Supporting Information for

# Synthesis and Structural Insights of Pro-Chiral 2-acetyl-*N*-aryl-2-(prop-2-yn-1-yl)pent-4-ynamides/-2-allyl-4-enamide derivatives through Kinetics and Energy Frameworks

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# 1 General Methods

## 1.1 Experimental techniques

The nomenclature of the synthesized molecules is done according to IUPAC. Also, the numbering in the carbon chain is based on the position of the carbon atom.

All the reactions are performed in an open-air atmosphere. All the solid and liquid reagents and needles are added to the RBF under the open-air atmosphere.

Percentages (%) refers to mass percentage.

The calculated yields refer to the limiting reagent component.

Paraffin oil baths (Silicone oil baths) are used to record the melting points. The temperature is set and controlled by using an adjustable contact thermometer. Melting points (M.P.) of all solid compounds were determined by utilizing an open capillary tube method and were uncorrected.

**Reagents**

All the reagents were purchased from TCI, Sigma-Aldrich, and Sisco Research Pvt. Ltd. and used without further purification. The reaction was performed using the conventional heating method.

Solvents

Solvents from the given companies were used with the corresponding quality grades and used without further purification.

The following solvents were used in thin-layer chromatography (TLC) and smart flash chromatography: DMF, DMSO, Ethyl acetate, n-hexane, methanol, dichloromethane

## 1.2 Analytical

**Thin Layer Chromatography (TLC)**

The progress of all chemical reactions was monitored by Thin-layer chromatography. For this purpose, TLC, on aluminium plates pre-coated with F252 silica gel 60 by Merck was used as the stationary phase. TLC plates were analyzed under Visible light ($\lambda$ =400 nm to 750 nm).

**Nuclear Magnetic Resonance (NMR) Spectroscopy**

NMR Spectra $^{1}$H NMR & $^{13}$C NMR were recorded on the Brucker Avance Neo 500 MHz/ 400 MHz & 128 MHz/ 101 MHz FT-NMR spectrometer with a proton noise decoupling mode with a standard 5 mm probe. The chemical shift values are given in $\delta$ (ppm) and the coupling constant (J) is provided in Hertz. For the solvent, deuterated DMSO-d6, the signal of solvents

was used in the $^{1}H$ NMR spectra (δ = 2.52 ppm) and $^{13}C$ NMR spectra (δ = 39 ppm) as an internal standard for calibration. The spectra were viewed by utilizing the Top Spin of the company Bruker. The following abbreviations were used for the clear assignment of the signals and the spin multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, dd = double of doublet, td = triplet of doublet, m = multiplet.

**Melting Points**

Melting points of the synthesized solid products were recorded using an open capillary method and were uncorrected.

**Mass Spectrometry**

Mass spectra were recorded using MS (ESI-TOF) *m/z*.

**Crystallization**

For the sample preparation, 150 mg of the **(5f)** was dissolved in 100 ml of ethyl acetate : n-Hexane (7:3): 1drop DMSO in a beaker and heated until **5f** properly dissolved and the amount of solution was half (50 ml), after that 150 mg of activated charcoal was added to eliminate coloured impurities from the compound. Once the charcoal treatment solution was filtered, it was kept in a clean beaker covered with aluminium foil for a couple of days. When the solvent was evaporated, a single crystal of compound **5f** developed over 10-15 days.

# 2 Materials and Methods

## 2.1 General Procedures for Synthesis of Pro-Chiral 2-acetyl-*N*-aryl-2-(prop-2-yn-1-yl)pent-4-ynamides/-2-allyl-4-enamides **5(a-n)**

In RBF (50 ml) mixture of 1mmol *N*-(substituted phenyl)-3-oxobutanamide **1(a-g)**, 2.5 mmol Propargyl bromide **2(a-b)** and $K_2CO_3$ (4 equi.) were stirred at room temperature for 8-10 hrs in 5 ml ACN. At the end of the reaction (monitored by TLC technique), 20-30 ml water is added to the reaction mixture and stirred for 1-1.5 hrs. Precipitation of targeted product **5(a-n)** separated by simple filtration. The precipitate was washed thoroughly twice with water (2×10) and n-Hexane (2×10 ml) to afford the desired product in pure form.

# 3 Analytical data of the synthesized compounds

## 3.1 2-acetyl-*N*-phenylpent-4-ynamide **(3a)**

MS (ESI-TOF) *m/z* calcd For CHNO $(M + H)^+$ : 215.10, Found: 215.18; % yield: 56%; MP: 124-126 °C; $^{1}H$ NMR (400 MHz, DMSO) δ 10.43 (s, 1H, -NH), 7.60 (d, *J* = 8 Hz, 2H, Ar-H), 7.33 (t, *J* = 8 Hz, 1H, Ar-H), 7.09 (t, *J* = 8 Hz, 1H, Ar-H), 3.85 (t, *J* = 8 Hz, 1H, -CH), 2.85 (t, *J* = 4 Hz, 1H, -C≡H), 2.63 - 2.60 (m, 2H, $-CH_2$), 2.20 (s, 3H, $-CH_3$); $^{13}C$ {1H}NMR (101 MHz, DMSO) δ 201.7 (-C=O), 165.8 (NH-C=O), 138.5, 128.7, 123.7, 119.3, 81.5, 72.4, 59.4, 28.3, 17.0.

## 3.2 2-acetyl-*N*-phenyl-2-(prop-2-yn-1-yl)pent-4-ynamide **(5a)**

MS (ESI-TOF) *m/z* calcd For CHNO $(M + H)^+$ :253.11, Found: 253.19; % yield: 89%; $^{1}H$ NMR (500 MHz, DMSO-D6) δ 9.63 (s, 1H, -NH), 7.57 (d, *J* = 5 Hz, 2H, Ar-H), 7.32 (t, *J* = 5 Hz, 2H, Ar-H), 7.11 (t, *J* = 5 Hz, 1H, Ar-H), 3.04 (t, *J* = 5 Hz, 2H, -C≡H), 2.97 - 2.91 (m, 4H, $-CH_2$), 2.19 (s, 3H, $-CH_3$); $^{13}C$ {1H}NMR (126 MHz, DMSO-D6) δ 202.4 (-C=O), 166.6 (NH-C=O), 138.3, 128.6, 124.3, 120.9, 79.3, 74.5, 62.6, 25.9, 21.4.

3.3 2-acetyl-2-(prop-2-yn-1-yl)-*N*-(*p*-tolyl)pent-4-ynamide **(5b)**

MS (ESI-TOF) *m/z* calcd For CHNO $(M + H)^+$ : 267.13, Found: 267.21; % yield: 93%; MP: 124-126 °C $^1$H NMR (400 MHz, DMSO) δ 9.55 (s, 1H, -NH), 7.44 (d, *J*= 8 Hz, 2H, Ar-H), 7.12 (d, *J*= 8 Hz, 2H, Ar-H), 3.07 - 2.90 (m, 6H, Alkyne), , 2.25 (s, 3H, -$CH_3$), 2.18 (s, 3H, -$CH_3$); $^{13}$C {1H}NMR (101 MHz, DMSO) δ 201.9 (-C=O), 166.0 (-NHC=O), 135.8, 133.3, 128.9, 121.0, 78.9 (C≡CH), 73.9 (C≡CH), 62.1 (CO$CH_2$CO), 25.8 (CO-$CH_3$), 20.9 (Ph-$CH_3$), 20.0 ($CH_2$C≡CH);

3.4 2-acetyl-2-(prop-2-yn-1-yl)-*N*-(*o*-tolyl)pent-4-ynamide **(5c)**

MS (ESI-TOF) *m/z* calcd For CHNO $(M + H)^+$ : 267.13, Found: 267.19; % yield: 88%; MP: 134-136 °C $^1$H NMR (500 MHz, DMSO-D6) δ 9.43 (s, 1H, -NH), 7.24 - 7.09 (m, 4H, Ar-H), 3.02 (d, *J* = 20 Hz, 4H, -$CH_2$), 2.93 (t, *J* = 5 Hz, 2H, ≡CH), 2.24 (s, 3H, -$CH_3$), 2.17 (s, 3H, -$CH_3$); $^{13}$C {1H}NMR (126 MHz, DMSO-D6) δ 202.6 (-C=O), 166.7 (NH-C=O), 135.9, 134.3, 130.3, 127.0, 126.6, 126.0, 79.43, 74.4, 62.1, 25.8 (-$CH_3$), 21.4 (-$CH_2$), 17.7 (-$CH_3$).

3.5 2-acetyl-*N*-(4-chlorophenyl)-2-(prop-2-yn-1-yl)pent-4-ynamide **(5d)**

MS (ESI-TOF) *m/z* calcd For CHNO $(M + H)^+$ : 287.07, Found: 287.11; % yield: 95% MP: 110-112 °C $^{13}$C {1H}NMR (126 MHz, DMSO-D6) δ 202.4 (-C=O), 166.6 (NH-C=O), 138.3, 128.6, 124.3 (Ar-C-Cl), 120.9, 79.3, 74.5, 62.6, 25.9, 21.4 (-$CH_3$).

3.6 2-acetyl-*N*-(2-chlorophenyl)-2-(prop-2-yn-1-yl)pent-4-ynamide **(5e)**

MS (ESI-TOF) *m/z* calcd For CHNO $(M + H)^+$ : 287.07, Found: 278.11; % yield: 91%; MP: 108-110 °C

3.7 2-acetyl-*N*-(2,4-dimethoxyphenyl)-2-(prop-2-yn-1-yl)pent-4-ynamide (**5f)**

MS (ESI-TOF) *m/z* calcd For CHNO $(M + H)^+$ : 313.13, Found: 313.34; % yield: 90%; MP: 108-110 °C $^1$H NMR (500 MHz, DMSO-D6) δ 9.02 (s, 1H, -NH), 7.18 (d, *J* = 5 Hz, 1H, Ar-H), 6.61 (d, *J* = 5 Hz, 1H, Ar-H), 6.49 (d, *J* = 10 Hz, 1H, Ar-H), 3.75 (s, 3H, -$OCH_3$), 3.75 (s, 3H, -$OCH_3$), 2.96 (d, *J* = 10 Hz, 4H, -$CH_2$), 2.88 (t, *J* = 5 Hz, 2H, -C≡H), 2.22 (s, 3H, -$CH_3$); $^{13}$C {1H}NMR (126 MHz, DMSO-D6) δ 202.7 (-C=O), 166.5 (NH-C=O), 158.3, 153.9, 126.7, 104.1, 98.8, 79.3, 74.2, 61.7, 55.5, 55.2, 25.6, 21.3.

3.8 2-acetyl-*N*-(4-chloro-2,5-dimethoxyphenyl)-2-(prop-2-yn-1-yl)pent-4-ynamide (**5g)**

MS (ESI-TOF) *m/z* calcd For CHNO $(M + H)^+$ : 347.10, Found: 347.14; % yield: 86%; MP: 132-134 °C $^1$H NMR (400 MHz, $CDCl_3$) δ 8.37 (s, 1H, -NH), 8.15 (s, 1H, Ar-H), 6.90 (s, 1H, Ar-H), 3.88 (s, 3H, -$OCH_3$), 3.85 (s, 3H, -$OCH_3$), 3.06 (d, *J* = 4 Hz, 4H, -$CH_2$), 2.37 (s, 3H, -$CH_3$), 2.10 (t, *J* = 4 Hz, 2H, -C≡H); $^{13}$C {1H}NMR (101 MHz, $CDCl_3$) δ 204.6 (-C=O), 165.6 (NH-C=O), 149.1, 142.3, 126.3, 116.7, 112.5, 105.1, 78.6, 72.6, 63.5, 56.8, 56.6, 26.9, 22.7.

3.9 2-acetyl-2-allyl-*N*-phenylpent-4-enamide **(5h)**

MS (ESI-TOF) *m/z* calcd For CHNO $(M + H)^+$: 257.14, Found: 257.23; % yield: 96%; MP: 112-114 °C $^1$H NMR (500 MHz, DMSO-D6) δ 9.50 (s, 1H, -NH), 7.57 (d, *J* = 5 Hz, 2H, Ar-H), 7.32, 7.30, 7.29 (t, *J* = 5 Hz, 2H, Ar-H), 7.09 (t, *J* = 5 Hz, 1H, Ar-H), 5.65 - 5.57 (m, 2H, -CH=C), 5.14 - 5.05 (m, 4H, =$CH_2$), 2.72 - 2.59 (m, 4H, -$CH_2$), 2.13 (-$CH_3$); $^{13}$C {1H}NMR (126 MHz, DMSO-D6) δ 205.0 (-C=O), 169.1 (NH-C=O), 138.5, 133.0, 128.5, 124.0, 120.9, 118.9, 63.7, 35.4, 26.7 (-$CH_3$).

3.10 2-acetyl-2-allyl-*N*-(*p*-tolyl)pent-4-enamide **(5i)**

MS (ESI-TOF) *m/z* calcd For CHNO $(M + H)^+$ : 271.16, Found: 271.11; % yield: 91%; MP: 106-108 °C $^1$H NMR (500 MHz, DMSO-D6) δ 9.41 (s, 1H, -NH), 7.43 (d, *J* = 10 Hz, 2H, Ar-

H), 7.10 (d, *J* = 10 Hz, 2H, Ar-H), 5.64 - 5.56 (m, 2H, -CH=C), 5.14 - 5.05 (m, 4H, $=CH_2$), 2.71 - 2.58 (m, 4H, $-CH_2$), 2.25 (s, 3H, $-CH_3$), 2.12 (s, 3H, $-CH_3$); $^{13}C$ {1H}NMR (126 MHz, DMSO-D6) δ 205.0 (-C=O), 169.0 (NH-C=O), 136.0, 133.1, 133.0, 128.9, 121.0, 118.8, 63.6, 35.4, 26.7, 20.5.

### 3.11 2-acetyl-2-allyl-*N*-(*o*-tolyl)pent-4-enamide **(5j)**

MS (ESI-TOF) *m/z* calcd For CHNO $(M + H)^+$ : 271.16, Found: 271.53; % yield: 93%; MP: 118-120 °C $^1H$ NMR (500 MHz, DMSO-D6) δ 9.27 (s, 1H, -NH), 7.24 - 7.12 (m, 4H, Ar-H), 5.70 - 5.62 (m, 2H, -CH=C), 5.19 - 5.10 (m, 4H, $=CH_2$), 2.73 - 2.61 (m, 4H, $-CH_2$), 2.18 (s, 3H, $-CH_3$), 2.17 (s, 3H, $-CH_3$); $^{13}C$ {1H}NMR (126 MHz, DMSO-D6) δ 205.19 (-C=O), 169.2 (NH-C=O), 136.0, 134.0, 133.1, 130.3, 126.9, 126.2, 126.0, 118.9, 63.0, 35.4, 26.7 ($-CH_3$), 17.9 ($-CH_3$).

### 3.12 2-acetyl-2-allyl-*N*-(4-chlorophenyl)pent-4-enamide **(5k)**

MS (ESI-TOF) *m/z* calcd For CHNO $(M + H)^+$ : 291.10 Found: 291.17; % yield: 94%; $^1H$ NMR (500 MHz, DMSO-D6) δ 9.64 (s, 1H, -NH), 7.62 (d, *J* = 10 Hz, 2H, Ar-H), 7.36 (d, *J* = 5 Hz, 2H, Ar-H), 5.64 - 5.56 (m, 2H, -CH=C), 5.14 - 5.05 (m, 4H, $=CH_2$), 2.71 - 2.59 (m, 4H, $-CH_2$), 2.13 (s, 3H, $-CH_3$); $^{13}C$ {1H}NMR (126 MHz, DMSO-D6) δ 204.9 (-C=O), 169.3 (NH-C=O), 137.6, 133.0, 128.4, 127.6, 122.4, 118.9, 63.8, 35.4, 26.7 ($-CH_3$).

### 3.13 2-acetyl-2-allyl-*N*-(2-chlorophenyl)pent-4-enamide **(5l)**

MS (ESI-TOF) *m/z* calcd For CHNO $(M + H)^+$ : 291.10, Found: 291.12; % yield: 85%;

## 4 NMR Spectra of 3a & 5(a-g)

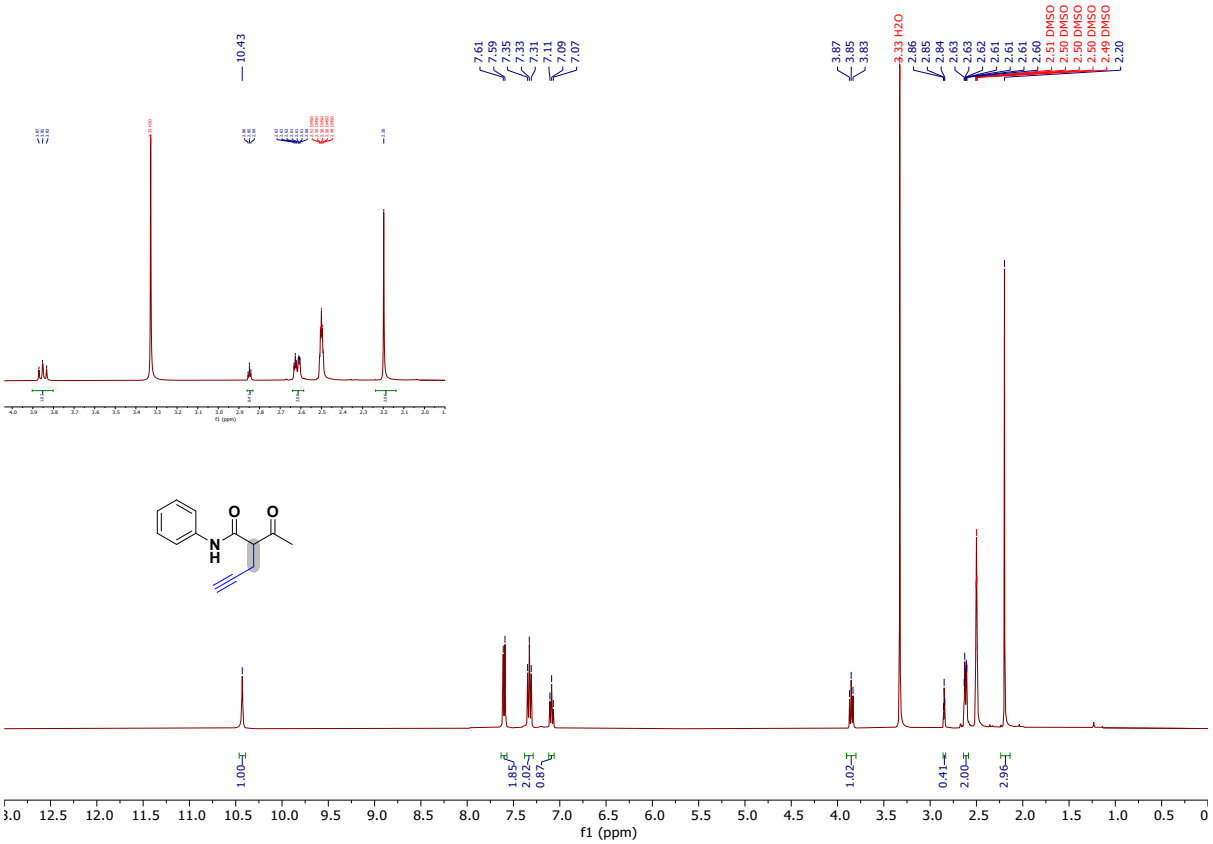


**Figure S1:** $^1H$ NMR spectra of compound **3a** (400 MHz, DMSO-$d_6$)

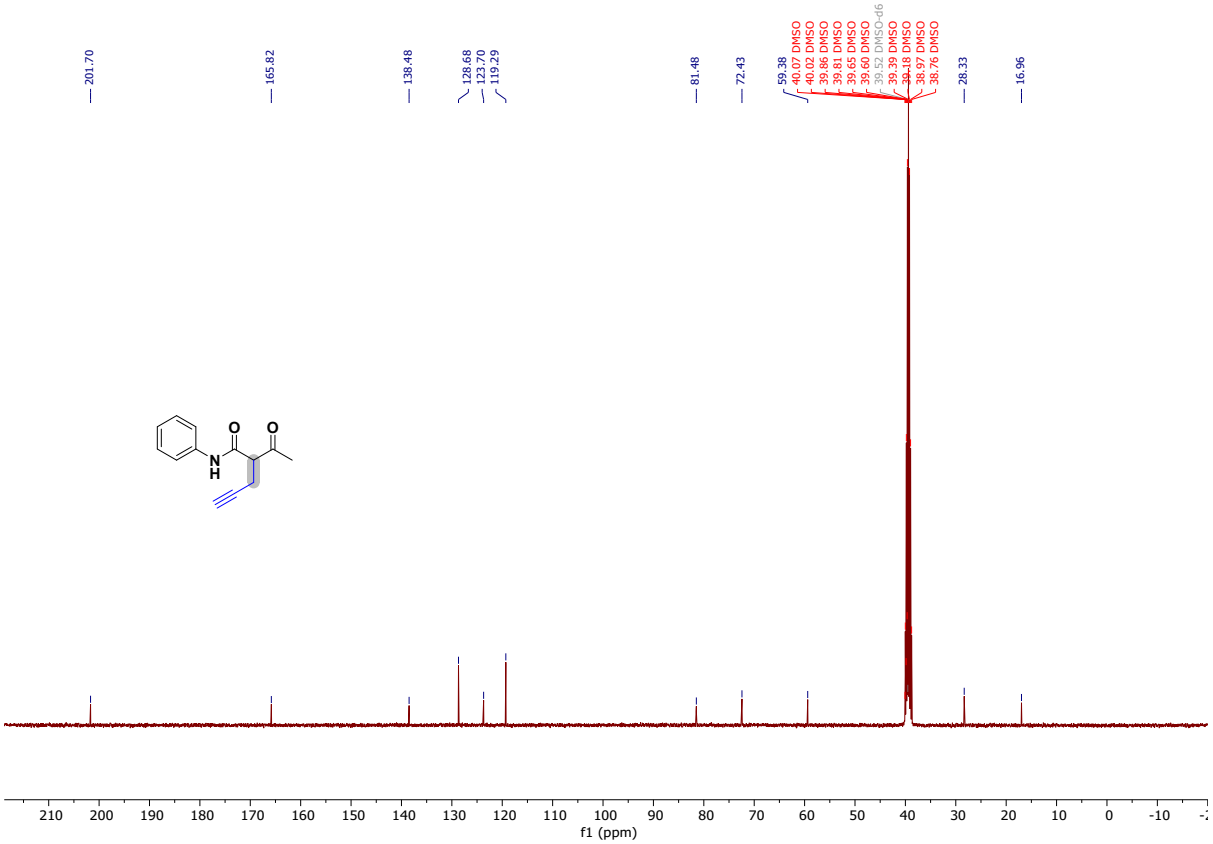


**Figure S2:** $^{13}$C NMR spectra of compound **3a** (101 MHz, DMSO-$d_6$)

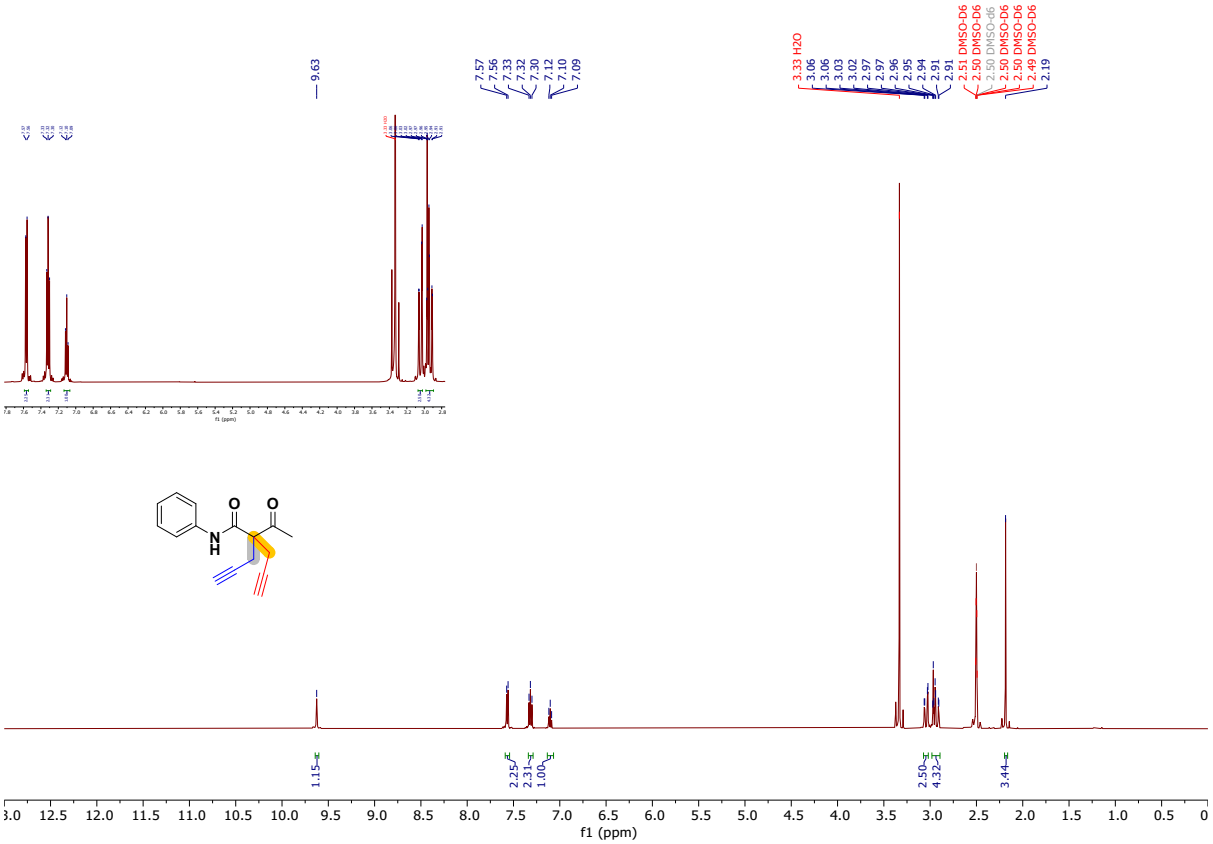


**Figure S3:** $^{1}$H NMR spectra of **5a** (500 MHz, DMSO-$d_6$)

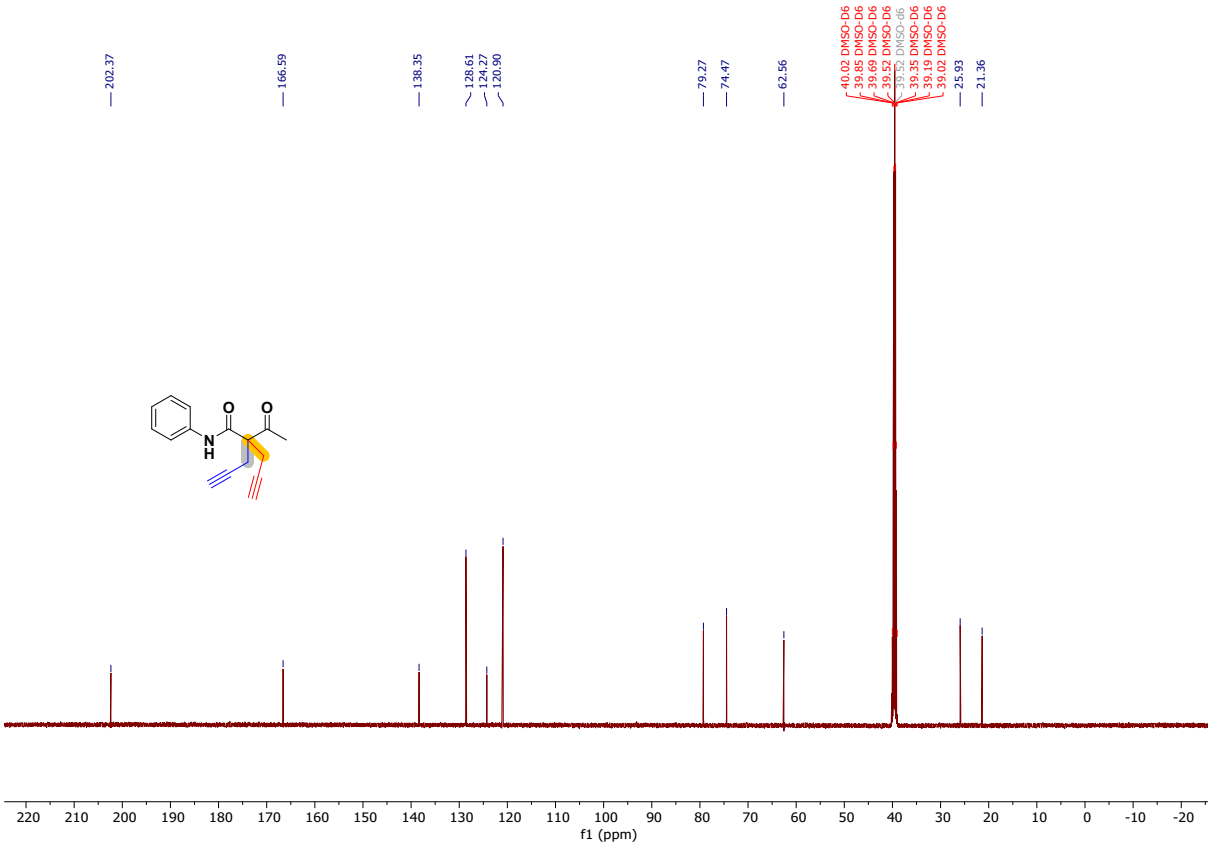


**Figure S4:** $^{13}$C NMR spectra of **5a** (126 MHz, DMSO-$d_6$)

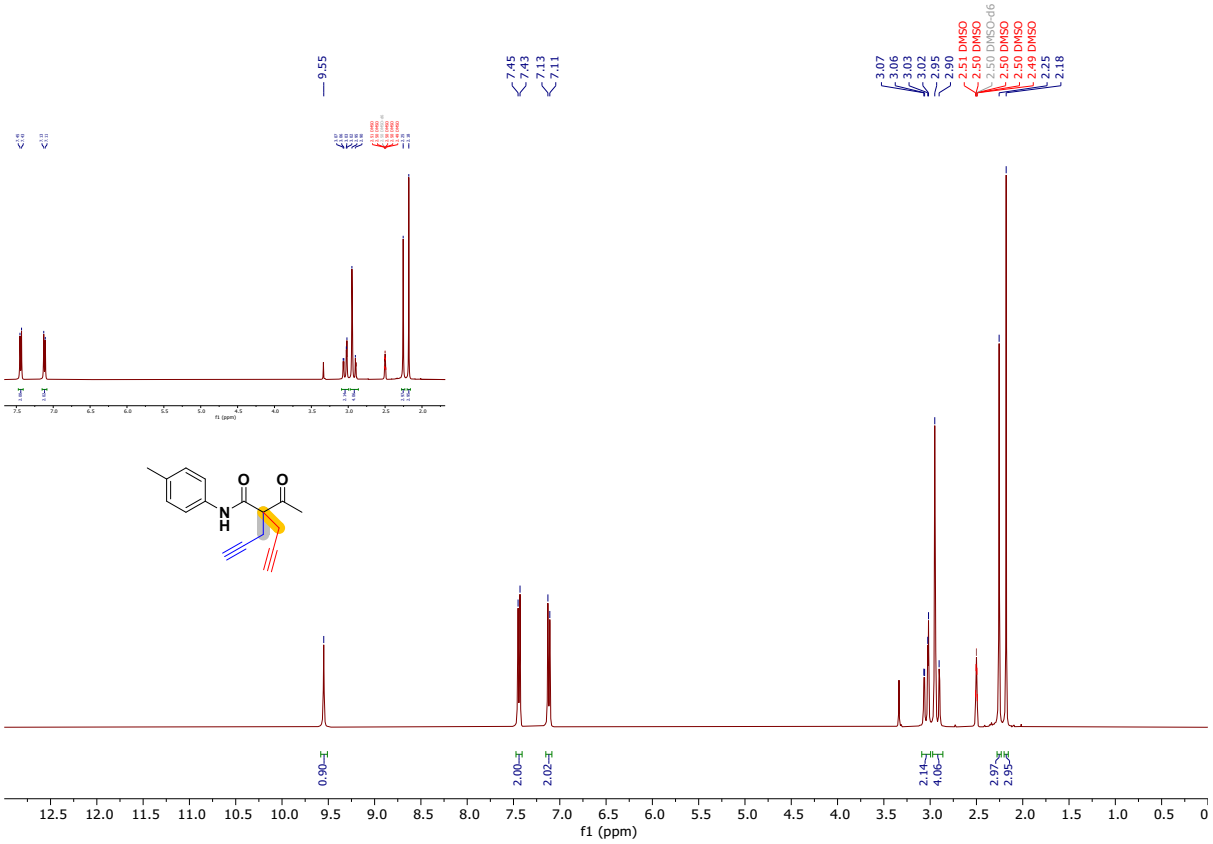


**Figure S5:** $^{1}$H NMR spectra of **5b** (400 MHz, DMSO-$d_6$)

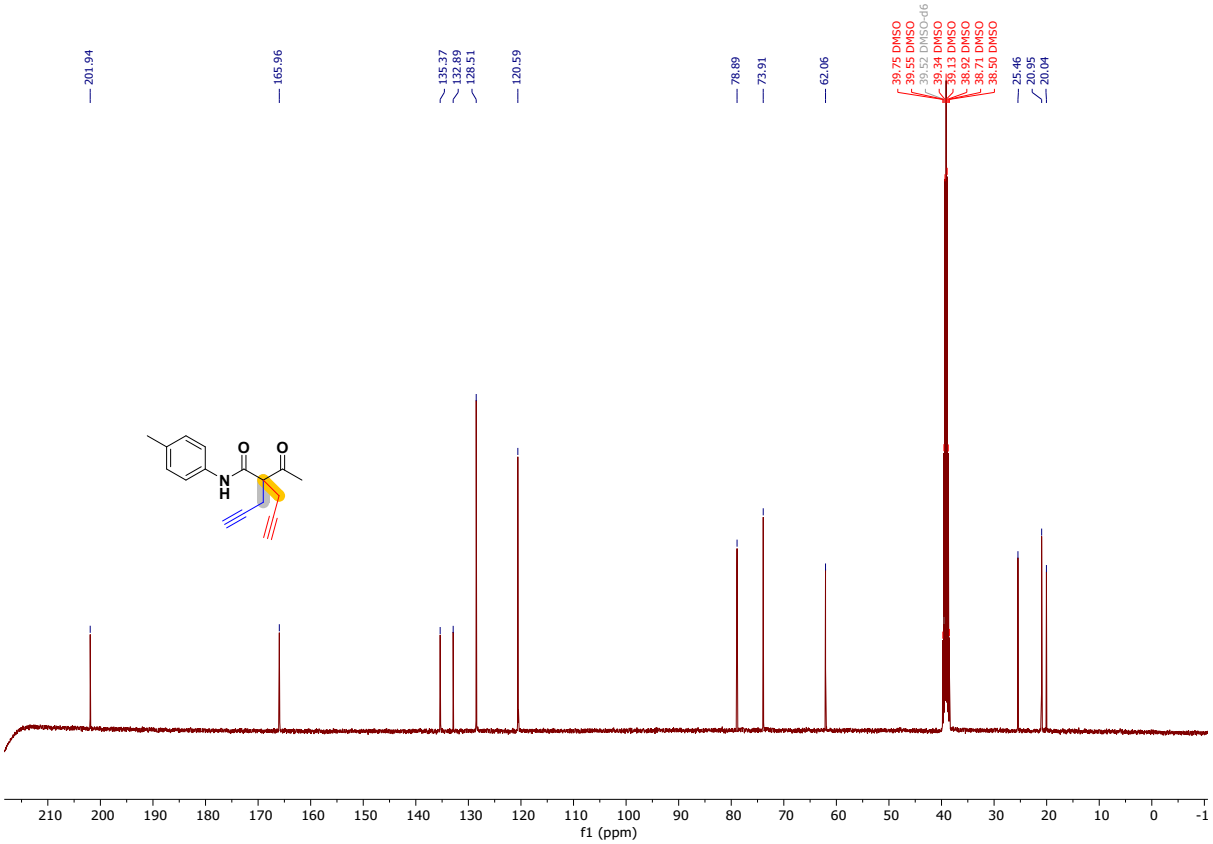


**Figure S6:** $^{13}$C NMR spectra of **5b** (101 MHz, DMSO-$d_6$)

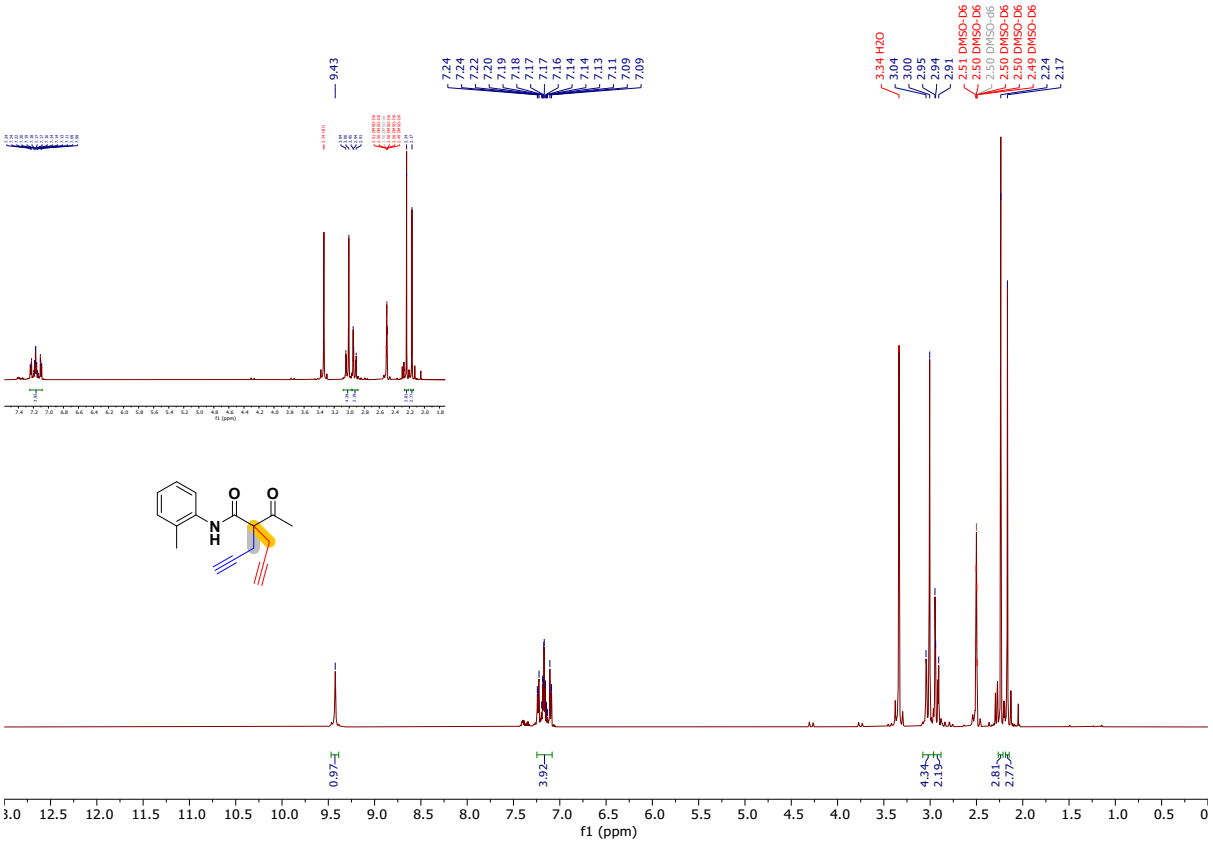


**Figure S7:** $^{1}$H NMR spectra of **5c** (500 MHz, DMSO-$d_6$)

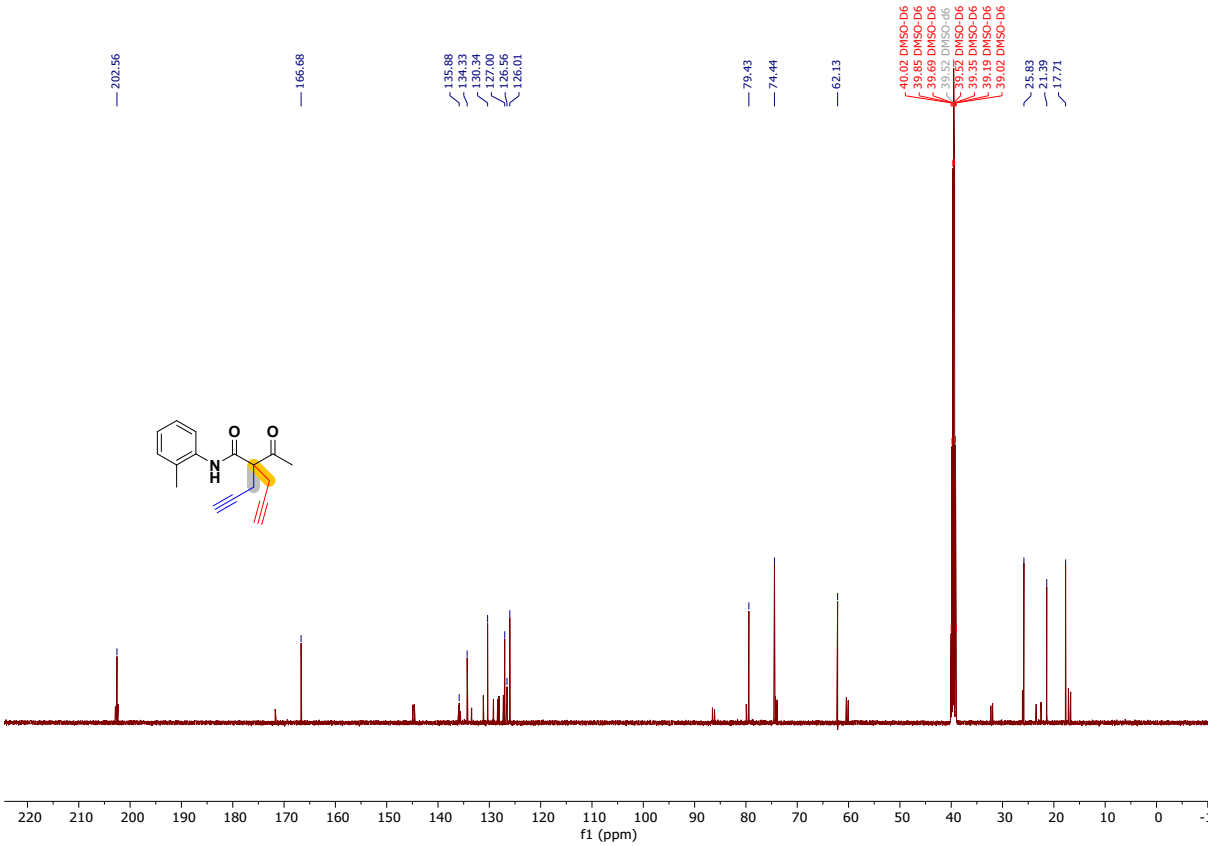


**Figure S8:** $^{13}$C NMR spectra of **5c** (126 MHz, DMSO-$d_6$)

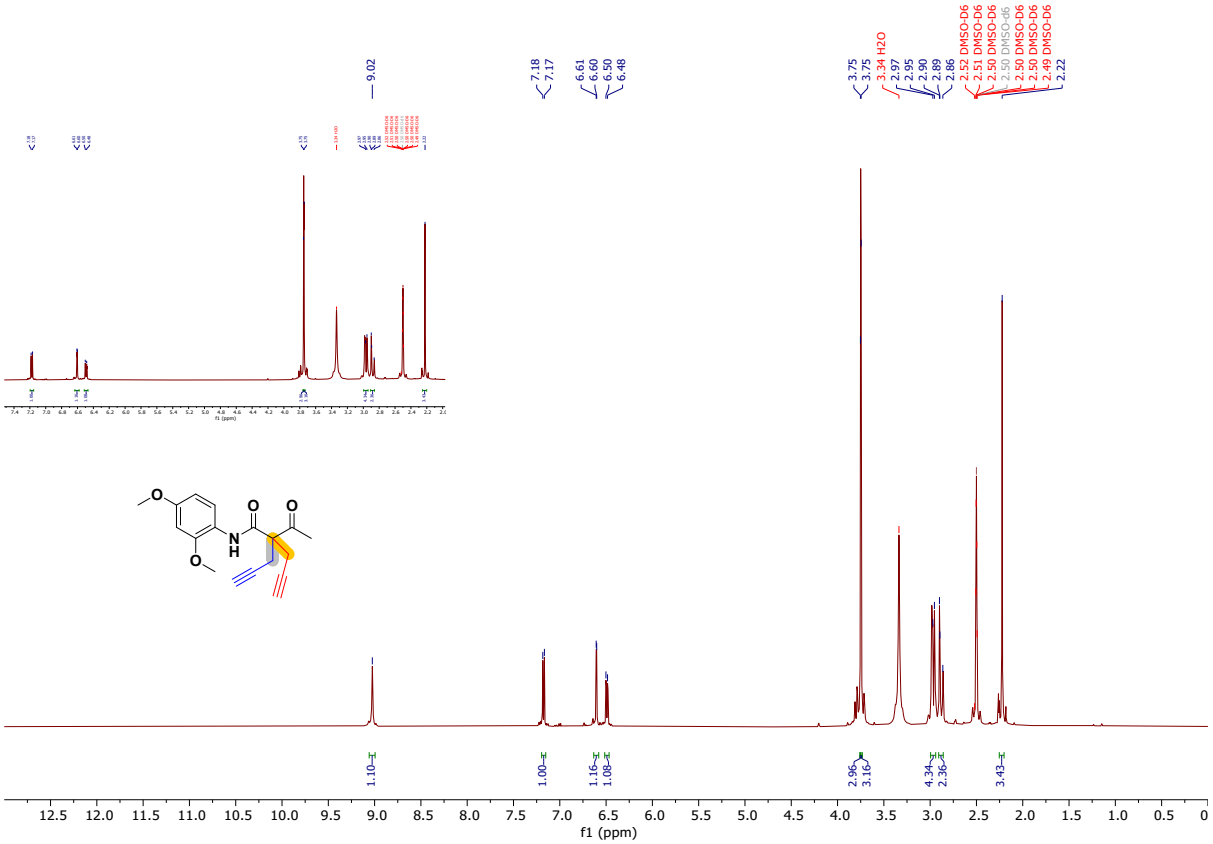


**Figure S9:** $^{1}$H NMR spectra of **5f** (500 MHz, DMSO-$d_6$)

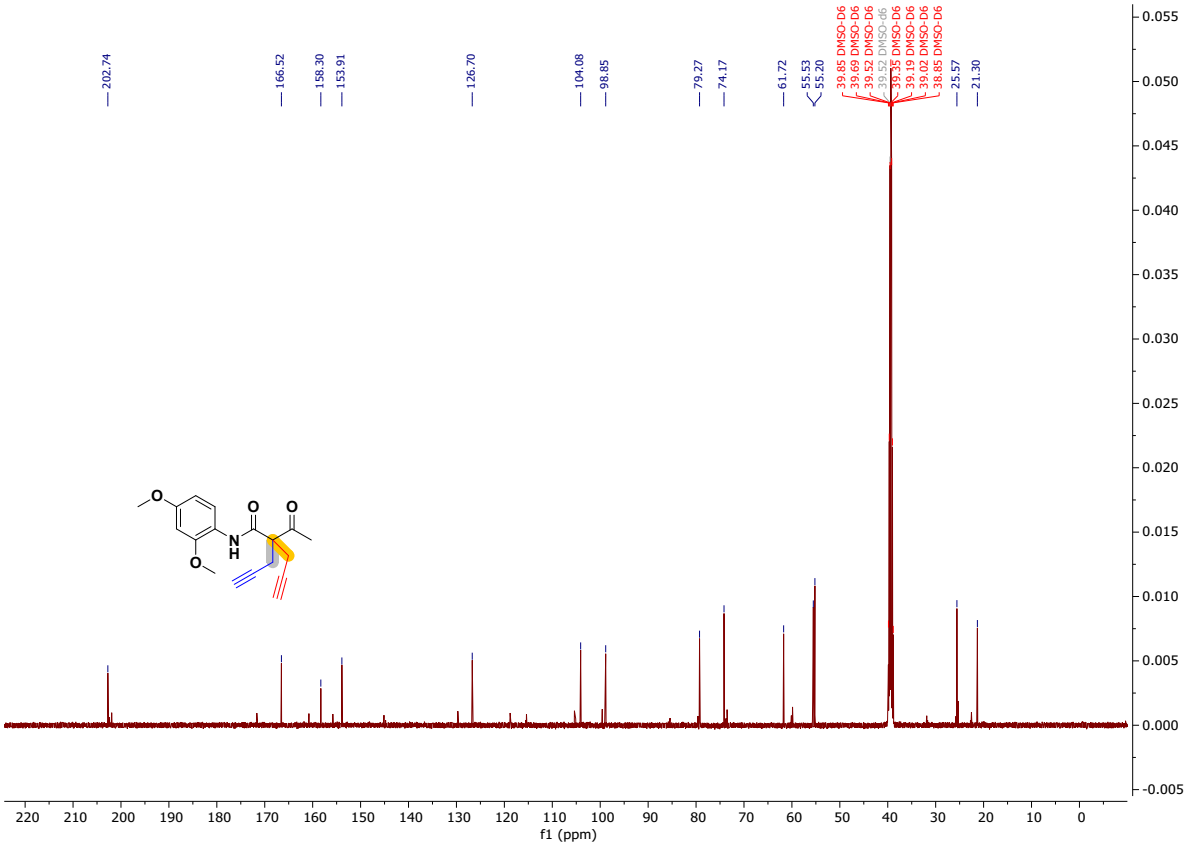


**Figure S10:** $^{13}$C NMR spectra of **5f** (126 MHz, DMSO-$d_6$)

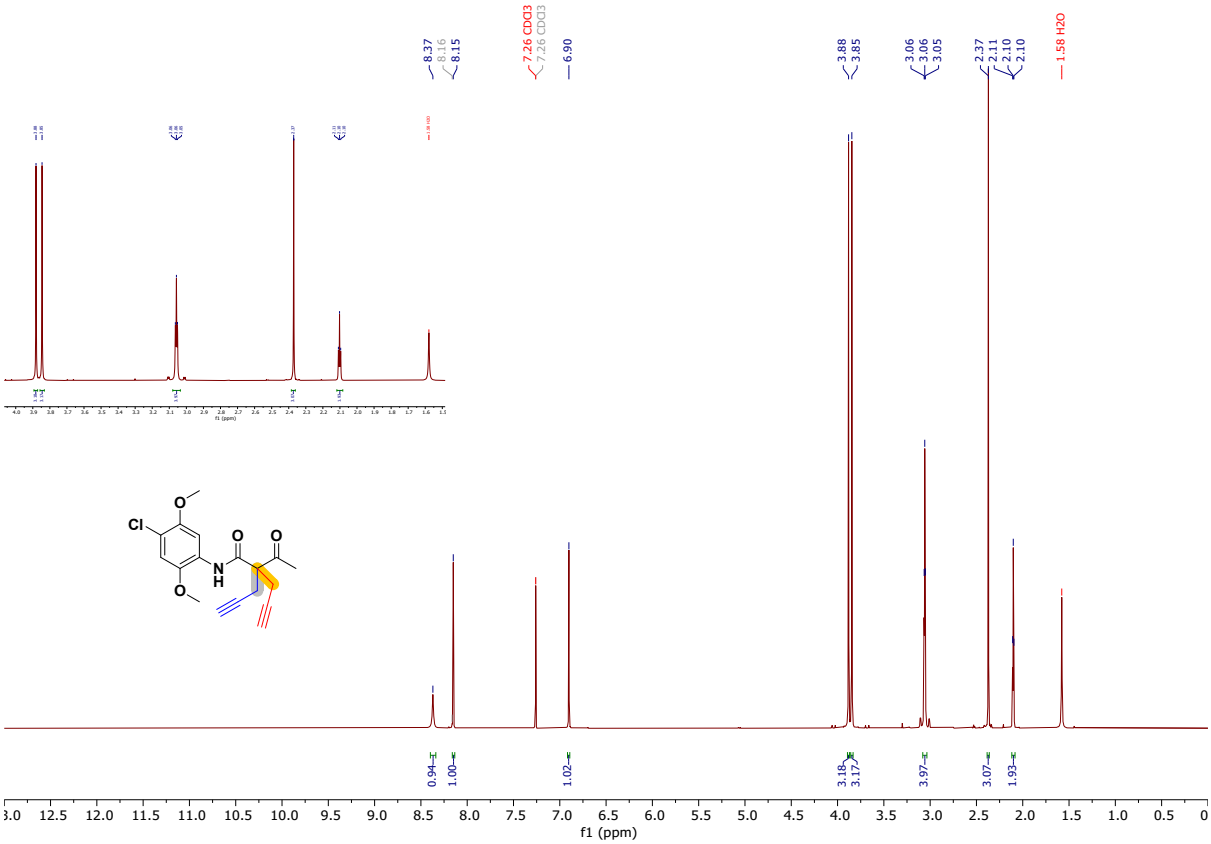


**Figure S11:** $^{1}$H NMR spectra of **5g** (400 MHz, $CDCl_3$)

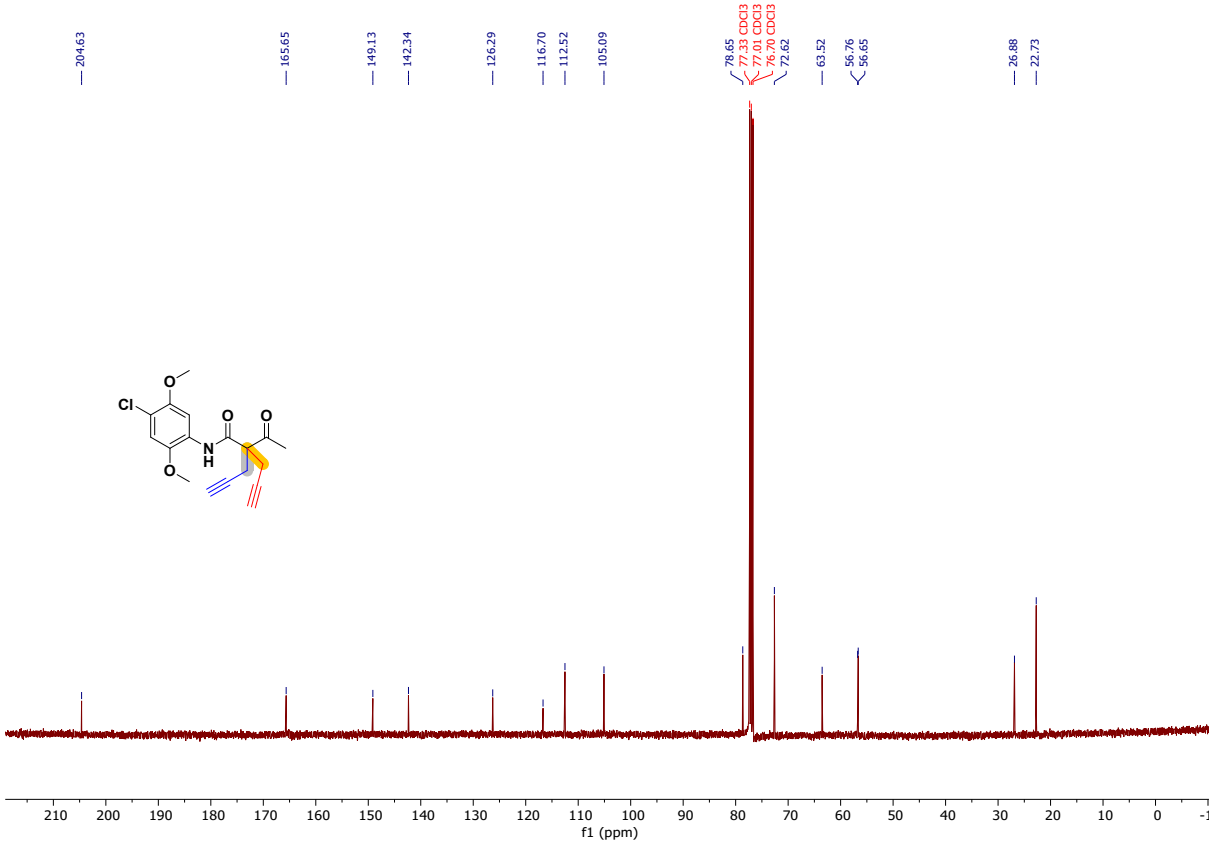


**Figure S12:** $^{13}C$ NMR spectra of **5g** (101 MHz, $CDCl_3$)

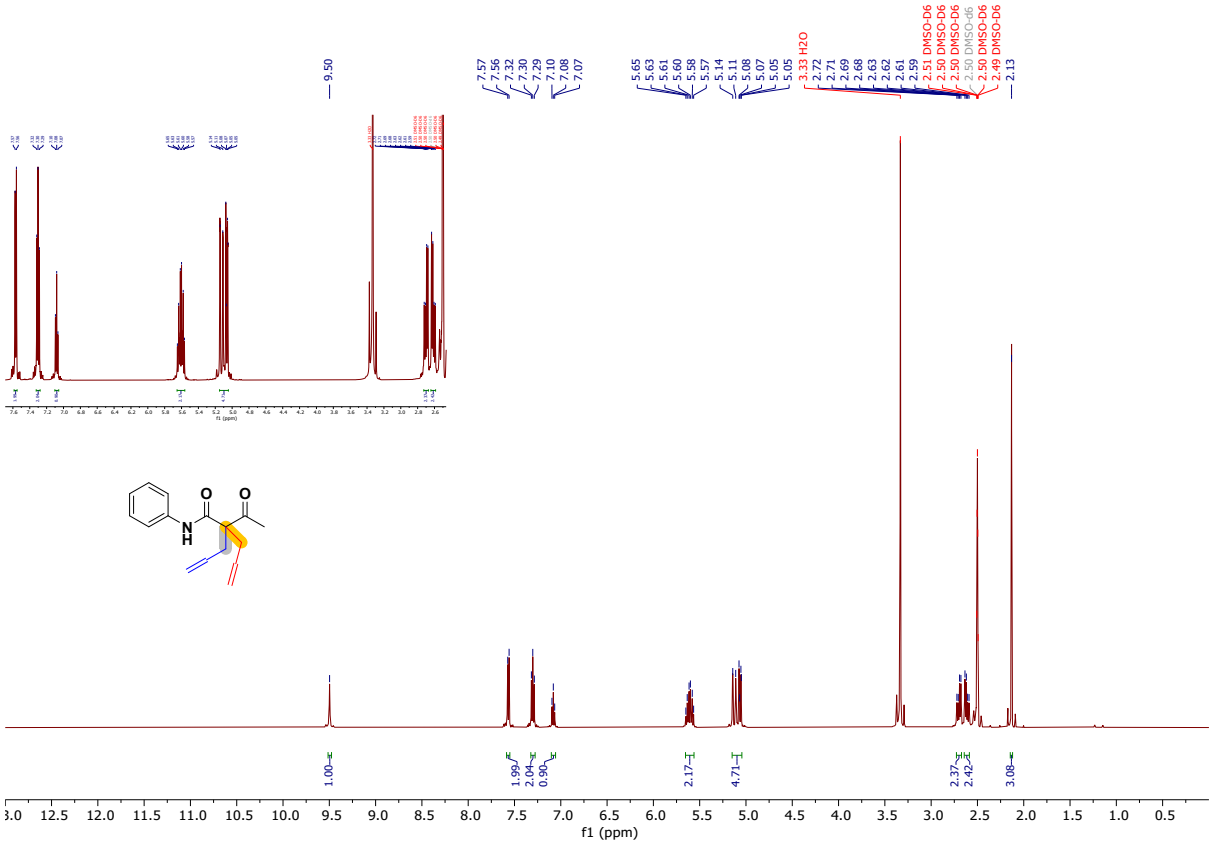


**Figure S13:** $^{1}H$ NMR spectra of **5h** (500 MHz, DMSO-$d_6$)

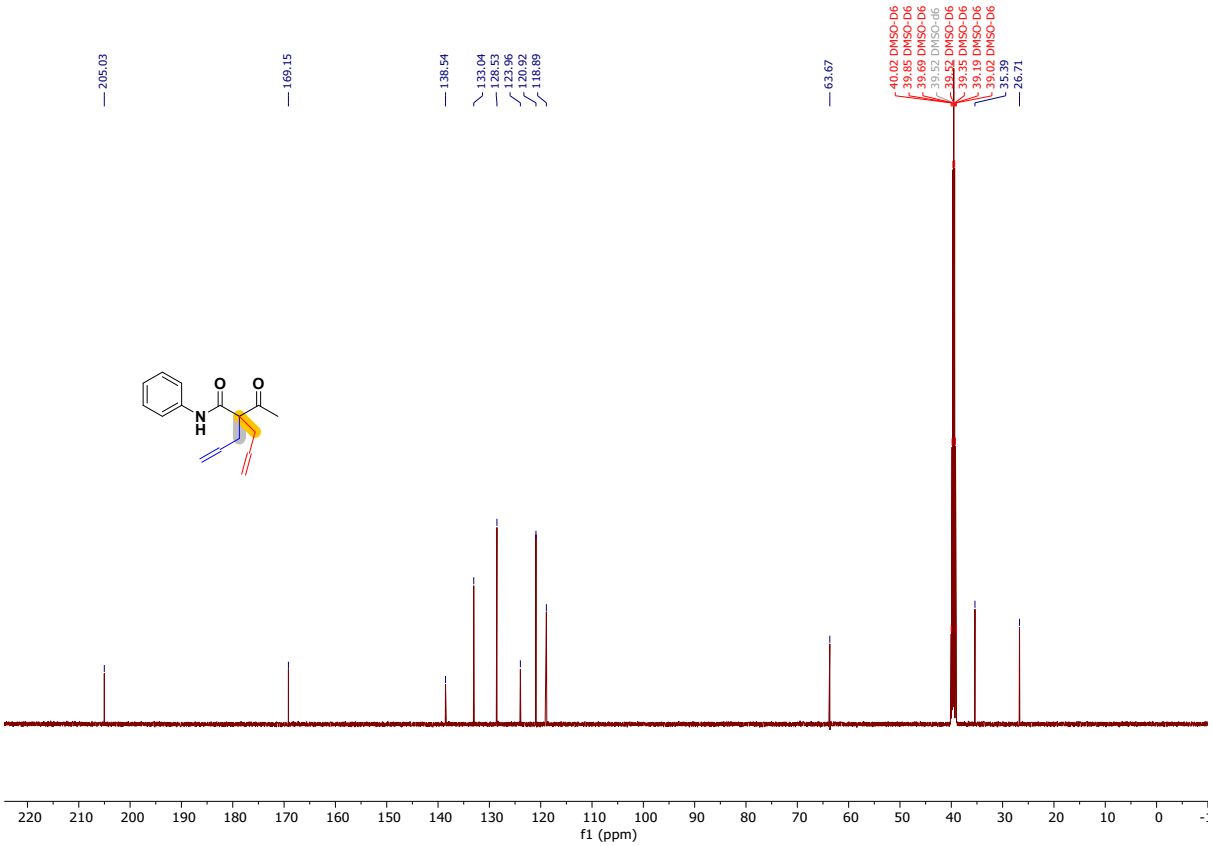


**Figure S14:** $^{13}$C NMR spectra of **5h** (126 MHz, DMSO-$d_6$)

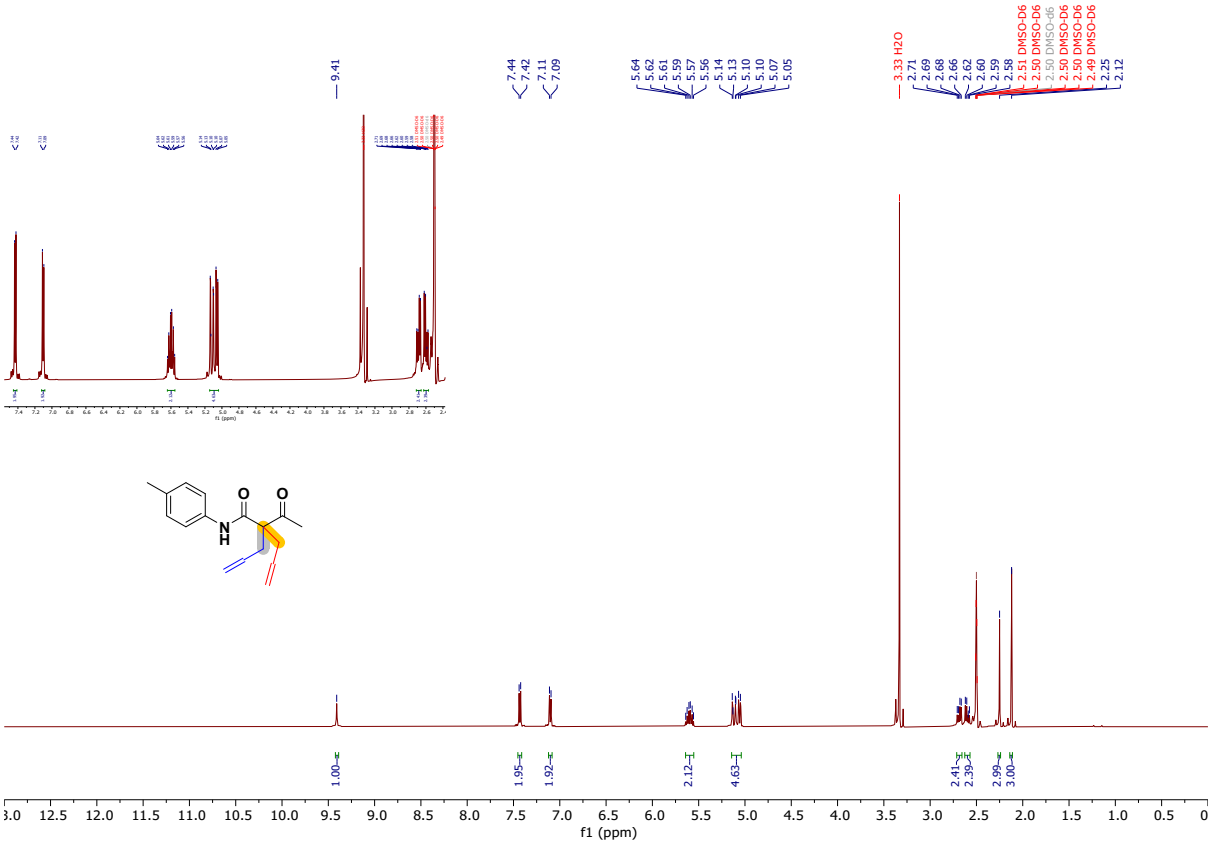


**Figure S15:** $^{1}$H NMR spectra of **5i** (500 MHz, DMSO-$d_6$)

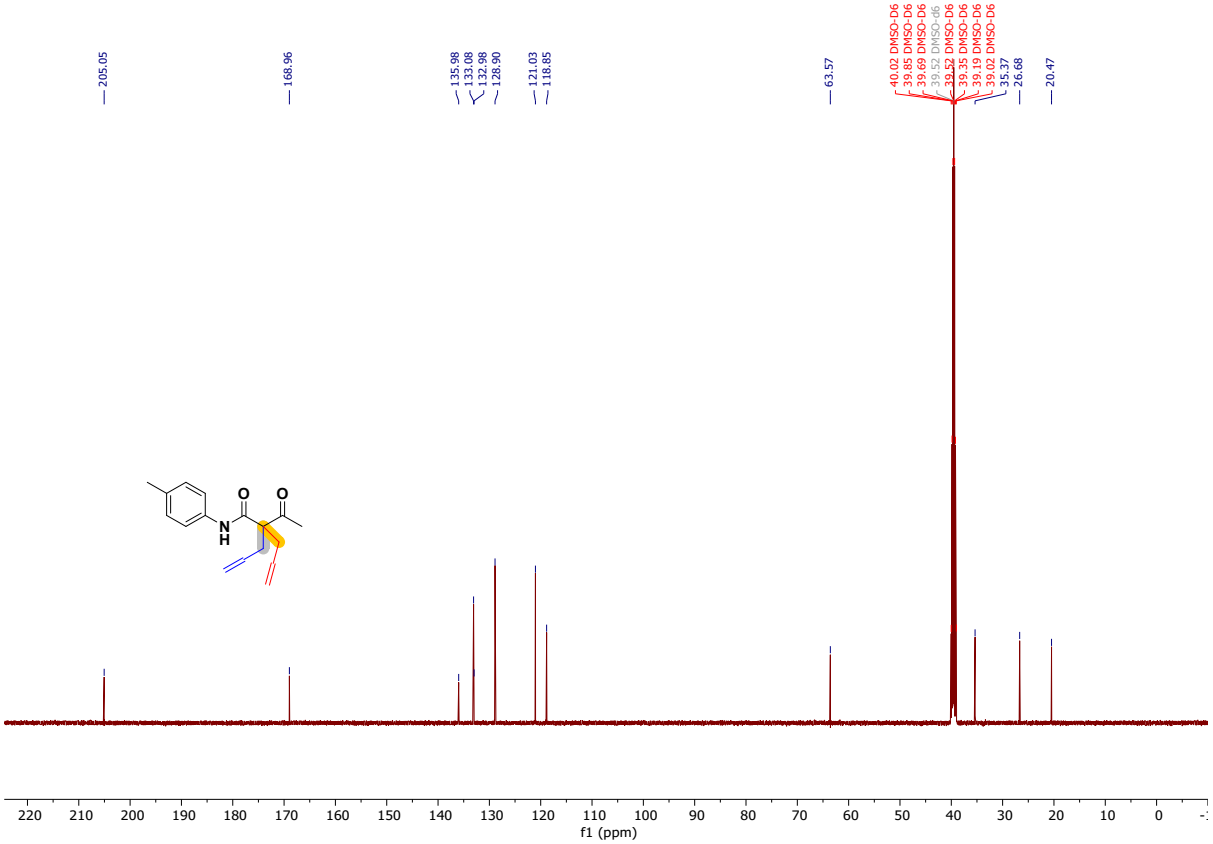


**Figure S16:** $^{13}$C NMR spectra of **5i** (126 MHz, DMSO-$d_6$)

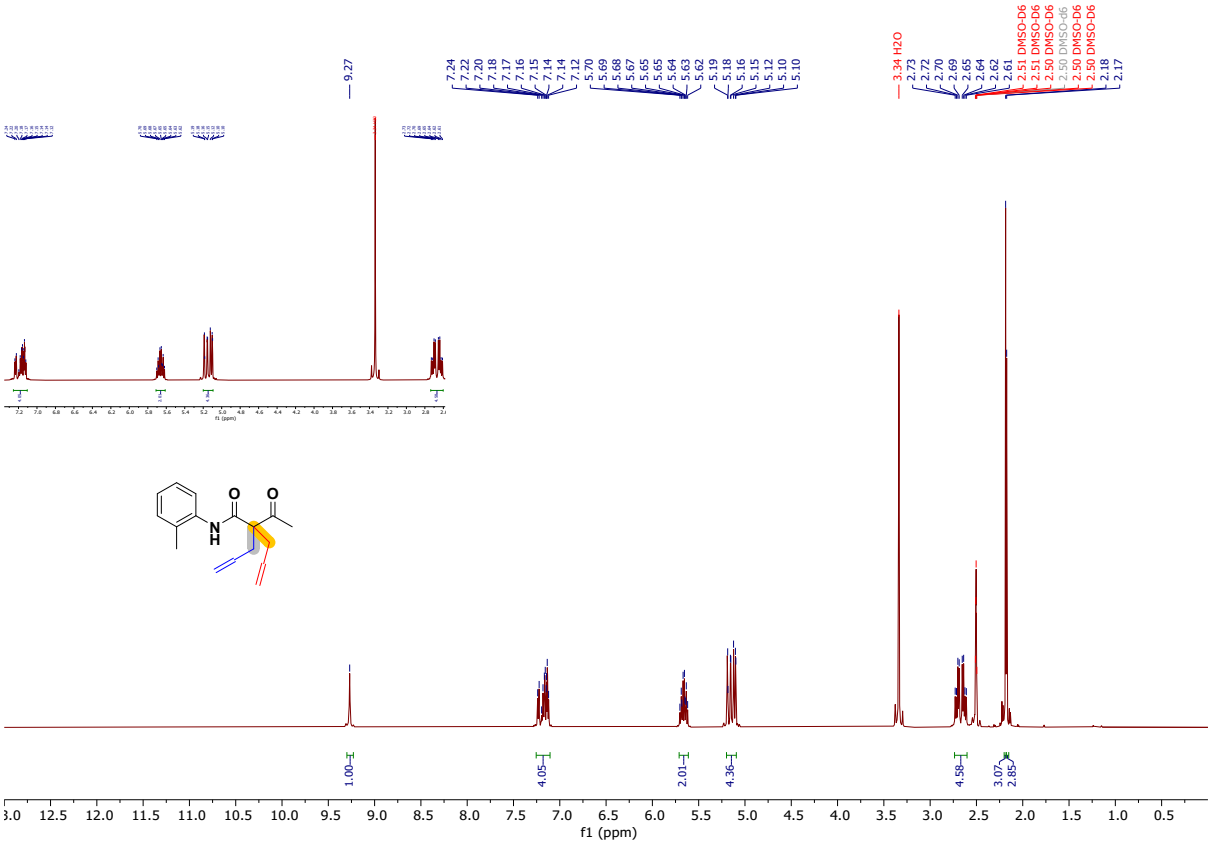


**Figure S17:** $^{1}$H NMR spectra of **5j** (500 MHz, DMSO-$d_6$)

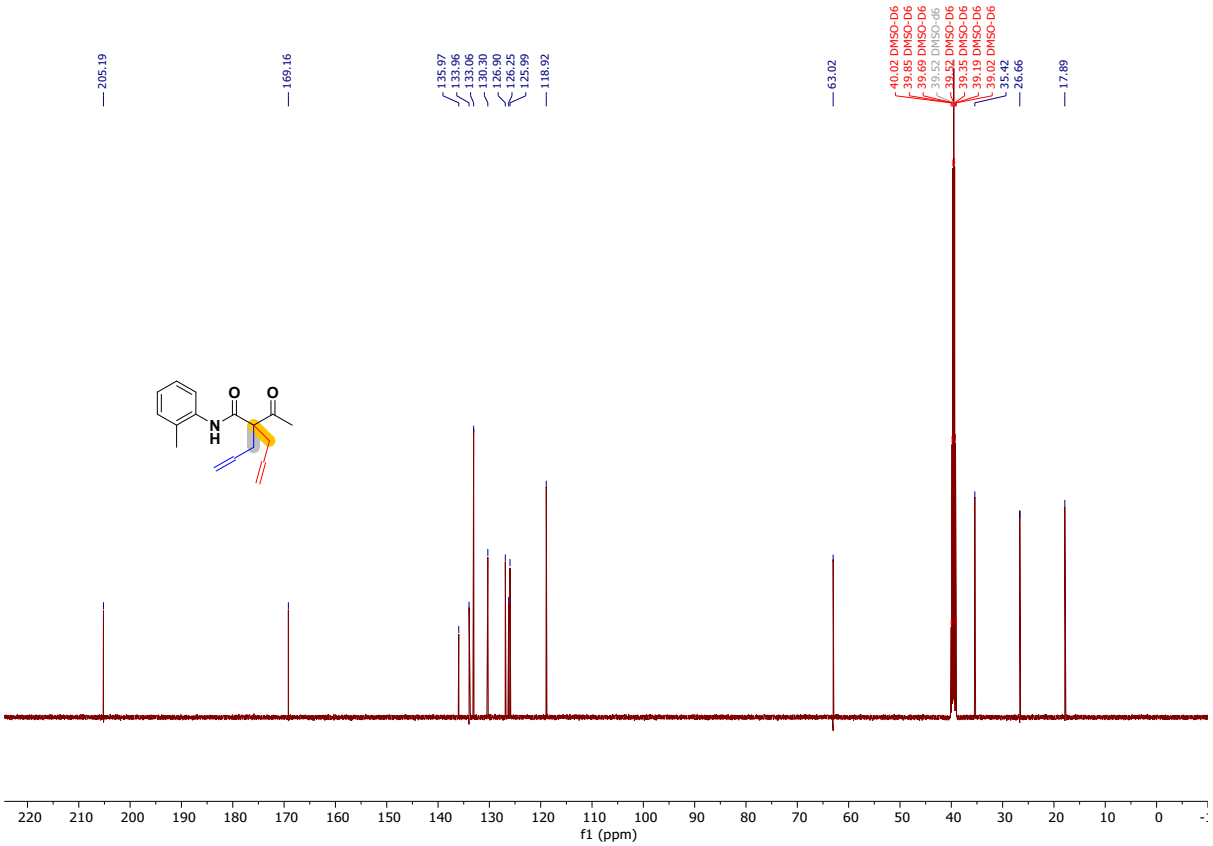


**Figure S18:** $^{13}$C NMR spectra of **5j** (126 MHz, DMSO-$d_6$)

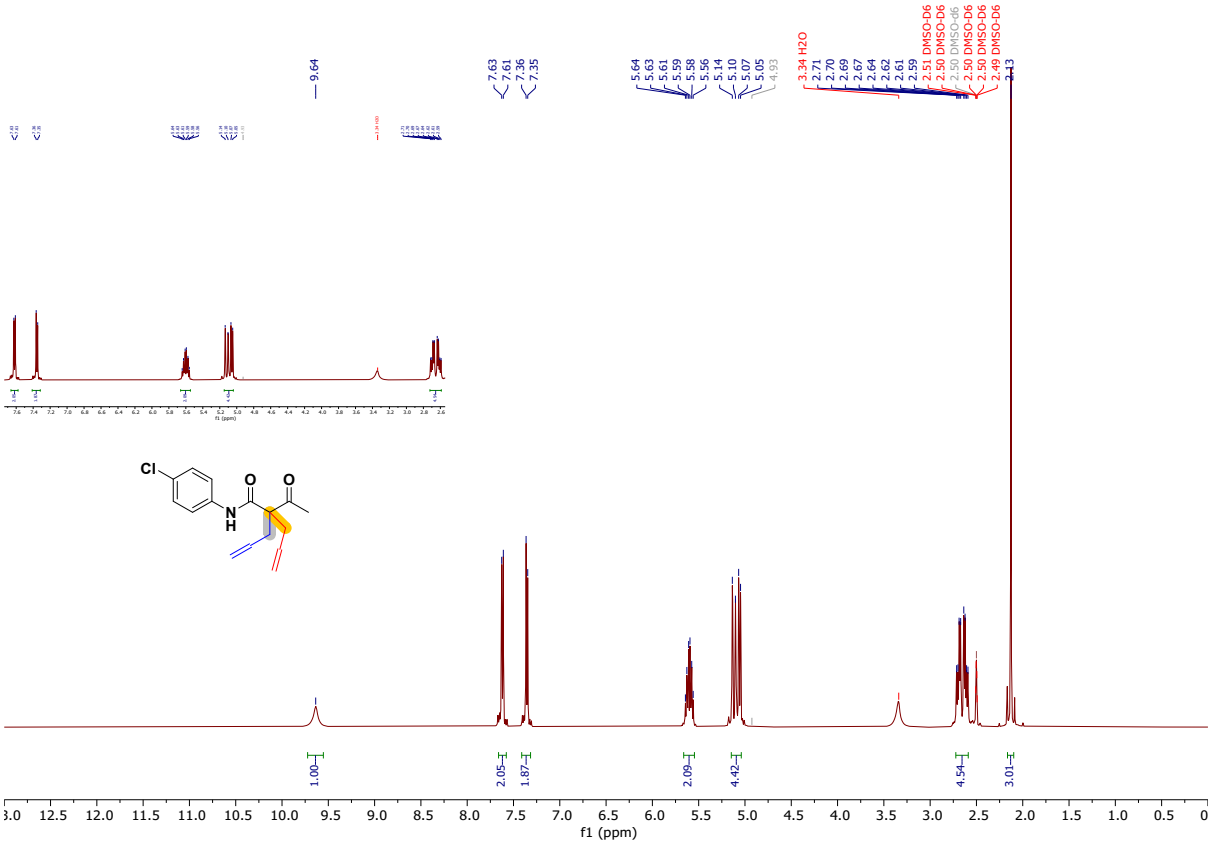


**Figure S19:** $^{1}$H NMR spectra of **5k** (500 MHz, DMSO-$d_6$)

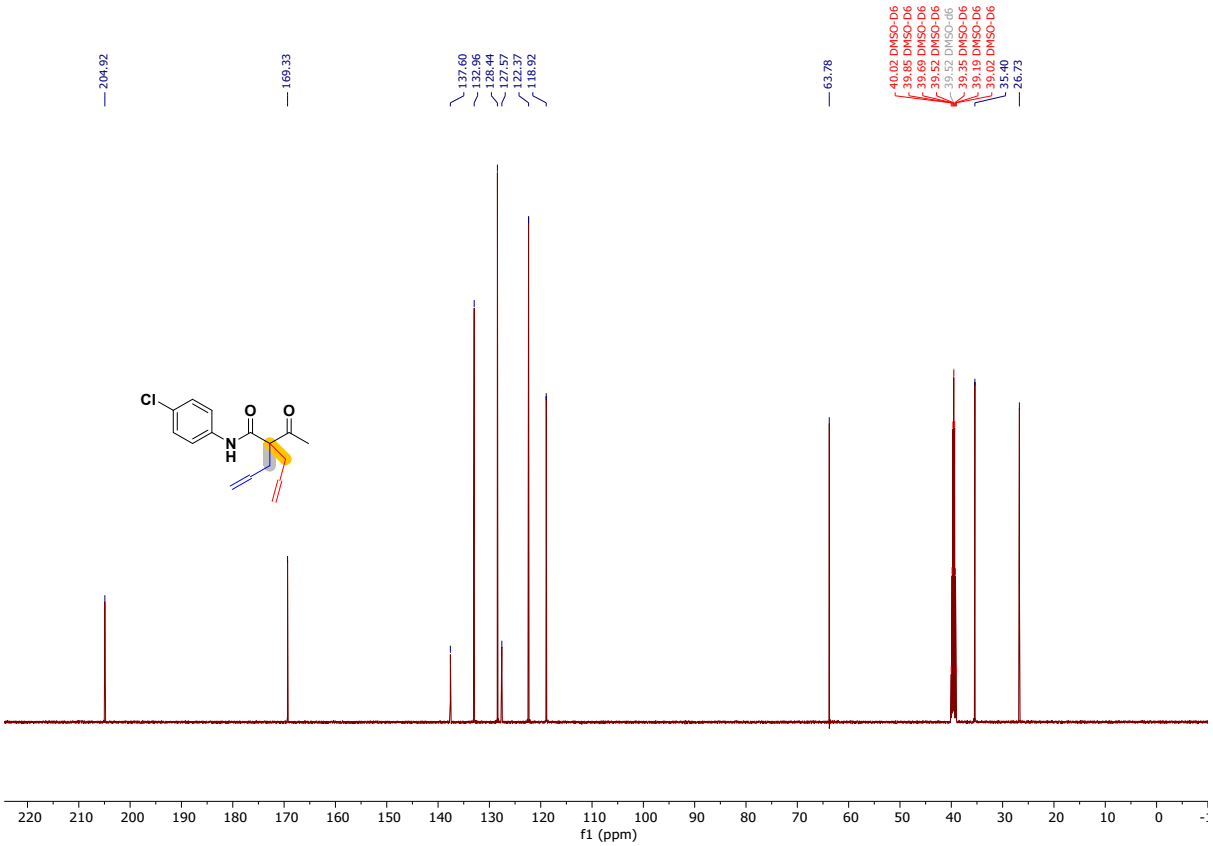


**Figure S20:** $^{13}$C NMR spectra of **5k** (126 MHz, DMSO-$d_6$)

# 5 Mass Analysis image

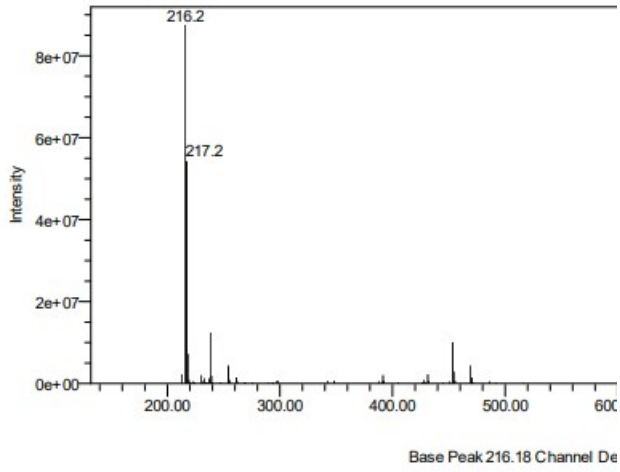


**Figure S21:** MS (ESI-TOF) *m/z* of **3a**

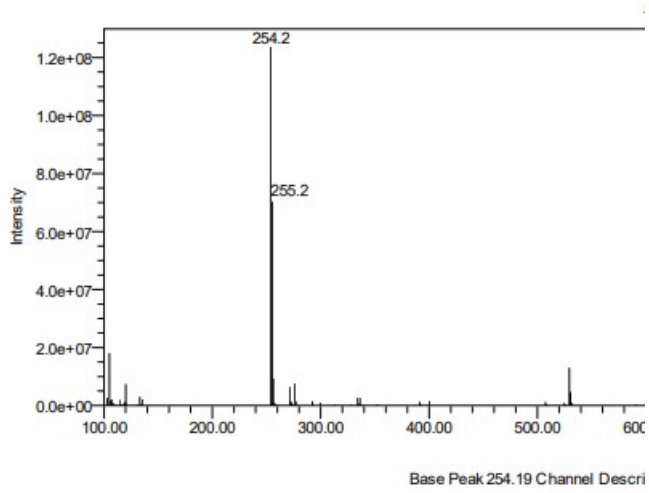


**Figure S22:** MS (ESI-TOF) *m/z* of **5a**

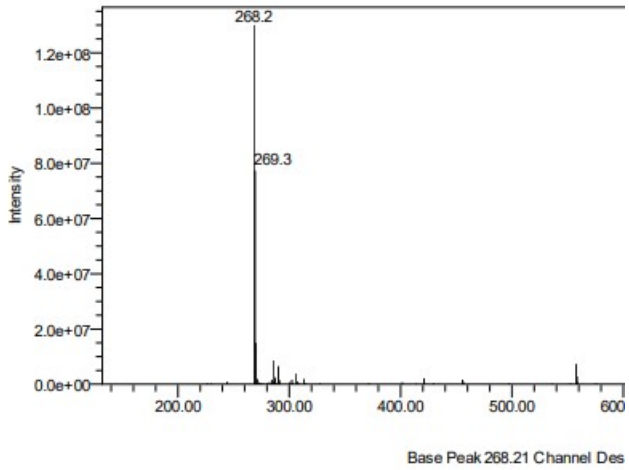


**Figure S23:** MS (ESI-TOF) *m/z* of **5b**

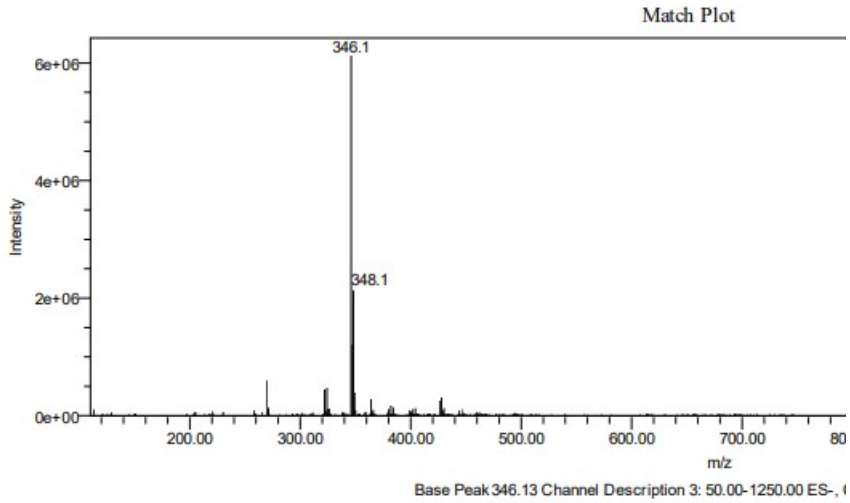


**Figure S24:** MS (ESI-TOF) *m/z* of **5g**

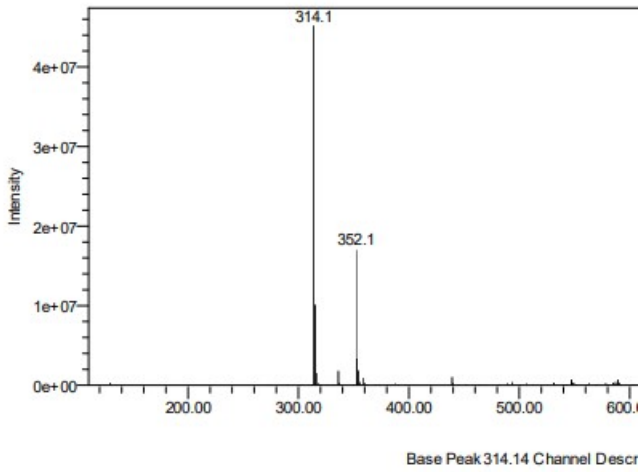


**Figure S25:** MS (ESI-TOF) *m/z* of **5h**

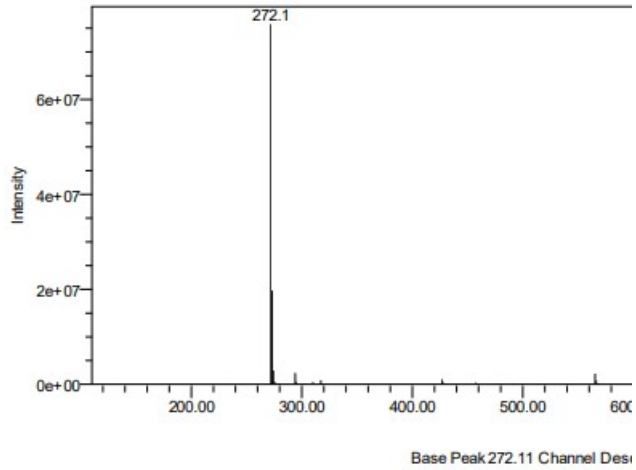


**Figure S26:** MS (ESI-TOF) *m/z* of **5i**

# 6 Crystallographic investigation

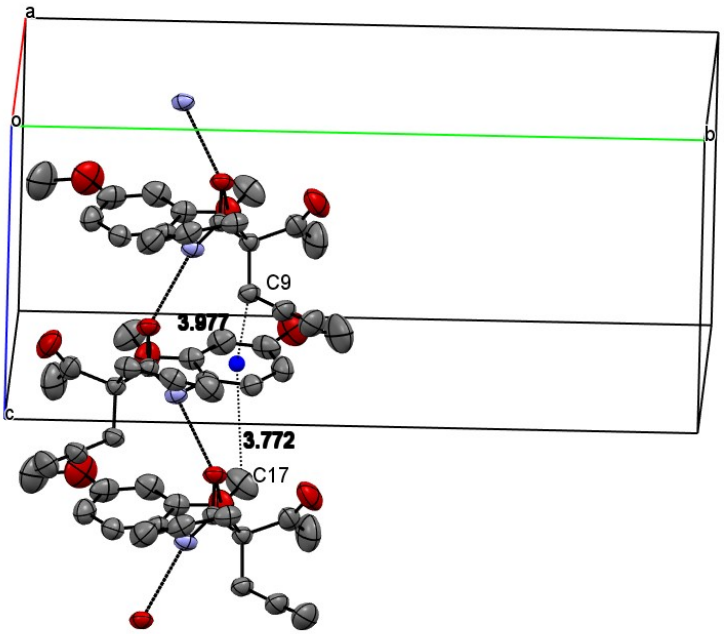


**Figure S27:** intermolecular sandwich type C-H…π internation

| | | |
|---|---|---|
| Crystal description | Colourless | |
| Crystal Size | 0.080 x 0.160 x 0.290 mm | |
| Empirical formula | $C_{18}H_{19}NO_4$ | |
| Formula weight | 313.34 | |
| Radiation, Wavelength | Mo *K*α, 0.71073 Å | |
| Unit cell dimension | a = 10.3767(5) Å | α = 90° |
| | b = 20.8762(10) Å | β = 113.4574(19)° |
| | c = 8.8540(3) Å | ɣ = 90° |
| Crystal system | Monoclinic | |
| Space group | p-1 21/c 1 | |
| Unit cell volume | 1759.50(14) $Å^3$ | |
| No. of molecule per unit cell, Z | 4 | |
| Temperature | 296(2) K | |
| Absorption coefficient | 0.084 $mm^{-1}$ | |
| F(000) | 644 | |
| Method of absorption correction | Multi-scan | |
| θ range for the entire data collection | 1.95 to 25.00° | |
| Density (calculated) | 1.183 $g/cm^3$ | |

**Table S1**: Preliminary Crystal data and structure refinement for **5f**

# 7 DFT Calculations

## 7.1 Optimization

The DFT studies were carried out using the B3LYP method with the 6-311G(d,p) basis set. The optimization of molecular structures using DFT showed excellent convergence for most of the systems, with all key parameters well within the defined thresholds. The mean maximum force across the systems was approximately 0.00003, significantly below the threshold of 0.000450. The RMS force also averaged at around 0.00052, comfortably meeting the threshold of 0.000300. For displacements, the mean maximum displacement was calculated at 0.00102, well within the allowable limit of 0.001800, and the mean RMS displacement was 0.00067, which also satisfied the threshold of 0.001200. These results indicate successful structural optimization for the majority of systems, with the exception of a few intermediates (INT-IIa, INT-IIb, INT-IIIb) and a transition state (TS-III) where slight deviations in force and displacement values were noted. Despite these exceptions, the overall convergence performance was robust and in line with the expectations for accurate molecular structure optimization.

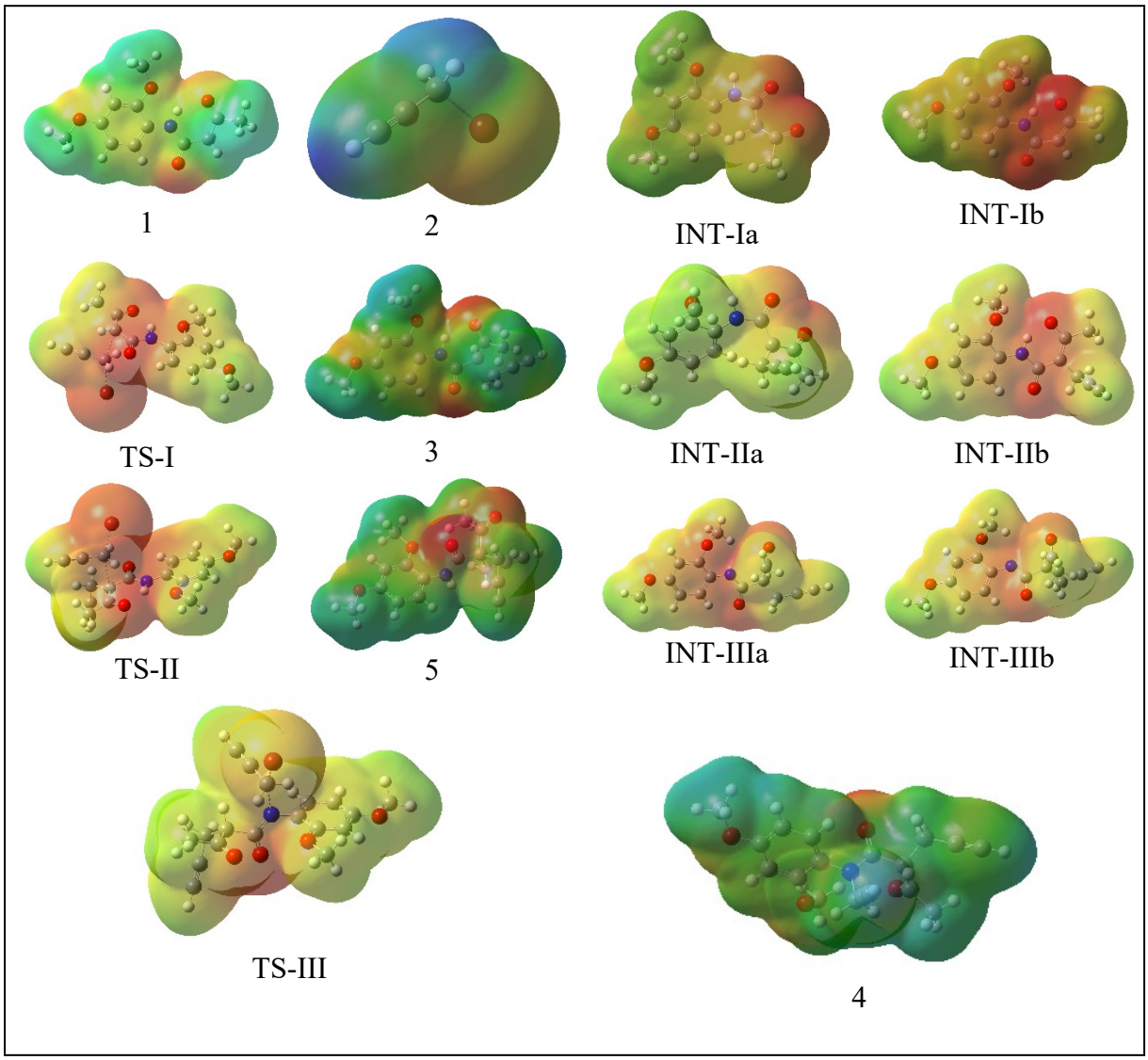


**Figure S28**. Electrostatic potential surface of all molecule

| | H (eV) | L (eV) | (ΔE) (eV) | χ (eV) | η (eV) | s ($eV^{-1}$) | μ (eV) | ω(eV) | ΔN max |
|---|---|---|---|---|---|---|---|---|---|
| 1a | -5.22 | -1.16 | 4.06 | 3.19 | 2.03 | 0.49 | −3.19 | 2.50 | 1.57 |
| INT Ia | -5.79 | -0.94 | 4.84 | 3.36 | 2.42 | 0.41 | −3.36 | 2.34 | 1.39 |
| INT Ib | -4.58 | -0.06 | 4.52 | 2.32 | 2.26 | 0.44 | -2.32 | 1.19 | 1.02 |
| 2 | -7.56 | -1.38 | 6.17 | 4.47 | 3.08 | 0.32 | -4.47 | 3.24 | 1.45 |
| TS-I | -5.29 | -2.58 | 2.71 | 3.94 | 1.35 | 0.73 | -3.94 | 5.71 | 2.90 |
| 3 | -5.61 | -1.37 | 4.24 | 3.49 | 2.12 | 0.47 | -3.49 | 2.87 | 1.64 |
| INT IIIa | -4.57 | -0.30 | 4.27 | 2.43 | 2.13 | 0.46 | −2.43 | 1.39 | 1.14 |
| INT IIIb | -4.58 | -0.64 | 3.93 | 2.61 | 1.96 | 0.50 | -2.61 | 1.73 | 1.32 |
| INT IIa | -4.48 | -0.01 | 4.47 | 2.25 | 2.23 | 0.44 | -2.25 | 1.13 | 1.00 |
| INT IIb | -4.51 | -0.05 | 4.45 | 2.28 | 2.22 | 0.44 | -2.28 | 1.16 | 1.02 |
| TS-II | -5.28 | -2.63 | 2.65 | 3.96 | 1.82 | 0.54 | −3.96 | 7.23 | 2.17 |
| TS-III | -5.41 | -2.23 | 3.18 | 3.82 | 1.59 | 0.62 | −3.82 | 4.59 | 2.40 |
| **4** | **-6.16** | **-1.32** | **4.84** | **3.74** | **2.42** | **0.41** | **−3.74** | **5.52** | **1.54** |
| **5** | **-6.10** | **-1.12** | **4.98** | **3.61** | **2.49** | **0.40** | **−3.61** | **5.14** | **1.45** |
| | HOMO(H), LUMO(L), Energy Gap (ΔE), Electronegativity (χ), Chemical Hardness (η), Chemical Softness (s), Chemical Potential (μ), Electrophilicity (ω), ΔN max | | | | | | | | |

**Table S2**: Quantum Chemical calculation

| **1** | | | |
|---|---|---|---|
| Item | Value | Threshold | Converged? |
| Maximum Force | 0.000009 | 0.000450 | YES |
| RMS Force | 0.000002 | 0.000300 | YES |
| Maximum Displacement | 0.001187 | 0.001800 | YES |
| RMS Displacement | 0.000200 | 0.001200 | YES |
| **2** | | | |
| Item | Value | Threshold | Converged? |
| Maximum Force | 0.000155 | 0.000450 | YES |
| RMS Force | 0.000058 | 0.000300 | YES |
| Maximum Displacement | 0.001106 | 0.001800 | YES |
| RMS Displacement | 0.000410 | 0.001200 | YES |
| **INT-Ia** | | | |
| Item | Value | Threshold | Converged? |
| Item | 0.000037 | 0.000450 | YES |
| Maximum Force | 0.000008 | 0.000300 | YES |
| RMS Force | 0.002716 | 0.001800 | YES |
| Maximum Displacement | 0.000590 | 0.001200 | YES |
| **INT-Ib** | | | |
| Item | Value | Threshold | Converged? |
| Item | 0.000002 | 0.000450 | YES |
| Maximum Force | 0.000001 | 0.000300 | YES |
| RMS Force | 0.000901 | 0.001800 | YES |
| Maximum Displacement | 0.000140 | 0.001200 | YES |
| **TS-I** | | | |
| Item | Value | Threshold | Converged? |
| Item | 0.000002 | 0.000450 | YES |
| Maximum Force | 0.000000 | 0.000300 | YES |

| | | | |
|---|---|---|---|
| RMS Force | 0.000982 | 0.001800 | YES |
| Maximum Displacement | 0.000193 | 0.001200 | YES |
| **3** | | | |
| Item | Value | Threshold | Converged? |
| Item | 0.000005 | 0.000450 | YES |
| Maximum Force | 0.000001 | 0.000300 | YES |
| RMS Force | 0.001858 | 0.001800 | YES |
| Maximum Displacement | 0.000522 | 0.001200 | YES |
| **INT-IIa** | | | |
| Item | Value | Threshold | Converged? |
| Item | 0.000013 | 0.000450 | YES |
| Maximum Force | 0.000003 | 0.000300 | YES |
| RMS Force | 0.002840 | 0.001800 | NO |
| Maximum Displacement | 0.000577 | 0.001200 | YES |
| **INT-IIb** | | | |
| Item | Value | Threshold | Converged? |
| Item | 0.000011 | 0.000450 | YES |
| Maximum Force | 0.000003 | 0.000300 | YES |
| RMS Force | 0.003145 | 0.001800 | NO |
| Maximum Displacement | 0.000622 | 0.001200 | YES |
| **TS-II** | | | |
| Item | Value | Threshold | Converged? |
| Item | 0.000009 | 0.000450 | YES |
| Maximum Force | 0.000001 | 0.000300 | YES |
| RMS Force | 0.001257 | 0.001800 | YES |
| Maximum Displacement | 0.000229 | 0.001200 | YES |
| **5** | | | |
| Item | Value | Threshold | Converged? |
| Item | 0.000051 | 0.000450 | YES |
| Maximum Force | 0.000009 | 0.000300 | YES |
| RMS Force | 0.001673 | 0.001800 | YES |
| Maximum Displacement | 0.000345 | 0.001200 | YES |
| **INT-IIIa** | | | |
| Item | Value | Threshold | Converged? |
| Item | 0.000015 | 0.000450 | YES |
| Maximum Force | 0.000003 | 0.000300 | YES |
| RMS Force | 0.000897 | 0.001800 | YES |
| Maximum Displacement | 0.000254 | 0.001200 | YES |
| **INT-IIIb** | | | |
| Item | Value | Threshold | Converged? |
| Item | 0.000058 | 0.000450 | YES |
| Maximum Force | 0.000012 | 0.000300 | YES |
| RMS Force | 0.007341 | 0.001800 | NO |
| Maximum Displacement | 0.001753 | 0.001200 | NO |
| **TS-III** | | | |
| Item | Value | Threshold | Converged? |
| Item | 0.000046 | 0.000450 | YES |
| Maximum Force | 0.000010 | 0.000300 | YES |
| RMS Force | 0.053944 | 0.001800 | NO |

| | | | |
|---|---|---|---|
| Maximum Displacement | 0.011020 | 0.001200 | NO |
| **4** | | | |
| Item | Value | Threshold | Converged? |
| Item | 0.000017 | 0.000450 | YES |
| Maximum Force | 0.000003 | 0.000300 | YES |
| RMS Force | 0.001416 | 0.001800 | YES |
| Maximum Displacement | 0.000242 | 0.001200 | YES |

**Table S3**: Optimized Parameter

| | |
|---|---|
| 1 | Electronic Energy (EE) = -821.71484 Hartree<br>Zero-point Energy Correction = 0.260508 Hartree<br>Thermal Correction to Energy = 0.277801 Hartree<br>Thermal Correction to Enthalpy = 0.278745 Hartree<br>Thermal Correction to Free Energy = 0.213889 Hartree<br>EE + Zero-point Energy = -821.45433 Hartree<br>EE + Thermal Energy Correction = -821.43704 Hartree<br>EE + Thermal Enthalpy Correction = -821.43609 Hartree<br>EE + Thermal Free Energy Correction = -821.50095 Hartree<br>E (Thermal) = 174.323 kcal/mol<br>Heat Capacity (Cv) = 62.761 cal/mol-kelvin<br>Entropy (S) = 136.5 cal/mol-kelvin |
| 2 | Electronic Energy (EE) = -2687.5987 Hartree<br>Zero-point Energy Correction = 0.047557 Hartree<br>Thermal Correction to Energy = 0.05216 Hartree<br>Thermal Correction to Enthalpy = 0.053104 Hartree<br>Thermal Correction to Free Energy = 0.018942 Hartree<br>EE + Zero-point Energy = -2687.5511 Hartree<br>EE + Thermal Energy Correction = -2687.5465 Hartree<br>EE + Thermal Enthalpy Correction = -2687.5456 Hartree<br>EE + Thermal Free Energy Correction = -2687.5797 Hartree<br>E (Thermal) = 32.731 kcal/mol<br>Heat Capacity (Cv) = 14.841 cal/mol-kelvin<br>Entropy (S) = 71.9 cal/mol-kelvin |
| 3 | Electronic Energy (EE) = -937.15369 Hartree<br>Zero-point Energy Correction = 0.297954 Hartree<br>Thermal Correction to Energy = 0.318605 Hartree<br>Thermal Correction to Enthalpy = 0.319549 Hartree<br>Thermal Correction to Free Energy = 0.246829 Hartree<br>EE + Zero-point Energy = -936.85574 Hartree<br>EE + Thermal Energy Correction = -936.83509 Hartree<br>EE + Thermal Enthalpy Correction = -936.83414 Hartree<br>EE + Thermal Free Energy Correction = -936.90686 Hartree<br>E (Thermal) = 199.928 kcal/mol<br>Heat Capacity (Cv) = 75.491 cal/mol-kelvin<br>Entropy (S) = 153.051 cal/mol-kelvin |
| 4 | Electronic Energy (EE) = -1052.5493 Hartree<br>Zero-point Energy Correction = 0.333979 Hartree<br>Thermal Correction to Energy = 0.358543 Hartree |

| | |
|---|---|
| | Thermal Correction to Enthalpy = 0.359487 Hartree<br>Thermal Correction to Free Energy = 0.276935 Hartree<br>EE + Zero-point Energy = -1052.2153 Hartree<br>EE + Thermal Energy Correction = -1052.1908 Hartree<br>EE + Thermal Enthalpy Correction = -1052.1898 Hartree<br>EE + Thermal Free Energy Correction = -1052.2724 Hartree<br>E (Thermal) = 224.989 kcal/mol<br>Heat Capacity (Cv) = 88.473 cal/mol-kelvin<br>Entropy (S) = 173.745 cal/mol-kelvin |
| INT-Ia | Electronic Energy (EE) = -821.22944 Hartree<br>Zero-point Energy Correction = 0.246727 Hartree<br>Thermal Correction to Energy = 0.263958 Hartree<br>Thermal Correction to Enthalpy = 0.264902 Hartree<br>Thermal Correction to Free Energy = 0.200415 Hartree<br>EE + Zero-point Energy = -820.98271 Hartree<br>EE + Thermal Energy Correction = -820.96548 Hartree<br>EE + Thermal Enthalpy Correction = -820.96454 Hartree<br>EE + Thermal Free Energy Correction = -821.02903 Hartree<br>E (Thermal) = 165.636 kcal/mol<br>Heat Capacity (Cv) = 62.699 cal/mol-kelvin<br>Entropy (S) = 135.725 cal/mol-kelvin |
| INT-Ib | Electronic Energy (EE) = -821.24668 Hartree<br>Zero-point Energy Correction = 0.24657 Hartree<br>Thermal Correction to Energy = 0.263605 Hartree<br>Thermal Correction to Enthalpy = 0.264549 Hartree<br>Thermal Correction to Free Energy = 0.200837 Hartree<br>EE + Zero-point Energy = -821.00011 Hartree<br>EE + Thermal Energy Correction = -820.98307 Hartree<br>EE + Thermal Enthalpy Correction = -820.98213 Hartree<br>EE + Thermal Free Energy Correction = -821.04584 Hartree<br>E (Thermal) = 165.415 kcal/mol<br>Heat Capacity (Cv) = 62.062 cal/mol-kelvin<br>Entropy (S) = 134.095 cal/mol-kelvin |
| TS-I | Zero-point correction= 0.290242 (Hartree/Particle)<br>Thermal correction to Energy= 0.313748<br>Thermal correction to Enthalpy= 0.314692<br>Thermal correction to Gibbs Free Energy= 0.232499<br>Sum of electronic and zero-point Energies= -3511.665052<br>Sum of electronic and thermal Energies= -3511.641546<br>Sum of electronic and thermal Enthalpies= -3511.640602<br>Sum of electronic and thermal Free Energies= -3511.722794 |
| INT-IIa | Electronic Energy (EE) = -936.64053 Hartree<br>Zero-point Energy Correction = 0.283654 Hartree<br>Thermal Correction to Energy = 0.304245 Hartree<br>Thermal Correction to Enthalpy = 0.305189 Hartree<br>Thermal Correction to Free Energy = 0.232805 Hartree<br>EE + Zero-point Energy = -936.35687 Hartree<br>EE + Thermal Energy Correction = -936.33628 Hartree<br>EE + Thermal Enthalpy Correction = -936.33534 Hartree<br>EE + Thermal Free Energy Correction = -936.40772 Hartree |

| | |
|---|---|
| | E (Thermal) = 190.916 kcal/mol<br>Heat Capacity (Cv) = 75.507 cal/mol-kelvin<br>Entropy (S) = 152.344 cal/mol-kelvin |
| INT-IIb | Electronic Energy (EE) = -936.67202 Hartree<br>Zero-point Energy Correction = 0.283775 Hartree<br>Thermal Correction to Energy = 0.304345 Hartree<br>Thermal Correction to Enthalpy = 0.305289 Hartree<br>Thermal Correction to Free Energy = 0.232767 Hartree<br>EE + Zero-point Energy = -936.38824 Hartree<br>EE + Thermal Energy Correction = -936.36767 Hartree<br>EE + Thermal Enthalpy Correction = -936.36673 Hartree<br>EE + Thermal Free Energy Correction = -936.43925 Hartree<br>E (Thermal) = 190.979 kcal/mol<br>Heat Capacity (Cv) = 74.873 cal/mol-kelvin<br>Entropy (S) = 152.635 cal/mol-kelvin |
| **TS-II** | Zero-point correction= 0.327653 (Hartree/Particle)<br>Thermal correction to Energy= 0.354388<br>Thermal correction to Enthalpy= 0.355333<br>Thermal correction to Gibbs Free Energy= 0.266780<br>Sum of electronic and zero-point Energies= -3627.110175<br>Sum of electronic and thermal Energies= -3627.083440<br>Sum of electronic and thermal Enthalpies= -3627.082496<br>Sum of electronic and thermal Free Energies= -3627.171049 |
| **5** | Zero-point correction= 0.290242 (Hartree/Particle)<br>Thermal correction to Energy= 0.313748<br>Thermal correction to Enthalpy= 0.314692<br>Thermal correction to Gibbs Free Energy= 0.232499<br>Sum of electronic and zero-point Energies= -3511.665052<br>Sum of electronic and thermal Energies= -3511.641546<br>Sum of electronic and thermal Enthalpies= -3511.640602<br>Sum of electronic and thermal Free Energies= -3511.722794 |
| **INT-IIIa** | Electronic Energy (EE) = -936.64554 Hartree<br>Zero-point Energy Correction = 0.283052 Hartree<br>Thermal Correction to Energy = 0.30364 Hartree<br>Thermal Correction to Enthalpy = 0.304584 Hartree<br>Thermal Correction to Free Energy = 0.232445 Hartree<br>EE + Zero-point Energy = -936.36249 Hartree<br>EE + Thermal Energy Correction = -936.3419 Hartree<br>EE + Thermal Enthalpy Correction = -936.34096 Hartree<br>EE + Thermal Free Energy Correction = -936.41309 Hartree<br>E (Thermal) = 190.537 kcal/mol<br>Heat Capacity (Cv) = 75.079 cal/mol-kelvin<br>Entropy (S) = 151.829 cal/mol-kelvin |
| **INT-IIIb** | Electronic Energy (EE) = -936.64521 Hartree<br>Zero-point Energy Correction = 0.283016 Hartree<br>Thermal Correction to Energy = 0.303649 Hartree<br>Thermal Correction to Enthalpy = 0.304594 Hartree<br>Thermal Correction to Free Energy = 0.231807 Hartree<br>EE + Zero-point Energy = -936.36219 Hartree<br>EE + Thermal Energy Correction = -936.34156 Hartree |

| | |
|---|---|
| | EE + Thermal Enthalpy Correction = -936.34062 Hartree<br>EE + Thermal Free Energy Correction = -936.4134 Hartree<br>E (Thermal) = 190.543 kcal/mol<br>Heat Capacity (Cv) = 75.061 cal/mol-kelvin<br>Entropy (S) = 153.191 cal/mol-kelvin |
| **TS-III** | Electronic Energy (EE) = -3627.4138 Hartree<br>Zero-point Energy Correction = 0.326748 Hartree<br>Thermal Correction to Energy = 0.353788 Hartree<br>Thermal Correction to Enthalpy = 0.354732 Hartree<br>Thermal Correction to Free Energy = 0.264634 Hartree<br>EE + Zero-point Energy = -3627.087 Hartree<br>EE + Thermal Energy Correction = -3627.06 Hartree<br>EE + Thermal Enthalpy Correction = -3627.059 Hartree<br>EE + Thermal Free Energy Correction = -3627.1491 Hartree<br>E (Thermal) = 222.005 kcal/mol<br>Heat Capacity (Cv) = 95.377 cal/mol-kelvin<br>Entropy (S) = 189.629 cal/mol-kelvin |
| **4** | Electronic Energy (EE) = -1052.5493 Hartree<br>Zero-point Energy Correction = 0.333979 Hartree<br>Thermal Correction to Energy = 0.358543 Hartree<br>Thermal Correction to Enthalpy = 0.359487 Hartree<br>Thermal Correction to Free Energy = 0.276935 Hartree<br>EE + Zero-point Energy = -1052.2153 Hartree<br>EE + Thermal Energy Correction = -1052.1908 Hartree<br>EE + Thermal Enthalpy Correction = -1052.1898 Hartree<br>EE + Thermal Free Energy Correction = -1052.2724 Hartree<br>E (Thermal) = 224.989 kcal/mol<br>Heat Capacity (Cv) = 88.473 cal/mol-kelvin<br>Entropy (S) = 173.745 cal/mol-kelvin |

**Table S4:** Thermochemical parameters and energy corrections obtained from DFT calculations, including electronic energy, zero-point energy, thermal corrections, and thermodynamic properties (E, Cv, S) at standard conditions.

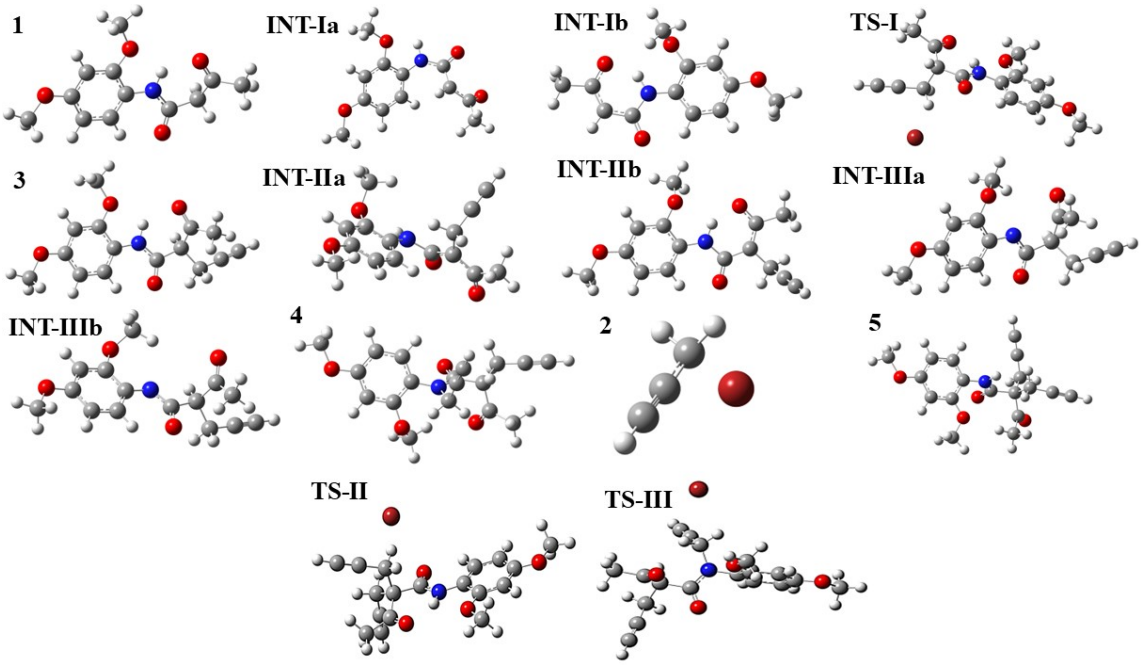


**Figure S29:** Optimized structure of all molecules

1

Input orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -3.123276 | -0.105714 | 0.094633 |
| 2 | 6 | 0 | -2.347666 | 1.060795 | -0.010837 |
| 3 | 6 | 0 | -0.967940 | 0.953627 | -0.123151 |
| 4 | 6 | 0 | -0.328400 | -0.311956 | -0.131402 |
| 5 | 6 | 0 | -1.118358 | -1.459963 | -0.025733 |
| 6 | 6 | 0 | -2.514437 | -1.361548 | 0.086633 |
| 7 | 7 | 0 | 1.080496 | -0.299293 | -0.251549 |
| 8 | 6 | 0 | 1.915127 | -1.376049 | -0.286889 |
| 9 | 6 | 0 | 3.405473 | -1.068350 | -0.508031 |
| 10 | 6 | 0 | 3.984279 | 0.167553 | 0.160455 |
| 11 | 6 | 0 | 5.354294 | 0.037882 | 0.777575 |
| 12 | 8 | 0 | 3.362610 | 1.247603 | 0.181898 |
| 13 | 8 | 0 | 1.553095 | -2.573890 | -0.208675 |
| 14 | 8 | 0 | -4.496060 | 0.111645 | 0.202289 |
| 15 | 6 | 0 | -5.369779 | -1.040496 | 0.315415 |
| 16 | 8 | 0 | -0.102663 | 2.038433 | -0.237664 |
| 17 | 6 | 0 | -0.644658 | 3.383127 | -0.196012 |
| 18 | 1 | 0 | -2.854698 | 2.016002 | -0.002640 |
| 19 | 1 | 0 | -0.634221 | -2.425388 | -0.030586 |
| 20 | 1 | 0 | -3.097014 | -2.270148 | 0.167310 |
| 21 | 1 | 0 | 1.510779 | 0.626016 | -0.263799 |
| 22 | 1 | 0 | 3.951287 | -1.966290 | -0.211838 |
| 23 | 1 | 0 | 3.557538 | -0.949030 | -1.593142 |

| | |
|---|---|
| | 24 1 0 6.069036 -0.375348 0.054929<br>25 1 0 5.702443 1.011724 1.125750<br>26 1 0 5.317844 -0.659764 1.624741<br>27 1 0 -6.376838 -0.630485 0.385351<br>28 1 0 -5.293357 -1.686473 -0.567396<br>29 1 0 -5.144259 -1.624418 1.215776<br>30 1 0 0.219144 4.041003 -0.280007<br>31 1 0 -1.330360 3.556467 -1.033246<br>32 1 0 -1.164616 3.567415 0.750916<br>--- |
| 2 | Input orientation:<br>---<br>Center Atomic Atomic Coordinates (Angstroms)<br>Number Number Type X Y Z<br>---<br>1 6 0 2.859328 -0.515662 -0.000082<br>2 6 0 1.837327 0.138365 0.000126<br>3 6 0 0.660684 0.964670 -0.000025<br>4 35 0 -1.057475 -0.158983 -0.000000<br>5 1 0 3.742228 -1.111764 0.000077<br>6 1 0 0.562636 1.576064 0.895757<br>7 1 0 0.562730 1.575884 -0.895940 |
| 3 | Input orientation:<br>---<br>Center Atomic Atomic Coordinates (Angstroms)<br>Number Number Type X Y Z<br>---<br>1 6 0 -3.841521 -0.379704 0.022024<br>2 6 0 -3.244554 0.880212 -0.161482<br>3 6 0 -1.860357 0.977012 -0.227731<br>4 6 0 -1.041457 -0.176198 -0.112689<br>5 6 0 -1.654276 -1.418993 0.067448<br>6 6 0 -3.052539 -1.526947 0.135566<br>7 7 0 0.354377 0.045326 -0.194542<br>8 6 0 1.356401 -0.872002 -0.129324<br>9 6 0 2.781554 -0.279926 -0.312782<br>10 6 0 3.006698 0.875731 0.673525<br>11 6 0 3.881775 0.682293 1.879590<br>12 8 0 2.412438 1.955361 0.465680<br>13 8 0 1.187168 -2.107979 0.024102<br>14 6 0 3.836283 -1.407976 -0.270488<br>15 6 0 5.166412 -0.965891 -0.698741<br>16 6 0 6.265010 -0.594900 -1.059596<br>17 8 0 -1.163153 2.166706 -0.406531<br>18 6 0 -1.908010 3.415611 -0.533931<br>19 8 0 -5.232407 -0.369067 0.076215<br>20 6 0 -5.931702 -1.634473 0.271151<br>21 1 0 -3.883563 1.748623 -0.246791<br>22 1 0 -1.036444 -2.300250 0.154080<br>23 1 0 -3.496011 -2.503711 0.276278 |

| | | | | | | |
|---|---|---|---|---|---|---|
| | 24 | 1 | 0 | 0.621567 | 1.023536 | -0.287073 |
| | 25 | 1 | 0 | 2.799152 | 0.179963 | -1.310180 |
| | 26 | 1 | 0 | 4.907300 | 0.437191 | 1.582045 |
| | 27 | 1 | 0 | 3.884344 | 1.594602 | 2.477686 |
| | 28 | 1 | 0 | 3.514427 | -0.151428 | 2.491355 |
| | 29 | 1 | 0 | 3.882880 | -1.841457 | 0.735586 |
| | 30 | 1 | 0 | 3.482772 | -2.217079 | -0.918802 |
| | 31 | 1 | 0 | 7.229743 | -0.272876 | -1.377943 |
| | 32 | 1 | 0 | -1.150873 | 4.187027 | -0.661610 |
| | 33 | 1 | 0 | -2.565306 | 3.386287 | -1.408248 |
| | 34 | 1 | 0 | -2.494127 | 3.610649 | 0.369280 |
| | 35 | 1 | 0 | -6.989871 | -1.377547 | 0.281016 |
| | 36 | 1 | 0 | -5.725285 | -2.328697 | -0.550070 |
| | 37 | 1 | 0 | -5.652005 | -2.095371 | 1.224218 |
| 4 | Input orientation: | | | | | |
| | --- | | | | | |
| | Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
| | --- | | | | | |
| | 1 | 6 | 0 | 4.025609 | -0.204404 | -0.258772 |
| | 2 | 6 | 0 | 3.411491 | 1.002288 | 0.108456 |
| | 3 | 6 | 0 | 2.033637 | 1.049059 | 0.303432 |
| | 4 | 6 | 0 | 1.246814 | -0.110025 | 0.146487 |
| | 5 | 6 | 0 | 1.874817 | -1.306643 | -0.211942 |
| | 6 | 6 | 0 | 3.255835 | -1.365345 | -0.424830 |
| | 7 | 7 | 0 | -0.171240 | -0.061092 | 0.400364 |
| | 8 | 6 | 0 | -1.058550 | -0.318419 | -0.622375 |
| | 9 | 6 | 0 | -2.556492 | -0.340481 | -0.282788 |
| | 10 | 6 | 0 | -3.104021 | 1.093711 | -0.160482 |
| | 11 | 6 | 0 | -4.274405 | 1.323868 | 0.756412 |
| | 12 | 8 | 0 | -2.595102 | 2.016197 | -0.826228 |
| | 13 | 8 | 0 | -0.665975 | -0.529141 | -1.794945 |
| | 14 | 6 | 0 | -0.585711 | 0.172617 | 1.810197 |
| | 15 | 6 | 0 | -3.308501 | -1.108961 | -1.423662 |
| | 16 | 6 | 0 | -4.711177 | -1.408022 | -1.134952 |
| | 17 | 6 | 0 | -0.736455 | -1.068783 | 2.578738 |
| | 18 | 6 | 0 | -0.863776 | -2.098411 | 3.208581 |
| | 19 | 6 | 0 | -5.873022 | -1.680653 | -0.909642 |
| | 20 | 8 | 0 | 1.452655 | 2.251712 | 0.733619 |
| | 21 | 6 | 0 | 0.809165 | 3.075067 | -0.311510 |
| | 22 | 8 | 0 | 5.400914 | -0.146580 | -0.432570 |
| | 23 | 6 | 0 | 6.113689 | -1.361334 | -0.819923 |
| | 24 | 1 | 0 | 4.009094 | 1.895219 | 0.242549 |
| | 25 | 1 | 0 | 1.275746 | -2.202071 | -0.328611 |
| | 26 | 1 | 0 | 3.710608 | -2.306773 | -0.703006 |
| | 27 | 1 | 0 | -2.728978 | -0.876264 | 0.655771 |
| | 28 | 1 | 0 | -4.006567 | 1.079263 | 1.792217 |
| | 29 | 1 | 0 | -4.593014 | 2.366075 | 0.701725 |
| | 30 | 1 | 0 | -5.105717 | 0.664378 | 0.482517 |
| | 31 | 1 | 0 | 0.171696 | 0.821713 | 2.256280 |

| | |
|---|---|
| | 32 1 0 -1.512508 0.751342 1.830010<br>33 1 0 -3.215731 -0.529895 -2.349121<br>34 1 0 -2.762413 -2.043059 -1.598525<br>35 1 0 -0.972668 -3.003560 3.761066<br>36 1 0 -6.893040 -1.921009 -0.715379<br>37 1 0 0.488527 3.983523 0.197513<br>38 1 0 1.533837 3.318426 -1.094425<br>39 1 0 -0.054738 2.559466 -0.737659<br>40 1 0 7.158804 -1.065540 -0.894215<br>41 1 0 6.000738 -2.141475 -0.060382<br>42 1 0 5.761384 -1.730385 -1.788439 |
| INT-Ia | Input orientation:<br>---<br>Center Atomic Atomic Coordinates (Angstroms)<br>Number Number Type X Y Z<br>---<br>1 6 0 -2.764897 -0.884037 -0.051898<br>2 6 0 -2.704367 0.500726 0.183202<br>3 6 0 -1.484399 1.160737 0.095787<br>4 6 0 -0.282694 0.467304 -0.228889<br>5 6 0 -0.383857 -0.905734 -0.488129<br>6 6 0 -1.609077 -1.587809 -0.389909<br>7 7 0 0.886127 1.236218 -0.331681<br>8 6 0 2.271840 0.911683 -0.313460<br>9 6 0 2.666542 -0.348755 0.216931<br>10 6 0 3.969063 -0.898393 0.229297<br>11 6 0 4.126555 -2.245282 0.951769<br>12 8 0 5.034318 -0.412922 -0.302979<br>13 8 0 3.032231 1.850137 -0.739027<br>14 1 0 1.896874 -0.933272 0.704404<br>15 8 0 -1.325729 2.533000 0.294983<br>16 6 0 -2.502840 3.341850 0.583840<br>17 8 0 -4.036458 -1.452691 0.074669<br>18 6 0 -4.177199 -2.881478 -0.169345<br>19 1 0 -3.619435 1.021568 0.432314<br>20 1 0 0.501419 -1.454181 -0.779965<br>21 1 0 -1.634241 -2.650958 -0.592148<br>22 1 0 0.727853 2.227852 -0.459516<br>23 1 0 3.194786 -2.614165 1.391156<br>24 1 0 4.506544 -2.999059 0.250002<br>25 1 0 4.875468 -2.147661 1.748413<br>26 1 0 -2.133709 4.361737 0.680337<br>27 1 0 -3.228845 3.283002 -0.233739<br>28 1 0 -2.973764 3.026279 1.520559<br>29 1 0 -5.233378 -3.098248 -0.013886<br>30 1 0 -3.893586 -3.137316 -1.196175<br>31 1 0 -3.571795 -3.464163 0.533672 |
| INT-Ib | Input orientation:<br>---<br>Center Atomic Atomic Coordinates (Angstroms) |

| | |
|---|---|
| | Number Number Type X Y Z<br>---<br>1 6 0 3.161514 0.064344 -0.091021<br>2 6 0 2.313497 1.172261 -0.230651<br>3 6 0 0.934663 0.997682 -0.221183<br>4 6 0 0.342488 -0.284496 -0.074364<br>5 6 0 1.216060 -1.381210 0.065681<br>6 6 0 2.608023 -1.211165 0.060590<br>7 7 0 -1.053042 -0.361980 -0.088264<br>8 6 0 -1.865358 -1.484317 0.096719<br>9 6 0 -3.282604 -1.237823 0.063153<br>10 6 0 -3.895534 0.006403 -0.116631<br>11 6 0 -5.417347 0.076872 -0.109133<br>12 8 0 -1.369114 -2.651751 0.286651<br>13 8 0 -3.262064 1.137281 -0.294718<br>14 1 0 -3.901270 -2.116859 0.201623<br>15 8 0 4.533269 0.341975 -0.115334<br>16 6 0 5.462257 -0.770744 0.021280<br>17 8 0 0.102250 2.122822 -0.407053<br>18 6 0 -0.308534 2.816485 0.826674<br>19 1 0 2.732593 2.164062 -0.353330<br>20 1 0 0.781065 -2.362546 0.182535<br>21 1 0 3.238895 -2.084651 0.171675<br>22 1 0 -1.592737 0.503903 -0.251272<br>23 1 0 -5.776149 0.494183 -1.058842<br>24 1 0 -5.884225 -0.900711 0.043344<br>25 1 0 -5.755619 0.756069 0.684054<br>26 1 0 6.455325 -0.325235 -0.025854<br>27 1 0 5.330997 -1.281204 0.981865<br>28 1 0 5.340713 -1.491174 -0.795218<br>29 1 0 -0.858677 3.698443 0.499168<br>30 1 0 -0.960069 2.176898 1.428715<br>31 1 0 0.570979 3.114314 1.406330 |
| TS-I | Input orientation:<br>---<br>Center Atomic Atomic Coordinates (Angstroms)<br>Number Number Type X Y Z<br>---<br>1 6 0 4.479580 -0.525344 0.147357<br>2 6 0 3.964840 0.370897 -0.801399<br>3 6 0 2.688174 0.891824 -0.649231<br>4 6 0 1.880419 0.531660 0.463503<br>5 6 0 2.417105 -0.360164 1.391316<br>6 6 0 3.706144 -0.890480 1.243165<br>7 7 0 0.600895 1.103724 0.530900<br>8 6 0 -0.359678 0.956291 1.505402<br>9 6 0 -1.615329 1.667149 1.282811<br>10 6 0 -1.861897 2.635047 0.269431<br>11 6 0 -3.125719 3.470714 0.377207<br>12 8 0 -1.101832 2.840720 -0.713430 |

| | | | | | | |
|---|---|---|---|---|---|---|
| | 13 | 8 | 0 | -0.192645 | 0.237447 | 2.511579 |
| | 14 | 6 | 0 | -2.760658 | -0.331422 | 0.220649 |
| | 15 | 6 | 0 | -4.095698 | 0.057164 | 0.459284 |
| | 16 | 6 | 0 | -5.239336 | 0.382266 | 0.667397 |
| | 17 | 8 | 0 | 2.113781 | 1.766956 | -1.525653 |
| | 18 | 6 | 0 | 2.853439 | 2.177913 | -2.676428 |
| | 19 | 8 | 0 | 5.749445 | -0.976705 | -0.103498 |
| | 20 | 6 | 0 | 6.332852 | -1.892664 | 0.822418 |
| | 21 | 1 | 0 | 4.584818 | 0.639381 | -1.645351 |
| | 22 | 1 | 0 | 1.815290 | -0.641553 | 2.240902 |
| | 23 | 1 | 0 | 4.075326 | -1.578740 | 1.990707 |
| | 24 | 1 | 0 | 0.331496 | 1.738644 | -0.225211 |
| | 25 | 1 | 0 | -2.282813 | 1.642753 | 2.133641 |
| | 26 | 1 | 0 | -2.844423 | 4.510526 | 0.574055 |
| | 27 | 1 | 0 | -3.660223 | 3.452677 | -0.576374 |
| | 28 | 1 | 0 | -3.792724 | 3.133223 | 1.170332 |
| | 29 | 1 | 0 | -2.192230 | -0.793341 | 1.009398 |
| | 30 | 1 | 0 | -6.247485 | 0.671770 | 0.848043 |
| | 31 | 1 | 0 | 2.202571 | 2.861473 | -3.217641 |
| | 32 | 1 | 0 | 3.771951 | 2.697416 | -2.388834 |
| | 33 | 1 | 0 | 3.097093 | 1.322847 | -3.313308 |
| | 34 | 1 | 0 | 7.325189 | -2.116511 | 0.435250 |
| | 35 | 1 | 0 | 6.422406 | -1.447283 | 1.817975 |
| | 36 | 1 | 0 | 5.750238 | -2.816733 | 0.886725 |
| | 37 | 1 | 0 | -2.242174 | 0.024127 | -0.652667 |
| | 38 | 35 | 0 | -3.052424 | -2.539657 | -0.860485 |
| INT-IIa | Input orientation: | | | | | |
| | Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
| | 1 | 6 | 0 | -3.282112 | -0.744515 | 0.041684 |
| | 2 | 6 | 0 | -3.181829 | 0.646633 | -0.112473 |
| | 3 | 6 | 0 | -1.947305 | 1.224799 | -0.378357 |
| | 4 | 6 | 0 | -0.768135 | 0.446801 | -0.501709 |
| | 5 | 6 | 0 | -0.896752 | -0.944879 | -0.360184 |
| | 6 | 6 | 0 | -2.136603 | -1.538205 | -0.080960 |
| | 7 | 7 | 0 | 0.423493 | 1.121113 | -0.814668 |
| | 8 | 6 | 0 | 1.732390 | 0.601393 | -1.091627 |
| | 9 | 6 | 0 | 2.305271 | -0.361279 | -0.196163 |
| | 10 | 6 | 0 | 3.404931 | -1.186520 | -0.583085 |
| | 11 | 6 | 0 | 4.035047 | -2.094859 | 0.484927 |
| | 12 | 8 | 0 | 3.899785 | -1.278460 | -1.763602 |
| | 13 | 8 | 0 | 2.292775 | 1.121636 | -2.113760 |
| | 14 | 6 | 0 | 1.838125 | -0.388685 | 1.265502 |
| | 15 | 6 | 0 | 2.654210 | 0.455365 | 2.161978 |
| | 16 | 6 | 0 | 3.331151 | 1.159119 | 2.888354 |
| | 17 | 8 | 0 | -4.563963 | -1.233343 | 0.312273 |
| | 18 | 6 | 0 | -4.734628 | -2.671667 | 0.465902 |
| | 19 | 8 | 0 | -1.855466 | 2.617597 | -0.590310 |

| | |
|---|---|
| | 20 6 0 -1.580106 3.417298 0.617939<br>21 1 0 -4.067221 1.266016 -0.032044<br>22 1 0 -0.019094 -1.568895 -0.476479<br>23 1 0 -2.187446 -2.614764 0.023547<br>24 1 0 0.268719 2.013100 -1.272037<br>25 1 0 3.344143 -2.888176 0.802384<br>26 1 0 4.920180 -2.565705 0.050318<br>27 1 0 4.327996 -1.540354 1.383796<br>28 1 0 0.799968 -0.054583 1.342990<br>29 1 0 1.836620 -1.413739 1.659692<br>30 1 0 3.925835 1.778940 3.518527<br>31 1 0 -5.795920 -2.816264 0.664268<br>32 1 0 -4.453110 -3.203753 -0.449460<br>33 1 0 -4.145494 -3.052562 1.307408<br>34 1 0 -1.534585 4.453034 0.282109<br>35 1 0 -2.386867 3.292529 1.346773<br>36 1 0 -0.625151 3.123163 1.063705 |
| INT-IIb | Input orientation:<br>---<br>Center Atomic Atomic Coordinates (Angstroms)<br>Number Number Type X Y Z<br>---<br>1 6 0 -3.804846 -0.361309 0.144321<br>2 6 0 -3.202413 0.877115 0.407170<br>3 6 0 -1.820767 1.007944 0.327629<br>4 6 0 -0.981765 -0.085631 -0.013497<br>5 6 0 -1.611844 -1.320221 -0.268006<br>6 6 0 -3.005300 -1.458003 -0.193734<br>7 7 0 0.395563 0.149855 -0.066519<br>8 6 0 1.415102 -0.746382 -0.382512<br>9 6 0 2.763433 -0.215140 -0.390989<br>10 6 0 3.080080 1.127346 -0.110833<br>11 6 0 4.538530 1.576742 -0.160879<br>12 8 0 2.205804 2.050854 0.189549<br>13 8 0 1.156117 -1.974227 -0.660525<br>14 6 0 3.854871 -1.224817 -0.729431<br>15 6 0 4.580529 -1.766079 0.436259<br>16 6 0 5.170752 -2.203002 1.406785<br>17 8 0 -5.200164 -0.392837 0.250803<br>18 6 0 -5.880270 -1.655905 0.001492<br>19 8 0 -1.215980 2.244735 0.636965<br>20 6 0 -1.282201 3.268354 -0.418015<br>21 1 0 -3.815847 1.727370 0.681890<br>22 1 0 -0.988520 -2.161884 -0.529572<br>23 1 0 -3.443489 -2.426731 -0.400713<br>24 1 0 0.738690 1.100219 0.150267<br>25 1 0 5.183385 0.949866 0.465707<br>26 1 0 4.938664 1.532780 -1.183160<br>27 1 0 4.597215 2.610742 0.187572<br>28 1 0 3.372153 -2.058239 -1.253618 |

| | | | | | | |
|---|---|---|---|---|---|---|
| | 29 | 1 | 0 | 4.587866 | -0.795049 | -1.426532 |
| | 30 | 1 | 0 | 5.681912 | -2.585651 | 2.259519 |
| | 31 | 1 | 0 | -6.939907 | -1.446119 | 0.142986 |
| | 32 | 1 | 0 | -5.705798 | -2.004806 | -1.022368 |
| | 33 | 1 | 0 | -5.557599 | -2.426468 | 0.710398 |
| | 34 | 1 | 0 | -0.805791 | 4.154629 | 0.000379 |
| | 35 | 1 | 0 | -0.738801 | 2.937566 | -1.308710 |
| | 36 | 1 | 0 | -2.322630 | 3.488507 | -0.677299 |
| **TS-II** | Input orientation: | | | | | |
| | Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
| | 1 | 6 | 0 | -4.360126 | -0.624412 | -0.123179 |
| | 2 | 6 | 0 | -3.845386 | 0.271829 | 0.825577 |
| | 3 | 6 | 0 | -2.568720 | 0.792757 | 0.673410 |
| | 4 | 6 | 0 | -1.760965 | 0.432593 | -0.439325 |
| | 5 | 6 | 0 | -2.297651 | -0.459231 | -1.367138 |
| | 6 | 6 | 0 | -3.586690 | -0.989548 | -1.218987 |
| | 7 | 7 | 0 | -0.481441 | 1.004656 | -0.506722 |
| | 8 | 6 | 0 | 0.479132 | 0.857224 | -1.481224 |
| | 9 | 6 | 0 | 1.734783 | 1.568082 | -1.258633 |
| | 10 | 6 | 0 | 1.981351 | 2.535980 | -0.245253 |
| | 11 | 6 | 0 | 3.245173 | 3.371647 | -0.353028 |
| | 12 | 8 | 0 | 1.221286 | 2.741653 | 0.737609 |
| | 13 | 8 | 0 | 0.312099 | 0.138380 | -2.487401 |
| | 14 | 6 | 0 | 2.880112 | -0.430490 | -0.196471 |
| | 15 | 6 | 0 | 4.215152 | -0.041903 | -0.435106 |
| | 16 | 6 | 0 | 5.358790 | 0.283199 | -0.643219 |
| | 17 | 8 | 0 | -1.994327 | 1.667889 | 1.549831 |
| | 18 | 6 | 0 | -2.733985 | 2.078846 | 2.700606 |
| | 19 | 8 | 0 | -5.629991 | -1.075773 | 0.127676 |
| | 20 | 6 | 0 | -6.213398 | -1.991732 | -0.798240 |
| | 21 | 1 | 0 | -4.465364 | 0.540313 | 1.669529 |
| | 22 | 1 | 0 | -1.695836 | -0.740621 | -2.216724 |
| | 23 | 1 | 0 | -3.955872 | -1.677807 | -1.966529 |
| | 24 | 1 | 0 | -0.212042 | 1.639576 | 0.249389 |
| | 25 | 1 | 0 | 2.963877 | 4.411459 | -0.549877 |
| | 26 | 1 | 0 | 3.779677 | 3.353609 | 0.600552 |
| | 27 | 1 | 0 | 3.912178 | 3.034156 | -1.146154 |
| | 28 | 1 | 0 | 2.311684 | -0.892408 | -0.985220 |
| | 29 | 1 | 0 | 6.366938 | 0.572703 | -0.823865 |
| | 30 | 1 | 0 | -2.083117 | 2.762405 | 3.241819 |
| | 31 | 1 | 0 | -3.652497 | 2.598348 | 2.413012 |
| | 32 | 1 | 0 | -2.977639 | 1.223779 | 3.337486 |
| | 33 | 1 | 0 | -7.205735 | -2.215578 | -0.411072 |
| | 34 | 1 | 0 | -6.302953 | -1.546350 | -1.793797 |
| | 35 | 1 | 0 | -5.630784 | -2.915801 | -0.862547 |
| | 36 | 1 | 0 | 2.361628 | -0.074941 | 0.676845 |
| | 37 | 35 | 0 | 3.171878 | -2.638725 | 0.884663 |

| | | | | | | |
|---|---|---|---|---|---|---|
| | 38 | 6 | 0 | 2.685084 | 1.533349 | -2.469964 |
| | 39 | 1 | 0 | 3.663081 | 1.842260 | -2.165013 |
| | 40 | 1 | 0 | 2.730695 | 0.537651 | -2.859072 |
| | 41 | 6 | 0 | 2.162153 | 2.487075 | -3.560170 |
| | 42 | 6 | 0 | 1.754267 | 3.230982 | -4.410531 |
| | 43 | 1 | 0 | 1.390931 | 3.893636 | -5.168012 |
| **5** | Input orientation: | | | | | |
| | --- | | | | | |
| | Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
| | --- | | | | | |
| | 1 | 6 | 0 | 2.142412 | -1.514639 | 0.311574 |
| | 2 | 1 | 0 | 1.641397 | -2.474147 | 0.379823 |
| | 3 | 6 | 0 | 3.537984 | -1.462806 | 0.199344 |
| | 4 | 1 | 0 | 4.109073 | -2.381119 | 0.186490 |
| | 5 | 6 | 0 | 4.156587 | -0.211375 | 0.097848 |
| | 6 | 6 | 0 | 3.397779 | 0.971083 | 0.118063 |
| | 7 | 1 | 0 | 3.921141 | 1.914287 | 0.042507 |
| | 8 | 6 | 0 | 2.010505 | 0.904119 | 0.243465 |
| | 9 | 6 | 0 | 1.370778 | -0.354701 | 0.334797 |
| | 10 | 6 | 0 | -0.924531 | -0.142374 | -0.514465 |
| | 11 | 6 | 0 | -2.440283 | -0.170344 | -0.213564 |
| | 12 | 6 | 0 | -2.787428 | -0.283933 | 1.307465 |
| | 13 | 1 | 0 | -2.443286 | -1.262842 | 1.667414 |
| | 14 | 1 | 0 | -2.239400 | 0.481090 | 1.871001 |
| | 15 | 6 | 0 | -4.220924 | -0.154311 | 1.579346 |
| | 16 | 6 | 0 | -5.409056 | -0.041736 | 1.800233 |
| | 17 | 1 | 0 | -6.452309 | 0.057000 | 1.994953 |
| | 18 | 6 | 0 | -3.066636 | -1.353818 | -1.015683 |
| | 19 | 1 | 0 | -4.156425 | -1.290635 | -0.919960 |
| | 20 | 1 | 0 | -2.837634 | -1.196128 | -2.074766 |
| | 21 | 6 | 0 | -2.589604 | -2.667632 | -0.580311 |
| | 22 | 6 | 0 | -2.192140 | -3.755656 | -0.215066 |
| | 23 | 1 | 0 | -1.845806 | -4.713637 | 0.098218 |
| | 24 | 6 | 0 | -2.999160 | 1.169084 | -0.765941 |
| | 25 | 6 | 0 | -2.494153 | 2.446934 | -0.141742 |
| | 26 | 1 | 0 | -2.732131 | 3.289836 | -0.793398 |
| | 27 | 1 | 0 | -1.416892 | 2.413403 | 0.046924 |
| | 28 | 1 | 0 | -2.997142 | 2.608925 | 0.820812 |
| | 29 | 6 | 0 | 1.795987 | 3.345131 | 0.199993 |
| | 30 | 1 | 0 | 2.490343 | 3.517104 | 1.028137 |
| | 31 | 1 | 0 | 0.962285 | 4.041913 | 0.262395 |
| | 32 | 1 | 0 | 2.314816 | 3.467192 | -0.755592 |
| | 33 | 6 | 0 | 6.396071 | -1.197098 | -0.057081 |
| | 34 | 1 | 0 | 6.311306 | -1.773342 | 0.869795 |
| | 35 | 1 | 0 | 7.405130 | -0.800163 | -0.155513 |
| | 36 | 1 | 0 | 6.161642 | -1.835626 | -0.914779 |
| | 37 | 7 | 0 | -0.052507 | -0.429922 | 0.489473 |
| | 38 | 1 | 0 | -0.403836 | -0.700391 | 1.396851 |
| | 39 | 8 | 0 | 5.526601 | -0.024358 | -0.025345 |

| | |
|---|---|
| | 40 8 0 1.189414 2.018329 0.296546<br>41 8 0 -0.553775 0.142825 -1.680669<br>42 8 0 -3.853471 1.174599 -1.666441 |
| **INT-IIIa** | Input orientation:<br>---<br>Center Atomic Atomic Coordinates (Angstroms)<br>Number Number Type X Y Z<br>---<br>1 6 0 -3.872255 -0.218099 0.119016<br>2 6 0 -3.212715 1.016425 0.190482<br>3 6 0 -1.824990 1.085353 0.091401<br>4 6 0 -1.024539 -0.084026 -0.085886<br>5 6 0 -1.730578 -1.309220 -0.172529<br>6 6 0 -3.127095 -1.385533 -0.070691<br>7 7 0 0.369308 0.080697 -0.136978<br>8 6 0 1.223652 -0.926723 -0.333599<br>9 6 0 2.706689 -0.459117 -0.410136<br>10 6 0 2.872425 0.939884 0.152582<br>11 6 0 2.829327 1.124450 1.653331<br>12 8 0 3.096411 1.911852 -0.602755<br>13 8 0 1.003764 -2.186758 -0.494785<br>14 6 0 3.627620 -1.511992 0.265439<br>15 6 0 5.057264 -1.270985 0.058827<br>16 6 0 6.240118 -1.056473 -0.120840<br>17 8 0 -1.265349 2.367765 0.241662<br>18 6 0 -0.503039 2.898173 -0.897522<br>19 8 0 -5.268512 -0.170335 0.238000<br>20 6 0 -6.006000 -1.421758 0.153999<br>21 1 0 -3.782752 1.927865 0.327170<br>22 1 0 -1.147312 -2.208309 -0.312714<br>23 1 0 -3.608021 -2.354584 -0.136522<br>24 1 0 2.975934 -0.401541 -1.473739<br>25 1 0 3.803570 0.859402 2.086633<br>26 1 0 2.627221 2.171692 1.889115<br>27 1 0 2.068291 0.489517 2.111713<br>28 1 0 3.407001 -1.559546 1.340347<br>29 1 0 3.326782 -2.483139 -0.145138<br>30 1 0 7.277778 -0.872854 -0.278266<br>31 1 0 -0.231090 3.916450 -0.613816<br>32 1 0 0.386389 2.291625 -1.067761<br>33 1 0 -1.132072 2.922616 -1.795718<br>34 1 0 -7.054719 -1.148641 0.267781<br>35 1 0 -5.853784 -1.908200 -0.816117<br>36 1 0 -5.714207 -2.109577 0.955654 |
| **INT-IIIb** | Input orientation:<br>---<br>Center Atomic Atomic Coordinates (Angstroms)<br>Number Number Type X Y Z<br>---<br>1 6 0 -3.942972 -0.260963 -0.080910 |

| | | | | | | |
|---|---|---|---|---|---|---|
| | 2 | 6 | 0 | -3.380932 | 0.992764 | -0.359902 |
| | 3 | 6 | 0 | -1.998741 | 1.147347 | -0.430374 |
| | 4 | 6 | 0 | -1.107447 | 0.051642 | -0.221457 |
| | 5 | 6 | 0 | -1.713578 | -1.193173 | 0.076891 |
| | 6 | 6 | 0 | -3.104628 | -1.356996 | 0.144382 |
| | 7 | 7 | 0 | 0.266678 | 0.303246 | -0.359464 |
| | 8 | 6 | 0 | 1.206433 | -0.609863 | -0.119013 |
| | 9 | 6 | 0 | 2.654514 | -0.062894 | -0.339683 |
| | 10 | 6 | 0 | 3.191299 | 0.418888 | 1.000786 |
| | 11 | 6 | 0 | 3.570161 | -0.622779 | 2.025660 |
| | 12 | 8 | 0 | 3.272291 | 1.641013 | 1.254460 |
| | 13 | 8 | 0 | 1.101632 | -1.835082 | 0.282860 |
| | 14 | 6 | 0 | 3.537442 | -1.158623 | -0.995800 |
| | 15 | 6 | 0 | 4.942226 | -0.774446 | -1.158402 |
| | 16 | 6 | 0 | 6.104266 | -0.441377 | -1.285181 |
| | 17 | 8 | 0 | -1.538715 | 2.430557 | -0.782034 |
| | 18 | 6 | 0 | -0.716547 | 3.134569 | 0.211496 |
| | 19 | 8 | 0 | -5.343610 | -0.304709 | -0.042014 |
| | 20 | 6 | 0 | -5.981139 | -1.577595 | 0.259544 |
| | 21 | 1 | 0 | -4.023636 | 1.849098 | -0.527326 |
| | 22 | 1 | 0 | -1.059452 | -2.036767 | 0.247800 |
| | 23 | 1 | 0 | -3.509874 | -2.337059 | 0.367596 |
| | 24 | 1 | 0 | 2.585965 | 0.811251 | -0.989323 |
| | 25 | 1 | 0 | 4.535589 | -1.072909 | 1.759584 |
| | 26 | 1 | 0 | 3.660699 | -0.164235 | 3.012689 |
| | 27 | 1 | 0 | 2.826342 | -1.426103 | 2.034250 |
| | 28 | 1 | 0 | 3.447292 | -2.073289 | -0.398917 |
| | 29 | 1 | 0 | 3.103099 | -1.396320 | -1.976050 |
| | 30 | 1 | 0 | 7.123894 | -0.153552 | -1.398285 |
| | 31 | 1 | 0 | -0.507879 | 4.112672 | -0.225416 |
| | 32 | 1 | 0 | -1.275587 | 3.260860 | 1.146573 |
| | 33 | 1 | 0 | 0.207852 | 2.584117 | 0.390159 |
| | 34 | 1 | 0 | -7.052039 | -1.377395 | 0.240125 |
| | 35 | 1 | 0 | -5.732908 | -2.334372 | -0.493090 |
| | 36 | 1 | 0 | -5.691035 | -1.941950 | 1.251486 |
| **TS-III** | Input orientation: | | | | | |
| | Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
| | 1 | 6 | 0 | 4.075815 | -0.973464 | -0.118510 |
| | 2 | 6 | 0 | 3.308027 | -0.623764 | 1.001190 |
| | 3 | 6 | 0 | 1.924330 | -0.503180 | 0.898437 |
| | 4 | 6 | 0 | 1.265417 | -0.736048 | -0.338650 |
| | 5 | 6 | 0 | 2.065977 | -1.070499 | -1.430203 |
| | 6 | 6 | 0 | 3.457432 | -1.199049 | -1.345149 |
| | 7 | 7 | 0 | -0.118967 | -0.542429 | -0.497520 |
| | 8 | 6 | 0 | -0.961427 | -1.531307 | -0.215942 |
| | 9 | 6 | 0 | -2.442112 | -1.195472 | -0.476138 |
| | 10 | 6 | 0 | -3.202383 | -0.767284 | 0.781333 |

| | | | | | | |
|---|---|---|---|---|---|---|
| | 11 | 6 | 0 | -4.669088 | -0.430243 | 0.610966 |
| | 12 | 8 | 0 | -2.661164 | -0.670410 | 1.866932 |
| | 13 | 8 | 0 | -0.664125 | -2.685767 | 0.175119 |
| | 14 | 6 | 0 | -0.556048 | 1.788300 | -0.509060 |
| | 15 | 6 | 0 | -1.073976 | 1.836541 | -1.826592 |
| | 16 | 6 | 0 | -1.515639 | 1.888566 | -2.947497 |
| | 17 | 8 | 0 | 1.125064 | -0.154068 | 1.948195 |
| | 18 | 6 | 0 | 1.729723 | 0.090857 | 3.216798 |
| | 19 | 8 | 0 | 5.426617 | -1.062075 | 0.103162 |
| | 20 | 6 | 0 | 6.267743 | -1.410265 | -0.995507 |
| | 21 | 1 | 0 | 3.823025 | -0.452308 | 1.936422 |
| | 22 | 1 | 0 | 1.576548 | -1.238165 | -2.383464 |
| | 23 | 1 | 0 | 4.023812 | -1.466296 | -2.226479 |
| | 24 | 1 | 0 | -5.245897 | -1.355868 | 0.518901 |
| | 25 | 1 | 0 | -5.023671 | 0.117125 | 1.483717 |
| | 26 | 1 | 0 | -4.841905 | 0.154454 | -0.295670 |
| | 27 | 1 | 0 | 0.507453 | 1.756902 | -0.357590 |
| | 28 | 1 | 0 | -1.905354 | 1.932572 | -3.936861 |
| | 29 | 1 | 0 | 0.913740 | 0.348865 | 3.889290 |
| | 30 | 1 | 0 | 2.241365 | -0.800906 | 3.591767 |
| | 31 | 1 | 0 | 2.437063 | 0.924455 | 3.166845 |
| | 32 | 1 | 0 | 7.282407 | -1.424718 | -0.601622 |
| | 33 | 1 | 0 | 6.016620 | -2.399614 | -1.390069 |
| | 34 | 1 | 0 | 6.199629 | -0.669363 | -1.798056 |
| | 35 | 1 | 0 | -1.191266 | 1.522871 | 0.315339 |
| | 36 | 35 | 0 | -0.621467 | 4.117026 | 0.123605 |
| | 37 | 6 | 0 | -3.177138 | -2.332691 | -1.247661 |
| | 38 | 1 | 0 | -4.062861 | -1.913549 | -1.734757 |
| | 39 | 1 | 0 | -2.519180 | -2.670944 | -2.052811 |
| | 40 | 6 | 0 | -3.598771 | -3.485802 | -0.454193 |
| | 41 | 6 | 0 | -4.004286 | -4.428066 | 0.176846 |
| | 42 | 1 | 0 | -4.344119 | -5.263701 | 0.740947 |
| | 43 | 1 | 0 | -2.476003 | -0.324935 | -1.139452 |
| **4** | Input orientation: | | | | | |
| | Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
| | 1 | 6 | 0 | 4.025609 | -0.204404 | -0.258772 |
| | 2 | 6 | 0 | 3.411491 | 1.002288 | 0.108456 |
| | 3 | 6 | 0 | 2.033637 | 1.049059 | 0.303432 |
| | 4 | 6 | 0 | 1.246814 | -0.110025 | 0.146487 |
| | 5 | 6 | 0 | 1.874817 | -1.306643 | -0.211942 |
| | 6 | 6 | 0 | 3.255835 | -1.365345 | -0.424830 |
| | 7 | 7 | 0 | -0.171240 | -0.061092 | 0.400364 |
| | 8 | 6 | 0 | -1.058550 | -0.318419 | -0.622375 |
| | 9 | 6 | 0 | -2.556492 | -0.340481 | -0.282788 |
| | 10 | 6 | 0 | -3.104021 | 1.093711 | -0.160482 |
| | 11 | 6 | 0 | -4.274405 | 1.323868 | 0.756412 |
| | 12 | 8 | 0 | -2.595102 | 2.016197 | -0.826228 |

| | | | | | | |
|---|---|---|---|---|---|---|
| | 13 | 8 | 0 | -0.665975 | -0.529141 | -1.794945 |
| | 14 | 6 | 0 | -0.585711 | 0.172617 | 1.810197 |
| | 15 | 6 | 0 | -3.308501 | -1.108961 | -1.423662 |
| | 16 | 6 | 0 | -4.711177 | -1.408022 | -1.134952 |
| | 17 | 6 | 0 | -0.736455 | -1.068783 | 2.578738 |
| | 18 | 6 | 0 | -0.863776 | -2.098411 | 3.208581 |
| | 19 | 6 | 0 | -5.873022 | -1.680653 | -0.909642 |
| | 20 | 8 | 0 | 1.452655 | 2.251712 | 0.733619 |
| | 21 | 6 | 0 | 0.809165 | 3.075067 | -0.311510 |
| | 22 | 8 | 0 | 5.400914 | -0.146580 | -0.432570 |
| | 23 | 6 | 0 | 6.113689 | -1.361334 | -0.819923 |
| | 24 | 1 | 0 | 4.009094 | 1.895219 | 0.242549 |
| | 25 | 1 | 0 | 1.275746 | -2.202071 | -0.328611 |
| | 26 | 1 | 0 | 3.710608 | -2.306773 | -0.703006 |
| | 27 | 1 | 0 | -2.728978 | -0.876264 | 0.655771 |
| | 28 | 1 | 0 | -4.006567 | 1.079263 | 1.792217 |
| | 29 | 1 | 0 | -4.593014 | 2.366075 | 0.701725 |
| | 30 | 1 | 0 | -5.105717 | 0.664378 | 0.482517 |
| | 31 | 1 | 0 | 0.171696 | 0.821713 | 2.256280 |
| | 32 | 1 | 0 | -1.512508 | 0.751342 | 1.830010 |
| | 33 | 1 | 0 | -3.215731 | -0.529895 | -2.349121 |
| | 34 | 1 | 0 | -2.762413 | -2.043059 | -1.598525 |
| | 35 | 1 | 0 | -0.972668 | -3.003560 | 3.761066 |
| | 36 | 1 | 0 | -6.893040 | -1.921009 | -0.715379 |
| | 37 | 1 | 0 | 0.488527 | 3.983523 | 0.197513 |
| | 38 | 1 | 0 | 1.533837 | 3.318426 | -1.094425 |
| | 39 | 1 | 0 | -0.054738 | 2.559466 | -0.737659 |
| | 40 | 1 | 0 | 7.158804 | -1.065540 | -0.894215 |
| | 41 | 1 | 0 | 6.000738 | -2.141475 | -0.060382 |
| | 42 | 1 | 0 | 5.761384 | -1.730385 | -1.788439 |