

## Supporting information

### **Near Infrared Light Activated Phenothiazine Based Cancer Cells Specific Phototherapeutic System: A Synergistic Approach to Chemo-Photothermal Therapy**

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## 1. General procedure and materials:

Anhydrous solvent dimethylformamide (DMF) was used without distillation. Dichloromethane was distilled from CaH<sub>2</sub> before use. Solvents for workup and column chromatography, such as petroleum ether (PE), ethyl acetate (EtOAc), and other chemicals, were obtained from commercial vendors and used without further purification. All commercial-grade reagents were used without further purification. HPLC-grade acetonitrile and water were used for photolysis and HPLC. Reactions were monitored by thin layer chromatography (TLC) using Merck silica gel 60 F254 pre-coated plates (0.25 mm). The spots were visualized by exposure to UV light and/or dipping into 2,4-dinitrophenylhydrazine (2,4-DNP) solution and KMnO<sub>4</sub> solution. Silica gel of particle size 60-120 and 100-200 mesh and petroleum ether/ethyl acetate as eluent were used for column chromatographic purification.

<sup>1</sup>H NMR (500 MHz and 400 MHz) and <sup>13</sup>C NMR (150 MHz and 100 MHz) spectra were recorded on a BRUKER-AC 400 MHz and a BRUKER-AC 500 MHz spectrometer. The spectra were recorded in deuteriochloroform (CDCl<sub>3</sub>), deuterated acetonitrile (CD<sub>3</sub>CN), deuterated dimethyl sulfoxide (DMSO-*d*<sub>6</sub>), deuterated acetic acid (CD<sub>3</sub>COOD) and deuterated water (D<sub>2</sub>O) as solvent at room temperature. Chemical shifts are reported in parts per million (ppm) from tetramethylsilane with the solvent resonance as internal standard (CDCl<sub>3</sub>: δH = 7.26 ppm, δC = 77.16 ppm, DMSO-*d*<sub>6</sub>: 3.313 ppm and 2.484 ppm and CD<sub>3</sub>CN: δH = 1.94 ppm). Data are reported as follows: chemical shifts, multiplicity (s = singlet, d = doublet, t = triplet, m = multiplet), coupling constant *J* (Hz). HRMS spectra were recorded on a 6545XT-LC/Q-TOF (Agilent) JEOL-Accu TOF JMS-T100L mass spectrometer. UV/vis absorption spectra were recorded on a Shimadzu UV-2450 UV/vis spectrophotometer and Shimadzu UV-2600 UV/vis spectrophotometer, fluorescence emission spectra were recorded on a Hitachi F-7000 fluorescence spectrophotometer. Photolysis of all the caged ester was carried out using a 125 W medium-pressure mercury lamp supplied by SAIC (India) and a red light (595 ± 5 nm) light source from Kessil. RP-HPLC was recorded using mobile phase Acetonitrile/water at a flow rate of 1 mL min<sup>-1</sup> (detection: UV 310 nm).

Chromatographic purification was done with 60–120 mesh silica gel (Merck). Precoated silica gel 60 F254 TLC sheets (Merck) were used for reaction monitoring.

The average particle size and polydispersity index (PDI) of nanoparticles were measured using Malvern ZetaSizer Nano ZS dynamic light scattering (DLS) with a scattering angle of 173°. The wavelength of 633 nm was fixed at room temperature. Each measurement was performed for 15 runs, and the reported value is the average of 3 independent measurements.

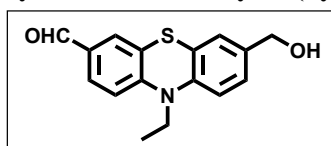
## 2. Experimental Procedure and spectroscopic data:

**Synthesis of 10-ethyl-10H-phenothiazine (2):** According to the method described in the literature, compound 2 was made.<sup>1</sup>

**Synthesis of 10-ethyl-10H-phenothiazine-3-carbaldehyde (3):** According to the literature described method, compound 3 was synthesized.<sup>2</sup>

**Synthesis of (10-ethyl-10H-phenothiazin-3-yl)methanol (4):** According to the method described in the literature, compound 4 was made.<sup>3</sup>

**Synthesis of 10-ethyl-7-(hydroxymethyl)-10H-phenothiazine-3-carbaldehyde (5):**



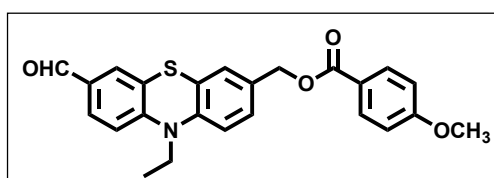
To a solution of DMF (0.5 mL, 3.89 mmol) at 0 °C was added POCl<sub>3</sub> (0.4 mL, 5.15 mmol) dropwise, and the reaction mixture was stirred for 10 min to form the Vilsmeier salt. Then, a solution of compound 4 (1.0 g, 3.88 mmol) in

chlorobenzene (5 mL) was added, and it was stirred at 60 °C for 13 hr. The progression of the reaction was monitored by TLC. After the reaction was finished, the mixture was extracted with EtOAc and then neutralised with a saturated NaHCO<sub>3</sub> solution. The product was purified by silica gel column chromatography using 30% EtOAc in hexane to get the pale yellow-coloured gel product. (Yield 0.51 g, 47%). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 9.78 (s, 1H), 7.62 (d, *J* = 8.4 Hz, 1H), 7.56 (d, *J* = 1.7 Hz, 1H), 7.13 (d, *J* = 8.3 Hz, 1H), 7.08 (s, 1H), 6.87 (dd, *J* = 15.5, 8.4 Hz, 2H), 4.41 (s, 2H), 3.96 (q, *J* = 6.9 Hz, 2H), 1.44 (t, *J* = 7.0 Hz, 3H). <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) δ 190.1, 150.2, 142.5, 136.4, 131.1, 130.3, 128.3, 126.5, 126.3, 124.3, 123.7, 115.6, 114.4, 64.5, 42.6, 12.9. HRMS (ESI<sup>+</sup>) calcd for C<sub>16</sub>H<sub>16</sub>NO<sub>2</sub>S [M+H]<sup>+</sup>, 286.0902; found: 286.0894.

**The general process for synthesizing caged esters (6a and 6b) is as follows:**

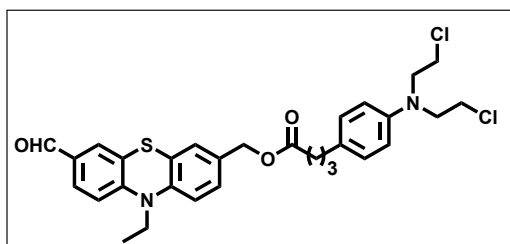
The corresponding acid (1.2 equiv) and 1.2 equiv of EDC-HCl were dissolved in dry DCM and cooled to 0°C. Compound 5 (200 mg, 0.70 mmol) and DMAP (cat.) were added to the reaction mixture after 5 minutes. Then, the reaction mixture was stirred at r.t for 8 h. Once the reaction was finished, it was extracted with DCM, washed with saturated NaHCO<sub>3</sub>, and then dried over Na<sub>2</sub>SO<sub>4</sub>. A rotary evaporator was used to remove the solvent, and the obtained residue was purified by column chromatography using EtOAc in hexane.

**Synthesis of (10-ethyl-7-formyl-10H-phenothiazin-3-yl)methyl 4-methoxybenzoate (6a):**



4-Methoxybenzoic acid was treated with compound 5 as the aforementioned procedure, and the crude residue was purified by chromatography on silica gel using 25% EtOAc in pet ether to give the yellow-coloured solid. (Yield 232 mg, 80%).  $^1\text{H NMR}$  (500 MHz,  $\text{CDCl}_3$ )  $\delta$  9.78 (s, 1H), 8.00 (d,  $J = 8.8$  Hz, 2H), 7.62 (dd,  $J = 8.4, 1.7$  Hz, 1H), 7.56 (d,  $J = 1.7$  Hz, 1H), 7.22 (dd,  $J = 8.3, 1.7$  Hz, 1H), 7.18 (d,  $J = 1.7$  Hz, 1H), 6.92 – 6.86 (m, 4H), 5.21 (s, 2H), 3.99 – 3.94 (m, 2H), 3.85 (s, 3H), 1.45 (d,  $J = 7.0$  Hz, 3H).  $^{13}\text{C NMR}$  (125 MHz,  $\text{CDCl}_3$ )  $\delta$  189.9, 166.2, 163.6, 150.1, 143.1, 131.9, 131.8, 131.3, 130.3, 128.3, 127.9, 127.6, 127.5, 124.3, 123.7, 122.6, 115.8, 114.2, 113.4, 65.6, 55.5, 42.6, 12.9. HRMS (ESI $^+$ ) calcd for  $\text{C}_{24}\text{H}_{22}\text{NO}_4\text{S}$  [M+H] $^+$ , 420.1270; found: 420.1263.

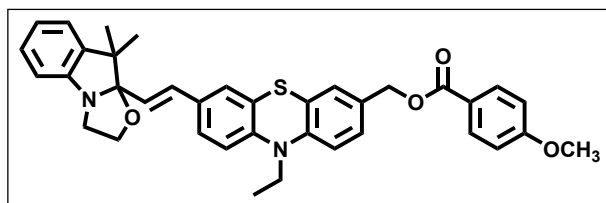
**Synthesis of (10-ethyl-7-formyl-10H-phenothiazin-3-yl)methyl 2-(4-(bis(2-chloroethyl)amino)phenyl)acetate (6b):**



Chlorambucil was treated with compound 5 as the aforementioned procedure, and the crude residue was purified by chromatography on silica gel using 25% EtOAc in pet ether to give the yellow-coloured solid. (Yield 285 mg, 75%).  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  9.78 (s, 1H), 7.62 (d,  $J = 8.4$  Hz, 1H), 7.56 (s, 1H), 7.14 (d,  $J =$

8.3 Hz, 1H), 7.10 (s, 1H), 7.04 (d,  $J = 8.4$  Hz, 2H), 6.88 (dd,  $J = 19.3, 8.4$  Hz, 2H), 6.63 (d,  $J = 8.4$  Hz, 2H), 4.98 (s, 2H), 3.96 (q,  $J = 6.9$  Hz, 2H), 3.69 (t,  $J = 6.4$  Hz, 4H), 3.61 (t,  $J = 6.3$  Hz, 4H), 2.54 (t,  $J = 7.5$  Hz, 2H), 2.34 (t,  $J = 7.4$  Hz, 2H), 1.99 – 1.81 (m, 2H), 1.44 (t,  $J = 6.9$  Hz, 3H).  $^{13}\text{C NMR}$  (125 MHz,  $\text{CDCl}_3$ )  $\delta$  189.8, 173.2, 149.9, 144.1, 143.0, 131.5, 131.2, 131.1, 130.2, 129.7, 128.2, 127.8, 127.5, 124.1, 123.6, 115.4, 114.4, 112.6, 65.2, 60.3, 53.8, 42.55, 40.4, 33.97, 33.60, 26.67, 21.02, 14.20, 12.80. HRMS (ESI $^+$ ) calcd for  $\text{C}_{30}\text{H}_{33}\text{Cl}_2\text{N}_2\text{O}_3\text{S}$  [M+H] $^+$ , 571.1583; found: 571.1586.

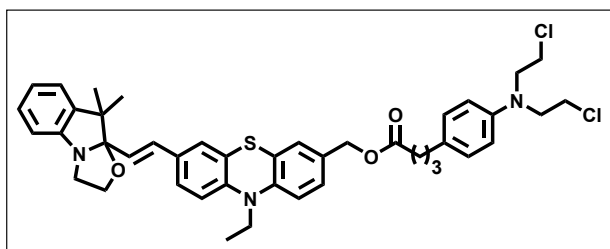
**Synthesis of (E)-(7-(2-(9,9-dimethyl-2,3-dihydrooxazolo[3,2-a]indol-9a(9H)-yl)vinyl)-10-ethyl-10H-phenothiazin-3-yl)methyl 4-methoxybenzoate (7a):**



Compound 6a (100 mg, 0.23 mmol) and 3H-Indolium, 1-(2-hydroxyethyl)-2,3,3-trimethyl-3H-indol-1-ium, iodide (49 mg, 0.24 mmol) was dissolved in 15 mL ACN. Then, piperidine (cat.) was added to the reaction mixture. The

mixture was refluxed to 80  $^\circ\text{C}$  under an argon atmosphere for 10 hours. The residue was purified by silica gel chromatography using 30% EtOAc in pet ether to get the yellow-coloured gel. (Yield 25 mg, 17%).  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.00 (d,  $J = 8.8$  Hz, 2H), 7.23 – 7.15 (m, 5H), 7.08 (d,  $J = 7.1$  Hz, 1H), 6.98 – 6.94 (m, 1H), 6.90 (d,  $J = 8.8$  Hz, 2H), 6.84 – 6.77 (m, 3H), 6.74 (d,  $J = 15.8$  Hz, 1H), 6.14 (d,  $J = 15.9$  Hz, 1H), 5.21 (s, 2H), 3.92 (dd,  $J = 13.5, 6.6$  Hz, 2H), 3.85 (s, 3H), 3.79 – 3.67 (m, 2H), 3.67 – 3.59 (m, 2H), 1.42 (d,  $J = 7.2$  Hz, 6H), 1.26 (s, 3H).  $^{13}\text{C NMR}$  (125 MHz,  $\text{CDCl}_3$ )  $\delta$  166.3, 163.6, 150.8, 144.7, 139.9, 131.9, 131.3, 131.0, 127.7, 127.6, 126.2, 125.4, 124.6, 122.5, 121.8, 115.0, 114.9, 113.8, 112.1, 110.1, 65.9, 63.6, 55.5, 48.1, 42.1, 20.5, 14.2, 13.0. HRMS (ESI $^+$ ) calcd for  $\text{C}_{37}\text{H}_{37}\text{N}_2\text{O}_4\text{S}$  [M+H] $^+$ , 605.2474; found: 605.2483.

**Synthesis of (E)-(7-(2-(9,9-dimethyl-2,3-dihydrooxazolo[3,2-a]indol-9a(9H)-yl)vinyl)-10-ethyl-10H-phenothiazin-3-yl)methyl 2-(4-(bis(2-chloroethyl)amino)phenyl)acetate (7b):**



Compound 6b (100 mg, 0.18 mmol) and 3H-Indolium, 1-(2-hydroxyethyl)-2,3,3-trimethyl-3H-indol-1-ium, iodide (39 mg, 0.59 mmol) was dissolved in 15 mL ACN. Then, piperidine (cat.) was added to the solution. The reaction mixture was refluxed to 80 °C under an argon atmosphere

for 10 hours. The crude was purified by silica gel chromatography using 30% EtOAc in pet ether to give the yellow-coloured gel. (Yield 20 mg, 15%). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.23 – 7.17 (m, 3H), 7.11 (s, 2H), 7.04 (d, *J* = 8.2 Hz, 2H), 6.95 (t, *J* = 7.4 Hz, 1H), 6.81 (t, *J* = 6.4 Hz, 4H), 6.74 (d, *J* = 15.9 Hz, 1H), 6.61 (d, *J* = 8.2 Hz, 2H), 6.14 (d, *J* = 15.8 Hz, 1H), 4.98 (s, 2H), 3.91 (q, *J* = 8.0 Hz, 2H), 3.77 (t, *J* = 7.8 Hz, 2H), 3.68 (d, *J* = 6.3 Hz, 4H), 3.62 (d, *J* = 5.9 Hz, 4H), 3.44 (t, *J* = 7.4 Hz, 2H), 2.54 (t, *J* = 7.5 Hz, 2H), 2.33 (t, *J* = 7.3 Hz, 2H), 1.92 (dd, *J* = 14.9, 7.4 Hz, 2H), 1.26 (s, 6H), 1.15 (s, 3H). <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) δ 173.5, 150.7, 144.7, 144.4, 144.2, 139.8, 131.2, 131.0, 130.6, 130.3, 129.8, 127.9, 127.7, 126.2, 125.3, 124.7, 124.4, 122.5, 121.8, 115.0, 114.8, 112.3, 112.1, 110.0, 65.5, 63.6, 53.7, 50.2, 48.0, 42.1, 40.6, 34.0, 33.7, 29.8, 28.5, 26.8, 20.4, 13.0. HRMS (ESI<sup>+</sup>) calcd for C<sub>43</sub>H<sub>48</sub>Cl<sub>2</sub>N<sub>3</sub>O<sub>3</sub>S [M+H]<sup>+</sup>, 756.2788; found: 756.2803.

**3. <sup>1</sup>H and <sup>13</sup>C NMR of all the compounds:**

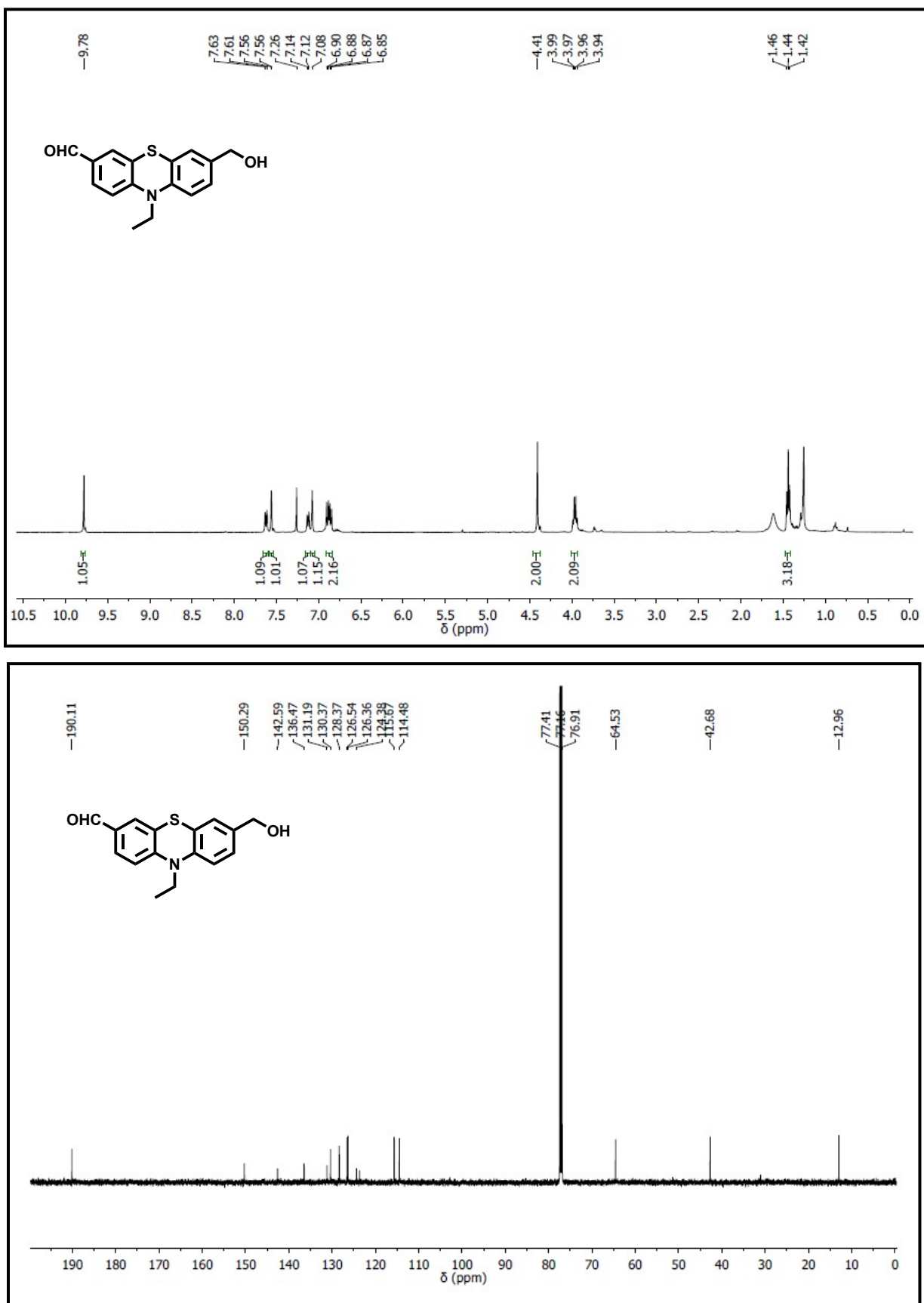


Fig. S1  $^1\text{H}$  (CDCl<sub>3</sub>, 400 MHz) and  $^{13}\text{C}$  (CDCl<sub>3</sub>, 126 MHz) NMR spectra of compound 5.

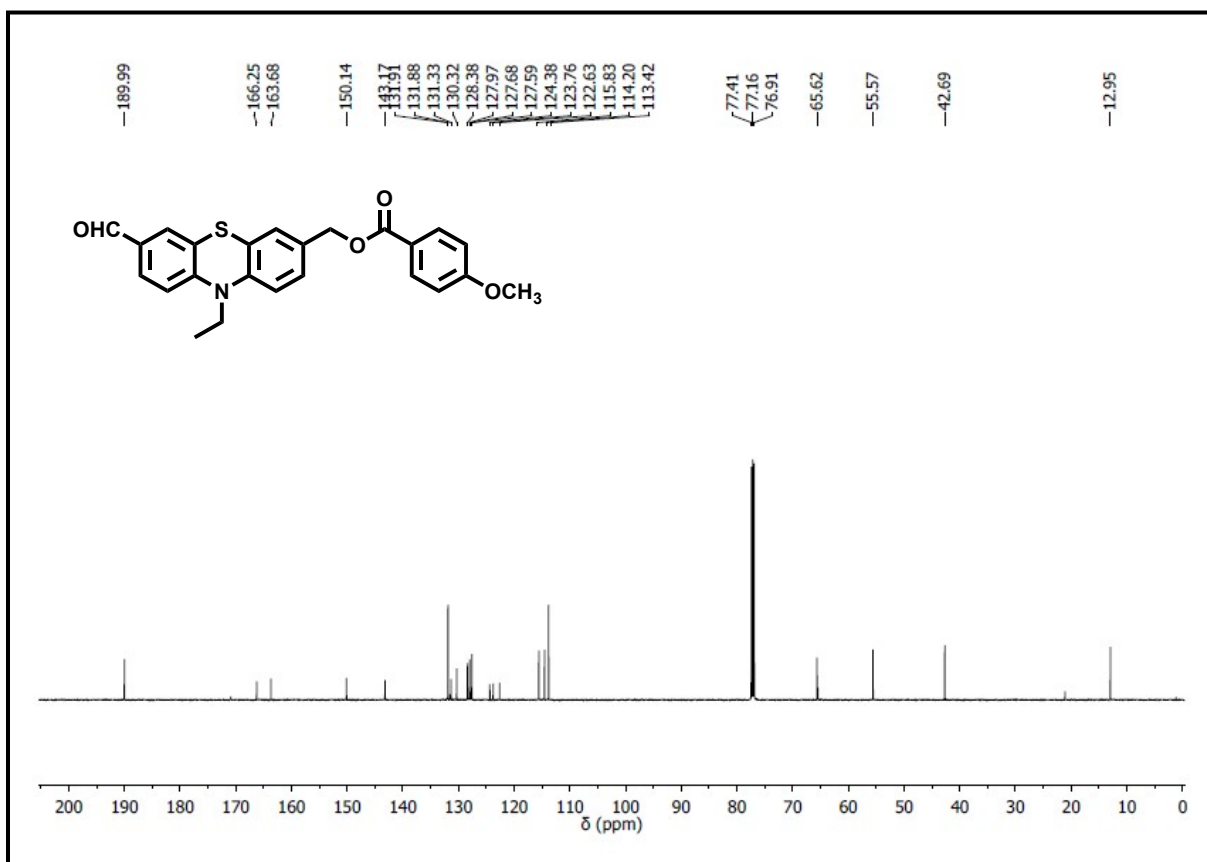
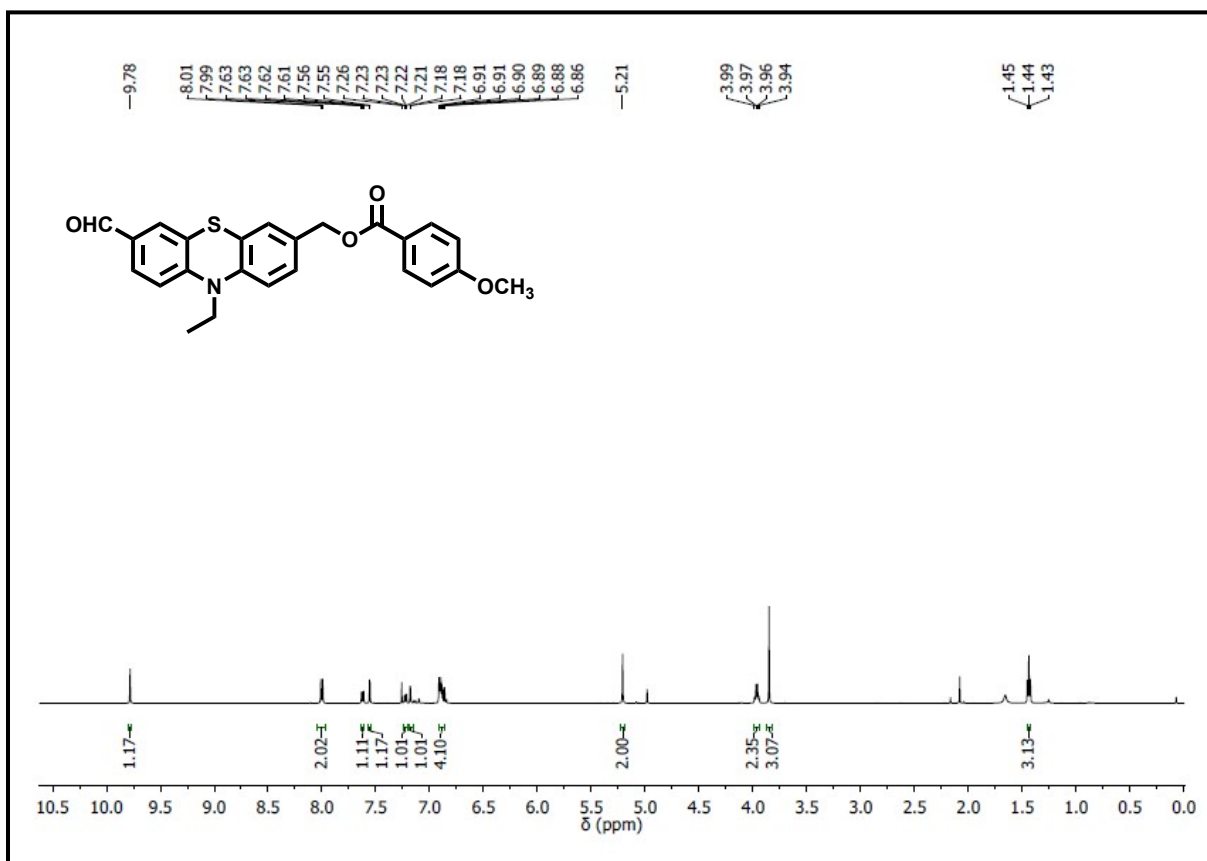
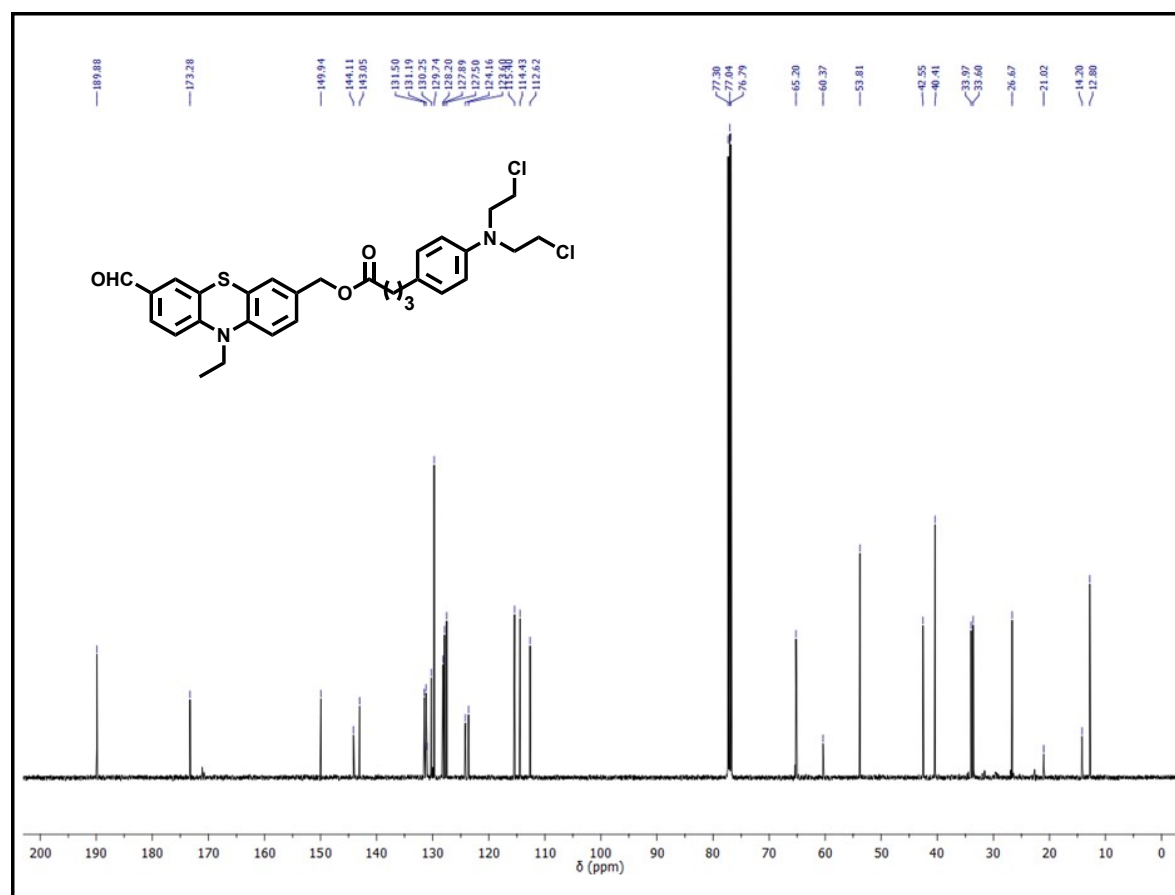
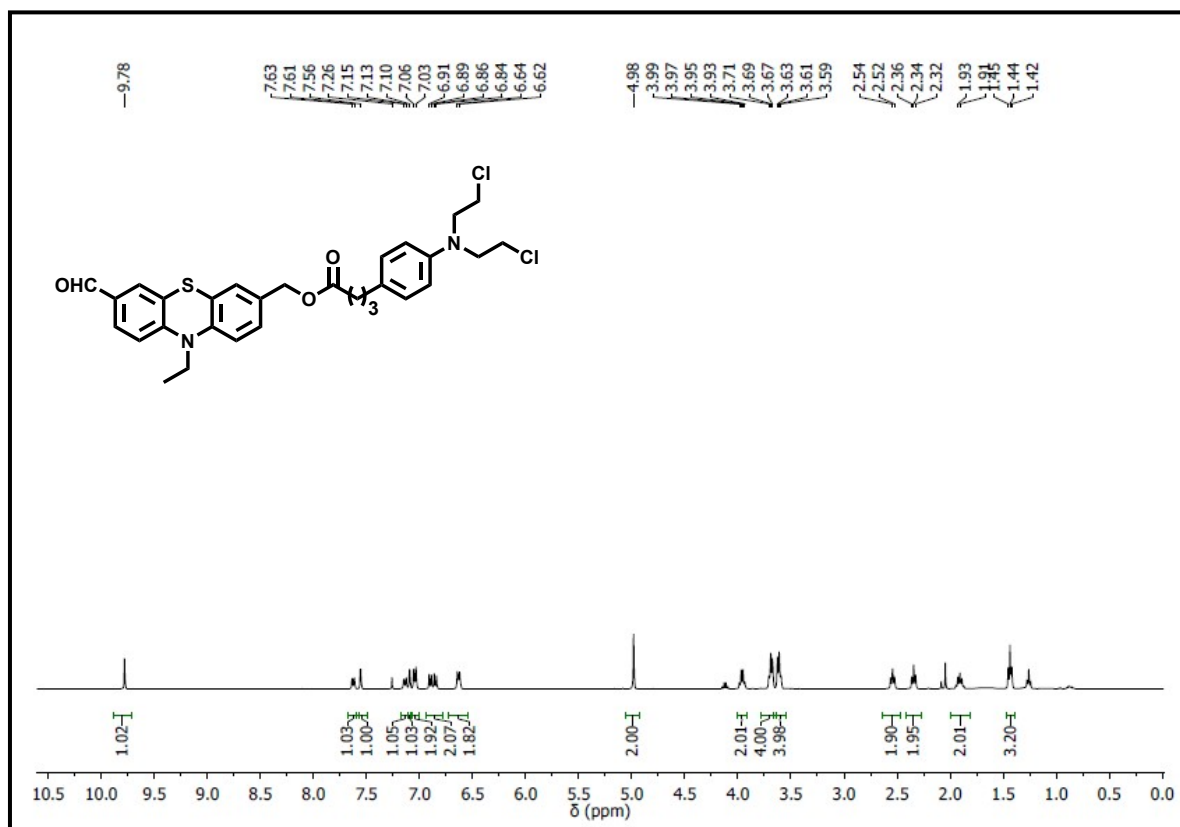


Fig. S2  $^1\text{H}$  (CDCl<sub>3</sub>, 400 MHz) and  $^{13}\text{C}$  (CDCl<sub>3</sub>, 126 MHz) NMR spectra of compound **6a**.



**Fig. S3** <sup>1</sup>H (CDCl<sub>3</sub>, 400 MHz) and <sup>13</sup>C (CDCl<sub>3</sub>, 125 MHz) NMR spectra of compound **6b**.



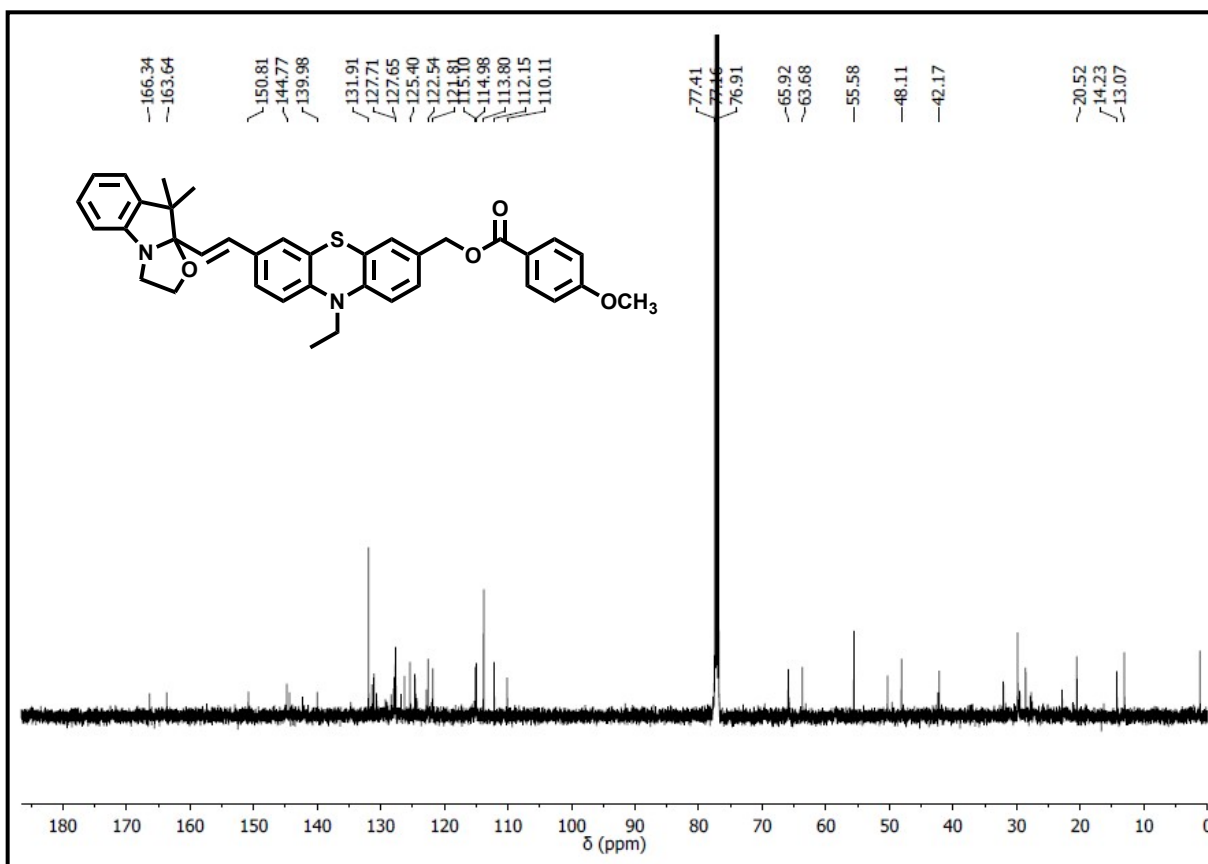
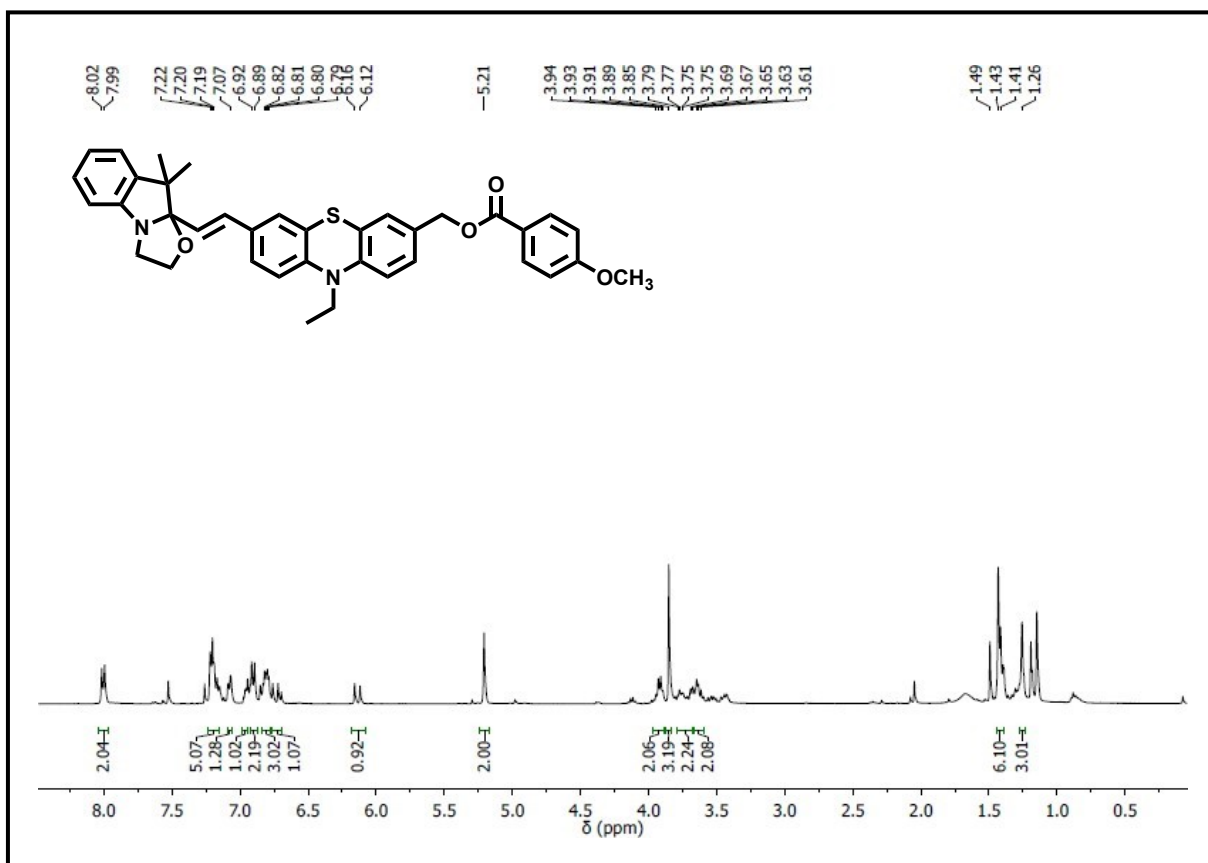


Fig. S4  $^1\text{H}$  (CDCl<sub>3</sub>, 400 MHz) and  $^{13}\text{C}$  (CDCl<sub>3</sub>, 126 MHz) NMR spectra of compound 7a.

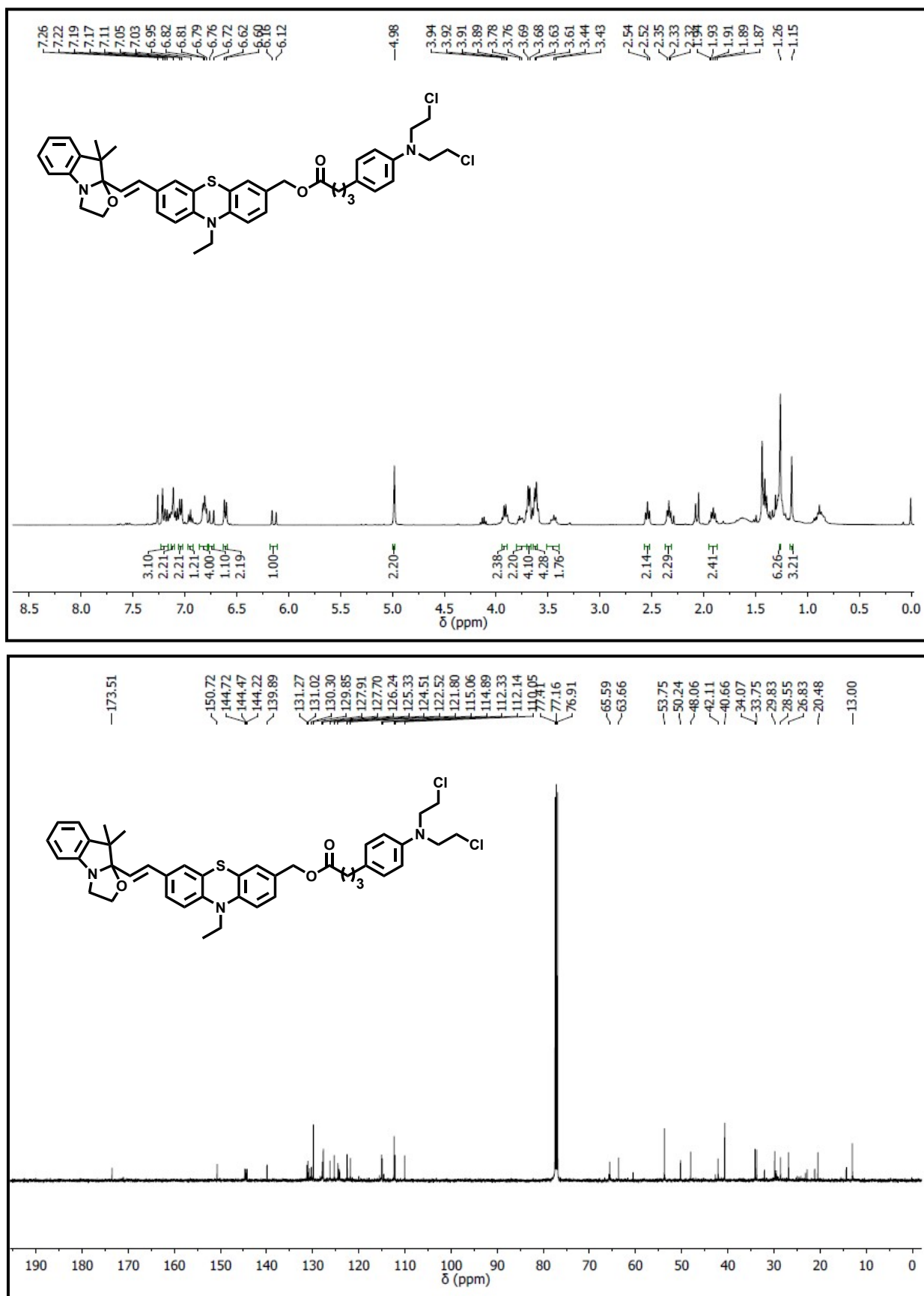


Fig. S5  $^1\text{H}$  (CDCl<sub>3</sub>, 400 MHz) and  $^{13}\text{C}$  (CDCl<sub>3</sub>, 126 MHz) NMR spectra of compound **7b**.

#### 4. HRMS spectra of all the compounds:

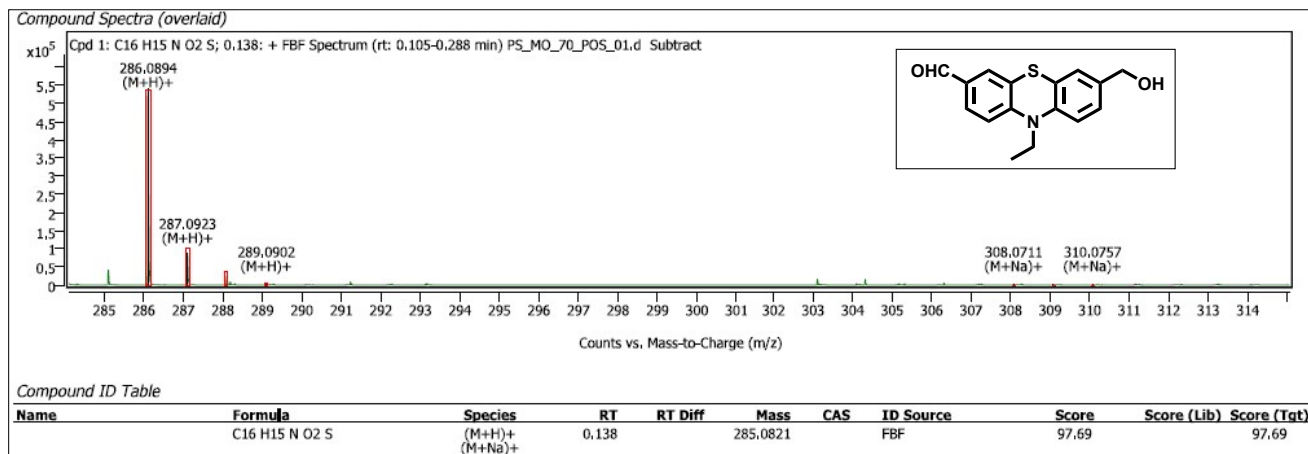


Fig. S6 HRMS of compound 5

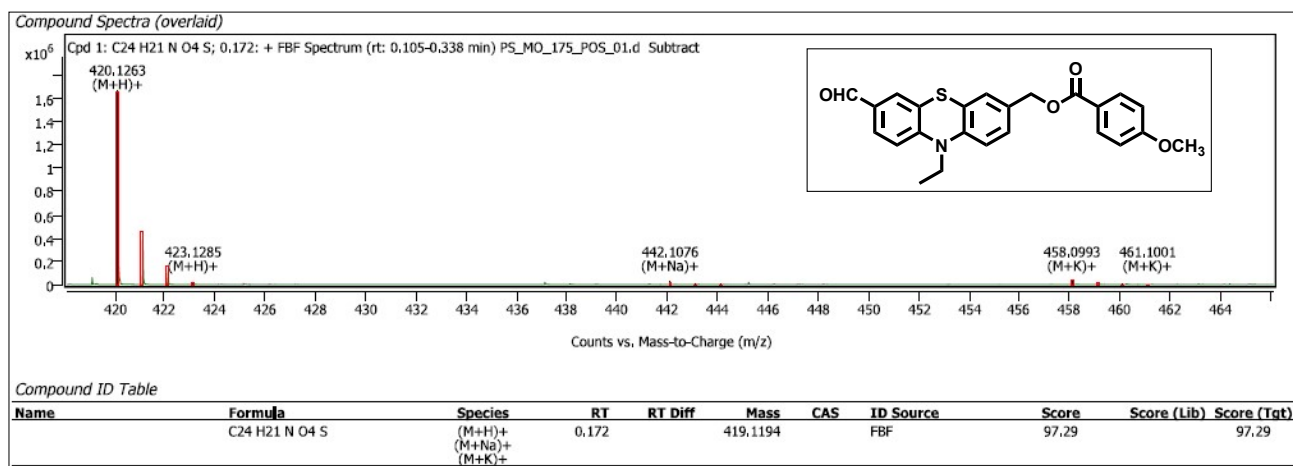


Fig. S7 HRMS of compound 6a

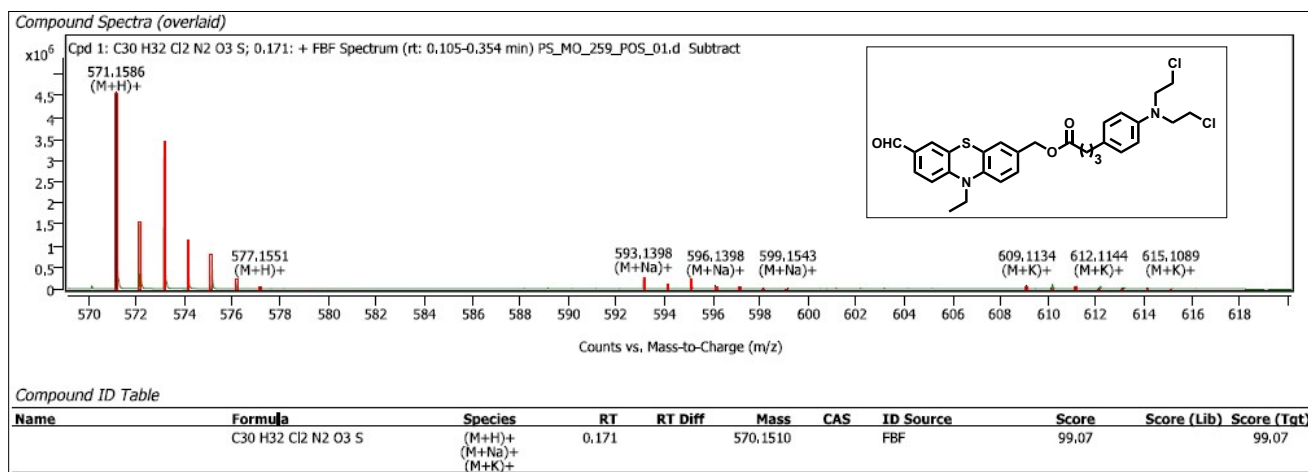


Fig. S8 HRMS of compound 6b

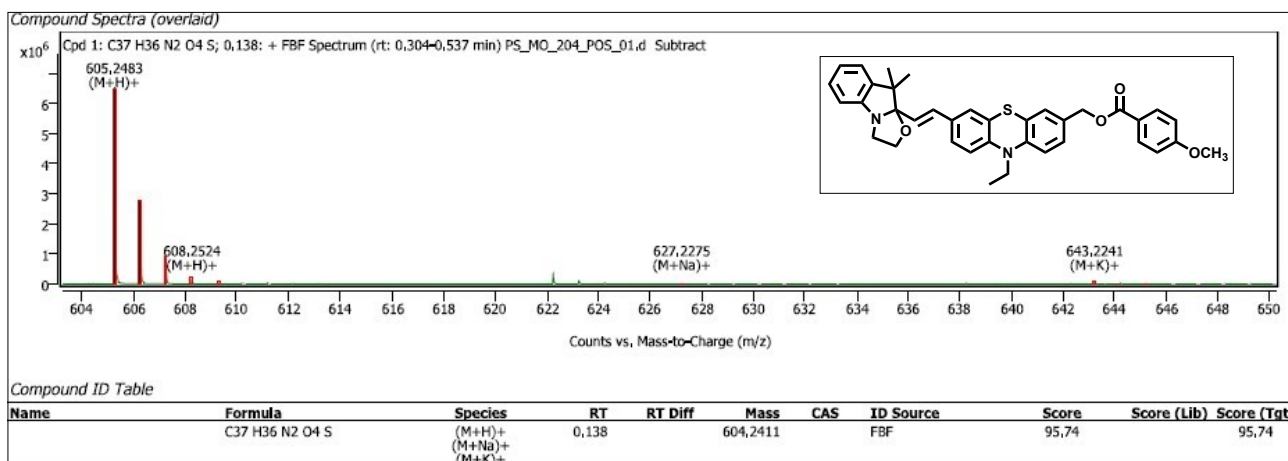


Fig. S9 HRMS of compound 7a

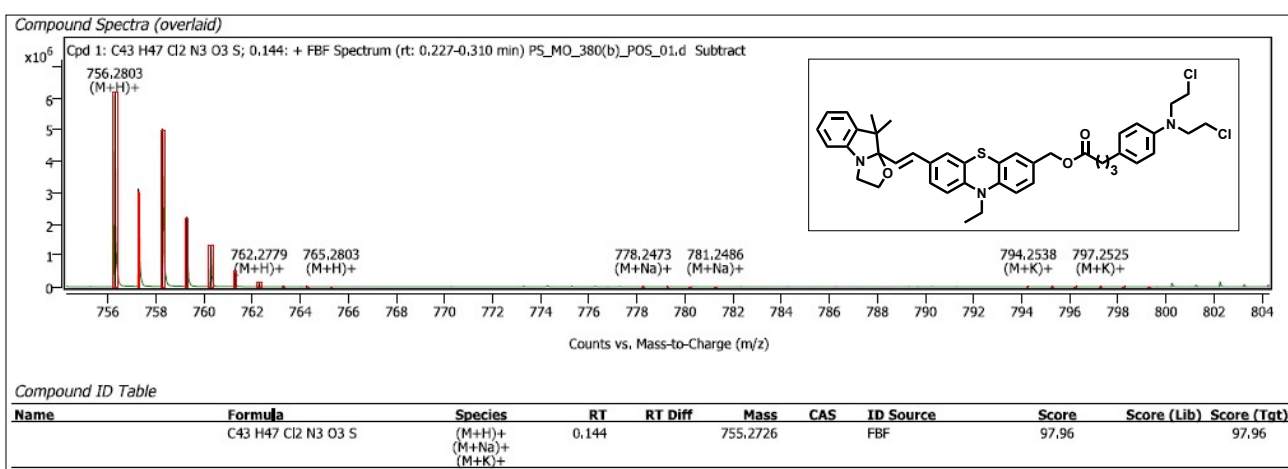
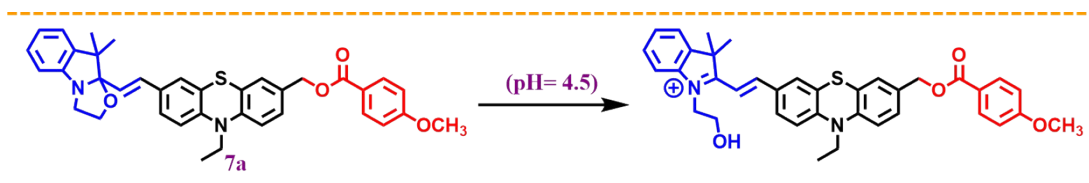
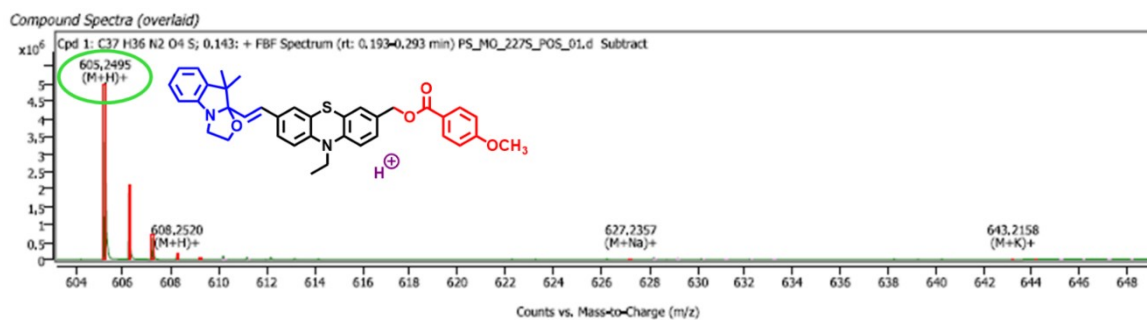


Fig. S10 HRMS of compound 7b

## 5. Characterization of photocage 7a in acidic pH (pH 4.5):

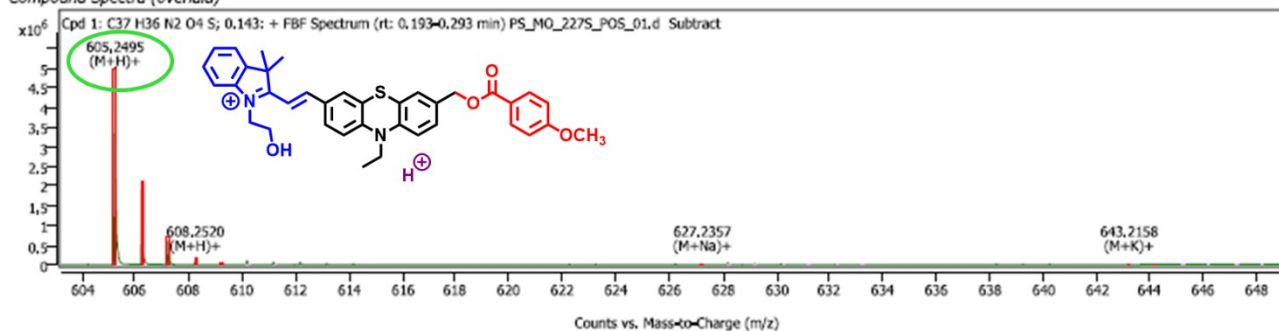




Compound ID Table

Name	Formula	Species	RT	RT Diff	Mass	CAS	ID Source	Score	Score (Lib)	Score (Tgt)
	C37 H36 N2 O4 S	(M+H)+ (M+Na)+ (M+K)+	0.143		604.2420		FBF	90.55		90.55

Compound Spectra (overlaid)

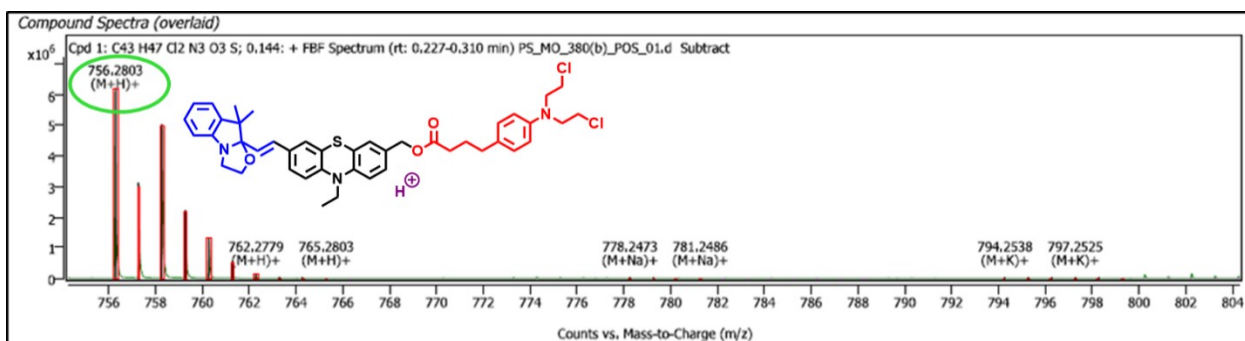
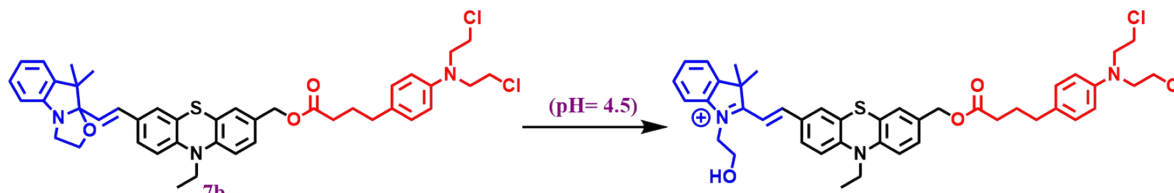


Compound ID Table

Name	Formula	Species	RT	RT Diff	Mass	CAS	ID Source	Score	Score (Lib)	Score (Tgt)
	C37 H36 N2 O4 S	(M+H)+ (M+Na)+ (M+K)+	0.143		604.2420		FBF	90.55		90.55

Fig. S11 HRMS spectra of photocage 7a in acidic pH (pH 4.5).

## 6. Characterization of photocage 7b in acidic pH (pH 4.5):



Compound ID Table

Name	Formula	Species	RT	RT Diff	Mass	CAS	ID Source	Score	Score (Lib)	Score (Tgt)
	C43 H47 Cl2 N3 O3 S	(M+H)+ (M+Na)+ (M+K)+	0.144		755.2726		FBF	97.96		97.96

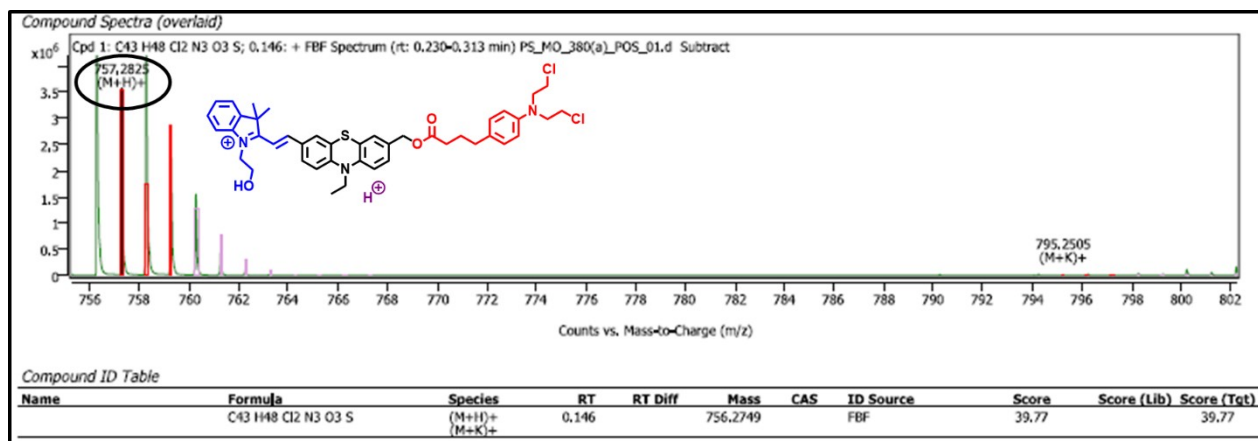


Fig. S12 HRMS spectra of photocage **7b** in acidic pH (pH 4.5).

## 7. Measurement of fluorescence quantum yields:

The quantum yields (QY) of PTZ photocage **7a** (PTZ-Ani) and **7b** (PTZ-Cbl) were calculated using the reference point approach. The standard sample, 9, 10-diphenyl anthracene ( $\Phi = 0.95$  in ethanol), was utilized to determine the fluorescence QY of **7a** and **7b**. A UV-vis spectrophotometer was used to measure the absorbance values of the solutions at the excitation wavelength. The Hitachi F- 7000 fluorescence spectrophotometer was used to capture both sample solutions' photoluminescence (PL) emission spectra at an excitation wavelength of 394 nm. Equation (1) was also used to compute the fluorescence quantum yield of photocage and DDS.

$$\frac{\Phi_S}{\Phi_R} = \frac{A_S}{A_R} \frac{(Abs)_R}{(Abs)_S} \frac{\eta_S^2}{\eta_R^2} \quad (1)$$

Where  $\Phi$  stands for quantum yield, Abs for absorbance, A for the area under the fluorescence curve, and  $\eta$  for the medium's refractive index. The parameters for the sample and reference are indicated by the subscripts S and R, respectively.

## 8. Fluorescence Lifetimes ( $\tau_F$ ) of the Photocage:

The TCSPC measurement, which is actually a time-resolved emission measurement, gives us the excited state decay dynamics of a fluorescent molecule through the excited state lifetime information. In the TCSPC measurement module, we have used a picosecond diode LASER unit with its peak wavelength at 375 nm excitation LASER source. The fluorescence signals generated are detected using the Hamamatsu MCP PMT (3809U) detector at the polarizer angle of  $\sim 54.7^\circ$ , which is called magic angle polarization. The TCSPC decays are collected in forward mode and analyzed with respect to the prompt (or instrument response function (IRF)) that has been taken. The IBH DAS-6 software has been utilized to fit the collected decays using the respective order of exponential equations to get the subsequent lifetime values and contributions. The average lifetime ( $\tau_{avg}$ ) has been calculated using the obtained lifetime information following the equation below:



$$\tau_{avg} = \sum a_i \tau_i \dots\dots\dots (2)$$

Where  $\tau_i$  is the lifetime component, and  $a_i$  is the respective amplitude. Contributions where ‘i’ represents the order of the exponential equation used to fit the lifetime decay trace, and  $\sum a_i = 1$ .

### 9. Photothermal Properties:

pH-dependent photothermal conversion was investigated by r.t thermometer (Fig. S13). We irradiated the solution (40  $\mu$ M) with 640 nm light at different pH, and then the solution temperature was monitored every 30 seconds.

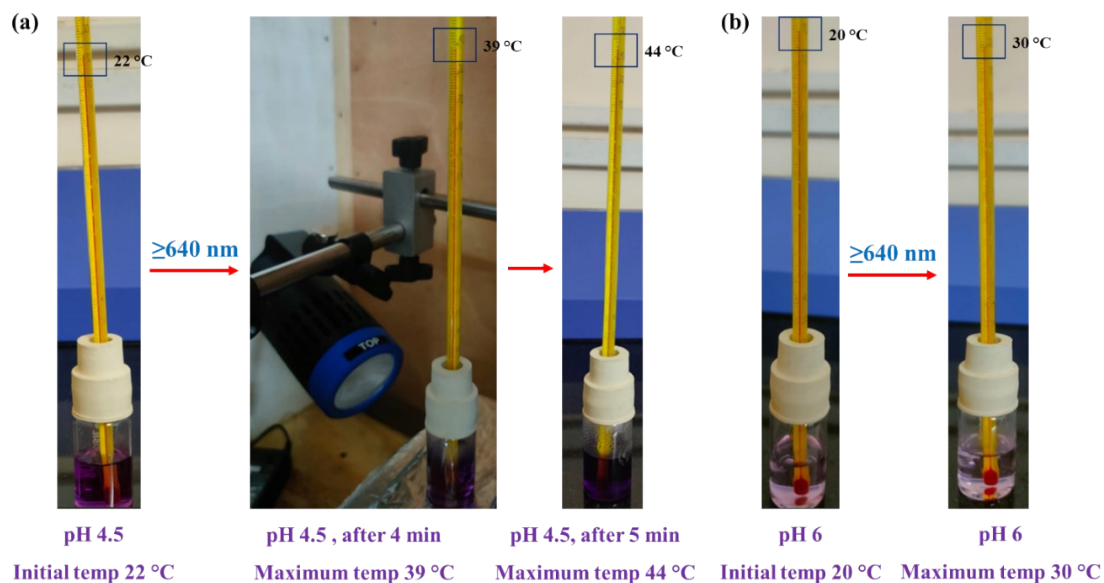


Fig. S13A Photographic image of temperature changes upon light irradiation

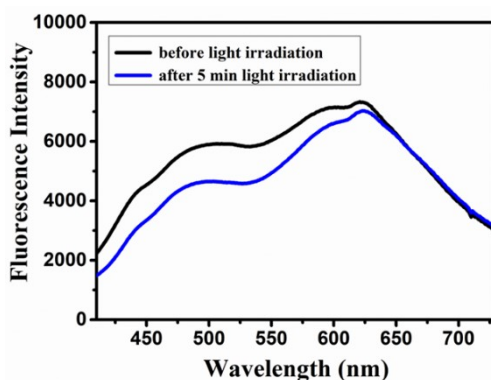


Fig. S13B Emission spectra of photocage 7a (pH 4.5) before and after 5 min of exposure to 640 nm light.

The solutions of 7a, 7b and 7a-OH (40  $\mu$ M) were irradiated by a 640 nm laser at power density (2.0 W  $\text{cm}^{-2}$ ). The temperature changes were monitored by the thermometer. Also, different concentrations of 7a were prepared (5  $\mu$ M, 10  $\mu$ M, 20  $\mu$ M, 30  $\mu$ M, 50  $\mu$ M, 70  $\mu$ M and 100  $\mu$ M) and irradiated by 40.0 W with 660 nm LED for 5 minutes. The temperature changes were monitored during irradiation. When its temperature reached a plateau, at this time point, the laser was shut off. Then the solution was cooled down to room temperature. The

temperature of the solution was recorded at an interval of 15 s during this process. The photothermal conversion efficiency<sup>4-6</sup> of **7a**, **7b** and **7a-OH** were determined according to Equation (3), and the other parameters in equation (3) were calculated from equation (4), (5) and (6).

$$\eta = \frac{hS(T_{Max} - T_{Surr}) - Q_{Dis}}{I(1 - 10^{-A_{640}})} \quad (3)$$

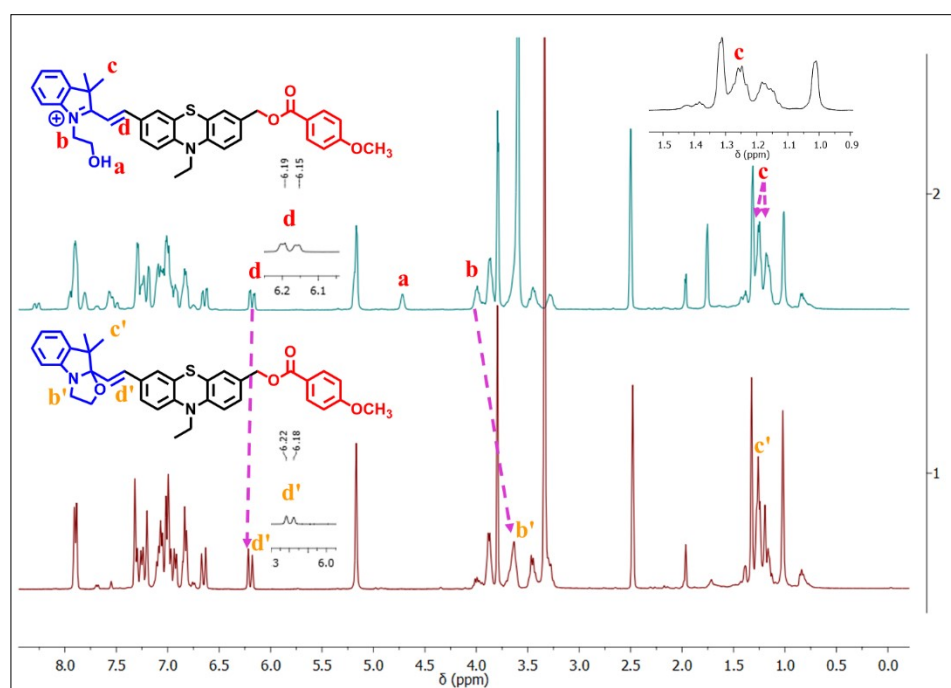
$$\tau_s = \frac{\sum_i m_i C_{p,i}}{hS} \quad (4)$$

$$t = \tau_s(-\ln \theta) \quad (5)$$

$$\theta = \frac{T - T_{Surr}}{T_{Max} - T_{Surr}} \quad (6)$$

In equation (a),  $\eta$  is the photothermal conversion efficiency,  $h$  is the heat transfer coefficient,  $S$  is the surface area of the container.  $Q_{Dis}$  represents heat dissipated from the laser mediated by the solvent and container.  $I$  is the laser power and  $A_{640}$  is the absorbance of the sample at 640 nm. In equation (b),  $m$  is the mass of the solution containing the photoactive material,  $C$  is the specific heat capacity of the solution ( $C_{water} = 4.2 \text{ J g}^{-1}$ ). In equation (c),  $\tau_s$  is the associated time constant. In equation (d),  $\theta$  is a dimensionless parameter, known as the driving force temperature.  $T_{max}$  and  $T_{Surr}$  are the maximum steady state temperature and the environmental temperature, respectively.

## 10. Characterisation of closed form and open form by <sup>1</sup>H NMR study of photocage **7a**:





**Fig. S14**  $^1\text{H}$  NMR spectra of PTZ-Ani (**7a**) in acid ( $\text{DMSO-d}_6 + \text{TFA}$ ) and basic ( $\text{DMSO-d}_6 + \text{NaOH}$  in  $\text{D}_2\text{O}$ ) surrounding.

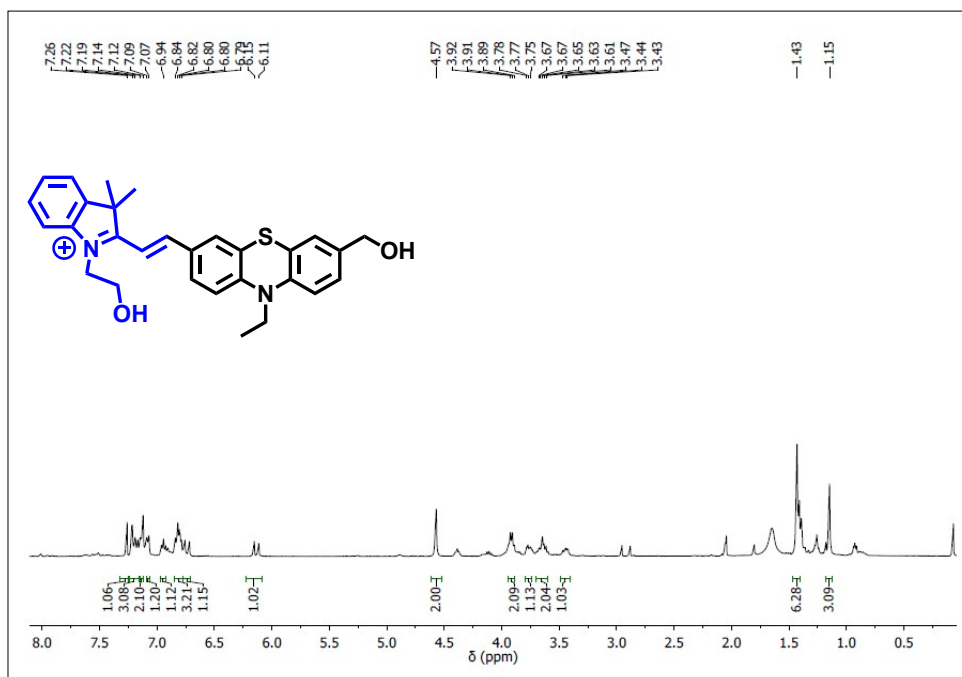
## 11. Characterisation of photoproduct for photolysis of photocage **7a** and **7b**:

The photoproduct was isolated and characterized by  $^1\text{H}$  NMR and HRMS spectroscopy.

### a) Photolysis of **7a** at 595 nm (pH 4.5):

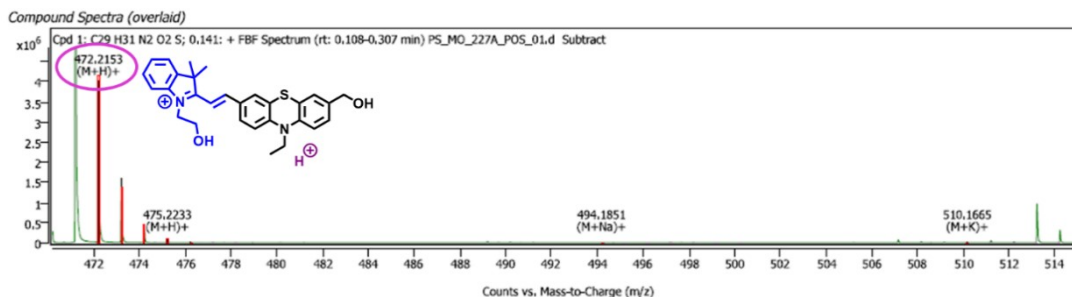
#### i) $^1\text{H}$ NMR of photoproduct **7a-OH**

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.26 (s, 1H), 7.24 – 7.15 (m, 3H), 7.13 (d,  $J = 9.6$  Hz, 2H), 7.08 (d,  $J = 7.1$  Hz, 1H), 6.95 (d,  $J = 7.3$  Hz, 1H), 6.85 – 6.78 (m, 3H), 6.74 (d,  $J = 15.9$  Hz, 1H), 6.13 (d,  $J = 15.9$  Hz, 1H), 4.57 (s, 2H), 3.94 – 3.88 (m, 2H), 3.79 – 3.74 (m, 1H), 3.70 – 3.60 (m, 2H), 3.49 – 3.40 (m, 1H), 1.43 (s, 6H), 1.15 (s, 3H).



**Fig. S15**  $^1\text{H}$  NMR (400 MHz) of photoproduct **7a-OH** in  $\text{CDCl}_3$ .

#### ii) HRMS spectra of photoproduct (**7a-OH**) during photolysis:



**Fig. S16** HRMS spectra of photoproduct **7a-OH** (photolysis in acidic pH).

## b) Photolysis of 7a and 7b at 640 nm (pH 4.5):

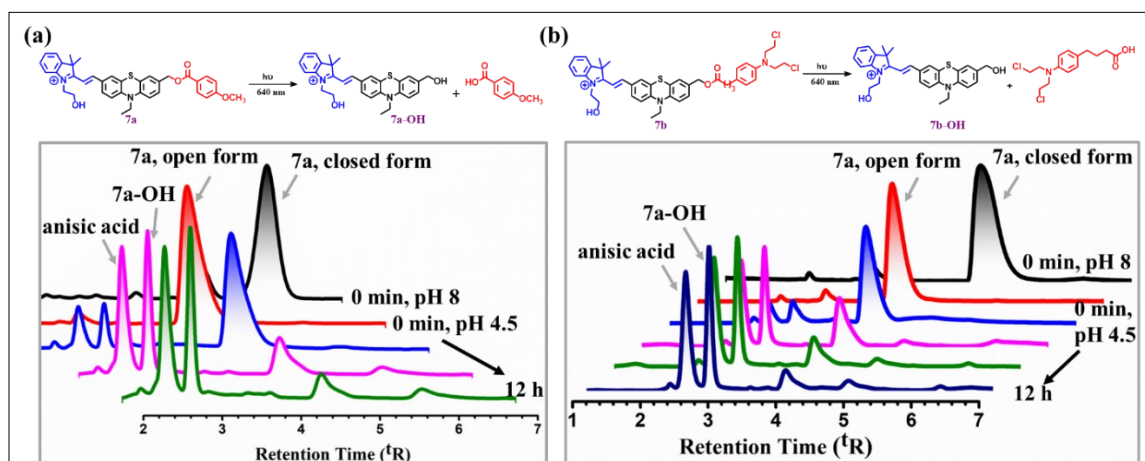


Fig. S17 HPLC diagram of photolysis of (a) PTZ Ani (7a) and (b) PTZ-Cbl (7b) at 640 nm (pH 4.5)

## b) Photolysis of 7b at 595 nm (pH 4.5):

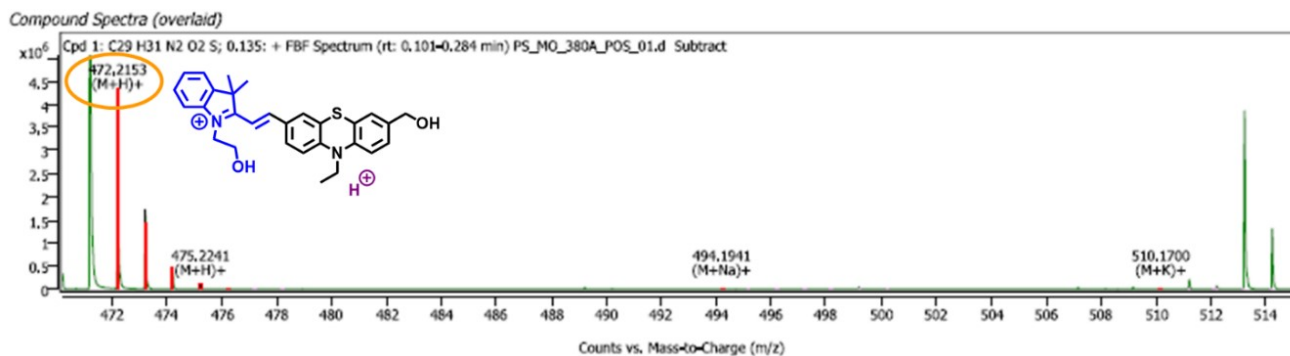


Fig. S18 HRMS spectra of photoproduct 7b-OH (photolysis in acidic pH).

## 12. Photochemical rate constant determination for the photodegradation of 7a and 7b:

A solution of  $1 \times 10^{-4}$  M of all the photocages was prepared in ACN/H<sub>2</sub>O (9:1 v/v). The solution of 6a, 6b, 12a, and 12b were then irradiated using a 125 W medium pressure Hg lamp with 1M CuSO<sub>4</sub> solution as a UV cut-off filter ( $\lambda \geq 365$  nm). On the other hand, the solutions of 18a, 18b1, and 18b3 were irradiated using a 125 W medium-pressure Hg lamp with 1M NaNO<sub>2</sub> solution as a UV cut-off filter ( $\lambda \geq 410$  nm). At regular intervals of time, 25  $\mu$ l of the aliquots were taken and analyzed by RP-HPLC using mobile phase acetonitrile-water at a flow rate of 1 mL/min (detection: UV 254 nm). Peak areas were determined by RP-HPLC, which indicated a gradual decrease of the caged ester with time. The reaction was followed until the consumption of the photocage was less than 10% of the initial area. Based on HPLC data for caged compounds, the natural logarithm of the concentration of caged compound ( $\ln C$ ) (from HPLC peak area) versus irradiation time was plotted. We observed an exponential correlation for the disappearance of the caged compounds, which suggested a first-order reaction.

### 13. Determination of incident photon flux ( $I_0$ ) of the UV lamp by potassium ferrioxalate actinometry and quantum yield calculation:

Potassium ferrioxalate actinometry was used to determine the incident photon flux ( $I_0$ ) of the UV lamp used for irradiation. The solution of potassium ferrioxalate, 1, 10-phenanthroline, and the buffer solution was prepared following the literature procedure.<sup>7</sup>

Degassed solution (0.006 M) of potassium ferrioxalate was irradiated using a 125 W medium-pressure Hg lamp as the visible light source ( $\geq 410$  nm) and 1M  $\text{NaNO}_2$  solution as a UV cut-off filter. At a regular interval of time (3 min), 1 ml of the aliquots was taken out, and to it, 3 ml of 1,10 phenanthroline solution and 2 ml of the sodium acetate buffer solution were added, and the whole solution was kept in the dark for 30 min. The absorbance of the red phenanthroline-ferrous complex formed was then measured spectrophotometrically at 510 nm. The amount of  $\text{Fe}^{2+}$  ions was determined from the calibration graph. The calibration graph was plotted by measuring the absorbance of the phenanthroline-ferrous complex at several known concentrations of  $\text{Fe}^{2+}$  ions in the dark. From the slope of the graph, the **molar absorptivity** of the phenanthroline-ferrous complex was calculated to be  $1.11 \times 10^4 \text{ M}^{-1} \text{ cm}^{-1}$  at 510 nm, which is found to be similar to the reported value.<sup>8</sup> Using the known **quantum yield**<sup>7</sup> ( $1.188 \pm 0.005$ ) for potassium ferrioxalate actinometer at 406.7 nm, the number of  $\text{Fe}^{2+}$  ions formed during photolysis and the fraction of light absorbed by the actinometer, the incident photon flux ( $I_0$ ) at 410 nm of the 125W Hg lamp was determined as  $2.886 \times 10^{16} \text{ photons s}^{-1} \text{ cm}^{-2}$ .

$$\Phi_{\text{act}} = k_{\text{act}} / [(I_0 / N_A) \times F] \quad (7)$$

Where  $k$  is the rate of reaction;  $I_0$  is photon flux;  $F$  is the fraction of light absorbed (molar absorptivity);  $N_A$  is Avogadro's no. We calculated the rate of reaction of the actinometer ( $k_{\text{act}}$ ), and then, from the above equation, we calculated the photochemical quantum yield by putting the value of  $k_{\text{act}}$ .

Further, the quantum yield for the photolysis of caged esters was calculated using equation (8).

$$(\Phi_p)_{\text{CG}} = (\Phi_p)_{\text{act}} \frac{(k_p)_{\text{CG}}}{(k_p)_{\text{act}}} \frac{(F_{\text{act}})}{(F_{\text{CG}})} \quad (8)$$

Where the subscript 'CG' and 'act' denote caged ester and actinometer, respectively. Potassium ferrioxalate was used as an actinometer.  $\Phi_p$  is the photolysis quantum yield,  $k_p$  is the photolysis rate constant, and  $F$  is the fraction of light absorbed.

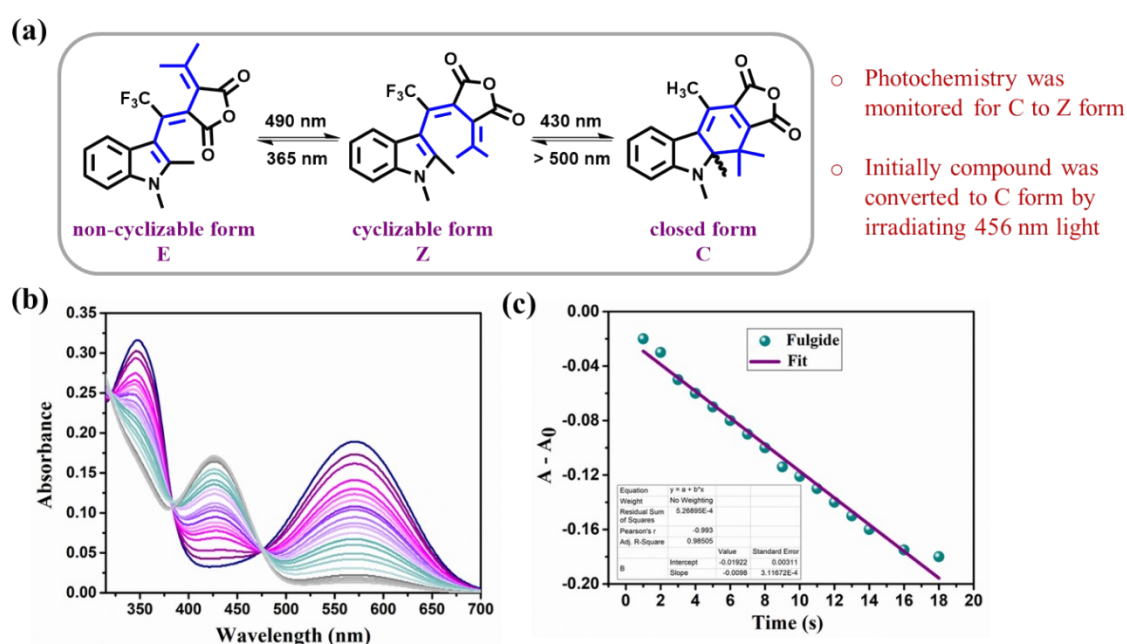
### 14. Determination of Photon Flux ( $I_0$ ) of the 595 nm LED light:

To determine the photon flux of the incident light source, indolyfulgide-based chemical actinometry was used. A fresh solution of compound indolyfulgide (3 ml,  $1 \times 10^{-3}$  M) was prepared in toluene and taken in a fluorescence cuvette (equipped with a stir bar). Then, 456 nm light irradiation was done to convert Z completely to C; as we have seen, the compound is already in the Z-isomeric form (checked with UV-Vis

spectrophotometer). Further, change in the absorption spectra was monitored (**Fig. S22**) with an increase in the light irradiation time. The photon flux was calculated for the conversion of **C** to **Z**, using **equation 9**, and was used to calculate photochemical-quantum yield.

$$I_0 = \frac{\Delta A V}{t \epsilon d \Phi} \quad (9)$$

Where  $I_0$  is the photon flux of the incident light ( $\text{Photon s}^{-1}\text{cm}^{-2}$ ),  $\Delta A$  is the absorbance decrease of the closed form **C** in time  $t$ ,  $V$  is the sample volume in  $\text{dm}^3$ ,  $\epsilon$  is the molar absorption coefficient of **C** at the wavelength used to monitor the photoreaction in  $\text{M}^{-1}\text{cm}^{-1}$ ,  $d$  is the optical pathway in  $\text{cm}$ , and  $\Phi$  is the quantum yield of the reaction.



**Fig. S19** (a) Working principle of fulgide actinometry, (b) change in the UV-vis spectrometry of the fulgide under red light ( $595 \pm 10 \text{ nm}$ ), (c) plot of  $(A - A_0)$  vs. time.

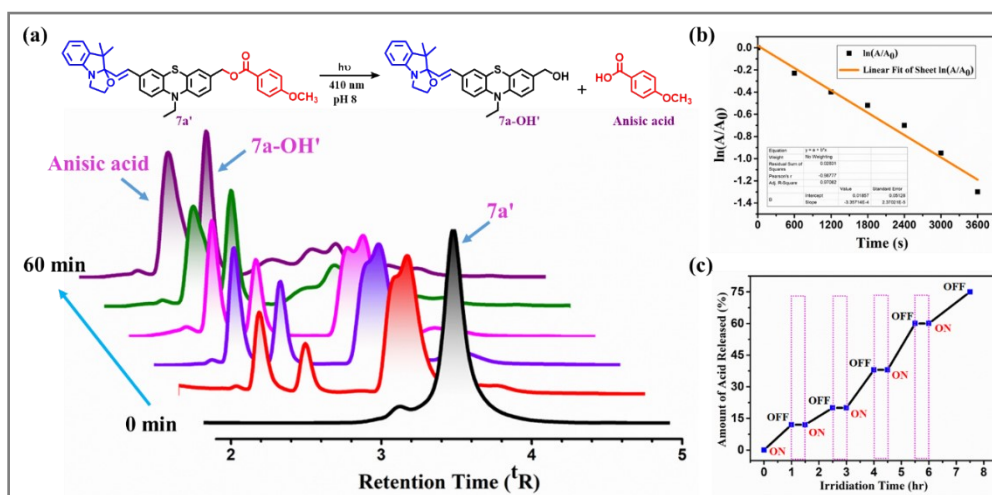
**Table S1: Calculated Photon Flux of the Light Sources:**

Incident Light	Slope ( $\Delta A/t$ )	Sample Volume ( $\text{cm}^3$ )	Photon Flux ( $\text{Photon s}^{-1}\text{cm}^{-2}$ )
$595 \pm 10 \text{ nm}$	$0.0098 \pm 0.0031$	3	$1.45 \times 10^{14}$

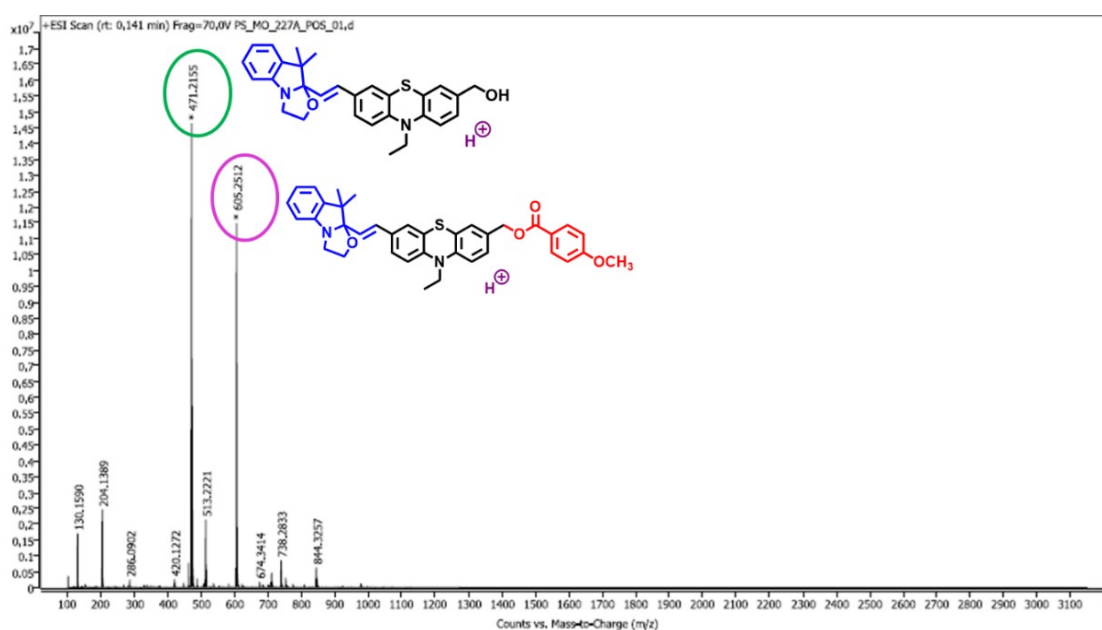
Footnote: estimated error limits were within  $\pm 10 \%$

## 15. Characterisation of photoproduct for photolysis of photocage 7a and 7b in pH 8:

### a) Photolysis of 7a at 410 nm (pH 8):



**Fig. S20** (a) HPLC diagram of photolysis of **7a** in basic pH, (b) rate of release from **7a** in basic pH, and (c) temporal control over the photouncaging of **7a**. “On” (switching on of light source) and “Off” (switching off of light source).



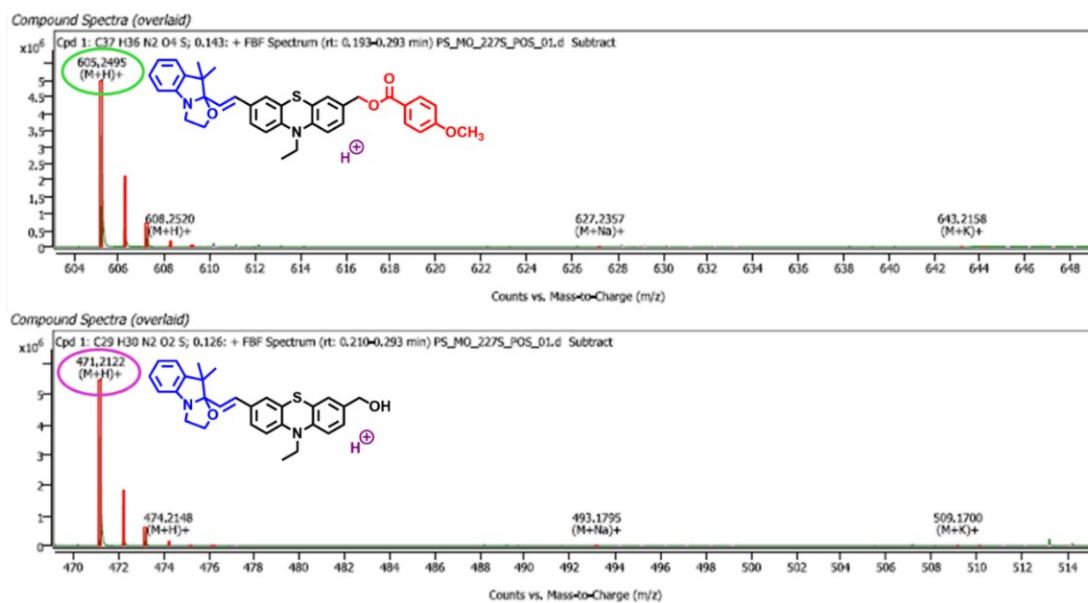
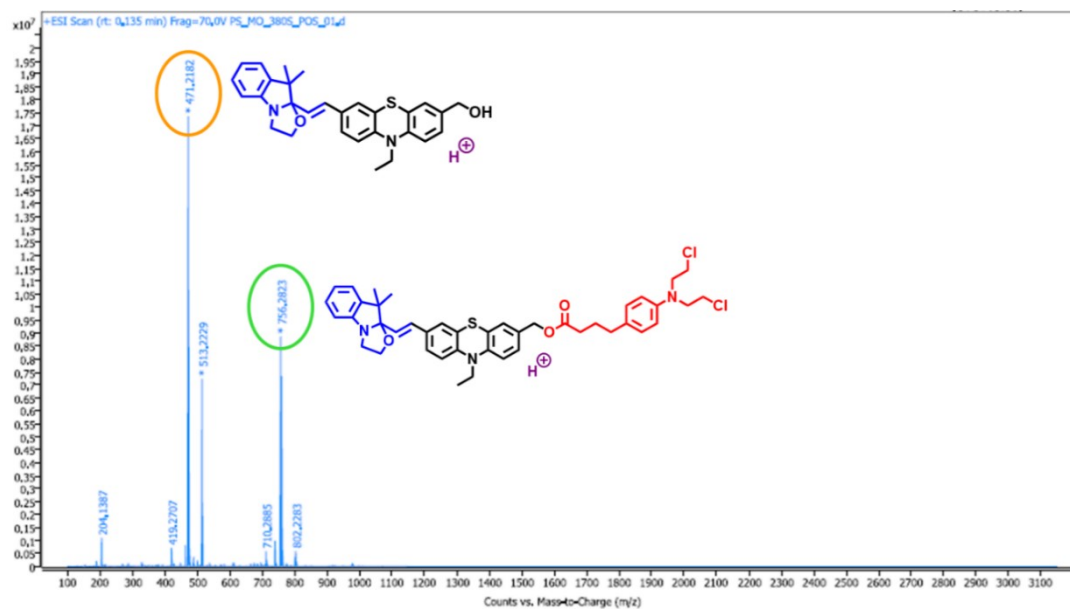


Fig. S21 HRMS spectra of photocage **7a** and its photoproduct (photolysis in basic pH).

b) Photolysis of **7b** at 410 nm (pH 8): HRMS analysis of photolysis mixture



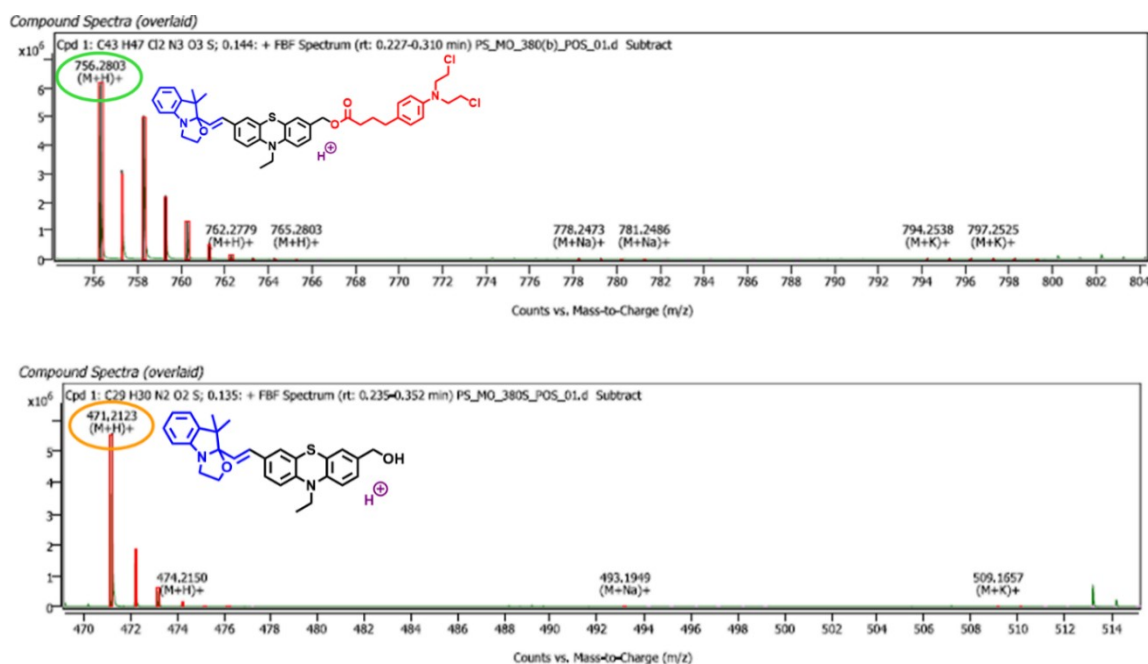
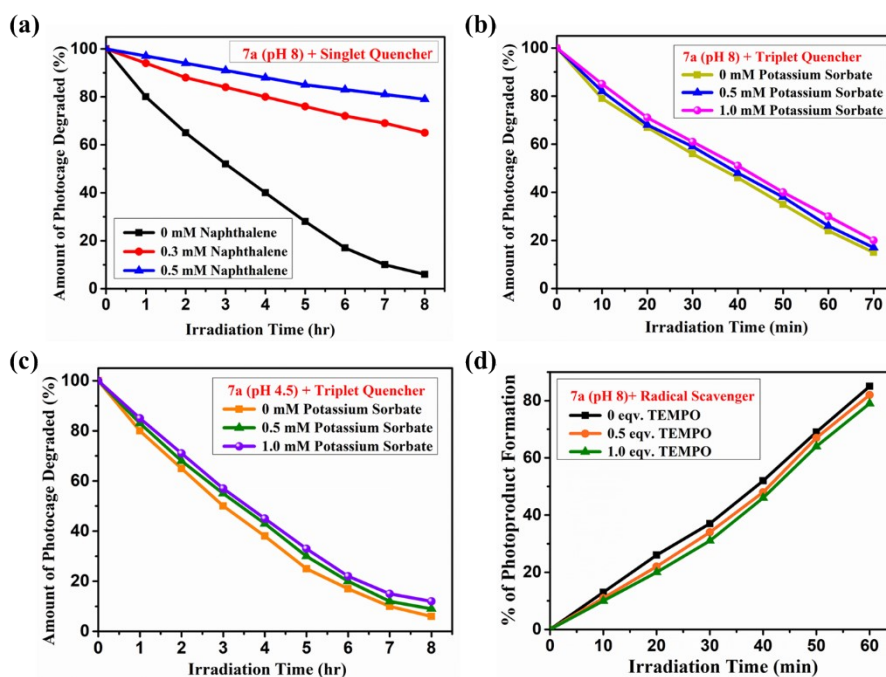


Fig. S22 HRMS spectra of photocage **7b** and its photoproduct (photolysis in basic pH).

## 16. Photorelease study of **7a** (in both the pH 4.5 and pH 8) in the presence of singlet quencher, triplet quencher and TEMPO:

To investigate the photorelease mechanism (whether it goes through singlet or triplet excited state) of phenothiazine photocage, we have done the photolysis of ( $1 \times 10^{-4}$  M) caged ester **7a** (pH 8) in the presence and absence of 0.5 mM singlet quencher (naphthalene) and the course of photolysis was monitored by HPLC. We observed (Fig. S21a) that photolysis is quenched in the presence of naphthalene. On the other hand, we observed that there is no change in photolysis of **7a** (in both pH 8 and pH 4.5) in the presence of 0.5 mM triplet quencher (potassium sorbate) (Fig. S21b, S21c). Hence, the photocleavage reaction of our phenothiazine photocage proceeds through a singlet excited state. Next, to know the excited state chemistry (whether it goes by a radical pair or by a solvent-separated ion pair), we conducted photolysis of photocage **7a** ( $1 \times 10^{-4}$  M conc. of acetonitrile/buffer (9:1 v/v)) in the presence of various concentrations of the radical scavenger TEMPO (2,2,6,6-Tetramethyl-1-piperidinyloxy) at pH 4.5 and pH 8 (Fig. S21d). The photodecomposition was monitored using RP-HPLC and HRMS analysis. No TEMPO-adduct photoproduct was detected in the HRMS, and there was no significant change in the rate of photodissociation in the presence or absence of TEMPO. The absence of the TEMPO-adduct photoproduct indicates the formation of a solvent-separated ion pair, leading to the formation of a solvent-captured photoproduct.





**Fig. S23** Photorelease study of photocage **7a** (pH 8,  $\lambda \geq 410$ ) in the presence of (a) singlet quencher, (b) triplet quencher, (c) photolysis of **7a** (pH 4.5,  $\lambda \geq 595$ ) in the presence of triplet quencher, (d) photorelease study of **7a** (pH 8,  $\lambda \geq 410$ ) in the presence of radical scavenger.

### 17. Hydrolytic stability of the PTZ-Cbl (**7b**) and nano-DDS (nano-PTZ-Cbl) under dark:

**Table S2.** Hydrolytic stability of nano-DDS under dark.

the photocage **7b** (pH 4.5), and

Caged esters	% of depleted
<b>7b</b>	8
<b>Nano-DDS</b>	10

### 18. Computational Data:

Geometry optimizations **7a** were performed at the ground state ( $S_0$ ) level using the B3LYP<sup>9-12</sup> functional and the def2-TZVP<sup>13</sup> basis set. The optimization was carried out using the RIJCOSX<sup>14</sup> approximation and the D3BJ<sup>15-16</sup> dispersion correction. The starting geometry for the optimization was obtained from the crystal structure of the compounds. All calculations were performed using the ORCA 5.0.3<sup>17</sup> software package. The optimized geometries were confirmed to be minima by verifying that no negative frequencies were present in the vibrational frequency calculations. Table S3 contains the HOMO-LUMO energies. We performed a transition state (TS) search by scanning the potential energy surface for **7a** along the coordinates up to the dissociation limit with the



difference in barrier height. The geometry corresponding to the highest energy point was optimized and subsequently confirmed using an Intrinsic Reaction Coordinate (IRC) calculation. The electron energies for **7a** were carried out using TDDFT<sup>18-20</sup> (Time-Dependent Density Functional Theory) and the CAM-B3LYP<sup>21</sup> functional with the def2-TZVP basis set at the S<sub>0</sub> geometry shown in Table 2.

**Table S3.** HOMO-LUMO energies were calculated using B3LYP/def2-TZVP at the optimized S<sub>0</sub> geometries for compounds **7a** (closed and open).

<b>7a</b>	<b>HOMO (eV)</b>	<b>LUMO (eV)</b>	<b>E<sub>H-L</sub> (eV)</b>
<b>Closed</b>	-5.15	-1.32	3.83
<b>Open</b>	-7.63	-5.64	1.99

**Table S4.** Singlet and triplet excitation energies calculated using CAM-B3LYP/def2-TZVP level for **7a**. Values in parentheses for singlet states indicate oscillator strength.

<b>State</b>	<b>7a (closed)</b>		<b>7a (open)</b>	
	<b>Singlet (eV)</b>	<b>Triplet (eV)</b>	<b>Singlet (eV)</b>	<b>Triplet (eV)</b>
1	3.419 (f=0.141)	2.749	1.900 (f=0.49)	1.137
2	3.457 (f=0.013)	3.377	2.026 (f=0.010)	2.020
3	3.932 (f=0.022)	3.441	2.687 (f=0.67)	2.190
4	3.950 (f=0.013)	3.459	2.870 (f=0.005)	2.491
5	3.992 (f=0.094)	3.602	3.128 (f=0.50)	2.869

## 19. Coordinates:

### i) Optimized Structure for Compound **7a** (closed form)

80

XYZ file generated by orca\_plot on BaseName=opt

```
C 3.756203 1.156247 0.406985
C 3.626496 0.175286 -0.582328
C 2.498880 -0.623752 -0.660984
```

C	1.458431	-0.500892	0.266982
C	1.581332	0.480718	1.258728
C	2.697881	1.301361	1.309912
N	0.310753	-1.312532	0.226699
C	-0.941459	-0.702384	0.445943
C	-1.072421	0.255916	1.463029
S	0.320750	0.613187	2.492438
C	-2.072223	-1.009089	-0.311760
C	-3.300703	-0.415217	-0.043396
C	-3.423264	0.533047	0.964090
C	-2.291619	0.872493	1.702329
C	0.371423	-2.596822	-0.464317
C	1.393739	-3.542386	0.157690
C	-4.725820	1.240790	1.242449
O	-5.835260	0.482812	0.746075
C	-6.510211	0.869674	-0.375800
C	-6.894341	2.298964	-0.492578
O	-6.820728	0.037510	-1.187615
C	-7.088421	2.838990	-1.769641
C	-7.509185	4.142126	-1.927292
C	-7.772425	4.935335	-0.804184
C	-7.603278	4.402846	0.475205
C	-7.159181	3.094915	0.618688
C	4.917597	2.035329	0.534288
C	6.014083	2.037770	-0.223514
C	7.146580	3.007228	-0.045781
O	7.076028	3.643786	1.241604
N	8.449431	2.319488	-0.042468
C	8.603389	1.835493	1.327695
C	7.870989	2.903670	2.169790
C	9.394207	3.251056	-0.527614
C	7.266426	4.103119	-1.160700

C	8.765437	4.317048	-1.173036
C	6.451390	5.349253	-0.823566
C	6.829516	3.550882	-2.529467
C	9.516976	5.324818	-1.746453
C	10.910287	5.268149	-1.667934
C	11.528336	4.201836	-1.024141
C	10.777627	3.178012	-0.446588
O	-8.190009	6.197840	-1.056959
C	-8.488677	7.049599	0.039764
H	4.409707	0.039393	-1.316117
H	2.428398	-1.354022	-1.453873
H	2.754294	2.062594	2.078666
H	-2.004367	-1.717133	-1.124873
H	-4.166747	-0.698156	-0.625470
H	-2.355554	1.614156	2.490609
H	0.559093	-2.470277	-1.538379
H	-0.612304	-3.050324	-0.373580
H	2.407655	-3.148929	0.105518
H	1.374381	-4.499849	-0.366217
H	1.152483	-3.715825	1.207076
H	-4.718885	2.235338	0.792435
H	-4.871936	1.361338	2.317811
H	-6.906312	2.213278	-2.632758
H	-7.652369	4.572322	-2.909329
H	-7.818318	4.989769	1.355312
H	-7.045785	2.684497	1.613107
H	4.866258	2.765025	1.335472
H	6.137660	1.336827	-1.039417
H	9.653529	1.734252	1.589488
H	8.124197	0.861591	1.424360
H	8.564219	3.599445	2.646436
H	7.234992	2.452541	2.935345

H	6.785447	5.797712	0.108581
H	5.393186	5.097021	-0.728100
H	6.547827	6.084958	-1.624344
H	7.370219	2.638023	-2.782691
H	7.044431	4.291251	-3.301096
H	5.758843	3.340777	-2.545145
H	9.033417	6.156533	-2.244609
H	11.509585	6.054173	-2.108329
H	12.608890	4.162492	-0.967939
H	11.268040	2.347826	0.045198
H	-8.797488	7.996885	-0.394708
H	-7.609116	7.207363	0.669925
H	-9.303501	6.643654	0.645561

ii) **Scanning Compound 7a (closed form) Up to the Dissociation Limit**

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Coordinates from ORCA-job neb\_MEP E -2237.754660567702

C	2.244215	-0.972378	0.515908
C	2.114508	-1.953339	-0.473405
C	0.986892	-2.752377	-0.552061
C	-0.053557	-2.629517	0.375905
C	0.069344	-1.647907	1.367651
C	1.185893	-0.827264	1.418835
N	-1.201235	-3.441157	0.335622
C	-2.453447	-2.831009	0.554866
C	-2.584409	-1.872709	1.571952
S	-1.191238	-1.515438	2.601361
C	-3.584211	-3.137714	-0.202837
C	-4.812691	-2.543842	0.065527
C	-4.935252	-1.595578	1.073013
C	-3.803607	-1.256132	1.811252
C	-1.140565	-4.725447	-0.355394

C	-0.118249	-5.671011	0.266613
C	-6.237808	-0.887835	1.351372
O	-7.347248	-1.645813	0.854998
C	-8.022199	-1.258951	-0.266877
C	-8.406329	0.170339	-0.383655
O	-8.332716	-2.091115	-1.078692
C	-8.600409	0.710365	-1.660718
C	-9.021173	2.013501	-1.818369
C	-9.284413	2.806710	-0.695261
C	-9.115266	2.274221	0.584128
C	-8.671169	0.966290	0.727611
C	3.405609	-0.093296	0.643211
C	4.502095	-0.090855	-0.114591
C	5.634592	0.878603	0.063142
O	5.564040	1.515161	1.350527
N	6.937443	0.190863	0.066455
C	7.091401	-0.293132	1.436618
C	6.359001	0.775045	2.278713
C	7.882219	1.122431	-0.418691
C	5.754438	1.974494	-1.051777
C	7.253449	2.188423	-1.064113
C	4.939402	3.220628	-0.714643
C	5.317528	1.422257	-2.420544
C	8.004988	3.196193	-1.637530
C	9.398299	3.139524	-1.559011
C	10.016348	2.073211	-0.915218
C	9.265639	1.049387	-0.337665
O	-9.701997	4.069215	-0.948036
C	-10.000665	4.920974	0.148687
H	2.897719	-2.089232	-1.207194
H	0.916410	-3.482647	-1.344950
H	1.242306	-0.066031	2.187589

H	-3.516355	-3.845758	-1.015950
H	-5.678735	-2.826781	-0.516547
H	-3.867542	-0.514469	2.599532
H	-0.952895	-4.598902	-1.429456
H	-2.124292	-5.178949	-0.264657
H	0.895667	-5.277554	0.214441
H	-0.137607	-6.628474	-0.257294
H	-0.359505	-5.844450	1.315999
H	-6.230873	0.106713	0.901358
H	-6.383924	-0.767287	2.426734
H	-8.418300	0.084653	-2.523835
H	-9.164357	2.443697	-2.800406
H	-9.330306	2.861144	1.464235
H	-8.557773	0.555872	1.722030
H	3.354270	0.636400	1.444395
H	4.625672	-0.791798	-0.930494
H	8.141541	-0.394373	1.698411
H	6.612209	-1.267034	1.533283
H	7.052231	1.470820	2.755359
H	5.723004	0.323916	3.044268
H	5.273459	3.669087	0.217504
H	3.881198	2.968396	-0.619177
H	5.035839	3.956333	-1.515421
H	5.858231	0.509398	-2.673768
H	5.532443	2.162626	-3.192173
H	4.246855	1.212152	-2.436222
H	7.521429	4.027908	-2.135686
H	9.997597	3.925548	-1.999406
H	11.096902	2.033867	-0.859016
H	9.756052	0.219201	0.154121
H	-10.309476	5.868260	-0.285785
H	-9.121104	5.078738	0.778848

H	-10.815489	4.515029	0.754484
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Coordinates from ORCA-job neb\_MEP E -2237.759243270616

C	2.311075	-0.909082	0.483750
C	2.169587	-1.889725	-0.515306
C	1.018017	-2.665398	-0.611046
C	-0.038484	-2.520483	0.308164
C	0.094961	-1.534353	1.306799
C	1.237457	-0.738356	1.377162
N	-1.201567	-3.310894	0.244016
C	-2.455127	-2.711256	0.491542
C	-2.579856	-1.742400	1.510831
S	-1.175675	-1.382838	2.542939
C	-3.603924	-3.032517	-0.248875
C	-4.840987	-2.450423	0.040765
C	-4.955310	-1.489229	1.048698
C	-3.807408	-1.132460	1.769026
C	-1.136731	-4.625544	-0.388822
C	-0.144026	-5.560752	0.300468
C	-6.269720	-0.801443	1.346963
O	-7.375742	-1.570860	0.881576
C	-8.028036	-1.247095	-0.274767
C	-8.578754	0.132338	-0.373399
O	-8.175725	-2.082555	-1.131730
C	-8.915139	0.630774	-1.647371
C	-9.462144	1.895300	-1.791771
C	-9.705332	2.695634	-0.657829
C	-9.401403	2.198268	0.620963
C	-8.841580	0.926183	0.751008
C	3.500535	-0.062347	0.627884
C	4.612918	-0.092042	-0.123147
C	5.774090	0.848252	0.069943

O	5.701828	1.480174	1.356984
N	7.057566	0.127530	0.087514
C	7.178934	-0.359684	1.457607
C	6.509325	0.764703	2.284007
C	8.035823	1.021809	-0.399986
C	5.931746	1.945698	-1.044501
C	7.441312	2.115023	-1.051017
C	5.154556	3.216027	-0.694137
C	5.482087	1.412701	-2.419521
C	8.231209	3.105367	-1.621383
C	9.629196	3.005098	-1.535210
C	10.213374	1.913887	-0.885082
C	9.424104	0.907169	-0.310559
O	-10.232494	3.915190	-0.895411
C	-10.485607	4.783695	0.188594
H	2.967185	-2.044504	-1.244667
H	0.939739	-3.398904	-1.413636
H	1.302737	0.024588	2.157224
H	-3.541772	-3.751034	-1.066606
H	-5.723780	-2.747249	-0.528150
H	-3.864223	-0.382677	2.563678
H	-0.917002	-4.546230	-1.471333
H	-2.137651	-5.067712	-0.313048
H	0.889735	-5.191859	0.238894
H	-0.178363	-6.556509	-0.169228
H	-0.401956	-5.666322	1.365413
H	-6.282881	0.203656	0.890862
H	-6.391849	-0.668219	2.434514
H	-8.735522	-0.002951	-2.517856
H	-9.718151	2.299222	-2.773005
H	-9.601768	2.787760	1.515140
H	-8.628857	0.538957	1.749136



H	3.468523	0.675166	1.436183
H	4.726477	-0.803594	-0.944365
H	8.228047	-0.532615	1.729516
H	6.630830	-1.308228	1.559709
H	7.255067	1.457957	2.709179
H	5.891605	0.364310	3.106069
H	5.505321	3.642403	0.253705
H	4.079562	2.994109	-0.597951
H	5.273601	3.966652	-1.491497
H	5.998394	0.474940	-2.674793
H	5.727943	2.152434	-3.196498
H	4.395585	1.236005	-2.443627
H	7.770869	3.959171	-2.126077
H	10.260440	3.780749	-1.975126
H	11.302205	1.840179	-0.821233
H	9.888953	0.054987	0.190229
H	-10.889469	5.709541	-0.241432
H	-9.561329	5.018064	0.746173
H	-11.227178	4.358669	0.888174

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Coordinates from ORCA-job neb\_MEP E -2237.758939839267

C	2.366310	-0.818252	0.460129
C	2.220123	-1.803491	-0.533529
C	1.053386	-2.553307	-0.643811
C	-0.015518	-2.377353	0.255153
C	0.119843	-1.382625	1.244928
C	1.279098	-0.611967	1.329293
N	-1.188203	-3.151485	0.180207
C	-2.437950	-2.541546	0.416621
C	-2.564125	-1.562982	1.425808
S	-1.164998	-1.192359	2.460817
C	-3.585435	-2.869186	-0.324036

C	-4.823792	-2.291156	-0.037093
C	-4.942296	-1.325662	0.966953
C	-3.794943	-0.956595	1.680950
C	-1.128868	-4.477476	-0.429574
C	-0.163842	-5.414471	0.295675
C	-6.265764	-0.656041	1.261976
O	-7.356117	-1.511788	0.922269
C	-8.110796	-1.281575	-0.192641
C	-8.746308	0.059342	-0.307161
O	-8.272817	-2.163375	-0.999043
C	-9.197880	0.483453	-1.572155
C	-9.832897	1.705082	-1.724537
C	-10.052869	2.533102	-0.605779
C	-9.629043	2.110125	0.665547
C	-8.979622	0.882339	0.802532
C	3.578675	-0.007901	0.622425
C	4.700373	-0.081353	-0.111386
C	5.893501	0.815180	0.090131
O	5.841747	1.441683	1.381075
N	7.149711	0.048088	0.103908
C	7.253440	-0.448590	1.472035
C	6.632214	0.699773	2.302249
C	8.159971	0.907682	-0.380654
C	6.091280	1.911654	-1.018862
C	7.605879	2.025841	-1.024858
C	5.360101	3.207229	-0.663133
C	5.623181	1.401222	-2.396407
C	8.431568	2.989120	-1.590816
C	9.824914	2.835824	-1.507862
C	10.368763	1.719517	-0.865343
C	9.543050	0.740052	-0.294938
O	-10.679354	3.703577	-0.848822

C	-10.930602	4.589020	0.221915
H	3.027776	-1.984772	-1.245341
H	0.973683	-3.293552	-1.439995
H	1.347658	0.156442	2.103778
H	-3.520644	-3.593268	-1.136530
H	-5.706272	-2.601615	-0.599463
H	-3.855243	-0.203218	2.471880
H	-0.885806	-4.418580	-1.508172
H	-2.136854	-4.905022	-0.367859
H	0.875856	-5.060180	0.250679
H	-0.201729	-6.417151	-0.158768
H	-0.446224	-5.499346	1.356266
H	-6.343931	0.296872	0.710034
H	-6.341891	-0.418865	2.335812
H	-9.037761	-0.173687	-2.428961
H	-10.179552	2.052173	-2.699651
H	-9.805333	2.722732	1.549168
H	-8.672727	0.550992	1.796224
H	3.559056	0.732908	1.428083
H	4.798646	-0.800433	-0.927938
H	8.294856	-0.666028	1.741641
H	6.666181	-1.373780	1.571368
H	7.407387	1.365993	2.718171
H	6.008386	0.323885	3.131071
H	5.724068	3.616153	0.287495
H	4.277490	3.024154	-0.569963
H	5.507580	3.957067	-1.456456
H	6.106264	0.447079	-2.655710
H	5.895152	2.135480	-3.169846
H	4.531184	1.262917	-2.420862
H	8.002607	3.862325	-2.090006
H	10.484120	3.589781	-1.944437

H	11.454148	1.604297	-0.804472
H	9.976119	-0.132116	0.199903
H	-11.436569	5.463180	-0.208289
H	-9.993968	4.916858	0.707223
H	-11.586802	4.131958	0.983768

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Coordinates from ORCA-job neb\_MEP E -2237.758466605143

C	2.420063	-0.729463	0.430706
C	2.267629	-1.720296	-0.556339
C	1.085509	-2.442739	-0.680576
C	0.005394	-2.233033	0.197290
C	0.145002	-1.229395	1.177404
C	1.321269	-0.485924	1.275475
N	-1.178337	-2.988249	0.111689
C	-2.422826	-2.365075	0.336493
C	-2.548006	-1.375636	1.334450
S	-1.152846	-0.996901	2.371995
C	-3.569769	-2.695915	-0.404789
C	-4.807665	-2.117255	-0.122086
C	-4.927987	-1.145960	0.877081
C	-3.780291	-0.768532	1.585233
C	-1.127607	-4.327718	-0.469491
C	-0.194353	-5.264482	0.296640
C	-6.259184	-0.493867	1.173526
O	-7.328478	-1.420333	0.970263
C	-8.161034	-1.297446	-0.105771
C	-8.890786	-0.007579	-0.238541
O	-8.310989	-2.226011	-0.860079
C	-9.453465	0.325894	-1.486060
C	-10.181584	1.493720	-1.644374
C	-10.386457	2.354514	-0.547611
C	-9.847044	2.022374	0.706796

C	-9.103719	0.849889	0.848694
C	3.653888	0.044357	0.610986
C	4.782987	-0.069962	-0.105966
C	6.006043	0.781877	0.108088
O	5.971098	1.400125	1.403583
N	7.233165	-0.031046	0.120045
C	7.316328	-0.537974	1.485772
C	6.739526	0.629772	2.320260
C	8.275765	0.791730	-0.359586
C	6.247671	1.877890	-0.993009
C	7.765397	1.934398	-0.996725
C	5.565928	3.198157	-0.630306
C	5.762406	1.394808	-2.374470
C	8.627506	2.868834	-1.556783
C	10.013882	2.661102	-1.475851
C	10.514173	1.520163	-0.841132
C	9.651369	0.569854	-0.276295
O	-11.113887	3.464642	-0.792769
C	-11.372948	4.366976	0.261724
H	3.084040	-1.929955	-1.250026
H	1.003082	-3.190446	-1.469445
H	1.394501	0.288213	2.043903
H	-3.504266	-3.426509	-1.211317
H	-5.690129	-2.437740	-0.679140
H	-3.841876	-0.010834	2.371829
H	-0.859562	-4.294725	-1.543018
H	-2.143359	-4.737935	-0.422267
H	0.851584	-4.927186	0.268046
H	-0.238124	-6.275820	-0.137684
H	-0.502081	-5.322510	1.351990
H	-6.406399	0.395994	0.536759
H	-6.292914	-0.155564	2.221926

H	-9.304871	-0.358204	-2.323747
H	-10.616306	1.770794	-2.606498
H	-10.005963	2.662458	1.573978
H	-8.705575	0.586894	1.830356
H	3.646652	0.786840	1.415341
H	4.866847	-0.793934	-0.919755
H	8.348276	-0.796991	1.755188
H	6.693294	-1.440077	1.580289
H	7.540172	1.267349	2.733042
H	6.106675	0.275159	3.151466
H	5.942081	3.586732	0.324186
H	4.476676	3.056754	-0.541858
H	5.745137	3.946775	-1.418185
H	6.209460	0.424961	-2.639969
H	6.062489	2.123688	-3.142590
H	4.666037	1.297647	-2.400089
H	8.231733	3.760720	-2.050348
H	10.701707	3.391572	-1.908145
H	11.594293	1.362269	-0.782358
H	10.050469	-0.321736	0.212446
H	-11.979860	5.177181	-0.162827
H	-10.439933	4.792330	0.672457
H	-11.936721	3.885551	1.080485

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Coordinates from ORCA-job neb\_MEP E -2237.757858026894

C	2.471558	-0.637680	0.403171
C	2.312978	-1.637479	-0.573703
C	1.116131	-2.332028	-0.710836
C	0.025479	-2.084398	0.143494
C	0.168947	-1.067705	1.109465
C	1.361958	-0.352487	1.220580
N	-1.168878	-2.820621	0.049175

C	-2.407598	-2.181734	0.255838
C	-2.533081	-1.176587	1.237341
S	-1.143189	-0.785201	2.277621
C	-3.551705	-2.517932	-0.488155
C	-4.789262	-1.936567	-0.215560
C	-4.913222	-0.955797	0.774418
C	-3.766986	-0.566767	1.477851
C	-1.128263	-4.175109	-0.497593
C	-0.228717	-5.107401	0.312978
C	-6.254996	-0.327061	1.070600
O	-7.289899	-1.311365	0.981317
C	-8.180857	-1.288268	-0.054120
C	-9.011184	-0.061590	-0.186648
O	-8.298511	-2.250163	-0.771711
C	-9.681762	0.173733	-1.402894
C	-10.508505	1.274820	-1.553204
C	-10.706730	2.163441	-0.477450
C	-10.056261	1.929880	0.746093
C	-9.214363	0.824761	0.878943
C	3.725863	0.098607	0.600601
C	4.859647	-0.056310	-0.101148
C	6.111674	0.748388	0.125660
O	6.093226	1.357967	1.425509
N	7.306688	-0.111240	0.136090
C	7.368851	-0.626221	1.499895
C	6.839596	0.560792	2.337682
C	8.381446	0.670879	-0.340059
C	6.399122	1.841862	-0.967522
C	7.917771	1.836930	-0.970417
C	5.771270	3.186395	-0.596514
C	5.895266	1.389177	-2.352533
C	8.816668	2.738948	-1.525826

C	10.193464	2.474318	-1.447845
C	10.647163	1.309919	-0.820612
C	9.746961	0.392353	-0.260044
O	-11.537716	3.200786	-0.711768
C	-11.813357	4.114303	0.328516
H	3.137624	-1.878928	-1.246887
H	1.030617	-3.090019	-1.489446
H	1.439899	0.430473	1.979666
H	-3.483771	-3.258252	-1.285442
H	-5.670635	-2.267610	-0.768232
H	-3.831481	0.199148	2.256164
H	-0.835591	-4.173155	-1.564961
H	-2.151490	-4.567187	-0.463906
H	0.822517	-4.785881	0.302613
H	-0.277278	-6.127967	-0.098657
H	-0.563428	-5.135922	1.361313
H	-6.464522	0.501690	0.371515
H	-6.264136	0.092965	2.089466
H	-9.537762	-0.533926	-2.221632
H	-11.029191	1.475470	-2.491328
H	-10.205191	2.593547	1.597225
H	-8.729868	0.635154	1.838365
H	3.732251	0.841655	1.404459
H	4.927611	-0.783421	-0.913504
H	8.389434	-0.927710	1.768568
H	6.709834	-1.502829	1.591412
H	7.665783	1.168787	2.745072
H	6.199557	0.229598	3.172877
H	6.161197	3.553363	0.361031
H	4.677059	3.088783	-0.510590
H	5.982278	3.931928	-1.379365
H	6.302249	0.403992	-2.625985



H	6.224430	2.111200	-3.115221
H	4.795872	1.336536	-2.378145
H	8.456385	3.648615	-2.014030
H	10.910229	3.178316	-1.876978
H	11.719958	1.107326	-0.764825
H	10.109797	-0.517734	0.222835
H	-12.515846	4.851236	-0.081858
H	-10.900156	4.635733	0.666255
H	-12.280919	3.614480	1.195476

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Coordinates from ORCA-job neb\_MEP E -2237.757007812971

C	2.524936	-0.552336	0.378481
C	2.358381	-1.563537	-0.584942
C	1.144911	-2.224522	-0.738583
C	0.042459	-1.932121	0.086176
C	0.191629	-0.899128	1.034056
C	1.403717	-0.218145	1.161345
N	-1.162558	-2.649559	-0.016463
C	-2.397279	-1.998848	0.175249
C	-2.520978	-0.971159	1.133175
S	-1.134646	-0.554421	2.169504
C	-3.544102	-2.350105	-0.558955
C	-4.781869	-1.765587	-0.295706
C	-4.905867	-0.765337	0.675160
C	-3.756370	-0.358271	1.363467
C	-1.131014	-4.018512	-0.527892
C	-0.260908	-4.943356	0.322268
C	-6.251886	-0.144956	0.971791
O	-7.271594	-1.150914	1.006178
C	-8.172134	-1.232068	-0.020725
C	-9.130946	-0.103294	-0.136017
O	-8.189863	-2.198277	-0.743280

C	-9.887510	0.025262	-1.317647
C	-10.819818	1.039983	-1.452988
C	-11.035788	1.948126	-0.396794
C	-10.300426	1.819102	0.793828
C	-9.354466	0.799638	0.911628
C	3.800530	0.142161	0.596030
C	4.936845	-0.049432	-0.092983
C	6.216223	0.707767	0.146247
O	6.214329	1.305753	1.451795
N	7.379865	-0.194948	0.150534
C	7.429025	-0.714581	1.513300
C	6.956960	0.492915	2.353447
C	8.482473	0.548596	-0.324268
C	6.545522	1.799741	-0.938016
C	8.062707	1.736654	-0.943820
C	5.971614	3.164675	-0.554344
C	6.023494	1.380622	-2.326770
C	8.994303	2.608315	-1.494035
C	10.359993	2.290179	-1.422388
C	10.769924	1.103313	-0.807100
C	9.836533	0.216557	-0.251309
O	-11.966925	2.899553	-0.617429
C	-12.243788	3.847948	0.391219
H	3.191560	-1.844353	-1.231497
H	1.056484	-2.995194	-1.504318
H	1.486816	0.576072	1.907990
H	-3.477017	-3.106476	-1.341085
H	-5.664132	-2.113657	-0.836593
H	-3.820416	0.423265	2.126271
H	-0.818388	-4.046853	-1.588960
H	-2.159839	-4.395668	-0.504618
H	0.794044	-4.634575	0.328611

H	-0.313303	-5.971779	-0.068604
H	-0.618877	-4.945889	1.363185
H	-6.510791	0.619555	0.217621
H	-6.232705	0.355201	1.953251
H	-9.723717	-0.694634	-2.121573
H	-11.408424	1.160319	-2.364273
H	-10.462272	2.497871	1.630619
H	-8.798657	0.686572	1.843807
H	3.821781	0.881648	1.402897
H	4.987218	-0.774196	-0.908542
H	8.437655	-1.059599	1.774929
H	6.733819	-1.562461	1.608627
H	7.812510	1.076327	2.736364
H	6.326240	0.190116	3.206050
H	6.376325	3.507648	0.405948
H	4.874507	3.109895	-0.468273
H	6.211782	3.907825	-1.331032
H	6.391405	0.383158	-2.611128
H	6.379813	2.096889	-3.082711
H	4.922901	1.370642	-2.351755
H	8.668048	3.535339	-1.973389
H	11.102295	2.969625	-1.847685
H	11.834234	0.858763	-0.756884
H	10.165476	-0.711083	0.222365
H	-13.012613	4.518838	-0.014459
H	-11.348341	4.440752	0.649490
H	-12.631063	3.366652	1.306928

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Coordinates from ORCA-job neb\_MEP E -2237.754941545028

C	2.589861	-0.471679	0.361421
C	2.415332	-1.502917	-0.578673
C	1.181666	-2.118692	-0.759301

C	0.059595	-1.765582	0.015690
C	0.213488	-0.704905	0.932302
C	1.450110	-0.070054	1.086955
N	-1.154596	-2.466906	-0.098705
C	-2.394818	-1.825573	0.095798
C	-2.524009	-0.762881	1.015287
S	-1.133203	-0.264506	2.012646
C	-3.552987	-2.229099	-0.594575
C	-4.799746	-1.665700	-0.325704
C	-4.931019	-0.630301	0.605920
C	-3.771757	-0.170874	1.249076
C	-1.118474	-3.852227	-0.567675
C	-0.278341	-4.760848	0.329374
C	-6.281674	-0.003579	0.889604
O	-7.324161	-0.981139	1.026576
C	-8.214618	-1.150689	-0.003578
C	-9.312106	-0.151500	-0.074590
O	-8.107650	-2.075426	-0.771137
C	-10.090586	-0.083906	-1.248673
C	-11.104317	0.851140	-1.373755
C	-11.384955	1.737494	-0.313664
C	-10.647271	1.649158	0.880006
C	-9.615668	0.713246	0.985719
C	3.890574	0.172557	0.605391
C	5.029598	-0.054327	-0.071110
C	6.336962	0.656159	0.175103
O	6.355672	1.239474	1.487958
N	7.474361	-0.282609	0.162179
C	7.534550	-0.796402	1.527692
C	7.142519	0.438777	2.362894
C	8.596007	0.428368	-0.321617
C	6.697002	1.749567	-0.901486

C	8.210968	1.637851	-0.920339
C	6.174117	3.129593	-0.500154
C	6.155521	1.363685	-2.292436
C	9.166331	2.486859	-1.466102
C	10.521090	2.122977	-1.412311
C	10.896684	0.913403	-0.819792
C	9.939260	0.050125	-0.268092
O	-12.369231	2.632822	-0.539862
C	-12.644101	3.628742	0.423100
H	3.260803	-1.842724	-1.179561
H	1.095856	-2.910531	-1.502977
H	1.536951	0.742514	1.813546
H	-3.491504	-3.012749	-1.349645
H	-5.684362	-2.054718	-0.833358
H	-3.834988	0.643373	1.977885
H	-0.779757	-3.911674	-1.618885
H	-2.148364	-4.224452	-0.562913
H	0.780489	-4.467199	0.351661
H	-0.335410	-5.799019	-0.033989
H	-0.659891	-4.729422	1.361441
H	-6.556907	0.710091	0.091461
H	-6.240666	0.559006	1.834983
H	-9.867244	-0.776803	-2.061916
H	-11.699945	0.932427	-2.285416
H	-10.871742	2.297677	1.727097
H	-9.046760	0.637055	1.913860
H	3.928233	0.904389	1.418853
H	5.061030	-0.770845	-0.894943
H	8.532975	-1.185311	1.765961
H	6.803132	-1.610083	1.648022
H	8.036305	1.010886	2.670652
H	6.563345	0.177665	3.263821

H	6.596774	3.447391	0.461105
H	5.076242	3.114219	-0.408743
H	6.437852	3.871806	-1.270188
H	6.489082	0.357707	-2.589374
H	6.534064	2.075289	-3.041999
H	5.055233	1.391257	-2.314105
H	8.867363	3.431762	-1.927798
H	11.281835	2.784568	-1.833142
H	11.952611	0.632781	-0.784238
H	10.242251	-0.894717	0.188380
H	-13.389319	4.297517	-0.027642
H	-11.740037	4.211506	0.673367
H	-13.061508	3.199683	1.351375

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Coordinates from ORCA-job neb\_MEP E -2237.728121473925

C	2.698193	-0.553467	0.447844
C	2.491170	-1.556217	-0.516582
C	1.243145	-2.144826	-0.697009
C	0.126421	-1.786378	0.087549
C	0.302341	-0.752766	1.030375
C	1.565929	-0.160738	1.202781
N	-1.104836	-2.461057	-0.046165
C	-2.348056	-1.821864	0.164025
C	-2.502188	-0.776334	1.102607
S	-1.074054	-0.296038	2.095668
C	-3.503463	-2.214204	-0.537886
C	-4.758948	-1.669405	-0.271645
C	-4.952439	-0.667271	0.681498
C	-3.777556	-0.208841	1.347868
C	-1.077893	-3.827912	-0.574192
C	-0.260612	-4.790933	0.286701
C	-6.388306	-0.094859	0.836127

O	-7.467249	-1.122735	0.860184
C	-8.609483	-1.296447	0.063994
C	-9.680772	-0.230526	-0.041436
O	-8.775112	-2.353529	-0.489801
C	-10.370240	-0.060001	-1.271121
C	-11.295356	0.965121	-1.442292
C	-11.613511	1.820038	-0.369054
C	-11.073460	1.547409	0.897692
C	-10.108292	0.543166	1.045171
C	4.016622	0.085815	0.662726
C	5.140930	-0.091685	-0.061055
C	6.450461	0.642671	0.164355
O	6.473919	1.225437	1.476731
N	7.613409	-0.270835	0.135677
C	7.717933	-0.770590	1.504477
C	7.310725	0.460462	2.337005
C	8.715785	0.464853	-0.362727
C	6.784095	1.747875	-0.915466
C	8.300279	1.668118	-0.950664
C	6.249212	3.120807	-0.506119
C	6.243413	1.359956	-2.305602
C	9.232375	2.542888	-1.498897
C	10.595719	2.211119	-1.457599
C	11.003083	1.005820	-0.877286
C	10.069274	0.117311	-0.324254
O	-12.433729	2.860949	-0.645401
C	-12.623777	3.871517	0.325313
H	3.321245	-1.892419	-1.142151
H	1.142844	-2.917054	-1.458879
H	1.684916	0.620072	1.959139
H	-3.434282	-2.979304	-1.308294
H	-5.629642	-2.038105	-0.814615

H	-3.818026	0.592531	2.094301
H	-0.727151	-3.843349	-1.622657
H	-2.110830	-4.186890	-0.599450
H	0.809921	-4.542151	0.303553
H	-0.370545	-5.814690	-0.104646
H	-0.628173	-4.775244	1.323670
H	-6.623900	0.541035	-0.020272
H	-6.424443	0.545415	1.737972
H	-10.161195	-0.728126	-2.110289
H	-11.777760	1.153467	-2.406230
H	-11.390691	2.118777	1.770103
H	-9.705267	0.335400	2.037741
H	4.079516	0.793962	1.495675
H	5.163258	-0.779395	-0.910655
H	8.733143	-1.126410	1.723478
H	7.015471	-1.604858	1.648901
H	8.194085	1.063699	2.614725
H	6.764507	0.192302	3.255900
H	6.687940	3.445934	0.445556
H	5.154011	3.092862	-0.393029
H	6.490647	3.864171	-1.282515
H	6.592545	0.361241	-2.609338
H	6.609715	2.081225	-3.052353
H	5.143034	1.371239	-2.325265
H	8.909883	3.484658	-1.951294
H	11.338255	2.893657	-1.878502
H	12.065958	0.750046	-0.851764
H	10.401043	-0.822307	0.123048
H	-13.144149	4.701303	-0.173852
H	-11.660453	4.245102	0.716084
H	-13.240535	3.520332	1.172093



Coordinates from ORCA-job neb\_MEP E -2237.664054436526

C	2.774707	-0.588611	0.441894
C	2.556384	-1.582352	-0.532024
C	1.308049	-2.172811	-0.699991
C	0.212678	-1.821725	0.112651
C	0.415296	-0.819932	1.079368
C	1.668730	-0.215885	1.229467
N	-1.051029	-2.455534	-0.054292
C	-2.241201	-1.810441	0.208529
C	-2.302503	-0.745904	1.170566
S	-0.893830	-0.391105	2.196882
C	-3.453071	-2.165912	-0.457280
C	-4.642461	-1.521556	-0.198014
C	-4.711374	-0.447515	0.750559
C	-3.492596	-0.102579	1.430923
C	-1.054391	-3.829145	-0.593272
C	-0.257597	-4.800275	0.277444
C	-5.891988	0.248319	0.951150
O	-8.117292	-1.494868	0.709716
C	-9.170575	-1.616806	0.000394
C	-10.104014	-0.424011	-0.103765
O	-9.460360	-2.633496	-0.648025
C	-10.667917	-0.105678	-1.353397
C	-11.443261	1.034614	-1.522941
C	-11.717134	1.870032	-0.425960
C	-11.231438	1.522870	0.844530
C	-10.415001	0.393509	0.988718
C	4.075701	0.069227	0.654197
C	5.192455	-0.099383	-0.075110
C	6.487814	0.644934	0.159014
O	6.495298	1.223643	1.471945
N	7.647509	-0.265867	0.132941

C	7.752932	-0.762822	1.503572
C	7.340125	0.466935	2.333894
C	8.745189	0.473575	-0.370156
C	6.808497	1.752120	-0.920269
C	8.323939	1.675140	-0.956840
C	6.267754	3.122455	-0.508032
C	6.262950	1.364356	-2.309081
C	9.251632	2.553908	-1.504497
C	10.615257	2.224871	-1.464420
C	11.027192	1.019481	-0.887237
C	10.097395	0.127226	-0.334795
O	-12.449091	2.986994	-0.693472
C	-12.617694	3.950122	0.317276
H	3.376006	-1.903513	-1.177114
H	1.191581	-2.926109	-1.478196
H	1.788843	0.562227	1.987517
H	-3.440502	-2.944626	-1.218265
H	-5.563825	-1.820222	-0.704112
H	-3.516247	0.690098	2.182826
H	-0.692898	-3.832989	-1.634921
H	-2.093196	-4.169259	-0.622883
H	0.817362	-4.574551	0.289305
H	-0.386840	-5.823294	-0.108413
H	-0.624386	-4.773490	1.314750
H	-6.801797	0.017524	0.390820
H	-5.940626	1.023725	1.721384
H	-10.465995	-0.770291	-2.196153
H	-11.845036	1.315920	-2.499085
H	-11.478228	2.125393	1.719774
H	-10.017820	0.134013	1.973060
H	4.128230	0.776601	1.487705
H	5.216413	-0.787836	-0.923087

H	8.769017	-1.114691	1.723892
H	7.053793	-1.600003	1.649690
H	8.218986	1.077712	2.606992
H	6.796965	0.198363	3.254375
H	6.707751	3.451908	0.441384
H	5.172848	3.090942	-0.391578
H	6.502038	3.866654	-1.285559
H	6.611804	0.366607	-2.616027
H	6.625895	2.086395	-3.056345
H	5.162147	1.376825	-2.326751
H	8.924767	3.494780	-1.955279
H	11.355168	2.910341	-1.884052
H	12.090227	0.766063	-0.863447
H	10.428914	-0.813565	0.109871
H	-13.112652	4.814923	-0.147163
H	-11.648546	4.276852	0.738138
H	-13.251826	3.580458	1.144190

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Coordinates from ORCA-job neb\_MEP E -2237.573146290797

C	2.836425	-0.615489	0.468473
C	2.650496	-1.608603	-0.490971
C	1.397421	-2.209516	-0.670935
C	0.278616	-1.860960	0.106523
C	0.458312	-0.837971	1.055812
C	1.725048	-0.241807	1.240246
N	-0.982561	-2.476217	-0.089129
C	-2.218159	-1.841307	0.199942
C	-2.308483	-0.809941	1.155743
S	-0.883754	-0.270008	2.096288
C	-3.393678	-2.151040	-0.510145
C	-4.611835	-1.506038	-0.258921
C	-4.708058	-0.513723	0.717316

C	-3.540756	-0.168217	1.414915
C	-1.019935	-3.865982	-0.597104
C	-0.228227	-4.841482	0.273576
C	-6.003756	0.237968	0.937934
O	-8.825821	-1.884003	1.133594
C	-9.719934	-1.808604	0.116866
C	-10.411410	-0.504244	-0.044971
O	-10.002341	-2.766755	-0.588211
C	-10.772905	-0.099836	-1.333974
C	-11.455729	1.104004	-1.520849
C	-11.789793	1.909866	-0.429411
C	-11.458254	1.488715	0.860803
C	-10.768581	0.283143	1.055174
C	4.128887	0.064249	0.686914
C	5.258302	-0.094599	-0.032597
C	6.560244	0.661133	0.171285
O	6.542299	1.223270	1.506152
N	7.689450	-0.308303	0.132522
C	7.884614	-0.742075	1.511134
C	7.446873	0.463469	2.325448
C	8.765345	0.473439	-0.380079
C	6.845784	1.762520	-0.923481
C	8.352470	1.677822	-0.963028
C	6.327266	3.148617	-0.529461
C	6.325760	1.392808	-2.328722
C	9.265059	2.576764	-1.502263
C	10.620980	2.255290	-1.456230
C	11.042368	1.042410	-0.895531
C	10.112921	0.141392	-0.364200
O	-12.451391	3.060951	-0.755022
C	-12.581291	4.040552	0.267628
H	3.465316	-1.938379	-1.128528

H	1.316284	-2.951786	-1.459456
H	1.834656	0.534061	1.996465
H	-3.383566	-2.874780	-1.320301
H	-5.481162	-1.787788	-0.851269
H	-3.580014	0.619565	2.165522
H	-0.677291	-3.901724	-1.637683
H	-2.037374	-4.270533	-0.604797
H	0.848729	-4.657325	0.245499
H	-0.386005	-5.865431	-0.081975
H	-0.551904	-4.789117	1.317905
H	-6.101217	1.001804	0.157842
H	-5.989194	0.739108	1.911683
H	-10.533029	-0.720738	-2.194805
H	-11.733562	1.416141	-2.525395
H	-11.741614	2.066548	1.735097
H	-10.542602	-0.045875	2.066723
H	4.133897	0.786796	1.502597
H	5.293041	-0.797626	-0.858255
H	8.895030	-1.080002	1.762966
H	7.211276	-1.585710	1.704549
H	8.296374	1.108191	2.573292
H	6.947239	0.174914	3.254700
H	6.790122	3.513838	0.393799
H	5.241787	3.130108	-0.383215
H	6.541597	3.890381	-1.307773
H	6.665080	0.398345	-2.644030
H	6.682450	2.104094	-3.083766
H	5.231095	1.403512	-2.365716
H	8.938240	3.505948	-1.957829
H	11.354609	2.943457	-1.869331
H	12.101550	0.797193	-0.879972
H	10.452575	-0.803139	0.046019

H	-12.969763	4.954096	-0.193545
H	-11.611922	4.282951	0.715915
H	-13.299014	3.717241	1.028017

iii) **Optimized Structure for Compound 7a (open form)**

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XYZ file generated by orca\_plot on BaseName=opt

C	3.619138	0.767587	0.331132
C	3.404375	-0.463331	-0.326705
C	2.207124	-1.122771	-0.228043
C	1.137216	-0.599343	0.537301
C	1.354922	0.623297	1.224997
C	2.550187	1.289189	1.096150
N	-0.065136	-1.248379	0.621566
C	-1.275401	-0.524136	0.812608
C	-1.297000	0.643525	1.583740
S	0.170299	1.184316	2.402814
C	-2.461704	-0.930217	0.203811
C	-3.646291	-0.233945	0.404592
C	-3.667216	0.914372	1.186800
C	-2.474914	1.356551	1.754203
C	-0.134296	-2.689805	0.324786
C	0.695752	-3.519018	1.297930
C	-4.934687	1.707336	1.406524
O	-6.084312	0.975957	0.993840
C	-6.589821	1.156276	-0.276309
C	-6.932546	2.538752	-0.669851
O	-6.775052	0.191147	-0.968466
C	-7.003942	2.851295	-2.034211
C	-7.368214	4.112998	-2.448799
C	-7.697612	5.095143	-1.504953
C	-7.651995	4.789821	-0.142049

C	-7.263404	3.520722	0.262285
C	4.829917	1.504638	0.275388
C	5.986467	1.146881	-0.383075
C	7.213999	1.817423	-0.462818
N	7.531415	3.065883	-0.090578
C	6.623784	4.067913	0.443333
C	6.470281	3.961386	1.961487
C	8.907029	3.337762	-0.307376
C	8.455258	1.141259	-1.047547
C	9.499265	2.220546	-0.883982
C	8.231178	0.796119	-2.533029
C	8.817650	-0.120933	-0.243467
C	10.843493	2.243304	-1.201263
C	11.577311	3.397868	-0.924332
C	10.968157	4.505077	-0.340314
C	9.612108	4.494053	-0.019111
O	5.227883	4.568439	2.271866
O	-8.050319	6.297909	-2.004870
C	-8.437674	7.329176	-1.104599
H	4.182616	-0.898239	-0.938423
H	2.074724	-2.049127	-0.764348
H	2.690924	2.224319	1.625166
H	-2.476775	-1.790852	-0.448100
H	-4.556649	-0.588188	-0.057755
H	-2.457121	2.259938	2.353012
H	0.149810	-2.880014	-0.713389
H	-1.172585	-2.983055	0.423630
H	1.756810	-3.276648	1.256013
H	0.581253	-4.577426	1.059996
H	0.349378	-3.357389	2.319105
H	-4.872391	2.661331	0.876915
H	-5.064062	1.923799	2.468626

H	-6.772899	2.081737	-2.758104
H	-7.419223	4.367889	-3.498648
H	-7.923895	5.523698	0.601259
H	-7.251420	3.285207	1.317999
H	4.801469	2.419843	0.848122
H	5.996767	0.188265	-0.883902
H	5.651921	3.946221	-0.030596
H	6.996182	5.049561	0.159770
H	7.304913	4.461154	2.461914
H	6.484991	2.906786	2.260718
H	7.954269	1.681043	-3.105855
H	7.449007	0.045487	-2.648619
H	9.152571	0.391900	-2.952135
H	8.963722	0.113085	0.811043
H	9.744557	-0.544204	-0.630479
H	8.037292	-0.877360	-0.327681
H	11.325695	1.386478	-1.653951
H	12.631385	3.432692	-1.163606
H	11.553599	5.389817	-0.130131
H	9.149426	5.357089	0.438635
H	5.175723	4.742660	3.217789
H	-8.683534	8.186980	-1.724536
H	-7.619709	7.590185	-0.427926
H	-9.315266	7.035063	-0.523342

**iv) Scanning Compound 7a (open form) Up to the Dissociation Limit**

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Coordinates from ORCA-job neb\_MEP E -2238.165309777203

C	2.129062	-0.997743	0.326569
C	1.914299	-2.228661	-0.331268
C	0.717048	-2.888101	-0.232606
C	-0.352860	-2.364673	0.532738



C	-0.135154	-1.142033	1.220434
C	1.060111	-0.476141	1.091587
N	-1.555212	-3.013709	0.617003
C	-2.765477	-2.289466	0.808045
C	-2.787076	-1.121805	1.579177
S	-1.319777	-0.581014	2.398251
C	-3.951780	-2.695547	0.199248
C	-5.136367	-1.999275	0.400029
C	-5.157292	-0.850958	1.182237
C	-3.964990	-0.408779	1.749640
C	-1.624372	-4.455135	0.320223
C	-0.794324	-5.284348	1.293367
C	-6.424763	-0.057994	1.401961
O	-7.574388	-0.789373	0.989277
C	-8.079897	-0.609054	-0.280872
C	-8.422622	0.773422	-0.674414
O	-8.265128	-1.574183	-0.973029
C	-8.494018	1.085965	-2.038774
C	-8.858290	2.347668	-2.453362
C	-9.187688	3.329813	-1.509516
C	-9.142071	3.024491	-0.146612
C	-8.753480	1.755392	0.257722
C	3.339841	-0.260692	0.270825
C	4.496391	-0.618449	-0.387638
C	5.723923	0.052093	-0.467381
N	6.041339	1.300553	-0.095141
C	5.133708	2.302583	0.438770
C	4.980205	2.196056	1.956924
C	7.416953	1.572432	-0.311939
C	6.965182	-0.624071	-1.052110
C	8.009189	0.455216	-0.888545
C	6.741102	-0.969211	-2.537592

C	7.327574	-1.886263	-0.248030
C	9.353417	0.477974	-1.205826
C	10.087235	1.632538	-0.928895
C	9.478081	2.739747	-0.344877
C	8.122032	2.728723	-0.023674
O	3.737807	2.803109	2.267303
O	-9.540395	4.532579	-2.009433
C	-9.927750	5.563846	-1.109162
H	2.692540	-2.663569	-0.942986
H	0.584648	-3.814457	-0.768911
H	1.200848	0.458989	1.620603
H	-3.966851	-3.556182	-0.452663
H	-6.046725	-2.353518	-0.062318
H	-3.947197	0.494608	2.348449
H	-1.340266	-4.645344	-0.717952
H	-2.662661	-4.748385	0.419067
H	0.266734	-5.041978	1.251450
H	-0.908823	-6.342756	1.055433
H	-1.140698	-5.122719	2.314542
H	-6.362467	0.896001	0.872352
H	-6.554138	0.158469	2.464063
H	-8.262975	0.316407	-2.762667
H	-8.909299	2.602559	-3.503211
H	-9.413971	3.758368	0.596696
H	-8.741496	1.519877	1.313436
H	3.311393	0.654513	0.843559
H	4.506691	-1.577065	-0.888465
H	4.161845	2.180891	-0.035159
H	5.506106	3.284231	0.155207
H	5.814837	2.695824	2.457351
H	4.994915	1.141456	2.256155
H	6.464193	-0.084287	-3.110418

H	5.958931	-1.719843	-2.653182
H	7.662495	-1.373430	-2.956698
H	7.473646	-1.652245	0.806480
H	8.254481	-2.309534	-0.635042
H	6.547216	-2.642690	-0.332244
H	9.835619	-0.378852	-1.658514
H	11.141309	1.667362	-1.168169
H	10.063523	3.624487	-0.134694
H	7.659350	3.591759	0.434072
H	3.685647	2.977330	3.213226
H	-10.173610	6.421650	-1.729099
H	-9.109785	5.824855	-0.432489
H	-10.805342	5.269733	-0.527905

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Coordinates from ORCA-job neb\_MEP E -2238.170280014257

C	2.172356	-0.954835	0.349050
C	1.949038	-2.183695	-0.325708
C	0.738848	-2.838115	-0.240188
C	-0.338479	-2.311923	0.527074
C	-0.116017	-1.084693	1.222476
C	1.095401	-0.426620	1.112976
N	-1.548677	-2.958761	0.595388
C	-2.762726	-2.239019	0.797266
C	-2.786074	-1.059689	1.566439
S	-1.314015	-0.514241	2.397636
C	-3.959729	-2.653324	0.194500
C	-5.152125	-1.957437	0.398162
C	-5.172614	-0.794651	1.174257
C	-3.972290	-0.345487	1.739947
C	-1.612777	-4.402842	0.305013
C	-0.790053	-5.235260	1.285890
C	-6.449040	-0.005962	1.389291

O	-7.595041	-0.734049	0.983334
C	-8.082878	-0.596165	-0.297852
C	-8.537468	0.759188	-0.686209
O	-8.148976	-1.564718	-1.012339
C	-8.674933	1.054548	-2.057668
C	-9.109583	2.301786	-2.471777
C	-9.440924	3.288849	-1.520344
C	-9.339655	2.994526	-0.148602
C	-8.887430	1.738407	0.254823
C	3.397998	-0.227293	0.303566
C	4.556020	-0.603634	-0.362097
C	5.802611	0.045269	-0.453168
N	6.146884	1.290881	-0.073851
C	5.256905	2.293492	0.484566
C	5.084122	2.155872	2.003107
C	7.526608	1.540328	-0.297759
C	7.029190	-0.650133	-1.058365
C	8.098389	0.411281	-0.892532
C	6.784964	-0.971459	-2.549687
C	7.377945	-1.929958	-0.270102
C	9.448536	0.413105	-1.220627
C	10.208622	1.558264	-0.937227
C	9.620349	2.676884	-0.334692
C	8.259496	2.687157	-0.001948
O	3.810105	2.676686	2.300251
O	-9.843333	4.473899	-2.014933
C	-10.177424	5.524777	-1.129479
H	2.734414	-2.623530	-0.942415
H	0.602292	-3.765823	-0.792397
H	1.241049	0.511263	1.655807
H	-3.976317	-3.526533	-0.457294
H	-6.072379	-2.315915	-0.065300

H	-3.953038	0.567976	2.341076
H	-1.321002	-4.597555	-0.741001
H	-2.661342	-4.700282	0.392720
H	0.284843	-5.008815	1.236851
H	-0.921100	-6.304707	1.059942
H	-1.130498	-5.055852	2.316927
H	-6.383545	0.957408	0.852811
H	-6.572312	0.224647	2.459866
H	-8.428922	0.280285	-2.786614
H	-9.210373	2.551580	-3.529486
H	-9.618810	3.729892	0.605288
H	-8.831945	1.507425	1.320325
H	3.375780	0.693094	0.887127
H	4.547019	-1.569807	-0.869698
H	4.273914	2.197261	0.004467
H	5.641801	3.285691	0.216474
H	5.894334	2.696029	2.527337
H	5.172974	1.086899	2.282486
H	6.517400	-0.065847	-3.113635
H	5.980704	-1.712798	-2.671134
H	7.702425	-1.390808	-2.988872
H	7.535982	-1.710160	0.796000
H	8.304575	-2.367316	-0.670832
H	6.580015	-2.682346	-0.359180
H	9.915897	-0.456568	-1.688334
H	11.271693	1.576689	-1.185929
H	10.229166	3.556915	-0.116960
H	7.810212	3.560322	0.473220
H	3.719156	2.786595	3.256023
H	-10.440126	6.386938	-1.756053
H	-9.324100	5.794618	-0.482464
H	-11.041960	5.261896	-0.495011

Coordinates from ORCA-job neb\_MEP E -2238.170005161882

C	2.212893	-0.917426	0.366602
C	1.979543	-2.139494	-0.316847
C	0.760269	-2.777459	-0.245728
C	-0.316660	-2.240447	0.514067
C	-0.089285	-1.014706	1.210406
C	1.134232	-0.375321	1.118937
N	-1.531149	-2.879464	0.574735
C	-2.742494	-2.152458	0.762159
C	-2.767584	-0.969458	1.524994
S	-1.299583	-0.423334	2.363501
C	-3.935913	-2.566808	0.152546
C	-5.128824	-1.870661	0.347733
C	-5.152917	-0.705919	1.121583
C	-3.955127	-0.254233	1.691057
C	-1.602524	-4.323505	0.286225
C	-0.777587	-5.160504	1.260986
C	-6.434882	0.077316	1.326489
O	-7.576525	-0.690240	0.982452
C	-8.115860	-0.596772	-0.281890
C	-8.640618	0.730966	-0.674517
O	-8.165142	-1.579267	-0.979186
C	-8.842478	0.996683	-2.044322
C	-9.336502	2.220748	-2.460429
C	-9.663852	3.212437	-1.512485
C	-9.503504	2.944034	-0.140915
C	-8.990801	1.711966	0.264529
C	3.451364	-0.210691	0.334344
C	4.601582	-0.600624	-0.337579
C	5.859191	0.025961	-0.430344
N	6.229806	1.259548	-0.037168

C	5.364072	2.269433	0.545285
C	5.206986	2.112556	2.063374
C	7.611560	1.486972	-0.270703
C	7.066856	-0.682618	-1.058450
C	8.157084	0.356249	-0.886621
C	6.802090	-0.974338	-2.552537
C	7.400165	-1.981935	-0.296055
C	9.503992	0.338178	-1.227152
C	10.287330	1.465225	-0.934521
C	9.725144	2.585655	-0.310807
C	8.367833	2.615892	0.034681
O	3.951237	2.661633	2.384993
O	-10.120616	4.375878	-2.010640
C	-10.429073	5.439927	-1.131928
H	2.764977	-2.587730	-0.927299
H	0.616389	-3.701011	-0.802992
H	1.286848	0.559428	1.665308
H	-3.949238	-3.442137	-0.496110
H	-6.047062	-2.233738	-0.116880
H	-3.940032	0.660493	2.290758
H	-1.320228	-4.520556	-0.761953
H	-2.651731	-4.616049	0.382421
H	0.298080	-4.939871	1.206745
H	-0.915532	-6.228736	1.033790
H	-1.111270	-4.981358	2.294103
H	-6.399219	1.013418	0.740002
H	-6.538232	0.360895	2.386431
H	-8.595624	0.219042	-2.769693
H	-9.485053	2.448979	-3.517432
H	-9.782865	3.680991	0.611304
H	-8.886353	1.500788	1.330676
H	3.445991	0.703089	0.928916

H	4.572495	-1.559911	-0.857171
H	4.374369	2.198099	0.074808
H	5.763885	3.258414	0.287292
H	6.038249	2.623341	2.584349
H	5.271747	1.037402	2.325550
H	6.545717	-0.054686	-3.098665
H	5.983068	-1.698637	-2.678230
H	7.707352	-1.402884	-3.007874
H	7.572464	-1.784112	0.772149
H	8.315065	-2.428269	-0.713649
H	6.588581	-2.719011	-0.390461
H	9.951182	-0.533007	-1.711506
H	11.348267	1.467884	-1.192609
H	10.351828	3.451248	-0.086176
H	7.938577	3.489869	0.526491
H	3.875451	2.758557	3.343469
H	-10.715281	6.290737	-1.763086
H	-9.555604	5.723807	-0.519010
H	-11.270988	5.185647	-0.464621

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Coordinates from ORCA-job neb\_MEP E -2238.169413805168

C	2.254614	-0.881173	0.393102
C	2.006148	-2.090574	-0.306557
C	0.778813	-2.713169	-0.249745
C	-0.295194	-2.171399	0.508822
C	-0.058829	-0.952959	1.214307
C	1.176998	-0.332133	1.143195
N	-1.514768	-2.801074	0.558878
C	-2.721877	-2.065837	0.735311
C	-2.748553	-0.886091	1.502105
S	-1.280437	-0.349067	2.350904
C	-3.909374	-2.471241	0.108825



C	-5.099623	-1.769708	0.292542
C	-5.130732	-0.610058	1.073853
C	-3.937392	-0.167937	1.660604
C	-1.596299	-4.243193	0.264897
C	-0.772736	-5.091120	1.231451
C	-6.417910	0.172706	1.256420
O	-7.555158	-0.629362	0.976114
C	-8.142777	-0.591845	-0.270229
C	-8.747628	0.700714	-0.660904
O	-8.167517	-1.588347	-0.948818
C	-9.013880	0.933054	-2.024818
C	-9.569593	2.129130	-2.442475
C	-9.895883	3.127013	-1.501732
C	-9.681443	2.886204	-0.132996
C	-9.105330	1.683086	0.273859
C	3.506468	-0.195923	0.370222
C	4.647454	-0.597268	-0.312864
C	5.916262	0.007008	-0.409655
N	6.313005	1.228664	-0.004694
C	5.471429	2.245042	0.600927
C	5.329754	2.068941	2.118300
C	7.696514	1.434577	-0.247049
C	7.105908	-0.713565	-1.060024
C	8.216341	0.302862	-0.882721
C	6.824780	-0.976369	-2.556626
C	7.424708	-2.030505	-0.322559
C	9.560007	0.265385	-1.234556
C	10.366249	1.373625	-0.932659
C	9.829592	2.495264	-0.289024
C	8.475830	2.545200	0.067752
O	4.085999	2.630861	2.462914
O	-10.398674	4.269199	-2.004024

C	-10.672962	5.354773	-1.139797
H	2.787265	-2.542510	-0.918537
H	0.624465	-3.627632	-0.818440
H	1.338876	0.594299	1.700916
H	-3.918634	-3.343021	-0.544672
H	-6.012610	-2.131786	-0.181384
H	-3.929847	0.740373	2.269415
H	-1.321995	-4.436767	-0.786521
H	-2.647062	-4.527985	0.368616
H	0.304663	-4.881634	1.171534
H	-0.921657	-6.156278	0.997858
H	-1.098275	-4.915762	2.268143
H	-6.402108	1.070775	0.611781
H	-6.504936	0.523242	2.298298
H	-8.763418	0.153114	-2.745158
H	-9.761621	2.332808	-3.496581
H	-9.964954	3.625028	0.615206
H	-8.955826	1.496820	1.338699
H	3.518292	0.708435	0.979498
H	4.597527	-1.548405	-0.846136
H	4.475471	2.196494	0.141073
H	5.885125	3.230658	0.351801
H	6.174650	2.560060	2.636360
H	5.382502	0.989402	2.364490
H	6.580725	-0.043907	-3.086507
H	5.993192	-1.685099	-2.688116
H	7.719622	-1.412540	-3.025158
H	7.610560	-1.853742	0.747101
H	8.328752	-2.483383	-0.756396
H	6.601331	-2.753710	-0.422318
H	9.987708	-0.606705	-1.734407
H	11.425033	1.360526	-1.199256

H	10.473972	3.345898	-0.057527
H	8.066814	3.419837	0.575221
H	4.022053	2.712298	3.423689
H	-10.968942	6.195232	-1.781325
H	-9.780052	5.641229	-0.556388
H	-11.498968	5.120947	-0.445649

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Coordinates from ORCA-job neb\_MEP E -2238.166023717949

C	2.305607	-0.867581	0.441206
C	2.026647	-2.043348	-0.303932
C	0.790125	-2.647968	-0.251032
C	-0.263820	-2.116919	0.543142
C	-0.005254	-0.928930	1.291095
C	1.245849	-0.331537	1.231986
N	-1.493929	-2.726889	0.583835
C	-2.688943	-1.972343	0.763018
C	-2.717332	-0.820280	1.569454
S	-1.232507	-0.348889	2.447153
C	-3.864546	-2.339785	0.093763
C	-5.043674	-1.622835	0.262354
C	-5.091319	-0.487979	1.077327
C	-3.907577	-0.090046	1.728393
C	-1.604187	-4.157508	0.246534
C	-0.792545	-5.048214	1.183350
C	-6.406251	0.283315	1.158993
O	-7.525302	-0.578634	0.937171
C	-8.218925	-0.606045	-0.262876
C	-8.901485	0.647505	-0.671926
O	-8.269190	-1.635021	-0.889504
C	-9.221052	0.854227	-2.033171
C	-9.802856	2.041676	-2.448999
C	-10.115034	3.047324	-1.509895

C	-9.886570	2.813093	-0.141973
C	-9.275391	1.625180	0.260494
C	3.571126	-0.201548	0.413331
C	4.696712	-0.598605	-0.301291
C	5.975884	-0.011393	-0.404521
N	6.393283	1.199427	0.011668
C	5.569776	2.218807	0.635618
C	5.443780	2.028872	2.152608
C	7.778358	1.391016	-0.235234
C	7.154920	-0.738545	-1.072352
C	8.280095	0.261126	-0.887853
C	6.869050	-0.978979	-2.571706
C	7.464867	-2.067877	-0.353798
C	9.622149	0.210686	-1.246395
C	10.444472	1.304097	-0.933310
C	9.925533	2.424432	-0.272708
C	8.573935	2.487368	0.090478
O	4.204437	2.589154	2.515179
O	-10.619442	4.189960	-2.011416
C	-10.855513	5.286967	-1.150039
H	2.788982	-2.478806	-0.951835
H	0.610233	-3.535200	-0.855040
H	1.436220	0.565947	1.827170
H	-3.872065	-3.191490	-0.583938
H	-5.949310	-1.951556	-0.247218
H	-3.891317	0.787354	2.382627
H	-1.340056	-4.326787	-0.811721
H	-2.659722	-4.425321	0.346846
H	0.288597	-4.859124	1.120685
H	-0.967467	-6.103834	0.924750
H	-1.108248	-4.891316	2.225906
H	-6.412500	1.089827	0.406202

H	-6.515681	0.759807	2.147828
H	-8.991206	0.070693	-2.758726
H	-10.020081	2.235078	-3.501950
H	-10.180183	3.547058	0.608084
H	-9.112869	1.437604	1.323575
H	3.610073	0.686289	1.045502
H	4.627481	-1.536526	-0.855574
H	4.568285	2.183603	0.186626
H	5.991583	3.201979	0.390302
H	6.294500	2.513643	2.666856
H	5.497718	0.946712	2.387477
H	6.636238	-0.037224	-3.089968
H	6.030020	-1.676974	-2.712291
H	7.759375	-1.418829	-3.045874
H	7.659140	-1.906571	0.716755
H	8.362442	-2.523437	-0.798586
H	6.634277	-2.781977	-0.457721
H	10.037457	-0.659913	-1.759511
H	11.502204	1.280589	-1.204175
H	10.582416	3.263222	-0.032451
H	8.179042	3.360707	0.611315
H	4.154503	2.672141	3.476575
H	-11.126034	6.135464	-1.791645
H	-9.952575	5.546235	-0.569768
H	-11.685436	5.084399	-0.451307

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**Coordinates from ORCA-job neb\_MEP E -2238.096357679249**

C	2.352263	-0.897537	0.447487
C	2.042146	-2.042488	-0.331527
C	0.799228	-2.636558	-0.266345
C	-0.221982	-2.127205	0.581680
C	0.078868	-0.987505	1.382466

C	1.329100	-0.391472	1.299779
N	-1.470684	-2.706984	0.620582
C	-2.636074	-1.932313	0.859299
C	-2.619322	-0.811517	1.714941
S	-1.104533	-0.464404	2.610394
C	-3.833653	-2.242514	0.201405
C	-4.971927	-1.477922	0.385465
C	-4.991245	-0.365140	1.227970
C	-3.782295	-0.041743	1.917798
C	-1.620010	-4.122533	0.236852
C	-0.827134	-5.046962	1.155507
C	-6.293325	0.381486	1.254587
O	-7.665905	-0.754003	0.799097
C	-8.450827	-0.723587	-0.369718
C	-9.109691	0.553257	-0.790250
O	-8.612632	-1.739883	-1.009457
C	-9.400341	0.823263	-2.153191
C	-9.896357	2.063951	-2.536778
C	-10.168697	3.053620	-1.568528
C	-9.982820	2.755004	-0.208768
C	-9.456256	1.515965	0.160201
C	3.615816	-0.225279	0.406633
C	4.729540	-0.606431	-0.328066
C	6.008432	-0.014144	-0.422699
N	6.420630	1.193551	0.001676
C	5.593262	2.209725	0.627935
C	5.466449	2.018266	2.145327
C	7.806678	1.388804	-0.241869
C	7.187958	-0.738744	-1.086744
C	8.311082	0.261464	-0.897240
C	6.900873	-0.979197	-2.585866
C	7.491591	-2.068596	-0.365268

C	9.653819	0.213585	-1.252612
C	10.473222	1.307510	-0.934562
C	9.951370	2.425542	-0.272177
C	8.599109	2.485779	0.088527
O	4.218823	2.562407	2.504668
O	-10.597879	4.244201	-2.037214
C	-10.845687	5.301711	-1.132623
H	2.780708	-2.458928	-1.018696
H	0.590763	-3.495170	-0.902159
H	1.548721	0.481253	1.920102
H	-3.897007	-3.080578	-0.486718
H	-5.908914	-1.736907	-0.101063
H	-3.693376	0.801804	2.613494
H	-1.353772	-4.266528	-0.824231
H	-2.681587	-4.371249	0.324192
H	0.256539	-4.873248	1.093441
H	-1.018062	-6.095313	0.881936
H	-1.138609	-4.899399	2.200738
H	-6.597598	0.912914	0.383327
H	-6.372025	1.044122	2.144429
H	-9.214306	0.061046	-2.914966
H	-10.073432	2.318848	-3.586046
H	-10.228732	3.479286	0.565797
H	-9.323537	1.265250	1.213341
H	3.660910	0.652322	1.052466
H	4.658289	-1.536414	-0.895373
H	4.591689	2.171551	0.179094
H	6.012058	3.194423	0.383640
H	6.309077	2.513692	2.662153
H	5.533236	0.936986	2.381141
H	6.666868	-0.037526	-3.103804
H	6.061355	-1.677033	-2.724531

H	7.789898	-1.419837	-3.061165
H	7.682347	-1.906607	0.705905
H	8.388689	-2.527957	-0.806678
H	6.658288	-2.779338	-0.471014
H	10.071057	-0.655198	-1.767030
H	11.531410	1.286423	-1.203326
H	10.606510	3.264698	-0.028917
H	8.201672	3.357348	0.610360
H	4.175348	2.671496	3.463804
H	-11.105442	6.178453	-1.739876
H	-9.952634	5.538101	-0.527021
H	-11.687390	5.072782	-0.455517

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Coordinates from ORCA-job neb\_MEP E -2238.066082484959

C	2.359380	-0.902242	0.442016
C	2.045194	-2.042832	-0.337164
C	0.796895	-2.634241	-0.270333
C	-0.209946	-2.129312	0.587647
C	0.106431	-1.008567	1.398005
C	1.350648	-0.401276	1.303855
N	-1.484373	-2.698564	0.610659
C	-2.618452	-1.927958	0.868033
C	-2.541015	-0.800300	1.740856
S	-1.041877	-0.494673	2.645213
C	-3.860101	-2.212461	0.243916
C	-4.967152	-1.411793	0.442223
C	-4.890052	-0.267771	1.303966
C	-3.648203	-0.016387	1.974141
C	-1.629298	-4.120098	0.229903
C	-0.832471	-5.039808	1.152942
C	-5.956781	0.613006	1.420323
O	-7.990514	-0.981794	0.560237



C	-8.672013	-0.857040	-0.516980
C	-9.225224	0.502977	-0.857624
O	-8.836813	-1.794672	-1.309493
C	-9.453105	0.828767	-2.209357
C	-9.909121	2.086712	-2.570842
C	-10.173045	3.056004	-1.582441
C	-9.982209	2.735558	-0.226400
C	-9.506481	1.466827	0.120540
C	3.625535	-0.223641	0.402970
C	4.732727	-0.605931	-0.330298
C	6.014693	-0.013315	-0.424441
N	6.423832	1.192827	0.000563
C	5.595661	2.209313	0.627781
C	5.468876	2.016776	2.145464
C	7.810053	1.388826	-0.242402
C	7.191494	-0.738587	-1.087258
C	8.314204	0.261086	-0.897774
C	6.902494	-0.978897	-2.586595
C	7.493312	-2.069204	-0.365590
C	9.656688	0.212949	-1.253123
C	10.475320	1.307086	-0.934564
C	9.953604	2.425406	-0.271724
C	8.601681	2.486148	0.088792
O	4.220484	2.559177	2.504353
O	-10.598925	4.255915	-2.037601
C	-10.847147	5.305470	-1.128820
H	2.780991	-2.460656	-1.025929
H	0.587110	-3.490932	-0.908218
H	1.563752	0.474018	1.922963
H	-3.940737	-3.050201	-0.447037
H	-5.931500	-1.638093	-0.024377
H	-3.575702	0.826837	2.664657

H	-1.356263	-4.263401	-0.828210
H	-2.690209	-4.371409	0.316532
H	0.251481	-4.867610	1.090158
H	-1.023842	-6.088496	0.879829
H	-1.141929	-4.894282	2.198914
H	-6.857579	0.470053	0.813940
H	-5.918679	1.415630	2.163697
H	-9.256397	0.065081	-2.964065
H	-10.074125	2.360490	-3.614920
H	-10.207697	3.460694	0.555895
H	-9.359631	1.208479	1.172147
H	3.666447	0.652661	1.050411
H	4.659377	-1.534792	-0.899133
H	4.594310	2.171379	0.178728
H	6.014836	3.193741	0.383745
H	6.310788	2.512837	2.662528
H	5.536349	0.935512	2.381099
H	6.668551	-0.037223	-3.104469
H	6.063002	-1.676841	-2.724904
H	7.791264	-1.419857	-3.061848
H	7.684219	-1.907706	0.705584
H	8.389989	-2.528774	-0.807353
H	6.659763	-2.779586	-0.471966
H	10.073666	-0.655743	-1.767782
H	11.533405	1.286132	-1.203414
H	10.609001	3.264200	-0.028416
H	8.203988	3.357534	0.610703
H	4.178315	2.673180	3.463117
H	-11.107743	6.185198	-1.732554
H	-9.954633	5.539917	-0.521172
H	-11.688826	5.072565	-0.452458

Coordinates from ORCA-job neb\_MEP E -2238.063299672122

C	2.416882	-0.901945	0.432184
C	2.084877	-2.040797	-0.341882
C	0.829854	-2.618104	-0.264781
C	-0.166576	-2.101983	0.598490
C	0.168019	-0.982491	1.401693
C	1.418449	-0.389380	1.298449
N	-1.449207	-2.661515	0.630965
C	-2.575342	-1.901113	0.924757
C	-2.479582	-0.768778	1.797737
S	-0.958726	-0.443359	2.655628
C	-3.840715	-2.194767	0.344214
C	-4.949505	-1.413444	0.593436
C	-4.861686	-0.283569	1.477912
C	-3.588129	-0.007519	2.083983
C	-1.599774	-4.080404	0.237058
C	-0.803706	-5.015130	1.146111
C	-5.961115	0.529272	1.683303
O	-8.107326	-0.962819	0.332118
C	-8.902002	-0.869356	-0.657389
C	-9.454505	0.494065	-0.991229
O	-9.213933	-1.821207	-1.390528
C	-9.650109	0.858021	-2.339289
C	-10.062042	2.137773	-2.676513
C	-10.321706	3.087030	-1.665749
C	-10.189424	2.718654	-0.313795
C	-9.753483	1.432422	0.008021
C	3.687891	-0.233423	0.388366
C	4.792194	-0.617396	-0.349036
C	6.074514	-0.027092	-0.438258
N	6.486561	1.175599	-0.000182
C	5.660872	2.190183	0.632754

C	5.533217	1.991478	2.148927
C	7.872308	1.370441	-0.240835
C	7.250699	-0.748182	-1.106324
C	8.374867	0.248442	-0.907768
C	6.962025	-0.977603	-2.607156
C	7.549534	-2.084087	-0.393167
C	9.717087	0.202270	-1.264229
C	10.537816	1.291901	-0.935266
C	10.018018	2.404058	-0.260773
C	8.666367	2.462961	0.100982
O	4.304696	2.572774	2.515288
O	-10.687108	4.316123	-2.089467
C	-10.922389	5.338893	-1.145284
H	2.811772	-2.469619	-1.033360
H	0.610061	-3.474986	-0.898708
H	1.645010	0.485437	1.913434
H	-3.936072	-3.025091	-0.354123
H	-5.927738	-1.631361	0.146942
H	-3.498312	0.835673	2.773249
H	-1.329420	-4.211116	-0.822970
H	-2.660392	-4.330960	0.323042
H	0.280910	-4.847890	1.083317
H	-1.001777	-6.058178	0.856339
H	-1.109646	-4.885994	2.195338
H	-6.888666	0.352178	1.113904
H	-5.918247	1.317744	2.442023
H	-9.460452	0.110517	-3.112141
H	-10.190540	2.446081	-3.716183
H	-10.423524	3.424529	0.483001
H	-9.643569	1.138247	1.054244
H	3.736542	0.640061	1.038077
H	4.715009	-1.542436	-0.924024

H	4.659776	2.158662	0.182832
H	6.082639	3.175390	0.396159
H	6.393441	2.455708	2.665623
H	5.565210	0.907179	2.377814
H	6.730326	-0.031621	-3.118162
H	6.120101	-1.671791	-2.749806
H	7.849041	-1.418054	-3.086238
H	7.740653	-1.928962	0.678944
H	8.444575	-2.544581	-0.837338
H	6.713135	-2.790633	-0.503058
H	10.132357	-0.661739	-1.788068
H	11.595682	1.272251	-1.205138
H	10.674600	3.239549	-0.009255
H	8.270135	3.329542	0.631944
H	4.271978	2.687312	3.474246
H	-11.138511	6.250018	-1.718782
H	-10.037637	5.515579	-0.507598
H	-11.787103	5.106457	-0.498992

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Coordinates from ORCA-job neb\_MEP E -2238.040546164884

C	2.444283	-0.896484	0.403751
C	2.128150	-2.059692	-0.339693
C	0.881020	-2.646868	-0.248305
C	-0.120602	-2.115192	0.601347
C	0.204668	-0.972861	1.379150
C	1.442968	-0.367266	1.254182
N	-1.392727	-2.677237	0.650499
C	-2.520474	-1.904865	0.943668
C	-2.427652	-0.797472	1.834779
S	-0.898116	-0.434913	2.651651
C	-3.776055	-2.163010	0.334604
C	-4.882769	-1.370420	0.581465

C	-4.805133	-0.293100	1.522379
C	-3.543091	-0.056613	2.152655
C	-1.551845	-4.094706	0.263659
C	-0.747726	-5.033537	1.161569
C	-5.864330	0.561096	1.822146
O	-8.603731	-1.128621	0.343190
C	-9.293822	-0.945139	-0.706438
C	-9.680921	0.462867	-1.056282
O	-9.643887	-1.868068	-1.463711
C	-9.780643	0.864815	-2.403696
C	-10.089727	2.175910	-2.728759
C	-10.331509	3.119345	-1.707839
C	-10.263905	2.722307	-0.359103
C	-9.936575	1.404199	-0.048168
C	3.707544	-0.227648	0.358591
C	4.814759	-0.621644	-0.365411
C	6.091765	-0.029536	-0.443304
N	6.499977	1.171020	0.003079
C	5.674924	2.185653	0.636614
C	5.546086	1.986336	2.151527
C	7.885271	1.365885	-0.234893
C	7.266550	-0.748132	-1.109738
C	8.388397	0.247428	-0.906613
C	6.976048	-0.973551	-2.609927
C	7.561734	-2.085666	-0.399419
C	9.729005	0.203131	-1.264495
C	10.548297	1.291968	-0.931816
C	10.028182	2.400246	-0.252190
C	8.677397	2.456895	0.111383
O	4.352894	2.630124	2.527791
O	-10.621911	4.372262	-2.114564
C	-10.903639	5.363480	-1.148806

H	2.862730	-2.501335	-1.014253
H	0.669523	-3.523559	-0.856811
H	1.663244	0.524431	1.846303
H	-3.869159	-2.985870	-0.373333
H	-5.848658	-1.599870	0.122198
H	-3.447333	0.793658	2.830280
H	-1.296534	-4.229560	-0.799636
H	-2.612693	-4.338594	0.366256
H	0.335555	-4.858661	1.099011
H	-0.938457	-6.074741	0.861018
H	-1.051743	-4.917337	2.212398
H	-6.628974	0.845126	1.110668
H	-5.880673	1.058532	2.794399
H	-9.612512	0.122115	-3.185995
H	-10.158359	2.511210	-3.765375
H	-10.469563	3.429331	0.443485
H	-9.881870	1.081187	0.993145
H	3.752770	0.652497	0.997720
H	4.741807	-1.550477	-0.933500
H	4.675347	2.161234	0.183525
H	6.101057	3.169989	0.405696
H	6.434006	2.402420	2.662310
H	5.522360	0.901178	2.376657
H	6.741746	-0.026345	-3.116881
H	6.134224	-1.667576	-2.752126
H	7.862325	-1.411775	-3.091414
H	7.752473	-1.933090	0.672855
H	8.455176	-2.547348	-0.844624
H	6.723284	-2.789195	-0.510870
H	10.142146	-0.658679	-1.792700
H	11.605042	1.274415	-1.203447
H	10.683286	3.235311	0.001769

H	8.279584	3.320094	0.645877
H	4.332853	2.742741	3.487338
H	-11.109944	6.288789	-1.701355
H	-10.045300	5.528916	-0.473597
H	-11.787896	5.098110	-0.543504

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Coordinates from ORCA-job neb\_MEP E -2237.967862929558

C	2.448853	-0.897002	0.397230
C	2.133837	-2.062471	-0.335226
C	0.897964	-2.647462	-0.243528
C	-0.113083	-2.109710	0.588949
C	0.205106	-0.954753	1.350530
C	1.438621	-0.361112	1.229235
N	-1.353742	-2.683012	0.667153
C	-2.506797	-1.896223	0.944958
C	-2.428722	-0.786140	1.793594
S	-0.906649	-0.400784	2.600500
C	-3.733833	-2.180495	0.347950
C	-4.862908	-1.423895	0.632765
C	-4.785170	-0.333898	1.491119
C	-3.550827	-0.011203	2.049094
C	-1.527943	-4.092669	0.275901
C	-0.729632	-5.040107	1.163963
C	-5.989873	0.523053	1.803985
O	-8.924221	-1.262756	0.450314
C	-9.450647	-0.961809	-0.788090
C	-9.709923	0.464145	-1.076179
O	-9.719210	-1.862247	-1.537729
C	-9.797013	0.874882	-2.413331
C	-10.086495	2.183492	-2.729897
C	-10.323226	3.117004	-1.711827
C	-10.261400	2.715252	-0.374826



C	-9.948449	1.398399	-0.069751
C	3.704616	-0.238628	0.353164
C	4.816149	-0.624571	-0.364271
C	6.083483	-0.031828	-0.437309
N	6.494313	1.164263	0.008281
C	5.671106	2.183920	0.637207
C	5.551959	1.982277	2.148784
C	7.878754	1.360020	-0.233076
C	7.260033	-0.745388	-1.105435
C	8.378473	0.249308	-0.902377
C	6.973032	-0.970921	-2.603018
C	7.558149	-2.081467	-0.400440
C	9.712088	0.206118	-1.259790
C	10.529315	1.288147	-0.928777
C	10.012248	2.389495	-0.252217
C	8.667740	2.444851	0.110272
O	4.362180	2.646209	2.538689
O	-10.607454	4.372134	-2.117837
C	-10.899870	5.361376	-1.138067
H	2.864135	-2.503724	-0.999282
H	0.688927	-3.523608	-0.836803
H	1.656360	0.523726	1.815569
H	-3.824550	-2.990840	-0.359871
H	-5.807271	-1.684812	0.176568
H	-3.455953	0.845224	2.706769
H	-1.285534	-4.228344	-0.781240
H	-2.580572	-4.323552	0.387503
H	0.343829	-4.865323	1.104960
H	-0.921635	-6.069634	0.858737
H	-1.036524	-4.927626	2.204179
H	-5.877765	1.505464	1.338413
H	-6.075533	0.673073	2.881866

H	-9.638081	0.144103	-3.194563
H	-10.148617	2.513611	-3.757962
H	-10.462964	3.411834	0.424653
H	-9.923769	1.089714	0.966703
H	3.753462	0.634394	0.987094
H	4.748221	-1.544632	-0.928864
H	4.680771	2.159328	0.187138
H	6.101025	3.156461	0.409042
H	6.431634	2.390343	2.655185
H	5.503633	0.910711	2.375386
H	6.740998	-0.032071	-3.105631
H	6.139188	-1.658921	-2.744290
H	7.853378	-1.404388	-3.077467
H	7.748179	-1.931453	0.662329
H	8.443586	-2.536492	-0.844343
H	6.726570	-2.777543	-0.510870
H	10.122981	-0.646820	-1.784433
H	11.576464	1.270522	-1.198405
H	10.661485	3.217277	-0.001320
H	8.276872	3.302354	0.639753
H	4.347530	2.757218	3.495403
H	-11.104040	6.274477	-1.690477
H	-10.048132	5.520607	-0.471529
H	-11.779223	5.085546	-0.550539

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