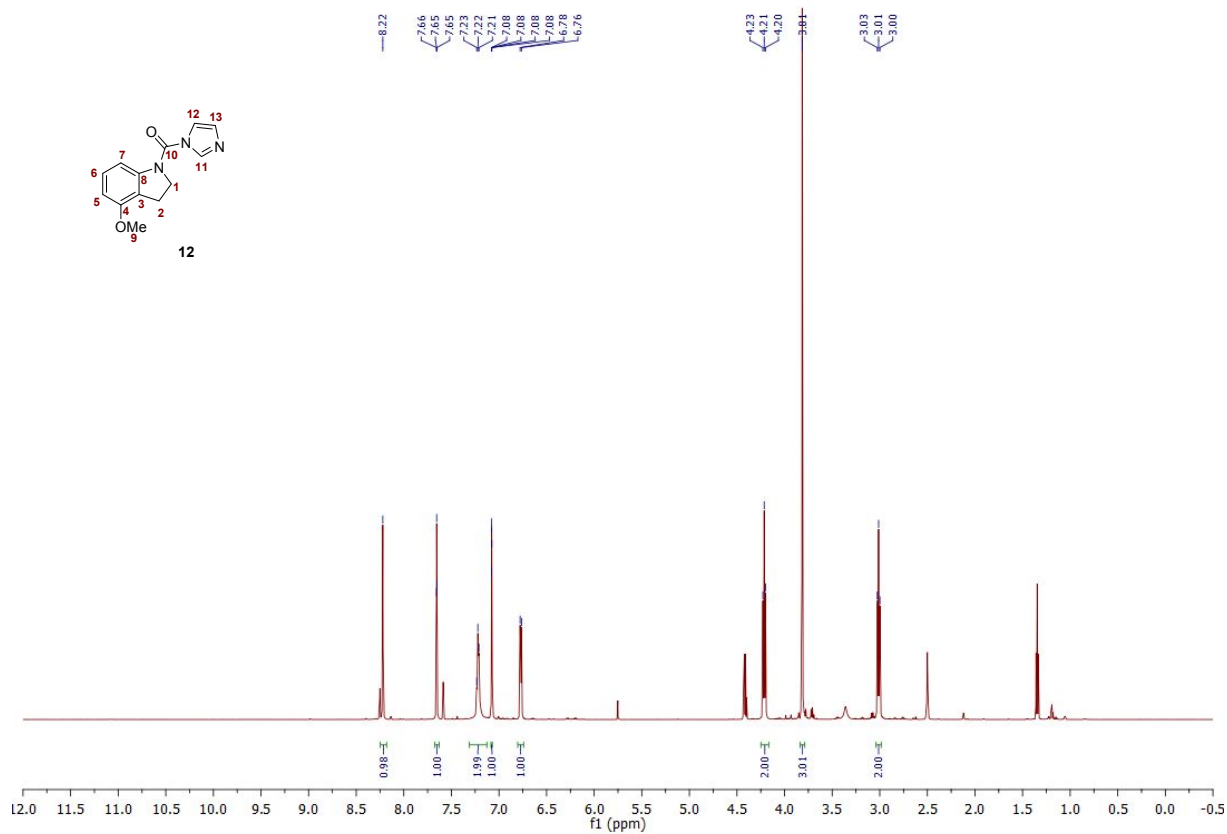


Figure S37. <sup>1</sup>H NMR spectrum of 12 in DMSO-d<sub>6</sub>.

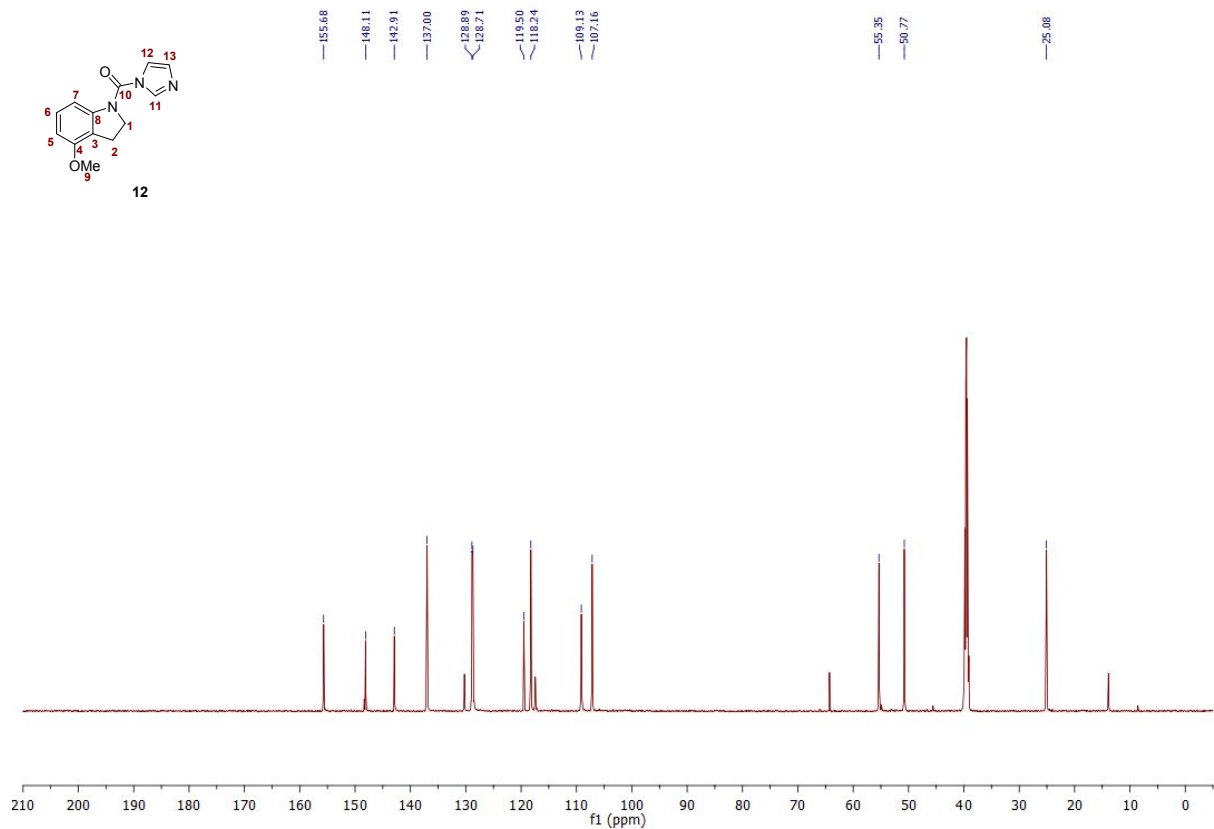


Figure S38. <sup>13</sup>C NMR spectrum of 12 in DMSO-d<sub>6</sub>.

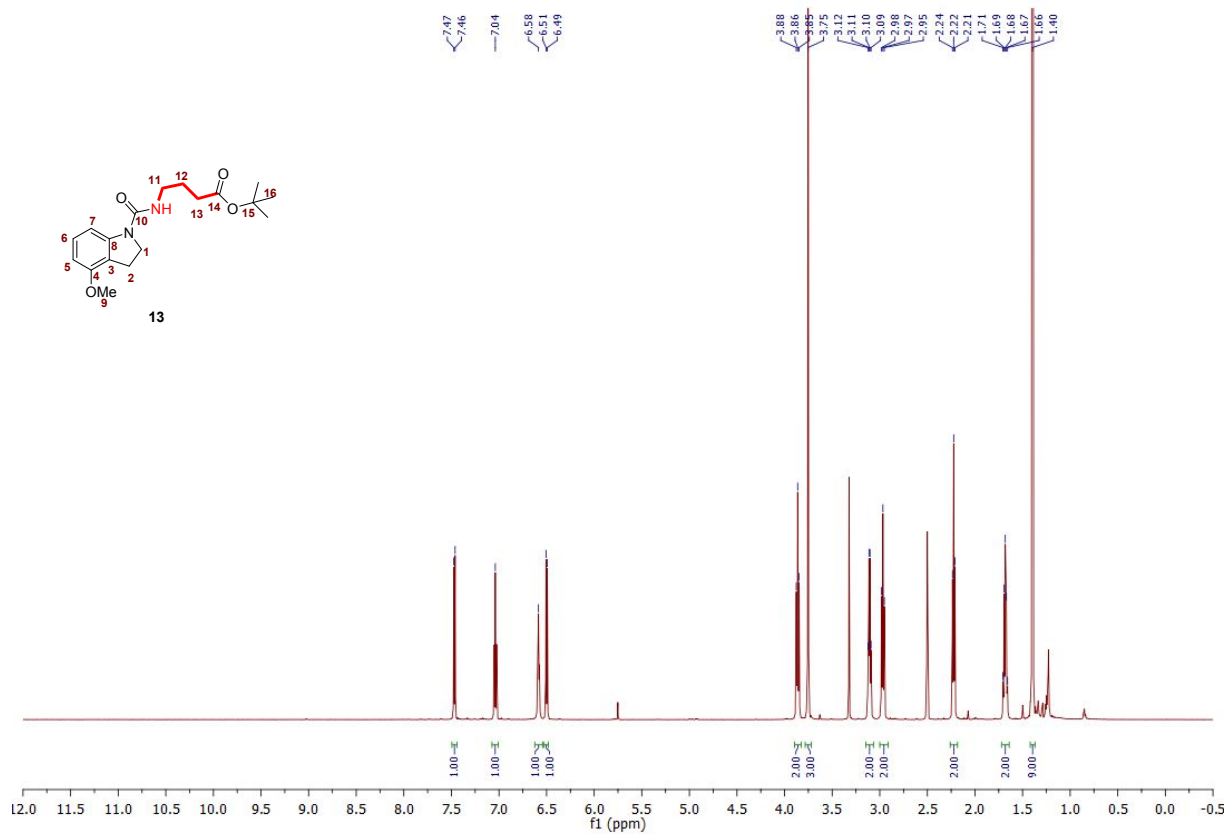


Figure S39. <sup>1</sup>H NMR spectrum of 13 in DMSO-d<sub>6</sub>.

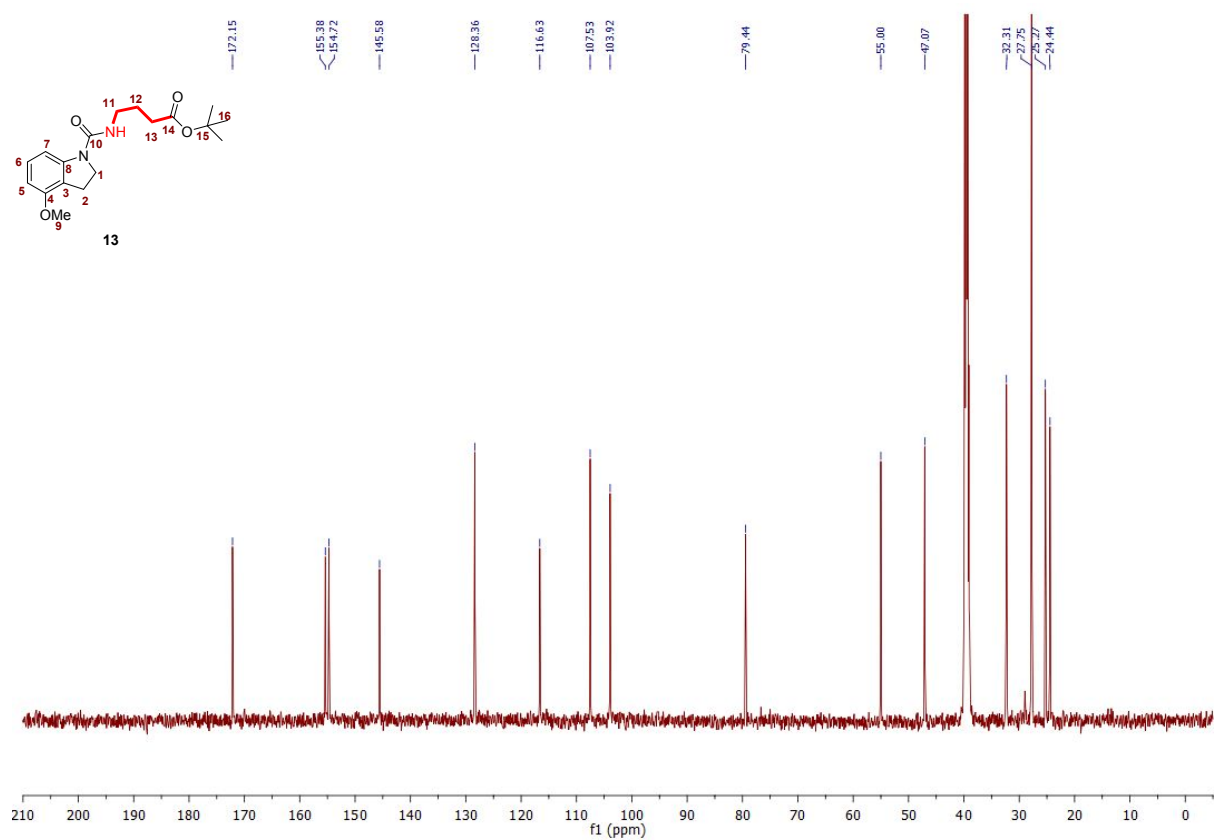


Figure S40. <sup>13</sup>C NMR spectrum of 13 in DMSO-d<sub>6</sub>.

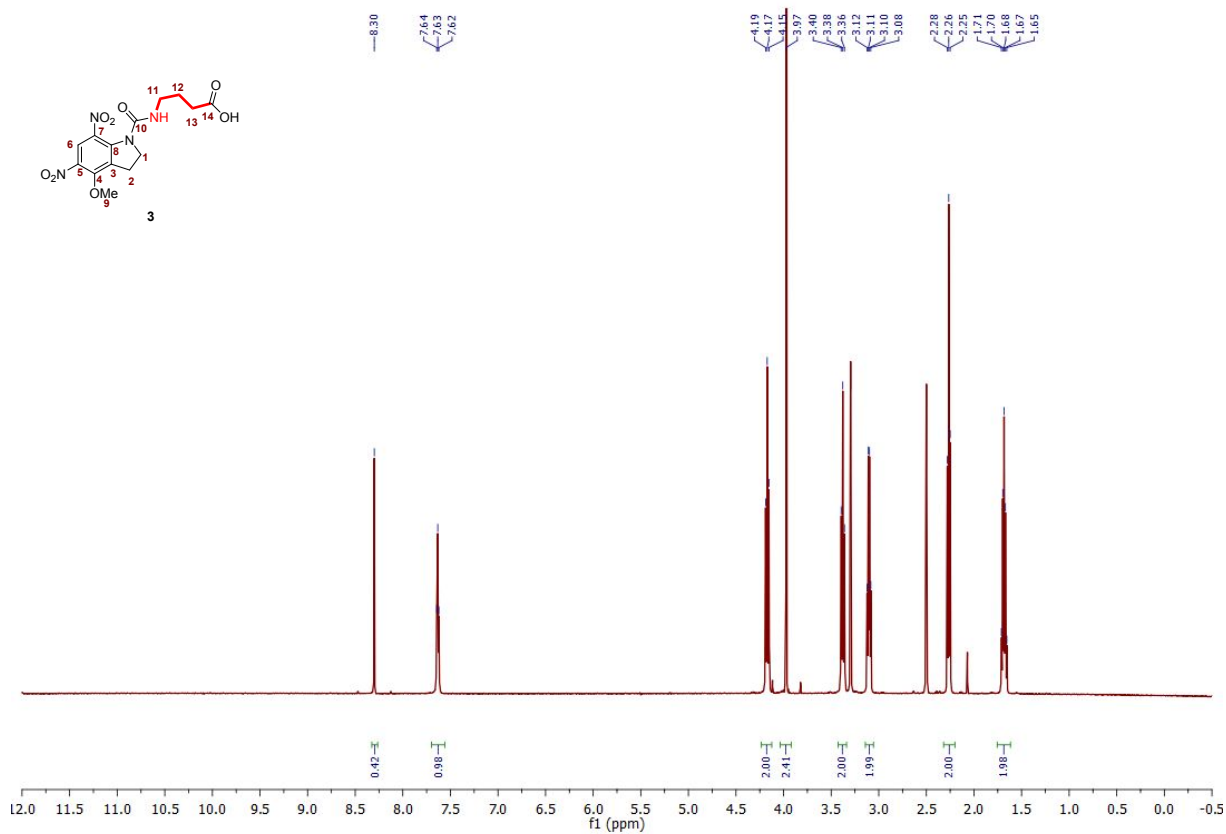


Figure S41. <sup>1</sup>H NMR spectrum of 3 in DMSO-d<sub>6</sub>.

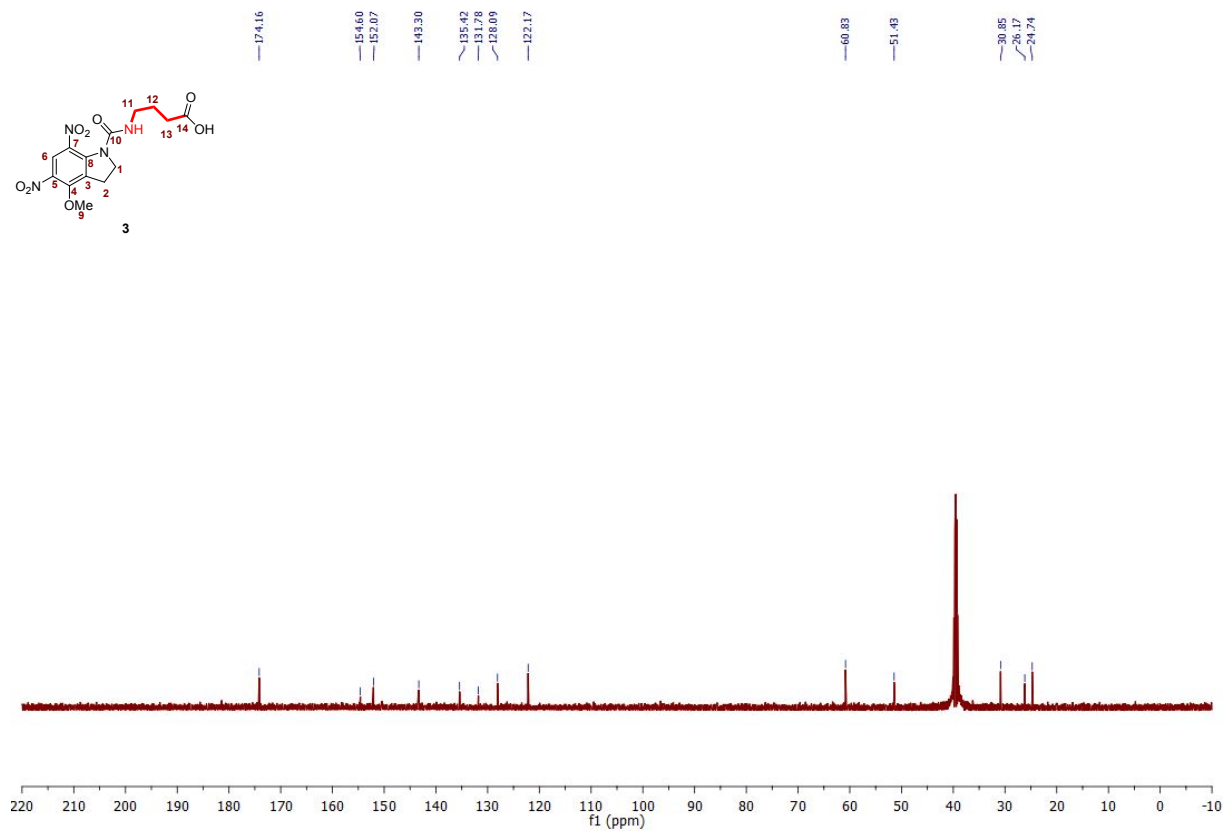


Figure S42. <sup>13</sup>C NMR spectrum of 3 in DMSO-d<sub>6</sub>.



## Computational row data in Table S2-S7

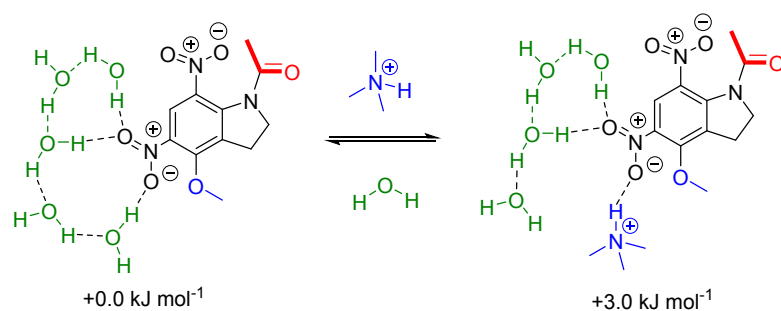


Figure S43. The consideration of the explicit solvent effect in water for the conformational study.

**Table S2.** Computed energies ( $E$ ), zero point energies, internal energies ( $U$ ), enthalpies ( $H$ ) and Gibbs free energies ( $G$ ) given in Hartree as well as entropies ( $S$ ) given in  $\text{J mol}^{-1} \text{K}^{-1}$  at B3LYP/6-31G(d,p) basis set with the consideration of PCM solvent method using the parameter set of water for the small molecules.

Number	File name	E	ZPE	U	H	G	S
GABA	001aaa_GABA_zw_b3lyp631dp_PCMw.log	-363.05699869	-362.917782	-362.909693	-362.908749	-362.951402	89.770
H <sub>2</sub> O	000haa_H2O_b3lyp631dp_PCMw.out	-76.42673000	-76.405409	-76.402574	-76.401630	-76.423071	45.127
H <sub>3</sub> O <sup>+</sup>	000c_H3Ocation_b3lyp631dp_PCMAcN.out	-76.82332900	-76.790173	-76.787333	-76.786389	-76.807567	44.573

**Table S3.** Computed energies ( $E$ ), zero point energies, internal energies ( $U$ ), enthalpies ( $H$ ) and Gibbs free energies ( $G$ ) given in Hartree as well as entropies ( $S$ ) given in  $J\ mol^{-1}\ K^{-1}$  at B3LYP/6-31G(d,p) basis set with the consideration of PCM solvent method using the parameter set of water for compound 1.

Number	States	conf	File name	E	ZPE	U	H	G	S
1	A(S <sub>0</sub> )		201aaa_DNIGABA_+H+_b3lyp631dp_PCMw.log	-1175.66001482	-1175.341754	-1175.319483	-1175.318539	-1175.395419	161.808
1	B(S1)		203aaa_DNIGABA_+H+_b3lyp631dp_PCMw_SP	-1175.53715919	-	-	-	-	-
1	C(S1)		205aaa_DNIGABA_+H+_TDb3lyp631dp_PCMw_OPT.log	-1175.63382582	-	-	-	-	-
1	D(T <sub>1</sub> )		207aaa_DNIGABA_+H+_b3lyp631dp_PCMw_TRIPLET.log	-1175.56520309	-1175.251202	-1175.228492	-1175.227548	-1175.305224	163.485
1	TS1		209aaa_DNIGABA_+H+_b3lyp631dp_PCMw_TRIPLET_TS1.log	-1175.5652010	-1175.250617	-1175.228717	-1175.227817	-1175.303417	158.762
1	E(T <sub>1</sub> )		221aaa_DNIGABA_+H+_INT_b3lyp631dp_PCMw.log	-1175.61316800	-1175.296614	-1175.274197	-1175.273253	-1175.350467	162.511
1	TS2		213caa_DNIGABA_+H+_b3lyp631dp_PCMw_TRIPLET_SCANopt_TS_FRQ.log	-1175.56858413	-1175.254000	-1175.232100	-1175.231200	-1175.306800	159.218
1	F(T <sub>1</sub> )		225baa_DNIGABA_+H+_INT_b3lyp631dp_PCMw_TRIPLET.log	-1175.59581453	-1175.282071	-1175.259314	-1175.258369	-1175.337213	165.941
1	TS3 <sup>c</sup>		225baa_DNIGABA_+H+_INT_b3lyp631dp_PCMw_TRIPLET.log	-1175.59581453	-1175.282071	-1175.259314	-1175.258369	-1175.337213	165.941
1	G(T <sub>1</sub> )		253aaa_DNI_VEGE_+H+_b3lyp631dp_PCMw_TRIPLET.log	-812.49568454	-812.324621	-812.310640	-812.309695	-812.367053	120.720
1	H(S <sub>0</sub> )		255aaa_DNI_VEGE_indole_b3lyp631dp_PCMw.out	-812.15036000	-811.988730	-811.975320	-811.974370	-812.029100	115.184
1	I(S <sub>0</sub> )		225baa_DNIGABA_+H+_INT_b3lyp631dp_PCMw_TRIPLET.log	-1175.59581453	-1175.282071	-1175.259314	-1175.258369	-1175.337213	165.941
1	TS4		221maa_DNIGABA_+H+_INT_B3LYP631dp_PCMw_TS.log	-1175.60057800	-1175.28476	-1175.26323	-1175.26229	-1175.33594	155.010

**Table S4.** Computed energies ( $E$ ), zero point energies, internal energies ( $U$ ), enthalpies ( $H$ ) and Gibbs free energies ( $G$ ) given in Hartree as well as entropies ( $S$ ) given in  $J\ mol^{-1}\ K^{-1}$  at B3LYP/6-31G(d,p) basis set with the consideration of PCM solvent method using the parameter set of water for compound 2a-l.

Number	States	conf	File name	E	ZPE	U	H	G	S
2a	A(S <sub>0</sub> )	l	101aaa_iDMPO_DNIGABA_+2H+_b3lyp631dp_PCMw.log	-1388.72193451	-1388.256843	-1388.228281	-1388.227337	-1388.318507	191.884
2a	B(S1)	l	103aaa_iDMPO_DNIGABA_+2H+_b3lyp631dp_PCMw_SP	-1388.59775561	-	-	-	-	-
2a	C(S1)	l	105aaa_iDMPO_DNIGABA_+2H+_TDb3lyp631dp_PCMw_OPT.log	-1388.69692928	-	-	-	-	-
2a	D(T <sub>1</sub> )	l	107aaa_iDMPO_DNIGABA_+2H+_b3lyp631dp_PCMw_TRIPLET.log	-1388.62711931	-1388.166603	-1388.137427	-1388.136483	-1388.229272	195.292
2a	TS1	l	111aaa_iDMPO_DNIGABA_+2H+_b3lyp631dp_PCMw_TRIPLET_TS1.log	-1388.62691590	-1388.166884	-1388.138446	-1388.137502	-1388.228349	191.203
2a	E(T <sub>1</sub> )	l	126aaa_iDMPO_DNIGABA_+2H+_INT_b3lyp631dp_PCMw_TRIPLET.log	-1388.62791912	-1388.166544	-1388.137997	-1388.137053	-1388.228355	192.162
2a	TS2	l	113aaa_iDMPO_DNIGABA_+2H+_b3lyp631dp_PCMw_TRIPLET_SCAN_vege_TS2.log	-1388.65484551	-1388.194869	-1388.166351	-1388.165406	-1388.257654	194.151
2a	F(T <sub>1</sub> )	l	114aaa_iDMPO_DNIGABA_+2H+_b3lyp631dp_PCMw_TRIPLET_SCAN_vege_SCAN2vege.log	-1388.65753745	-1388.197699	-1388.168367	-1388.167423	-1388.262174	199.420
2a	TS3 <sup>c</sup>	l	114aaa_iDMPO_DNIGABA_+2H+_b3lyp631dp_PCMw_TRIPLET_SCAN_vege_SCAN2vege_TS_FRQ.log	-1388.62810435	-1388.172788	-1388.142431	-1388.141487	-1388.240511	208.413
2a	G(T <sub>1</sub> )	l	153aaa_iDMPO_DNI_VEGE_+2H+_b3lyp631dp_PCMw_TRIPLET.log	-1025.55282554	-1025.235419	-1025.214726	-1025.213782	-1025.287064	154.235
2a	H(S <sub>0</sub> )	l	155baa_iDMPO_DNI_VEGE_indole+H+_b3lyp631dp_PCMw.log	-1025.22356477	-1024.915674	-1024.89585	-1024.894906	-1024.964387	146.235
2a	I(S <sub>0</sub> )	l	121aaa_iDMPO_DNIGABA_+2H+_INT_b3lyp631dp_PCMw.log	-1388.67658606	-1388.214628	-1388.185468	-1388.184524	-1388.277553	195.797
2a	TS4	l	121aba_iDMPO_DNIGABA_+2H+_INT_b3lyp631dp_PCMw_SCAN_CN_jof2_FRQ.log	-1388.66324723	-1388.201066	-1388.173014	-1388.172070	-1388.261020	-187.211

**Table S5.** Computed energies ( $E$ ), zero point energies, internal energies ( $U$ ), enthalpies ( $H$ ) and Gibbs free energies ( $G$ ) given in Hartree as well as entropies ( $S$ ) given in  $\text{J mol}^{-1} \text{K}^{-1}$  at B3LYP/6-31G(d,p) basis set with the consideration of PCM solvent method using the parameter set of water for compound **2a-II**.

Number	States	conf	File name	E	ZPE	U	H	G	S
2a	A(S <sub>0</sub> )	II	101baa_iDMPO_DNIGABA_+2H+_b3lyp631dp_PCMw.log	-1388.72982567	-1388.264726	-1388.236386	-1388.235442	-1388.324707	187.875
2a	B(S1)	II	103baa_iDMPO_DNIGABA_+2H+_b3lyp631dp_PCMw_SP.log	-1388.60523500	-	-	-	-	-
2a	C(S1)	II	105baa_iDMPO_DNIGABA_+2H+_TDb3lyp631dp_PCMw_OPT.log	-1388.67686051	-	-	-	-	-
2a	D(T <sub>1</sub> )	II	107baa_iDMPO_DNIGABA_+2H+_b3lyp631dp_PCMw_TRIPLET_f.log	-1388.64105800	-1388.180824	-1388.152073	-1388.151129	-1388.242347	191.985
2a	TS1	II	111baa_iDMPO_DNIGABA_+2H+_b3lyp631dp_PCMw_TRIPLET_TS_f.log	-1388.63473900	-1388.175452	-1388.147253	-1388.146308	-1388.235833	188.420
2a	E(T <sub>1</sub> )	II	126baa_iDMPO_DNIGABA_+2H+_INT_b3lyp631dp_PCMw_TRIPLET.log	-1388.63603556	-1388.174551	-1388.146193	-1388.145249	-1388.234784	188.444
2a	TS2	II	113baa_iDMPO_DNIGABA_+2H+_b3lyp631dp_PCMw_TRIPLET_SCANvege_TS2.log	-1388.66396477	-1388.204049	-1388.175625	-1388.174680	-1388.266467	193.181
2a	F(T <sub>1</sub> )	II	114baa_iDMPO_DNIGABA_+2H+_b3lyp631dp_PCMw_TRIPLET_SCANvege_SCAN2vege.log	-1388.66655781	-1388.206491	-1388.177367	-1388.176423	-1388.269829	196.589
2a	TS3 <sup>c</sup>	II	114baa_iDMPO_DNIGABA_+2H+_b3lyp631dp_PCMw_TRIPLET_SCANvege_SCAN2vege_TS_FRQ.log	-1388.63822041	-1388.182177	-1388.152278	-1388.151334	-1388.247410	202.209
2a	G(T <sub>1</sub> )	II	153baa_iDMPO_DNI_VEGE_+2H+_b3lyp631dp_PCMw_log	-1025.54325700	-1025.227112	-1025.206442	-1025.205498	-1025.276904	150.286
2a	H(S <sub>0</sub> )	II	155baa_iDMPO_DNI_VEGE_indole+H+_b3lyp631dp_PCMw.log	-1025.22356477	-1024.915674	-1024.89585	-1024.894906	-1024.964387	146.235
2a	I(S <sub>0</sub> )	II	121baa_iDMPO_DNIGABA_+2H+_INT_b3lyp631dp_PCMw.log	-1388.68471369	-1388.222392	-1388.193587	-1388.192643	-1388.283972	192.218
2a	TS4	I	121bba_iDMPO_DNIGABA_+2H+_INT_b3lyp631dp_PCMw_SCAN_CN_f_FRQ.log	-1388.67292523	-1388.211167	-1388.182939	-1388.181995	-1388.271727	188.857

**Table S6.** Computed energies ( $E$ ), zero point energies, internal energies ( $U$ ), enthalpies ( $H$ ) and Gibbs free energies ( $G$ ) given in Hartree as well as entropies ( $S$ ) given in  $\text{J mol}^{-1} \text{K}^{-1}$  at B3LYP/6-31G(d,p) basis set with the consideration of PCM solvent method using the parameter set of water for compound **2b-I**.

Number	States	conf	File name	E	ZPE	U	H	G	S
2b	A(S <sub>0</sub> )	I	701aaa_iDMBO_DNIGABA_+2H+_b3lyp631dp_PCMw.log	-1428.04303910	-1427.54917	-1427.51928	-1427.518336	-1427.612682	198.57
2b	B(S1)	I	703aaa_iDMBO_DNIGABA_+2H+_TD_b3lyp631dp_PCMw_sp.log	-1427.91717320	-	-	-	-	-
2b	C(S1)	I	705aaa_iDMBO_DNIGABA_+2H+_TD_b3lyp631dp_PCMw_opt.log	-1427.93880490	-	-	-	-	-
2b	D(T <sub>1</sub> )	I	707aaa_iDMBO_DNIGABA_+2H+_b3lyp631dp_PCMw_TRIPLET_opt.log	-1427.94833328	-1427.458867	-1427.428457	-1427.427513	-1427.523319	201.64
2b	TS1	I	709aaa_iDMBO_DNIGABA_+2H+_b3lyp631dp_PCMw_TRIPLET_opt_TS_OCFRQ.log	-1427.94821119	-1427.459159	-1427.429547	-1427.428603	-1427.522402	197.416
2b	E(T <sub>1</sub> )	I	710aaa_iDMBO_DNIGABA_+2H+_b3lyp631dp_PCMw_TRIPLET_SCAN_vege.log	-1427.95132297	-1427.461383	-1427.431434	-1427.430490	-1427.525218	199.371
2b	TS2	I	713baa_iDMBO_DNIGABA_+2H+_b3lyp631dp_PCMw_TRIPLET_SCAN_vege_TS_CN_FRQ.log	-1427.95048329	-1427.461898	-1427.432515	-1427.431571	-1427.524145	194.839
2b	F(T <sub>1</sub> )	I	721aaa_iDMBO_DNIGABA_+2H+_INT_b3lyp631dp_PCMw.log	-1427.99722623	-1427.506222	-1427.475837	-1427.474893	-1427.570789	201.83
2b	TS3 <sup>c</sup>	I	722aba_iDMBO_DNIGABA_+2H+_INT_b3lyp631dp_PCMw_SCAN_FRQ.log	-1427.94965327	-1427.465749	-1427.433943	-1427.432999	-1427.537560	220.067
2b	G(T <sub>1</sub> )	I	725aaa_iDMBO_DNI_+H+_b3lyp631dp_PCMw.log	-1064.85881801	-1064.514603	-1064.492216	-1064.491272	-1064.568232	161.976
2b	H(S <sub>0</sub> )	I	727aaa_iDMBO_DNI_indole_+H+_b3lyp631dp_PCMw.log	-1064.53329073	-1064.196898	-1064.175542	-1064.174598	-1064.248875	156.329
2b	I(S <sub>0</sub> )	I	721baa_iDMBO_DNIGABA_INT_+2H+_b3lyp631dp_PCMw_uj.log	-1427.99698845	-1427.505729	-1427.475727	-1427.474783	-1427.568847	197.974
2b	TS4	I	721naa_iDMBO_DNIGABA_+2H+_INT_b3lyp631dp_PCMw_TS_FRQ.log	-1427.98434734	-1427.494825	-1427.467524	-1427.46658	-1427.554214	184.440

**Table S7.** Computed energies ( $E$ ), zero point energies, internal energies ( $U$ ), enthalpies ( $H$ ) and Gibbs free energies ( $G$ ) given in Hartree as well as entropies ( $S$ ) given in  $\text{J mol}^{-1} \text{K}^{-1}$  at B3LYP/6-31G(d,p) basis set with the consideration of PCM solvent method using the parameter set of water for compound **2b-II**.

Number	States	conf	File name	E	ZPE	U	H	G	S
2b	A(S <sub>0</sub> )	II	701baa_iDMBO_DNIGABA_+2H+_b3lyp631dp_PCMw.log	-1428.04427742	-1427.55089	-1427.521067	-1427.520123	-1427.613312	196.133
2b	B(S1)	II	703baa_iDMBO_DNIGABA_+2H+_TD_b3lyp631dp_PCMw_sp.log	-1427.92650183	-	-	-	-	-
2b	C(S1)	II	705baa_iDMBO_DNIGABA_+2H+_TD_b3lyp631dp_PCMw_opt.log	-1427.949102510	-	-	-	-	-
2b	D(T <sub>1</sub> )	II	707baa_iDMBO_DNIGABA_+2H+_b3lyp631dp_PCMw_TRIPLET_opt.log	-1427.95862200	-1427.468928	-1427.439512	-1427.438568	-1427.530441	193.363
2b	TS1	II	709baa_iDMBO_DNIGABA_+2H+_b3lyp631dp_PCMw_TRIPLET_opt_TS_OC_FRQ.log	-1427.94848320	-1427.460302	-1427.430608	-1427.429663	-1427.523439	197.368
2b	E(T <sub>1</sub> )	II	710baa_iDMBO_DNIGABA_+2H+_b3lyp631dp_PCMw_TRIPLET_SCAN_vege.log	-1427.95224369	-1427.462076	-1427.432479	-1427.431535	-1427.524074	194.766
2b	TS2	II	713baa_iDMBO_DNIGABA_+2H+_b3lyp631dp_PCMw_TRIPLET_SCAN_vege_TS_CN_FRQ.log	-1427.95048337	-1427.461898	-1427.432515	-1427.431571	-1427.524145	194.839
2b	F(T <sub>1</sub> )	II	721baa_iDMBO_DNIGABA_+2H+_INT_b3lyp631dp_PCMw.log	-1427.99922835	-1427.508294	-1427.478123	-1427.477179	-1427.571385	198.273
2b	TS3 <sup>c</sup>	II	722bba_iDMBO_DNIGABA_+2H+_INT_b3lyp631dp_TRIPLET_PCMw_TS_FRQ.log	-1427.95100731	-1427.466759	-1427.435373	-1427.434429	-1427.535374	212.457
2b	G(T <sub>1</sub> )	II	725baa_iDMBO_DNI_+H+_b3lyp631dp_PCMw.log	-1064.85818307	-1064.513355	-1064.49152	-1064.490576	-1064.564641	155.882
2b	H(S <sub>0</sub> )	II	727baa_iDMBO_DNI_indole_+H+_b3lyp631dp_PCMw.log	-1064.53526452	-1064.198602	-1064.177645	-1064.176701	-1064.248322	150.740
2b	I(S <sub>0</sub> )	II	721baa_iDMBO_DNIGABA_+2H+_INT_b3lyp631dp_PCMw.log	-1427.99922813	-1427.508294	-1427.478123	-1427.477179	-1427.571385	198.273

## Computed XYZ coordinates for structures

**GABA:** 001aaa\_GABA\_zw\_b3lyp631dp\_PCMw.log

orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.903765	0.083080	0.006432
2	8	0	-1.845879	1.337852	0.112546
3	6	0	-0.553602	-0.695852	0.097998
4	1	0	-0.579912	-1.526754	-0.616411
5	1	0	-0.506030	-1.156064	1.095693
6	6	0	0.680131	0.181295	-0.124950
7	1	0	0.611811	1.046638	0.541728
8	1	0	0.674693	0.572453	-1.150042
9	6	0	1.973374	-0.581071	0.120950
10	7	0	3.179004	0.319980	-0.068538
11	1	0	3.167820	1.098458	0.596333
12	1	0	4.057613	-0.187738	0.065567
13	1	0	2.040720	-0.962894	1.141255
14	1	0	3.197151	0.722344	-1.009893
15	1	0	2.106965	-1.411612	-0.574381
16	8	0	-2.929205	-0.632777	-0.139129

1\_A(S0) 201aaa\_DNIGABA\_+H+\_b3lyp631dp\_PCMw.log

orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.253723	-0.186744	0.189078
2	6	0	1.205513	-1.206627	0.051605
3	6	0	2.558994	-0.949812	-0.143288
4	6	0	2.956312	0.416167	-0.212466
5	6	0	2.028351	1.435013	-0.012869
6	6	0	0.689820	1.148732	0.223532
7	6	0	-0.905467	-2.195795	0.559070
8	6	0	0.524849	-2.551457	0.097222
9	1	0	2.362108	2.463050	-0.023263
10	1	0	-1.667632	-2.751346	0.016979
11	1	0	1.012286	-3.244867	0.784850
12	7	0	-1.027556	-0.733498	0.286750
13	1	0	0.524753	-3.015462	-0.895172
14	1	0	-1.036145	-2.370165	1.630798
15	6	0	-2.173003	-0.110558	-0.194910
16	8	0	-2.127349	0.995723	-0.715796
17	8	0	3.366550	-2.024049	-0.311936
18	6	0	4.336496	-2.299060	0.723348
19	1	0	4.804274	-3.241130	0.438861
20	1	0	5.093203	-1.515272	0.774784
21	1	0	3.834465	-2.411107	1.688624
22	7	0	-0.155067	2.264561	0.639168
23	8	0	0.054804	3.367029	0.132198
24	8	0	-0.982608	2.050165	1.522964
25	6	0	-3.472200	-0.886641	-0.036206
26	1	0	-3.513289	-1.336998	0.961295
27	1	0	-3.471375	-1.717996	-0.753301
28	6	0	-4.685817	0.015468	-0.281300
29	1	0	-4.586613	0.493180	-1.260175
30	1	0	-4.703377	0.815046	0.466910
31	6	0	-5.978583	-0.787951	-0.216099
32	7	0	-7.172710	0.101580	-0.474515
33	1	0	-7.132677	0.525786	-1.406108
34	1	0	-8.049516	-0.424191	-0.415538
35	1	0	-6.014598	-1.572878	-0.973243
36	1	0	-7.229773	0.863930	0.207238
37	7	0	4.314768	0.838108	-0.537876
38	8	0	4.606035	2.027434	-0.379043
39	8	0	5.102972	0.000908	-0.983845
40	1	0	-6.139285	-1.236927	0.765140

1\_C(S1) 205aaa\_DNIGABA\_+H+\_TDb3lyp631dp\_PCMw\_OPT.log

orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.290289	-0.382221	-0.002927
2	6	0	1.374807	-1.269429	-0.016399
3	6	0	2.719545	-0.799683	-0.005749
4	6	0	2.868495	0.589119	-0.029589
5	6	0	1.747033	1.475947	0.103457
6	6	0	0.461450	1.015096	0.132340
7	6	0	-0.651987	-2.530196	0.053838
8	6	0	0.883736	-2.679330	-0.048220
9	1	0	1.937261	2.538294	0.176878
10	1	0	-1.193196	-3.063002	-0.730876
11	1	0	1.308163	-3.270178	0.769147
12	7	0	-0.885086	-1.079156	-0.077851
13	1	0	1.171284	-3.181328	-0.980325
14	1	0	-1.034006	-2.870247	1.023834
15	6	0	-2.106394	-0.482280	-0.599507
16	8	0	-2.009293	0.236128	-1.571201
17	8	0	3.643013	-1.767222	0.044764
18	6	0	4.868601	-1.621355	0.795135
19	1	0	5.100304	-2.622413	1.157756
20	1	0	5.667620	-1.250506	0.154606
21	1	0	4.718221	-0.943381	1.639246
22	7	0	-0.667828	1.857236	0.373405
23	8	0	-0.619961	3.087252	0.029859
24	8	0	-1.634666	1.307567	1.041104
25	6	0	-3.381775	-0.953366	0.047657
26	1	0	-3.212333	-1.072112	1.121258
27	1	0	-3.623270	-1.947737	-0.354166
28	6	0	-4.521671	0.032146	-0.231855
29	1	0	-4.647925	0.142883	-1.313048
30	1	0	-4.236187	1.009472	0.171128
31	6	0	-5.820440	-0.447818	0.403414
32	7	0	-6.943266	0.520796	0.113542
33	1	0	-7.120025	0.604385	-0.892036
34	1	0	-7.817706	0.219731	0.553058
35	1	0	-6.141498	-1.413524	0.009724
36	1	0	-6.731421	1.458683	0.466844
37	7	0	4.155902	1.228821	-0.241268
38	8	0	4.316426	2.370548	0.197951
39	8	0	5.003824	0.616002	-0.898387
40	1	0	-5.748224	-0.514871	1.489878

1\_D(T1) 207aaa\_DNIGABA\_+H+\_b3lyp631dp\_PCMw\_TRIPLET.log

orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.306301	-0.395049	-0.052552
2	6	0	-1.405112	-1.271992	-0.034644
3	6	0	-2.733388	-0.789459	-0.030117
4	6	0	-2.863733	0.610107	0.024367
5	6	0	-1.759379	1.499251	-0.051308
6	6	0	-0.461669	1.019429	-0.124300
7	6	0	0.615125	-2.537658	0.098944
8	6	0	-0.920580	-2.686416	0.012492
9	1	0	-1.938646	2.564620	-0.051705
10	1	0	1.028030	-2.921138	1.036990
11	1	0	-1.233176	-3.240573	-0.879209
12	7	0	0.857322	-1.081621	0.036908
13	1	0	-1.326119	-3.223954	0.875911
14	1	0	1.142154	-3.022741	-0.728233
15	6	0	2.127542	-0.444861	0.555611
16	8	0	2.082859	-0.128595	1.729507
17	8	0	-3.690278	-1.734334	-0.067016
18	6	0	-4.871484	-1.575922	-0.881679
19	1	0	-5.126314	-2.579714	-1.221648
20	1	0	-5.688328	-1.155208	-0.295573
21	1	0	-4.659520	-0.936151	-1.742555
22	7	0	0.650961	1.833568	-0.263848
23	8	0	0.557692	3.097630	-0.150254
24	8	0	1.793183	1.241626	-0.575314
25	6	0	3.361501	-0.814283	-0.230573
26	1	0	3.152112	-0.703032	-1.296729
27	1	0	3.567848	-1.876599	-0.041216
28	6	0	4.556059	0.042752	0.202690
29	1	0	4.722276	-0.085725	1.276847
30	1	0	4.310272	1.094921	0.028847
31	6	0	5.810703	-0.342186	-0.570284
32	7	0	6.977942	0.521362	-0.151291
33	1	0	7.176435	0.428048	0.849489
34	1	0	7.831381	0.266548	-0.656199
35	1	0	6.112609	-1.374043	-0.383600
36	1	0	6.798383	1.512548	-0.336476
37	7	0	-4.163218	1.247046	0.225729
38	8	0	-4.334906	2.373236	-0.243185
39	8	0	-4.998606	0.641060	0.902020
40	1	0	5.694298	-0.197548	-1.645370



1\_TS1 209aaa\_DNIGABA\_+H+\_b3lyp631dp\_PCMw\_TRIPLET\_TS1.log

orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.354984	-0.360576	0.060678
2	6	0	-1.403176	-1.268246	0.090436
3	6	0	-2.727016	-0.820018	0.020052
4	6	0	-2.924516	0.593496	-0.017277
5	6	0	-1.850257	1.502678	-0.065090
6	6	0	-0.553926	1.026261	-0.024980
7	6	0	0.709854	-2.416382	0.285901
8	6	0	-0.824849	-2.664474	0.127793
9	1	0	-2.055085	2.564132	-0.093228
10	1	0	1.060252	-2.654846	1.293172
11	1	0	-1.043019	-3.204587	-0.799226
12	7	0	0.866541	-0.965659	0.039557
13	1	0	-1.225959	-3.257974	0.952818
14	1	0	1.304857	-2.979968	-0.434873
15	6	0	2.063123	-0.010965	0.210402
16	8	0	2.028565	0.030989	1.561083
17	8	0	-3.668631	-1.780175	-0.007622
18	6	0	-4.787008	-1.707528	-0.918425
19	1	0	-4.968582	-2.733856	-1.238872
20	1	0	-5.665113	-1.305310	-0.414802
21	1	0	-4.537787	-1.090742	-1.785752
22	7	0	0.595906	1.840945	0.065578
23	8	0	0.639380	3.039823	-0.204965
24	8	0	1.832948	1.049893	-0.425174
25	6	0	3.344501	-0.649636	-0.381302
26	1	0	3.249607	-0.708935	-1.469949
27	1	0	3.415638	-1.666544	0.014417
28	6	0	4.581935	0.160756	0.024419
29	1	0	4.634917	0.202975	1.117876
30	1	0	4.484751	1.188086	-0.342522
31	6	0	5.852237	-0.466864	-0.534611
32	7	0	7.072885	0.313521	-0.101184
33	1	0	7.162299	0.336953	0.918863
34	1	0	7.931758	-0.101474	-0.473408
35	1	0	5.999009	-1.486657	-0.175860
36	1	0	7.036862	1.284104	-0.427058
37	7	0	-4.237978	1.195496	0.129792
38	8	0	-4.410084	2.337699	-0.308817
39	8	0	-5.107871	0.557328	0.732962
40	1	0	5.864144	-0.470949	-1.625506

1\_E(T1) 221aaa\_DNIGABA\_+H+\_INT\_b3lyp631dp\_PCMw.log

orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.448736	0.526105	-0.447648
2	6	0	1.642079	1.360285	-0.249963
3	6	0	2.861857	0.820867	0.026210
4	6	0	2.948803	-0.639161	0.095819
5	6	0	1.886787	-1.468761	-0.045847
6	6	0	0.594011	-0.933049	-0.349387
7	6	0	-0.349318	2.611261	-0.673389
8	6	0	1.176156	2.788026	-0.443839
9	1	0	2.010015	-2.539863	0.032165
10	1	0	-0.947610	3.097699	0.106361
11	1	0	1.661889	3.247484	-1.310747
12	7	0	-0.650631	1.177363	-0.663437
13	1	0	1.376327	3.428156	0.417708
14	1	0	-0.681211	3.035099	-1.628075
15	6	0	-2.492774	-0.924657	0.036853
16	8	0	-2.219684	-1.060806	1.198651
17	8	0	4.024826	1.457024	0.292351
18	6	0	4.010109	2.788232	0.827472
19	1	0	5.037331	2.983151	1.135143
20	1	0	3.713659	3.523679	0.076694
21	1	0	3.349540	2.848289	1.696888
22	7	0	-0.386065	-1.825320	-0.528131
23	8	0	-0.335160	-3.051000	-0.421666
24	8	0	-1.637195	-1.308700	-0.993262
25	6	0	-3.749107	-0.353908	-0.565565
26	1	0	-3.453587	0.568012	-1.079090
27	6	0	-4.814113	-0.089632	0.503115
28	1	0	-4.405613	0.584224	1.262826
29	1	0	-5.069064	-1.029189	1.004050
30	6	0	-6.060933	0.520905	-0.125955
31	1	0	-6.520616	-0.145844	-0.857044
32	1	0	-5.853308	1.479608	-0.603554
33	1	0	-4.109753	-1.042738	-1.336916
34	7	0	-7.116285	0.789942	0.921318
35	1	0	-6.786194	1.447740	1.633729
36	1	0	-7.957679	1.195064	0.501252
37	1	0	-7.399986	-0.067481	1.405367
38	7	0	4.251748	-1.289071	0.277752
39	8	0	5.204013	-0.853487	-0.365551
40	8	0	4.304543	-2.260852	1.034910

orientation:

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.219480	-0.127404	-0.354246
2	6	0	-1.155213	-1.221668	-0.405860
3	6	0	-2.493058	-1.026638	-0.246471
4	6	0	-2.957817	0.345943	-0.035664
5	6	0	-2.107968	1.416827	-0.007489
6	6	0	-0.713382	1.212566	-0.171274
7	6	0	1.122602	-1.948645	-0.541177
8	6	0	-0.342454	-2.465556	-0.673830
9	1	0	-2.493541	2.417834	0.127595
10	1	0	1.605890	-2.327396	0.366570
11	1	0	-0.540454	-2.847491	-1.681051
12	7	0	1.032579	-0.477197	-0.451433
13	1	0	-0.555528	-3.275388	0.027831
14	1	0	1.749718	-2.228139	-1.391996
15	6	0	2.157565	0.930664	0.356477
16	8	0	1.941159	0.916935	1.540606
17	8	0	-3.375328	-2.053405	-0.387782
18	6	0	-3.608863	-2.857625	0.787961
19	1	0	-4.289307	-3.649389	0.474474
20	1	0	-2.675745	-3.298313	1.150883
21	1	0	-4.073509	-2.256652	1.572021
22	7	0	0.133083	2.271471	-0.202961
23	8	0	-0.186136	3.451492	-0.083883
24	8	0	1.442767	2.022680	-0.491428
25	6	0	3.488491	0.766694	-0.344962
26	1	0	3.326583	0.528789	-1.397089
27	6	0	4.357252	-0.284194	0.356260
28	1	0	3.896607	-1.273920	0.267186
29	1	0	4.417365	-0.045106	1.422924
30	6	0	5.754944	-0.312153	-0.250953
31	1	0	6.270823	0.642243	-0.133655
32	1	0	5.741925	-0.580250	-1.308418
33	1	0	3.976996	1.747865	-0.296990
34	7	0	6.614363	-1.345788	0.438236
35	1	0	6.232971	-2.290057	0.327429
36	1	0	7.565010	-1.353046	0.058037
37	1	0	6.689331	-1.162075	1.443144
38	7	0	-4.373400	0.644492	0.159950
39	8	0	-5.094451	-0.227753	0.647806
40	8	0	-4.776414	1.768398	-0.156329

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1\_F(T1) 225baa\_DNIGABA\_+H+\_INT\_b3lyp631dp\_PCMw\_TRIPLET.log

orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.528007	0.663602	0.167301
2	6	0	1.711879	1.432517	0.013440
3	6	0	2.981976	0.854895	-0.116547
4	6	0	3.026471	-0.560326	-0.147213
5	6	0	1.864218	-1.346106	0.034031
6	6	0	0.629784	-0.763882	0.183211
7	6	0	-0.190127	2.801479	0.298419
8	6	0	1.343999	2.881681	0.087001
9	1	0	1.960760	-2.423213	0.031982
10	1	0	-0.512336	3.272612	1.236075
11	1	0	1.614737	3.416253	-0.830217
12	7	0	-0.586240	1.393583	0.333328
13	1	0	1.861486	3.386819	0.909935
14	1	0	-0.755503	3.300559	-0.498764
15	6	0	-2.754604	-0.843012	0.288310
16	8	0	-2.849644	-0.950991	1.484718
17	8	0	4.012203	1.717431	-0.173883
18	6	0	5.238688	1.472618	0.547784
19	1	0	5.577985	2.452605	0.884234
20	1	0	5.053856	0.830254	1.412802
21	1	0	5.982311	1.015385	-0.103889
22	7	0	-0.509354	-1.587266	0.428256
23	8	0	-0.416352	-2.810313	0.635211
24	8	0	-1.635175	-1.179924	-0.432809
25	6	0	-3.814244	-0.333378	-0.662764
26	1	0	-3.428790	0.592133	-1.106371
27	6	0	-5.147083	-0.096457	0.052802
28	1	0	-5.000541	0.622904	0.864546
29	1	0	-5.487649	-1.032663	0.507215
30	6	0	-6.197343	0.419890	-0.923255
31	1	0	-6.409359	-0.298075	-1.716600
32	1	0	-5.909744	1.370529	-1.375269
33	1	0	-3.918321	-1.050616	-1.484041
34	7	0	-7.509398	0.669464	-0.216584
35	1	0	-7.419277	1.389407	0.506588
36	1	0	-8.229674	0.985310	-0.872077
37	1	0	-7.863182	-0.177648	0.238235
38	7	0	4.232432	-1.296975	-0.476504
39	8	0	5.072385	-0.742566	-1.194911
40	8	0	4.336761	-2.459304	-0.070698

1\_G(T1) 253aaa\_DNI\_VEGE\_+H+\_b3lyp631dp\_PCMw\_TRIPLET.log

orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.714477	-0.232256	0.038143
2	6	0	0.678118	-1.211125	0.064436
3	6	0	-0.682635	-0.863821	-0.017142
4	6	0	-0.985828	0.551303	-0.000685
5	6	0	-0.018452	1.525104	-0.064781
6	6	0	1.361232	1.175672	-0.058108
7	6	0	2.819045	-2.178917	0.141001
8	6	0	1.317929	-2.553470	0.116177
9	1	0	-0.314688	2.567335	-0.076519
10	1	0	3.335875	-2.518970	1.047507
11	1	0	1.041835	-3.160532	-0.754490
12	7	0	2.931849	-0.727577	0.076253
13	1	0	1.002373	-3.116989	1.002030
14	1	0	3.383087	-2.600969	-0.700612
15	8	0	-1.515049	-1.871517	-0.133093
16	7	0	2.326748	2.083549	-0.104575
17	8	0	2.328050	3.278637	-0.176122
18	7	0	-2.355596	1.040176	0.236654
19	8	0	-2.712218	2.058508	-0.343030
20	8	0	-3.016742	0.410395	1.059820
21	6	0	-2.859649	-1.800495	-0.682567
22	1	0	-3.009607	-2.773007	-1.146731
23	1	0	-3.573303	-1.639512	0.122867
24	1	0	-2.924335	-1.010537	-1.431809

1\_H(S0) 253aaa\_DNI\_VEGE\_+H+\_b3lyp631dp\_PCMw\_TRIPLET.log

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.675352	-0.211839	-0.030491
2	6	0	-0.662112	-1.203408	-0.109349
3	6	0	0.695212	-0.832949	-0.106322
4	6	0	0.984940	0.564740	-0.069511
5	6	0	-0.020978	1.526801	0.049567
6	6	0	-1.367047	1.166473	0.074231
7	6	0	-2.664706	-2.223136	-0.091921
8	6	0	-1.321626	-2.478937	-0.138667
9	1	0	0.242084	2.576026	0.086209
10	7	0	-2.872372	-0.852214	-0.021356
11	8	0	1.572509	-1.844213	-0.115942
12	7	0	-2.440268	2.073624	0.171767
13	8	0	-2.134511	3.265481	0.269508
14	7	0	2.326927	1.081345	-0.300214
15	8	0	2.624046	2.176798	0.184441
16	8	0	3.085198	0.423946	-1.021538
17	6	0	2.796506	-1.809556	0.649399
18	1	0	2.923404	-2.820600	1.037553
19	1	0	3.636048	-1.538246	0.011096
20	1	0	2.713656	-1.105258	1.480744
21	1	0	-0.852804	-3.448644	-0.198685

22	1	0	-3.506320	-2.899122	-0.101896
23	1	0	-3.768316	-0.391779	0.044458

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1\_I(S0) 221baa\_DNIGABA\_+H+\_INT\_b3lyp631dp\_PCMw.log

Input orientation:

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Center Atomic Atomic Coordinates (Angstroms)  
Number Number Type X Y Z

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1	6	0	1.886375	0.062498	0.194941
2	6	0	3.170533	-0.514572	-0.200620
3	6	0	4.273704	0.223488	-0.472349
4	6	0	4.153655	1.677877	-0.337085
5	6	0	2.990443	2.289452	0.017744
6	6	0	1.819207	1.523911	0.319744
7	6	0	1.459655	-2.139326	0.069915
8	6	0	2.969795	-2.002937	-0.268006
9	1	0	2.953627	3.365023	0.117652
10	1	0	0.884437	-2.582502	-0.751394
11	1	0	3.605043	-2.523561	0.456057
12	7	0	0.924480	-0.795308	0.333406
13	1	0	3.215263	-2.405199	-1.255502
14	1	0	1.277856	-2.766791	0.949861
15	6	0	-1.254553	1.083836	0.153779
16	8	0	-1.113929	1.436557	-0.985319
17	8	0	5.430048	-0.402398	-0.832489
18	6	0	5.854119	-0.223270	-2.197638
19	1	0	6.712402	-0.882158	-2.330359
20	1	0	5.056572	-0.511522	-2.889572
21	1	0	6.161273	0.807732	-2.392083
22	7	0	0.740255	2.215903	0.708446
23	8	0	0.600262	3.433832	0.796880
24	8	0	-0.367220	1.437880	1.170940
25	6	0	-2.355783	0.244086	0.744093
26	1	0	-1.881122	-0.651396	1.159703
27	6	0	-3.411998	-0.110597	-0.306667
28	1	0	-2.933669	-0.646383	-1.132901
29	1	0	-3.839506	0.808880	-0.719258
30	6	0	-4.512190	-0.967922	0.308004
31	1	0	-5.048977	-0.443830	1.100014
32	1	0	-4.126749	-1.908142	0.705114
33	1	0	-2.790479	0.791673	1.587876
34	7	0	-5.545613	-1.340647	-0.729106
35	1	0	-5.137531	-1.893547	-1.488979
36	1	0	-6.297244	-1.900532	-0.316509
37	1	0	-5.978270	-0.512875	-1.150344
38	7	0	5.315048	2.560594	-0.474383
39	8	0	6.426412	2.092171	-0.221949
40	8	0	5.118759	3.731547	-0.808771

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1\_TS3 213caa\_DNIGABA\_+H+\_b3lyp631dp\_PCMw\_TRIPLET\_SCANopt\_TS\_FRQ.log

Input orientation:

-----  
Center Atomic Atomic Coordinates (Angstroms)  
Number Number Type X Y Z  
-----

C	0.39518200	0.38884500	-0.08692100
C	1.49537500	1.24301700	0.07157900
C	2.79819400	0.72116600	0.10705700
C	2.91363800	-0.68015400	0.01209500
C	1.80255400	-1.54928600	-0.09453100
C	0.53128100	-1.01871800	-0.16494500
C	-0.55976500	2.45206900	0.27186400
C	0.98289900	2.64622100	0.24722900
H	1.95896000	-2.61862500	-0.11866000
H	-0.98429200	2.62812300	1.26704400
H	1.27924700	3.29352000	-0.58470800
N	-0.78795800	1.04458600	-0.07953100
H	1.36487600	3.10534100	1.16380800
H	-1.08940500	3.09492700	-0.43608200
C	-2.12122800	0.04465500	0.35224900
O	-2.00516600	-0.14938700	1.57247600
O	3.85466100	1.52854600	0.37003800
C	4.39929700	2.25744200	-0.75375700
H	4.83611500	1.56136600	-1.47250400
H	3.63072100	2.86846800	-1.23545600
N	-0.63106800	-1.79313500	-0.20837600
O	-0.65029300	-3.04524400	-0.23623200
O	-1.79457500	-1.10687600	-0.57961900
C	-3.35965200	0.67264800	-0.27931100
H	-3.23450200	0.72451500	-1.36433800
H	-3.44023300	1.69545300	0.10267400
C	-4.61379500	-0.12776100	0.10127000
H	-4.69618500	-0.15939100	1.19264500
H	-4.50929300	-1.15926200	-0.25177300
C	-5.86344000	0.50112400	-0.50093900
N	-7.10236800	-0.26206100	-0.08947800
H	-7.22331400	-0.26475700	0.92766300
H	-7.94626600	0.15121000	-0.49618800
H	-6.01084600	1.52753800	-0.16169400
H	-7.06383300	-1.23897700	-0.39544000
N	4.22613100	-1.32311200	0.06380700
O	4.27993800	-2.46023000	0.54005600
O	5.19851900	-0.71331700	-0.38045400
H	-5.84565200	0.48887200	-1.59167100
H	5.17282800	2.90220300	-0.33802000

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1\_TS3 213caa\_DNIGABA\_+H+\_b3lyp631dp\_PCMw\_TRIPLET\_SCANopt\_TS\_FRQ.log  
Input orientation:

-----  
Center Atomic Atomic Coordinates (Angstroms)  
Number Number Type X Y Z  
-----

C	1.71447700	-0.23225600	0.03814300
C	0.67811800	-1.21112500	0.06443600
C	-0.68263500	-0.86382100	-0.01714200
C	-0.98582800	0.55130300	-0.00068500
C	-0.01845200	1.52510400	-0.06478100
C	1.36123200	1.17567200	-0.05810800
C	2.81904500	-2.17891700	0.14100100
C	1.31792900	-2.55347000	0.11617700
H	-0.31468800	2.56733500	-0.07651900
H	3.33587500	-2.51897000	1.04750700
H	1.04183500	-3.16053200	-0.75449000
N	2.93184900	-0.72757700	0.07625300
H	1.00237300	-3.11698900	1.00203000
H	3.38308700	-2.60096900	-0.70061200
O	-1.51504900	-1.87151700	-0.13309300
N	2.32674800	2.08354900	-0.10457500
O	2.32805000	3.27863700	-0.17612200
N	-2.35559600	1.04017600	0.23665400
O	-2.71221800	2.05850800	-0.34303000
O	-3.01674200	0.41039500	1.05982000
C	-2.85964900	-1.80049500	-0.68256700
H	-3.00960700	-2.77300700	-1.14673100
H	-3.57330300	-1.63951200	0.12286700
H	-2.92433500	-1.01053700	-1.43180900

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orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.025728	0.337132	0.139481
2	6	0	0.194532	-0.304406	-0.131602
3	6	0	1.366917	0.403521	-0.354110
4	6	0	1.299794	1.822443	-0.317596
5	6	0	0.106193	2.465367	-0.004774
6	6	0	-1.044332	1.735624	0.268785
7	6	0	-1.450998	-1.960725	0.346802
8	6	0	-0.022962	-1.794467	-0.216384
9	1	0	0.083579	3.544513	0.055756
10	1	0	-2.032974	-2.692321	-0.208655
11	1	0	0.705219	-2.366727	0.360674
12	7	0	-2.053597	-0.601844	0.223083
13	1	0	0.041184	-2.129061	-1.257658
14	1	0	-1.434495	-2.247872	1.401964
15	6	0	-3.367648	-0.347583	-0.161234
16	8	0	-3.710303	0.754178	-0.566514
17	8	0	2.481863	-0.294696	-0.716725
18	6	0	3.426702	-0.590699	0.328005
19	1	0	3.748359	0.338514	0.805684
20	1	0	2.958718	-1.244391	1.071179
21	7	0	-2.175614	2.479143	0.820077
22	8	0	-2.374665	3.618498	0.399541
23	8	0	-2.817588	1.944306	1.721406
24	6	0	-4.333924	-1.516315	-0.047803
25	1	0	-4.184011	-2.023505	0.911460
26	1	0	-4.089261	-2.248692	-0.827826
27	6	0	-5.786294	-1.054829	-0.203621
28	1	0	-5.896298	-0.518925	-1.151089
29	1	0	-6.035543	-0.350252	0.596751
30	6	0	-6.731733	-2.249665	-0.163168
31	7	0	-8.165608	-1.802270	-0.326709
32	1	0	-8.308362	-1.313048	-1.215250
33	1	0	-8.810743	-2.597270	-0.308237
34	1	0	-6.538064	-2.954920	-0.972686
35	1	0	-8.448958	-1.163453	0.422133
36	7	0	2.443872	2.678442	-0.609898
37	8	0	2.223048	3.870815	-0.837168
38	8	0	3.573565	2.182921	-0.623532
39	1	0	-6.685532	-2.782683	0.787576
40	6	0	4.594939	-1.276523	-0.391222
41	1	0	4.839088	-0.654557	-1.256391
42	1	0	5.963946	-0.205834	0.714331
43	7	0	5.847564	-1.198567	0.487394
44	6	0	5.746914	-1.930258	1.799015
45	1	0	4.885019	-1.565909	2.354619
46	1	0	5.654248	-2.996463	1.603660
47	1	0	6.657396	-1.731983	2.362722
48	6	0	7.092147	-1.605427	-0.255424
49	1	0	7.130157	-1.063197	-1.198842
50	1	0	7.951393	-1.348850	0.362202
51	1	0	7.066892	-2.678762	-0.430457
52	6	0	4.269852	-2.694589	-0.842129
53	1	0	4.040903	-3.355492	-0.002525
54	1	0	3.379428	-2.637916	-1.471922

55 1 0 5.068805 -3.135042 -1.440992

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2a\_I\_A(S1) 101aba\_iDMPO\_DNIGABA\_+2H+\_b3lyp631dp\_PCMw.log (2<sup>nd</sup> isomer)

orientation:

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.129125	-0.191940	0.605018
2	6	0	0.138189	-0.649433	0.188749
3	6	0	1.147125	0.213237	-0.208233
4	6	0	0.871703	1.610855	-0.191611
5	6	0	-0.340109	2.078646	0.295949
6	6	0	-1.323329	1.198185	0.740548
7	6	0	-1.109526	-2.499082	1.008218
8	6	0	0.163328	-2.157415	0.209754
9	1	0	-0.513268	3.143386	0.361160
10	1	0	-1.656760	-3.358682	0.628069
11	1	0	1.061457	-2.559373	0.681088
12	7	0	-1.955418	-1.279732	0.863206
13	1	0	0.116238	-2.553557	-0.810924
14	1	0	-0.891780	-2.660163	2.067867
15	6	0	-3.337842	-1.441725	0.730151
16	8	0	-3.842846	-2.493002	1.098013
17	8	0	2.299346	-0.332549	-0.688002
18	6	0	3.432724	-0.350090	0.201110
19	1	0	3.582353	0.642753	0.633084
20	1	0	3.252577	-1.076238	1.000147
21	7	0	-2.444826	1.785632	1.465348
22	8	0	-2.697087	2.976110	1.284354
23	8	0	-3.050414	1.063575	2.262488
24	6	0	-4.158875	-0.371621	0.026661
25	1	0	-3.522574	0.317323	-0.534621
26	1	0	-4.677413	0.211554	0.794412
27	6	0	-5.188181	-1.024097	-0.910395
28	1	0	-5.771063	-1.754081	-0.341760
29	1	0	-4.672074	-1.565167	-1.711138
30	6	0	-6.106311	0.036075	-1.507181
31	7	0	-7.139690	-0.594819	-2.410772
32	1	0	-7.726820	-1.262728	-1.902319
33	1	0	-7.761438	0.111361	-2.814900
34	1	0	-6.661612	0.574289	-0.737687
35	1	0	-6.704111	-1.098797	-3.189286
36	7	0	1.811076	2.615904	-0.677270
37	8	0	1.390316	3.764476	-0.834807
38	8	0	2.973501	2.280014	-0.919672
39	1	0	-5.564939	0.757454	-2.120972
40	6	0	4.618214	-0.748934	-0.686569
41	1	0	4.588898	-0.095545	-1.561854
42	1	0	5.848053	0.628832	0.225359
43	7	0	5.926401	-0.371534	0.017612
44	6	0	6.160576	-1.067646	1.331993
45	1	0	5.330087	-0.865175	2.005508
46	1	0	6.258645	-2.136591	1.154972
47	1	0	7.081795	-0.674419	1.759170
48	6	0	7.124453	-0.515298	-0.883321
49	1	0	6.918443	-0.010866	-1.826004
50	1	0	7.975456	-0.051245	-0.387190
51	1	0	7.321262	-1.572152	-1.048682

52	6	0	4.573689	-2.208170	-1.120965
53	1	0	4.626497	-2.895961	-0.273388
54	1	0	3.615451	-2.369182	-1.619561
55	1	0	5.361095	-2.453467	-1.835643

2a\_IL\_A(S1) 101baa\_iDMPO\_DNIGABA\_+2H+\_b3llyp631dp\_PCMw.log

orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.027963	0.206709	0.214893
2	6	0	0.149098	-0.548511	0.069073
3	6	0	1.387330	0.049982	-0.110646
4	6	0	1.438375	1.468556	-0.158024
5	6	0	0.284723	2.225392	0.028381
6	6	0	-0.937354	1.608745	0.260346
7	6	0	-1.666266	-2.033425	0.502581
8	6	0	-0.192998	-2.018024	0.040995
9	1	0	0.348429	3.304599	0.028871
10	1	0	-2.271353	-2.738391	-0.062970
11	1	0	0.435164	-2.620050	0.699331
12	7	0	-2.134910	-0.635892	0.274228
13	1	0	-0.083333	-2.412352	-0.975109
14	1	0	-1.750276	-2.268057	1.567254
15	6	0	-3.397359	-0.292951	-0.206793
16	8	0	-3.610216	0.803454	-0.703560
17	8	0	2.472084	-0.741823	-0.357049
18	6	0	3.218073	-1.213436	0.788021
19	1	0	3.455742	-0.376222	1.450514
20	1	0	2.635402	-1.951369	1.345903
21	7	0	-2.035780	2.474691	0.686916
22	8	0	-2.109557	3.596803	0.187767
23	8	0	-2.776838	2.051098	1.570921
24	6	0	-4.476253	-1.356425	-0.073172
25	1	0	-4.420520	-1.812008	0.921452
26	1	0	-4.271533	-2.157850	-0.794763
27	6	0	-5.864008	-0.761286	-0.331289
28	1	0	-5.869130	-0.277635	-1.312481
29	1	0	-6.071148	0.015402	0.412170
30	6	0	-6.938847	-1.839199	-0.272855
31	7	0	-8.300111	-1.247882	-0.561747
32	1	0	-8.330615	-0.807912	-1.486439
33	1	0	-9.030462	-1.965444	-0.541376
34	1	0	-6.780854	-2.618054	-1.020423
35	1	0	-8.556358	-0.533137	0.126094
36	7	0	2.668405	2.208218	-0.390967
37	8	0	2.578808	3.397457	-0.691452
38	8	0	3.756481	1.627015	-0.269962
39	1	0	-7.009563	-2.303687	0.711811
40	6	0	4.463185	-1.885090	0.225469
41	1	0	4.135768	-2.571956	-0.558447
42	1	0	4.597054	-0.166511	-0.895460
43	7	0	5.292674	-0.826227	-0.518235
44	6	0	6.202157	-0.016930	0.361700
45	1	0	5.642023	0.358635	1.215218
46	1	0	7.030356	-0.641352	0.690450
47	1	0	6.575050	0.821270	-0.224106
48	6	0	6.042297	-1.408838	-1.680604

49	1	0	5.328679	-1.874977	-2.358238
50	1	0	6.569775	-0.603545	-2.190238
51	1	0	6.755093	-2.145835	-1.313088
52	6	0	5.261499	-2.645524	1.276921
53	1	0	5.532948	-2.021888	2.131395
54	1	0	4.643123	-3.468376	1.642879
55	1	0	6.168353	-3.084156	0.855116

2a\_IL\_A(S1) 101bba\_iDMPO\_DNIGABA\_+2H+\_b3lyp631dp\_PCMw.log (2<sup>nd</sup> isomer)

orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.128037	-0.248436	-0.681449
2	6	0	-0.131633	-0.801492	-0.364599
3	6	0	-1.226732	-0.016775	-0.045916
4	6	0	-1.057395	1.396596	-0.044264
5	6	0	0.153348	1.956819	-0.428532
6	6	0	1.230568	1.154270	-0.792908
7	6	0	1.310429	-2.548973	-1.079935
8	6	0	-0.037142	-2.307239	-0.374729
9	1	0	0.251596	3.031672	-0.483925
10	1	0	1.892710	-3.365990	-0.660174
11	1	0	-0.862858	-2.785767	-0.902935
12	7	0	2.048087	-1.268972	-0.876113
13	1	0	-0.028987	-2.692476	0.651170
14	1	0	1.181389	-2.721878	-2.152080
15	6	0	3.430688	-1.327280	-0.663892
16	8	0	4.032836	-2.330160	-1.018189
17	8	0	-2.376588	-0.638396	0.345052
18	6	0	-3.362754	-0.903895	-0.680310
19	1	0	-3.569760	0.007937	-1.247239
20	1	0	-2.997184	-1.672534	-1.366722
21	7	0	2.359921	1.829654	-1.423950
22	8	0	2.514935	3.030696	-1.209295
23	8	0	3.070275	1.163735	-2.182208
24	6	0	4.124336	-0.216845	0.110661
25	1	0	3.404867	0.404730	0.650353
26	1	0	4.639539	0.425463	-0.610445
27	6	0	5.147281	-0.819978	1.087190
28	1	0	5.813708	-1.484603	0.530595
29	1	0	4.630319	-1.425583	1.839679
30	6	0	5.950734	0.281210	1.767851
31	7	0	6.990317	-0.310042	2.691394
32	1	0	7.641050	-0.917957	2.185027
33	1	0	7.545878	0.422322	3.142490
34	1	0	6.495896	0.892566	1.047161
35	1	0	6.562234	-0.869834	3.435042
36	7	0	-2.111852	2.324474	0.335059
37	8	0	-1.810212	3.505095	0.501359
38	8	0	-3.267773	1.901000	0.475098
39	1	0	5.328719	0.932263	2.383746
40	6	0	-4.589194	-1.429908	0.050967
41	1	0	-4.251110	-2.223507	0.721273
42	1	0	-4.258751	0.192620	1.269134
43	7	0	-5.102774	-0.328928	0.993762
44	6	0	-6.023643	0.668147	0.349758
45	1	0	-5.570882	1.046141	-0.564121

46	1	0	-6.976734	0.188290	0.136949
47	1	0	-6.166101	1.489863	1.049521
48	6	0	-5.712711	-0.898054	2.241896
49	1	0	-4.963382	-1.498969	2.754919
50	1	0	-6.031672	-0.074001	2.878292
51	1	0	-6.569725	-1.512020	1.968492
52	6	0	-5.662281	-1.969166	-0.886557
53	1	0	-5.963914	-1.240474	-1.641847
54	1	0	-5.254946	-2.841256	-1.402999
55	1	0	-6.547184	-2.300089	-0.338355

2a\_I\_C(S1) 105aaa\_iDMPO\_DNIGABA\_+2H+\_TDb3lyp631dp\_PCMw\_OPT\_f.log

orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.016459	0.069127	-0.131871
2	6	0	0.251963	-0.493270	-0.339586
3	6	0	1.413824	0.312456	-0.346314
4	6	0	1.210701	1.681558	-0.158232
5	6	0	-0.078590	2.226889	0.147091
6	6	0	-1.192864	1.436752	0.187928
7	6	0	-1.381638	-2.236307	-0.331248
8	6	0	0.118198	-1.962415	-0.592254
9	1	0	-0.163183	3.284505	0.357033
10	1	0	-1.866218	-2.805325	-1.126821
11	1	0	0.770364	-2.556202	0.053979
12	7	0	-1.983079	-0.892294	-0.240653
13	1	0	0.387123	-2.207858	-1.627428
14	1	0	-1.540531	-2.766380	0.615779
15	6	0	-3.353003	-0.566469	-0.601227
16	8	0	-3.521008	0.306432	-1.426022
17	8	0	2.595545	-0.277499	-0.662244
18	6	0	3.512133	-0.566671	0.416590
19	1	0	3.629680	0.317908	1.046302
20	1	0	3.116786	-1.395973	1.010984
21	7	0	-2.468535	1.912842	0.627871
22	8	0	-2.774081	3.139231	0.446349
23	8	0	-3.166435	1.057596	1.304306
24	6	0	-4.411942	-1.451510	0.000925
25	1	0	-4.138241	-1.684822	1.033630
26	1	0	-4.421559	-2.401355	-0.552657
27	6	0	-5.783905	-0.772169	-0.073370
28	1	0	-6.006934	-0.521736	-1.114898
29	1	0	-5.735899	0.165989	0.489588
30	6	0	-6.868553	-1.679171	0.493832
31	7	0	-8.221056	-1.010871	0.410337
32	1	0	-8.479111	-0.797931	-0.557932
33	1	0	-8.955942	-1.610607	0.796351
34	1	0	-6.955865	-2.614370	-0.061201
35	1	0	-8.240693	-0.129540	0.932194
36	7	0	2.290752	2.649817	-0.314289
37	8	0	1.964567	3.812583	-0.563119
38	8	0	3.458841	2.270235	-0.209240
39	1	0	-6.706439	-1.907888	1.548159
40	6	0	4.824791	-0.928901	-0.290604
41	1	0	5.017956	-0.132665	-1.013292
42	1	0	5.902033	0.107488	1.126693

43	7	0	5.986955	-0.820661	0.701183
44	6	0	5.951239	-1.818772	1.827600
45	1	0	4.996114	-1.750295	2.344282
46	1	0	6.093958	-2.816993	1.419577
47	1	0	6.760167	-1.577420	2.515253
48	6	0	7.326948	-0.838935	0.013238
49	1	0	7.319390	-0.105202	-0.791279
50	1	0	8.086679	-0.582060	0.749657
51	1	0	7.511941	-1.836520	-0.378841
52	6	0	4.766998	-2.277048	-0.997431
53	1	0	4.573766	-3.099892	-0.304887
54	1	0	3.936883	-2.237522	-1.705851
55	1	0	5.674038	-2.488649	-1.566148

2a\_I\_C(S1) 105baa\_iDMPO\_DNIGABA\_+2H+\_TDb3lyp631dp\_PCMw\_OPT\_f.log

orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.899241	0.058222	-0.241675
2	6	0	0.208148	-0.757598	-0.629264
3	6	0	1.457635	-0.194724	-0.844627
4	6	0	1.603595	1.195743	-0.680216
5	6	0	0.546498	1.986541	-0.176054
6	6	0	-0.691852	1.437226	0.055970
7	6	0	-1.735671	-2.131320	-0.444590
8	6	0	-0.250828	-2.165917	-0.844996
9	1	0	0.723312	3.032807	0.040605
10	1	0	-2.388707	-2.543122	-1.213237
11	1	0	0.311807	-2.885746	-0.245602
12	7	0	-2.037784	-0.686196	-0.256671
13	1	0	-0.123745	-2.452029	-1.895134
14	1	0	-1.926232	-2.651417	0.498139
15	6	0	-3.373860	-0.156826	-0.351951
16	8	0	-3.528954	0.991443	-0.698931
17	8	0	2.541710	-0.902605	-1.245605
18	6	0	3.097328	-1.893793	-0.347658
19	1	0	2.509227	-1.949474	0.571908
20	1	0	3.042011	-2.861509	-0.851114
21	7	0	-1.670708	2.260343	0.769756
22	8	0	-1.716329	3.455076	0.498192
23	8	0	-2.328800	1.701873	1.645337
24	6	0	-4.483184	-1.120523	-0.012101
25	1	0	-4.244382	-1.607996	0.940361
26	1	0	-4.504101	-1.915504	-0.767870
27	6	0	-5.837156	-0.406043	0.051897
28	1	0	-6.041410	0.074268	-0.909684
29	1	0	-5.794631	0.384218	0.808204
30	6	0	-6.944420	-1.397815	0.391941
31	7	0	-8.281352	-0.700137	0.471703
32	1	0	-8.534827	-0.259710	-0.418199
33	1	0	-9.028173	-1.359889	0.708091
34	1	0	-7.050126	-2.173949	-0.367587
35	1	0	-8.285435	0.031463	1.188920
36	7	0	2.882194	1.777971	-0.933291
37	8	0	3.000148	2.569946	-1.935592
38	8	0	3.534928	1.936511	0.219407
39	1	0	-6.788654	-1.872256	1.361950

40	6	0	4.573216	-1.592693	-0.076060
41	1	0	5.027747	-1.320500	-1.031758
42	1	0	4.164559	0.456335	0.460906
43	7	0	4.768895	-0.359196	0.803299
44	6	0	4.393106	-0.547348	2.240169
45	1	0	3.382202	-0.945628	2.309260
46	1	0	5.097072	-1.220846	2.726324
47	1	0	4.424430	0.430221	2.720210
48	6	0	6.161452	0.186421	0.691837
49	1	0	6.387358	0.358360	-0.359883
50	1	0	6.194646	1.131790	1.231835
51	1	0	6.876750	-0.512189	1.123350
52	6	0	5.271093	-2.829014	0.494277
53	1	0	4.763152	-3.218204	1.380392
54	1	0	5.267675	-3.612940	-0.266219
55	1	0	6.312997	-2.627259	0.748399

2a\_I\_D(T1) 107aaa\_iDMPO\_DNIGABA\_+2H+\_b3lyp631dp\_PCMw\_TRIPLET.log

orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.969094	0.093251	-0.130602
2	6	0	0.325873	-0.406546	-0.374207
3	6	0	1.438938	0.446356	-0.367391
4	6	0	1.167104	1.811320	-0.160029
5	6	0	-0.118373	2.323251	0.102469
6	6	0	-1.210211	1.466462	0.189689
7	6	0	-1.265352	-2.171054	-0.647741
8	6	0	0.248126	-1.867264	-0.700595
9	1	0	-0.254550	3.381013	0.275832
10	1	0	-1.664472	-2.518230	-1.605304
11	1	0	0.807424	-2.474550	0.018043
12	7	0	-1.899007	-0.879459	-0.308841
13	1	0	0.668051	-2.076347	-1.689976
14	1	0	-1.529315	-2.906837	0.118188
15	6	0	-3.333537	-0.590792	-0.646106
16	8	0	-3.511518	-0.009823	-1.694103
17	8	0	2.672649	-0.033601	-0.703508
18	6	0	3.479439	-0.527580	0.383851
19	1	0	3.603270	0.263206	1.129905
20	1	0	2.991581	-1.392936	0.843577
21	7	0	-2.466295	1.892311	0.592151
22	8	0	-2.716569	3.136511	0.700377
23	8	0	-3.348554	0.968528	0.882117
24	6	0	-4.330470	-1.417642	0.121410
25	1	0	-4.028096	-1.451426	1.170540
26	1	0	-4.281152	-2.443485	-0.270293
27	6	0	-5.745942	-0.851840	-0.041997
28	1	0	-6.006097	-0.828371	-1.104953
29	1	0	-5.748915	0.179077	0.324966
30	6	0	-6.756139	-1.691110	0.730075
31	7	0	-8.146617	-1.117128	0.587859
32	1	0	-8.456289	-1.113332	-0.388317
33	1	0	-8.830112	-1.661411	1.121743
34	1	0	-6.809989	-2.717201	0.363422
35	1	0	-8.191897	-0.151834	0.927837
36	7	0	2.249733	2.801897	-0.226109

37	8	0	1.963201	3.914568	-0.665062
38	8	0	3.369427	2.472737	0.162464
39	1	0	-6.542515	-1.709544	1.799767
40	6	0	4.820125	-0.897487	-0.263321
41	1	0	5.138949	-0.028408	-0.844639
42	1	0	5.823533	-0.168537	1.380309
43	7	0	5.888984	-1.028139	0.826927
44	6	0	5.681208	-2.171869	1.783591
45	1	0	4.692495	-2.097742	2.231719
46	1	0	5.786342	-3.109925	1.242917
47	1	0	6.441702	-2.102279	2.559612
48	6	0	7.283770	-1.047649	0.259534
49	1	0	7.399074	-0.198240	-0.411932
50	1	0	7.985850	-0.969034	1.088176
51	1	0	7.439367	-1.983277	-0.273179
52	6	0	4.731965	-2.123097	-1.163298
53	1	0	4.414731	-3.015683	-0.618291
54	1	0	3.978126	-1.913408	-1.925048
55	1	0	5.671653	-2.329266	-1.678808

2a\_IL\_D(T1) 107baa\_iDMPO\_DNIGABA\_+2H+\_b3lyp631dp\_PCMw\_TRIPLET\_f.log

orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.027823	0.086196	0.061722
2	6	0	0.133264	-0.730684	-0.164905
3	6	0	1.395412	-0.195015	-0.339069
4	6	0	1.521404	1.229596	-0.346279
5	6	0	0.380586	2.040274	0.008116
6	6	0	-0.849140	1.484166	0.230978
7	6	0	-1.787339	-2.140234	0.057913
8	6	0	-0.276997	-2.165923	-0.240378
9	1	0	0.534721	3.101714	0.134321
10	1	0	-2.370594	-2.687534	-0.681308
11	1	0	0.270216	-2.789452	0.471818
12	7	0	-2.150729	-0.699450	0.023126
13	1	0	-0.073935	-2.569975	-1.238976
14	1	0	-2.017084	-2.535882	1.051858
15	6	0	-3.459331	-0.226577	-0.281884
16	8	0	-3.603204	0.910853	-0.685557
17	8	0	2.458965	-1.024412	-0.546551
18	6	0	3.137704	-1.543859	0.622304
19	1	0	3.059648	-0.837268	1.454265
20	1	0	2.679323	-2.488066	0.930407
21	7	0	-1.878892	2.353939	0.808649
22	8	0	-1.927212	3.520014	0.429655
23	8	0	-2.587029	1.863303	1.685853
24	6	0	-4.588550	-1.211024	-0.077378
25	1	0	-4.491992	-1.661617	0.917363
26	1	0	-4.481301	-2.030740	-0.798772
27	6	0	-5.948926	-0.527562	-0.250114
28	1	0	-6.005011	-0.082806	-1.248359
29	1	0	-6.041443	0.287853	0.474539
30	6	0	-7.083034	-1.527743	-0.057399
31	7	0	-8.421034	-0.853391	-0.245159
32	1	0	-8.522070	-0.472099	-1.190596
33	1	0	-9.192700	-1.510085	-0.097236



34	1	0	-7.045489	-2.339935	-0.784820
35	1	0	-8.551236	-0.078717	0.412490
36	7	0	2.707525	1.895968	-0.630162
37	8	0	2.814149	3.112030	-0.250552
38	8	0	3.646398	1.321471	-1.313357
39	1	0	-7.092748	-1.953350	0.946961
40	6	0	4.581905	-1.809741	0.215402
41	1	0	4.553780	-2.377362	-0.718223
42	1	0	4.514961	0.112796	-0.629500
43	7	0	5.251964	-0.490116	-0.158979
44	6	0	5.736999	0.319952	1.004153
45	1	0	4.953100	0.391077	1.756747
46	1	0	6.626229	-0.139859	1.432465
47	1	0	5.971219	1.317844	0.635257
48	6	0	6.340079	-0.675361	-1.170631
49	1	0	5.919199	-1.155373	-2.053313
50	1	0	6.732573	0.305921	-1.436099
51	1	0	7.134876	-1.290600	-0.749545
52	6	0	5.351179	-2.597290	1.271978
53	1	0	5.315609	-2.119861	2.254073
54	1	0	4.901425	-3.588682	1.362515
55	1	0	6.396005	-2.737686	0.986254

2a\_I\_TS1 111aaa\_iDMPO\_DNIGABA\_+2H+\_b3lyp631dp\_PCMw\_TRIPLET\_TS.log

orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.945833	0.104834	-0.090762
2	6	0	0.344451	-0.395009	-0.339749
3	6	0	1.451758	0.465591	-0.333963
4	6	0	1.179397	1.828643	-0.117548
5	6	0	-0.113489	2.338639	0.132975
6	6	0	-1.196463	1.475781	0.197433
7	6	0	-1.268090	-2.137734	-0.640610
8	6	0	0.253807	-1.857558	-0.662933
9	1	0	-0.253279	3.398051	0.293420
10	1	0	-1.661533	-2.419706	-1.622262
11	1	0	0.783113	-2.468476	0.075473
12	7	0	-1.885478	-0.858548	-0.241010
13	1	0	0.695799	-2.080681	-1.638966
14	1	0	-1.554712	-2.912603	0.076131
15	6	0	-3.337693	-0.501505	-0.545197
16	8	0	-3.481702	-0.023920	-1.660501
17	8	0	2.683408	-0.006312	-0.681915
18	6	0	3.500537	-0.516632	0.390159
19	1	0	3.655948	0.272780	1.131771
20	1	0	3.003023	-1.370610	0.860609
21	7	0	-2.486287	1.878787	0.509630
22	8	0	-2.797943	3.107105	0.580363
23	8	0	-3.362454	0.916507	0.790212
24	6	0	-4.335200	-1.372707	0.183881
25	1	0	-4.061673	-1.427939	1.240179
26	1	0	-4.255237	-2.384527	-0.235749
27	6	0	-5.758626	-0.834530	-0.003033
28	1	0	-5.980032	-0.768229	-1.072974
29	1	0	-5.805506	0.178306	0.408857
30	6	0	-6.777335	-1.731041	0.688205

31	7	0	-8.173397	-1.177793	0.515895
32	1	0	-8.439664	-1.131410	-0.472026
33	1	0	-8.868060	-1.760022	0.991910
34	1	0	-6.794337	-2.739085	0.271092
35	1	0	-8.253803	-0.231166	0.899388
36	7	0	2.258818	2.820589	-0.175322
37	8	0	1.963473	3.946162	-0.576340
38	8	0	3.386764	2.483851	0.183568
39	1	0	-6.605819	-1.796737	1.763499
40	6	0	4.817589	-0.917447	-0.287067
41	1	0	5.131862	-0.063568	-0.892968
42	1	0	5.883456	-0.173567	1.309691
43	7	0	5.916583	-1.045349	0.772839
44	6	0	5.720390	-2.164580	1.760231
45	1	0	4.738733	-2.077283	2.221365
46	1	0	5.816115	-3.116002	1.241612
47	1	0	6.492423	-2.076494	2.523162
48	6	0	7.291702	-1.102549	0.161661
49	1	0	7.407391	-0.258238	-0.516222
50	1	0	8.022027	-1.041027	0.966774
51	1	0	7.405706	-2.043461	-0.372331
52	6	0	4.684445	-2.156973	-1.162090
53	1	0	4.381039	-3.037439	-0.590279
54	1	0	3.903555	-1.952855	-1.897670
55	1	0	5.601332	-2.380279	-1.710362

2a\_II\_TS1 111baa\_iDMPO\_DNIGABA\_+2H+\_b3lyp631dp\_PCMw\_TRIPLET\_TS\_f.log

orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.066291	-0.003126	-0.332592
2	6	0	0.204160	-0.685628	-0.369615
3	6	0	1.415425	-0.029190	-0.230408
4	6	0	1.401824	1.375376	-0.007086
5	6	0	0.147632	2.063457	0.037655
6	6	0	-1.054747	1.401905	-0.128524
7	6	0	-1.512006	-2.248209	-0.903826
8	6	0	-0.005537	-2.140744	-0.637677
9	1	0	0.158541	3.131220	0.192001
10	1	0	-1.742111	-2.447653	-1.955361
11	1	0	0.284682	-2.743041	0.230523
12	7	0	-2.050414	-0.906720	-0.566767
13	1	0	0.596013	-2.484929	-1.483751
14	1	0	-2.012752	-3.002229	-0.292144
15	6	0	-3.512878	-0.731465	-0.799632
16	8	0	-3.878002	-0.596399	-1.934923
17	8	0	2.568263	-0.708805	-0.470858
18	6	0	3.224965	-1.399372	0.620170
19	1	0	3.201917	-0.779968	1.520321
20	1	0	2.720345	-2.348827	0.818560
21	7	0	-2.264588	2.195170	-0.086055
22	8	0	-2.168090	3.417924	-0.028751
23	8	0	-3.351527	1.595616	-0.095822
24	6	0	-4.368878	-0.994739	0.409356
25	1	0	-3.955558	-0.454841	1.264606
26	1	0	-4.266953	-2.065007	0.638953
27	6	0	-5.834165	-0.632205	0.147765

28	1	0	-6.187042	-1.169910	-0.737634
29	1	0	-5.906627	0.438947	-0.066935
30	6	0	-6.701006	-0.982603	1.351584
31	7	0	-8.146739	-0.642114	1.076688
32	1	0	-8.507913	-1.153123	0.265434
33	1	0	-8.742843	-0.877831	1.875142
34	1	0	-6.675649	-2.048843	1.581524
35	1	0	-8.270916	0.357387	0.888748
36	7	0	2.563699	2.132502	0.107408
37	8	0	2.471479	3.391824	-0.117989
38	8	0	3.658615	1.606071	0.572214
39	1	0	-6.417872	-0.420651	2.242730
40	6	0	4.643050	-1.669334	0.132106
41	1	0	4.560592	-2.008309	-0.903338
42	1	0	4.650933	0.406895	-0.071826
43	7	0	5.391648	-0.334939	0.047337
44	6	0	6.098475	0.060028	1.308740
45	1	0	5.407152	-0.008285	2.146796
46	1	0	6.959345	-0.586595	1.469031
47	1	0	6.421870	1.093645	1.195559
48	6	0	6.314981	-0.280903	-1.128226
49	1	0	5.734124	-0.432444	-2.037357
50	1	0	6.790596	0.699237	-1.152439
51	1	0	7.072648	-1.058595	-1.030803
52	6	0	5.374619	-2.728166	0.950437
53	1	0	5.396351	-2.495233	2.017353
54	1	0	4.852983	-3.679743	0.823364
55	1	0	6.399252	-2.868911	0.598336

2a\_I\_TS2 113aaa\_iDMPO\_DNIGABA\_+2H+\_b3lyp631dp\_PCMw\_TRIPLET\_SCAN\_vege\_TS2.log

orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.036637	0.307728	-0.790163
2	6	0	0.303929	-0.148689	-0.958821
3	6	0	1.394142	0.598264	-0.527084
4	6	0	1.124866	1.849219	0.076010
5	6	0	-0.191068	2.326242	0.246900
6	6	0	-1.263953	1.567213	-0.157866
7	6	0	-1.270283	-1.652286	-1.883940
8	6	0	0.256899	-1.458972	-1.686170
9	1	0	-0.346535	3.296312	0.698811
10	1	0	-1.554705	-1.714521	-2.942210
11	1	0	0.701971	-2.272052	-1.102993
12	7	0	-1.969358	-0.514302	-1.289008
13	1	0	0.803914	-1.410525	-2.633686
14	1	0	-1.645186	-2.571208	-1.416232
15	6	0	-4.623724	0.857433	0.007684
16	8	0	-4.946569	1.393379	-1.020975
17	8	0	2.661991	0.169458	-0.798787
18	6	0	3.270190	-0.670187	0.198983
19	1	0	3.169140	-0.200672	1.181771
20	1	0	2.776517	-1.647260	0.205628
21	7	0	-2.590303	2.088026	-0.023015
22	8	0	-2.800921	3.277964	0.270543
23	8	0	-3.446333	1.108085	0.674891
24	6	0	-5.413659	-0.185160	0.771189

25	1	0	-6.464129	-0.048207	0.504273
26	1	0	-5.298001	-0.008248	1.844412
27	6	0	-4.948002	-1.612322	0.417297
28	1	0	-3.882100	-1.715703	0.642472
29	1	0	-5.076633	-1.783652	-0.656440
30	6	0	-5.753211	-2.635224	1.210853
31	7	0	-5.286321	-4.040265	0.909553
32	1	0	-4.296849	-4.166957	1.142267
33	1	0	-5.816070	-4.731469	1.448263
34	1	0	-5.635868	-2.499533	2.286837
35	1	0	-5.399491	-4.274754	-0.081098
36	7	0	2.194037	2.728774	0.528206
37	8	0	1.946756	3.936276	0.596805
38	8	0	3.283021	2.233815	0.832227
39	1	0	-6.815291	-2.604533	0.964020
40	6	0	4.744642	-0.770435	-0.210665
41	1	0	5.115589	0.252651	-0.310025
42	1	0	5.309899	-0.780667	1.773906
43	7	0	5.554733	-1.348709	0.956953
44	6	0	5.227642	-2.774438	1.313122
45	1	0	4.162228	-2.864552	1.514501
46	1	0	5.516759	-3.421190	0.487648
47	1	0	5.792843	-3.034958	2.206527
48	6	0	7.037279	-1.172051	0.759310
49	1	0	7.235224	-0.129078	0.517117
50	1	0	7.538035	-1.444826	1.686974
51	1	0	7.368260	-1.822600	-0.047054
52	6	0	4.953200	-1.531884	-1.513343
53	1	0	4.589191	-2.560649	-1.456036
54	1	0	4.377050	-1.018750	-2.285992
55	1	0	5.997647	-1.535573	-1.829889

2a\_II\_TS2 113baa\_iDMPO\_DNIGABA\_+2H+\_b3lyp631dp\_PCMw\_TRIPLET\_SCANvege\_TS2.log

orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.923300	0.188192	-0.795664
2	6	0	0.360731	-0.405490	-0.995058
3	6	0	1.534233	0.273295	-0.653674
4	6	0	1.395562	1.579925	-0.119815
5	6	0	0.133182	2.178071	0.077194
6	6	0	-1.017351	1.495151	-0.227270
7	6	0	-1.402394	-1.764644	-1.817249
8	6	0	0.141942	-1.725318	-1.686084
9	1	0	0.082242	3.181175	0.476575
10	1	0	-1.735455	-1.823422	-2.861497
11	1	0	0.513442	-2.575308	-1.106749
12	7	0	-1.952315	-0.548759	-1.231132
13	1	0	0.641367	-1.752956	-2.660729
14	1	0	-1.848179	-2.629316	-1.309763
15	6	0	-4.424528	1.136457	-0.015206
16	8	0	-4.682203	1.663770	-1.066391
17	8	0	2.779404	-0.192643	-0.905287
18	6	0	3.110230	-1.580334	-0.695470
19	1	0	2.513226	-1.992359	0.122262
20	1	0	2.924749	-2.161087	-1.601674
21	7	0	-2.280578	2.144919	-0.078513

22	8	0	-2.368828	3.359145	0.177834
23	8	0	-3.226850	1.281308	0.648393
24	6	0	-5.333414	0.226254	0.783113
25	1	0	-6.355359	0.447875	0.466635
26	1	0	-5.237270	0.464269	1.846567
27	6	0	-5.006514	-1.261676	0.541701
28	1	0	-3.982257	-1.471524	0.865013
29	1	0	-5.066004	-1.480432	-0.529577
30	6	0	-5.995249	-2.134207	1.307168
31	7	0	-5.728007	-3.601344	1.067103
32	1	0	-4.795073	-3.875701	1.389102
33	1	0	-6.405479	-4.186767	1.564371
34	1	0	-5.925500	-1.982494	2.385099
35	1	0	-5.791773	-3.839744	0.072924
36	7	0	2.537142	2.402564	0.249387
37	8	0	2.373260	3.623014	0.262680
38	8	0	3.617280	1.877062	0.563367
39	1	0	-7.024011	-1.956395	0.991048
40	6	0	4.605696	-1.619781	-0.394658
41	1	0	5.124471	-1.150359	-1.234156
42	1	0	4.316344	0.145931	0.626756
43	7	0	4.901227	-0.694602	0.789363
44	6	0	4.510700	-1.243420	2.130186
45	1	0	3.475211	-1.577548	2.103920
46	1	0	5.169627	-2.070061	2.388735
47	1	0	4.613777	-0.443432	2.861994
48	6	0	6.326395	-0.223527	0.795046
49	1	0	6.539738	0.256182	-0.159104
50	1	0	6.447865	0.492274	1.606992
51	1	0	6.987456	-1.074819	0.948984
52	6	0	5.117167	-3.041669	-0.195539
53	1	0	4.565493	-3.578358	0.579794
54	1	0	4.993326	-3.586095	-1.134691
55	1	0	6.180724	-3.055912	0.050602

2a\_I\_F(T1) 114aaa\_iDMPO\_DNIGABA\_+2H+\_b3lyp631dp\_PCMw\_TRIPLET\_SCAN\_vege\_SCAN2vege.log

orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.794009	0.021174	-0.625585
2	6	0	0.543936	-0.447292	-0.776202
3	6	0	1.643454	0.361197	-0.508871
4	6	0	1.384755	1.687907	-0.091004
5	6	0	0.069820	2.174360	0.068334
6	6	0	-1.010459	1.359076	-0.173508
7	6	0	-1.044151	-2.077275	-1.418718
8	6	0	0.486173	-1.852856	-1.294638
9	1	0	-0.078112	3.199123	0.379977
10	1	0	-1.357426	-2.282511	-2.450666
11	1	0	0.950507	-2.565063	-0.604125
12	7	0	-1.734238	-0.870883	-0.965378
13	1	0	1.009471	-1.949535	-2.251641
14	1	0	-1.399888	-2.926061	-0.821594
15	6	0	-4.307133	0.577606	0.036940
16	8	0	-4.633562	1.010297	-1.038280
17	8	0	2.899405	-0.103214	-0.774887
18	6	0	3.594279	-0.731470	0.317743

19	1	0	3.543137	-0.090182	1.201916
20	1	0	3.132400	-1.699430	0.537313
21	7	0	-2.333771	1.889161	-0.056473
22	8	0	-2.546698	3.100579	0.128858
23	8	0	-3.180103	0.972818	0.721542
24	6	0	-5.031140	-0.464297	0.858560
25	1	0	-5.105586	-0.106119	1.890771
26	1	0	-4.385600	-1.350561	0.884119
27	6	0	-6.406913	-0.796232	0.273894
28	1	0	-6.291358	-1.123119	-0.764309
29	1	0	-7.028077	0.105521	0.263890
30	6	0	-7.084252	-1.886199	1.095604
31	7	0	-8.444298	-2.220596	0.529914
32	1	0	-8.380093	-2.560154	-0.434337
33	1	0	-8.905943	-2.950776	1.079720
34	1	0	-6.515043	-2.816904	1.092672
35	1	0	-9.064386	-1.404983	0.526408
36	7	0	2.457528	2.638479	0.163568
37	8	0	2.183834	3.840209	0.088693
38	8	0	3.579529	2.209635	0.449536
39	1	0	-7.251061	-1.578544	2.128998
40	6	0	5.040622	-0.877304	-0.171046
41	1	0	5.358724	0.111924	-0.509040
42	1	0	5.719657	-0.464607	1.729570
43	7	0	5.950518	-1.173431	1.026567
44	6	0	5.727094	-2.512427	1.676206
45	1	0	4.680047	-2.612398	1.954082
46	1	0	6.013619	-3.296561	0.978863
47	1	0	6.350903	-2.560549	2.567266
48	6	0	7.406865	-0.973435	0.700418
49	1	0	7.533250	0.010357	0.251361
50	1	0	7.972097	-1.039529	1.628854
51	1	0	7.728360	-1.752590	0.012620
52	6	0	5.190390	-1.892112	-1.296679
53	1	0	4.869438	-2.892532	-0.996129
54	1	0	4.544713	-1.568256	-2.115506
55	1	0	6.210844	-1.940195	-1.680816

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2a\_II\_F(T1) 114baa\_iDMPO\_DNIGABA\_+2H+\_b3lyp631dp\_PCMw\_TRIPLET\_SCANvege\_SCAN2vege.log

orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.664619	-0.166273	-0.691561
2	6	0	0.651086	-0.705264	-0.826791
3	6	0	1.784796	0.083335	-0.608390
4	6	0	1.572640	1.442926	-0.265324
5	6	0	0.277577	1.986953	-0.130562
6	6	0	-0.832059	1.201022	-0.312894
7	6	0	-1.032785	-2.270861	-1.413805
8	6	0	0.507061	-2.124313	-1.308980
9	1	0	0.169557	3.031367	0.125999
10	1	0	-1.365656	-2.494785	-2.435666
11	1	0	0.929370	-2.852519	-0.610471
12	7	0	-1.650754	-1.018114	-0.997986
13	1	0	1.004521	-2.273322	-2.273430
14	1	0	-1.425414	-3.080132	-0.785545
15	6	0	-4.182102	0.614290	-0.035839

16	8	0	-4.501171	1.027205	-1.121329
17	8	0	3.052363	-0.343453	-0.814732
18	6	0	3.466417	-1.663834	-0.408796
19	1	0	2.926286	-1.969457	0.491203
20	1	0	3.277557	-2.388919	-1.203267
21	7	0	-2.131614	1.786623	-0.222873
22	8	0	-2.295404	3.014291	-0.106592
23	8	0	-3.013153	0.950315	0.606951
24	6	0	-4.963620	-0.340886	0.837866
25	1	0	-4.888357	-0.013565	1.879405
26	1	0	-4.451077	-1.309347	0.777632
27	6	0	-6.421107	-0.457052	0.381628
28	1	0	-6.448228	-0.754143	-0.671282
29	1	0	-6.905643	0.522375	0.455812
30	6	0	-7.172831	-1.472281	1.234029
31	7	0	-8.617837	-1.566082	0.803826
32	1	0	-8.702717	-1.850784	-0.176454
33	1	0	-9.129207	-2.252515	1.365761
34	1	0	-6.758607	-2.476838	1.138948
35	1	0	-9.100828	-0.668119	0.905813
36	7	0	2.664861	2.375941	-0.037994
37	8	0	2.423641	3.574949	-0.183720
38	8	0	3.781143	1.964853	0.317228
39	1	0	-7.187411	-1.195113	2.289203
40	6	0	4.972917	-1.581915	-0.180979
41	1	0	5.427895	-1.234605	-1.111907
42	1	0	4.630968	0.313389	0.544950
43	7	0	5.266524	-0.459111	0.817555
44	6	0	4.954386	-0.789097	2.247945
45	1	0	3.934178	-1.159940	2.326835
46	1	0	5.658404	-1.536492	2.608157
47	1	0	5.053305	0.125576	2.830670
48	6	0	6.665193	0.069614	0.684264
49	1	0	6.829621	0.372796	-0.348693
50	1	0	6.769529	0.928963	1.345496
51	1	0	7.373652	-0.706213	0.970193
52	6	0	5.570299	-2.925155	0.221162
53	1	0	5.091451	-3.346428	1.107988
54	1	0	5.424459	-3.626324	-0.603902
55	1	0	6.645288	-2.852229	0.398568

2a\_I\_I(S0) 121aaa\_iDMPO\_DNIGABA\_+2H+\_INT\_b3lyp631dp\_PCMw.log

orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.882250	-0.090804	0.218361
2	6	0	0.474856	-0.550398	-0.089515
3	6	0	1.504868	0.298584	-0.311984
4	6	0	1.232993	1.731842	-0.238069
5	6	0	0.001325	2.234150	0.046483
6	6	0	-1.093845	1.357601	0.332949
7	6	0	-1.100533	-2.322188	0.068039
8	6	0	0.408768	-2.049767	-0.179234
9	1	0	-0.153695	3.302967	0.093070
10	1	0	-1.583353	-2.810990	-0.785931
11	1	0	1.037282	-2.533353	0.575384
12	7	0	-1.766536	-1.033820	0.298279

13	1	0	0.746559	-2.408074	-1.156700
14	1	0	-1.275731	-2.967190	0.936276
15	6	0	-4.115765	0.610218	0.100104
16	8	0	2.731437	-0.149119	-0.732946
17	6	0	3.631982	-0.580316	0.298743
18	1	0	3.789385	0.235821	1.011536
19	1	0	3.212363	-1.446345	0.820747
20	7	0	-2.249698	1.939455	0.680714
21	8	0	-2.513809	3.137439	0.749471
22	8	0	-3.280300	1.056492	1.127509
23	6	0	-5.111841	-0.355100	0.683515
24	1	0	-5.579623	0.114421	1.555697
25	1	0	-4.530880	-1.205592	1.057112
26	6	0	-6.153554	-0.794805	-0.349741
27	1	0	-5.645559	-1.212929	-1.224473
28	1	0	-6.725904	0.074613	-0.689514
29	6	0	-7.088910	-1.833381	0.258575
30	7	0	-8.139421	-2.263701	-0.737751
31	1	0	-7.719531	-2.667123	-1.580617
32	1	0	-8.760216	-2.973306	-0.338171
33	1	0	-6.557113	-2.739382	0.552608
34	1	0	-8.725780	-1.477610	-1.033260
35	7	0	2.302978	2.710634	-0.429797
36	8	0	2.002776	3.811883	-0.894356
37	8	0	3.445959	2.391580	-0.095053
38	1	0	-7.628868	-1.444731	1.122995
39	6	0	4.931815	-0.930400	-0.437109
40	1	0	5.192976	-0.062692	-1.048269
41	1	0	6.049377	-0.158443	1.111363
42	7	0	6.080115	-1.030164	0.574121
43	6	0	5.954811	-2.151605	1.570260
44	1	0	4.999496	-2.076464	2.085169
45	1	0	6.034159	-3.102096	1.046972
46	1	0	6.767094	-2.053180	2.288891
47	6	0	7.427939	-1.055450	-0.097094
48	1	0	7.489701	-0.215528	-0.787539
49	1	0	8.191801	-0.965525	0.673669
50	1	0	7.543878	-1.997923	-0.627864
51	6	0	4.803988	-2.167990	-1.315804
52	1	0	4.560976	-3.063851	-0.738987
53	1	0	3.981328	-1.987677	-2.010634
54	1	0	5.701658	-2.352973	-1.908343
55	8	0	-4.006529	0.981371	-1.036003

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**2a\_I\_TS4** 121aba\_iDMPO\_DNIGABA\_+2H+\_INT\_b3lyp631dp\_PCMw.log

orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.906223	-0.139386	-0.233518
2	6	0	-0.442725	-0.627719	0.066988
3	6	0	-1.488612	0.199955	0.293862
4	6	0	-1.245951	1.638310	0.222999
5	6	0	-0.023533	2.167523	-0.051193
6	6	0	1.091052	1.314070	-0.333579
7	6	0	1.166175	-2.367640	-0.100843
8	6	0	-0.348381	-2.125866	0.146644
9	1	0	0.109645	3.239423	-0.095333



10	1	0	1.657017	-2.855865	0.748833
11	1	0	-0.967670	-2.614384	-0.612439
12	7	0	1.808557	-1.064807	-0.317572
13	1	0	-0.680240	-2.497544	1.121179
14	1	0	1.354444	-3.000594	-0.975250
15	6	0	4.129610	0.629159	-0.082037
16	8	0	-2.704557	-0.266926	0.722035
17	6	0	-3.613581	-0.714727	-0.295222
18	1	0	-3.657348	0.020798	-1.104375
19	1	0	-3.278371	-1.677445	-0.695256
20	7	0	2.238462	1.921593	-0.664701
21	8	0	2.479909	3.125172	-0.718540
22	8	0	3.290034	1.063407	-1.111064
23	6	0	5.148507	-0.310995	-0.666893
24	1	0	5.594024	0.164922	-1.547095
25	1	0	4.587861	-1.180295	-1.028644
26	6	0	6.212282	-0.714268	0.358921
27	1	0	5.725290	-1.150790	1.236572
28	1	0	6.756538	0.174175	0.695640
29	6	0	7.178327	-1.717351	-0.260915
30	7	0	8.248941	-2.122472	0.724475
31	1	0	7.850100	-2.560894	1.560023
32	1	0	8.898625	-2.795948	0.308177
33	1	0	6.674989	-2.637546	-0.560793
34	1	0	8.801725	-1.317830	1.034448
35	7	0	-2.341017	2.591080	0.400243
36	8	0	-2.076809	3.694691	0.879870
37	8	0	-3.468452	2.248769	0.035442
38	1	0	7.700451	-1.303289	-1.124583
39	6	0	-4.968662	-0.826938	0.415822
40	1	0	-5.162125	0.144873	0.876169
41	1	0	-5.912074	-0.240322	-1.319969
42	7	0	-6.081403	-0.976118	-0.627604
43	6	0	-6.078042	-2.281176	-1.377475
44	1	0	-5.098150	-2.445603	-1.820434
45	1	0	-6.325629	-3.085391	-0.687855
46	1	0	-6.830725	-2.217696	-2.161731
47	6	0	-7.443983	-0.696340	-0.051382
48	1	0	-7.422151	0.272208	0.445316
49	1	0	-8.161304	-0.683886	-0.870507
50	1	0	-7.699005	-1.483410	0.654661
51	6	0	-4.995773	-1.923965	1.472550
52	1	0	-4.783528	-2.909375	1.050496
53	1	0	-4.210764	-1.697377	2.196640
54	1	0	-5.943271	-1.959807	2.013634
55	8	0	4.006034	0.989649	1.056035

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**2a\_II\_I(S0)** 121baa\_iDMPO\_DNIGABA\_+2H+\_INT\_b3lyp631dp\_PCMw.log

orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.873195	-0.313223	0.285238
2	6	0	0.452908	-0.890815	0.042568
3	6	0	1.552811	-0.130107	-0.173488
4	6	0	1.392084	1.321353	-0.144220
5	6	0	0.196536	1.927792	0.091087
6	6	0	-0.971258	1.149351	0.364024

7	6	0	-1.280476	-2.516669	0.134295
8	6	0	0.260118	-2.382222	-0.012550
9	1	0	0.127314	3.006327	0.114985
10	1	0	-1.747052	-2.954376	-0.755939
11	1	0	0.782140	-2.890558	0.804768
12	7	0	-1.839293	-1.173908	0.329880
13	1	0	0.634465	-2.805350	-0.949965
14	1	0	-1.570553	-3.148032	0.981062
15	6	0	-4.046898	0.683289	0.036099
16	8	0	2.765706	-0.648187	-0.545264
17	6	0	3.461348	-1.477324	0.404279
18	1	0	3.464095	-0.999534	1.389454
19	1	0	2.983770	-2.456350	0.494353
20	7	0	-2.085009	1.831840	0.665315
21	8	0	-2.249346	3.047957	0.703305
22	8	0	-3.200774	1.047217	1.087828
23	6	0	-5.153500	-0.175748	0.585282
24	1	0	-5.539735	0.293305	1.496237
25	1	0	-4.686270	-1.119530	0.889786
26	6	0	-6.258986	-0.400220	-0.451102
27	1	0	-5.831914	-0.868046	-1.343755
28	1	0	-6.674416	0.566009	-0.755613
29	6	0	-7.360775	-1.278889	0.129512
30	7	0	-8.480958	-1.461745	-0.866504
31	1	0	-8.157783	-1.927018	-1.719967
32	1	0	-9.235284	-2.033461	-0.475639
33	1	0	-7.003033	-2.279394	0.376403
34	1	0	-8.891561	-0.564379	-1.142128
35	7	0	2.536451	2.213098	-0.307236
36	8	0	2.346006	3.319626	-0.804980
37	8	0	3.641800	1.829188	0.101857
38	1	0	-7.813396	-0.835612	1.017732
39	6	0	4.863034	-1.681113	-0.156683
40	1	0	4.752717	-2.037241	-1.183666
41	1	0	4.779491	0.334587	-0.559011
42	7	0	5.541934	-0.312526	-0.305509
43	6	0	6.138299	0.231831	0.959881
44	1	0	5.401520	0.185606	1.759180
45	1	0	7.021690	-0.347706	1.220073
46	1	0	6.411091	1.270371	0.779517
47	6	0	6.539155	-0.297019	-1.426979
48	1	0	6.028549	-0.562388	-2.351704
49	1	0	6.956569	0.705929	-1.504773
50	1	0	7.330683	-1.013426	-1.211797
51	6	0	5.688979	-2.675465	0.650447
52	1	0	5.742770	-2.413130	1.709373
53	1	0	5.216133	-3.656985	0.570164
54	1	0	6.703408	-2.770564	0.257301
55	8	0	-3.865691	1.038553	-1.095770

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2a\_I\_G(T1) 153aaa\_iDMPO\_DNI\_VEGE\_+2H+\_b3lyp631dp\_PCMw\_TRIPLET.log

orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.486194	1.279825	0.024985
2	6	0	1.056928	1.149354	0.024465
3	6	0	0.470536	-0.127038	0.039621
4	6	0	1.359932	-1.265543	0.054844
5	6	0	2.725943	-1.177561	0.022045
6	6	0	3.337550	0.103697	0.021251
7	6	0	1.781668	3.404061	0.013712
8	6	0	0.497771	2.542590	-0.000487
9	1	0	3.329418	-2.076899	0.006200
10	1	0	1.866282	4.068793	-0.855890
11	1	0	-0.140273	2.750258	0.863744
12	7	0	2.928394	2.517608	0.018506
13	1	0	-0.099379	2.727800	-0.899418
14	1	0	1.852489	4.057562	0.893412
15	8	0	-0.812537	-0.430540	0.003498
16	6	0	-1.885985	0.537460	0.020763
17	1	0	-1.819906	1.125179	0.938784
18	1	0	-1.805402	1.184025	-0.853685
19	7	0	4.656147	0.270979	0.012578
20	8	0	5.575027	-0.494636	0.008019
21	7	0	0.796891	-2.631663	0.123459
22	8	0	1.303814	-3.471074	-0.613412
23	8	0	-0.099365	-2.830261	0.933218
24	6	0	-3.156690	-0.327781	-0.009099
25	1	0	-3.037097	-1.095026	0.759758
26	1	0	-4.066105	0.894583	1.383711
27	7	0	-4.344353	0.506458	0.476599
28	6	0	-4.703177	1.674350	-0.405358
29	1	0	-3.840639	2.328880	-0.516567
30	1	0	-5.028854	1.299884	-1.373321
31	1	0	-5.514113	2.217848	0.076297
32	6	0	-5.557224	-0.346398	0.751781
33	1	0	-5.262237	-1.183549	1.382375
34	1	0	-6.290017	0.273030	1.266027
35	1	0	-5.964694	-0.700321	-0.192367
36	6	0	-3.394656	-0.982439	-1.364121
37	1	0	-3.530958	-0.251179	-2.164088
38	1	0	-2.509736	-1.576331	-1.603267
39	1	0	-4.246591	-1.663601	-1.346697

2a\_I\_H(S0) 153baa\_iDMPO\_DNI\_VEGE\_+2H+\_b3lyp631dp\_PCMw\_.log

orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.632077	0.959745	0.094975
2	6	0	1.239345	1.229583	-0.210244
3	6	0	0.342044	0.157296	-0.353973
4	6	0	0.903830	-1.132154	-0.217030
5	6	0	2.258665	-1.411718	0.051010
6	6	0	3.140799	-0.376819	0.226516
7	6	0	2.519720	3.188503	-0.040900
8	6	0	1.098251	2.700426	-0.345456
9	1	0	2.598569	-2.438701	0.122732
10	1	0	2.984067	3.777278	-0.848656
11	1	0	0.357427	3.130134	0.338460
12	7	0	3.353563	2.053740	0.200348
13	1	0	0.777466	2.972360	-1.361563
14	1	0	2.593693	3.848982	0.838865
15	8	0	-0.949400	0.227867	-0.682172
16	6	0	-1.798539	1.343557	-0.304790
17	1	0	-1.572656	1.645743	0.720108
18	1	0	-1.642333	2.182817	-0.984108
19	7	0	4.550743	-0.550085	0.539169
20	8	0	4.900251	-1.713683	0.557925
21	7	0	0.031006	-2.315817	-0.384071
22	8	0	0.451952	-3.191177	-1.123137
23	8	0	-1.016179	-2.352003	0.255480
24	6	0	-3.232852	0.851921	-0.467818
25	1	0	-3.353677	0.514270	-1.499691
26	1	0	-2.589072	-0.977256	0.239982
27	7	0	-3.443084	-0.416354	0.369378
28	6	0	-3.586094	-0.179536	1.846965
29	1	0	-2.755985	0.426610	2.204059
30	1	0	-4.533564	0.319846	2.038457
31	1	0	-3.567572	-1.149359	2.341799
32	6	0	-4.580333	-1.249755	-0.155549
33	1	0	-4.381212	-1.496205	-1.197205
34	1	0	-4.638534	-2.158735	0.441157
35	1	0	-5.507328	-0.686763	-0.067566
36	6	0	-4.241284	1.952004	-0.153677
37	1	0	-4.085826	2.389873	0.834732
38	1	0	-4.127821	2.744243	-0.897103
39	1	0	-5.267999	1.588124	-0.223162

2a\_II\_G(T1) 155baa\_iDMPO\_DNI\_VEGE\_indole+H+\_b3lyp631dp\_PCMw.log

orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.554484	1.010264	0.079876
2	6	0	1.183842	1.260647	-0.234505
3	6	0	0.326413	0.160330	-0.411128
4	6	0	0.874442	-1.150820	-0.277201
5	6	0	2.223171	-1.366624	0.003167
6	6	0	3.087250	-0.294196	0.198052
7	6	0	2.276451	3.227411	-0.059367
8	6	0	1.046253	2.695291	-0.323273
9	1	0	2.605800	-2.374743	0.090670
10	7	0	3.180327	2.206574	0.183899
11	1	0	2.593809	4.258375	-0.024518
12	8	0	-0.962757	0.248682	-0.778058
13	6	0	-1.790503	1.379953	-0.454415
14	1	0	-1.502906	1.795689	0.514608
15	1	0	-1.697209	2.152856	-1.220789
16	7	0	4.461203	-0.410495	0.500555
17	8	0	4.895311	-1.559781	0.594474
18	7	0	0.051940	-2.349004	-0.403385
19	8	0	0.618247	-3.394008	-0.722285
20	8	0	-1.164119	-2.307515	-0.157426
21	6	0	-3.225486	0.855386	-0.469006
22	1	0	-3.431643	0.483657	-1.475605
23	1	0	-2.450430	-0.934795	0.191422
24	7	0	-3.309300	-0.396415	0.409791
25	6	0	-3.297105	-0.131268	1.886707
26	1	0	-2.457110	0.513216	2.139268
27	1	0	-4.235010	0.338761	2.175886
28	1	0	-3.187790	-1.087475	2.396861
29	6	0	-4.466970	-1.274220	0.032294
30	1	0	-4.389077	-1.520819	-1.025804
31	1	0	-4.416251	-2.182378	0.631162
32	1	0	-5.399263	-0.749332	0.234302
33	6	0	-4.236977	1.931149	-0.093716
34	1	0	-4.031620	2.371545	0.884435
35	1	0	-4.183365	2.727963	-0.839449
36	1	0	-5.258680	1.546294	-0.103669
37	1	0	4.162769	2.319263	0.389443
38	1	0	0.163750	3.268464	-0.552789

2a\_I\_E(T1) 126aaa\_iDMPO\_DNIGABA\_+2H+\_INT\_b3lyp631dp\_PCMw\_TRIPLET\_vege.log

orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
C	-1.03412100	0.48234300	0.05715500		
C	0.12604800	-0.23010900	-0.22622200		
C	1.34709100	0.44538100	-0.32608400		
C	1.32105900	1.85129700	-0.16796400		
C	0.13614900	2.56772300	0.08965400		
C	-1.05567200	1.87674600	0.22450100		

C	-1.78776500	-1.68671400	-0.31826000
C	-0.23335400	-1.68224700	-0.41844600
H	0.16673700	3.64457100	0.17678900
H	-2.25941400	-1.88334800	-1.28423900
H	0.20574100	-2.31111400	0.36208200
N	-2.14283600	-0.31708300	0.12001800
H	0.11644300	-2.06486800	-1.38077700
H	-2.16252100	-2.40803200	0.41072500
C	-3.49349800	0.38834000	-0.01295500
O	2.46174600	-0.24194600	-0.70572100
C	3.28645300	-0.76981900	0.35077300
H	3.49990500	0.01928600	1.07693200
H	2.76481600	-1.59540400	0.84538000
N	-2.29969000	2.47331100	0.42488900
O	-2.49790400	3.69920100	0.56282100
O	-3.32099200	1.59951400	0.86281600
C	-4.64296500	-0.33900300	0.69717800
H	-5.40079100	0.42499400	0.89835800
H	-4.29201500	-0.71006800	1.66492900
C	-5.26162500	-1.45804500	-0.15064200
H	-4.55043000	-2.27824000	-0.29349600
H	-5.50301400	-1.05822100	-1.14016000
C	-6.51832600	-1.99334100	0.52465200
N	-7.15728200	-3.08392700	-0.30456000
H	-6.52068200	-3.87359700	-0.44748900
H	-7.99970200	-3.44983900	0.14904200
H	-6.30522400	-2.43689900	1.49820100
H	-7.43343300	-2.74195200	-1.23000500
N	2.53425200	2.65285000	-0.31010600
O	2.39917100	3.83850700	-0.62106600
O	3.62756400	2.11973600	-0.10587100
H	-7.27739200	-1.21962400	0.64817800
C	4.56735900	-1.23177400	-0.35563700
H	4.89598800	-0.39724000	-0.98011600
H	5.69795600	-0.51127200	1.20544200
N	5.68957000	-1.38819600	0.67595000
C	5.48392800	-2.49297300	1.67715300
H	4.51927800	-2.36785100	2.16493500
H	5.53232300	-3.45048100	1.16290200
H	6.28002800	-2.42598700	2.41727900
C	7.04576600	-1.49347600	0.03043100
H	7.17020300	-0.65946600	-0.65855500
H	7.79831000	-1.44749700	0.81616700
H	7.11714300	-2.44216300	-0.49718200
C	4.36097000	-2.47611300	-1.20927400
H	4.03061300	-3.33410900	-0.61853600
H	3.57398200	-2.24736600	-1.93108300
H	5.25495400	-2.74824700	-1.77319800
O	-3.56619500	0.61824400	-1.28071900

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orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
C	0.48105800	0.48781900	1.05250700		
C	-0.82947200	-0.09812100	1.10152700		
C	-1.93091700	0.54591800	0.56857100		
C	-1.72072600	1.82986600	-0.02439400		
C	-0.47082600	2.43216700	-0.07896800		
C	0.65071200	1.77782000	0.44071500		
C	0.79168300	-1.43791200	2.17703700		
C	-0.72087000	-1.39806600	1.83662400		
H	-0.36332400	3.41070200	-0.52947200		
H	0.98344100	-1.46638400	3.25747000		
H	-1.02358000	-2.24869100	1.21708700		
N	1.42498800	-0.23860800	1.63716300		
H	-1.35852400	-1.40869500	2.72687500		
H	1.30166800	-2.31434000	1.75833300		
C	4.80064800	0.29186100	-0.46360700		
O	5.21867400	1.07331400	0.38577600		
O	-3.18098100	0.03492800	0.72808800		
C	-3.64888000	-0.89783100	-0.26803900		
H	-3.51395500	-0.46392600	-1.26276900		
H	-3.08460300	-1.83209400	-0.19254500		
N	1.93161000	2.32217000	0.35533900		
O	2.07101600	3.47129100	-0.01384800		
O	3.60115600	0.31096500	-0.96429800		
C	5.64907100	-0.83809900	-1.06985300		
H	5.73282000	-0.66098000	-2.14775400		
H	5.10358300	-1.78012200	-0.94874500		
C	7.03070000	-0.90606700	-0.41023200		
H	6.91266500	-1.04227000	0.66933500		
H	7.55439200	0.04334400	-0.56025900		
C	7.83993000	-2.05595500	-0.99810100		
N	9.20107100	-2.14821500	-0.34531700		
H	9.12513700	-2.30206200	0.66461200		
H	9.74640000	-2.92437100	-0.73160800		
H	7.35998200	-3.02183600	-0.83334500		
H	9.74732900	-1.29315600	-0.48509600		
N	-2.83684600	2.59168000	-0.59393500		
O	-2.75176400	3.81911600	-0.56900500		
O	-3.78157600	1.96909300	-1.07864700		
H	8.02201600	-1.92998600	-2.06627300		
C	-5.13551700	-1.08840100	0.06092000		
H	-5.56821100	-0.08822100	0.14130500		
H	-5.58007500	-1.13413400	-1.95078900		
N	-5.85005500	-1.70630700	-1.14488500		
C	-5.44540100	-3.12052300	-1.46543900		
H	-4.36441900	-3.17255400	-1.57849000		
H	-5.77783600	-3.77520100	-0.66265400		
H	-5.92695000	-3.40272800	-2.40034400		
C	-7.34737100	-1.58727300	-1.03845500		
H	-7.60117200	-0.54866000	-0.83266300		
H	-7.77909600	-1.89920300	-1.98812700		
H	-7.70051100	-2.23384100	-0.23844100		
C	-5.36559700	-1.86453000	1.35135500		
H	-4.93898500	-2.86980900	1.31198300		
H	-4.86190300	-1.32090100	2.15334000		

H -6.42320000 -1.93062300 1.61293700

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2a\_I\_TS4 121aba\_iDMPO\_DNIGABA\_+2H+\_INT\_b3lyp631dp\_PCMw\_SCAN\_CN\_jof2\_FRQ.log

orientation:

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
C	-1.05281400	0.35680200	0.17861200		
C	0.21187400	-0.28142200	-0.09372400		
C	1.34164600	0.44684200	-0.29552100		
C	1.24504900	1.90365900	-0.22982700		
C	0.06632200	2.54810300	0.02626700		
C	-1.10884300	1.79275600	0.27186000		
C	-1.61260200	-1.83382200	-0.04265200		
C	-0.06018100	-1.76277800	-0.17599500		
H	0.03163500	3.62795700	0.06904500		
H	-2.08547400	-2.17722200	-0.96902200		
H	0.42891800	-2.30697800	0.63806200		
N	-2.06806100	-0.45740800	0.23804800		
H	0.29758400	-2.19225200	-1.11583700		
H	-1.93645900	-2.49969100	0.76181600		
C	-3.73027100	0.54191000	-0.13152400		
O	2.50370000	-0.15479100	-0.69492400		
C	3.35129800	-0.66485600	0.34711400		
H	3.62336300	0.14822900	1.02721400		
H	2.82697700	-1.44864700	0.90318800		
N	-2.26582600	2.41737400	0.60824800		
O	-2.41637200	3.62863900	0.73842600		
O	-3.33370000	1.63162300	0.91745500		
C	-4.79138500	-0.25842600	0.59116400		
H	-5.60158900	0.44608500	0.81658300		
H	-4.39567600	-0.62341000	1.53997500		
C	-5.31644100	-1.39739700	-0.29119600		
H	-4.50706800	-2.09999300	-0.51446700		
H	-5.66326500	-0.98276100	-1.24307800		
C	-6.45172700	-2.13692000	0.40704400		
N	-6.96492400	-3.26541000	-0.45658600		
H	-6.22452100	-3.93688900	-0.68138100		
H	-7.71232000	-3.78403300	0.01331600		
H	-6.12965700	-2.59269700	1.34433800		
H	-7.34427100	-2.92172800	-1.34397100		
N	2.41999200	2.74913100	-0.40771300		
O	2.24658100	3.90374600	-0.80679100		
O	3.52765000	2.27954300	-0.13308800		
H	-7.30627700	-1.48819900	0.60432700		
C	4.58371000	-1.20586000	-0.38902000		
H	4.92502200	-0.40921600	-1.05519200		
H	5.81341500	-0.48187000	1.09637600		
N	5.73667900	-1.37822400	0.60571300		
C	5.51180000	-2.42831600	1.66011100		
H	4.58370000	-2.22093500	2.18904500		
H	5.47252600	-3.40537200	1.18341100		
H	6.34818100	-2.38657500	2.35627300		
C	7.05811800	-1.59058300	-0.08341500		
H	7.19400200	-0.81150000	-0.83171700		
H	7.84353700	-1.53211400	0.66865100		
H	7.06207800	-2.57359400	-0.54932000		
C	4.29402100	-2.46937900	-1.18861100		



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H      3.95181400 -3.29122300 -0.55477400
H      3.48971200 -2.23256800 -1.88805100
H      5.15432400 -2.79876900 -1.77389800
O      -3.70069300  0.85571900 -1.29220500

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**2a\_IL\_H(S0)** 155baa\_iDMPO\_DNI\_VEGE\_indole+H+\_b3lyp631dp\_PCMw.log

Input orientation:

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.576565	0.982234	0.124017
2	6	0	1.210106	1.248964	-0.195096
3	6	0	0.347343	0.158783	-0.405387
4	6	0	0.886128	-1.158718	-0.299152
5	6	0	2.231166	-1.389911	-0.013372
6	6	0	3.100258	-0.328099	0.214549
7	6	0	2.313420	3.203848	0.036756
8	6	0	1.082138	2.686196	-0.249890
9	1	0	2.606815	-2.402290	0.052536
10	7	0	3.208942	2.171627	0.262228
11	1	0	2.636866	4.231606	0.099311
12	8	0	-0.938224	0.264294	-0.780339
13	6	0	-1.761552	1.392609	-0.435784
14	1	0	-1.479286	1.782754	0.545372
15	1	0	-1.657232	2.183351	-1.182280
16	7	0	4.470955	-0.460519	0.525089
17	8	0	4.897153	-1.614504	0.594373
18	7	0	0.057271	-2.348188	-0.461133
19	8	0	0.619670	-3.388708	-0.800929
20	8	0	-1.160469	-2.304932	-0.223958
21	6	0	-3.199592	0.877739	-0.474649
22	1	0	-3.399844	0.531982	-1.491642
23	1	0	-2.441048	-0.932928	0.148027
24	7	0	-3.298315	-0.394550	0.372612
25	6	0	-3.296505	-0.165565	1.855613
26	1	0	-2.454617	0.467188	2.130545
27	1	0	-4.233803	0.303262	2.148684
28	1	0	-3.197276	-1.134603	2.343116
29	6	0	-4.458290	-1.255473	-0.035452
30	1	0	-4.373312	-1.476700	-1.098602
31	1	0	-4.418078	-2.178264	0.541441
32	1	0	-5.388926	-0.729715	0.171861
33	6	0	-4.207420	1.950479	-0.081288
34	1	0	-4.007311	2.365580	0.908938
35	1	0	-4.142800	2.764874	-0.806884
36	1	0	-5.231373	1.572522	-0.108802
37	1	0	4.190357	2.272989	0.478306
38	1	0	0.205103	3.270424	-0.472382

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**2a\_IL\_TS4** 121bba\_iDMPO\_DNIGABA\_+2H+\_INT\_b3lyp631dp\_PCMw\_SCAN\_CN\_f\_FRQ.log

Input orientation:

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z

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1	6	0	-0.953014	0.226629	0.113948
2	6	0	0.228540	-0.543163	-0.202326
3	6	0	1.423991	0.075462	-0.424152
4	6	0	1.474100	1.536583	-0.351823
5	6	0	0.374117	2.295322	-0.063645
6	6	0	-0.861029	1.662813	0.217193
7	6	0	-1.769341	-1.878788	-0.095623
8	6	0	-0.230130	-1.984523	-0.320415
9	1	0	0.450527	3.372333	-0.009319
10	1	0	-2.331574	-2.172301	-0.988348
11	1	0	0.226986	-2.630651	0.433351
12	7	0	-2.052532	-0.464349	0.199507
13	1	0	0.003335	-2.405234	-1.302340
14	1	0	-2.115881	-2.503706	0.732611
15	6	0	-3.621542	0.739974	-0.095676
16	8	0	2.570967	-0.539167	-0.809094
17	6	0	2.900348	-1.844188	-0.300450
18	1	0	2.524333	-1.955007	0.719984
19	1	0	2.464753	-2.626381	-0.926180
20	7	0	-1.928892	2.406786	0.596402
21	8	0	-1.945628	3.625642	0.736118
22	8	0	-3.066515	1.737430	0.944876
23	6	0	-4.736759	0.039372	0.648323
24	1	0	-5.450045	0.825115	0.927121
25	1	0	-4.349597	-0.396535	1.570281
26	6	0	-5.428223	-1.004157	-0.237197
27	1	0	-4.725832	-1.804313	-0.491656
28	1	0	-5.739029	-0.530156	-1.173581
29	6	0	-6.636604	-1.591789	0.481539
30	7	0	-7.336665	-2.610031	-0.388151
31	1	0	-6.717268	-3.389144	-0.630890
32	1	0	-8.153341	-3.005563	0.087025
33	1	0	-6.357614	-2.112591	1.398541
34	1	0	-7.666113	-2.194124	-1.264818
35	7	0	2.715537	2.282102	-0.535767
36	8	0	2.632602	3.427344	-0.976168
37	8	0	3.797638	1.769079	-0.213778
38	1	0	-7.381148	-0.831053	0.719864
39	6	0	4.420300	-1.958427	-0.368752
40	1	0	4.720421	-1.793836	-1.406340
41	1	0	4.450599	0.036352	0.134789
42	7	0	5.037656	-0.778913	0.388444
43	6	0	4.992815	-0.897276	1.883829
44	1	0	3.980949	-1.136889	2.205725
45	1	0	5.686066	-1.671583	2.206684
46	1	0	5.287912	0.062979	2.304299
47	6	0	6.427831	-0.466408	-0.083388
48	1	0	6.402082	-0.289010	-1.157613
49	1	0	6.772241	0.428245	0.433705
50	1	0	7.084098	-1.304256	0.147227
51	6	0	4.921880	-3.316128	0.108475
52	1	0	4.582625	-3.553718	1.119248
53	1	0	4.532083	-4.082335	-0.566024
54	1	0	6.011450	-3.378771	0.075338
55	8	0	-3.589368	1.060310	-1.254566

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orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
C	-1.00599300	0.38479900	0.10364900		
C	0.09530900	-0.44490800	-0.08092200		
C	1.37421500	0.11655900	-0.16876700		
C	1.46972100	1.52606500	-0.08617500		
C	0.34437800	2.35877300	0.07005700		
C	-0.90873000	1.78372600	0.18613200		
C	-1.94226000	-1.72496900	-0.19773400		
C	-0.39157000	-1.86778700	-0.20990700		
H	0.46720000	3.43194500	0.10389100		
H	-2.38027600	-1.93188700	-1.17695900		
H	-0.06132400	-2.48280200	0.63279200		
N	-2.18641300	-0.30603000	0.15073500		
H	-0.02954600	-2.34269100	-1.12555700		
H	-2.41654300	-2.36770500	0.54608000		
C	-3.45555200	0.50778900	-0.08044200		
O	2.45142500	-0.66227400	-0.46956500		
C	2.99033700	-1.49709700	0.57981900		
H	3.12432200	-0.90733900	1.49148500		
H	2.31812200	-2.33159700	0.79575900		
N	-2.10046400	2.49900700	0.28985200		
O	-2.19319400	3.74267000	0.35121000		
O	-3.21587900	1.74554900	0.72794900		
C	-4.70252400	-0.06989100	0.60189400		
H	-5.39558400	0.77001100	0.71439900		
H	-4.43786300	-0.40816900	1.60828800		
C	-5.37812300	-1.18067900	-0.21280900		
H	-4.74737100	-2.07453500	-0.25460200		
H	-5.51819200	-0.83054200	-1.24016600		
C	-6.72236000	-1.54114500	0.40930300		
N	-7.41197800	-2.62981600	-0.37893600		
H	-6.86000500	-3.49263900	-0.40006300		
H	-8.32226600	-2.86157500	0.02901400		
H	-6.61832800	-1.92138900	1.42638900		
H	-7.57582000	-2.34732700	-1.34987000		
N	2.75436000	2.20813700	-0.17885700		
O	2.75314000	3.38929100	-0.52025400		
O	3.78859000	1.59231800	0.11739700		
H	-7.40645600	-0.69142000	0.41917400		
C	4.30252300	-2.05292700	0.04281300		
H	4.09562900	-2.48965700	-0.93709100		
H	4.62853400	-0.11480900	-0.56483700		
N	5.24714200	-0.87906900	-0.25493500		
C	5.98522900	-0.35464300	0.94293300		
H	5.28369900	-0.18109100	1.75626500		
H	6.74473400	-1.07516200	1.23961600		
H	6.45215100	0.58753700	0.66128300		
C	6.19204300	-1.18517300	-1.38027500		
H	5.61183900	-1.42839800	-2.26905900		
H	6.80676400	-0.30530500	-1.56483500		
H	6.82229400	-2.02665000	-1.09624600		
C	4.92069600	-3.10128000	0.95962000		
H	5.05185200	-2.73681400	1.98090600		
H	4.25100600	-3.96364100	0.99240700		
H	5.88321000	-3.45179200	0.58101500		

O -3.44587500 0.66576600 -1.36544100

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2b\_II\_F(T1) 114baa\_iDMPO\_DNIGABA\_+2H+\_b3lyp631dp\_PCMw\_TRIPLET\_SCANvege\_SCAN2vege\_SCAN.log

orientation:

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
C	-0.32886800	0.05642800	-1.08042100		
C	0.98014000	-0.53301700	-1.10430500		
C	2.09485000	0.19350000	-0.69195900		
C	1.88365700	1.54542700	-0.26859900		
C	0.63075500	2.13917700	-0.25344700		
C	-0.49879500	1.41155100	-0.63488000		
C	-0.68597500	-1.97963400	-1.97035900		
C	0.83853700	-1.90687100	-1.70222000		
H	0.52413800	3.16560400	0.07361900		
H	-0.92281800	-2.13419200	-3.03111400		
H	1.16228100	-2.70142900	-1.02449800		
N	-1.29497200	-0.72734700	-1.54817300		
H	1.42322200	-2.00415500	-2.62317500		
H	-1.17456300	-2.80141200	-1.43163800		
C	-4.76934700	0.32746200	0.37714800		
O	-5.10615500	1.12041600	-0.49760900		
O	3.36814500	-0.23338200	-0.74582000		
C	3.72508100	-1.61499500	-0.52306400		
H	3.08599900	-2.04536300	0.25157800		
H	3.62024900	-2.19321800	-1.44303900		
N	-1.78031500	1.95163800	-0.57678200		
O	-1.92347800	3.13378900	-0.34015100		
O	-3.56633300	0.15832800	0.83213500		
C	-5.76884700	-0.60639200	1.09259200		
H	-5.79154000	-0.32495000	2.15129400		
H	-5.38394700	-1.63027900	1.04789100		
C	-7.16210800	-0.50472100	0.46376700		
H	-7.10871000	-0.78835300	-0.59227800		
H	-7.50013400	0.53533000	0.50146700		
C	-8.14695700	-1.40476000	1.20079400		
N	-9.52854000	-1.29757200	0.59525100		
H	-9.53445500	-1.59080300	-0.38616800		
H	-10.20080600	-1.88732400	1.09380300		
H	-7.86997000	-2.45831000	1.14221000		
H	-9.88103200	-0.33643800	0.63025500		
N	2.99130100	2.39321000	0.18986600		
O	2.88981100	3.59887900	-0.01456500		
O	3.94480600	1.88426500	0.78937800		
H	-8.25299200	-1.12555300	2.25013900		
C	5.19604300	-1.60477800	-0.11985100		
H	5.75780100	-1.12033200	-0.92203500		
H	4.77848200	0.14563500	0.88407700		
N	5.38130400	-0.67110800	1.08154300		
C	4.92823700	-1.23774400	2.39590700		
H	3.91086900	-1.61316900	2.30344300		
H	5.60259600	-2.03781200	2.69509000		
H	4.95372000	-0.43533300	3.13185100		
C	6.78665300	-0.14873200	1.17566800		
H	7.03640000	0.35119700	0.24096100		
H	6.83370800	0.55900600	2.00209900		

H	7.46771000	-0.97829500	1.35795800
C	5.73303700	-3.01104500	0.11840400
H	5.14335700	-3.56269000	0.85408600
H	5.69149700	-3.55840000	-0.82599400
H	6.77655900	-2.99421200	0.43818600

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**2b\_II\_TS3** 114baa\_iDMPO\_DNIGABA\_+2H+\_b3lyp631dp\_PCMw\_TRIPLET\_SCANvege\_SCAN2vege\_TS\_FRQ.log

orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
C	-0.32886800	0.05642800	-1.08042100		
C	0.98014000	-0.53301700	-1.10430500		
C	2.09485000	0.19350000	-0.69195900		
C	1.88365700	1.54542700	-0.26859900		
C	0.63075500	2.13917700	-0.25344700		
C	-0.49879500	1.41155100	-0.63488000		
C	-0.68597500	-1.97963400	-1.97035900		
C	0.83853700	-1.90687100	-1.70222000		
H	0.52413800	3.16560400	0.07361900		
H	-0.92281800	-2.13419200	-3.03111400		
H	1.16228100	-2.70142900	-1.02449800		
N	-1.29497200	-0.72734700	-1.54817300		
H	1.42322200	-2.00415500	-2.62317500		
H	-1.17456300	-2.80141200	-1.43163800		
C	-4.76934700	0.32746200	0.37714800		
O	-5.10615500	1.12041600	-0.49760900		
O	3.36814500	-0.23338200	-0.74582000		
C	3.72508100	-1.61499500	-0.52306400		
H	3.08599900	-2.04536300	0.25157800		
H	3.62024900	-2.19321800	-1.44303900		
N	-1.78031500	1.95163800	-0.57678200		
O	-1.92347800	3.13378900	-0.34015100		
O	-3.56633300	0.15832800	0.83213500		
C	-5.76884700	-0.60639200	1.09259200		
H	-5.79154000	-0.32495000	2.15129400		
H	-5.38394700	-1.63027900	1.04789100		
C	-7.16210800	-0.50472100	0.46376700		
H	-7.10871000	-0.78835300	-0.59227800		
H	-7.50013400	0.53533000	0.50146700		
C	-8.14695700	-1.40476000	1.20079400		
N	-9.52854000	-1.29757200	0.59525100		
H	-9.53445500	-1.59080300	-0.38616800		
H	-10.20080600	-1.88732400	1.09380300		
H	-7.86997000	-2.45831000	1.14221000		
H	-9.88103200	-0.33643800	0.63025500		
N	2.99130100	2.39321000	0.18986600		
O	2.88981100	3.59887900	-0.01456500		
O	3.94480600	1.88426500	0.78937800		
H	-8.25299200	-1.12555300	2.25013900		
C	5.19604300	-1.60477800	-0.11985100		
H	5.75780100	-1.12033200	-0.92203500		
H	4.77848200	0.14563500	0.88407700		
N	5.38130400	-0.67110800	1.08154300		
C	4.92823700	-1.23774400	2.39590700		
H	3.91086900	-1.61316900	2.30344300		
H	5.60259600	-2.03781200	2.69509000		
H	4.95372000	-0.43533300	3.13185100		

C	6.78665300	-0.14873200	1.17566800
H	7.03640000	0.35119700	0.24096100
H	6.83370800	0.55900600	2.00209900
H	7.46771000	-0.97829500	1.35795800
C	5.73303700	-3.01104500	0.11840400
H	5.14335700	-3.56269000	0.85408600
H	5.69149700	-3.55840000	-0.82599400
H	6.77655900	-2.99421200	0.43818600

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**2b\_I\_A(S0)** 701aaa\_iDMBO\_DNIGABA\_+2H+\_b3lyp631dp\_PCMw.log

orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.404595	0.345372	0.156827
2	6	0	-0.153215	-0.230946	-0.114108
3	6	0	0.984392	0.536206	-0.332290
4	6	0	0.840496	1.949466	-0.288250
5	6	0	-0.385716	2.530247	0.019271
6	6	0	-1.497765	1.741151	0.287784
7	6	0	-1.711450	-1.972534	0.355357
8	6	0	-0.294080	-1.730018	-0.207341
9	1	0	-0.464636	3.606573	0.082710
10	1	0	-2.255872	-2.731375	-0.201975
11	1	0	0.462471	-2.267291	0.366797
12	7	0	-2.383682	-0.646325	0.236346
13	1	0	-0.212999	-2.055987	-1.250207
14	1	0	-1.679277	-2.262050	1.409559
15	6	0	-3.705916	-0.459860	-0.155134
16	8	0	-4.102209	0.622114	-0.565798
17	8	0	2.133740	-0.092642	-0.696489
18	6	0	3.070183	-0.393868	0.364878
19	1	0	3.305359	0.526187	0.905072
20	1	0	2.615311	-1.114166	1.055549
21	7	0	-2.667563	2.423512	0.835798
22	8	0	-2.921216	3.554159	0.420095
23	8	0	-3.288800	1.853027	1.730119
24	6	0	-4.615721	-1.673642	-0.039595
25	1	0	-4.442831	-2.171301	0.920889
26	1	0	-4.338593	-2.395821	-0.818189
27	6	0	-6.086616	-1.275248	-0.195412
28	1	0	-6.220384	-0.755556	-1.148866
29	1	0	-6.359425	-0.570318	0.596853
30	6	0	-6.989214	-2.501338	-0.136062
31	7	0	-8.437935	-2.101567	-0.296889
32	1	0	-8.601785	-1.630628	-1.191712
33	1	0	-9.057639	-2.915904	-0.261062
34	1	0	-6.776654	-3.210007	-0.937825
35	1	0	-8.736034	-1.460214	0.444252
36	7	0	1.942884	2.863854	-0.563881
37	8	0	1.659695	4.034906	-0.833603
38	8	0	3.099001	2.437937	-0.518165
39	1	0	-6.921647	-3.020717	0.821023
40	6	0	4.322217	-0.972247	-0.301984
41	1	0	4.640938	-0.221517	-1.033442
42	1	0	6.538408	-2.532597	-0.179141
43	6	0	4.021329	-2.295474	-1.020683

44	1	0	3.754169	-3.081541	-0.305976
45	1	0	3.183565	-2.160762	-1.707444
46	1	0	4.866942	-2.648389	-1.620365
47	6	0	5.395197	-1.106269	0.786856
48	1	0	5.614270	-0.145117	1.257100
49	6	0	7.653121	-1.922628	1.429915
50	1	0	7.169078	-2.625777	2.105574
51	1	0	8.570890	-2.352449	1.031647
52	1	0	7.865113	-0.985675	1.943810
53	6	0	7.378317	-0.737555	-0.728149
54	1	0	6.732609	-0.635950	-1.597321
55	1	0	7.547640	0.233861	-0.265140
56	1	0	8.324907	-1.187937	-1.021792
57	7	0	6.722968	-1.636909	0.282623
58	1	0	5.071945	-1.806444	1.561086

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**2b\_II\_A(S0)** 701baa\_iDMBO\_DNIGABA\_+2H+\_b3lyp631dp\_PCMw.log

orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.367836	0.105583	0.182286
2	6	0	-0.266886	-0.756928	0.088363
3	6	0	1.033936	-0.300039	-0.093858
4	6	0	1.215776	1.113339	-0.199663
5	6	0	0.133888	1.979605	-0.037913
6	6	0	-1.145473	1.495487	0.186422
7	6	0	-2.206363	-2.048072	0.600622
8	6	0	-0.728992	-2.189243	0.173120
9	1	0	0.302363	3.046868	-0.073217
10	1	0	-2.861110	-2.728600	0.060745
11	1	0	-0.151089	-2.770832	0.893666
12	7	0	-2.546992	-0.629380	0.284621
13	1	0	-0.636228	-2.682073	-0.800779
14	1	0	-2.332440	-2.212908	1.674329
15	6	0	-3.777508	-0.199019	-0.205058
16	8	0	-3.898627	0.883914	-0.759888
17	8	0	1.988098	-1.247447	-0.225637
18	6	0	3.127601	-1.259186	0.667636
19	1	0	3.311735	-0.256445	1.053440
20	1	0	2.875704	-1.901852	1.518481
21	7	0	-2.159047	2.477200	0.564576
22	8	0	-2.118272	3.583534	0.026458
23	8	0	-2.949509	2.159831	1.450843
24	6	0	-4.943036	-1.154644	-0.006553
25	1	0	-4.922444	-1.545332	1.016838
26	1	0	-4.807969	-2.017838	-0.670822
27	6	0	-6.279300	-0.468772	-0.307146
28	1	0	-6.266843	-0.087420	-1.332528
29	1	0	-6.406240	0.393485	0.355765
30	6	0	-7.435164	-1.443957	-0.119969
31	7	0	-8.753303	-0.779422	-0.442405
32	1	0	-8.793574	-0.471504	-1.418481
33	1	0	-9.539401	-1.417936	-0.291516
34	1	0	-7.358566	-2.308307	-0.781164
35	1	0	-8.913102	0.043989	0.145836
36	7	0	2.485646	1.738402	-0.511841
37	8	0	2.600032	2.954559	-0.380090

38	8	0	3.409088	1.015855	-0.932214
39	1	0	-7.515442	-1.794338	0.910124
40	6	0	4.327231	-1.822509	-0.109633
41	1	0	4.238119	-1.450005	-1.135271
42	1	0	5.117217	0.622578	-0.045707
43	6	0	4.299292	-3.357396	-0.150756
44	1	0	4.447907	-3.782417	0.847658
45	1	0	3.332649	-3.704213	-0.525253
46	1	0	5.080032	-3.746781	-0.809874
47	6	0	5.649850	-1.324493	0.490203
48	1	0	5.613287	-1.320548	1.581718
49	6	0	6.642540	0.117813	-1.304486
50	1	0	6.023533	-0.437121	-2.007000
51	1	0	6.729181	1.154699	-1.625870
52	1	0	7.628645	-0.339093	-1.226972
53	6	0	6.848529	0.795351	1.067846
54	1	0	6.295212	0.857906	2.003958
55	1	0	7.766039	0.224006	1.206749
56	1	0	7.078488	1.794006	0.699245
57	7	0	5.996700	0.091920	0.051745
58	1	0	6.488305	-1.952502	0.184498

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**2b\_I\_D(T1)** 707aaa\_iDMBO\_DNIGABA\_+2H+\_b3lyp631dp\_PCMw\_TRIPLET\_opt.log

orientation:

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.359699	0.071706	-0.135345
2	6	0	-0.063308	-0.413064	-0.403116
3	6	0	1.043457	0.449927	-0.405289
4	6	0	0.759694	1.807927	-0.171783
5	6	0	-0.528780	2.306555	0.110045
6	6	0	-1.610926	1.439395	0.196130
7	6	0	-1.643284	-2.188447	-0.672874
8	6	0	-0.133030	-1.871273	-0.742279
9	1	0	-0.672317	3.361021	0.297253
10	1	0	-2.053721	-2.522517	-1.630368
11	1	0	0.440666	-2.479721	-0.035987
12	7	0	-2.282458	-0.907863	-0.304310
13	1	0	0.276689	-2.067675	-1.738481
14	1	0	-1.891055	-2.939039	0.083931
15	6	0	-3.729107	-0.628664	-0.608499
16	8	0	-3.932000	-0.066011	-1.663361
17	8	0	2.273530	-0.005220	-0.767067
18	6	0	3.100640	-0.535921	0.297944
19	1	0	3.118289	0.180253	1.123101
20	1	0	2.678417	-1.484885	0.649962
21	7	0	-2.871869	1.847787	0.602249
22	8	0	-3.141188	3.087549	0.717745
23	8	0	-3.740830	0.908051	0.895791
24	6	0	-4.700622	-1.472104	0.175213
25	1	0	-4.380881	-1.501954	1.219240
26	1	0	-4.643100	-2.496535	-0.218679
27	6	0	-6.126596	-0.926828	0.034900
28	1	0	-6.407937	-0.918290	-1.022894
29	1	0	-6.135837	0.107801	0.391000
30	6	0	-7.110765	-1.769571	0.836199
31	7	0	-8.511151	-1.215029	0.713615



32	1	0	-8.838897	-1.225770	-0.256625
33	1	0	-9.177875	-1.761846	1.265734
34	1	0	-7.158289	-2.800813	0.483270
35	1	0	-8.562890	-0.246654	1.043842
36	7	0	1.833724	2.806661	-0.231745
37	8	0	1.540447	3.916967	-0.674673
38	8	0	2.952350	2.488443	0.168059
39	1	0	-6.876773	-1.771667	1.901838
40	6	0	4.502898	-0.734080	-0.286338
41	1	0	4.802352	0.244990	-0.676340
42	1	0	6.923101	-1.938268	-0.295967
43	6	0	4.500204	-1.763391	-1.425674
44	1	0	4.252807	-2.763102	-1.052557
45	1	0	3.756190	-1.484692	-2.174468
46	1	0	5.463557	-1.818384	-1.943460
47	6	0	5.424629	-1.123058	0.877343
48	1	0	5.407076	-0.374410	1.672348
49	6	0	7.669268	-1.892576	1.614044
50	1	0	7.227552	-2.855243	1.865257
51	1	0	8.699063	-2.023686	1.286031
52	1	0	7.627067	-1.219379	2.469482
53	6	0	7.512788	0.005973	0.030648
54	1	0	6.974618	0.386751	-0.834107
55	1	0	7.467406	0.720664	0.851801
56	1	0	8.547817	-0.197538	-0.239062
57	7	0	6.881723	-1.279834	0.488100
58	1	0	5.123888	-2.084743	1.299976

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orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.373188	0.014839	-0.172654
2	6	0	0.278469	-0.880082	-0.188356
3	6	0	-1.035034	-0.449545	-0.097055
4	6	0	-1.244588	0.956319	0.097865
5	6	0	-0.162235	1.862517	0.001288
6	6	0	1.126749	1.417195	-0.164764
7	6	0	2.294972	-2.125570	-0.481999
8	6	0	0.775903	-2.294492	-0.269594
9	1	0	-0.366342	2.924834	0.044600
10	1	0	2.883641	-2.752987	0.184663
11	1	0	0.304178	-2.844298	-1.087048
12	7	0	2.552617	-0.684980	-0.186375
13	1	0	0.559649	-2.836910	0.657003
14	1	0	2.590038	-2.328868	-1.515029
15	6	0	3.790925	-0.189082	0.288869
16	8	0	3.838285	0.872658	0.880116
17	8	0	-1.990450	-1.393954	-0.093584
18	6	0	-3.230923	-1.197825	-0.827402
19	1	0	-3.350643	-0.146709	-1.086732
20	1	0	-3.131744	-1.761078	-1.761543
21	7	0	2.137678	2.419616	-0.501023
22	8	0	2.065516	3.514238	0.051151
23	8	0	2.951087	2.118770	-1.372027
24	6	0	4.999653	-1.060148	0.020489
25	1	0	4.997463	-1.356389	-1.035025
26	1	0	4.904912	-1.986507	0.600629
27	6	0	6.295894	-0.332645	0.391315
28	1	0	6.253018	-0.031827	1.442395
29	1	0	6.384189	0.582202	-0.203475
30	6	0	7.503400	-1.231110	0.149841
31	7	0	8.781492	-0.515105	0.518434
32	1	0	8.795252	-0.247708	1.507435
33	1	0	9.600264	-1.107010	0.351873
34	1	0	7.473424	-2.136101	0.758063
35	1	0	8.906541	0.339495	-0.032646
36	7	0	-2.515779	1.524042	0.376510
37	8	0	-2.951217	2.098060	-0.738081
38	8	0	-3.335806	0.947029	1.193164
39	1	0	7.604315	-1.514017	-0.898923
40	6	0	-4.396568	-1.741997	0.012409
41	1	0	-4.169004	-1.506431	1.057359
42	1	0	-4.881802	0.690035	0.488433
43	6	0	-4.534099	-3.264192	-0.127582
44	1	0	-4.825778	-3.542510	-1.146113
45	1	0	-3.580983	-3.751325	0.095638
46	1	0	-5.286356	-3.655248	0.563236
47	6	0	-5.703228	-1.033825	-0.383200
48	1	0	-5.745384	-0.862240	-1.461153
49	6	0	-6.487053	0.188143	1.647250
50	1	0	-5.948052	-0.559449	2.227710
51	1	0	-6.430411	1.153266	2.149663
52	1	0	-7.527223	-0.112740	1.521561
53	6	0	-6.574852	1.307363	-0.555550
54	1	0	-5.996874	1.478057	-1.463034

55	1	0	-7.560136	0.911026	-0.802325
56	1	0	-6.674506	2.239473	-0.000136
57	7	0	-5.848141	0.315844	0.297774
58	1	0	-6.579462	-1.623549	-0.107251

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**2b\_I\_TS1** 709aaa\_iDMBO\_DNIGABA\_+2H+\_b3lyp631dp\_PCMw\_TRIPLET\_opt\_TS\_OCFRQ.log

orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.343479	0.076271	0.116444
2	6	0	0.052190	-0.409609	0.392310
3	6	0	-1.052216	0.456651	0.390191
4	6	0	-0.770789	1.812801	0.143178
5	6	0	0.522148	2.311244	-0.132384
6	6	0	1.599106	1.441349	-0.198550
7	6	0	1.652822	-2.164035	0.687908
8	6	0	0.135147	-1.867371	0.736319
9	1	0	0.666185	3.366499	-0.315245
10	1	0	2.062293	-2.443512	1.663629
11	1	0	-0.416756	-2.483882	0.019407
12	7	0	2.275707	-0.893850	0.266921
13	1	0	-0.288828	-2.069898	1.724880
14	1	0	1.917481	-2.946710	-0.028981
15	6	0	3.736070	-0.558491	0.539388
16	8	0	3.916460	-0.066302	1.641574
17	8	0	-2.280549	0.006059	0.758792
18	6	0	-3.109194	-0.539720	-0.297730
19	1	0	-3.132413	0.168002	-1.129950
20	1	0	-2.683814	-1.490458	-0.640796
21	7	0	2.884676	1.832809	-0.541930
22	8	0	3.199197	3.059889	-0.635915
23	8	0	3.748636	0.863623	-0.826563
24	6	0	4.707304	-1.438191	-0.213593
25	1	0	4.405980	-1.489522	-1.262455
26	1	0	4.630189	-2.450233	0.206124
27	6	0	6.139014	-0.910520	-0.062597
28	1	0	6.398516	-0.873634	1.000269
29	1	0	6.174636	0.112707	-0.448902
30	6	0	7.127988	-1.790094	-0.816394
31	7	0	8.531981	-1.246536	-0.682338
32	1	0	8.841196	-1.237051	0.293882
33	1	0	9.203418	-1.812256	-1.209000
34	1	0	7.156644	-2.809927	-0.429893
35	1	0	8.599155	-0.286699	-1.034144
36	7	0	-1.844339	2.810760	0.190735
37	8	0	-1.546403	3.934197	0.597802
38	8	0	-2.968900	2.482011	-0.184614
39	1	0	6.915428	-1.823656	-1.885925
40	6	0	-4.508371	-0.736677	0.294111
41	1	0	-4.808047	0.244757	0.677884
42	1	0	-6.930611	-1.941652	0.320271
43	6	0	-4.498338	-1.757362	1.441042
44	1	0	-4.249171	-2.758953	1.074325
45	1	0	-3.752451	-1.470787	2.185018
46	1	0	-5.459651	-1.811545	1.962648
47	6	0	-5.434238	-1.136061	-0.862784
48	1	0	-5.418760	-0.394829	-1.664745

49	6	0	-7.681636	-1.906552	-1.588164
50	1	0	-7.241996	-2.871379	-1.834699
51	1	0	-8.710803	-2.034141	-1.256864
52	1	0	-7.640534	-1.238552	-2.447741
53	6	0	-7.518484	0.001304	-0.016643
54	1	0	-6.977214	0.386978	0.843974
55	1	0	-7.475158	0.710791	-0.842379
56	1	0	-8.552838	-0.199405	0.257719
57	7	0	-6.890306	-1.288127	-0.467925
58	1	0	-5.135657	-2.101879	-1.277478

2b\_II\_TS1 709baa\_iDMBO\_DNIGABA\_+2H+\_b3lyp631dp\_PCMw\_TRIPLET\_opt\_TS\_OC\_FRQ.log

orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.312033	-0.198530	0.003523
2	6	0	0.155234	-0.987066	0.083513
3	6	0	-1.124429	-0.398771	0.127997
4	6	0	-1.148195	1.016432	0.157888
5	6	0	0.026107	1.811222	0.041552
6	6	0	1.269881	1.219094	-0.064736
7	6	0	2.092434	-2.380916	0.197513
8	6	0	0.546130	-2.432737	0.143303
9	1	0	-0.064453	2.887434	0.041427
10	1	0	2.494988	-2.727486	1.154698
11	1	0	0.189274	-2.974945	-0.739163
12	7	0	2.429915	-0.953830	0.039953
13	1	0	0.120806	-2.933439	1.018303
14	1	0	2.574345	-2.952231	-0.600794
15	6	0	3.768861	-0.326336	0.467818
16	8	0	3.773897	-0.067149	1.668123
17	8	0	-2.161340	-1.254499	0.206911
18	6	0	-3.264215	-1.173617	-0.731414
19	1	0	-3.335764	-0.167357	-1.142270
20	1	0	-3.038262	-1.857169	-1.556699
21	7	0	2.461364	1.914926	-0.202541
22	8	0	2.524549	3.173404	-0.090161
23	8	0	3.540989	1.196941	-0.560581
24	6	0	4.943974	-0.878481	-0.312690
25	1	0	4.730841	-0.815598	-1.382554
26	1	0	5.036880	-1.940809	-0.051620
27	6	0	6.235572	-0.135052	0.048199
28	1	0	6.385558	-0.183829	1.131562
29	1	0	6.125962	0.919399	-0.223611
30	6	0	7.429373	-0.745871	-0.674525
31	7	0	8.702200	-0.010007	-0.324244
32	1	0	8.889308	-0.038699	0.682434
33	1	0	9.512905	-0.419785	-0.796684
34	1	0	7.591439	-1.787369	-0.392956
35	1	0	8.655978	0.975767	-0.598964
36	7	0	-2.382366	1.760796	0.345548
37	8	0	-2.391577	2.960662	0.082810
38	8	0	-3.371625	1.153908	0.799960
39	1	0	7.330782	-0.685023	-1.759350
40	6	0	-4.543011	-1.603638	0.003648
41	1	0	-4.458831	-1.225486	1.027827
42	1	0	-5.100176	0.899404	-0.073849

43	6	0	-4.669440	-3.132863	0.063354
44	1	0	-4.817391	-3.555791	-0.936024
45	1	0	-3.759363	-3.568590	0.483888
46	1	0	-5.512820	-3.432044	0.691471
47	6	0	-5.782295	-0.984662	-0.660219
48	1	0	-5.686837	-0.980563	-1.748086
49	6	0	-6.737318	0.531135	1.091553
50	1	0	-6.207382	-0.073625	1.825267
51	1	0	-6.758457	1.571197	1.413252
52	1	0	-7.751094	0.155940	0.954755
53	6	0	-6.742147	1.246756	-1.276929
54	1	0	-6.139208	1.258031	-2.183655
55	1	0	-7.705234	0.773412	-1.467019
56	1	0	-6.887303	2.261526	-0.908783
57	7	0	-6.019338	0.455176	-0.226046
58	1	0	-6.689368	-1.534442	-0.404080

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**2b\_I\_E(T1)** 710aaa\_iDMBO\_DNIGABA\_+2H+\_b3lyp631dp\_PCMw\_TRIPLET\_SCAN\_vege.log

orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.303156	0.139708	-0.053250
2	6	0	-0.032677	-0.350130	-0.333171
3	6	0	1.060680	0.525364	-0.346300
4	6	0	0.787912	1.892161	-0.101449
5	6	0	-0.508735	2.384653	0.146159
6	6	0	-1.569661	1.497113	0.192613
7	6	0	-1.672744	-2.098577	-0.583788
8	6	0	-0.139404	-1.825222	-0.633619
9	1	0	-0.662583	3.443780	0.297614
10	1	0	-2.087874	-2.318301	-1.570500
11	1	0	0.384259	-2.426947	0.115473
12	7	0	-2.261400	-0.835639	-0.085856
13	1	0	0.290087	-2.072516	-1.608030
14	1	0	-1.936113	-2.912110	0.095336
15	6	0	-3.697463	-0.362128	-0.233439
16	8	0	-3.771460	-0.053234	-1.486932
17	8	0	2.285703	0.072349	-0.721415
18	6	0	3.122144	-0.466625	0.330126
19	1	0	3.213543	0.278626	1.124238
20	1	0	2.661198	-1.375638	0.735134
21	7	0	-2.905218	1.860675	0.373770
22	8	0	-3.315748	3.023181	0.577658
23	8	0	-3.768423	0.796081	0.724883
24	6	0	-4.698172	-1.359315	0.350989
25	1	0	-4.504574	-1.483364	1.420549
26	1	0	-4.519155	-2.322212	-0.139082
27	6	0	-6.141008	-0.902965	0.095721
28	1	0	-6.280273	-0.744761	-0.979003
29	1	0	-6.314959	0.055359	0.596153
30	6	0	-7.131498	-1.943705	0.602374
31	7	0	-8.555378	-1.486611	0.383742
32	1	0	-8.744567	-1.304059	-0.606351
33	1	0	-9.226357	-2.194011	0.697022
34	1	0	-7.031738	-2.894114	0.076004
35	1	0	-8.757668	-0.624821	0.899115

36	7	0	1.854865	2.889872	-0.132539
37	8	0	1.539501	4.050338	-0.410187
38	8	0	3.006282	2.537171	0.129569
39	1	0	-7.030852	-2.121585	1.674109
40	6	0	4.485061	-0.765574	-0.302077
41	1	0	4.807619	0.173385	-0.765250
42	1	0	6.818600	-2.139304	-0.332763
43	6	0	4.383034	-1.860092	-1.374007
44	1	0	4.121669	-2.826305	-0.928850
45	1	0	3.609243	-1.597423	-2.097970
46	1	0	5.313966	-1.981113	-1.937707
47	6	0	5.447398	-1.124003	0.838186
48	1	0	5.523205	-0.316565	1.569967
49	6	0	7.690558	-1.957738	1.512383
50	1	0	7.198963	-2.847373	1.902633
51	1	0	8.678054	-2.209446	1.128987
52	1	0	7.768985	-1.195182	2.286446
53	6	0	7.536108	-0.214957	-0.241788
54	1	0	6.980715	0.092355	-1.124878
55	1	0	7.557254	0.588750	0.493530
56	1	0	8.548422	-0.500561	-0.522851
57	1	0	5.115198	-2.028996	1.352503
58	7	0	6.865506	-1.406931	0.381717

2b\_II\_E(T1) 710baa\_iDMBO\_DNIGABA\_+2H+\_b3lyp631dp\_PCMw\_TRIPLET\_SCAN\_vege.log

orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.282857	0.173517	0.028269
2	6	0	-0.152995	0.970886	0.129011
3	6	0	1.121652	0.388975	0.171506
4	6	0	1.169154	-1.036972	0.162780
5	6	0	0.005002	-1.833392	0.049778
6	6	0	-1.234529	-1.230316	-0.027185
7	6	0	-2.137295	2.334360	0.206549
8	6	0	-0.581337	2.417173	0.168569
9	1	0	0.097695	-2.910022	0.045812
10	1	0	-2.545212	2.628734	1.176627
11	1	0	-0.238830	2.954624	-0.721143
12	7	0	-2.435056	0.902990	-0.029410
13	1	0	-0.179192	2.939888	1.039931
14	1	0	-2.614327	2.934642	-0.570694
15	6	0	-3.718251	0.156863	0.244951
16	8	0	-3.696149	0.045473	1.540786
17	8	0	2.161713	1.240999	0.281141
18	6	0	3.244925	1.205355	-0.680268
19	1	0	3.319217	0.214748	-1.128362
20	1	0	2.998707	1.914544	-1.478035
21	7	0	-2.456014	-1.905445	-0.061286
22	8	0	-2.594617	-3.145415	-0.097638
23	8	0	-3.552791	-1.120998	-0.511669
24	6	0	-4.930142	0.809969	-0.419512
25	1	0	-4.794960	0.799315	-1.505104
26	1	0	-4.955758	1.854363	-0.091846
27	6	0	-6.230101	0.103438	-0.011546
28	1	0	-6.314998	0.115267	1.080297
29	1	0	-6.193632	-0.943813	-0.329206

30	6	0	-7.435217	0.794877	-0.636865
31	7	0	-8.720458	0.115486	-0.224808
32	1	0	-8.845489	0.126955	0.791742
33	1	0	-9.535191	0.578588	-0.637682
34	1	0	-7.524790	1.834275	-0.317699
35	1	0	-8.742012	-0.863597	-0.523844
36	7	0	2.403374	-1.774183	0.336033
37	8	0	2.420184	-2.975440	0.074583
38	8	0	3.399237	-1.165101	0.775919
39	1	0	-7.408779	0.761483	-1.727091
40	6	0	4.533993	1.621958	0.045122
41	1	0	4.466493	1.218007	1.060617
42	1	0	5.087638	-0.877082	-0.119839
43	6	0	4.656690	3.149588	0.141811
44	1	0	4.785864	3.598761	-0.848765
45	1	0	3.752311	3.570727	0.588738
46	1	0	5.509603	3.436270	0.762992
47	6	0	5.765250	1.024972	-0.651961
48	1	0	5.657084	1.056319	-1.738190
49	6	0	6.737605	-0.551746	1.037005
50	1	0	6.215357	0.025936	1.797559
51	1	0	6.761010	-1.602804	1.321002
52	1	0	7.750290	-0.172408	0.904142
53	6	0	6.716108	-1.182027	-1.355689
54	1	0	6.098509	-1.167814	-2.252416
55	1	0	7.673024	-0.696369	-1.546408
56	1	0	6.873505	-2.207125	-1.023158
57	7	0	6.005913	-0.428672	-0.269122
58	1	0	6.676022	1.565343	-0.388752

2b\_I\_F(T1) 721aaa\_iDMBO\_DNIGABA\_+2H+\_INT\_b3lyp631dp\_PCMw\_TS\_f.log

orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.180637	-0.354686	0.146098
2	6	0	-0.234929	-0.644580	0.385301
3	6	0	-1.191447	0.314342	0.403199
4	6	0	-0.766799	1.693710	0.171430
5	6	0	0.526444	2.041444	-0.066111
6	6	0	1.545392	1.038570	-0.142226
7	6	0	1.163612	-2.553604	0.608154
8	6	0	-0.325960	-2.117283	0.676633
9	1	0	0.791852	3.075826	-0.233880
10	1	0	1.525648	-2.961114	1.559132
11	1	0	-0.938120	-2.644270	-0.062166
12	7	0	1.971409	-1.373119	0.274531
13	1	0	-0.774119	-2.304676	1.657404
14	1	0	1.342574	-3.325249	-0.149046
15	6	0	4.413556	0.038175	0.469218
16	8	0	-2.484207	0.044837	0.757561
17	6	0	-3.334568	-0.460155	-0.292924
18	1	0	-3.324753	0.244878	-1.128995
19	1	0	-2.961127	-1.432219	-0.637518
20	7	0	2.774619	1.457158	-0.470149
21	8	0	3.164514	2.602441	-0.687312
22	8	0	3.739279	0.425272	-0.692018
23	6	0	5.384930	-1.063814	0.130570

24	1	0	4.984009	-1.657363	-0.693585
25	1	0	5.459605	-1.698744	1.016993
26	6	0	6.768645	-0.486123	-0.233421
27	1	0	7.146302	0.112410	0.602404
28	1	0	6.676904	0.173231	-1.103055
29	6	0	7.738734	-1.620346	-0.545352
30	7	0	9.105773	-1.078645	-0.887524
31	1	0	9.518063	-0.567790	-0.101225
32	1	0	9.754072	-1.832315	-1.133879
33	1	0	7.876184	-2.288092	0.306247
34	1	0	9.068705	-0.435477	-1.684118
35	7	0	-1.742960	2.783681	0.145026
36	8	0	-1.374171	3.898073	0.522158
37	8	0	-2.874611	2.536656	-0.275163
38	1	0	7.416352	-2.206695	-1.406869
39	6	0	-4.744033	-0.592518	0.294524
40	1	0	-5.006671	0.402014	0.672309
41	1	0	-7.190224	-1.742612	0.312497
42	6	0	-4.780682	-1.606204	1.447167
43	1	0	-4.571876	-2.619715	1.087672
44	1	0	-4.024489	-1.346290	2.190322
45	1	0	-5.744474	-1.617357	1.967100
46	8	0	4.245887	0.575925	1.528984
47	6	0	-5.678295	-0.961872	-0.865053
48	1	0	-5.645951	-0.215814	-1.661977
49	6	0	-7.739498	0.212627	-0.015483
50	1	0	-7.184140	0.586729	0.841319
51	1	0	-7.689403	0.922816	-0.840268
52	1	0	-8.775293	0.030419	0.266301
53	6	0	-7.940139	-1.684349	-1.596193
54	1	0	-7.522932	-2.658942	-1.843430
55	1	0	-8.973115	-1.788257	-1.268353
56	1	0	-7.880232	-1.016204	-2.454537
57	1	0	-5.399238	-1.930952	-1.285733
58	7	0	-7.137591	-1.086764	-0.473016

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orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.086281	-0.321430	0.362499
2	6	0	0.247139	-0.890968	0.157879
3	6	0	1.364848	-0.136806	0.034491
4	6	0	1.210849	1.316015	0.108579
5	6	0	0.004500	1.916597	0.313600
6	6	0	-1.178620	1.137013	0.498593
7	6	0	-1.481876	-2.520589	0.137017
8	6	0	0.061697	-2.378038	0.034996
9	1	0	-0.062252	2.993934	0.370858
10	1	0	-1.924239	-2.945932	-0.771219
11	1	0	0.572769	-2.922205	0.835790
12	7	0	-2.052795	-1.183032	0.343712
13	1	0	0.459899	-2.753803	-0.912625
14	1	0	-1.792215	-3.165763	0.966350
15	6	0	-4.238124	0.701349	0.019248
16	8	0	2.571837	-0.707975	-0.275408
17	6	0	3.321482	-1.260217	0.834611
18	1	0	3.696543	-0.434160	1.449642
19	1	0	2.669729	-1.877104	1.459818
20	7	0	-2.301503	1.814659	0.780483
21	8	0	-2.461140	3.028583	0.864481
22	8	0	-3.437526	1.019760	1.120571
23	6	0	-5.369894	-0.173662	0.485646
24	1	0	-5.795994	0.262315	1.395200
25	1	0	-4.918293	-1.129721	0.774848
26	6	0	-6.427920	-0.354008	-0.607033
27	1	0	-5.962790	-0.787583	-1.497757
28	1	0	-6.828382	0.624641	-0.891030
29	6	0	-7.555860	-1.251803	-0.111670
30	7	0	-8.625693	-1.403796	-1.166540
31	1	0	-8.260031	-1.843916	-2.016198
32	1	0	-9.396177	-1.987739	-0.828923
33	1	0	-7.208196	-2.259543	0.119713
34	1	0	-9.024520	-0.499220	-1.435964
35	7	0	2.353943	2.214416	0.000410
36	8	0	2.161385	3.367623	-0.375119
37	8	0	3.474056	1.786231	0.324301
38	1	0	-8.051487	-0.838292	0.767722
39	6	0	4.452965	-2.115351	0.260410
40	1	0	3.984133	-2.994205	-0.198662
41	1	0	4.579414	0.501559	-0.592032
42	6	0	5.363178	-2.635469	1.385428
43	1	0	5.824130	-1.837449	1.972984
44	1	0	4.783108	-3.254621	2.075902
45	1	0	6.162800	-3.256686	0.973006
46	8	0	-4.006161	1.100137	-1.088545
47	6	0	5.175365	-1.453838	-0.933030
48	1	0	6.128126	-1.947906	-1.134080
49	6	0	6.459408	0.394808	0.239137
50	1	0	6.070922	0.108593	1.212374
51	1	0	7.395242	-0.125600	0.037182
52	1	0	6.613440	1.472600	0.210989
53	6	0	5.908680	0.572189	-2.156926
54	1	0	5.138589	0.356969	-2.896037

55	1	0	6.047138	1.648247	-2.063478
56	1	0	6.847185	0.093522	-2.435789
57	1	0	4.547627	-1.543561	-1.818984
58	7	0	5.468186	0.031038	-0.825593

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**2b\_I\_TS4** 721naa\_iDMBO\_DNIGABA\_+2H+\_INT\_b3lyp631dp\_PCMw\_TS\_FRQ.log

orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.302227	-0.313153	-0.025782
2	6	0	-0.081224	-0.632031	0.235595
3	6	0	-1.021605	0.341919	0.362939
4	6	0	-0.589773	1.732206	0.220574
5	6	0	0.708730	2.082421	-0.020153
6	6	0	1.690064	1.068423	-0.183049
7	6	0	1.346333	-2.553771	0.338053
8	6	0	-0.153293	-2.130594	0.398180
9	1	0	0.987616	3.122418	-0.118786
10	1	0	1.708612	-2.926979	1.302619
11	1	0	-0.722437	-2.592609	-0.414975
12	7	0	2.105836	-1.337460	-0.005936
13	1	0	-0.633531	-2.420092	1.336907
14	1	0	1.537137	-3.331008	-0.406956
15	6	0	3.961572	-0.685235	0.399964
16	8	0	-2.298599	0.058162	0.746905
17	6	0	-3.194725	-0.382876	-0.295360
18	1	0	-3.198180	0.361147	-1.096649
19	1	0	-2.851764	-1.344073	-0.697620
20	7	0	2.966145	1.399587	-0.490762
21	8	0	3.404785	2.534835	-0.655571
22	8	0	3.831908	0.365083	-0.729739
23	6	0	4.803064	-1.795652	-0.189062
24	1	0	4.578430	-1.913039	-1.250478
25	1	0	4.502289	-2.714302	0.320189
26	6	0	6.307425	-1.572359	0.057733
27	1	0	6.831966	-2.491377	-0.223173
28	1	0	6.472954	-1.411841	1.128473
29	6	0	6.871864	-0.399671	-0.740678
30	7	0	8.348693	-0.229500	-0.464964
31	1	0	8.890900	-1.037502	-0.784692
32	1	0	8.722988	0.595704	-0.941694
33	1	0	6.778114	-0.557318	-1.816026
34	1	0	8.536031	-0.113221	0.535586
35	7	0	-1.553275	2.827338	0.285291
36	8	0	-1.150462	3.928329	0.670886
37	8	0	-2.712681	2.606920	-0.071708
38	1	0	6.398164	0.547655	-0.483443
39	6	0	-4.587756	-0.513871	0.331263
40	1	0	-4.842521	0.481508	0.712251
41	1	0	-7.078366	-1.506464	0.454338
42	6	0	-4.596850	-1.524050	1.487782
43	1	0	-4.397065	-2.538914	1.127332
44	1	0	-3.825009	-1.262491	2.213947
45	1	0	-5.549464	-1.532642	2.027743
46	8	0	3.956348	-0.284642	1.533860
47	6	0	-5.550859	-0.892867	-0.802662
48	1	0	-5.495657	-0.188692	-1.635967

49	6	0	-7.560785	0.428774	-0.057849
50	1	0	-6.975646	0.871761	0.744521
51	1	0	-7.506003	1.046888	-0.953394
52	1	0	-8.595466	0.311001	0.259589
53	6	0	-7.840357	-1.603135	-1.447309
54	1	0	-7.478925	-2.621491	-1.579598
55	1	0	-8.879317	-1.609608	-1.122150
56	1	0	-7.736851	-1.039259	-2.373432
57	1	0	-5.321742	-1.892473	-1.178866
58	7	0	-7.009104	-0.929831	-0.389878

2b\_I\_G(T1) 725aaa\_iDMBO\_DNI\_+H+\_b3lyp631dp\_PCMw.log

orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	3.069405	1.109090	0.108814
2	6	0	1.644020	1.180199	-0.148418
3	6	0	0.887564	0.005384	-0.253490
4	6	0	1.604868	-1.193676	-0.087055
5	6	0	2.995319	-1.295222	0.153506
6	6	0	3.742146	-0.152837	0.269408
7	6	0	2.645872	3.295661	-0.107644
8	6	0	1.287758	2.606365	-0.297377
9	1	0	3.464929	-2.268418	0.244886
10	1	0	2.980433	3.878005	-0.981685
11	1	0	0.551547	2.931240	0.449656
12	7	0	3.639146	2.292073	0.141984
13	1	0	0.828770	2.801950	-1.276143
14	1	0	2.682976	4.017866	0.722902
15	8	0	-0.404343	-0.023479	-0.615018
16	6	0	-1.419491	0.328911	0.375806
17	1	0	-1.333354	-0.374408	1.207575
18	1	0	-1.243961	1.346826	0.735357
19	7	0	5.178109	-0.138738	0.525733
20	8	0	5.657917	-1.249399	0.628125
21	7	0	0.866665	-2.465912	-0.205921
22	8	0	1.322730	-3.279644	-0.997973
23	8	0	-0.118318	-2.606192	0.505521
24	6	0	-2.769754	0.211054	-0.335230
25	1	0	-2.791510	-0.792118	-0.775036
26	1	0	-5.380912	0.964204	-0.484710
27	6	0	-2.915679	1.264056	-1.443397
28	1	0	-2.964124	2.275741	-1.026214
29	1	0	-2.059596	1.214208	-2.119388
30	1	0	-3.807818	1.099827	-2.055994
31	6	0	-3.854667	0.309252	0.747944
32	1	0	-3.760104	-0.493124	1.482596
33	6	0	-6.265457	0.499740	1.306312
34	1	0	-6.057249	1.481291	1.728808
35	1	0	-7.265057	0.478286	0.875917
36	1	0	-6.163814	-0.272075	2.068253
37	6	0	-5.571016	-1.083812	-0.468645
38	1	0	-4.903273	-1.213502	-1.317233
39	1	0	-5.431758	-1.888168	0.252848
40	1	0	-6.603554	-1.056869	-0.812938
41	7	0	-5.269267	0.222102	0.212887
42	1	0	-3.794340	1.267302	1.269324

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**2b\_II\_G(T1)** 725baa\_iDMBO\_DNI\_+H+\_b3lyp631dp\_PCMw.log

orientation:

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	3.297815	0.446909	-0.065846
2	6	0	2.067051	1.191682	0.032847
3	6	0	0.810838	0.548907	0.148183
4	6	0	0.872734	-0.861416	0.067503
5	6	0	2.076767	-1.608744	0.015139
6	6	0	3.297073	-0.989894	-0.049052
7	6	0	3.915982	2.598364	-0.137603
8	6	0	2.390338	2.625004	-0.008783
9	1	0	2.023142	-2.691810	0.007872
10	1	0	4.313143	3.094787	-1.037486
11	1	0	2.030467	3.141840	0.893017
12	7	0	4.349080	1.233503	-0.167648
13	1	0	1.892298	3.130155	-0.849500
14	1	0	4.448077	3.094771	0.691267
15	8	0	-0.220031	1.365703	0.289624
16	6	0	-1.495973	1.057509	0.926187
17	1	0	-1.506343	0.031922	1.289134
18	1	0	-1.532860	1.717143	1.796671
19	7	0	4.563012	-1.686104	-0.125631
20	8	0	4.458731	-2.898432	-0.077719
21	7	0	-0.351671	-1.675834	-0.006302
22	8	0	-0.385625	-2.715802	0.628058
23	8	0	-1.245734	-1.248822	-0.744998
24	6	0	-2.627154	1.395139	-0.059693
25	1	0	-2.345829	0.987817	-1.035961
26	1	0	-3.208110	-1.129576	-0.116277
27	6	0	-2.791882	2.916515	-0.200102
28	1	0	-3.144421	3.361663	0.736214
29	1	0	-1.837187	3.380223	-0.459655
30	1	0	-3.511510	3.154075	-0.987681
31	6	0	-3.948558	0.753404	0.398978
32	1	0	-4.018250	0.721093	1.488147
33	6	0	-4.634947	-0.704571	-1.519681
34	1	0	-3.988817	-0.092834	-2.146641
35	1	0	-4.621422	-1.736483	-1.866914
36	1	0	-5.651362	-0.312442	-1.530535
37	6	0	-5.019119	-1.471731	0.805389
38	1	0	-4.556231	-1.525323	1.789495
39	1	0	-5.986567	-0.974493	0.866743
40	1	0	-5.133962	-2.470763	0.387706
41	7	0	-4.129312	-0.671548	-0.103636
42	1	0	-4.806532	1.314472	0.026404

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orientation:

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-3.037202	-1.136153	0.100000
2	6	0	-1.650632	-1.203790	-0.227605
3	6	0	-0.907383	-0.023313	-0.349173
4	6	0	-1.588029	1.209832	-0.159895
5	6	0	-2.950312	1.267134	0.137555
6	6	0	-3.696584	0.098774	0.287392
7	6	0	-2.474731	-3.292936	-0.134624
8	6	0	-1.323886	-2.595546	-0.377413
9	1	0	-3.438870	2.224324	0.263908
10	7	0	-3.505213	-2.408138	0.154453
11	8	0	0.391434	-0.085285	-0.738503
12	6	0	1.366814	-0.285539	0.311292
13	1	0	1.277461	0.530623	1.033260
14	1	0	1.169167	-1.240271	0.813052
15	7	0	-5.075365	0.059488	0.603535
16	8	0	-5.619089	1.152061	0.764229
17	7	0	-0.891512	2.487589	-0.280644
18	8	0	-1.566560	3.481932	-0.564168
19	8	0	0.325149	2.526769	-0.082166
20	6	0	2.745367	-0.279893	-0.356627
21	1	0	2.802052	0.661757	-0.914152
22	1	0	5.346440	-0.944611	-0.415543
23	6	0	2.907637	-1.461586	-1.323702
24	1	0	2.909901	-2.414833	-0.783710
25	1	0	2.077480	-1.473218	-2.032742
26	1	0	3.826658	-1.399872	-1.916188
27	6	0	3.790489	-0.270450	0.767344
28	1	0	3.658520	0.583449	1.435317
29	6	0	6.187842	-0.476506	1.395645
30	1	0	5.968655	-1.459198	1.810071
31	1	0	7.199808	-0.453932	0.994705
32	1	0	6.064155	0.293471	2.156332
33	6	0	5.549111	1.102111	-0.404598
34	1	0	4.888613	1.240536	-1.257297
35	1	0	5.414167	1.908748	0.315126
36	1	0	6.583880	1.062075	-0.740698
37	7	0	5.222822	-0.198476	0.275520
38	1	0	3.724124	-1.186671	1.358401
39	1	0	-2.661067	-4.356277	-0.142275
40	1	0	-0.363438	-3.014575	-0.634080
41	1	0	-4.461303	-2.661419	0.357784

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2b\_II\_H(S0) 727baa\_iDMBO\_DNI\_indole\_+H+\_b3lyp631dp\_PCMw.log

orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-3.267680	0.507742	0.015175
2	6	0	-2.048345	1.237926	0.078923
3	6	0	-0.817126	0.566645	0.099962
4	6	0	-0.858044	-0.866050	0.090902
5	6	0	-2.065413	-1.568876	-0.008559
6	6	0	-3.286816	-0.905928	-0.048893
7	6	0	-3.757677	2.695245	0.031302
8	6	0	-2.393121	2.632860	0.081941
9	1	0	-2.056059	-2.650960	-0.021520
10	7	0	-4.279625	1.407918	-0.013477
11	8	0	0.277155	1.345023	0.153431
12	6	0	1.402415	1.145922	-0.736127
13	1	0	1.397460	0.135360	-1.142065
14	1	0	1.269955	1.839237	-1.573784
15	7	0	-4.546261	-1.544025	-0.127060
16	8	0	-4.521332	-2.773550	-0.189578
17	7	0	0.323821	-1.679059	0.279774
18	8	0	0.305670	-2.856106	-0.070353
19	8	0	1.313638	-1.153441	0.831145
20	6	0	2.690467	1.467851	0.039402
21	1	0	2.535303	1.117131	1.064566
22	1	0	3.049534	-1.077856	0.068503
23	6	0	2.955132	2.979817	0.083800
24	1	0	3.179040	3.371238	-0.914292
25	1	0	2.074135	3.504314	0.463030
26	1	0	3.798324	3.210536	0.740619
27	6	0	3.890415	0.725338	-0.569940
28	1	0	3.817037	0.683014	-1.658790
29	6	0	4.678405	-0.782540	1.267266
30	1	0	4.158837	-0.130088	1.966708
31	1	0	4.634801	-1.811772	1.620159
32	1	0	5.714402	-0.464307	1.153911
33	6	0	4.693718	-1.593981	-1.071034
34	1	0	4.113051	-1.598621	-1.992343
35	1	0	5.694124	-1.203088	-1.255250
36	1	0	4.752440	-2.600991	-0.659991
37	7	0	4.005501	-0.708808	-0.073624
38	1	0	4.833843	1.212588	-0.317464
39	1	0	-4.419258	3.548151	0.022667
40	1	0	-1.710868	3.467121	0.126820
41	1	0	-5.259186	1.169571	-0.072645

orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
C	0.79735000	1.06179200	1.47817800		
C	-0.55111900	0.57555200	1.46249600		
C	-1.48061400	1.04351300	0.54866500		
C	-1.04040300	2.03347300	-0.38094200		
C	0.26375900	2.52607900	-0.38507300		
C	1.20072000	2.05681400	0.52914500		
C	0.72651000	-0.40029000	3.19485700		
C	-0.70222100	-0.40328900	2.58811300		
H	0.55085300	3.28801700	-1.09860600		
H	0.74095100	-0.08691000	4.24676600		
H	-0.99468700	-1.39816900	2.23684400		
N	1.56070500	0.52477500	2.43018500		
H	-1.46779500	-0.07776500	3.30044400		
H	1.19869800	-1.39058700	3.16942500		
C	4.81827600	-0.19798200	-0.74828000		
O	-2.78396400	0.66763800	0.63307500		
C	-3.15394100	-0.56181000	-0.03530200		
H	-2.93746800	-0.45970900	-1.10198900		
H	-2.57143700	-1.39467400	0.37587700		
N	2.54477900	2.51260400	0.55732700		
O	2.81158400	3.40558600	-0.23882100		
O	3.55721000	-0.01163700	-0.69145000		
C	5.42515700	-1.56869100	-0.77120700		
H	5.15949700	-2.02299700	-1.73400500		
H	4.93154900	-2.17294700	-0.00255100		
C	6.94736300	-1.53210800	-0.57188400		
H	7.17556900	-1.11901700	0.41660600		
H	7.39594800	-0.86859000	-1.31745200		
C	7.53873500	-2.93247900	-0.69564600		
N	9.03842400	-2.89973300	-0.50914100		
H	9.29862900	-2.51991800	0.40662000		
H	9.44250500	-3.83850400	-0.57441900		
H	7.15166700	-3.61110400	0.06554200		
H	9.49638500	-2.32178900	-1.22047500		
N	-1.95478200	2.60111200	-1.37179200		
O	-1.73647300	3.75577300	-1.74776900		
O	-2.87782000	1.90028600	-1.79057600		
H	7.36430900	-3.36802500	-1.68035000		
C	-4.65333900	-0.76166100	0.20847200		
H	-5.14057800	0.15411900	-0.14500400		
H	-6.76851200	-2.44342000	0.44003400		
C	-4.96094900	-0.96589000	1.69756900		
H	-4.55138500	-1.91483600	2.06000400		
H	-4.51475000	-0.15866600	2.28150000		
H	-6.03588700	-0.95062400	1.90486600		
O	5.45881600	0.88096500	-0.79322100		
C	-5.09126200	-1.94268600	-0.66555100		
H	-4.90630800	-1.74894100	-1.72436600		
C	-7.46540000	-1.17914700	-1.02662500		
H	-7.29250400	-0.28750200	-0.42830100		
H	-7.24569300	-0.98212700	-2.07549500		
H	-8.49662000	-1.50882000	-0.91078100		
C	-6.86074600	-3.57152700	-1.26991500		
H	-6.25128500	-4.36065800	-0.83215200		

H	-7.91836500	-3.80000200	-1.15041500
H	-6.61840400	-3.44360500	-2.32423700
H	-4.55737800	-2.85259900	-0.38120900
N	-6.56335200	-2.28254400	-0.55158600

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**2b\_I\_TS3** 722aba\_iDMBO\_DNIGABA\_+2H+\_INT\_b3lyp631dp\_TRIPLET\_PCMw\_SCAN\_FRQ.log

orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
C	0.79735000	1.06179200	1.47817800		
C	-0.55111900	0.57555200	1.46249600		
C	-1.48061400	1.04351300	0.54866500		
C	-1.04040300	2.03347300	-0.38094200		
C	0.26375900	2.52607900	-0.38507300		
C	1.20072000	2.05681400	0.52914500		
C	0.72651000	-0.40029000	3.19485700		
C	-0.70222100	-0.40328900	2.58811300		
H	0.55085300	3.28801700	-1.09860600		
H	0.74095100	-0.08691000	4.24676600		
H	-0.99468700	-1.39816900	2.23684400		
N	1.56070500	0.52477500	2.43018500		
H	-1.46779500	-0.07776500	3.30044400		
H	1.19869800	-1.39058700	3.16942500		
C	4.81827600	-0.19798200	-0.74828000		
O	-2.78396400	0.66763800	0.63307500		
C	-3.15394100	-0.56181000	-0.03530200		
H	-2.93746800	-0.45970900	-1.10198900		
H	-2.57143700	-1.39467400	0.37587700		
N	2.54477900	2.51260400	0.55732700		
O	2.81158400	3.40558600	-0.23882100		
O	3.55721000	-0.01163700	-0.69145000		
C	5.42515700	-1.56869100	-0.77120700		
H	5.15949700	-2.02299700	-1.73400500		
H	4.93154900	-2.17294700	-0.00255100		
C	6.94736300	-1.53210800	-0.57188400		
H	7.17556900	-1.11901700	0.41660600		
H	7.39594800	-0.86859000	-1.31745200		
C	7.53873500	-2.93247900	-0.69564600		
N	9.03842400	-2.89973300	-0.50914100		
H	9.29862900	-2.51991800	0.40662000		
H	9.44250500	-3.83850400	-0.57441900		
H	7.15166700	-3.61110400	0.06554200		
H	9.49638500	-2.32178900	-1.22047500		
N	-1.95478200	2.60111200	-1.37179200		
O	-1.73647300	3.75577300	-1.74776900		
O	-2.87782000	1.90028600	-1.79057600		
H	7.36430900	-3.36802500	-1.68035000		
C	-4.65333900	-0.76166100	0.20847200		
H	-5.14057800	0.15411900	-0.14500400		
H	-6.76851200	-2.44342000	0.44003400		
C	-4.96094900	-0.96589000	1.69756900		
H	-4.55138500	-1.91483600	2.06000400		
H	-4.51475000	-0.15866600	2.28150000		
H	-6.03588700	-0.95062400	1.90486600		
O	5.45881600	0.88096500	-0.79322100		
C	-5.09126200	-1.94268600	-0.66555100		
H	-4.90630800	-1.74894100	-1.72436600		



C	-7.46540000	-1.17914700	-1.02662500
H	-7.29250400	-0.28750200	-0.42830100
H	-7.24569300	-0.98212700	-2.07549500
H	-8.49662000	-1.50882000	-0.91078100
C	-6.86074600	-3.57152700	-1.26991500
H	-6.25128500	-4.36065800	-0.83215200
H	-7.91836500	-3.80000200	-1.15041500
H	-6.61840400	-3.44360500	-2.32423700
H	-4.55737800	-2.85259900	-0.38120900
N	-6.56335200	-2.28254400	-0.55158600

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**2b\_II\_TS3** 722aba\_iDMBO\_DNIGABA\_+2H+\_INT\_b3lyp631dp\_TRIPLET\_PCMw\_SCAN\_FRQ.log

orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
C	0.55667600	-0.25280600	1.12695300		
C	-0.75828200	-0.80650600	0.97473900		
C	-1.81076900	-0.05415400	0.47942300		
C	-1.53638600	1.30412100	0.12943300		
C	-0.27720000	1.87655500	0.27765500		
C	0.78927900	1.11749600	0.76275100		
C	0.75569300	-2.34539400	1.93476100		
C	-0.72449600	-2.21150900	1.49253000		
H	-0.12034100	2.91269700	0.00557000		
H	0.86160800	-2.55900900	3.00629300		
H	-0.98810600	-2.94475800	0.72337400		
N	1.44352300	-1.08925100	1.65453300		
H	-1.43065900	-2.34847200	2.31851500		
H	1.28641600	-3.15224700	1.41412700		
C	5.17972400	0.35230400	-0.29127400		
O	-3.07209900	-0.55348800	0.45368000		
C	-3.42161000	-1.44223700	-0.64413000		
H	-3.48183600	-0.84363900	-1.55921200		
H	-2.64311400	-2.19711400	-0.78055900		
N	2.08127600	1.64013800	0.88020600		
O	2.25106600	2.83291800	0.72723900		
O	3.96580500	-0.06131500	-0.50591200		
C	6.22388400	-0.45965600	-1.06477300		
H	6.21319500	-0.09614300	-2.09966700		
H	5.91674400	-1.50956600	-1.09571200		
C	7.61578000	-0.29631000	-0.44323000		
H	7.61063300	-0.69211700	0.57816900		
H	7.85342600	0.76949100	-0.37687400		
C	8.66494200	-1.02348300	-1.27530900		
N	10.03956900	-0.85426600	-0.66875900		
H	10.07546900	-1.21650300	0.28874100		
H	10.75057400	-1.35283600	-1.21131600		
H	8.48299100	-2.09805300	-1.32193000		
H	10.31717200	0.13105600	-0.63482400		
N	-2.58142200	2.17502200	-0.40438100		
O	-2.47224100	3.38185300	-0.21730900		
O	-3.50653800	1.66113100	-1.04980800		
H	8.72953300	-0.63195700	-2.29151200		
C	-4.74951800	-2.11458000	-0.29598900		
H	-4.55098600	-2.79385500	0.54179300		
H	-5.01926100	0.64212700	-0.41527600		

C	-5.23000800	-2.98611900	-1.46862800
H	-5.36126400	-2.42636300	-2.39784100
H	-4.50053900	-3.77699500	-1.66502000
H	-6.18188600	-3.46431600	-1.22340200
O	5.45565500	1.30249000	0.43780400
C	-5.79359100	-1.14607400	0.29949200
H	-6.78319500	-1.60679500	0.31203400
C	-6.49761200	0.15745100	-1.76457400
H	-5.79977500	-0.37124300	-2.40805500
H	-7.45991400	-0.35363300	-1.74783300
H	-6.61988200	1.17895100	-2.12207100
C	-6.79555200	1.11103600	0.49273000
H	-6.33728000	1.18485500	1.47767500
H	-6.83664200	2.09354400	0.02486100
H	-7.79588100	0.68611800	0.57076200
H	-5.51091800	-0.91342000	1.32585500
N	-5.95368700	0.20845300	-0.36696500

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**2b\_I\_C(S1)** 705aaa\_iDMBO\_DNIGABA\_+2H+\_TD\_b3lyp631dp\_PCMw\_opt.log

orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
C	-1.37719700	0.10547400	-0.18784700		
C	-0.08313700	-0.38699300	-0.42297800		
C	1.03952300	0.47304800	-0.40252300		
C	0.76966100	1.81852400	-0.14853900		
C	-0.54366400	2.29453700	0.16849200		
C	-1.61897300	1.45213000	0.17629600		
C	-1.62791900	-2.20945000	-0.45087600		
C	-0.14915600	-1.85094100	-0.72803000		
H	-0.67781100	3.33815700	0.41987400		
H	-2.09629500	-2.78052700	-1.25455100		
H	0.54295800	-2.43624600	-0.11694600		
N	-2.29462100	-0.90069000	-0.31241300		
H	0.11040800	-2.04369200	-1.77666000		
H	-1.74322000	-2.77220100	0.48330400		
C	-3.68926900	-0.63997900	-0.62309400		
O	-3.92972700	0.24245700	-1.41940600		
O	2.25317100	-0.02327600	-0.74516900		
C	3.11908200	-0.44614200	0.34070300		
H	3.18513900	0.35856000	1.07586500		
H	2.69172400	-1.33862000	0.81270900		
N	-2.91598300	1.85208100	0.63525300		
O	-3.28454700	3.06618600	0.48736800		
O	-3.54805100	0.95289300	1.32043600		
C	-4.68306200	-1.58819900	-0.00479100		
H	-4.35099100	-1.84489900	1.00509100		
H	-4.68537000	-2.51838300	-0.59053400		
C	-6.08061700	-0.95846200	0.01023000		
H	-6.37308900	-0.70240100	-1.01276900		
H	-6.03155800	-0.02764400	0.58493000		
C	-7.09901400	-1.91041300	0.62501600		
N	-8.48008400	-1.29745000	0.60447800		
H	-8.78728900	-1.09181500	-0.35095600		
H	-9.17279500	-1.92734500	1.01865800		
H	-7.17406700	-2.84801800	0.07216500		

H	-8.51348500	-0.41921600	1.13082500
N	1.81319100	2.83430300	-0.23178500
O	1.45232500	3.97670300	-0.52637400
O	2.98129600	2.51273200	-0.01261300
H	-6.87905900	-2.13245600	1.67024200
C	4.48851500	-0.74263400	-0.27718500
H	4.79171300	0.17790400	-0.78787200
H	6.83113200	-2.08993500	-0.22841400
C	4.41502800	-1.89308400	-1.29170400
H	4.17963000	-2.84265400	-0.79867600
H	3.63525600	-1.68892100	-2.02785100
H	5.34911200	-2.01596000	-1.84962600
C	5.45301200	-1.02149900	0.88399400
H	5.52082500	-0.16997500	1.56472400
C	7.69624300	-1.80926800	1.60806300
H	7.21407100	-2.68925800	2.03108100
H	8.69098100	-2.06214100	1.24467300
H	7.75475000	-1.01282900	2.34916200
C	7.53850700	-0.16007500	-0.23707300
H	6.97840100	0.10245500	-1.13160800
H	7.56163200	0.67947400	0.45676000
H	8.55036700	-0.45652600	-0.50839700
N	6.87311600	-1.32117500	0.44720400
H	5.12648400	-1.89537100	1.45278600

2b\_II\_C(S1) 705baa\_iDMBO\_DNIGABA\_+2H+\_TD\_b3lyp631dp\_PCMw\_opt.log

orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
C	-1.33725900	-0.00526600	0.34031000		
C	-0.24846700	-0.89691300	0.54920100		
C	1.09210800	-0.46975400	0.57780200		
C	1.31993000	0.90500200	0.35854600		
C	0.23130700	1.79420100	0.21107900		
C	-1.08466300	1.38637600	0.23242200		
C	-2.27317400	-2.14840600	0.59444000		
C	-0.74477900	-2.29534600	0.66158900		
H	0.45020700	2.85054400	0.11422100		
H	-2.72997600	-2.77784100	-0.16975100		
H	-0.40471000	-2.76317500	1.59080000		
N	-2.49097200	-0.71904100	0.25043400		
H	-0.36281400	-2.91578700	-0.15836000		
H	-2.75547200	-2.35327800	1.55500100		
C	-3.70451000	-0.26284200	-0.40539500		
O	-3.61362800	0.55834700	-1.28416000		
O	1.95600800	-1.46896400	0.77953800		
C	3.39116800	-1.31718900	0.96068700		
H	3.60805600	-0.32257900	1.34390000		
H	3.63165900	-2.04487800	1.74049900		
N	-2.12084800	2.40381200	0.31134300		
O	-1.88362400	3.50621600	-0.17712200		
O	-3.15495700	2.11208500	0.91638500		
C	-4.97696500	-0.89428700	0.09159200		
H	-5.02248200	-0.73429800	1.17607800		
H	-4.92342400	-1.97971000	-0.05350200		
C	-6.20404500	-0.31066400	-0.61592500		

H	-6.11758400	-0.48279900	-1.69314900
H	-6.23223200	0.77216600	-0.45935400
C	-7.48007300	-0.95313700	-0.08299600
N	-8.69469700	-0.39299400	-0.78377500
H	-8.65569500	-0.54926400	-1.79563200
H	-9.55321300	-0.83455200	-0.44176600
H	-7.49949600	-2.03058000	-0.25265600
H	-8.78942900	0.61587600	-0.63178600
N	2.62480000	1.50640900	0.29340100
O	3.25797800	1.67559700	1.40980400
O	3.24083000	1.27814000	-0.85630600
H	-7.62453500	-0.76019900	0.98083800
C	4.15626800	-1.66178600	-0.32729800
H	3.65633500	-1.15998100	-1.16204100
H	4.70715800	0.78698300	-0.56550400
C	4.16822200	-3.17368400	-0.58866500
H	4.72594800	-3.70532000	0.19034600
H	3.14709200	-3.56464500	-0.59785900
H	4.62794000	-3.40171500	-1.55450600
C	5.59161100	-1.11259700	-0.21019300
H	5.95939500	-1.20719000	0.81435900
C	6.11068500	0.50274400	-2.02946300
H	5.44592600	-0.08962000	-2.65821500
H	6.03101600	1.55431500	-2.30429200
H	7.13967800	0.15975600	-2.14457700
C	6.56977100	1.13198300	0.31616200
H	6.12383700	1.12253000	1.31013300
H	7.56550400	0.68720000	0.33678800
H	6.62783400	2.15828700	-0.04650200
N	5.69058300	0.34950800	-0.60257400
H	6.27773600	-1.66609900	-0.85380200

2b\_I\_TS2 713baa\_iDMBO\_DNIGABA\_+2H+\_b3lyp631dp\_PCMw\_TRIPLET\_SCAN\_vege\_TS\_CN\_FRQ.log

orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
C	-1.28253500	0.23812800	-0.05559800		
C	-0.12490700	1.01528100	0.06404400		
C	1.14741500	0.41881600	0.12364500		
C	1.16935500	-1.00068300	0.12743100		
C	-0.01084300	-1.78539300	0.01023400		
C	-1.24217700	-1.17934000	-0.08851000		
C	-2.07777700	2.38483500	0.13826700		
C	-0.52563300	2.46173300	0.11299700		
H	0.07238500	-2.86259900	0.02396400		
H	-2.49235800	2.66874400	1.11284500		
H	-0.16937600	3.00124300	-0.77151200		
N	-2.40976500	0.97588700	-0.10789100		
H	-0.11396500	2.97244800	0.98812700		
H	-2.55740400	3.00789100	-0.62129300		
C	-3.82939800	0.07202400	0.35143500		
O	-3.73173600	-0.07743900	1.57650300		
O	2.19017400	1.26357300	0.23514700		
C	3.30397100	1.19868700	-0.69072800		
H	3.37192100	0.20383800	-1.12939500		
H	3.09454700	1.90736500	-1.49909300		

N	-2.45158900	-1.87393000	-0.12175000
O	-2.55835600	-3.12045000	-0.10191700
O	-3.56394600	-1.12302200	-0.53144700
C	-5.00595100	0.76990900	-0.32140400
H	-4.85435800	0.78747900	-1.40405600
H	-5.01956400	1.80389100	0.03761900
C	-6.32401000	0.07188100	0.04636000
H	-6.42929800	0.06344100	1.13628000
H	-6.29363700	-0.96991900	-0.29077300
C	-7.50942000	0.78757300	-0.58889200
N	-8.80971000	0.12125500	-0.20267500
H	-8.94875200	0.12508300	0.81213700
H	-9.61270000	0.59803100	-0.62282100
H	-7.58898000	1.82441000	-0.25884100
H	-8.83856700	-0.85478700	-0.51082900
N	2.39212100	-1.75728000	0.31494000
O	2.39255100	-2.95614900	0.04421900
O	3.38750900	-1.16445300	0.77544100
H	-7.46762800	0.76622000	-1.67890000
C	4.57713200	1.59701400	0.07137800
H	4.48146000	1.18473400	1.08124200
H	5.11371000	-0.90345100	-0.09913800
C	4.70997300	3.12275400	0.18377300
H	4.86696100	3.57861900	-0.79967500
H	3.79873700	3.54808600	0.61229900
H	5.55000200	3.39675500	0.82773600
C	5.81968000	0.99589100	-0.60172200
H	5.73912700	1.03939700	-1.69003300
C	6.74652600	-0.60612400	1.08971400
H	6.21868700	-0.02725400	1.84554300
H	6.75162300	-1.65948800	1.36606400
H	7.76608600	-0.23886300	0.97659200
C	6.75932100	-1.21487200	-1.30934500
H	6.15608700	-1.18713800	-2.21545000
H	7.72337000	-0.73628500	-1.48079300
H	6.90222600	-2.24399900	-0.98294300
N	6.03864500	-0.46376300	-0.22788300
H	6.72785100	1.52577600	-0.31013500

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## References

- (1) Molnár-Perl, I.; Vasanits, A. Stability and Characteristics of the O-Phthaldialdehyde/3-Mercaptopropionic Acid and o-Phthaldialdehyde/N-Acetyl-L-Cysteine Reagents and Their Amino Acid Derivatives Measured by High-Performance Liquid Chromatography. *J. Chromatogr. A* **1999**, *835* (1-2), 73-91. [https://doi.org/10.1016/S0021-9673\(98\)01088-7](https://doi.org/10.1016/S0021-9673(98)01088-7).