Supporting information

Photocaging of Aminoacids and Short Peptides by Arylidenethiazoles: Mechanism, Photochemical Charachteristics and Biological Behaviour

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Table of contents

1. EXPERIMENTAL SECTION

Materials and general methods. All reagents were purchased from Acros Organics and used without further purification. ^{1}H, and ^{13}C NMR, spectra were recorded with Bruker Avance II (Karlsruhe, Germany) (400 MHz for ^{1}H, and 100 MHz for ^{13}C, NMR) spectrometer and Bruker Avance NEO spectrometer (Karlsruhe, Germany; 600 MHz for ^{1}H and 150 MHz for ^{13}C). Chemical shifts are reported in parts per million (ppm) relative to TMS in ^{1}H NMR, to the residual solvent signals in ^{13}C, and NMR spectra as external reference. Coupling constants (*J*) values are given in Hertz (Hz). Signal splitting patterns are described as a singlet (s), doublet (d), triplet (t), quartet (q), sextet (sext), quintet (quint), multiplet (m), broad (br), doublet of doublets (dd), doublet of triplets (dt) or AA'XX' - spin system of para-substituted benzene with two different substituents.

High-resolution mass spectra were obtained using an Agilent 6545 Q-TOF (Agilent Technologies Inc., Santa Clara, CA, USA) equipped with an ESI source operating in positive ionization mode. Samples were infused at 3 µL/min and spectra were obtained in positive (or negative) ionization mode with a resolution of 15000 (FWHM) using leucine encephalin as lock mass. The abbreviation $[M]^+$ refers to the molecular ion. The Fourier-transform infrared (FTIR) spectra were obtained using a Bruker Alpha (NPVO, ZnSe) spectrometer (Ettlingen, Germany).

UV-Vis absorption spectra were recorded on a Shimadzu UV-1800 spectrophotometer (Kyoto, Japan). Fluorescence of the sample solutions was measured using a Hitachi F-7000 spectrophotometer (Tokyo, Japan). The absorption and emission spectra were recorded in 1,4-Dioxane, EtOH, MeOH, MeCN, DMSO and MeCN-H_2O (9:1, v/v), DMSO-H_2O (1:1, v/v), DMSO-buff (1:1, v/v) mixtures in 10.00 mm quartz cells. The excitation wavelength was at the absorption maxima. Atmospheric oxygen contained in solutions was not removed. Concentration of the compounds in the solution was 5×10^{-5} M and 2.5×10^{-6} M, 5×10^{-6} M for absorption and fluorescence measurements, respectively. The relative fluorescence quantum yields (QY) were determined using quinine sulphate (5×10^{-6} M) in 0.1 M H_2SO_4 as a standard ($\Phi_F = 0.546$). All solvents were of spectroscopic grade.

Melting points were determined on a Stuart SMP3 apparatus (Staffordshire, ST15 OSA, UK). The reactions were monitored by analytical thin-layer chromatography (TLC) on aluminium-backed silica-gel plates (Sorbfil UV–254). Visualization of components was accomplished by short wavelength UV-light (254 nm). Solvents were dried and distilled according to the common procedures. All compounds are >95% pure by HPLC.

3-(4-Methoxyphenyl)-2-(5-methyl-4-phenylthiazol-2-yl)acrylonitrile (3b). Yellow powder (0.209 g, 65% yield); mp = 89-91 °C; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.09 (s, 1H), 7.96 and 6.99 (AA`XX`, 4H, *J* = 8.8 Hz), 7.70 (d, 2H, *J* = 7.2 Hz), 7.47 (t, 2H, *J* = 7.4 Hz), 7.38 (t, 1H, *J* = 7.4 Hz), 3.88 (s, 3H), 2.61 (s, 3H). $^{13}C\{1H\}$ NMR ($CDCl_3$, 101 MHz): δ 162.3, 158.7, 152.5, 143.0, 134.5, 132.1, 129.7, 128.7, 128.5, 128.0, 125.6, 117.5, 114.6, 101.9, 55.5, 12.9. FT-IR (neat) v_{max} (cm^{-1}): 3054, 3005, 2970, 2932, 2842, 2214. HRMS (ESI-TOF) m/z: $[M+H]^+$ Calcd. for $C_{20}H_{16}N_2OSH$ 333.1056; Found 333.1069.

3-(4-Bromophenyl)-2-(5-methyl-4-phenylthiazol-2-yl)acrylonitrile (3c). Light-yellow powder (0.239 g, 63% yield); mp = 145-147 °C; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.10 (s, 1H), 7.82 and 7.61 (AA'XX', 4H, *J* = 8.5 Hz), 7.69 (d, 2H, *J* = 7.3 Hz), 7.47 (t, 2H, *J* = 7.4 Hz), 7.39 (t, 1H, *J* = 7.3 Hz), 2.63 (s, 3H). $^{13}C\{1H\}$ NMR ($CDCl_3$, 101 MHz): δ 157.7, 153.0, 141.6, 134.3, 132.4, 131.7, 131.2, 130.8, 128.6, 128.5, 128.1, 126.0, 116.7, 105.4, 12.9. FT-IR (neat) v_{max} (cm^{-1}): 3076, 3061, 2224. HRMS (ESI-TOF) m/z: $[M+H]^+$ Calcd. for $C_{19}H_{13}BrN_2SH$ 381.0056; Found 381.0061.

2-(5-(Bromomethyl)-4-phenylthiazol-2-yl)-3-(4-bromophenyl)acrylonitrile (4c). Yellow powder (0.405 g, 88% yield); mp = 130-132 °C; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.19 (s, 1H), 7.84 and 7.64 (AA'XX', 4H, *J* = 8.6 Hz), 7.77 (d, 2H, *J* = 7.0 Hz), 7.53 (t, 2H, *J* = 7.3 Hz), 7.48 (m, 1H), 4.81 (s, 2H). $^{13}C\{1H\}$ NMR ($CDCl_3$, 101 MHz): δ 161.2, 155.2, 143.2, 133.2, 132.6, 131.9, 131.4, 131.3, 129.1, 128.9, 128.6, 126.7, 116.3, 105.1, 24.4. FT-IR (KBr) v_{max} (cm^{-1}): 3093, 3060, 3022, 2851, 2221. HRMS (ESI-TOF) m/z: $[M+H]^+$ Calcd. for $C_{19}H_{12}Br_2N_2SH$ 458.9161; Found 458.9159.

General Procedure for the synthesis of compounds 6-8. $NaHCO_3$ (1.0 mmol, 0.084 g) was added to a solution of compound **3** (1.0 mmol, 0.406 g) in DMF (2.0 mL). The mixture was stirred at room temperature for 10 min, then *Boc*-protected amino acids or peptides **5** were added and stirring continued until the starting compound **3** was consumed. The resulting mixture was poured into distilled water and extracted with dichloromethane (3 x 25 ml). The combined organic extracts were washed with water, brine, dried with anhydrous sulphate, filtered and concentrated under reduced pressure. The residue was purified by silica gel column chromatography (elution with petroleum ether/ethyl acetate = 4/3) to give the resulting compound.

(2-(1-Cyano-2-(4-cyanophenyl)vinyl)-4-phenylthiazol-5-yl)methyl(*tert*-butoxycarbonyl)glycinate (6a). Yellow powder (0.250 g, 50% yield); mp = 101-103 °C; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.25 (s, 1H), 8.05 (d, 2H, *J* = 8.5 Hz), 7.78 (d, 2H, *J* = 8.1 Hz), 7.68 (d, 2H, *J* = 7.0 Hz), 7.49 (m, 3H), 5.43 (s, 2H), 5.01 (br s, 1H), 4.01 (d, 2H, *J* = 5.6 Hz), 1.46 (s, 9H). $^{13}C\{^{1}H\}$ NMR ($CDCl_3$, 101 MHz): δ 170.2, 161.0, 156.8, 155.7, 141.6, 136.5, 1 33.0, 132.8, 130.2, 129.3, 129.0, 128.9, 128.8, 118.0, 115.8, 114.7, 107.9, 80.3, 58.9, 42.4, 28.3. FT-IR (neat) v_{max} (cm^{-1}): 3393, 3021, 2276, 1754, 1667. HRMS (ESI-TOF) m/z: $[M+H]^+$ Calcd. for $C_{27}H_{24}N_4O_4SH$ 501.1591; Found 501.1596.

(2-(1-Cyano-2-(4-cyanophenyl)vinyl)-4-phenylthiazol-5-yl)methyl 4-((*tert*-butoxycarbonyl)-amino)butanoate (6b). Yellow powder (0.286 g, 54% yield); mp = 113-115 °C; ^{1}H NMR (DMSO-d_6, 400 MHz): δ 8.42 (s, 1H), 8.17 and 8.05 (AA'XX', 4H, *J* = 8.4 Hz), 7.71 (d, 2H, *J* = 7.1 Hz), 7.55 (t, 2H, *J* = 7.3 Hz), 7.50 (m, 1H), 6.83 (m, 1H), 5.38 (s, 2H), 2.94 (m, 2H), 2.39 (t, 2H, *J* = 7.4 Hz), 1.65 (q, 2H, *J* = 7.0 Hz), 1.35 (s, 9H), $^{13}C\{^1H\}$ NMR (DMSO-d$_6$, 101 MHz): δ 172.4, 160.8, 155.6, 154.4, 143.7, 136.7, 132.9 (2C), 130.3, 130.1, 128.9, 128.8, 128.6, 118.3, 115.6, 113.3, 107.9, 77.5, 57.8, 30.6, 28.2, 24.7. FT-IR (neat) v_{max} (cm^{-1}): 3317, 2971, 2227, 1732, 1686. HRMS (ESI-TOF) m/z: $[M+H]^+$ Calcd. for $C_{29}H_{28}N_4O_4SH$ 529.1904; Found 529.1901.

(2-(1-Cyano-2-(4-cyanophenyl)vinyl)-4-phenylthiazol-5-yl)methyl N2,N$_6$-bis(tert-butoxy-carbonyl)lysinate (6c). Dark yellow oil (0.329 g, 49% yield); ^1H NMR (CDCl$_3$, 400 MHz): δ 8.25 (s, 1H), 8.05 (d, 2H, *J* = 7.7 Hz), 7.78 (d, 2H, *J* = 8.1 Hz), 8.25 (s, 1H), 7.69 (d, 2H, *J* = 7.7 Hz), 7.50 (m, 3H), 5.46 and 5.37 (AB, 2H, *J* = 13.3 Hz), 5.10 (s, 1H), 4.54 (br s, 1H), 4.33 (br s, 1H), 3.08 (s, 2H), 1.82 (m, 1H), 1.64 (m, 2H), 1.46 (m, 21H). $^{13}C\{^1H\}$ NMR (CDCl$_3$, 101 MHz): δ 172.6, 160.9, 156.6, 156.1, 155.5, 141.7, 136.5, 133.1, 132.8, 130.3, 129.2, 129.1, 128.9, 128.8, 118.0, 115.8, 114.7, 108.0, 80.2, 58.9, 53.4, 39.9, 29.7, 28.4, 28.3, 22.5, 22.1. FT-IR (KBr) v_{max} (cm^{-1}): 3369, 3064, 2976, 2930, 2863, 2229, 1745, 1707. HRMS (ESI-TOF) *m/z*: $[M+H]^+$ Calcd. for $C_{36}H_{41}N_5O_6SH$ 672.2837; Found 672.2850.

1-(*tert*-Butyl) 2-((2-(1-cyano-2-(4-cyanophenyl)vinyl)-4-phenylthiazol-5-yl)methyl)pyrrolidine-1,2-dicarboxylate (6d). Yellow oil (0.378 g, 70% yield); ^1H NMR (CDCl$_3$, 600 MHz): δ 8.24 (s, 1H), 8.05 and 7.78 (AA'XX', 4H, *J* = 7.7 Hz), 7.70 (d, 2H, *J* = 7.3 Hz), 7.49 (m, 3H), 5.52 and 5.35 (AB, 1H, *J* = 13.2 Hz), 5.44 and 5.39 (AB, 1H, *J* = 13.1 Hz), 4.36 (m, 1H), 3.50 (m, 2H), 2.26 (m, 2H), 1.94 (m, 3H), 1.46 (s, 4.17H), 1.34 (s, 4.83H). $^{13}C\{^1H\}$ NMR (CDCl$_3$, 151 MHz): δ 173.0, 172.7, 160.9, 160.7, 156.8, 156.4, 154.4, 153.6, 141.6, 141.4, 136.6, 136.5, 133.1, 133.0, 132.8, 130.3, 130.2, 129.7, 129.3, 129.2, 129.1, 128.9, 128.8, 118.0 (2C), 115.9, 115.8, 114.7, 114.6, 108.0, 107.9, 80.1, 59.0, 58.8, 58.7, 58.5, 46.6, 46.4, 30.9, 29.9, 29.7, 28.4, 28.3, 24.5, 23.7. FT-IR (KBr) v_{max} (cm^{-1}): 2975, 2930, 2879, 2228, 1749, 1694. HRMS (ESI-TOF) *m/z*: [M+H]+ Calcd. for $C_{30}H_{28}N_4O_4SH$ 541.1904; Found 541.1921.

(2-(1-Cyano-2-(4-cyanophenyl)vinyl)-4-phenylthiazol-5-yl)methyl acetyltryptophanate (6e). Yellow powder (0.343 g, 60% yield); mp = 104-106 °C; ^1H NMR (CDCl$_3$, 400 MHz): δ 8.20 (s, 1H), 8.10 (s, 1H), 8.04 (d, 2H, *J* = 7.0 Hz), 7.78 (d, 2H, *J* = 6.8 Hz), 7.58 (m, 2H), 7.52 (d, 1H, *J* = 8.0 Hz), 7.46 (m, 3H), 7.31 (d, 1H, *J* = 7.9 Hz), 7.15 (t, 1H, *J* = 7.0 Hz), 7.06 (t, 1H, *J* = 7.2 Hz), 6.91 (s, 1H), 6.03 (d, 1H, *J* = 7.3 Hz), 5.35 and 5.24 (AB, 2H, *J* = 13.5 Hz), 5.02 (m, 1H), 3.31 (m, 2H), 2.00 (s, 3H). $^{13}C\{^1H\}$ NMR (CDCl$_3$, 101 MHz): δ 171.9, 169.8, 160.9, 156.7, 141.6, 136.5, 136.2, 133.0, 132.8, 130.2, 129.2, 128.9 (2C), 128.8, 127.5, 122.7, 122.4, 119.9, 118.4, 118.0, 115.9, 114.7, 111.4, 109.7, 107.9, 58.9, 53.1, 27.9, 23.2. FT-IR (KBr) v_{max} (cm^{-1}): 3406, 3058, 2925, 2852, 2228, 1742, 1656. HRMS (ESI-TOF) *m/z*: $[M+H]^+$ Calcd. for $C_{33}H_{25}N_5O_3SH$ 572.1751; Found 572.1766.

(2-(1-Cyano-2-(4-cyanophenyl)vinyl)-4-phenylthiazol-5-yl)methyl (*tert*-butoxycarbonyl)-glycylleucinate (6f). Yellow oil (0.246 g, 40% yield); ^1H NMR (CDCl$_3$, 600 MHz): δ 8.26 (s, 1H), 8.05 and 7.78 (AA'XX', 4H, J = 8.3 Hz), 7.69 (d, 2H, J = 7.3 Hz), 7.52 (t, 2H, *J* = 7.4 Hz), 7.47 (t, 1H, *J* = 7.3 Hz), 6.50 (s, 1H), 5.43 and 5.37 (AB, 2H, *J* = 13.3 Hz), 5.10 (br s, 1H), 4.69 (m, 1H), 3.83 (m, 2H), 1.67 (m, 3H), 1.46 (s, 9H), 0.94 (d, 6H, *J* = 5.8 Hz). $^{13}C\{^1H\}$ NMR (CDCl$_3$, 151 MHz): δ 172.5, 169.5, 160.9, 156.8, 156.1, 141.7, 136.5, 133.0, 132.8, 130.3, 129.3, 128.9, 128.8, 118.0, 115.9, 114.7, 107.9, 80.6, 59.0, 50.7, 44.5, 41.2, 29.7, 28.3, 24.9, 22.8, 21.8. FT-IR (KBr) v_{max} (cm^{-1}): 3357, 3063, 2959, 2927, 2870, 2853, 2229, 1744, 1710, 1679. HRMS (ESI-TOF) *m/z*: $[M+H]^+$ Calcd. for $C_{33}H_{35}N_5O_5SH$ 614.2432; Found 614.2432.

(2-(1-Cyano-2-(4-cyanophenyl)vinyl)-4-phenylthiazol-5-yl)methyl (*tert*-butoxycarbonyl)glycyl-phenylalanylleucinate (6g). Yellow oil (0.312 g, 41% yield); ^1H NMR (CDCl$_3$, 600 MHz): δ 8.26 (s, 1H), 8.05 and 7.78 (AA'XX', 4H, *J* = 8.4 Hz), 7.69 (d, 2H, *J* = 7.2 Hz), 7.52 (t, 2H, *J* = 7.4 Hz), 7.47 (t, 1H, *J* = 7.3 Hz), 7.27 (m, 2H), 7.21 (m, 3H), 6.54 (d, 1H, *J* = 7.6 Hz), 6.39 (br s, 1H), 5.40 and 5.36 (AB, 2H, *J* = 13.3 Hz), 5.00 (br s , 1H), 4.71 (m, 1H), 4.57 (m, 1H), 3.74 (m, 2H), 3.19 (m, 1H), 3.04 (dd, *J* = 14.0 Hz, *J* = 6.9 Hz, 1H), 1.60 (m, 1H), 1.51 (m, 2H), 1.41 (s, 9H), 0.89 (d, 6H, *J* = 6.2 Hz). $^{13}C\{^1H\}$ NMR (CDCl$_3$, 151 MHz): δ 171.9, 170.5, 169.3, 160.9, 156.6, 156.2, 136.5, 136.1, 133.1, 132.8, 130.2, 129.3, 129.2, 129.1, 128.9, 128.8, 128.7, 128.0, 127.2, 118.0, 115.9, 114.6, 108.0, 80.7, 59.0, 54.0, 51.0, 44.6, 40.9, 37.5, 28.2, 24.7, 22.7, 21.8. FT-IR (KBr) v_{max} (cm^{-1}): 3307, 3064, 2959, 2927, 2870, 2229, 1749, 1656. HRMS (ESI-TOF) *m/z*: $[M+H]^+$ Calcd. for $C_{42}H_{44}N_6O_6SH$ 761.3116; Found 761.3104.

(2-(1-Cyano-2-(4-methoxyphenyl)vinyl)-4-phenylthiazol-5-yl)methyl (*tert*-butoxycarbonyl)glycinate (7). Orange oil (0.247 g, 49% yield); ^1H NMR (CDCl$_3$, 400 MHz): δ 8.16 (s, 1H), 7.98 and 7.00 (AA'XX', 4H, *J* = 8.8 Hz), 7.69 (d, 2H, *J* = 7.1 Hz), 7.48 (m, 3H), 5.40 (s, 2H), 5.01 (br s, 1H), 4.00 (d, 2H, *J* = 5.6 Hz), 3.89 (s, 3H), 1.46 (s, 9H). $^{13}C\{^1H\}$ NMR (CDCl$_3$, 151 MHz): δ 170.2, 163.0, 162.7, 156.3, 155.7, 144.5, 133.4, 132.5, 129.0, 128.9, 128.8, 126.8, 125.3, 117.2, 114.7, 101.5, 80.3, 59.0, 55.6, 42.5, 28.3. FT-IR (KBr) v_{max} (cm^{-1}): 3386, 3059, 2974, 2928, 2850, 2216, 1752, 1714. HRMS (ESI-TOF) *m/z*: $[M+H]^+$ Calcd. for $C_{27}H_{27}N_3O_5SH$ 506.1744; Found 506.1761.

(2-(2-(4-Bromophenyl)-1-cyanovinyl)-4-phenylthiazol-5-yl)methyl (*tert*-butoxycarbonyl)glycinate (8). Yellow oil (0.199 g, 36% yield); ^1H NMR (CDCl$_3$, 400 MHz): δ 8.20 (s, 1H), 7.86 and 7.66 (AA'XX', 4H, *J* = 8.5 Hz), 7.71 (d, 2H, *J* = 6.8 Hz), 7.51 (m, 3H), 5.44 (s, 2H), 5.04 (br s, 1H), 4.03 (d, 2H, *J* = 5.3 Hz), 3.89 (s, 3H), 1.48 (s, 9H). $^{13}C\{^1H\}$ NMR (CDCl$_3$, 101 MHz): δ 170.2, 161.8, 156.6, 155.7, 143.2, 133.2, 132.6, 131.4, 131.3, 129.1, 128.9, 128.8, 128.0, 126.6, 116.3, 105.2, 80.3, 58.9, 42.4, 28.3. FT-IR (KBr) v_{max} (cm^{-1}): 3418, 3060, 2976, 2926, 2197, 1753, 1714. HRMS (ESI-TOF) *m/z*: $[M+H]^+$ Calcd. for $C_{26}H_{24}BrN_3O_4SH$ 554.0744; Found 554.0753.

2. NMR ^1H and ^{13}C spectra of new compounds

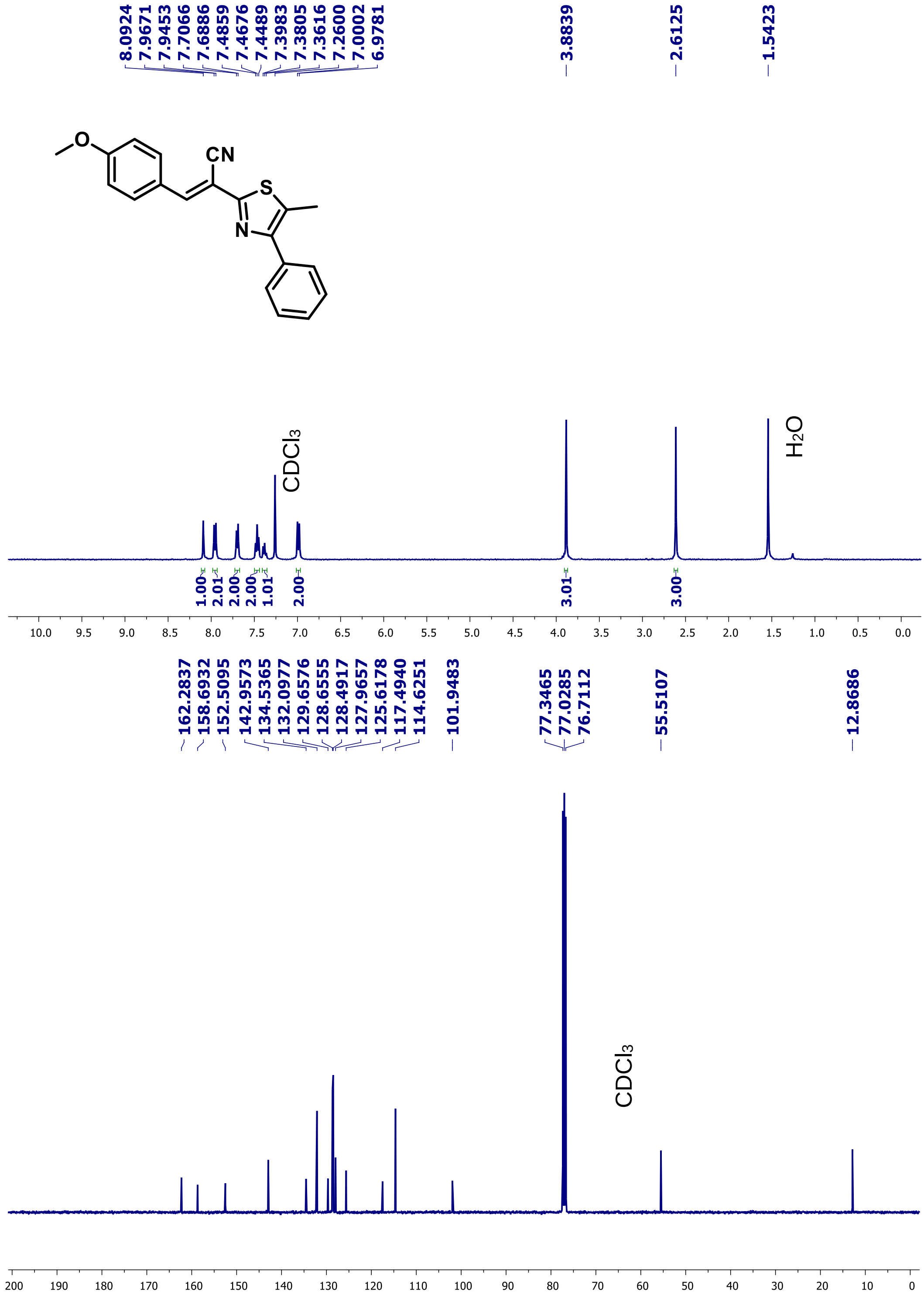


Fig. S1. ^{1}H NMR (400 MHz, $CDCl_3$, TMS) and ^{13}C NMR (101 MHz, $CDCl_3$) spectra of 3-(4-methoxyphenyl)-2-(5-methyl-4-phenylthiazol-2-yl)acrylonitrile **3b**.

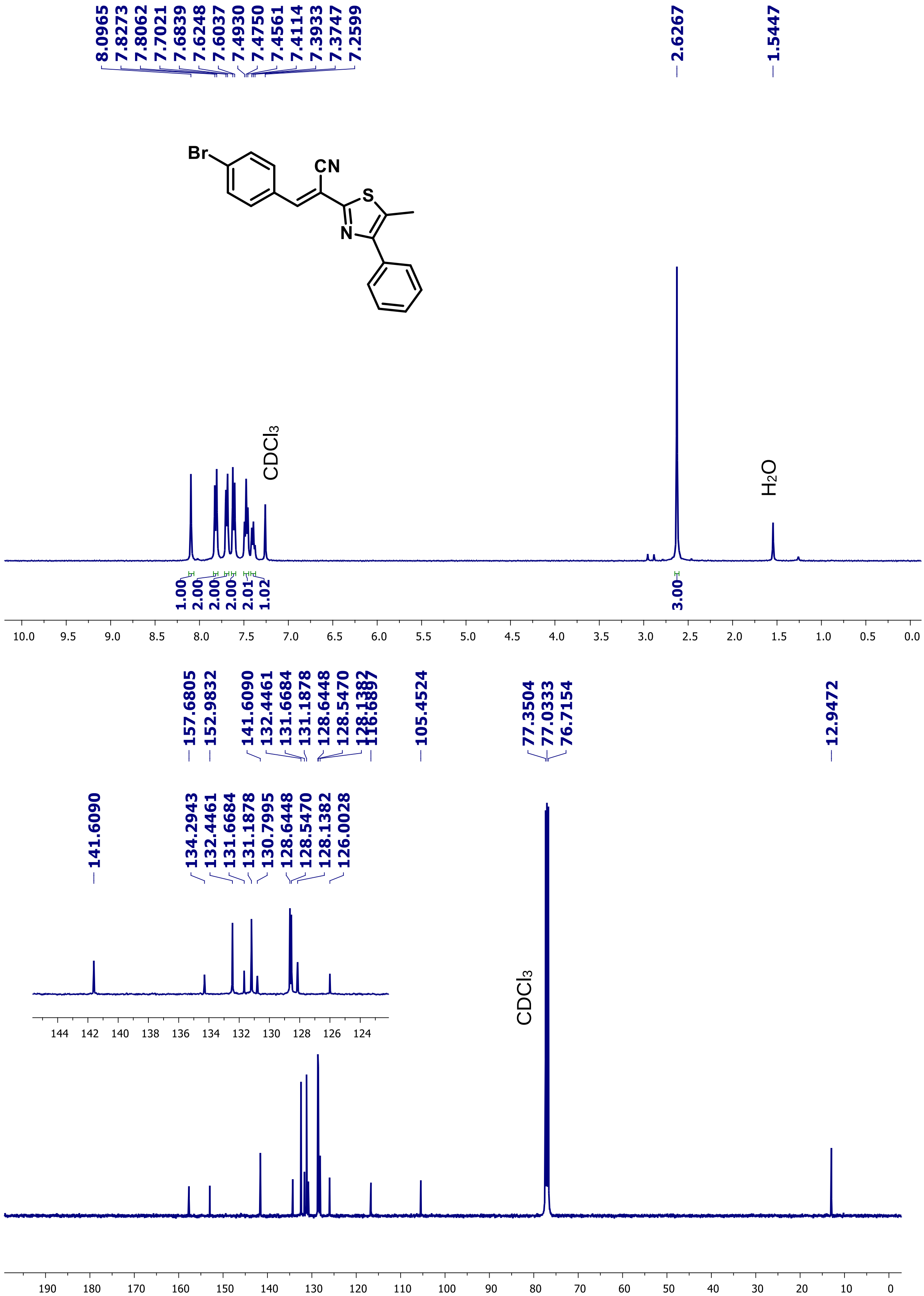


Fig. S2. ^{1}H NMR (400 MHz, $CDCl_3$, TMS) and ^{13}C NMR (101 MHz, $CDCl_3$) spectra of 3-(4-bromophenyl)-2-(5-methyl-4-phenylthiazol-2-yl)acrylonitrile **3c**.

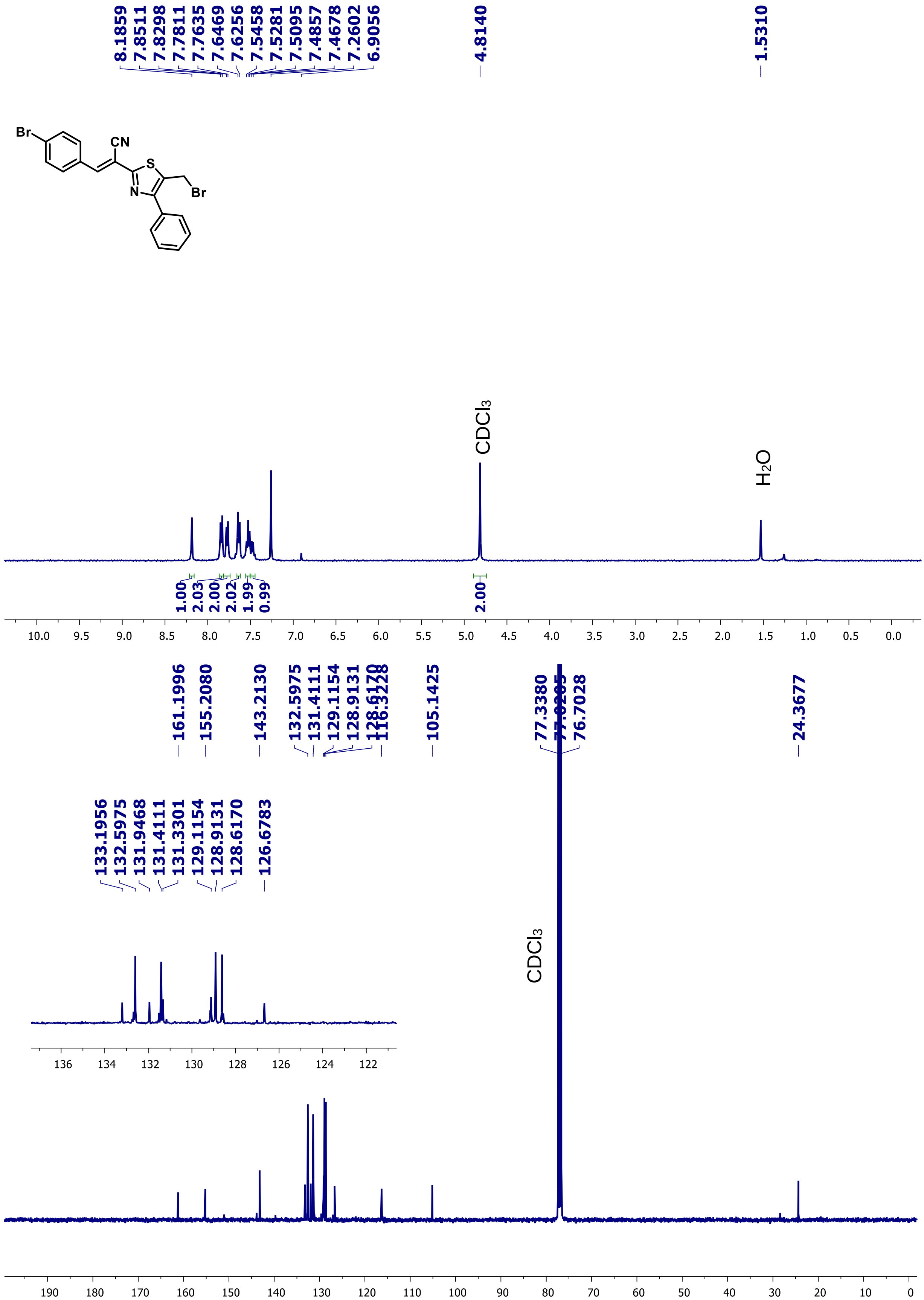


Fig. S3. ^{1}H NMR (400 MHz, $CDCl_3$, TMS) and ^{13}C NMR (101 MHz, $CDCl_3$) spectra of 2-(5-(bromomethyl)-4-phenylthiazol-2-yl)-3-(4-bromophenyl)acrylonitrile **4c**.

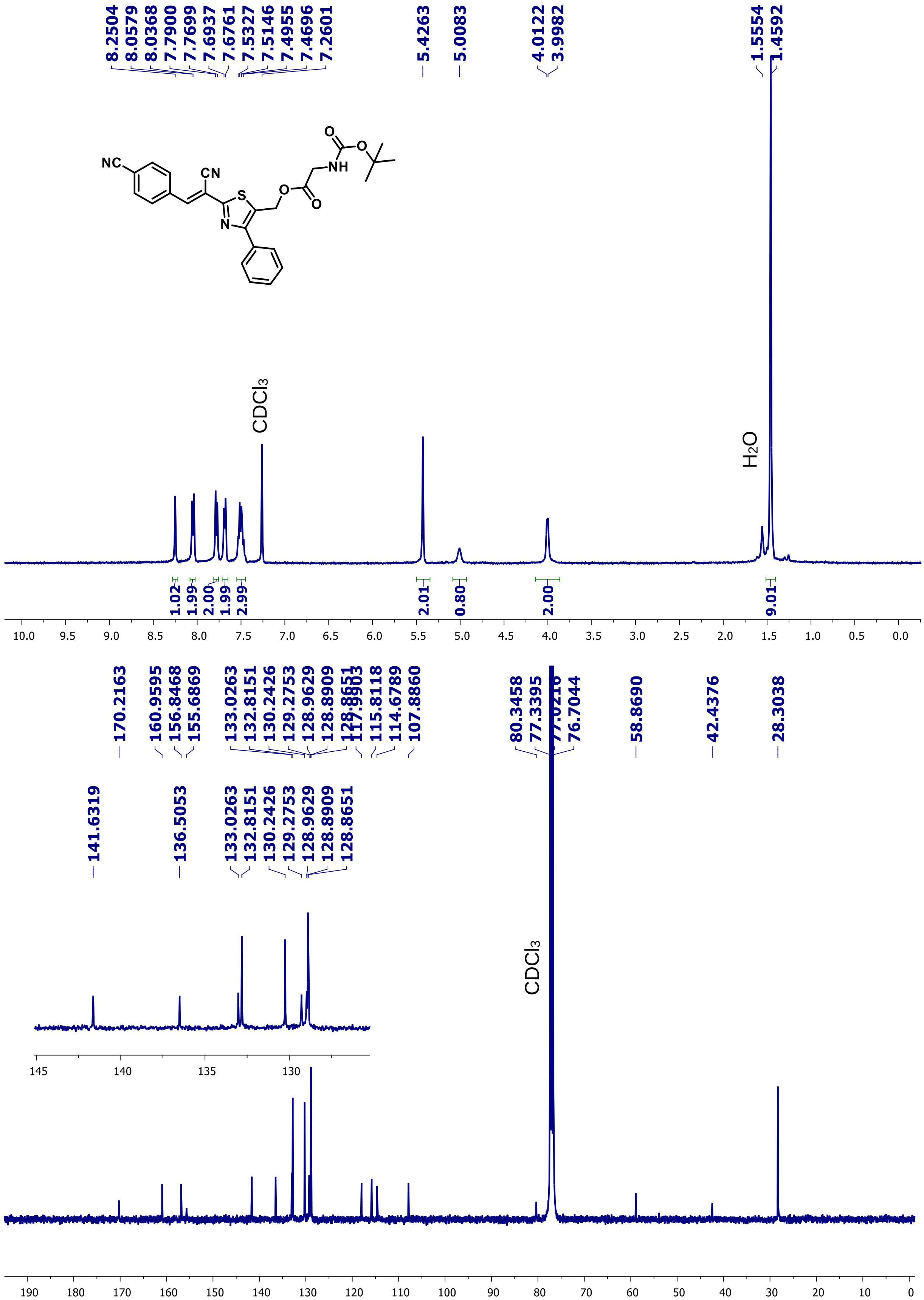


Fig. S4. ^{1}H NMR (400 MHz, $CDCl_3$, TMS) and ^{13}C NMR (101 MHz, $CDCl_3$) spectra of (2-(1-cyano-2-(4-cyanophenyl)vinyl)-4-phenylthiazol-5-yl)methyl (*tert*-butoxycarbonyl)glycinate **6a**.

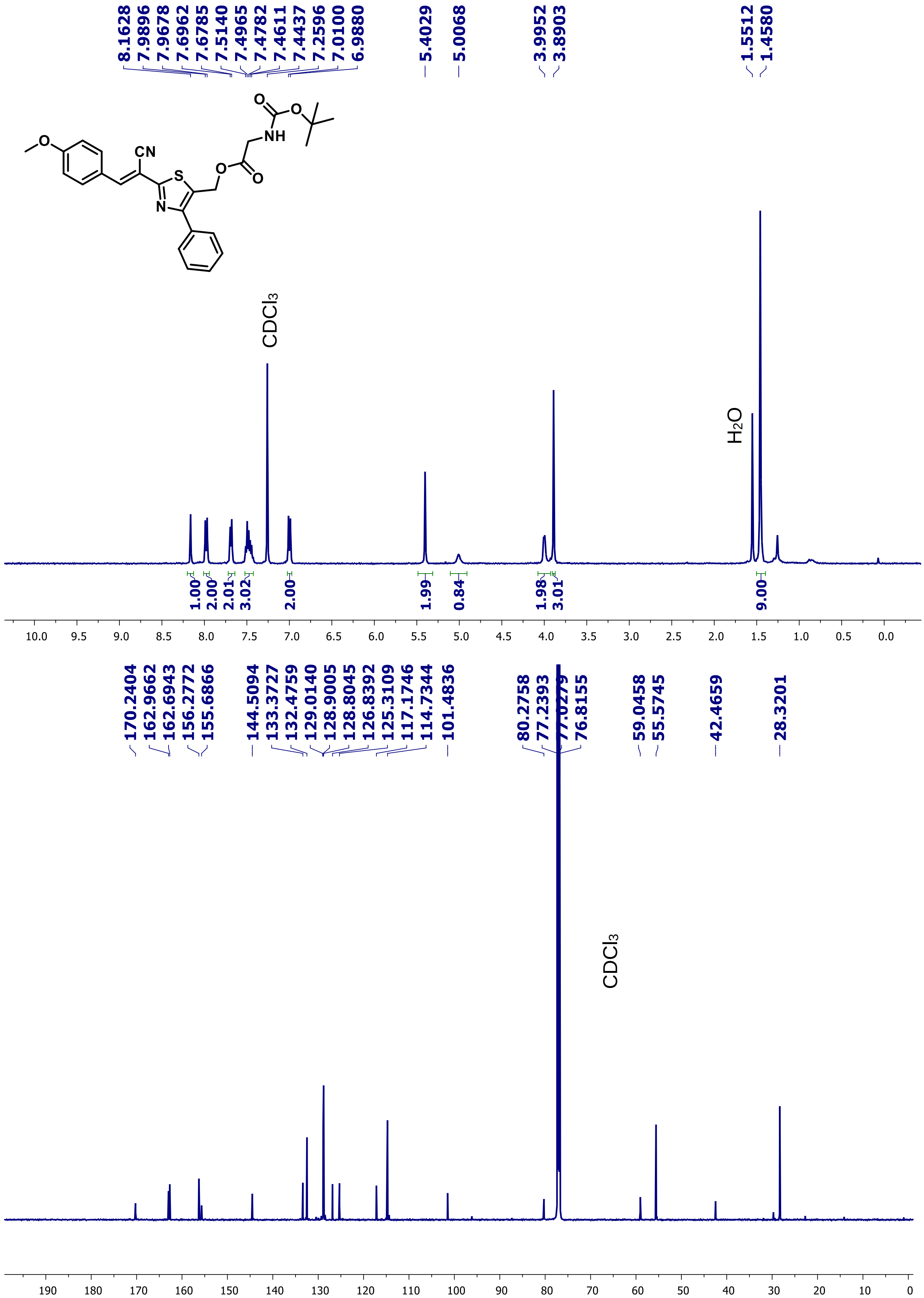


Fig. S5. ^{1}H NMR (400 MHz, $CDCl_3$, TMS) and ^{13}C NMR (151 MHz, $CDCl_3$) spectra of (2-(1-cyano-2-(4-methoxyphenyl)vinyl)-4-phenylthiazol-5-yl)methyl (*tert*-butoxycarbonyl)glycinate **7**.

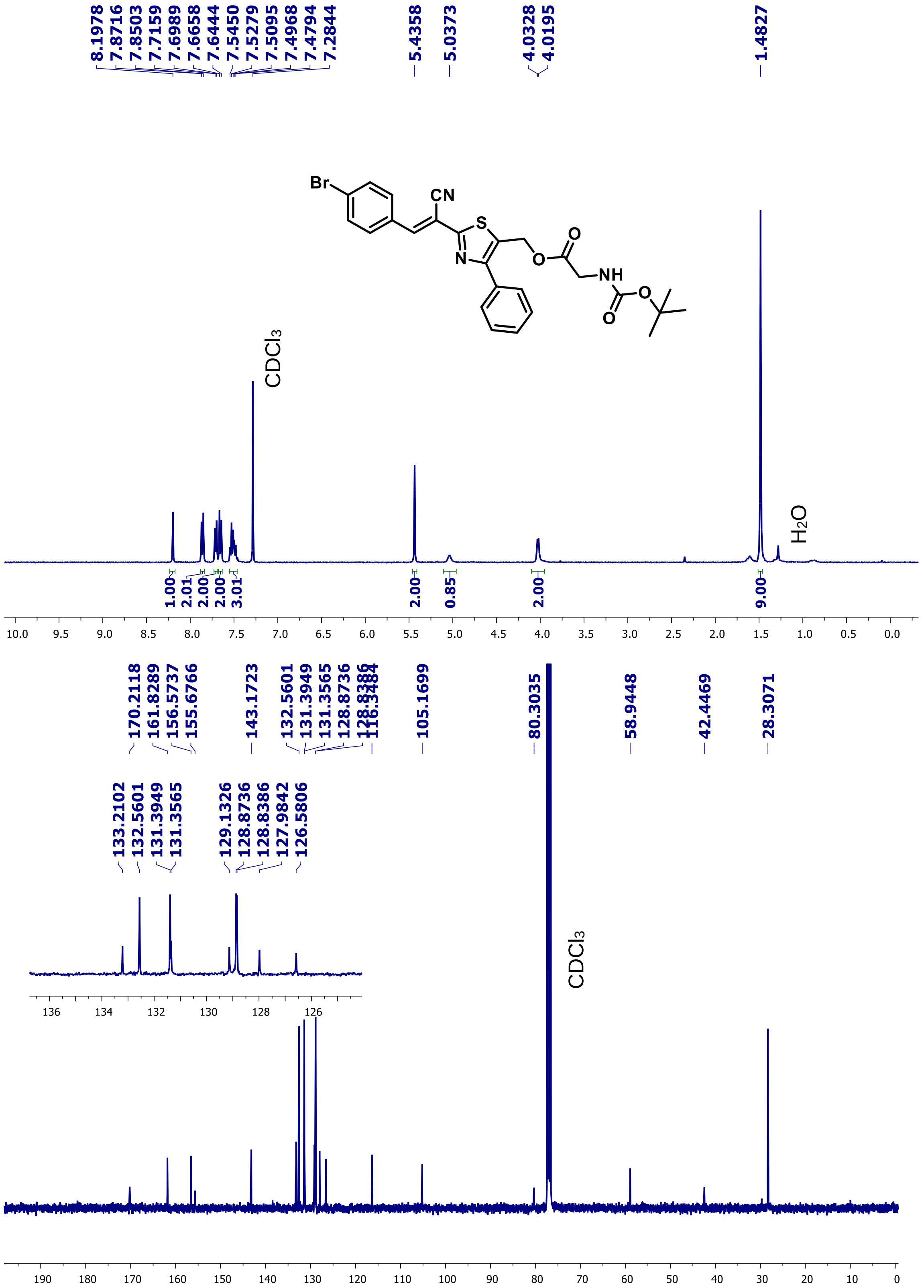


Fig. S6. ^{1}H NMR (400 MHz, $CDCl_3$, TMS) and ^{13}C NMR (101 MHz, $CDCl_3$) spectra of (2-(2-(4-bromophenyl)-1-cyanovinyl)-4-phenylthiazol-5-yl)methyl (*tert*-butoxycarbonyl)glycinate **8**.

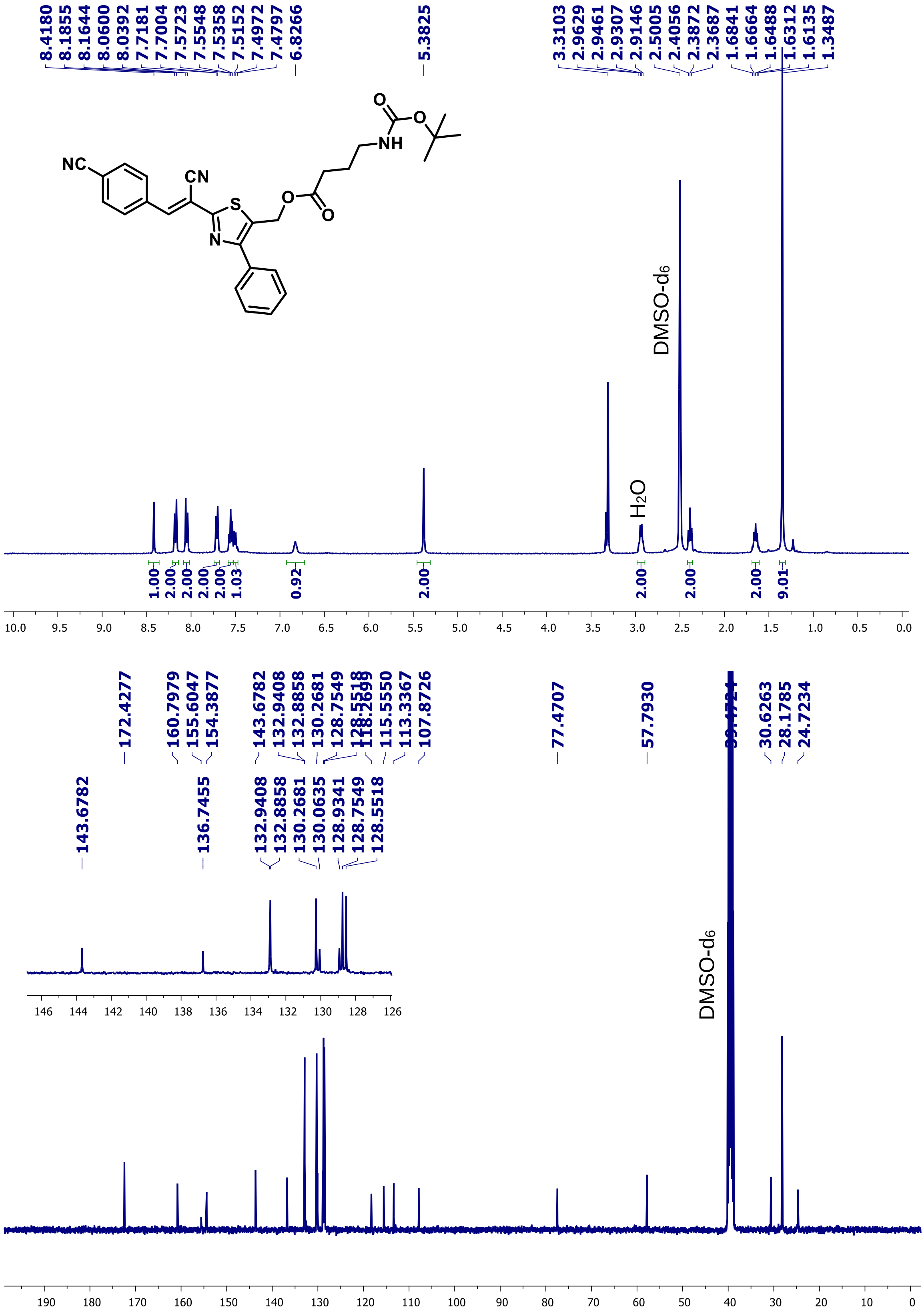


Fig. S7. ^{1}H NMR (400 MHz, DMSO-d$_6$, TMS) and ^{13}C NMR (101 MHz, DMSO-d$_6$) spectra of (2-(1-cyano-2-(4-cyanophenyl)vinyl)-4-phenylthiazol-5-yl)methyl 4-((*tert*-butoxycarbonyl)amino)butanoate **6b**.

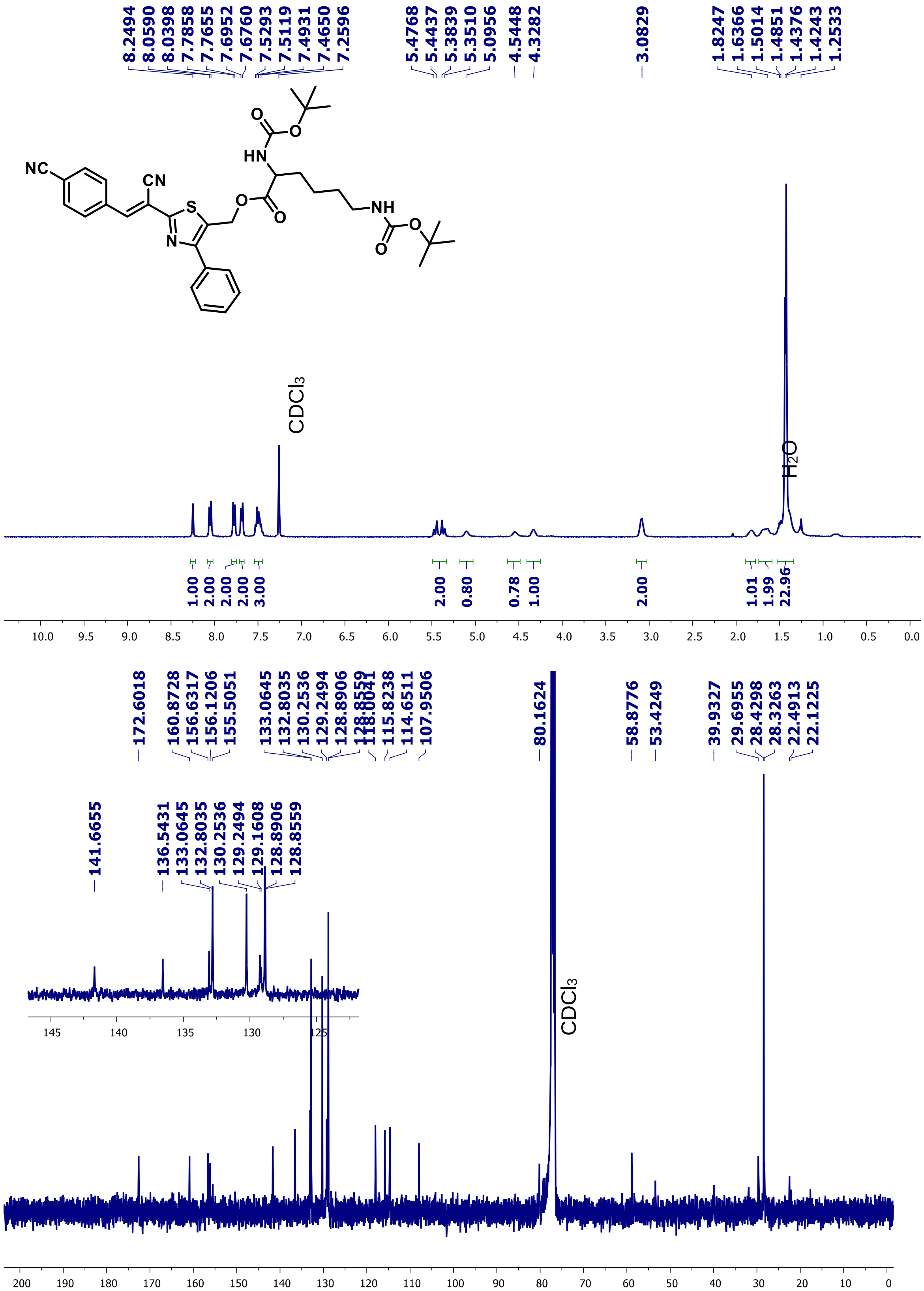


Fig. S8. ^{1}H NMR (400 MHz, $CDCl_3$, TMS) and ^{13}C NMR (101 MHz, $CDCl_3$) spectra of (2-(1-cyano-2-(4-cyanophenyl)vinyl)-4-phenylthiazol-5-yl)methyl N2,N6-bis(*tert*-butoxycarbonyl)lysinate **6c**.

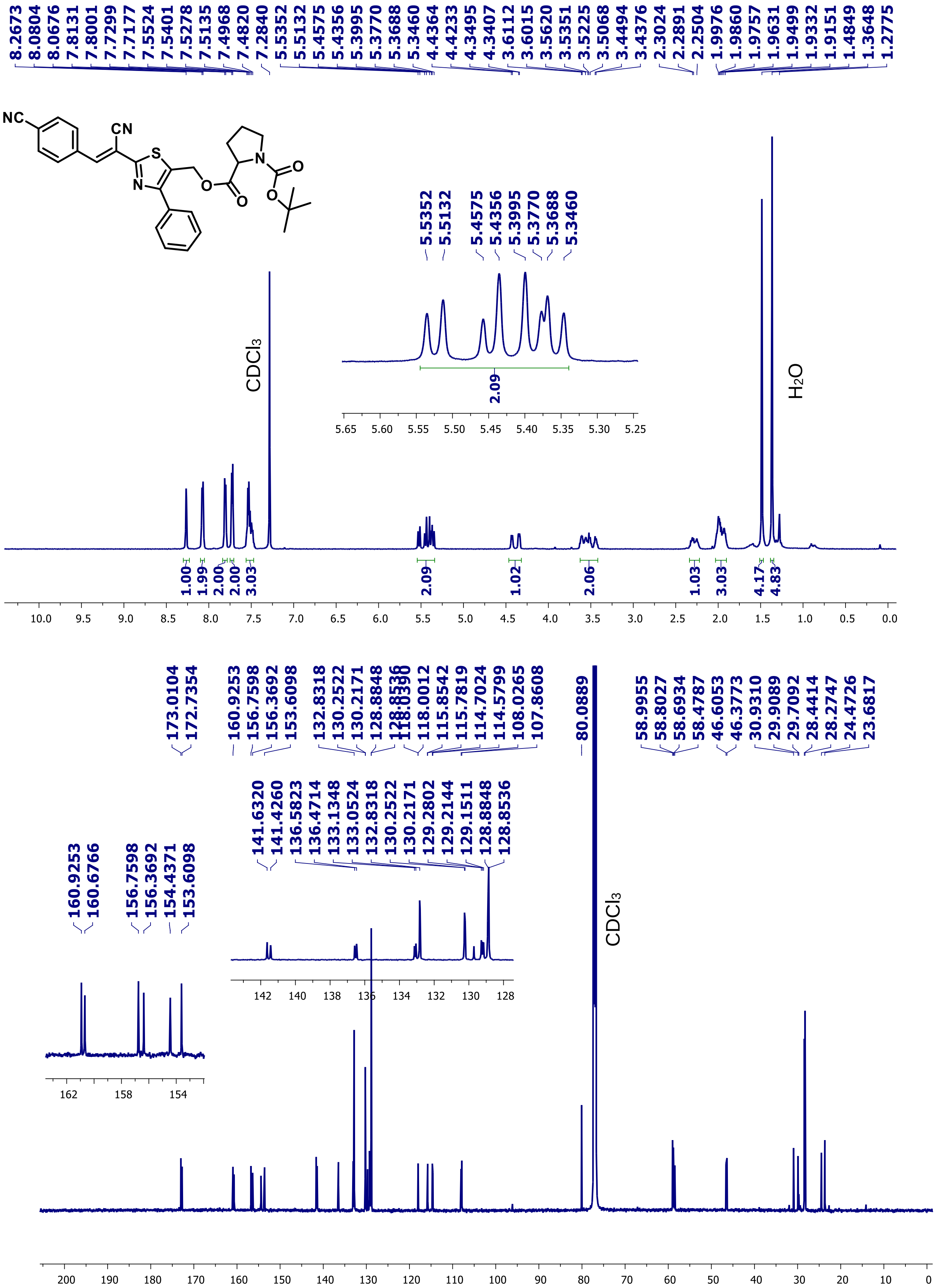


Fig. S9. Fig. S9. ^{1}H NMR (600 MHz, $CDCl_3$, TMS) and ^{13}C NMR (151 MHz, $CDCl_3$) spectra of 1-(*tert*-butyl) 2-((2-(1-cyano-2-(4-cyanophenyl)vinyl)-4-phenylthiazol-5-yl)methyl) pyrrolidine-1,2-dicarboxylate **6d**.

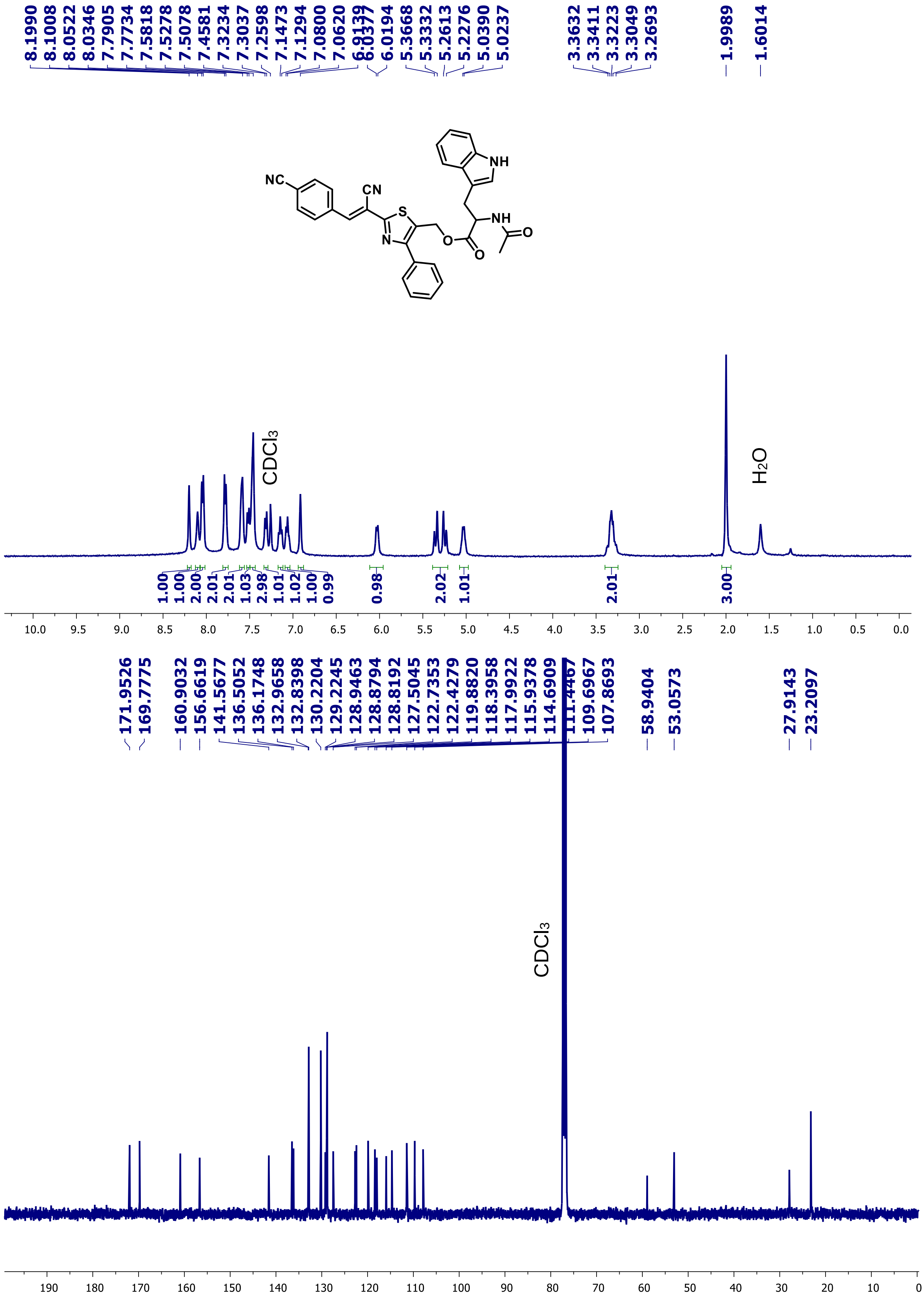


Fig. S10. ^{1}H NMR (400 MHz, $CDCl_3$, TMS) and ^{13}C NMR (101 MHz, $CDCl_3$) spectra of (2-(1-cyano-2-(4-cyanophenyl)vinyl)-4-phenylthiazol-5-yl)methyl acetyltryptophanate **6e**.

3.

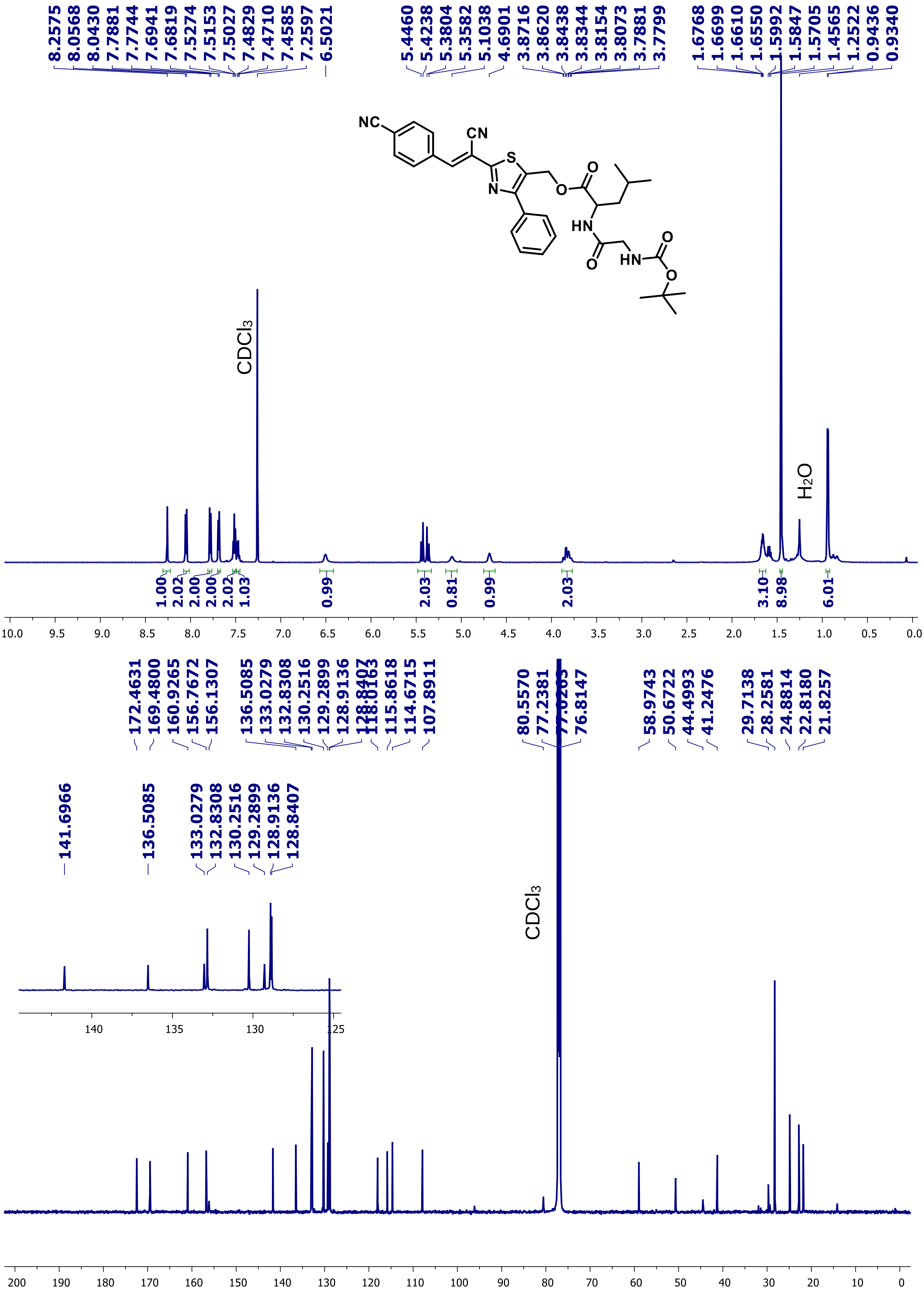


Fig. S11. ^{1}H NMR (600 MHz, $CDCl_3$, TMS) and ^{13}C NMR (151 MHz, $CDCl_3$) spectra of (2-(1-cyano-2-(4-cyanophenyl)vinyl)-4-phenylthiazol-5-yl)methyl (*tert*-butoxycarbonyl)glycylleucinate **6f**.

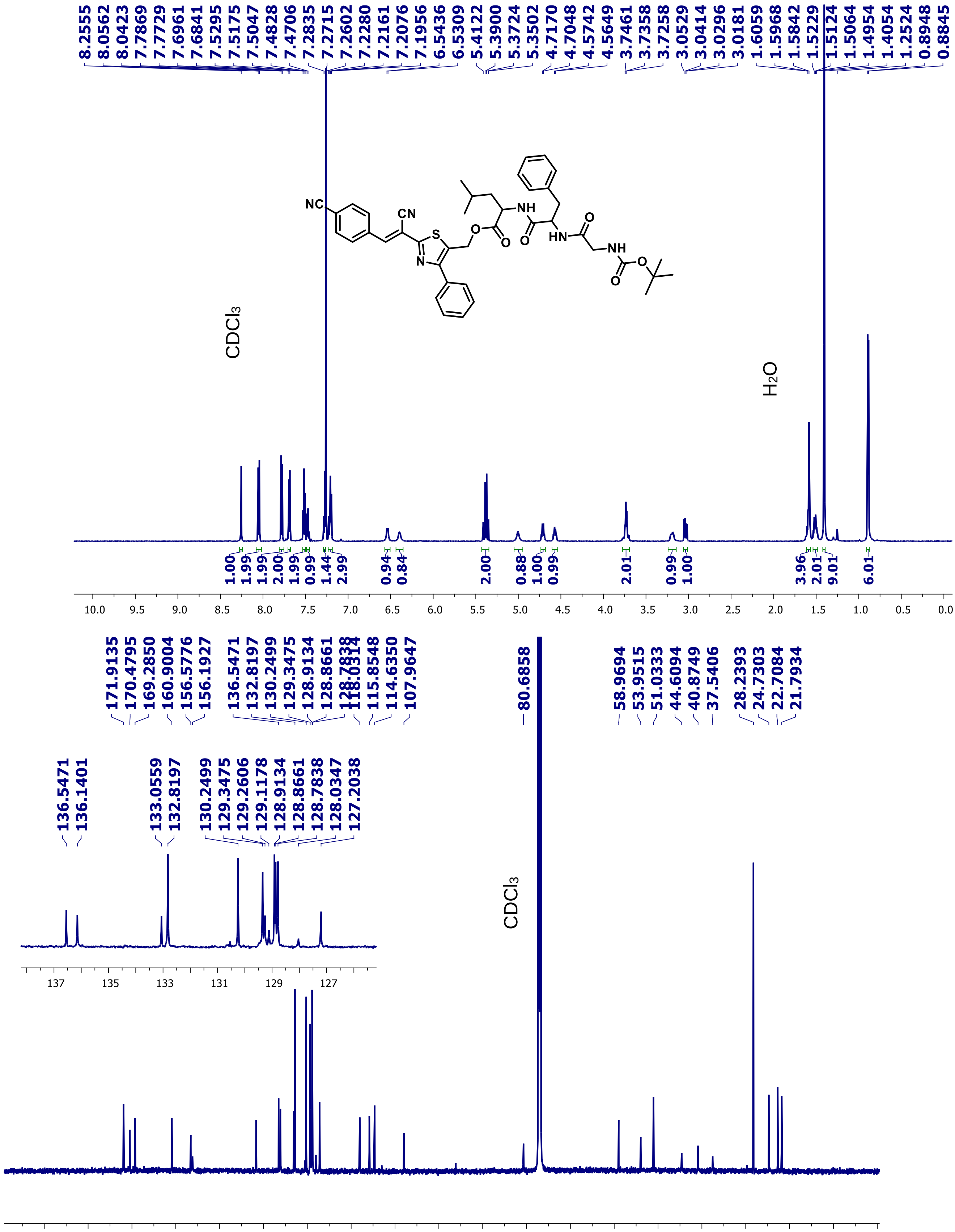


Fig. S12. ^{1}H NMR (600 MHz, $CDCl_3$, TMS) and ^{13}C NMR (151 MHz, $CDCl_3$) spectra of (2-(1-cyano-2-(4-cyanophenyl)vinyl)-4-phenylthiazol-5-yl)methyl (*tert*-butoxycarbonyl)glycylphenylalanylleucinate **6g**.

3. Photophysical properties of MPAT 3a-c in organic solvents and in binary mixtures with water and buffer pH 7.4.

Table S1. Photophysical properties of MPTA **3a-c** in different solvents.[a]

Entry	Compd	Solvent	λ_{max}, nm	ε, M^{-1} cm^{-1}	λ_{em}, nm	QY,[c] %	SS, cm^{-1}
1	**3a**[b]	Dioxd	279, 377	15500, 20960	477	25.3	5561
2		MeOH	277, 377	14000, 16500	503	27.4	6645
3		MeCN	277, 374	19600, 20800	507	25.7	7014
4		DMSO	278, 380	17300, 17700	519	24.7	7048
5	**3b**	Diox[d]	278, 375	8960, 31900	-[e]	-	-
6		MeOH	237, 274, 375	17400, 8000, 30000	429	0.5	3356
7		MeCN	238, 277, 375	17400, 9200, 28100	-[e]	-	-
8		DMSO	275, 381	10000, 26800	-[e]	-	-
9	**3c**	Diox	280, 370	14100, 25600	463	0.6	5429
10		MeOH	278, 364	13800, 23200	465	0.7	5967
		MeCN	277, 365	15300, 22000	479	0.8	6595
		DMSO	277, 373	16300, 21000	493	1.6	6526

a - For absorption **3b** and **3c**: $c = 5.0 \times 10^{-5}$ M; for fluorescence: $c = 2.5 \times 10^{-6}$ M (**3a** $c = 5.0 \times 10^{-6}$ M); b – from ref.[29]; c – Relative QY, determined relative to the standard (quinine sulphate solution; $c = 5.0 \times 10^{-5}$ M in 0.1 M H_2SO_4; $\Phi_F = 54.0$ %); d – 1,4-Dioxane. e – non-fluorescent .

4. Quantum Mechanical Calculation for MPTAs 3a-c. Computation details.

The molecular geometry of the ground state of all the main rotamers of the investigated molecules was fully optimized in *vacuo* and in implicit solvents (*vide infra*) at the Density Functional Theory (DFT) level, using a combination of the hybrid functionals B3LYP[1] and M06-2X[2] with the triple-ζ basis set 6-311++G**. The D3 version of Grimme's semi-empirical dispersion with Becke-Johnson damping GD3BJ [3] was also included in the case of B3LYP. The optimised geometries were submitted to vibrational analysis. The vibrational frequencies and thermochemical parameters were computed in harmonic approximation at $T = 298.15$ K and $p = 1$ atm, using the same level of theory employed for the optimisation. No imaginary frequencies were found.

Solvent effects were taken into account via the implicit polarizable continuum model in its integral equation formalism (IEF-PCM). [4] For geometry optimisations and frequency calculations, the PCM molecular cavity was built according to the universal force field (UFF) [5] radii within the value used in the last implementation of the PCM (based on a continuum surface charge formalism). For topological analysis and the evaluation of energetics, SMD parameterisation was employed. [6] The solvent used were acetonitrile (MeCN), chloroform ($CHCl_3$), dimethylsulhoxide (DMSO), methanol (MeOH) and water (H_2O). The standard values for dielectric constants and refractive indexes were always assumed. In the case of water, a local micro-explicit solvation about the proton-donor/proton-acceptor centres of the organic molecules was also combined with the implicit model.

The UV-vis absorption spectra for the equilibrium geometries of the rotamers with $\Delta G < 2.5$ kJ·mol^{-1} were calculated at time-dependent density functional theory (TD-DFT) level, accounting for $S_0 \rightarrow S_n$ (n = 1 to 20); the energy of the first 20 triplet states was also computed. The nature of the vertical excited electronic state was analysed both *in vacuo* and in the solvated phase. This investigation was performed by employing the long-range corrected functionals ω-B97X[D] [7] and CAM-B3LYP [8] coupled with the 6-311++G** basis set. In the case of the solvated phase, state-specific (SS) [9] treatment of the solvent effects was considered, both within the non-equilibrium (neq) and equilibrium (eq) solvation regimes of all non-dark electronic transitions were also simulated, including the Duschinsky and Herzberg–Teller effects. The first singlet excited state $S(\pi,\pi^*)$ state geometry was optimised using analytical gradients and the first transitions $S_1 \rightarrow S_0$ of the emission. In this case, SS (both eq and neq) treatment of the solvent effects was considered. The properties of the corresponding non-optimised ground state were also computed. Solvent effects were taken into account via IEF-PCM(UFF).

The atomic charge population analysis, electric multiple moments, electronic density, and electrostatic potential were also computed using Mulliken's and the CHELPG procedure [10] for the optimised and vertically de-excited ground state and the vertically excited and relaxed S_1 states.

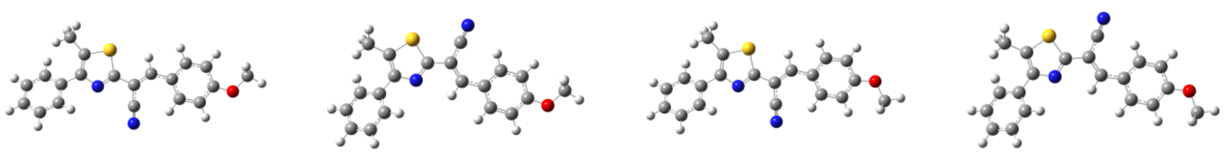
To investigate the presence and nature of possible intramolecular H-bonding interactions, two different approaches were used: first on one hand, topological analysis based on Bader's atoms in molecules (AIM) theory [11] was used, and second, the -covalent interaction (NCI) index combined with the second derivative of the reduced density gradient along the second main axis of variation were employed.[12] These procedures were applied both to the ground and first singlet excited states.

The different photo-reaction pathways were investigated by means of a relaxed scan of the ground state potential energy surface along with the selected internal coordinates (interatomic distances). Each coordinate was elongated of + 3 Å (step 0.1 Å) starting from the equilibrium value. For each point, the electronic energy of the ground state and the singlet and triplet excited states was computed at TD-DFT level.

The self-consistent field (SCF) algorithm used was the quadratically convergent procedure designed by Bacskay,[13] a method that is acknowledged to be slower but more reliable than the regular SCF with DIIS extrapolation. For all calculations, the integration grid for the electronic density was set to 250 radial shells and 974 angular points for all the atomic species. The accuracy for the two-electron integrals and their derivatives was set to 10^{-14} a.u.. The convergence criteria for the SCF were set to 10^{-12} for a root mean square (RMS) change in the density matrix and 10^{-10} for a maximum change in the density matrix. The convergence criteria for geometry optimizations were set to 2×10^{-6} a.u. for a maximum force, 1×10^{-6} a.u. for an RMS force, 6×10^{-6} a.u. for a maximum displacement and 4×10^{-6} a.u. for an RMS displacement. For the AIM analysis, the number of paths in each interbasin surface was set equal to 500, the number of points in each interbasin surface path as well as the max number of points of a path equal to 1000, the stepsize 1×10^{-4} bohr, the maximal number of interactions to 512, the criterion for gradient-norm (displacement) convergence to 1×10^{-7} a.u. (1×10^{-8} a.u.), and the minimal distance between CPs to 1×10^{-3} bohr. The search of the CPs was made staring from the nuclear positions, the midpoint of each atom pairs, the centre of any triangle defined by three atoms and tetrahaedron defined by four atoms

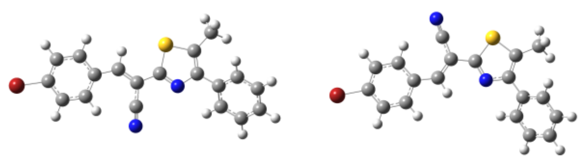
The location of BCPs and subsequent calculation of SF values were performed using a modified version of the PROAIMV program. [14] All the other calculations were performed using the GAUSSIAN G169.C01 software package. [15] The calculation of the NCI was performed using homemade code.

Table S2. MPTAs **3b-c** rotamers thermochemical characteristics in different solvents
Rotamers **3b**



A B C D

Rotamers **3c**



A B

Differences of thermochemicals at T = 298.15K and p = 1.00 atm (in units of kJ·mol^{-1}).

Compd		**3b**					**3c**				
		E	ZPE	E+ZPE	H	G	E	ZPE	E+ZPE	H	G
DMSO	A	0.9	0.1	0.9	1.0	0.5	0.7	0.1	0.9	0.9	1.2
	B	0.5	0.3	0.8	0.7	1.4	0.0	0.0	0.0	0.0	0.0
	C	1.4	0.0	1.3	1.4	0.7					
	D	0.0	0.1	0.0	0.0	0.0					
MeCN	A	1.0	0.1	1.0	1.1	0.6	A	0.9	0.1	1.0	1.1
	B	0.5	0.3	0.8	0.7	1.3	B	0.0	0.0	0.0	0.0
	C	1.5	0.0	1.4	1.5	0.7					
	D	0.0	0.1	0.0	0.0	0.0					
MeOH	A	1.1	0.1	1.1	1.2	0.6	A	1.0	0.1	1.1	1.1
	B	0.5	0.3	0.7	0.7	1.3	B	0.0	0.0	0.0	0.0
	C	1.6	0.0	1.5	1.6	0.6					
	D	0.0	0.1	0.0	0.0	0.0					

Table S3. Theoretical and experimental values of maxima absorption and emission of MPTAs **3a-c** in DMSO.

Entry	Comp	λ_{abs}, nm		λ_{em}, nm	
		Exp	Calc	Exp	Calc
1	**3a**	380	372	519	511
2	**3b**	381	381	-	514
3	**3c**	373	373	493	492

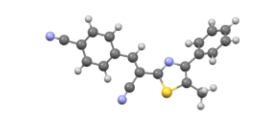
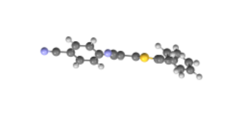
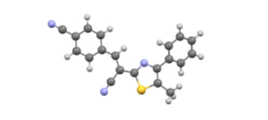
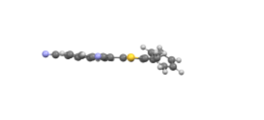
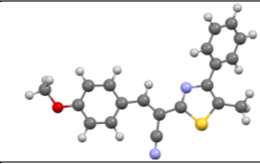
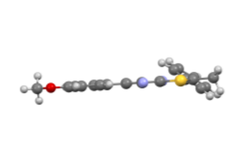
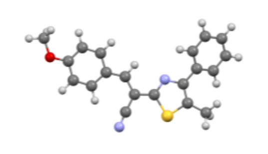
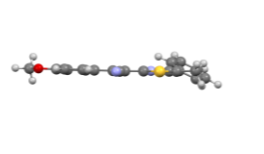
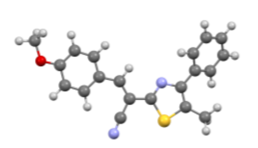
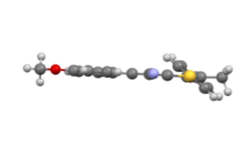
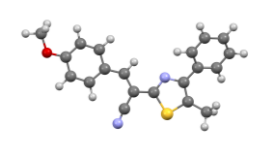
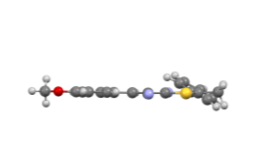
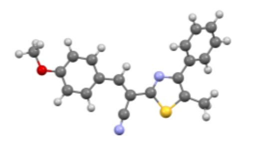
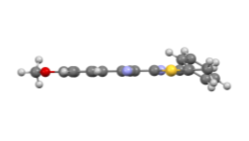
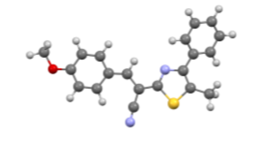
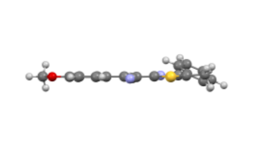
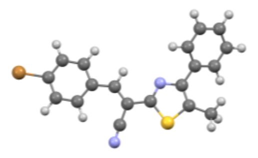
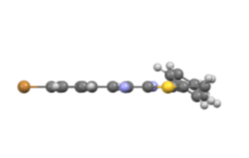
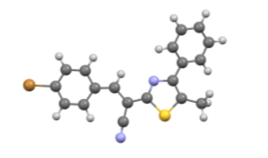
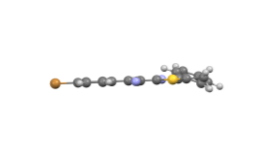
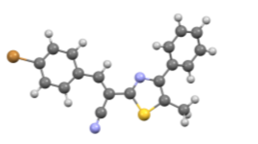
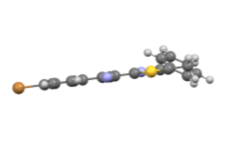
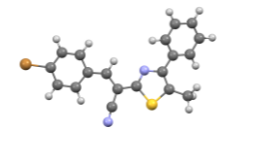
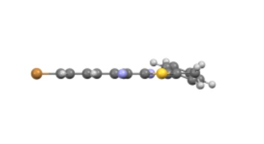
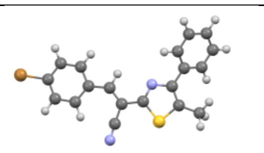
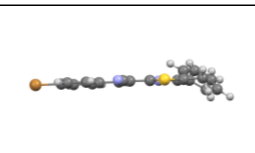
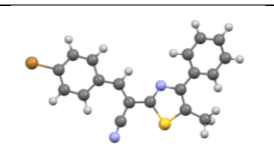
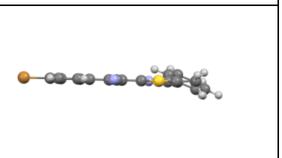
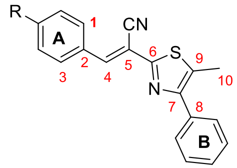
Compd	*Solvent*	S_0		S_{1r}	
3a	DMSO				
3b	DMSO				
	MeCN				
	MeOH				
3c	DMSO				
	MeCN				
	MeOH				

Fig. S13. Optimized geometries of the investigated MPTAs **3a-c** in their *GS* and *ES* in DMSO, depicted from two orthogonal viewpoints. Level of theory: DFT/IEF-PCM(UFF). Legend of colours: white (H), grey (C), lilac (N), yellow (S), red (O), and brown (Br).

Table S4. Selected bonds lengths (in Å) torsion (°) for the *GS* (S_0) optimized geometries of MPTAs **3a-c** in DMSO, MeCN and MeOH



Entry	Compd	Solv	C2-C4	C4-C5	C5-C6	C7-C8	C7-C9	C9-C10	θ_A	θ_B	θ_C	N···HC(4)	N···HC_{Ar}
1	**3a**	DMSO	1.464	1.352	1.473	1.479	1.377	1.498	28.88	34.98	3.03	2.497	2.649
2	**3b**	DMSO	1.444	1.369	1.469	1.477	1.382	1.498	0.07	35.49	0.54	2.457	2.643
3		MeCN	1.444	1.369	1.469	1.477	1.382	1.498	0.07	35.49	0.54	2.457	2.643
4		MeOH	1.444	1.369	1.469	1.477	1.382	1.498	0.07	35.49	0.54	2.457	2.643
5	**3c**	DMSO	1.451	1.365	1.470	1.477	1.384	1.498	0.85	35.52	0.59	2.413	2.483
6		MeCN	1.451	1.365	1.470	1.477	1.384	1.498	0.85	37.82	0.59	2.412	2.482
7		MeOH	1.451	1.365	1.470	1.477	1.384	1.498	0.85	35.52	0.59	2.412	2.481

Table S5. Selected bonds lengths (in Å) torsion (°) for the *ES* (*S_1*) optimized geometries of MPTAs **3a-c** in DMSO, MeCN and $CHCl_3$

Entry	Compd	Solv	C2-C4	C4-C5	C5-C6	C7-C8	C7-C9	C9-C10	θ_A	θ_B	θ_C	N···HC(4)	N···HC_{Ar}
1	**3a**	DMSO	1.399	1.436	1.407	1.474	1.412	1.490	0.64	36.20	0.09	2.383	2.638
2	**3b**	DMSO	1.407	1.439	1.420	1.465	1.413	1.492	1.11	27.70	0.02	2.417	2.642
3		MeCN	1.407	1.439	1.420	1.465	1.413	1.492	1.11	27.70	0.02	2.416	2.541
4		MeOH	1.407	1.439	1.420	1.465	1.413	1.492	1.10	27.65	0.03	2.416	2.541
5	**3c**	DMSO	1.408	1.430	1.428	1.457	1.418	1.491	0.20	22.43	0.30	2.413	2.483
6		MeCN	1.409	1.430	1.428	1.457	1.418	1.491	0.21	22.35	0.27	2.412	2.482
7		MeOH	1.409	1.430	1.428	1.457	1.418	1.491	0.22	22.33	0.26	2.412	2.481

Table S6. Computed photophysical characteristics[a] of compounds **3a-c** in DMSO, MeCN, MeOH.

Compd	Solvent	$c_{(HL)}$	f_{01}	$c_{(LH)}$	f_{10}	μ_0	μ_{1v}	μ_{1r}	$\theta_{0\text{-}1v}$	$\theta_{0\text{-}1r}$
3a[b]	DMSO	0.6305	1.255	0.6808	1.271	12.6	16.8	14.6	11.6	11.3
	MeCN	0.6408	1.1625	0.6824	1.2366	8.8	15.5	15.2	7.6	8.8
3b	MeCN	0.7051	1.091	0.7063	0.883	6.3	9.3	9.2	36.4	35.7
	MeOH	0.7051	1.090	0.7063	1.042	6.3	9.3	9.1	36.4	35.7
	DMSO	0.7050	0.950	0.7060	0.949	4.9	14.8	13.7	22.1	19.3
3c	MeCN	0.7050	0.946	0.7060	0.945	4.9	14.8	13.7	22.1	19.3
	MeOH	0.7050	0.944	0.70603	0.943	4.9	14.8	13.7	22.1	19.3

a - absorption wavelength (λ_{01}, nm) and oscillator strength (f_{01}), emission wavelength (λ_{10}, nm) and oscillator strength (f10), modulus of the electric dipole moments of the ground state ($\mu_{0,}$, D), and of the relaxed excited state (μ_{1r}, D), and angles formed by the directions of the electric dipole moment vectors ($\theta_{0,1v}$, deg) and $\theta_{0,1r}$, deg)); b – from ref. 29.

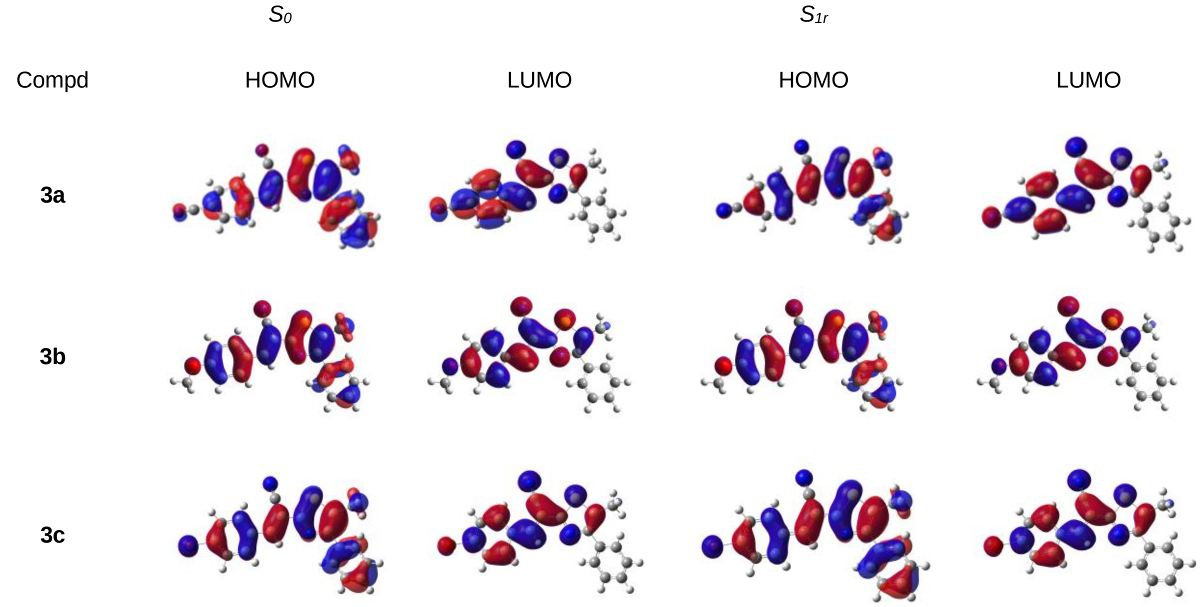


Fig. S14. Frontier molecular orbitals (FMOs), HOMO and LUMO, in the ground and excited states for MPTAs **3a-c** in DMSO at (TD-)DFT ω-B97X-D/6−311++G**//IEF-PCM(UFF) (|Isovalue(MO)| = 0.02 a.u.; |Isovalue| = 0.0004 a.u.).

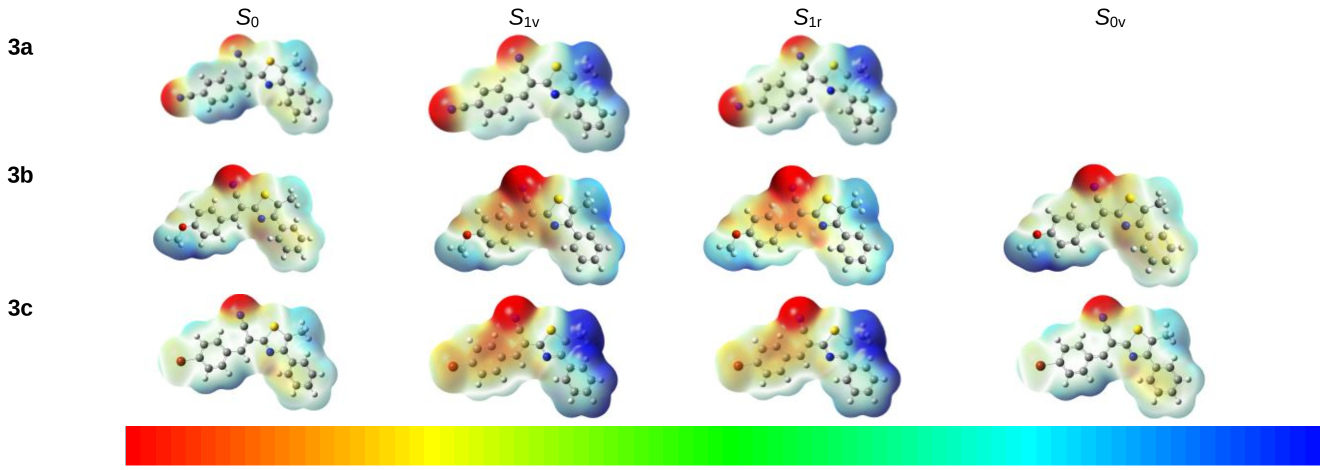


Fig. S15. Plot of MEPs of MPTAs **3a-c** in DMSO calculated by TD-DFT at the ω-B97X-D / 6−311++G** // IEF-PCM(UFF) level of theory, for ground and excited states in dioxane. Map colours: Red (negative potential), blue (positive potential). Elements: Hydrogen (white), carbon (grey), nitrogen (blue), oxygen (red), sulfur (yellow), bromine (brown). (Range, –0.04 to 0.04; density |Isovalue| = 0.0004 a.u.).

5. Photophysical properties of hybrids 6a-g, 7, 8 in organic solvents and in binary mixtures with water and buffer pH 7.4.

Table S7. Photophysical properties of hybrids **6a-g**, **7**, **8** in different organic solvent and in binary mixtures with water and buffer pH 7.4.[a]

Entry	Compound	Solvent	λ_{max}, nm	ε, M^{-1} cm^{-1}	λ_{em}, nm	QY,[b] %	SS, nm/cm^{-1}
1	**6a**	MeOH	229, 280, 361	19100, 17500, 23300	494	10.4	133/7458
		MeCN	231, 277, 363	17900, 17400, 19900	496	9.2	133/7694
		MeCN-H_2O (9:1, v/v)	231, 275, 361	18800, 17500, 19100	501	9.5	140/7895
2		DMSO	278, 369	16400, 18200	509	3.6	140/7454
		DMSO-H_2O (1:1, v/v)	278, 363	15500, 17800	513	4.9	150/7904
3		DMSO-buff (1:1, v/v)	277, 369	16100, 17600	518	2.9	149/7795
4	**6b**	$CHCl_3$	292, 372	16200, 22300	473	9.6	101/5740
5		DMSO	278, 371	17000, 19400	509	4.3	138/7308
6		DMSO-buff (1:1, v/v)	279, 369	16700, 18300	516	2.6	147/7720
7	**6c**	DMSO	277, 370	15900, 17400	508	3.6	138/7342
8		DMSO-buff (1:1, v/v)	280, 372	15300, 16400	517	2.5	145/7539
9	**6d**	DMSO	277, 367	16000, 17000	507	4.1	140/7524
10		DMSO-H_2O (1:1, v/v)	277, 363	14600, 16300	508	2.4	145/7863
11		DMSO-buff (1:1, v/v)	278, 371	16000, 16500	513	0.9	142/7461
12	**6e**	DMSO	282, 369	17700, 14700	506	0.5	137/7337
13		DMSO-buff (1:1, v/v)	281, 370	19100, 15900	516	3.8	146/7647
14	**6f**	DMSO	278, 368	16000, 17600	510	4.2	142/7566
15		DMSO-buff (1:1, v/v)	278, 370	15100, 16400	518	2.9	148/7722
16	**6g**	DMSO	275, 369	12500, 12900	508	3.7	139/7415
17		DMSO-H_2O (1:1, v/v)	276, 369	11600, 11500	508	2.6	139/7415
18		DMSO-buff (1:1, v/v)	276, 371	12200, 11800	518	2.6	147/7649
19	**7**	MeOH	238, 272, 373	16500, 6900, 26600	430	0.7	57/3554
20		MeCN	246, 280, 371	9400, 5800, 25000	-[c]	-[c]	-[c]
21		MeCN-H_2O (9:1, v/v)	246, 279, 372	10200, 6200, 25000	-	-	-
22		DMSO	378	21400	-	-	-
23		DMSO-H_2O (1:1, v/v)	377	21000	-	-	-
24		DMSO-buff (1:1, v/v)	277, 380	6900, 21400	-	-	-
25	**8**	MeOH	273, 357	10500, 18500	434	0.7	77/4970
26		MeCN	273, 357	11600, 17000	405	0.4	48/3320
27		MeCN-H_2O (9:1, v/v)	271, 356	11900, 15400	406	0.3	50/3459
28		DMSO	273, 364	11500, 14300	469	0.6	105/6151
29		DMSO-H_2O (1:1, v/v)	271, 358	10200, 11900	410	0.2	52/3542
30		DMSO-buff (1:1, v/v)	277, 367	10200, 14400	486	0.3	119/6671

a – for absorption: $c = 5 \times 10^{-5}$ M; for fluorescence $c = 2.5 \times 10^{-6}$ M; b – Relative quantum yield, determined relative to the standard (quinine sulfate solution) $c = 5\times10^{-5}$M in 0.1 M H_2SO_4; $\Phi_F = 54.0$ %). c – Emission is not registered.

6. Quantum Mechanical Calculation data for hybrids 6a, 7, 8

Table S8. Thermochemical characteristics of hybrids **6a, 7, 8** rotamers in DMSO and $CHCl_3$
(Energy differences at T = 298.15 K and p = 1.00 atm (in kJ/mol))

		DMSO					$CHCl_3$				
		E	ZPE	*E*+ZPE	*H*	*G*	*E*	ZPE	*E*+ZPE	*H*	*G*
6a	A	4.3	0.3	3.2	4.0	1.3	9.1	0.8	8.2	8.7	9.3
	B	4.0	0.1	2.7	3.4	2.3	4.9	0.0	3.2	4.0	1.0
	C	2.3	1.3	2.1	2.3	2.2	9.0	1.0	8.3	8.6	6.9
	D	2.0	0.8	1.4	1.6	2.5	4.9	0.5	3.7	4.1	2.2
	E	3.1	1.4	3.1	3.3	3.5	7.0	1.1	6.3	6.7	5.7
	F	2.7	0.5	1.8	2.4	1.0	2.5	0.9	1.7	2.2	1.0
	G	0.3	1.8	0.6	0.7	0.3	3.5	2.0	3.8	3.8	3.4
	H	0.1	1.8	0.4	0.3	3.5	0.0	2.0	0.2	0.0	3.8
	I	4.4	0.6	3.5	4.0	4.5	9.5	0.4	8.2	8.9	7.4
	J	3.9	0.0	2.5	3.2	1.3	4.6	0.3	3.1	3.9	1.8
	K	2.1	1.0	1.7	1.9	1.3	9.2	1.0	8.5	8.7	9.1
	L	1.7	1.1	1.4	1.6	2.3	4.7	0.8	3.7	4.0	3.5
	M	3.0	1.4	2.9	3.2	3.8	6.8	1.5	6.5	6.8	8.2
	N	2.6	0.8	2.0	2.5	1.2	2.4	0.9	1.5	2.0	1.4
	O	0.3	1.5	0.4	0.5	0.0	3.5	1.6	3.4	3.5	1.2
	P	0.0	1.4	0.0	0.0	1.2	0.4	1.3	0.0	0.0	0.0
7	A	4.0	0.6	3.0	4.6	3.6	8.8	0.7	7.9	8.5	10.5
	B	3.9	0.0	2.3	4.0	1.4	4.5	0.5	3.4	4.0	7.0
	C	2.4	1.0	1.8	3.0	0.7	8.9	1.3	8.6	8.8	10.4
	D	2.1	0.6	1.0	0.0	6.0	4.8	0.0	3.2	3.9	0.0
	E	3.0	0.8	2.1	3.6	1.6	6.8	0.7	5.8	6.4	7.0
	F	2.4	0.7	1.5	2.9	1.7	2.3	0.6	1.2	1.8	3.7
	G	0.4	1.4	0.1	1.3	0.0	3.4	1.9	3.7	3.7	7.7
	H	0.0	1.6	0.0	1.0	2.2	0.0	1.6	0.0	0.0	4.3
8	A	4.2	0.5	3.2	3.8	3.7	9.2	0.4	8.0	8.8	8.0
	B	3.7	0.0	2.3	3.0	1.2	4.5	0.0	2.9	3.9	0.0
	C	2.3	1.2	2.1	2.2	2.2	9.1	0.9	8.4	8.9	7.6
	D	1.8	1.1	1.5	1.6	2.7	4.5	0.8	3.7	4.1	3.3
	E	2.8	1.3	2.6	3.0	1.9	6.7	1.0	6.1	6.7	5.4
	F	2.3	0.7	1.6	2.1	1.7	2.0	0.8	1.2	1.8	0.8
	G	0.3	1.5	0.4	0.5	0.0	3.5	1.7	3.6	3.8	3.1
	H	0.0	1.5	0.0	0.0	1.6	0.0	1.6	0.0	0.0	2.7

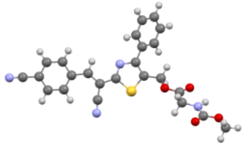
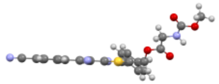
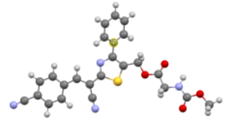
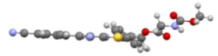
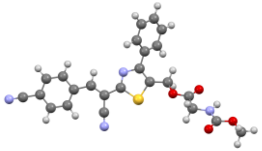
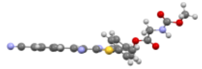
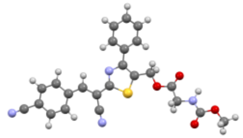
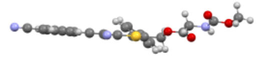
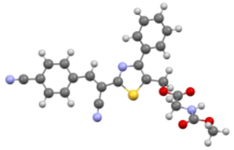
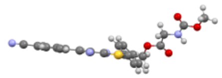
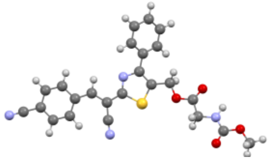
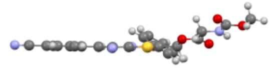
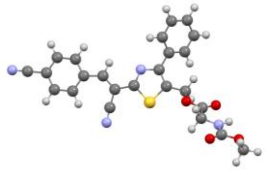
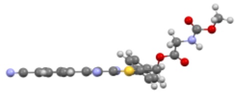
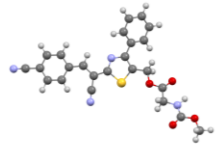
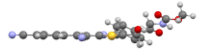
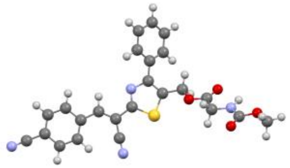
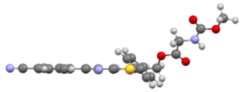
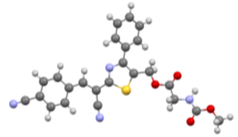
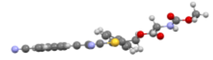
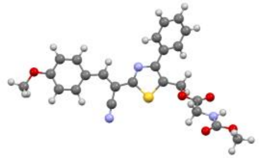
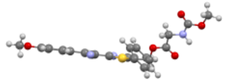
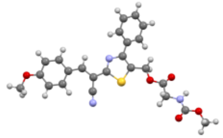
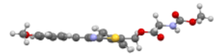
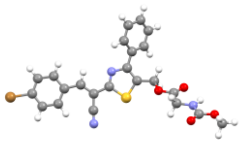
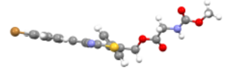
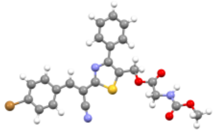
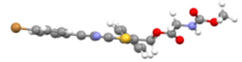
Compd	Solvent	S_0		S_{1r}	
6a	MeCN				
	$CHCl_3$				
	DMSO				
	H_2O				
	MeOH				
7	DMSO				
8	DMSO				

Fig. S16. Optimized geometries of the hybrids **6a**, **7** and **8** in their *GS* and *ES* in DMSO, depicted from two orthogonal viewpoints. Level of theory: DFT/IEF-PCM(UFF). Legend of colours: white (H), grey (C), lilac (N), yellow (S), red (O), and brown (Br).

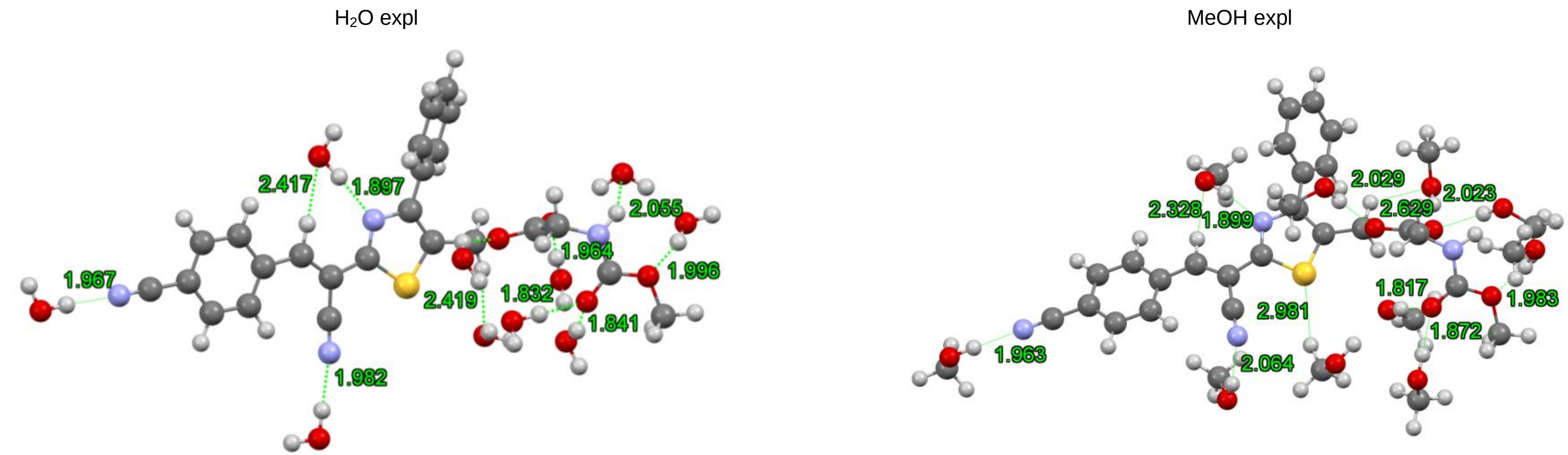
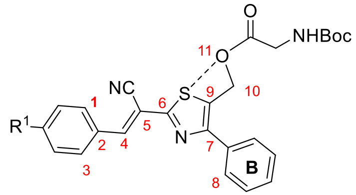


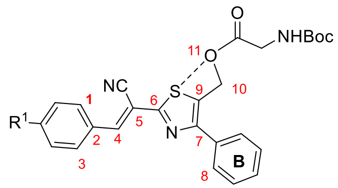
Fig. S17. Optimized geometries of the investigated hybrid **6a**. Level of theory: DFT/IEF-PCM(UFF). Legend of colours: white (H), grey (C), lilac (N), yellow (S), red (O).

Table S9. Selected bonds lengths (in Å) torsion (°) for the *GS* (S_0) optimized geometries of hybrids **6a, 7** and **8** in DMSO, MeCN and MeOH



Entry	Compd	Solv	C2-C4	C4-C5	C5-C6	C7-C8	C7-C9	C9-C10	C10-O11	θ_A	θ_B	S…O11	N···HC4	N···HC$_{Ar}$
1	**6a**	DMSO	1.453	1.364	1.470	1.477	1.383	1.489	1.458	0.17	42.07	3.080	2.455	2.722
2		MeCN	1.453	1.364	1.470	1.477	1.383	1.489	1.458	0.14	42.07	3.080	2.455	2.722
3		$CHCl_3$	1.454	1.364	1.470	1.476	1.383	1.489	1.456	2.89	41.23	3.062	2.453	2.709
4		MeOH	1.453	1.364	1.470	1.477	1.383	1.489	1.458	0.13	42.05	3.080	2.455	2.721
5		H_2O	1.453	1.364	1.470	1.477	1.383	1.489	1.458	0.20	42.07	3.080	2.456	2.722
6	**7**	DMSO	1.443	1.370	1.468	1.477	1.381	1.487	1.462	0.77	43.36	3.150	2.450	2.793
7	**8**	DMSO	1.450	1.365	1.470	1.477	1.382	1.488	1.458	0.30	42.48	3.101	2.457	2.722

Table S10. Selected bonds lengths (in Å) torsion (°) for the *ES* (S_1) optimized geometries of of hybrids **6a, 7** and **8** in DMSO, MeCN and MeOH



Entry	Compd	Solv	C2-C4	C4-C5	C5-C6	C7-C8	C7-C9	C9-C10	C10-O11	θ_A	θ_B	S…O11	N···HC(4)	N···HC$_{Ar}$
1	**6a**	DMSO	1.398	1.426	1.410	1.467	1.408	1.488	1.435	0.74	34.48	2.856	2.577	2.380
2		MeCN	1.401	1.426	1.410	1.467	1.408	1.488	1.435	0.73	31.21	2.855	2.380	2.577
3		$CHCl_3$	1.398	1.422	1.414	1.465	1.407	1.488	1.434	0.42	29.80	2.855	2.555	2.855
4		MeOH	1.398	1.426	1.410	1.467	1.408	1.488	1.435	0.73	31.19	2.855	2.380	2.576
5		H_2O	1.397	1.426	1.410	1.467	1.408	1.488	1.435	0.77	31.37	2.855	2.380	2.578
6	**7**	DMSO	1.398	1.426	1.410	1.467	1.408	1.488	1.435	0.74	34.48	2.856	2.577	2.380
7	**8**	DMSO	1.398	1.431	1.408	1.471	1.400	1.488	1.439	1.67	36.23	2.910	2.393	2.635

Table S11. Computed photophysical characteristicsa of hybrids **6a**, **7**, **8** in different solvents**.**

Compd	Solvent	$c_{(HL)}$	λ_{01}	f_{01}	$c_{(LH)}$	λ_{10}	f_{10}	μ_0	μ_{1v}	μ_{1r}	$\theta_{0\text{-}1v}$	$\theta_{0\text{-}1r}$
6a	MeCN	0.66360	364	1.4383	-0.6848	496	1.453	8.0	13.4	14.6	17.0	17.9
	$CHCl_3$	0.66654	369	1.4055	-0.6850	473	1.433	7.6	13.1	14.0	17.4	17.7
	DMSO	0.66348	367	1.4392	-0.6848	505	1.454	8.0	13.4	14.7	17.0	17.9
	H_2O*	0.66545	377	1.5014	-0.6848	508	1.454	8.0	13.4	14.7	16.9	18.0
	MeOH*	0.65972	361	1.4879	-0.6848	493	1.453	8.0	13.4	14.6	17.0	17.9
7	MeCN	0.67841	356	1.3912	0.6868	407	1.461	6.3	6.3	6.3	1.2	1.2
	$CHCl_3$	0.67755	359	1.4066	0.6865	423	1.452	5.9	5.9	5.9	1.2	1.2
	DMSO	0.67743	361	1.4001	0.6865	465	1.460	6.3	6.3	6.3	1.2	1.2
	H_2O	0.67777	357	1.3904	0.6866	436	1.453	6.4	6.3	6.3	1.2	1.2
	MeOH	0.67783	355	1.3908	0.6865	432	1.460	6.3	6.2	6.2	1.1	1.1
8	MeCN	0.68625	373	1.4520	0.6953	432	1.301	6.2	8.5	7.5	9.9	42.5
	$CHCl_3$	0.68615	362	1.4461	0.6891	414	1.188	6.0	7.9	7.9	7.9	53.7
	DMSO	0.68625	374	1.4520	0.6955	433	1.305	6.2	8.5	7.5	10.0	41.9
	H_2O	0.68624	374	1.4519	0.6958	434	1.311	6.2	8.6	7.5	10.0	41.0
	MeOH	0.68625	373	1.4520	0.6953	432	1.299	6.2	8.5	7.6	9.8	42.7

a - absorption wavelength (λ_{01}, nm) and oscillator strength (f_{01}), emission wavelength (λ_{10}, nm) and oscillator strength (f_{10}), modulus of the electric dipole moments of the ground state (μ_0, D), of the vertical FC excited state (μ_{1v}, D), and of the relaxed excited state (μ_{1r}, D), and angles formed by the directions of the electric dipole moment vectors ($\theta_{0,1v}$, deg) and $\theta_{0,1r}$, deg)). *Explicit micro solvation including 10 solvent molecules with a further embedding implicit solvation (PCM).

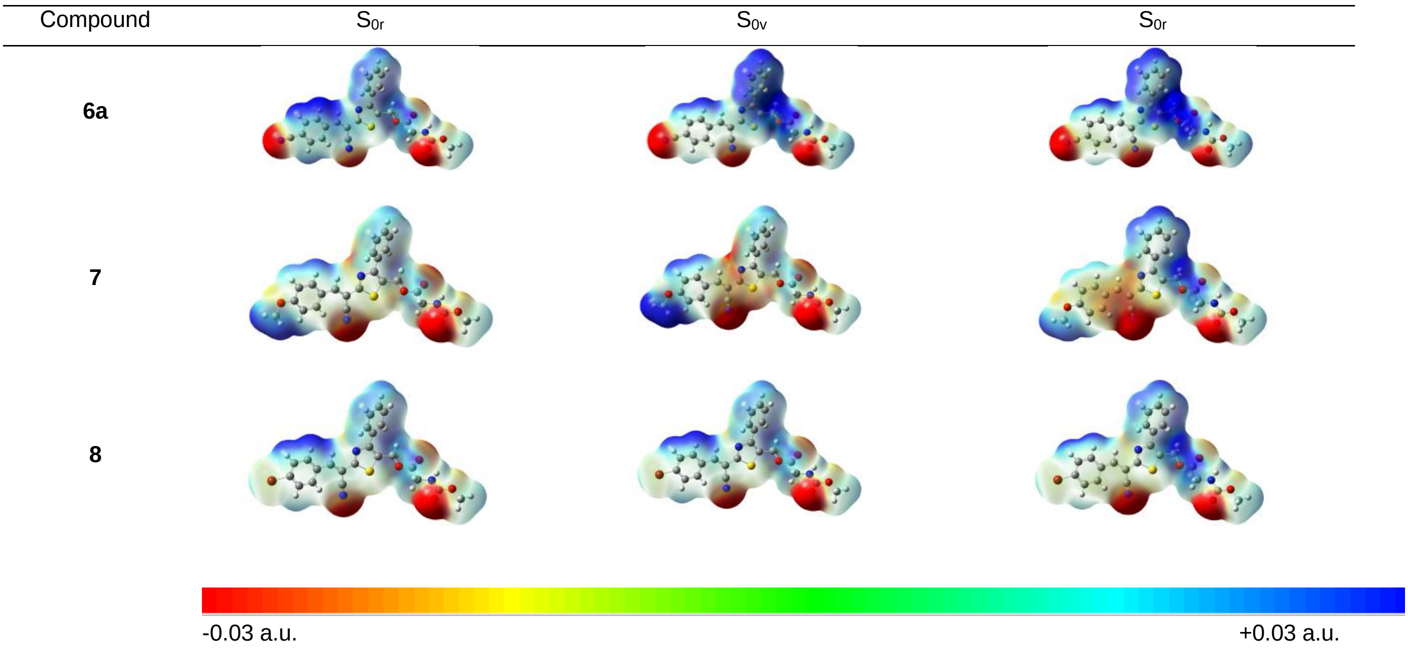


Fig. S18. Plot of MEPs of hybrids **6a, 7, 8** in DMSO calculated by TD-DFT at the ω-B97X-D / 6−311++G** // IEF-PCM(UFF) level of theory, for ground and excited states in DMSO. Map colours: Red (negative potential), blue (positive potential). Elements: Hydrogen (white), carbon (grey), nitrogen (blue), oxygen (red), sulfur (yellow), bromine (brown). (Range, –0.05 to 0.05; density |Isovalue| = 0.0003 a.u.).

7. Photodissociation of hybrids 6a-g, 7 and 8

HPLC-HRMS analysis of the photodissociacion of hybrids 6a-g, 7 and **8**

Photorelease investigations were performed on a reactor Acceled, Penn Photon Devices, LLC 1055 Mensch Dam Road Pennsburg, PA 18073, USA equipped with LED (365 nm) in aerated conditions.

General procedure for photolysis of hybrids 6a-g, 7 and **8:**

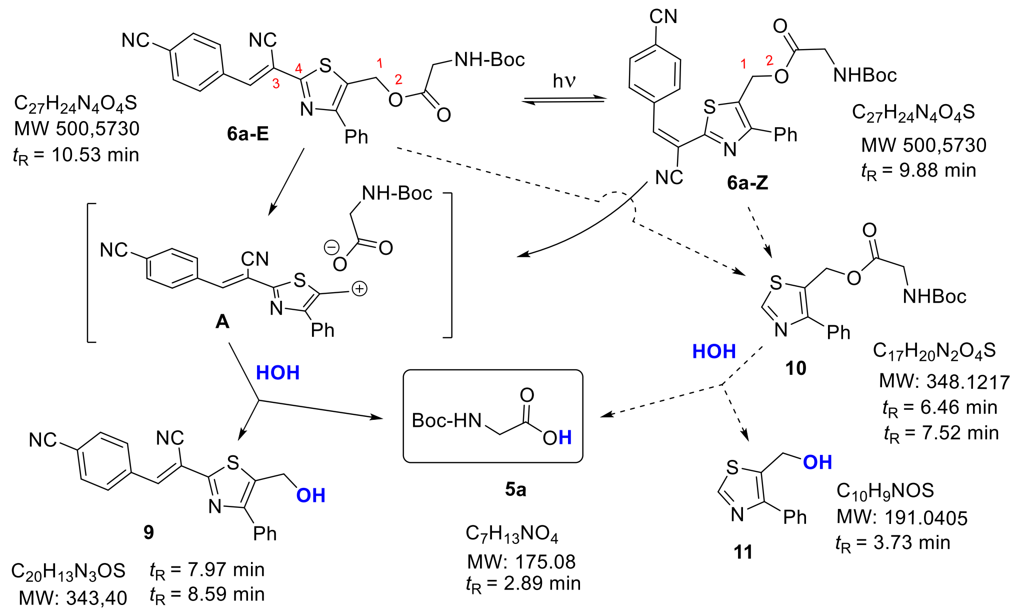
Compound **6** (2 mg) was dissolved in a quartz tube in MeCN-H_2O (7:3, v/v) (10 ml). The solution (c = 4.2×10^{-4}M) was irradiated (365 nm) in a photoreactor (intensity of 50% power). At regular interval of time, an 1 mL aliquots were taken and injected into Agilent 6545 Q-TOF (Agilent Technologies Inc., Santa Clara, CA, USA) with LC/MS system.

HPLC-HRMS analysis of the photodissociation of compounds **6a**, **7** and **8** was performed on an Agilent 1290 Infinity II HPLC system connected with a quadrupole time-of-flight (Q-TOF) accurate mass spectrometer detector (Agilent 6545 Q-TOF LC-MS, Agilent Technologies, Santa Clara, USA). Chromatographic separations were performed using a "Zorbax Eclipse Plus C18" (2.1 mm × 50 mm, 1.8 µm, Agilent Technologies, p/n 959757-902) column with an additional 5 mm guard column. The column thermostat temperature was 35°C and the injected volume was 1 µL. The mobile phase was prepared from solvent A, containing 0.1% (v/v) formic acid in water and solvent B, containing 0.1% formic acid (v/v) in acetonitrile. Gradient elution was carried out according to the following program: the concentration of solvent B changed linearly over 15 min from 5% to 100%, which was kept for 2 min. Flow rate was kept 0.4 mL/min.

The Q-TOF instrument was operated with an electrospray ion source in positive ion mode using the following conditions: drying gas temperature, 350 °C (nitrogen, 10 L/min); nebulizer pressure, 40 psi; capillary voltage, 3500 V; and fragment or voltage, 90 V. Ions were scanned in the *m/z* range of 100–1700 and the acquisition rate was 1.5 spectra/s.

The elemental composition of the detected compounds was confirmed by measuring the accurate mass with an error of no more than 5 ppm and the nature of the isotopic distribution. Determination of the yield of Boc-Gly in the course of reactions was carried out by LC-HRMS on an Agilent 1290 Infinity II HPLC system connected with a Q-TOF accurate mass spectrometer Agilent 6545 Q-TOF LC-MS (Agilent Technologies, USA) under the analysis conditions used to study the reaction progress.

The detection of releasing of Boc-Gly in the analyzed solutions was carried out on the basis of the exact masses and retention times of the peak of the corresponding reference standards (if necessary, give the manufacturer and purity). The compound (Boc-Gly) were quantified using their corresponding standard calibration curves plotted for m/z = 76.039346 ion with a concentration range of approximately 3 - 77 µg/mL.



Scheme S1. Scheme of a photodissociation of hybrid **6a** in a MeCN-H_2O (7:3, v/v) mixture based on experimental, quantum-mechanical calculation data and literature data.

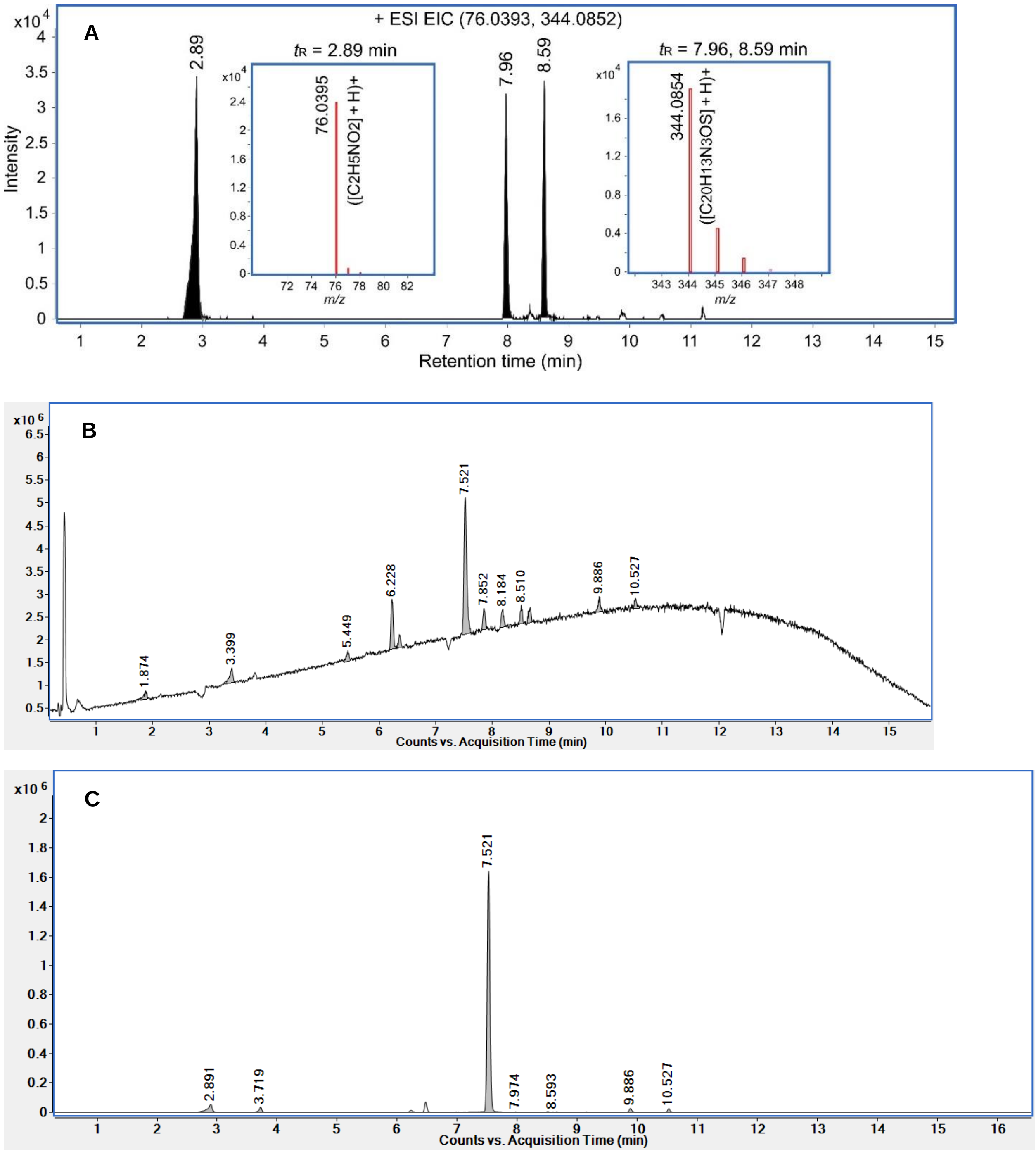
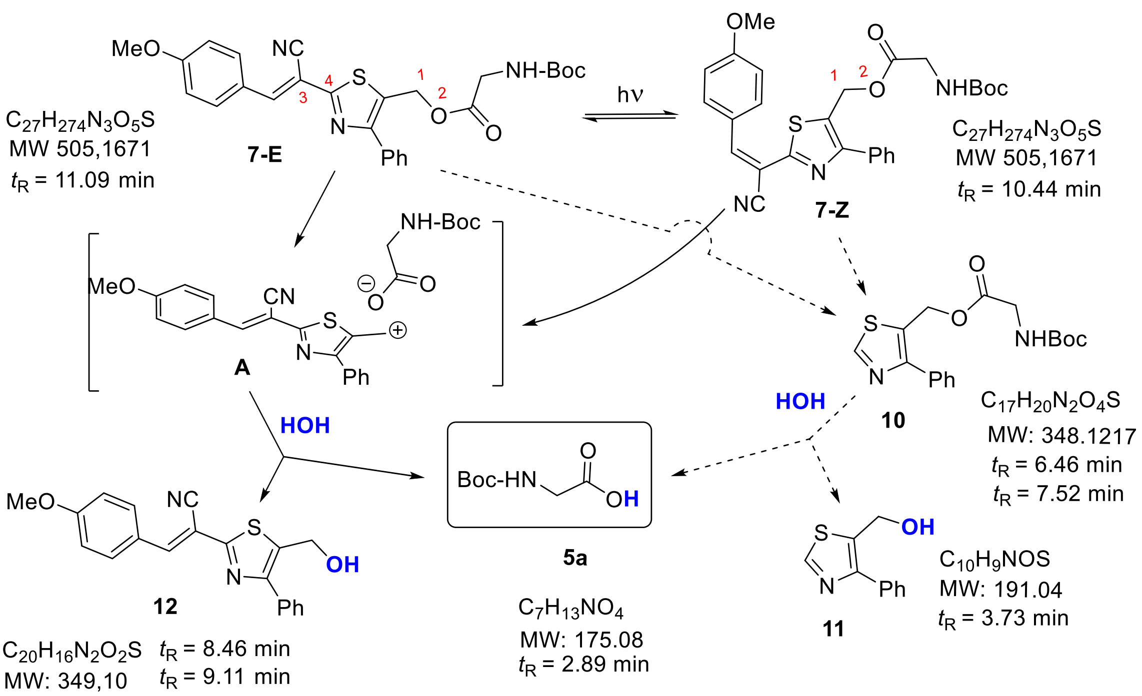
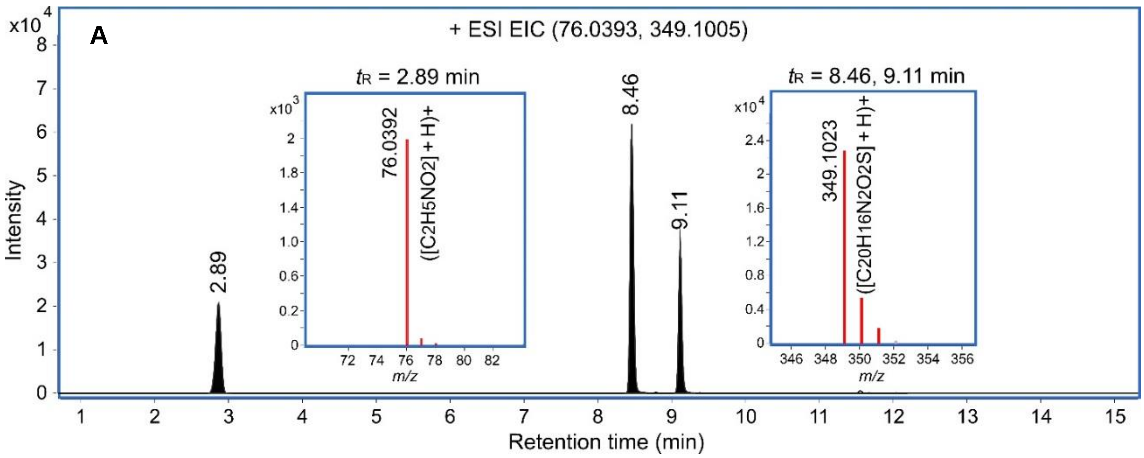
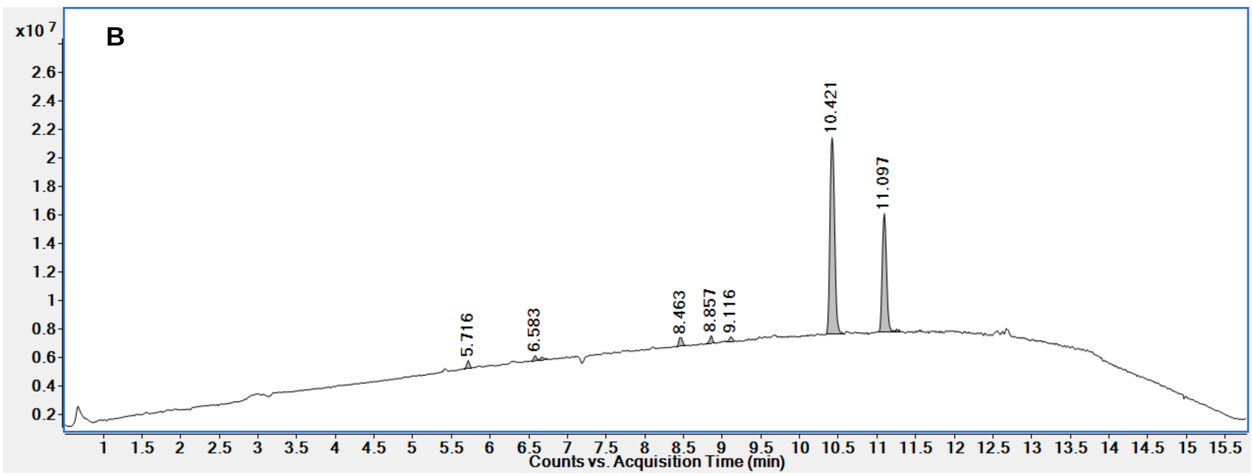


Fig. S19. (A) The extracted ion chromatograms at t_R = 2.89 min and 7.96, 8.59 min after 5 min irradiation (50% power, λ_{ir} = 365 nm) of a hybrid **6a** solution in a MeCN-H_2O (7:3, v/v) mixture and corresponding mass spectra; (B) The total ion chromatograms irradiation (50% power, λ_{ir} = 365 nm) of a hybrid **6a** solution in a MeCN-H_2O (7:3, v/v) and (C) compound ion chromatograms for hybrid **6a**, and photodissociation products **5a**, **9-11** at the end of experiment**.** (It should be noted that the intensity of the peaks depends on the ionization efficiency and therefore it is not correct to relate it to the amount of substance.).



Scheme S2. Photodissociation of hybrid **7** in a MeCN-H_2O (7:3, v/v) mixture based on experimental, quantum-mechanical calculation data and literature data.





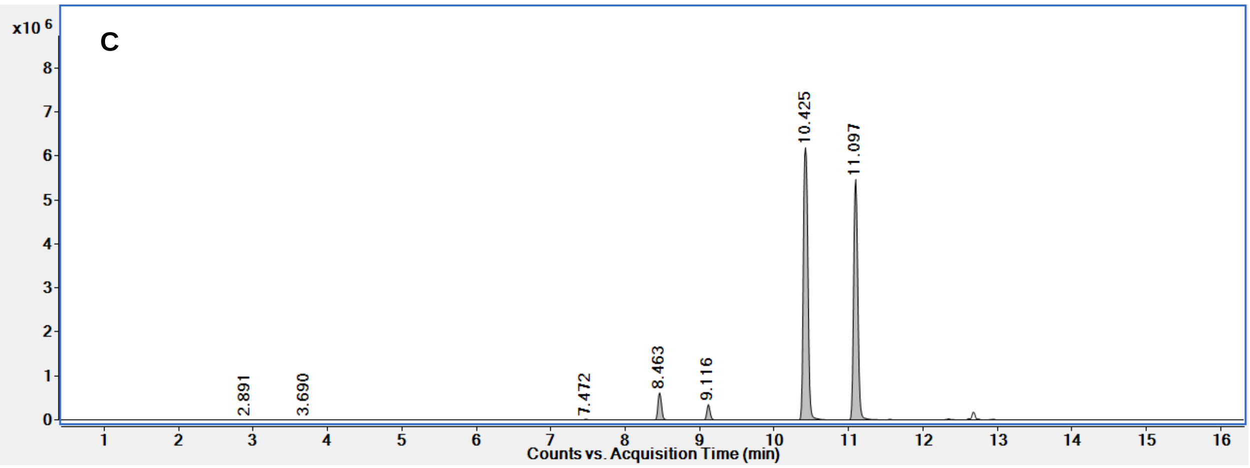
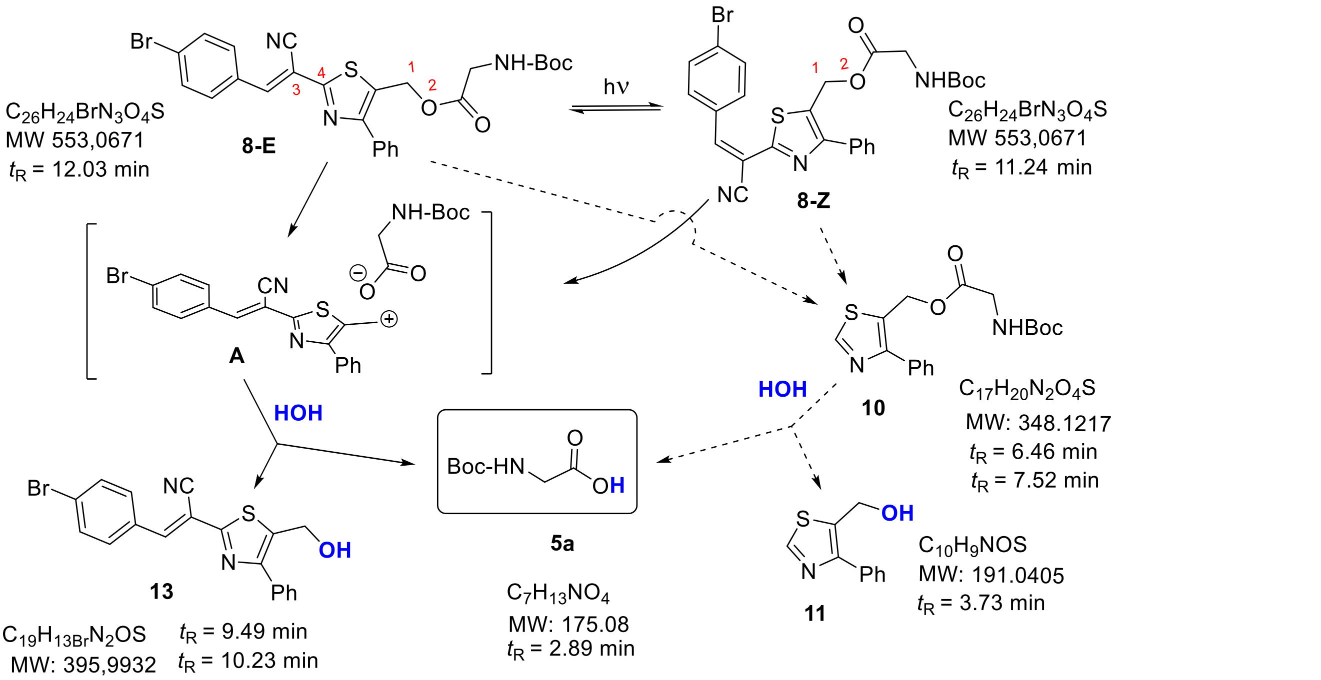


Fig. S20. (A) The extracted ion chromatograms at t_R = 2.89 min and 8.46, 9.11 min after irradiation 5 min (50% power, λ_{ir} = 365 nm) of a hybrid **7** solution in a MeCN-H_2O (7:3, v/v) mixture and corresponding mass spectra; (B) The total ion chromatograms after 5 min irradiation (50% power, λ_{ir} = 365 nm) of a hybrid **7** solution in a MeCN-H_2O (7:3, v/v) and (C) compounds ion chromatograms for hybrid **6a**, and photoissociation products **5a**, **7,10-12** at the end of experiment**.** (It should be noted that the intensity of the peaks depends on the ionization efficiency and therefore it is not correct to relate it to the amount of substance).



Scheme S3. Photodissociation of hybrid **8** in a MeCN-H_2O (7:3, v/v) mixture based on experimental, quantum-mechanical calculation data and literature data.

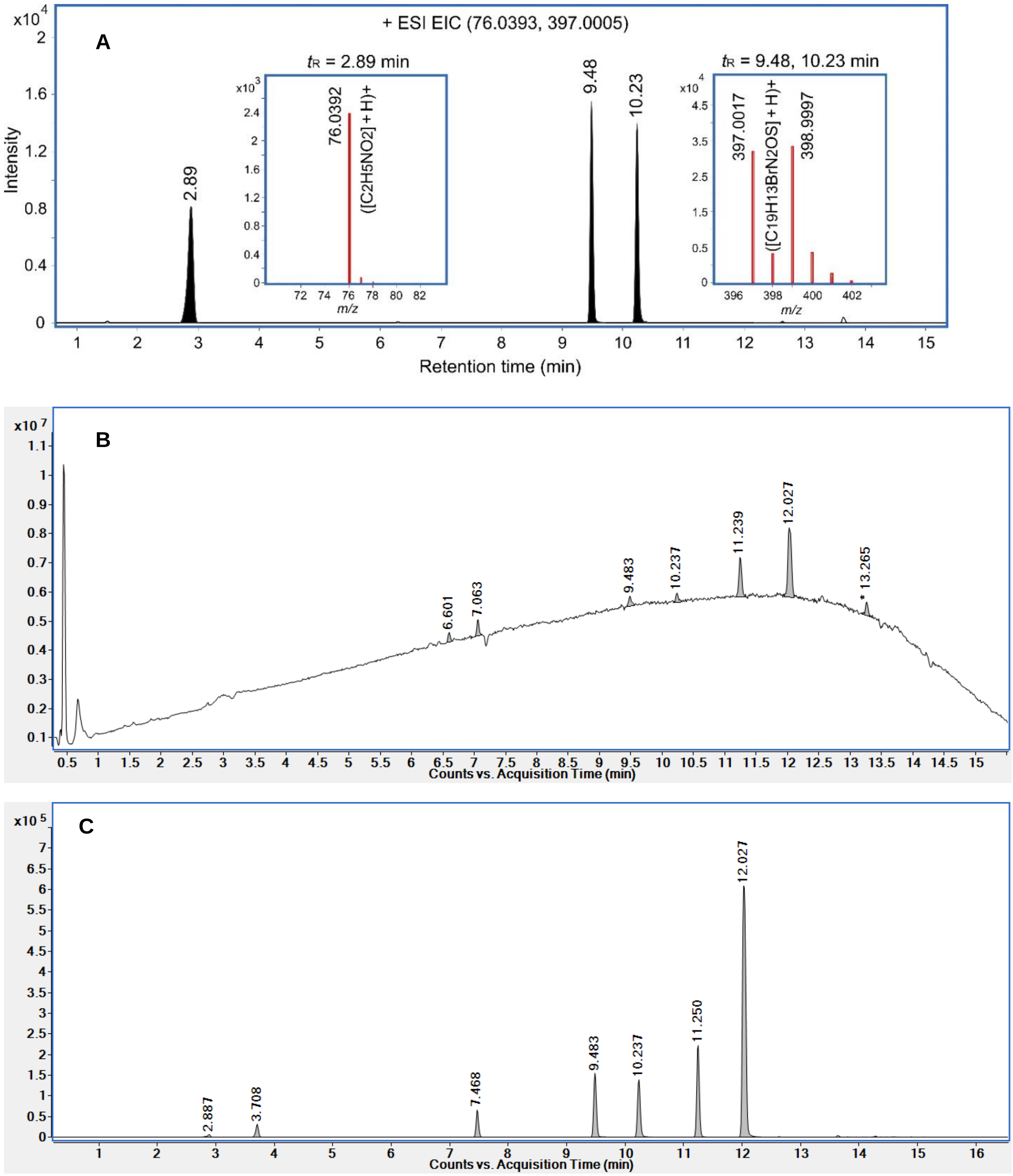
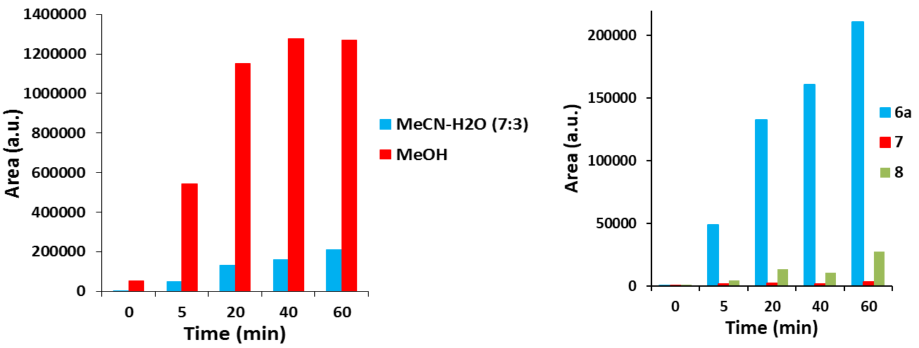
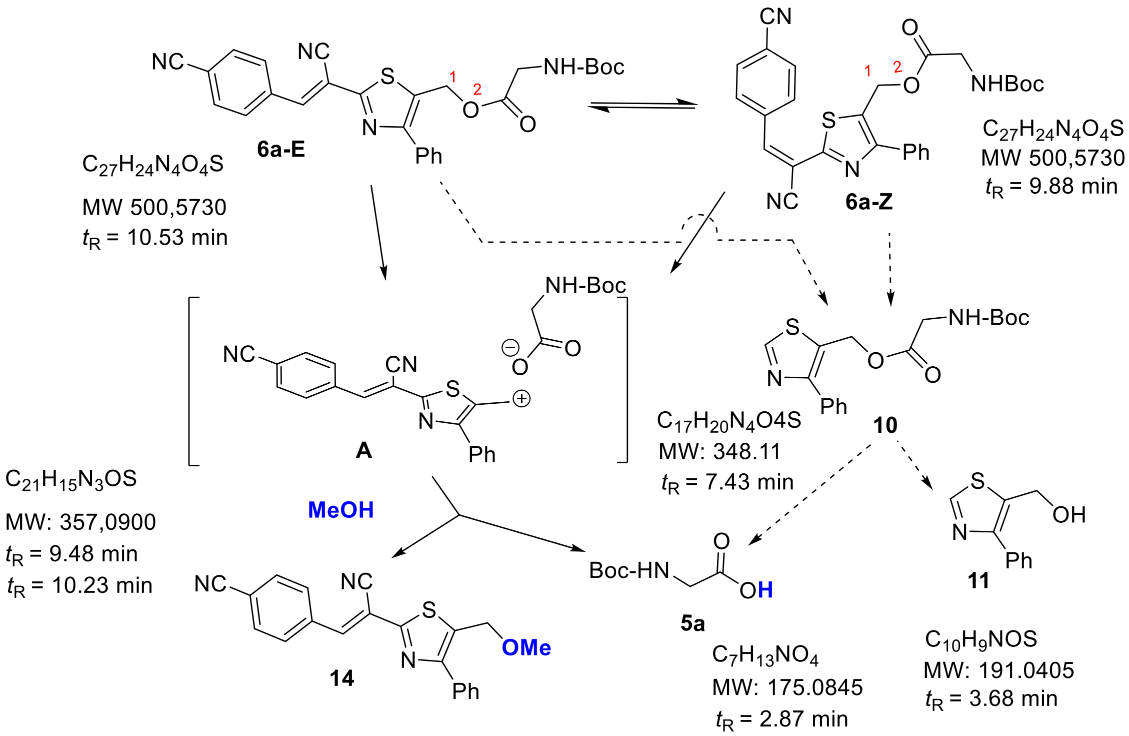


Fig. S21. (A) The extracted ion chromatograms at t_R = 2.89 min and 9.48, 10.23 min after irradiation (50% power, λ_{ir} = 365 nm) of a hybrid **8** solution in a MeCN-H_2O (7:3, v/v) mixture and corresponding mass spectra. (B) The total ion chromatograms irradiation (50% power, λ_{ir} = 365 nm) of a hybrid **8** solution in a MeCN-H_2O (7:3, v/v) and (C) compound ion chromatograms for hybrid **6a**, and photoissociation products **5a**, **10, 11, 13** at the end of experiment**.** (It should be noted that the intensity of the peaks depends on the ionization efficiency and therefore it is not correct to relate it to the amount of substance).

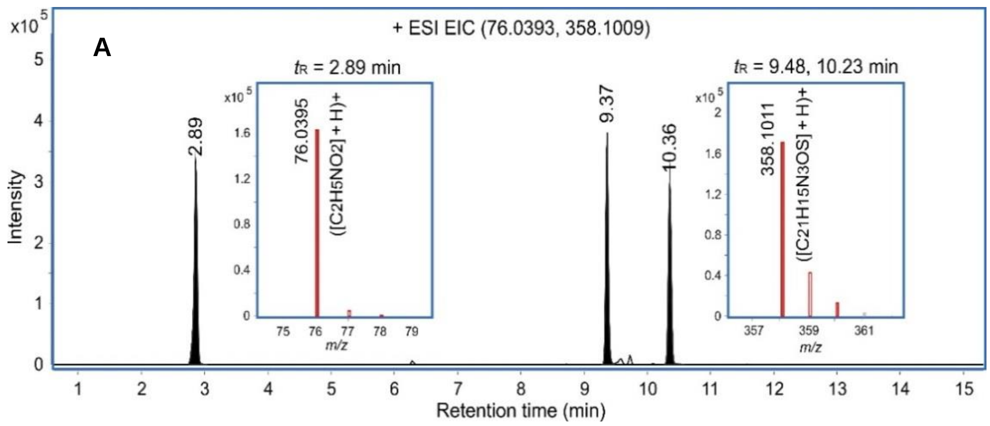


a *b*

Fig. S22. (*a*) Evaluation of *N*-Boc-gly **5a** releasing during hybrids **6a** photodissociation in MeCN-H_2O (7:3, v/v) and MeOH. (*b*) Evaluation of Boc-gly **5a** releasing during hybrids **6a, 7, 8** photodissociation in MeCN-H_2O (7:3, v/v);



Scheme S4. Photodissociation of hybrid **6a** in MeOH based on experimental, quantum-mechanical calculation data and literature data.



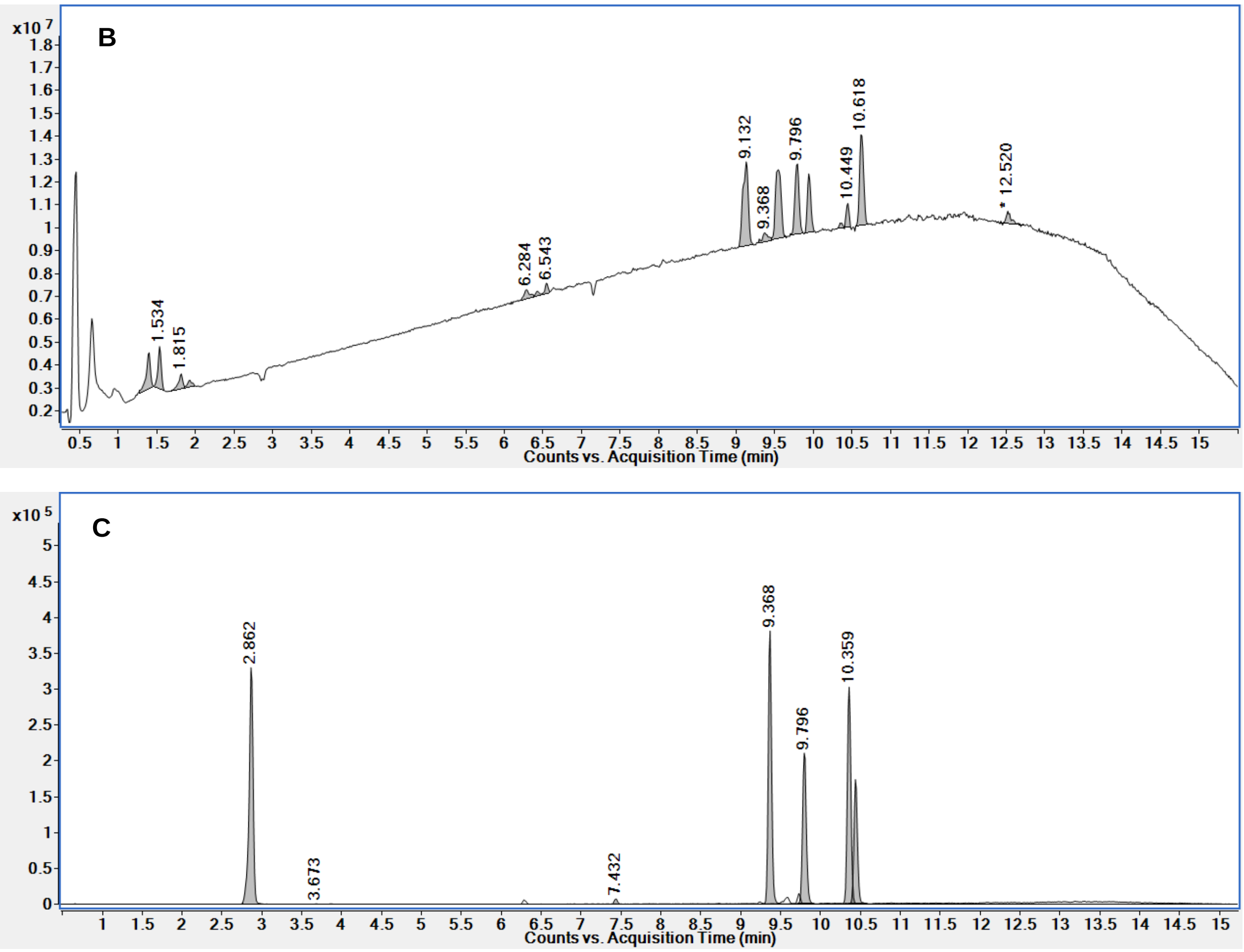


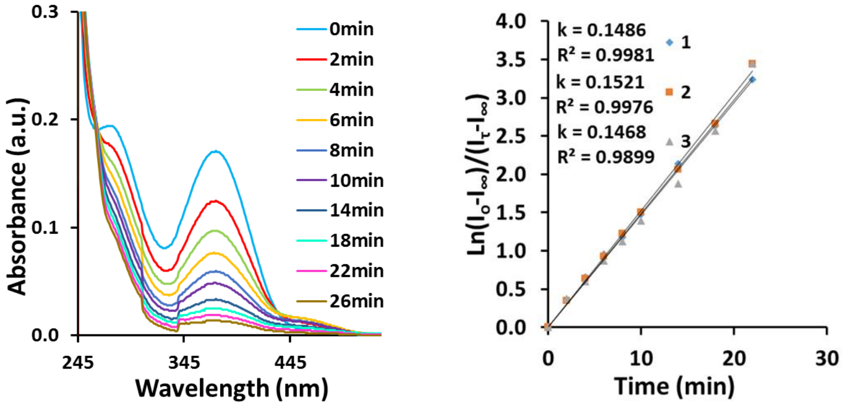
Fig. S23. (A) The extracted ion chromatograms at t_R = 3.94 min and 10.38 min after 5 min of an irradiation (50% power, λ_{ir} = 365 nm) of a hybrid 6a solution in MeOH and corresponding mass spectra. (B) The total ion chromatograms irradiation (50% power, λ_{ir} = 365 nm) of a hybrid **6a** solution in a MeOH and (C) compounds ion chromatograms for hybrid **6a**, and photodissociation products **5a**, **10,11,14** at the end of experiment**.** (It should be noted that the intensity of the peaks depends on the ionization efficiency and therefore it is not correct to relate it to the amount of substance).

Table S12. Evaluation of the yields of *N*-Boc-glycine **5a** during photoreleasing from photo cage **6a** in MeCN-H_2O mixture upon irradiation with sampling at time intervals of 30-60 minutes.

Entry	Time, min.	Yields of *N-Boc*-glycine, %
1	30	21.8
2	60	35.8
3	120	47.5
4	180	54.9
5	240	62.5
6	300	73.0
7	360	89.0

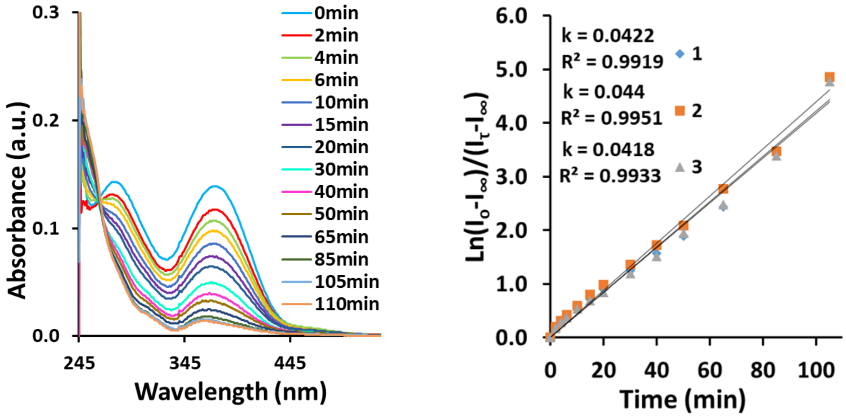
Kinetic investigations. The kinetic equation describing the time evolution of the concentrations coincided with that of the first-order reaction, wherein, in absorption spectra is proportional to the fluorescence intensity hybrids **6a-g, 7** and **8**. The rate constant (*k*) was determined using the derived equation: $\ln(I_0 – I_\infty)/(I_\tau - I_\infty) = k\tau$; where I_0 is the initial intensity of the PTB solution, I_∞ is the intensity of this solution at the end of the transformation, and I_t is intensity of the sample at time *t*. The observed rate constant (*k*) and standard deviation were determined from several kinetic experiments for each sample. (c = 10^{-5} M in DMSO/buff (1:1, v/v), I_{ir} = 20% and 50%).

6a
I = 50%
λ_{ir} = 365 nm



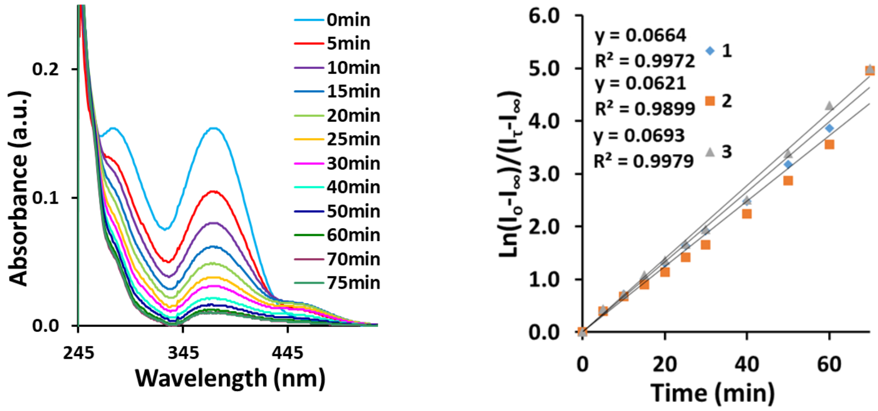
k = 0.149±0.003 $\tau_{1/2}$ = 4.65 min

6a
I = 50%
λ_{ir} = 420 nm



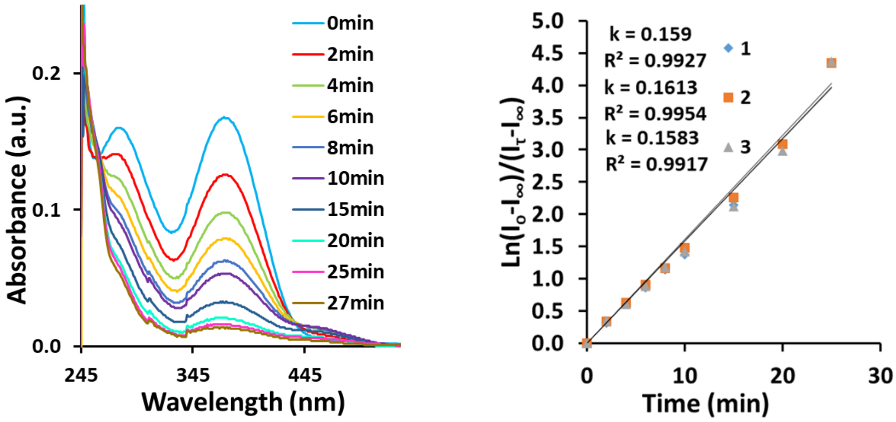
k = 0.042±0.001 $\tau_{1/2}$ = 16.24 min

6a
I = 20%
λ_{ir} = 365 nm



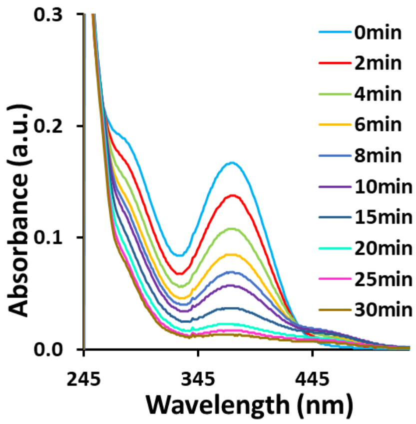
k = 0.066 ±0.004 $\tau_{1/2}$ = 10.51 min

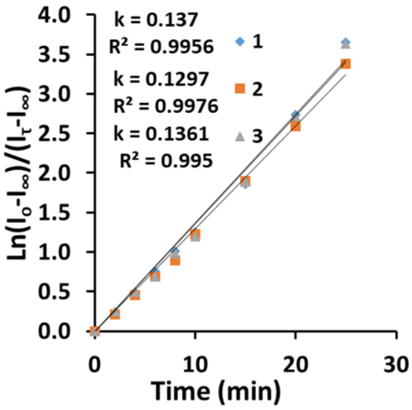
6b
I = 50%
λ_{ir} = 365 nm



k = 0.160 ±0.0002 τ1/2 = 4.34 min

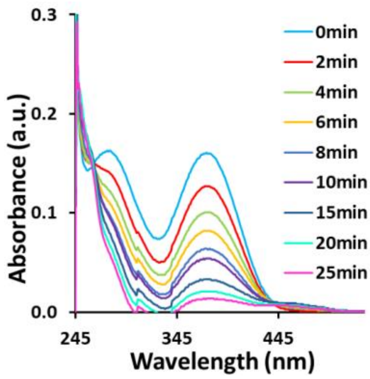
6c
I = 50%
λ_{ir} = 365 nm

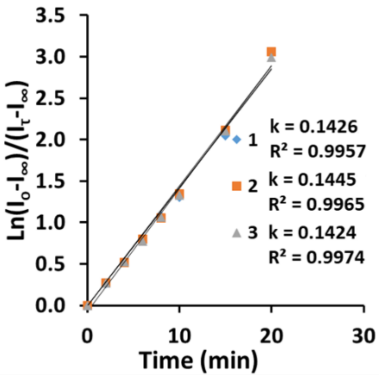




k = 0.134 ±0.004 $\tau_{1/2}$ = 5.16 min

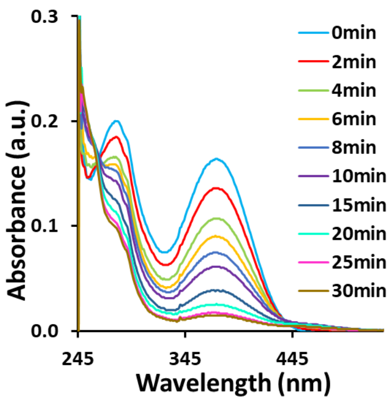
6d
I = 50%
λ_{ir} = 365 nm

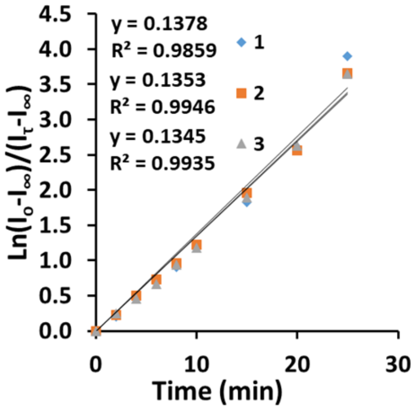




k = 0.143 ±0.001 $\tau_{1/2}$ = 4.84 min

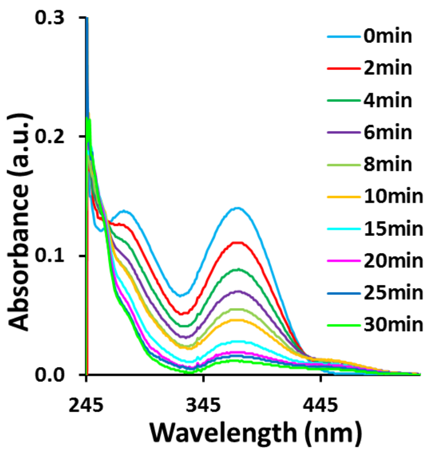
6e
I = 50%
λ_{ir} = 365 nm

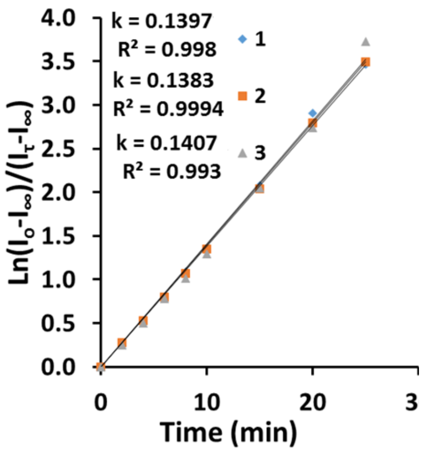




k = 0.136 ±0.002 $\tau_{1/2}$ = 5.10 min

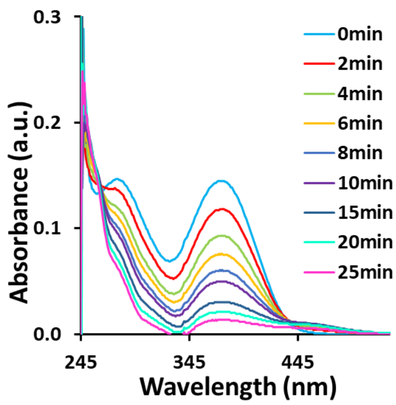
6f
I = 50%
λ_{ir} = 365 nm

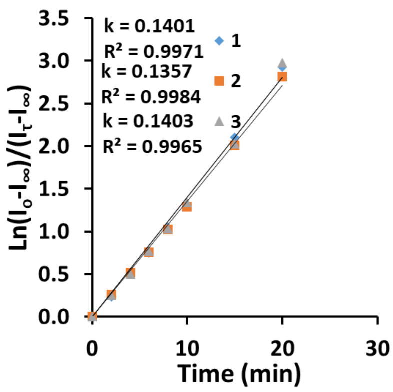




k = 0.140 ±0.001 $\tau_{1/2}$ = 5.00 min

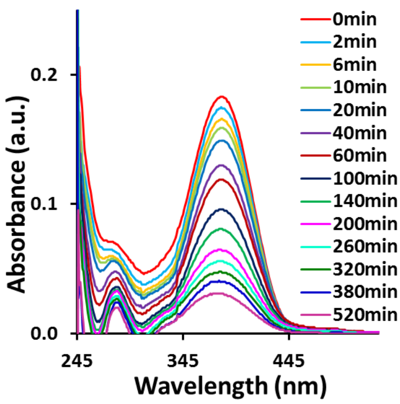
6g
I = 50%
λ_{ir} = 365 nm

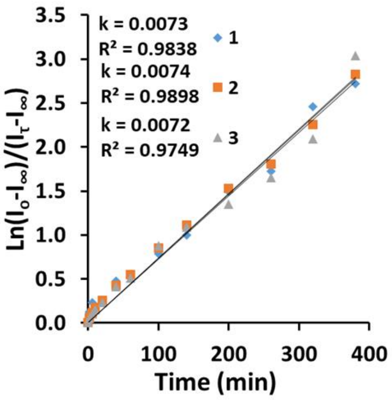




k = 0.1387 ±0.0026 $\tau_{1/2}$ = 4.99

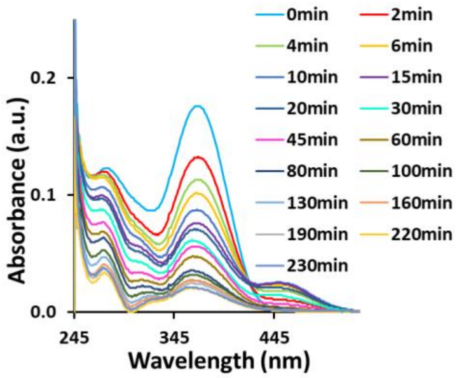
7
I = 50%
λ_{ir} = 365 nm

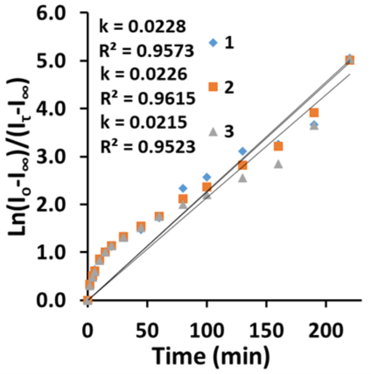




k = 0.0073 ±0.0001 $\tau_{1/2}$ = 94.95 min

8
I = 50%
λ_{ir} = 365 nm





k = 0.0223 ±0.0007 $\tau_{1/2}$ = 31.08 min

Fig. S24. Evolution of the absorption of hybrids **6a-g**, **7** and **8** in (c = 1.0 ×10^{-5} M) solutions in a binary mixture of solvents DMSO-buffer (pH 7.5) upon irradiation (Left). Plot of $\ln[(I_0 - I_\infty)/(I_\tau - I_\infty)]$ versus τ for hybrids **6a-g**, **7** and **8** (Right).

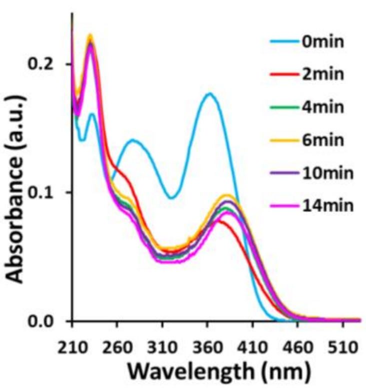
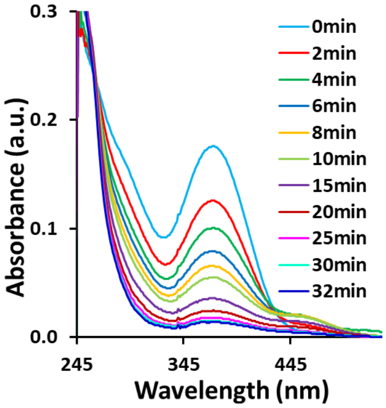
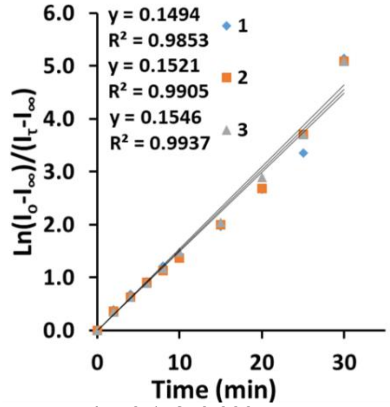


Fig. S25. Evaluation of the absorption of hybrid **6a** (c = 1.0 × 10^{-5} M) solution in MeOH upon irradiation (λ_{ir} = 365 nm).

Potassium Sorbate Experiment. Potassium sorbate solution in in DMSO-buffer (pH 7.5) (1:1, v/v) (c = 1x10^{-5} M), 0.5 and 1.0 equiv. were added into cuvettes with a solution of of hybrids **6a, 8** in DMSO-buffer (pH 7.5) (1:1, v/v) (c = 1x10^{-5} M). The absorption spectra were recorded after irradiation at regular time intervals.

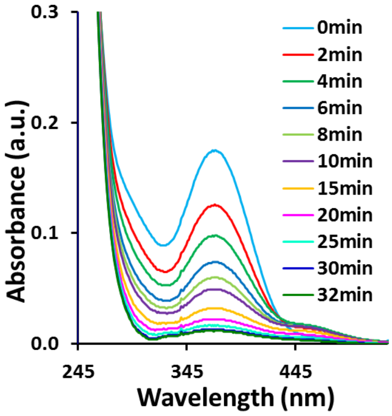


a

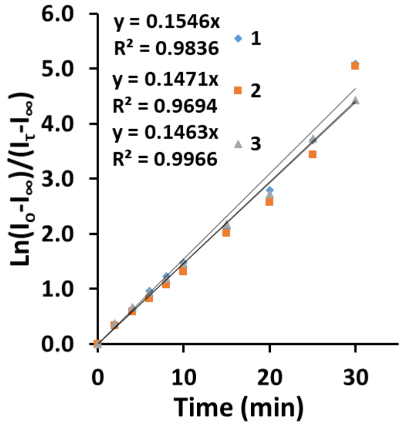


k = 0.152±0.003 $\tau_{1/2}$ = 4.56 min

b



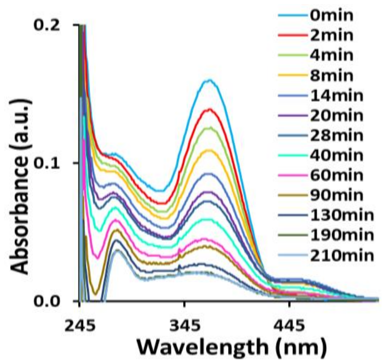
c

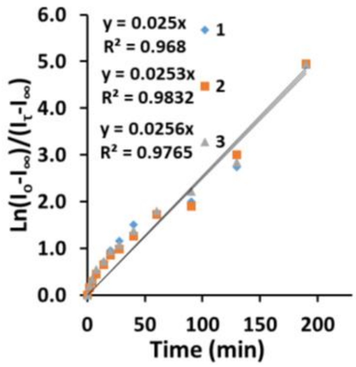


k = 0.149±0.006 $\tau_{1/2}$ = 4.64 min

c

d





k = 0.0253±0.0003 $\tau_{1/2}$ = 27.4 min

e

f

Fig. S26. Evaluation of the (*a*) absorption maxima recorded during photodissociation of hybrids **6a** solutions in DMSO-buffer (pH 7.5) (1:1, v/v) at the present 0.5 equiv. of potassium sorbate and 1.0 equiv. of potassium sorbate. (e) Evaluation of the absorption maxima recorded during photodissociation of hybrids **8** solutions in DMSO-buffer (pH 7.5) (1:1, v/v) at the present 0.5 equiv. of potassium sorbate. (*b*) Plot of ln[($I_0 - I_\infty$)/($I_\tau - I_\infty$)] versus τ for hybrid **6a** at the present (b) 0.5 equiv. of potassium sorbate and (d) 1.0 equiv. of potassium sorbate. (f) Plot of ln[($I_0 - I_\infty$)/($I_\tau - I_\infty$)] versus τ for hybrid **8** at the present 0.5 equiv. of potassium (c = 1×10^{-5} M).

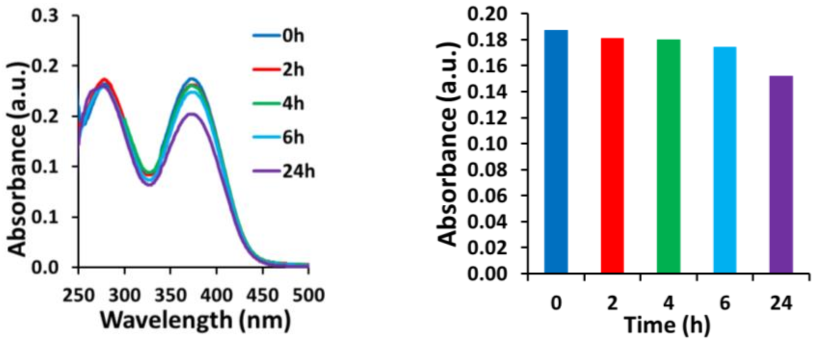
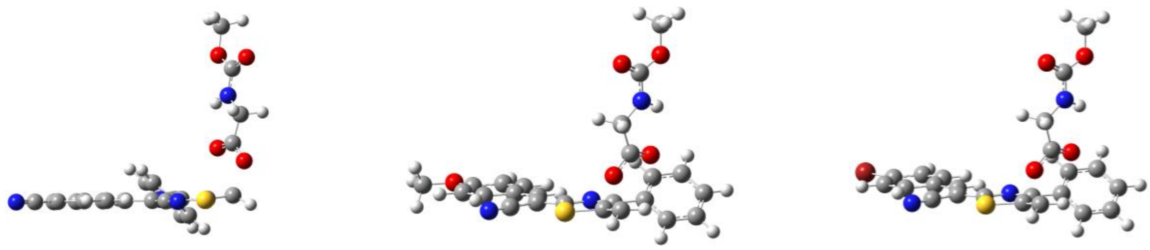


Fig. S27. (*a*,*b*) Evaluation of the absorption maxima recorded during hydrolytic dissociation of hybrid **6a** in solutions in DMSO-buffer (pH 7.5) mixture (9:1, v/v) ($c = 1.0 \times 10^{-5}$ M).



6a **7** **8**

Fig. S28. Structures of the complex **B** formed after breaking the C-O bond during photodissociation of photocages **6a**, **7** and **8**. (Passing from d = 1.80 Å to 1.81 Å, the detached acid fragment becomes “perpendicular” to the remaining fluorophore fragment). (in DMSO)

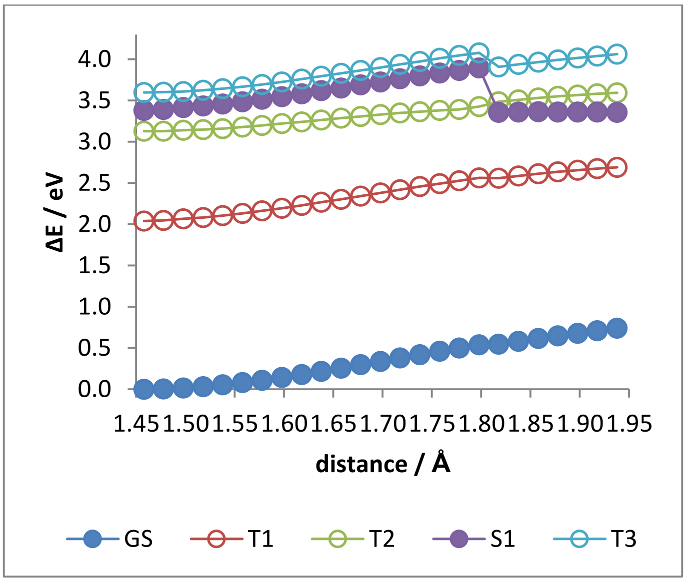


Fig. S29. Potential Energy Surface (PES) scan of the S_0 (GS)), and excited states S_1 and T_1-T_3 calculated in TD(DFT) for hybrid **6a**.

Table S13. The amount of charge assigned to acid fragment formed during the photodissociation in the different electronic state (hybrid **6a**).

	S_0	T_1	T_2	S_1
q(acid)/|e|	-0.493	-0.474	-0.494	-0.470

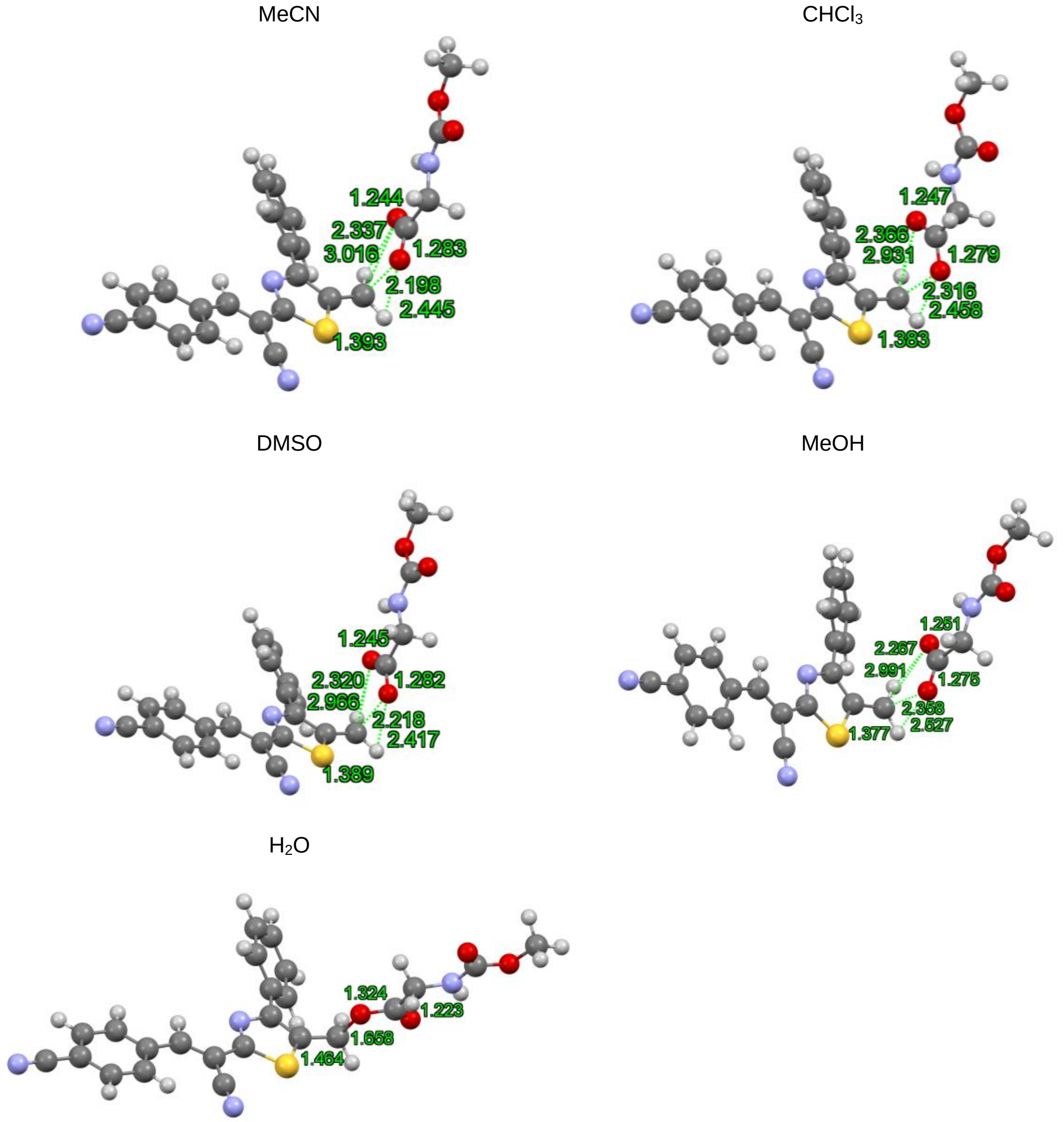


Fig. S30. Structure of the state **A** during the breaking the C–O bond upon UV-irradiation of photocourier **6a** in MeCN, $CHCl_3$, DMSO, MeOH and H_2O. Level of theory: DFT/IEF-PCM(UFF). Legend of colours: white (H), grey (C), lilac (N), yellow (S), red (O).

8. Biological experiments

Materials and methods. We used Vero cell cultures (green monkey kidney epithelium) and human fibroblast cultures obtained from the Russian Collection of Cell Cultures of the Institute of Cytology of the Russian Academy of Sciences.

Cells were cultured in T-25 ventilated culture flasks (JetBiofil, China) in DMEM nutrient medium (HiMedia, India) supplemented with 3% fetal calf serum (Biolot, Russia) and gentamicin-streptamycin solution (Biolot, Russia). Cells were maintained in a humidified incubator with 5% CO_2. Cells were passengered every three days (or when 90% confluence was reached) using trypsin-Versene solution (ServiceBio, China).

MTT-test. The MTT test is an available test for screening the cytotoxicity of various substances in cell cultures. This method is based on the study of mitochondrial activity associated with cell viability. Under normal conditions, cell mitochondrial enzymes are able to reduce the yellow tetrazolium dye 3-(4,5-dimethylthiazol-2-yl)-2,5-diphenyl-tetrazolium bromide to insoluble formazan, which has a purple color.

The test substances were prepared in working concentrations from a solution in DMSO by dissolving them in a complete nutrient medium to the required concentration. For the study, the cells were seeded into a 96-well plate (JetBiofil, China) and grown to 70%

monolayer, after which the medium was taken with a multichannel dispenser and replaced with the prepared medium with the addition of the test substance.

Incubation with the test substance was carried out for 24 hours or for 30 min, 4 h and 24 h after which the medium was taken and replaced with a complete nutrient medium with the addition of MTT (at a concentration of 1 mg/ml), after which they were incubated for 2 hours. Next, the medium was removed and 100 μl of DMSO was poured into the wells of the plate. After complete dissolution of the dye, the intensity of staining was assessed using a plate photometer at a wavelength of 570 nm.

Statistical processing. The results were analyzed using a python script available in the repository at the link: https://github.com/arteys/MTT_assay_multi. Raw data is also given in this repository. Statistical processing was carried out using the Statannotations 3 library, using a two-tailed Mann-Whitney-Wilcoxon test, taking into account the Bonferroni correction for multiple comparisons. The designation ns corresponds to the absence of statistical significance, * significance at 1.00e-02 < p <= 5.00e-02, ** reliability at 1.00e-03 < p <= 1.00e-02, *** reliability at 1.00e-04 < p <= 1.00e-03, **** reliability at p <= 1.00e-04.

Confocal and optical microscopy. Microscopic examination was performed using the equipment of the Shared Research Center of Scientific Equipment SRC IIP UrB RAS. After staining and washing, living cells were examined using a confocal laser scanning microscope LSM-710 (Carl Zeiss) has a multichannel QUASAR detector (34 channels). The images were obtained using an immersion lens 40x/1.3 Oil. To obtain an informative fluorescent image in special software ZEN a special lambda mode (λ-mode) was used, which allows determining the emission range with the maximum contrast for this preparation.

To minimize the light effect on the sample, the initial focus adjustment was carried out under illumination with a laser with a wavelength of 633 mm, as the lowest energy available. The emission spectra of substances were also extracted from images obtained in the lambda mode. However, it is necessary to clarify that the confocal microscope is not a spectrofluorometer, and the fluorescence spectra obtained with it can be unreliable. The images were processed using FIJI, a Python script was written to process the lambda images obtained with the confocal microscope, allowing the processing of the .lsm file format. The script is available on the Github (https://github.com/arteys/PyLSM).

The initial focus adjustment on a confocal microscope was carried out using the light of a laser with a wavelength of 633 nm, as the least energetic available. To study the phenomenon of a decrease in the brightness of the dye under the action of light radiation (photobleaching), the cells were stained with a dye according to the procedure described above. The light exposure was carried out with the same laser intensity, which is necessary to obtain an image with adequate contrast. Without changing the laser intensity, a series of images was recorded sequentially for 30 seconds. Then, the integrated fluorescence intensity was determined from the images and graphs were plotted.

Cell staining. To clarify the localization of the tested substance, cells were additionally stained with fluorescent dyes staining known cell organelles.

Additional cell staining and colocalization experiments. To clarify the localization of the tested substance, cells were additionally stained with fluorescent dyes staining known cell organelles. The colocalisation of mitochondrial dye with the tested substance was assessed using ImagJ (FIJI), specifically the JACoP BIOP plugin. Noise was removed from the images using the standard Despeckle function, as well as the background using the Subtract Background function at default settings. Next, the JACoP BIOP plugin was used to obtain a fluorogram (colocalisation scatterplot) as well as numerical data (namely Manders overlap coefficient).

Preliminary cells grown in specialized confocal dishes were stained with the investigated substance, for this purpose a solution of the substance at a concentration of 10 μM in nutrient medium was added to the cells, after which they were incubated for half an hour. Then the medium was removed, the cells were washed three times with phosphate buffer, after which the cells were stained with commercial dye.

MitoTracker Red CMXRos (Thermo Scientific, USA) was used to stain mitochondria. For staining, a solution of the dye at a concentration of 100 nM in DMEM nutrient medium was prepared and added to the cells, incubation was carried out for 30 minutes, then the cells were washed three times with phosphate buffer and studied using a confocal microscope. Excitation wavelength - 561 nm, emission was recorded in the range of 600-650 nm.

All work with photosensitive substances was performed in a Bioinnelix laminar flow cabinet (BioinnLabs, Russia) using red LED illumination (625 nm) to minimize the effect of light on the substance.

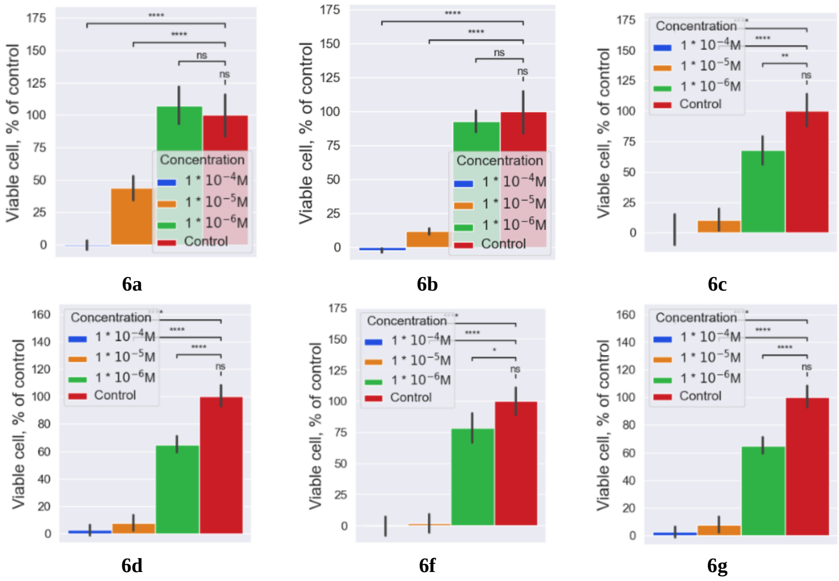
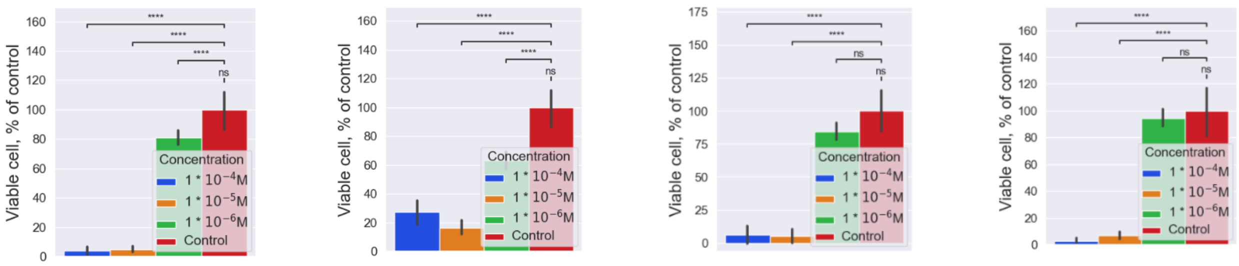


Fig. S31. Results of the MTT test (percentage of *Vero* cell survival) for hybrides **6a-d**,**f** and **g** (c = 10^{-4}, 10^{-5}, and 10^{-6} M).



6a **6c** **6d** **6f**

Fig. S32. Results of the MTT test (percentage of cell RD survival) for hybrids **6a**, **6c**, **6d**, and **6f** (c = 10^{-4}, 10^{-5} and 10^{-6} M).

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10. Cartesian coordinates (Å) of the optimized structures

GS and ES optimized geometries (S_0) for compounds 3b and 3c

Mol3b-A_s0r_dmso

6	-5.511354	1.137769	-0.310704
6	-4.132384	1.316383	-0.307417
6	-3.233584	0.233144	-0.196859
6	-3.788492	-1.066784	-0.089821
6	-5.158047	-1.257386	-0.092516
6	-6.033869	-0.159887	-0.202369
1	-6.160110	1.999499	-0.397413
1	-3.736380	2.324010	-0.392462
1	-3.148118	-1.933734	-0.005207
1	-5.579283	-2.253640	-0.011110
6	-1.823247	0.550038	-0.205621
1	-1.625723	1.613974	-0.314218
6	-0.703704	-0.229726	-0.101974
6	0.653607	0.321858	-0.146956
6	2.889782	0.343442	-0.067861
6	2.702037	1.692711	-0.288691
6	4.186910	-0.348555	0.072905
6	4.350011	-1.637015	-0.466751
6	5.268163	0.240708	0.749489
6	5.567095	-2.308036	-0.349803
1	3.516080	-2.102775	-0.980810
6	6.486681	-0.432170	0.864633
1	5.151175	1.214694	1.211132
6	6.642660	-1.706545	0.312867
1	5.677298	-3.299975	-0.777592
1	7.309749	0.036545	1.395394
6	-0.751249	-1.649263	0.061727
7	-0.773457	-2.806322	0.195589
16	0.990961	2.029584	-0.395162
7	1.729202	-0.408756	-0.003752
1	7.589845	-2.229181	0.403876
6	3.700614	2.793026	-0.478015
1	3.902863	3.322958	0.459898
1	4.645348	2.384075	-0.843628
1	3.343244	3.529241	-1.203065
8	-7.355514	-0.455143	-0.195311
6	-8.299663	0.618304	-0.303791
1	-8.172532	1.154141	-1.249716
1	-9.281742	0.148631	-0.275674
1	-8.197247	1.312796	0.535977

Mol3b-A_s0r_mecn

6	-5.511207	1.137870	-0.308501
6	-4.132213	1.316486	-0.305150
6	-3.233402	0.233056	-0.197181
6	-3.788275	-1.067114	-0.092950
6	-5.157830	-1.257708	-0.095764
6	-6.033713	-0.160001	-0.202927
1	-6.160007	1.999782	-0.393121
1	-3.736289	2.324335	-0.388072
1	-3.147849	-1.934230	-0.010495
1	-5.579083	-2.254132	-0.016560
6	-1.822992	0.549946	-0.205608
1	-1.625511	1.614079	-0.312444
6	-0.703470	-0.229933	-0.103353
6	0.653795	0.321788	-0.147991
6	2.889943	0.343808	-0.068085
6	2.702030	1.693013	-0.289322
6	4.186912	-0.348250	0.073369
6	4.348780	-1.638321	-0.462846
6	5.269195	0.242259	0.747215
6	5.565651	-2.309577	-0.345405
1	3.513925	-2.105164	-0.974373
6	6.487487	-0.430915	0.862889
1	5.153229	1.217425	1.206575
6	6.642265	-1.706825	0.314393
1	5.674829	-3.302797	-0.770479
1	7.311314	0.038795	1.391597
6	-0.751030	-1.649716	0.058689
7	-0.773703	-2.806902	0.191167

16	0.990958	2.029679	-0.396494
7	1.729396	-0.408473	-0.004293
1	7.589282	-2.229700	0.405814
6	3.700425	2.793522	-0.478714
1	3.904688	3.321819	0.459699
1	4.644366	2.385089	-0.846990
1	3.341734	3.531044	-1.201776
8	-7.355352	-0.455256	-0.196147
6	-8.299476	0.618220	-0.302619
1	-8.172061	1.156312	-1.247265
1	-9.281555	0.148431	-0.276018
1	-8.197557	1.310890	0.538758

Mol3b-A_s0r_meoh

6	-5.511146	1.137869	-0.308216
6	-4.132145	1.316465	-0.304847
6	-3.233351	0.232996	-0.197273
6	-3.788239	-1.067198	-0.093462
6	-5.157800	-1.257768	-0.096295
6	-6.033665	-0.160024	-0.203058
1	-6.159940	1.999815	-0.392537
1	-3.736217	2.324344	-0.387436
1	-3.147812	-1.934342	-0.011310
1	-5.579072	-2.254208	-0.017406
6	-1.822916	0.549866	-0.205634
1	-1.625431	1.614036	-0.312126
6	-0.703403	-0.230035	-0.103659
6	0.653837	0.321742	-0.148181
6	2.889968	0.343888	-0.068111
6	2.702014	1.693088	-0.289381
6	4.186914	-0.348172	0.073465
6	4.348571	-1.638500	-0.462190
6	5.269352	0.242522	0.746895
6	5.565404	-2.309794	-0.344665
1	3.513544	-2.105527	-0.973259
6	6.487602	-0.430702	0.862661
1	5.153529	1.217859	1.205924
6	6.642185	-1.706849	0.314675
1	5.674407	-3.303228	-0.769285
1	7.311544	0.039146	1.391070
6	-0.750987	-1.649885	0.057946
7	-0.773886	-2.807104	0.190028
16	0.990930	2.029703	-0.396644
7	1.729450	-0.408423	-0.004427
1	7.589169	-2.229770	0.406172
6	3.700357	2.793636	-0.478843
1	3.904687	3.321966	0.459541
1	4.644280	2.385235	-0.847203
1	3.341590	3.531134	-1.201897
8	-7.355325	-0.455256	-0.196329
6	-8.299395	0.618255	-0.302294
1	-8.172100	1.156716	-1.246756
1	-9.281499	0.148506	-0.275755
1	-8.197381	1.310633	0.539324

Mol3b-A_s1r_dmso

6	-5.496914	1.164600	-0.092460
6	-4.149094	1.371530	0.130714
6	-3.181472	0.320254	0.013099
6	-3.683238	-0.971991	-0.363069
6	-5.027533	-1.178032	-0.590522
6	-5.953968	-0.121483	-0.455614
1	-6.187725	1.991463	0.015017
1	-3.806481	2.363392	0.410917
1	-3.000517	-1.802114	-0.486447
1	-5.397253	-2.156157	-0.881108
6	-1.823189	0.620124	0.234639
1	-1.595544	1.667735	0.415096
6	-0.696886	-0.277068	0.292867
6	0.622311	0.209842	0.133510
6	2.856039	0.273293	0.006532
6	2.609940	1.631124	-0.304082
6	4.171979	-0.365155	0.074280
6	4.274834	-1.744274	-0.211439
6	5.338188	0.337908	0.440226
6	5.507046	-2.388273	-0.162499
1	3.378468	-2.289877	-0.481934

6	6.567844	-0.314601	0.498284
1	5.282536	1.382093	0.719097
6	6.660029	-1.676065	0.190002
1	5.571629	-3.445674	-0.398664
1	7.453956	0.238001	0.793477
6	-0.816830	-1.657149	0.572916
7	-0.909773	-2.801668	0.808270
16	0.911060	1.939739	-0.269824
7	1.746981	-0.490093	0.231961
1	7.620613	-2.179648	0.231054
6	3.563748	2.717791	-0.676461
1	3.943225	3.240047	0.211954
1	4.421044	2.312228	-1.218666
1	3.077786	3.465326	-1.308226
8	-7.249176	-0.434979	-0.692881
6	-8.244815	0.589285	-0.573669
1	-8.057141	1.398453	-1.286738
1	-9.192132	0.105092	-0.806014
1	-8.271950	0.987617	0.445624

Mol3b-A_s1r_mecn

6	-5.496291	1.164702	-0.092925
6	-4.148105	1.370732	0.129199
6	-3.181483	0.318663	0.011799
6	-3.684538	-0.973500	-0.362632
6	-5.029193	-1.178659	-0.589054
6	-5.954589	-0.121260	-0.454673
1	-6.186362	1.992232	0.014239
1	-3.804499	2.362578	0.408292
1	-3.002630	-1.804376	-0.485355
1	-5.399909	-2.156799	-0.878310
6	-1.822666	0.617799	0.232007
1	-1.594529	1.665438	0.411773
6	-0.696682	-0.279488	0.289939
6	0.622567	0.208114	0.131921
6	2.856323	0.273168	0.005997
6	2.609587	1.631323	-0.303053
6	4.172287	-0.364749	0.074256
6	4.275051	-1.744584	-0.208538
6	5.338844	0.339110	0.437897
6	5.507298	-2.388351	-0.159176
1	3.378427	-2.290774	-0.476896
6	6.568510	-0.313199	0.496384
1	5.283447	1.383818	0.714762
6	6.660524	-1.675326	0.190885
1	5.571739	-3.446278	-0.392989
1	7.454825	0.240013	0.789823
6	-0.816427	-1.660113	0.567373
7	-0.909239	-2.805082	0.800540
16	0.910600	1.939011	-0.269264
7	1.747389	-0.491106	0.229846
1	7.621165	-2.178769	0.232301
6	3.562771	2.719090	-0.673981
1	3.942914	3.239684	0.215140
1	4.419695	2.314995	-1.217883
1	3.076020	3.467757	-1.303794
8	-7.250349	-0.433823	-0.691050
6	-8.244671	0.591529	-0.572308
1	-8.056552	1.399909	-1.286215
1	-9.192712	0.108248	-0.803672
1	-8.270934	0.990961	0.446613

Mol3b-A_s1r_meoh

6	-5.496107	1.164772	-0.093507
6	-4.147748	1.370574	0.127904
6	-3.181489	0.318170	0.010888
6	-3.685082	-0.974122	-0.362269
6	-5.029908	-1.179063	-0.587969
6	-5.954930	-0.121313	-0.454074
1	-6.185871	1.992603	0.013311
1	-3.803752	2.362542	0.406097
1	-3.003496	-1.805332	-0.484500
1	-5.401026	-2.157341	-0.876238
6	-1.822469	0.617154	0.230319
1	-1.594156	1.664869	0.409361
6	-0.696567	-0.280080	0.288276
6	0.622749	0.207786	0.131099

6	2.856560	0.273372	0.005944
6	2.609681	1.631681	-0.302456
6	4.172447	-0.364523	0.074369
6	4.274974	-1.744616	-0.207436
6	5.339241	0.339410	0.437248
6	5.507127	-2.388502	-0.157933
1	3.378192	-2.290869	-0.475098
6	6.568803	-0.313032	0.495892
1	5.284133	1.384291	0.713458
6	6.660549	-1.675392	0.191324
1	5.571348	-3.446615	-0.390959
1	7.455266	0.240247	0.788754
6	-0.816149	-1.660983	0.564450
7	-0.908716	-2.806197	0.796473
16	0.910690	1.939143	-0.268880
7	1.747592	-0.491204	0.228936
1	7.621126	-2.178945	0.232882
6	3.562695	2.719856	-0.672702
1	3.943572	3.239275	0.216790
1	4.419168	2.316422	-1.217818
1	3.075522	3.469362	-1.301181
8	-7.250924	-0.433698	-0.689712
6	-8.244850	0.592010	-0.571316
1	-8.056793	1.399848	-1.285868
1	-9.193147	0.108879	-0.801969
1	-8.270626	0.992197	0.447332

Mol3b-B_s0r_dmso

6	-4.598860	-1.922619	-0.062406
6	-3.263561	-1.562523	-0.048051
6	-2.856475	-0.207040	-0.133043
6	-3.870051	0.770497	-0.233273
6	-5.215614	0.421788	-0.248512
6	-5.590185	-0.930514	-0.163293
1	-4.900177	-2.962440	0.002828
1	-2.506395	-2.336916	0.029929
1	-3.617265	1.819947	-0.300783
1	-5.961024	1.202625	-0.326446
6	-1.435565	0.051778	-0.109967
1	-0.814838	-0.836527	-0.028475
6	-0.712716	1.212884	-0.173265
6	0.755432	1.177586	-0.136035
6	2.822240	0.337769	-0.016219
6	3.172873	1.672230	-0.095827
6	3.751973	-0.806615	0.070326
6	3.444206	-2.004719	-0.598958
6	4.937744	-0.739448	0.821031
6	4.308167	-3.097693	-0.534234
1	2.525331	-2.067131	-1.172068
6	5.802370	-1.834573	0.883976
1	5.173913	0.159092	1.379739
6	5.493748	-3.015997	0.204392
1	4.057745	-4.012962	-1.062121
1	6.711708	-1.766345	1.473285
6	-1.303972	2.506515	-0.279842
7	-1.741748	3.583619	-0.366415
16	1.726040	2.641511	-0.192440
7	1.463476	0.082162	-0.051573
1	6.166118	-3.866868	0.254628
6	4.524530	2.316664	-0.151644
1	4.865111	2.633448	0.840886
1	5.260047	1.614247	-0.550675
1	4.513450	3.200761	-0.794793
8	-6.871362	-1.369570	-0.170824
6	-7.929760	-0.407769	-0.272507
1	-7.858499	0.152023	-1.210380
1	-8.852561	-0.985828	-0.258178
1	-7.912088	0.281915	0.577201

Mol3b-B_s0r_mecn

6	-4.598860	-1.922619	-0.062406
6	-3.263561	-1.562523	-0.048051
6	-2.856475	-0.207040	-0.133043
6	-3.870051	0.770497	-0.233273
6	-5.215614	0.421788	-0.248512
6	-5.590185	-0.930514	-0.163293
1	-4.900177	-2.962440	0.002828

1	-2.506395	-2.336916	0.029929
1	-3.617265	1.819947	-0.300783
1	-5.961024	1.202625	-0.326446
6	-1.435565	0.051778	-0.109967
1	-0.814838	-0.836527	-0.028475
6	-0.712716	1.212884	-0.173265
6	0.755432	1.177586	-0.136035
6	2.822240	0.337769	-0.016219
6	3.172873	1.672230	-0.095827
6	3.751973	-0.806615	0.070326
6	3.444206	-2.004719	-0.598958
6	4.937744	-0.739448	0.821031
6	4.308167	-3.097693	-0.534234
1	2.525331	-2.067131	-1.172068
6	5.802370	-1.834573	0.883976
1	5.173913	0.159092	1.379739
6	5.493748	-3.015997	0.204392
1	4.057745	-4.012962	-1.062121
1	6.711708	-1.766345	1.473285
6	-1.303972	2.506515	-0.279842
7	-1.741748	3.583619	-0.366415
16	1.726040	2.641511	-0.192440
7	1.463476	0.082162	-0.051573
1	6.166118	-3.866868	0.254628
6	4.524530	2.316664	-0.151644
1	4.865111	2.633448	0.840886
1	5.260047	1.614247	-0.550675
1	4.513450	3.200761	-0.794793
8	-6.871362	-1.369570	-0.170824
6	-7.929760	-0.407769	-0.272507
1	-7.858499	0.152023	-1.210380
1	-8.852561	-0.985828	-0.258178
1	-7.912088	0.281915	0.577201

Mol3b-B_s0r_meoh

6	-4.598860	-1.922619	-0.062406
6	-3.263561	-1.562523	-0.048051
6	-2.856475	-0.207040	-0.133043
6	-3.870051	0.770497	-0.233273
6	-5.215614	0.421788	-0.248512
6	-5.590185	-0.930514	-0.163293
1	-4.900177	-2.962440	0.002828
1	-2.506395	-2.336916	0.029929
1	-3.617265	1.819947	-0.300783
1	-5.961024	1.202625	-0.326446
6	-1.435565	0.051778	-0.109967
1	-0.814838	-0.836527	-0.028475
6	-0.712716	1.212884	-0.173265
6	0.755432	1.177586	-0.136035
6	2.822240	0.337769	-0.016219
6	3.172873	1.672230	-0.095827
6	3.751973	-0.806615	0.070326
6	3.444206	-2.004719	-0.598958
6	4.937744	-0.739448	0.821031
6	4.308167	-3.097693	-0.534234
1	2.525331	-2.067131	-1.172068
6	5.802370	-1.834573	0.883976
1	5.173913	0.159092	1.379739
6	5.493748	-3.015997	0.204392
1	4.057745	-4.012962	-1.062121
1	6.711708	-1.766345	1.473285
6	-1.303972	2.506515	-0.279842
7	-1.741748	3.583619	-0.366415
16	1.726040	2.641511	-0.192440
7	1.463476	0.082162	-0.051573
1	6.166118	-3.866868	0.254628
6	4.524530	2.316664	-0.151644
1	4.865111	2.633448	0.840886
1	5.260047	1.614247	-0.550675
1	4.513450	3.200761	-0.794793
8	-6.871362	-1.369570	-0.170824
6	-7.929760	-0.407769	-0.272507
1	-7.858499	0.152023	-1.210380
1	-8.852561	-0.985828	-0.258178
1	-7.912088	0.281915	0.577201

Mol3b-B_s1r_dmso

6	-4.583449	-1.948998	-0.050171
6	-3.250642	-1.617498	-0.005571
6	-2.800291	-0.253663	-0.098317
6	-3.820844	0.744251	-0.239450
6	-5.165649	0.409903	-0.285310
6	-5.564738	-0.937437	-0.191497
1	-4.907443	-2.982169	0.021028
1	-2.507775	-2.402353	0.102639
1	-3.550142	1.788509	-0.315507
1	-5.900310	1.198235	-0.394084
6	-1.415786	-0.007162	-0.051947
1	-0.769447	-0.872264	0.040189
6	-0.696517	1.237904	-0.108112
6	0.722878	1.196893	-0.080673
6	2.790572	0.340076	0.015432
6	3.151117	1.704300	-0.064658
6	3.722412	-0.788673	0.074698
6	3.323521	-2.030605	-0.465585
6	4.993074	-0.690935	0.677660
6	4.179366	-3.127094	-0.429595
1	2.343003	-2.111703	-0.920159
6	5.842291	-1.794900	0.719638
1	5.304986	0.231745	1.149813
6	5.444129	-3.013983	0.160671
1	3.862982	-4.071350	-0.861378
1	6.812378	-1.706306	1.198035
6	-1.285076	2.518167	-0.178814
7	-1.705843	3.612093	-0.236709
16	1.726661	2.684295	-0.139509
7	1.451371	0.084774	-0.007804
1	6.110231	-3.870379	0.191118
6	4.500067	2.336300	-0.145834
1	4.898839	2.555856	0.853535
1	5.207727	1.675326	-0.651171
1	4.456801	3.282032	-0.691799
8	-6.849110	-1.363742	-0.225621
6	-7.896512	-0.395749	-0.366429
1	-7.794679	0.151484	-1.309181
1	-8.824456	-0.965595	-0.368005
1	-7.892188	0.305378	0.474411

Mol3b-B_s1r_mecn

6	-4.582993	-1.949179	-0.051680
6	-3.250175	-1.617582	-0.007635
6	-2.799964	-0.253752	-0.099689
6	-3.820624	0.744166	-0.239552
6	-5.165450	0.409733	-0.284780
6	-5.564393	-0.937613	-0.191653
1	-4.906948	-2.982393	0.019036
1	-2.507172	-2.402454	0.099659
1	-3.549980	1.788488	-0.314984
1	-5.900200	1.198135	-0.392487
6	-1.415433	-0.007042	-0.053774
1	-0.768779	-0.871973	0.037778
6	-0.696624	1.238070	-0.109537
6	0.722903	1.196924	-0.081693
6	2.790602	0.340253	0.015235
6	3.151114	1.704474	-0.064496
6	3.722206	-0.788538	0.074818
6	3.322834	-2.030687	-0.464692
6	4.993111	-0.690913	0.677426
6	4.178429	-3.127321	-0.428491
1	2.342061	-2.111670	-0.918709
6	5.842028	-1.795028	0.719659
1	5.305296	0.231863	1.149208
6	5.443397	-3.014259	0.161311
1	3.861682	-4.071725	-0.859686
1	6.812235	-1.706562	1.197851
6	-1.285154	2.518353	-0.180161
7	-1.705771	3.612300	-0.238469
16	1.726749	2.684531	-0.139846
7	1.451363	0.084882	-0.008764
1	6.109275	-3.870826	0.191996
6	4.500061	2.336661	-0.144938
1	4.898161	2.556498	0.854668
1	5.208187	1.675831	-0.649781
1	4.457017	3.282341	-0.691050
8	-6.848863	-1.364034	-0.225104

6	-7.896179	-0.395952	-0.364619
1	-7.794788	0.152165	-1.306931
1	-8.824198	-0.965706	-0.366285
1	-7.891512	0.304504	0.476816

molG3b-B_s1r_meoh

6	-4.582961	-1.949662	-0.058034
6	-3.250010	-1.618296	-0.015898
6	-2.799947	-0.254193	-0.104439
6	-3.820828	0.744263	-0.238498
6	-5.165803	0.410072	-0.281733
6	-5.564588	-0.937565	-0.192351
1	-4.906809	-2.983092	0.009948
1	-2.506824	-2.403570	0.087065
1	-3.550301	1.788841	-0.310815
1	-5.900748	1.198898	-0.384934
6	-1.415294	-0.007674	-0.060548
1	-0.768603	-0.872873	0.028118
6	-0.696481	1.237489	-0.114793
6	0.723048	1.196392	-0.085028
6	2.790815	0.340151	0.014944
6	3.151135	1.704496	-0.064294
6	3.722391	-0.788500	0.075897
6	3.323177	-2.031188	-0.462603
6	4.993196	-0.690355	0.678687
6	4.178759	-3.127768	-0.425228
1	2.342520	-2.112574	-0.916782
6	5.842099	-1.794422	0.722079
1	5.305348	0.232787	1.149739
6	5.443613	-3.014168	0.164739
1	3.862103	-4.072559	-0.855638
1	6.812210	-1.705499	1.200374
6	-1.284859	2.517733	-0.186904
7	-1.705439	3.611644	-0.246400
16	1.726769	2.684272	-0.142044
7	1.451568	0.084620	-0.011030
1	6.109507	-3.870686	0.196318
6	4.500045	2.337025	-0.142974
1	4.897385	2.555624	0.857193
1	5.208666	1.676973	-0.648166
1	4.457199	3.283380	-0.687900
8	-6.849207	-1.363797	-0.224275
6	-7.896767	-0.395149	-0.357483
1	-7.797780	0.156572	-1.297951
1	-8.824852	-0.964804	-0.358970
1	-7.889942	0.302123	0.486589

Mol3b-C_s0r_dmso

6	-5.498314	1.103094	0.102229
6	-4.131234	1.300336	0.031291
6	-3.216744	0.220457	0.118064
6	-3.754590	-1.074612	0.278425
6	-5.126800	-1.285992	0.350308
6	-6.010338	-0.196465	0.263192
1	-6.189209	1.936403	0.035259
1	-3.747939	2.308629	-0.093657
1	-3.104051	-1.935371	0.347840
1	-5.497837	-2.295199	0.472693
6	-1.810403	0.545386	0.032351
1	-1.625956	1.608272	-0.105830
6	-0.681623	-0.225404	0.094044
6	0.668533	0.331915	-0.027031
6	2.905635	0.362400	-0.067350
6	2.700669	1.709239	-0.288337
6	4.210838	-0.324405	0.008188
6	4.346899	-1.618891	-0.524585
6	5.326990	0.275412	0.615252
6	5.570669	-2.285594	-0.469090
1	3.486255	-2.092810	-0.984308
6	6.552120	-0.393161	0.668787
1	5.233589	1.254467	1.071399
6	6.680370	-1.673635	0.124064
1	5.659348	-3.282390	-0.890538
1	7.402591	0.083806	1.146327
6	-0.712359	-1.642094	0.283604
7	-0.723310	-2.796764	0.437942
16	0.984921	2.038882	-0.304863

7	1.753267	-0.393525	0.064756
1	7.632792	-2.192895	0.167170
6	3.683069	2.811695	-0.540253
1	3.937102	3.347236	0.381751
1	4.606627	2.403642	-0.957404
1	3.282379	3.543028	-1.247361
8	-7.359365	-0.301054	0.323007
6	-7.943316	-1.600490	0.484812
1	-7.620579	-2.058067	1.425267
1	-9.019770	-1.437008	0.505384
1	-7.683930	-2.251298	-0.356114

Mol3b-C_s0r_mecn

6	-5.498120	1.103122	0.102216
6	-4.131003	1.300188	0.031401
6	-3.216616	0.220238	0.118076
6	-3.754616	-1.074766	0.278274
6	-5.126876	-1.285960	0.350039
6	-6.010283	-0.196375	0.262962
1	-6.188969	1.936475	0.035346
1	-3.747605	2.308481	-0.093341
1	-3.104146	-1.935566	0.347714
1	-5.498023	-2.295136	0.472406
6	-1.810179	0.545006	0.032520
1	-1.625584	1.607916	-0.105362
6	-0.681483	-0.225867	0.094068
6	0.668610	0.331620	-0.026761
6	2.905645	0.362473	-0.067008
6	2.700533	1.709318	-0.287898
6	4.210886	-0.324246	0.008332
6	4.346540	-1.619069	-0.523634
6	5.327377	0.275873	0.614446
6	5.570305	-2.285753	-0.468434
1	3.485446	-2.093365	-0.982096
6	6.552497	-0.392704	0.667715
1	5.234217	1.255136	1.070200
6	6.680378	-1.673479	0.123660
1	5.658633	-3.282895	-0.889134
1	7.403237	0.084450	1.144602
6	-0.712376	-1.642683	0.283046
7	-0.723854	-2.797401	0.436773
16	0.984731	2.038758	-0.304400
7	1.753412	-0.393604	0.064934
1	7.632781	-2.192794	0.166617
6	3.682808	2.811875	-0.539893
1	3.937140	3.347330	0.382098
1	4.606239	2.403897	-0.957406
1	3.281916	3.543309	-1.246799
8	-7.359370	-0.300837	0.322639
6	-7.943229	-1.600202	0.484630
1	-7.620324	-2.057724	1.425079
1	-9.019692	-1.436747	0.505346
1	-7.683987	-2.251123	-0.356286

Mol3b-C_s0r_meoh

6	-5.498034	1.103127	0.102285
6	-4.130904	1.300120	0.031509
6	-3.216559	0.220135	0.118114
6	-3.754624	-1.074845	0.278201
6	-5.126903	-1.285963	0.349931
6	-6.010263	-0.196347	0.262930
1	-6.188859	1.936504	0.035475
1	-3.747462	2.308413	-0.093144
1	-3.104187	-1.935671	0.347597
1	-5.498095	-2.295133	0.472228
6	-1.810083	0.544844	0.032620
1	-1.625439	1.607767	-0.105129
6	-0.681417	-0.226053	0.094097
6	0.668651	0.331500	-0.026658
6	2.905660	0.362501	-0.066894
6	2.700484	1.709342	-0.287765
6	4.210917	-0.324181	0.008381
6	4.346423	-1.619134	-0.523272
6	5.327528	0.276059	0.614142
6	5.570189	-2.285807	-0.468170
1	3.485164	-2.093575	-0.981262
6	6.552647	-0.392516	0.667322

1	5.234452	1.255403	1.069741
6	6.680395	-1.673407	0.123528
1	5.658389	-3.283082	-0.888581
1	7.403483	0.084714	1.143965
6	-0.712360	-1.642917	0.282860
7	-0.724059	-2.797652	0.436376
16	0.984662	2.038700	-0.304249
7	1.753479	-0.393636	0.065002
1	7.632793	-2.192741	0.166438
6	3.682701	2.811942	-0.539818
1	3.937077	3.347443	0.382141
1	4.606119	2.403980	-0.957380
1	3.281758	3.543346	-1.246733
8	-7.359366	-0.300739	0.322599
6	-7.943251	-1.600065	0.484515
1	-7.620348	-2.057669	1.424933
1	-9.019711	-1.436578	0.505259
1	-7.684051	-2.250958	-0.356445

Mol3b-C_s1r_dmso

6	5.352754	1.334056	-0.282056
6	3.998971	1.523274	-0.428998
6	3.061420	0.442160	-0.293581
6	3.612046	-0.845455	0.009372
6	4.976686	-1.036144	0.161560
6	5.863762	0.047885	0.015184
1	6.049430	2.158938	-0.389677
1	3.619742	2.515207	-0.656678
1	2.956683	-1.696411	0.137705
1	5.346873	-2.026427	0.396245
6	1.687374	0.720246	-0.431561
1	1.434447	1.766907	-0.578561
6	0.570431	-0.188702	-0.431553
6	-0.747284	0.289051	-0.230484
6	-2.975555	0.330098	-0.021663
6	-2.735864	1.699500	0.239604
6	-4.284753	-0.325234	-0.019305
6	-4.360646	-1.693961	0.319605
6	-5.471405	0.351708	-0.368176
6	-5.586046	-2.352400	0.338118
1	-3.448880	-2.219731	0.577584
6	-6.694425	-0.315547	-0.358671
1	-5.437440	1.385521	-0.686490
6	-6.759186	-1.665800	0.001628
1	-5.629687	-3.401078	0.614512
1	-7.597039	0.216316	-0.641673
6	0.687577	-1.574696	-0.683117
7	0.769896	-2.724608	-0.894974
16	-1.043571	2.025986	0.135867
7	-1.865803	-0.426433	-0.265662
1	-7.714506	-2.180817	0.013176
6	-3.689268	2.785832	0.614265
1	-4.106837	3.277221	-0.274654
1	-4.521651	2.386632	1.198412
1	-3.190254	3.557229	1.205968
8	7.208855	-0.037557	0.139119
6	7.796434	-1.308115	0.447135
1	7.577071	-2.037835	-0.338835
1	8.869593	-1.130407	0.497488
1	7.435402	-1.678524	1.412070

Mol3b-C_s1r_mecn

6	5.351916	1.334620	-0.278737
6	3.997850	1.522925	-0.424556
6	3.061353	0.440752	-0.291117
6	3.613272	-0.847047	0.008265
6	4.978233	-1.036850	0.159281
6	5.864225	0.048269	0.015200
1	6.047786	2.160391	-0.384740
1	3.617643	2.515078	-0.649679
1	2.958818	-1.699003	0.134461
1	5.349382	-2.027440	0.391145
6	1.686890	0.718189	-0.427564
1	1.433572	1.764983	-0.572820
6	0.570183	-0.190722	-0.427788
6	-0.747758	0.287711	-0.228732
6	-2.976200	0.330308	-0.021808

6	-2.736130	1.700138	0.237224
6	-4.285311	-0.324742	-0.019522
6	-4.360979	-1.693922	0.317990
6	-5.472304	0.352478	-0.367004
6	-5.586302	-2.352366	0.336641
1	-3.448951	-2.219883	0.574560
6	-6.695227	-0.314830	-0.357397
1	-5.438690	1.386532	-0.684488
6	-6.759696	-1.665457	0.001630
1	-5.629712	-3.401355	0.611871
1	-7.598046	0.217219	-0.639392
6	0.687072	-1.577286	-0.676358
7	0.768900	-2.727711	-0.885483
16	-1.043748	2.025832	0.134373
7	-1.866351	-0.427106	-0.263400
1	-7.714987	-2.180525	0.013240
6	-3.689233	2.787611	0.609561
1	-4.108010	3.276131	-0.280367
1	-4.520842	2.390264	1.196105
1	-3.189570	3.560941	1.198174
8	7.209592	-0.036207	0.138349
6	7.798252	-1.306820	0.443460
1	7.579314	-2.035146	-0.343953
1	8.871305	-1.128409	0.493902
1	7.437836	-1.679661	1.407720

Mol3b-C_s1r_meoh

6	5.351586	1.334855	-0.277150
6	3.997410	1.522830	-0.422450
6	3.061314	0.440229	-0.289933
6	3.613739	-0.847682	0.007860
6	4.978826	-1.037166	0.158333
6	5.864409	0.048384	0.015268
1	6.047147	2.160981	-0.382415
1	3.616815	2.515105	-0.646403
1	2.959629	-1.700031	0.133139
1	5.350354	-2.027909	0.388947
6	1.686700	0.717447	-0.425744
1	1.433235	1.764318	-0.570138
6	0.570070	-0.191420	-0.426197
6	-0.747952	0.287320	-0.228004
6	-2.976458	0.330477	-0.021928
6	-2.736295	1.700481	0.236242
6	-4.285529	-0.324516	-0.019624
6	-4.361053	-1.693789	0.317638
6	-5.472645	0.352663	-0.366874
6	-5.586314	-2.352302	0.336373
1	-3.448916	-2.219723	0.573849
6	-6.695495	-0.314734	-0.357206
1	-5.439180	1.386734	-0.684282
6	-6.759809	-1.665421	0.001649
1	-5.629597	-3.401352	0.611382
1	-7.598391	0.217265	-0.639052
6	0.686867	-1.578212	-0.673613
7	0.768532	-2.728820	-0.881733
16	-1.043849	2.025836	0.133864
7	-1.866585	-0.427282	-0.262530
1	-7.715055	-2.180570	0.013282
6	-3.689314	2.788395	0.607582
1	-4.108642	3.275659	-0.282775
1	-4.520574	2.391799	1.195147
1	-3.189419	3.562581	1.194865
8	7.209876	-0.035748	0.138036
6	7.798965	-1.306473	0.441656
1	7.580037	-2.034068	-0.346443
1	8.871986	-1.127817	0.492002
1	7.438922	-1.680440	1.405630

Mol3b-D_s0r_dmso

6	-4.589981	-1.982502	0.369735
6	-3.255234	-1.598201	0.301777
6	-2.867724	-0.250080	0.140233
6	-3.898527	0.718766	0.047868
6	-5.229212	0.349702	0.114353
6	-5.589934	-1.002544	0.275303
1	-4.837557	-3.028672	0.493906
1	-2.486490	-2.361670	0.375449

1	-3.660723	1.766441	-0.076668
1	-6.015684	1.093323	0.043182
6	-1.450345	0.020018	0.082393
1	-0.817738	-0.859318	0.169301
6	-0.743781	1.183700	-0.063891
6	0.724745	1.162112	-0.098034
6	2.803380	0.344616	-0.048361
6	3.136039	1.677754	-0.197122
6	3.747685	-0.787878	0.035667
6	3.416942	-2.015002	-0.566758
6	4.970830	-0.680479	0.718685
6	4.294112	-3.097491	-0.503746
1	2.469531	-2.108003	-1.086754
6	5.848608	-1.765188	0.780001
1	5.227108	0.242159	1.226948
6	5.516310	-2.976025	0.166578
1	4.025357	-4.035768	-0.979684
1	6.787133	-1.665505	1.316709
6	-1.352023	2.467403	-0.193522
7	-1.801736	3.537577	-0.302074
16	1.676557	2.630622	-0.259524
7	1.447160	0.076755	-0.006201
1	6.198903	-3.818786	0.215489
6	4.476514	2.330774	-0.345508
1	4.867045	2.680948	0.616940
1	5.196412	1.622301	-0.762084
1	4.422023	3.194397	-1.013702
8	-6.919000	-1.256268	0.327547
6	-7.354586	-2.612803	0.487073
1	-6.988904	-3.030510	1.430352
1	-8.442698	-2.571333	0.499991
1	-7.017587	-3.230578	-0.351264

Mol3b-D_s0r_mecn

6	-4.589981	-1.982502	0.369735
6	-3.255234	-1.598201	0.301777
6	-2.867724	-0.250080	0.140233
6	-3.898527	0.718766	0.047868
6	-5.229212	0.349702	0.114353
6	-5.589934	-1.002544	0.275303
1	-4.837557	-3.028672	0.493906
1	-2.486490	-2.361670	0.375449
1	-3.660723	1.766441	-0.076668
1	-6.015684	1.093323	0.043182
6	-1.450345	0.020018	0.082393
1	-0.817738	-0.859318	0.169301
6	-0.743781	1.183700	-0.063891
6	0.724745	1.162112	-0.098034
6	2.803380	0.344616	-0.048361
6	3.136039	1.677754	-0.197122
6	3.747685	-0.787878	0.035667
6	3.416942	-2.015002	-0.566758
6	4.970830	-0.680479	0.718685
6	4.294112	-3.097491	-0.503746
1	2.469531	-2.108003	-1.086754
6	5.848608	-1.765188	0.780001
1	5.227108	0.242159	1.226948
6	5.516310	-2.976025	0.166578
1	4.025357	-4.035768	-0.979684
1	6.787133	-1.665505	1.316709
6	-1.352023	2.467403	-0.193522
7	-1.801736	3.537577	-0.302074
16	1.676557	2.630622	-0.259524
7	1.447160	0.076755	-0.006201
1	6.198903	-3.818786	0.215489
6	4.476514	2.330774	-0.345508
1	4.867045	2.680948	0.616940
1	5.196412	1.622301	-0.762084
1	4.422023	3.194397	-1.013702
8	-6.919000	-1.256268	0.327547
6	-7.354586	-2.612803	0.487073
1	-6.988904	-3.030510	1.430352
1	-8.442698	-2.571333	0.499991
1	-7.017587	-3.230578	-0.351264

Mol3b-D_s0r_meoh

6	-4.589981	-1.982502	0.369735

6	-3.255234	-1.598201	0.301777
6	-2.867724	-0.250080	0.140233
6	-3.898527	0.718766	0.047868
6	-5.229212	0.349702	0.114353
6	-5.589934	-1.002544	0.275303
1	-4.837557	-3.028672	0.493906
1	-2.486490	-2.361670	0.375449
1	-3.660723	1.766441	-0.076668
1	-6.015684	1.093323	0.043182
6	-1.450345	0.020018	0.082393
1	-0.817738	-0.859318	0.169301
6	-0.743781	1.183700	-0.063891
6	0.724745	1.162112	-0.098034
6	2.803380	0.344616	-0.048361
6	3.136039	1.677754	-0.197122
6	3.747685	-0.787878	0.035667
6	3.416942	-2.015002	-0.566758
6	4.970830	-0.680479	0.718685
6	4.294112	-3.097491	-0.503746
1	2.469531	-2.108003	-1.086754
6	5.848608	-1.765188	0.780001
1	5.227108	0.242159	1.226948
6	5.516310	-2.976025	0.166578
1	4.025357	-4.035768	-0.979684
1	6.787133	-1.665505	1.316709
6	-1.352023	2.467403	-0.193522
7	-1.801736	3.537577	-0.302074
16	1.676557	2.630622	-0.259524
7	1.447160	0.076755	-0.006201
1	6.198903	-3.818786	0.215489
6	4.476514	2.330774	-0.345508
1	4.867045	2.680948	0.616940
1	5.196412	1.622301	-0.762084
1	4.422023	3.194397	-1.013702
8	-6.919000	-1.256268	0.327547
6	-7.354586	-2.612803	0.487073
1	-6.988904	-3.030510	1.430352
1	-8.442698	-2.571333	0.499991
1	-7.017587	-3.230578	-0.351264

Mol3b-D_s1r_dmso

6	-4.570564	-2.011921	0.363812
6	-3.236750	-1.656840	0.320330
6	-2.805545	-0.297482	0.152240
6	-3.844581	0.688606	0.029986
6	-5.176783	0.333965	0.073221
6	-5.562785	-1.013423	0.239743
1	-4.840904	-3.052504	0.492872
1	-2.480989	-2.430911	0.416934
1	-3.590055	1.731536	-0.100516
1	-5.953334	1.086342	-0.021187
6	-1.423128	-0.037373	0.113942
1	-0.763437	-0.892669	0.203994
6	-0.720127	1.210663	-0.026679
6	0.699148	1.183046	-0.061403
6	2.777624	0.348116	-0.020684
6	3.120736	1.710497	-0.175208
6	3.722509	-0.769215	0.045521
6	3.314530	-2.035867	-0.426241
6	5.015806	-0.635461	0.590606
6	4.182652	-3.122334	-0.381047
1	2.317007	-2.144162	-0.835911
6	5.877545	-1.729213	0.642604
1	5.336471	0.308886	1.011311
6	5.469390	-2.973792	0.151033
1	3.858816	-4.086451	-0.760242
1	6.865492	-1.612526	1.076318
6	-1.324703	2.481596	-0.124158
7	-1.761173	3.567493	-0.209381
16	1.684646	2.674981	-0.229440
7	1.441488	0.080943	0.026458
1	6.145110	-3.822314	0.188873
6	4.458144	2.349492	-0.344280
1	4.896732	2.620722	0.625339
1	5.150845	1.671455	-0.847642
1	4.380833	3.267616	-0.932108
8	-6.895684	-1.250453	0.269116
6	-7.357329	-2.597512	0.431036

1	-7.015066	-3.013933	1.383928
1	-8.444624	-2.537448	0.423902
1	-7.015030	-3.227385	-0.396409

Mol3b-D_s1r_mecn

6	-4.570249	-2.011897	0.363807
6	-3.236435	-1.656747	0.320407
6	-2.805345	-0.297417	0.152287
6	-3.844400	0.688597	0.029959
6	-5.176591	0.333879	0.073121
6	-5.562518	-1.013488	0.239648
1	-4.840556	-3.052488	0.492892
1	-2.480609	-2.430753	0.417105
1	-3.589873	1.731536	-0.100528
1	-5.953195	1.086186	-0.021350
6	-1.422939	-0.037151	0.114032
1	-0.763076	-0.892314	0.204213
6	-0.720213	1.210906	-0.026632
6	0.699124	1.183209	-0.061225
6	2.777547	0.348253	-0.020328
6	3.120719	1.710605	-0.174901
6	3.722297	-0.769134	0.045684
6	3.313842	-2.035823	-0.425577
6	5.015892	-0.635526	0.590140
6	4.181797	-3.122406	-0.380635
1	2.316041	-2.143980	-0.834599
6	5.877441	-1.729408	0.641943
1	5.336898	0.308821	1.010585
6	5.468824	-2.973995	0.150772
1	3.857586	-4.086549	-0.759445
1	6.865595	-1.612854	1.075227
6	-1.324943	2.481762	-0.124314
7	-1.761530	3.567588	-0.209728
16	1.684666	2.675167	-0.229226
7	1.441379	0.081103	0.026672
1	6.144399	-3.822643	0.188475
6	4.458152	2.349561	-0.344131
1	4.896802	2.621048	0.625401
1	5.150847	1.671436	-0.847391
1	4.380827	3.267557	-0.932171
8	-6.895439	-1.250644	0.268922
6	-7.356814	-2.597718	0.430798
1	-7.014554	-3.014112	1.383726
1	-8.444126	-2.537859	0.423579
1	-7.014335	-3.227542	-0.396633

Mol3b-D_s1r_meoh

6	-4.570129	-2.011888	0.363794
6	-3.236315	-1.656715	0.320421
6	-2.805268	-0.297396	0.152297
6	-3.844327	0.688593	0.029953
6	-5.176515	0.333849	0.073095
6	-5.562415	-1.013509	0.239617
1	-4.840426	-3.052482	0.492883
1	-2.480465	-2.430698	0.417143
1	-3.589797	1.731536	-0.100521
1	-5.953138	1.086132	-0.021389
6	-1.422866	-0.037071	0.114057
1	-0.762935	-0.892182	0.204284
6	-0.720248	1.210995	-0.026621
6	0.699115	1.183268	-0.061161
6	2.777516	0.348304	-0.020197
6	3.120710	1.710646	-0.174783
6	3.722216	-0.769103	0.045745
6	3.313579	-2.035807	-0.425322
6	5.015923	-0.635549	0.589962
6	4.181472	-3.122434	-0.380474
1	2.315673	-2.143912	-0.834096
6	5.877401	-1.729479	0.641692
1	5.337057	0.308798	1.010308
6	5.468608	-2.974072	0.150678
1	3.857117	-4.086587	-0.759134
1	6.865634	-1.612976	1.074814
6	-1.325041	2.481820	-0.124380
7	-1.761675	3.567617	-0.209878
16	1.684671	2.675236	-0.229155
7	1.441336	0.081161	0.026742

1	6.144128	-3.822767	0.188331
6	4.458153	2.349588	-0.344066
1	4.896824	2.621173	0.625434
1	5.150848	1.671430	-0.847287
1	4.380824	3.267536	-0.932187
8	-6.895345	-1.250712	0.268865
6	-7.356614	-2.597792	0.430715
1	-7.014350	-3.014184	1.383651
1	-8.443933	-2.538012	0.423470
1	-7.014071	-3.227591	-0.396717

Mol3c-A_s0r-s1v_dmso

6	-4.646861	1.247229	-0.000286
6	-3.268772	1.430266	-0.017166
6	-2.377491	0.334772	-0.007652
6	-2.924577	-0.966222	0.018353
6	-4.301064	-1.160907	0.035368
6	-5.150628	-0.052764	0.026219
1	-5.315091	2.100028	-0.007591
1	-2.870933	2.439990	-0.038203
1	-2.284509	-1.837038	0.024319
1	-4.707747	-2.165007	0.054982
6	-0.960036	0.651354	-0.027844
1	-0.760656	1.719399	-0.062109
6	0.151368	-0.139531	-0.009280
6	1.513511	0.401626	-0.042418
6	3.748959	0.387317	-0.013182
6	3.573378	1.753275	-0.124284
6	5.039740	-0.328064	0.038427
6	5.169766	-1.573213	-0.602242
6	6.147185	0.196201	0.725777
6	6.380695	-2.264467	-0.572521
1	4.315365	-1.988993	-1.125496
6	7.359411	-0.496908	0.753312
1	6.056627	1.133427	1.263096
6	7.482496	-1.727070	0.101967
1	6.465572	-3.221963	-1.077503
1	8.203519	-0.079151	1.293434
6	0.097654	-1.569405	0.047481
7	0.070554	-2.732334	0.093318
16	1.867161	2.117294	-0.163693
7	2.581008	-0.352198	0.019187
1	8.424983	-2.265361	0.124745
6	4.583183	2.852165	-0.250409
1	4.825196	3.292448	0.723659
1	5.508046	2.463890	-0.683222
1	4.214177	3.655154	-0.893890
35	-7.034787	-0.325306	0.050217

Mol3c-A_s0r-s1v_mecn

6	-4.646743	1.247283	0.000195
6	-3.268609	1.430361	-0.016639
6	-2.377325	0.334928	-0.007425
6	-2.924412	-0.966102	0.018249
6	-4.300852	-1.160809	0.035243
6	-5.150468	-0.052691	0.026434
1	-5.314947	2.100099	-0.006968
1	-2.870883	2.440144	-0.037417
1	-2.284231	-1.836844	0.024000
1	-4.707580	-2.164900	0.054541
6	-0.959817	0.651366	-0.027450
1	-0.760293	1.719409	-0.061380
6	0.151464	-0.139655	-0.009037
6	1.513606	0.401508	-0.042044
6	3.749031	0.387415	-0.012846
6	3.573374	1.753317	-0.124613
6	5.039794	-0.327988	0.038570
6	5.169258	-1.573570	-0.601305
6	6.147648	0.196510	0.725071
6	6.380099	-2.264946	-0.571806
1	4.314388	-1.989700	-1.123500
6	7.359779	-0.496747	0.752410
1	6.057459	1.133975	1.262030
6	7.482342	-1.727288	0.101721
1	6.464500	-3.222854	-1.076080
1	8.204200	-0.078852	1.291942

6	0.097478	-1.569569	0.047295
7	0.068968	-2.732467	0.092647
16	1.867115	2.117289	-0.162990
7	2.581140	-0.352156	0.019723
1	8.424735	-2.265752	0.124413
6	4.583041	2.852224	-0.251847
1	4.825752	3.292893	0.721884
1	5.507602	2.463842	-0.685208
1	4.213562	3.654976	-0.895369
35	-7.034600	-0.325257	0.049923

Mol3c-A_s0r-s1v_meoh

6	-4.646687	1.247309	0.000232
6	-3.268553	1.430386	-0.016557
6	-2.377263	0.334959	-0.007351
6	-2.924353	-0.966067	0.018270
6	-4.300797	-1.160768	0.035222
6	-5.150422	-0.052660	0.026420
1	-5.314902	2.100118	-0.006925
1	-2.870832	2.440176	-0.037290
1	-2.284158	-1.836802	0.024023
1	-4.707529	-2.164858	0.054486
6	-0.959742	0.651359	-0.027333
1	-0.760163	1.719398	-0.061213
6	0.151492	-0.139712	-0.008931
6	1.513634	0.401446	-0.041925
6	3.749039	0.387409	-0.012773
6	3.573369	1.753302	-0.124627
6	5.039805	-0.327979	0.038585
6	5.169119	-1.573698	-0.601028
6	6.147776	0.196644	0.724788
6	6.379952	-2.265076	-0.571593
1	4.314102	-1.989979	-1.122854
6	7.359898	-0.496620	0.752068
1	6.057676	1.134205	1.261598
6	7.482323	-1.727292	0.101614
1	6.464224	-3.223125	-1.075619
1	8.204413	-0.078646	1.291394
6	0.097390	-1.569638	0.047314
7	0.068387	-2.732521	0.092546
16	1.867102	2.117256	-0.162892
7	2.581173	-0.352180	0.019836
1	8.424702	-2.265783	0.124283
6	4.583025	2.852206	-0.252021
1	4.825818	3.292971	0.721652
1	5.507549	2.463777	-0.685418
1	4.213512	3.654904	-0.895595
35	-7.034543	-0.325217	0.049853

Mol3c-A_s1r-s0v_dmso

6	-4.610685	1.267495	-0.076776
6	-3.241195	1.443442	-0.095575
6	-2.332466	0.336156	-0.026220
6	-2.912984	-0.970421	0.065472
6	-4.286976	-1.146708	0.084242
6	-5.133532	-0.033352	0.013146
1	-5.274767	2.122692	-0.130559
1	-2.836317	2.448776	-0.165113
1	-2.280130	-1.845070	0.122123
1	-4.703990	-2.145164	0.154214
6	-0.948164	0.611851	-0.050224
1	-0.700402	1.666504	-0.116761
6	0.175839	-0.268294	-0.006602
6	1.501138	0.257922	-0.023708
6	3.738560	0.357058	0.009224
6	3.487061	1.752408	-0.055835
6	5.043635	-0.285171	0.030397
6	5.140906	-1.634591	-0.391360
6	6.216134	0.369476	0.474727
6	6.366498	-2.287169	-0.399841
1	4.243000	-2.142099	-0.721329
6	7.437271	-0.294984	0.475056
1	6.169910	1.378943	0.858156
6	7.521534	-1.620647	0.030728
1	6.427286	-3.315588	-0.740294
1	8.325353	0.216390	0.831031
6	0.098998	-1.678086	0.048149

7	0.075906	-2.849004	0.091925
16	1.790988	2.039895	-0.086108
7	2.620403	-0.437981	0.008986
1	8.478437	-2.132356	0.027383
6	4.435581	2.900883	-0.154734
1	4.824754	3.181051	0.832650
1	5.286424	2.649083	-0.792677
1	3.941112	3.781022	-0.571048
35	-7.017530	-0.284492	0.039485

Mol3c-A_s1r-s0v_mecn

6	-4.610128	1.267533	-0.076641
6	-3.240564	1.443014	-0.095301
6	-2.332233	0.335512	-0.026078
6	-2.913076	-0.970826	0.065339
6	-4.287158	-1.146690	0.083970
6	-5.133382	-0.033142	0.012995
1	-5.273968	2.122927	-0.130308
1	-2.835377	2.448260	-0.164625
1	-2.280416	-1.845624	0.121886
1	-4.704478	-2.145029	0.153781
6	-0.947693	0.610735	-0.049959
1	-0.699708	1.665365	-0.116320
6	0.175993	-0.269462	-0.006521
6	1.501330	0.257187	-0.023610
6	3.738696	0.357507	0.009218
6	3.486797	1.752722	-0.055446
6	5.043687	-0.284574	0.030282
6	5.140193	-1.634905	-0.389018
6	6.216887	0.370651	0.472206
6	6.365629	-2.287657	-0.397779
1	4.241657	-2.142864	-0.716516
6	7.437824	-0.294020	0.472308
1	6.171302	1.380768	0.853966
6	7.521285	-1.620528	0.030195
1	6.425803	-3.316760	-0.736241
1	8.326432	0.217714	0.826455
6	0.099141	-1.679284	0.048063
7	0.075938	-2.850174	0.091634
16	1.790529	2.039520	-0.085563
7	2.620727	-0.438071	0.008724
1	8.478079	-2.132442	0.026723
6	4.434772	2.901753	-0.153952
1	4.824276	3.181566	0.833418
1	5.285430	2.650936	-0.792540
1	3.939677	3.781922	-0.569494
35	-7.017481	-0.283842	0.039276

Mol3c-A_s1r-s0v_meoh

6	-4.610156	1.267561	-0.076199
6	-3.240593	1.443279	-0.094968
6	-2.332133	0.335911	-0.026236
6	-2.912727	-0.970534	0.064820
6	-4.286797	-1.146653	0.083581
6	-5.133177	-0.033208	0.013095
1	-5.274126	2.122877	-0.129528
1	-2.835605	2.448622	-0.164017
1	-2.279913	-1.845256	0.120998
1	-4.703924	-2.145093	0.153095
6	-0.947563	0.611242	-0.050145
1	-0.699676	1.665913	-0.116129
6	0.175988	-0.269069	-0.007111
6	1.501503	0.257341	-0.023941
6	3.739000	0.357897	0.008974
6	3.486856	1.753121	-0.054925
6	5.043649	-0.284569	0.030233
6	5.139034	-1.636196	-0.385521
6	6.217958	0.371187	0.468692
6	6.364063	-2.289619	-0.394103
1	4.239818	-2.144518	-0.710499
6	7.438492	-0.294124	0.468898
1	6.173695	1.382370	0.847646
6	7.520678	-1.621933	0.030407
1	6.423224	-3.319694	-0.729771
1	8.327883	0.218140	0.820292
6	0.099052	-1.678868	0.046936
7	0.075438	-2.849787	0.090087

16	1.790653	2.039980	-0.084869
7	2.620761	-0.437693	0.007953
1	8.477209	-2.134331	0.027030
6	4.434400	2.902621	-0.152744
1	4.826767	3.179431	0.834309
1	5.283199	2.653955	-0.794681
1	3.937954	3.783932	-0.564170
35	-7.017300	-0.284171	0.039388

Mol3c-B_s0r-s1v_dmso

6	-3.919958	-1.571211	0.088994
6	-2.557531	-1.293140	0.077737
6	-2.074586	0.032464	0.015712
6	-3.018027	1.081532	-0.036385
6	-4.382322	0.815356	-0.025580
6	-4.821758	-0.508882	0.037316
1	-4.272068	-2.594758	0.137098
1	-1.849836	-2.115200	0.118138
1	-2.698574	2.113206	-0.086706
1	-5.095832	1.629787	-0.066127
6	-0.632741	0.197825	0.009687
1	-0.069138	-0.730306	0.041489
6	0.153299	1.312980	-0.028085
6	1.617982	1.193065	-0.030220
6	3.629686	0.226269	-0.001414
6	4.057184	1.541699	-0.038731
6	4.491146	-0.973198	0.013048
6	4.092092	-2.123282	-0.691195
6	5.700006	-1.005376	0.728154
6	4.890208	-3.266964	-0.694904
1	3.154806	-2.108239	-1.237020
6	6.498345	-2.151387	0.722723
1	6.006141	-0.145184	1.312558
6	6.099398	-3.284536	0.008903
1	4.570108	-4.144262	-1.248904
1	7.426832	-2.160400	1.285372
6	-0.360320	2.645779	-0.066587
7	-0.727912	3.750796	-0.097489
16	2.671533	2.596843	-0.056543
7	2.259183	0.054381	-0.008535
1	6.720503	-4.174901	0.005782
6	5.443665	2.105725	-0.102074
1	5.831751	2.339606	0.895888
1	6.121904	1.385751	-0.566076
1	5.467955	3.026668	-0.690469
35	-6.691788	-0.867309	0.052093

Mol3c-B_s0r-s1v_mecn

6	-3.919958	-1.571211	0.088994
6	-2.557531	-1.293140	0.077737
6	-2.074586	0.032464	0.015712
6	-3.018027	1.081532	-0.036385
6	-4.382322	0.815356	-0.025580
6	-4.821758	-0.508882	0.037316
1	-4.272068	-2.594758	0.137098
1	-1.849836	-2.115200	0.118138
1	-2.698574	2.113206	-0.086706
1	-5.095832	1.629787	-0.066127
6	-0.632741	0.197825	0.009687
1	-0.069138	-0.730306	0.041489
6	0.153299	1.312980	-0.028085
6	1.617982	1.193065	-0.030220
6	3.629686	0.226269	-0.001414
6	4.057184	1.541699	-0.038731
6	4.491146	-0.973198	0.013048
6	4.092092	-2.123282	-0.691195
6	5.700006	-1.005376	0.728154
6	4.890208	-3.266964	-0.694904
1	3.154806	-2.108239	-1.237020
6	6.498345	-2.151387	0.722723
1	6.006141	-0.145184	1.312558
6	6.099398	-3.284536	0.008903
1	4.570108	-4.144262	-1.248904
1	7.426832	-2.160400	1.285372
6	-0.360320	2.645779	-0.066587
7	-0.727912	3.750796	-0.097489
16	2.671533	2.596843	-0.056543

7	2.259183	0.054381	-0.008535
1	6.720503	-4.174901	0.005782
6	5.443665	2.105725	-0.102074
1	5.831751	2.339606	0.895888
1	6.121904	1.385751	-0.566076
1	5.467955	3.026668	-0.690469
35	-6.691788	-0.867309	0.052093

Mol3c-B_s0r-s1v_meoh

6	-3.919958	-1.571211	0.088994
6	-2.557531	-1.293140	0.077737
6	-2.074586	0.032464	0.015712
6	-3.018027	1.081532	-0.036385
6	-4.382322	0.815356	-0.025580
6	-4.821758	-0.508882	0.037316
1	-4.272068	-2.594758	0.137098
1	-1.849836	-2.115200	0.118138
1	-2.698574	2.113206	-0.086706
1	-5.095832	1.629787	-0.066127
6	-0.632741	0.197825	0.009687
1	-0.069138	-0.730306	0.041489
6	0.153299	1.312980	-0.028085
6	1.617982	1.193065	-0.030220
6	3.629686	0.226269	-0.001414
6	4.057184	1.541699	-0.038731
6	4.491146	-0.973198	0.013048
6	4.092092	-2.123282	-0.691195
6	5.700006	-1.005376	0.728154
6	4.890208	-3.266964	-0.694904
1	3.154806	-2.108239	-1.237020
6	6.498345	-2.151387	0.722723
1	6.006141	-0.145184	1.312558
6	6.099398	-3.284536	0.008903
1	4.570108	-4.144262	-1.248904
1	7.426832	-2.160400	1.285372
6	-0.360320	2.645779	-0.066587
7	-0.727912	3.750796	-0.097489
16	2.671533	2.596843	-0.056543
7	2.259183	0.054381	-0.008535
1	6.720503	-4.174901	0.005782
6	5.443665	2.105725	-0.102074
1	5.831751	2.339606	0.895888
1	6.121904	1.385751	-0.566076
1	5.467955	3.026668	-0.690469
35	-6.691788	-0.867309	0.052093

Mol3c-B_s1r-s0v_dmso

6	-3.904314	-1.581321	0.042126
6	-2.546273	-1.334681	0.034401
6	-2.017028	-0.000363	0.010173
6	-2.969187	1.072488	-0.004868
6	-4.331203	0.824179	0.002964
6	-4.798674	-0.496764	0.026761
1	-4.277989	-2.598829	0.060432
1	-1.853279	-2.170714	0.046997
1	-2.632079	2.099862	-0.022891
1	-5.033333	1.650384	-0.008890
6	-0.617374	0.156817	0.002650
1	-0.028674	-0.753703	0.015113
6	0.178296	1.345017	-0.016578
6	1.599349	1.200034	-0.018026
6	3.605802	0.206815	0.009016
6	4.054220	1.551485	-0.036419
6	4.446854	-0.983316	0.018504
6	3.901594	-2.201874	-0.453427
6	5.773803	-0.980885	0.504987
6	4.666353	-3.361610	-0.467679
1	2.881197	-2.209142	-0.816828
6	6.529432	-2.148768	0.498574
1	6.201847	-0.082079	0.926934
6	5.984976	-3.341049	0.005620
1	4.239019	-4.284367	-0.846466
1	7.542069	-2.133614	0.887785
6	-0.316657	2.665113	-0.033877
7	-0.657681	3.787613	-0.049165
16	2.700398	2.621865	-0.053972
7	2.247175	0.046992	0.002711

1	6.580752	-4.248037	-0.002281
6	5.437457	2.103078	-0.119109
1	5.892683	2.180324	0.877085
1	6.076393	1.462486	-0.731601
1	5.432845	3.105603	-0.552396
35	-6.669110	-0.827903	0.037743

molG3c-B_s1r-s0v_mecn

6	-3.904165	-1.581280	0.042773
6	-2.546151	-1.334555	0.035189
6	-2.017010	-0.000279	0.010415
6	-2.969097	1.072494	-0.005341
6	-4.331152	0.824099	0.002339
6	-4.798573	-0.496771	0.026698
1	-4.277860	-2.598774	0.061523
1	-1.853083	-2.170529	0.048353
1	-2.631979	2.099861	-0.023813
1	-5.033294	1.650289	-0.010063
6	-0.617273	0.157063	0.003062
1	-0.028456	-0.753392	0.016037
6	0.178171	1.345157	-0.016435
6	1.599404	1.199861	-0.017906
6	3.605926	0.206794	0.008981
6	4.054327	1.551383	-0.036168
6	4.446743	-0.983340	0.018393
6	3.900799	-2.202143	-0.452310
6	5.774217	-0.980937	0.503630
6	4.665363	-3.361950	-0.466745
1	2.879999	-2.209364	-0.814540
6	6.529619	-2.148900	0.497074
1	6.202769	-0.082003	0.924781
6	5.984465	-3.341354	0.005228
1	4.237501	-4.284852	-0.844575
1	7.542613	-2.133776	0.885363
6	-0.316632	2.665296	-0.033875
7	-0.657339	3.787885	-0.049259
16	2.700519	2.621854	-0.053535
7	2.247125	0.046981	0.002526
1	6.580069	-4.248456	-0.002751
6	5.437565	2.103143	-0.118893
1	5.892944	2.180467	0.877235
1	6.076551	1.462769	-0.731566
1	5.432725	3.105693	-0.552156
35	-6.669045	-0.827838	0.037520

Mol3c-B_s1r-s0v_meoh

6	-3.904105	-1.581220	0.043047
6	-2.546091	-1.334462	0.035513
6	-2.016995	-0.000208	0.010517
6	-2.969071	1.072539	-0.005519
6	-4.331129	0.824119	0.002108
6	-4.798528	-0.496740	0.026693
1	-4.277798	-2.598713	0.061972
1	-1.852998	-2.170416	0.048899
1	-2.631950	2.099901	-0.024173
1	-5.033290	1.650290	-0.010515
6	-0.617224	0.157189	0.003215
1	-0.028375	-0.753246	0.016372
6	0.178145	1.345251	-0.016387
6	1.599435	1.199849	-0.017869
6	3.605952	0.206783	0.008985
6	4.054377	1.551336	-0.036086
6	4.446675	-0.983372	0.018369
6	3.900496	-2.202223	-0.451996
6	5.774304	-0.981028	0.503248
6	4.664974	-3.362069	-0.466524
1	2.879572	-2.209386	-0.813867
6	6.529607	-2.149032	0.496615
1	6.203017	-0.082083	0.924208
6	5.984217	-3.341507	0.005053
1	4.236934	-4.284993	-0.844096
1	7.542704	-2.133961	0.884640
6	-0.316588	2.665412	-0.033887
7	-0.657195	3.788028	-0.049335
16	2.700581	2.621858	-0.053373
7	2.247098	0.046993	0.002485
1	6.579751	-4.248655	-0.002982

6	5.437619	2.103131	-0.118831
1	5.893088	2.180406	0.877265
1	6.076593	1.462859	-0.731626
1	5.432711	3.105720	-0.552018
35	-6.669000	-0.827860	0.037436

GS and ES optimized geometries (S_0) for compounds 6, 7 and 8

Mol6a-A_s0_acn.out

6	-6.101760	-2.925447	-0.691704
6	-4.865766	-2.297878	-0.752680
6	-4.654042	-1.030748	-0.164689
6	-5.732923	-0.412376	0.504046
6	-6.972018	-1.032957	0.572991
6	-7.164255	-2.290985	-0.026319
1	-6.248660	-3.896102	-1.150681
1	-4.046004	-2.790075	-1.265515
1	-5.612751	0.551157	0.977617
1	-7.792861	-0.549763	1.090192
6	-3.317860	-0.471242	-0.298232
1	-2.618769	-1.144820	-0.786502
6	-2.799968	0.735467	0.067197
6	-1.396693	1.098621	-0.157734
6	0.420027	2.395204	-0.176435
6	0.991918	1.242294	-0.676449
6	1.104841	3.680457	0.066185
6	0.833215	4.398420	1.243442
6	2.014657	4.212530	-0.861667
6	1.476692	5.609362	1.496271
1	0.122255	3.995987	1.957226
6	2.658966	5.424989	-0.605443
1	2.194184	3.699025	-1.800692
6	2.395590	6.124222	0.575012
1	1.263308	6.150673	2.412779
1	3.356169	5.826658	-1.333997
6	-8.445159	-2.926755	0.044449
7	-9.486867	-3.443699	0.101454
6	-3.571517	1.769202	0.691341
7	-4.184804	2.618602	1.197624
16	-0.207484	-0.015389	-0.806016
7	-0.922937	2.287684	0.119899
1	2.895481	7.067258	0.772821
6	2.410750	0.982676	-1.046216
1	2.548281	0.852229	-2.123007
1	3.050082	1.798311	-0.706461
8	2.821374	-0.248380	-0.383719
6	4.057469	-0.682805	-0.658035
8	4.838696	-0.116323	-1.399468
6	4.348683	-1.971737	0.080439
1	4.220253	-1.792680	1.153762
1	3.599473	-2.715661	-0.212967
7	5.692082	-2.406032	-0.236331
1	6.233678	-1.832410	-0.869429
6	6.284490	-3.520902	0.252117
8	7.427876	-3.880174	-0.022271
8	5.457225	-4.194759	1.084186
6	5.990895	-5.402912	1.662280
1	6.251467	-6.116575	0.878395
1	6.871920	-5.178277	2.266527
1	5.191168	-5.797705	2.286839

Mol6a-A_s0_chl.out

6	-6.046854	-2.956474	-0.698685
6	-4.817887	-2.315079	-0.753643
6	-4.624859	-1.041031	-0.174123
6	-5.717804	-0.429501	0.477914
6	-6.950244	-1.064319	0.539939
6	-7.123445	-2.329822	-0.048783
1	-6.178894	-3.932625	-1.150723
1	-3.987865	-2.802244	-1.255158
1	-5.613504	0.540593	0.941872
1	-7.782029	-0.585739	1.043971
6	-3.293477	-0.467713	-0.298326
1	-2.584668	-1.132360	-0.785490
6	-2.788617	0.742053	0.074938
6	-1.386589	1.115481	-0.139260
6	0.417499	2.428700	-0.165726

6	1.009160	1.267943	-0.624216
6	1.084067	3.727098	0.051595
6	0.747612	4.496390	1.178512
6	2.039635	4.222313	-0.850290
6	1.374513	5.719592	1.410300
1	-0.003421	4.124554	1.867035
6	2.666884	5.447522	-0.615091
1	2.267536	3.671268	-1.757026
6	2.340394	6.196691	0.517616
1	1.109812	6.301272	2.287840
1	3.399624	5.820299	-1.323896
6	-8.397147	-2.981063	0.016100
7	-9.432000	-3.511664	0.067989
6	-3.574529	1.765493	0.698667
7	-4.206073	2.599414	1.207663
16	-0.174923	-0.006014	-0.737321
7	-0.928278	2.314046	0.114183
1	2.826744	7.150052	0.699093
6	2.436178	1.013933	-0.967280
1	2.602446	0.923417	-2.044693
1	3.070053	1.814415	-0.582742
8	2.824698	-0.241779	-0.342350
6	4.065814	-0.673562	-0.609481
8	4.859454	-0.087777	-1.320017
6	4.339476	-1.984647	0.096044
1	4.207529	-1.831055	1.173406
1	3.581804	-2.712206	-0.216695
7	5.677629	-2.427099	-0.227112
1	6.235591	-1.837774	-0.830861
6	6.254809	-3.562980	0.236286
8	7.394196	-3.927657	-0.034026
8	5.406883	-4.250440	1.040170
6	5.925091	-5.477822	1.589060
1	6.189266	-6.171256	0.788253
1	6.803384	-5.277694	2.205915
1	5.116473	-5.883537	2.195350

Mol6a-A_s0_dmso.out

6	-6.102705	-2.925208	-0.691524
6	-4.866555	-2.297935	-0.752596
6	-4.654468	-1.030973	-0.164381
6	-5.733030	-0.412501	0.504782
6	-6.972260	-1.032774	0.573867
6	-7.164881	-2.290602	-0.025767
1	-6.249900	-3.895727	-1.150688
1	-4.047005	-2.790216	-1.265670
1	-5.612491	0.550817	0.978697
1	-7.792851	-0.549544	1.091427
6	-3.318194	-0.471729	-0.298051
1	-2.619131	-1.145632	-0.785894
6	-2.800260	0.735136	0.066818
6	-1.396929	1.098144	-0.158056
6	0.419934	2.394557	-0.176453
6	0.991577	1.241815	-0.677049
6	1.104989	3.679629	0.066674
6	0.835044	4.396199	1.245175
6	2.013354	4.212871	-0.861928
6	1.478636	5.607019	1.498397
1	0.125438	3.992722	1.959734
6	2.657801	5.425197	-0.605310
1	2.191726	3.700317	-1.801688
6	2.396020	6.123107	0.576293
1	1.266624	6.147219	2.415880
1	3.353896	5.827767	-1.334424
6	-8.445938	-2.926026	0.045133
7	-9.487811	-3.442642	0.102247
6	-3.571793	1.769362	0.690137
7	-4.184717	2.619517	1.195620
16	-0.207990	-0.015653	-0.806943
7	-0.923027	2.287127	0.119990
1	2.896032	7.066014	0.774411
6	2.410278	0.982285	-1.047350
1	2.547086	0.850629	-2.124064
1	3.049488	1.798568	-0.708939
8	2.821783	-0.247787	-0.383576
6	4.057156	-0.683088	-0.659280
8	4.837603	-0.117831	-1.402571
6	4.348844	-1.971470	0.079942

1	4.221010	-1.791827	1.153195
1	3.599565	-2.715617	-0.212756
7	5.692215	-2.405748	-0.237161
1	6.232394	-1.833832	-0.873004
6	6.285098	-3.520035	0.251806
8	7.428101	-3.879861	-0.024032
8	5.459269	-4.192549	1.086211
6	5.993637	-5.399939	1.665364
1	6.252919	-6.114827	0.882180
1	6.875482	-5.174466	2.268085
1	5.194741	-5.793693	2.291616

Mol6a-A_s0_H2O.out

6	-6.104121	-2.924767	-0.690881
6	-4.867804	-2.297812	-0.752180
6	-4.655365	-1.030861	-0.164076
6	-5.733646	-0.412044	0.505238
6	-6.973020	-1.031961	0.574574
6	-7.165995	-2.289787	-0.025001
1	-6.251598	-3.895278	-1.149960
1	-4.048454	-2.790317	-1.265325
1	-5.612778	0.551234	0.979156
1	-7.793394	-0.548497	1.092252
6	-3.318985	-0.472002	-0.298008
1	-2.620125	-1.146249	-0.785636
6	-2.800742	0.734848	0.066484
6	-1.397340	1.097535	-0.158530
6	0.419884	2.393500	-0.176588
6	0.990942	1.241016	-0.678377
6	1.105483	3.678170	0.067362
6	0.838063	4.392708	1.247682
6	2.011860	4.213020	-0.862268
6	1.482046	5.603214	1.501571
1	0.130306	3.987818	1.963295
6	2.656725	5.425006	-0.604985
1	2.188435	3.701910	-1.803150
6	2.397364	6.120967	0.578323
1	1.272069	6.141781	2.420483
1	3.351300	5.828812	-1.334863
6	-8.447219	-2.924809	0.046144
7	-9.489291	-3.441028	0.103507
6	-3.571904	1.769545	0.689440
7	-4.184087	2.620551	1.194436
16	-0.209034	-0.015972	-0.808729
7	-0.923016	2.286300	0.120230
1	2.897729	7.063578	0.776953
6	2.409363	0.981461	-1.049616
1	2.545034	0.847939	-2.126207
1	3.048567	1.798553	-0.713204
8	2.822063	-0.247299	-0.383986
6	4.056468	-0.683760	-0.661565
8	4.835746	-0.120288	-1.407548
6	4.348995	-1.971124	0.079094
1	4.222732	-1.790074	1.152255
1	3.599274	-2.715560	-0.211735
7	5.691989	-2.405899	-0.239186
1	6.230561	-1.835815	-0.878034
6	6.285964	-3.518736	0.251428
8	7.428607	-3.879042	-0.025982
8	5.462263	-4.189224	1.089317
6	5.997912	-5.395003	1.670764
1	6.255644	-6.112030	0.889028
1	6.880843	-5.167751	2.271234
1	5.200269	-5.787087	2.299636

Mol6a-A_s0_meoh.out

6	-6.100807	-2.925755	-0.692671
6	-4.864936	-2.297934	-0.753511
6	-4.653331	-1.031054	-0.164937
6	-5.732234	-0.413216	0.504260
6	-6.971202	-1.034058	0.573068
6	-7.163327	-2.291822	-0.026822
1	-6.247610	-3.896212	-1.152104
1	-4.045156	-2.789751	-1.266695
1	-5.612161	0.550103	0.978300
1	-7.792064	-0.551264	1.090616
6	-3.317268	-0.471240	-0.298345

1	-2.618025	-1.144525	-0.786812
6	-2.799655	0.735495	0.067378
6	-1.396427	1.098938	-0.157322
6	0.419948	2.395977	-0.176158
6	0.992342	1.242924	-0.675290
6	1.104330	3.681547	0.065958
6	0.831568	4.400450	1.242372
6	2.014831	4.213006	-0.861571
6	1.474658	5.611683	1.494744
1	0.119971	3.998543	1.955813
6	2.658741	5.425767	-0.605806
1	2.195179	3.698802	-1.800056
6	2.394270	6.125913	0.573854
1	1.260382	6.153741	2.410602
1	3.356475	5.826962	-1.334113
6	-8.444099	-2.927879	0.043847
7	-9.485689	-3.445059	0.100773
6	-3.571552	1.768954	0.691557
7	-4.185261	2.617979	1.197945
16	-0.206673	-0.015169	-0.804554
7	-0.923065	2.288233	0.119831
1	2.893838	7.069196	0.771307
6	2.411357	0.983508	-1.044516
1	2.549486	0.853809	-2.121329
1	3.050531	1.798918	-0.703884
8	2.821611	-0.247978	-0.382651
6	4.057485	-0.682832	-0.657458
8	4.838755	-0.116375	-1.398840
6	4.348252	-1.972271	0.080306
1	4.219858	-1.793816	1.153725
1	3.598723	-2.715738	-0.213510
7	5.691471	-2.406882	-0.236695
1	6.233064	-1.833454	-0.869974
6	6.283739	-3.521894	0.251707
8	7.426937	-3.881475	-0.022852
8	5.456403	-4.195507	1.083988
6	5.990046	-5.403692	1.662016
1	6.250602	-6.117318	0.878092
1	6.871118	-5.179121	2.266207
1	5.190331	-5.798488	2.286586

Mol6a-B_s0_acn.out

6	-7.336794	-0.192122	0.787742
6	-6.023321	0.214163	0.599857
6	-5.046732	-0.667687	0.085221
6	-5.436280	-1.986223	-0.237406
6	-6.746836	-2.402553	-0.053360
6	-7.704006	-1.508171	0.460026
1	-8.074104	0.496609	1.183445
1	-5.739906	1.230334	0.853090
1	-4.722469	-2.694794	-0.632712
1	-7.035122	-3.416856	-0.304093
6	-3.705733	-0.128039	-0.066358
1	-3.594679	0.907657	0.241234
6	-2.552109	-0.689928	-0.528268
6	-1.310708	0.096112	-0.569000
6	0.052150	1.839966	-0.311275
6	0.970534	0.944200	-0.827584
6	0.321490	3.235195	0.090139
6	-0.232759	3.732846	1.281842
6	1.110207	4.085511	-0.701467
6	0.016811	5.044911	1.682741
1	-0.850859	3.081630	1.890793
6	1.359568	5.398981	-0.297335
1	1.501453	3.733496	-1.650492
6	0.817802	5.880913	0.896871
1	-0.411164	5.414971	2.609274
1	1.966933	6.046515	-0.921854
6	-9.055504	-1.941339	0.648987
7	-10.154570	-2.293614	0.802688
6	-2.450171	-2.037649	-0.994659
7	-2.312433	-3.125909	-1.385182
16	0.193057	-0.574270	-1.169768
7	-1.222445	1.338090	-0.165523
1	1.010952	6.902240	1.209804
6	2.431180	1.124341	-1.052783
1	2.701129	1.107025	-2.112044
1	2.773445	2.063803	-0.617740

8	3.118453	0.021008	-0.391867
6	4.445878	-0.030650	-0.552846
8	5.095829	0.776234	-1.191558
6	5.026362	-1.228267	0.168581
1	4.762917	-1.154454	1.229655
1	4.545164	-2.132906	-0.219775
7	6.459482	-1.252342	-0.029833
1	6.867774	-0.517289	-0.592140
6	7.299414	-2.184114	0.478702
8	8.516264	-2.196239	0.302736
8	6.629936	-3.105660	1.208966
6	7.432653	-4.147898	1.798842
1	7.941346	-4.721725	1.021856
1	8.166938	-3.720503	2.484321
1	6.728675	-4.778752	2.339152

Mol6a-B_s0_chl.out

6	-7.344581	-0.186667	0.770298
6	-6.030691	0.219038	0.584820
6	-5.050401	-0.666192	0.083253
6	-5.437940	-1.987875	-0.228800
6	-6.749330	-2.402993	-0.047039
6	-7.710337	-1.505743	0.453471
1	-8.084953	0.504650	1.155962
1	-5.749006	1.237968	0.829599
1	-4.721380	-2.699282	-0.614228
1	-7.036006	-3.419784	-0.289811
6	-3.708834	-0.127445	-0.066718
1	-3.597929	0.911214	0.231334
6	-2.553505	-0.694234	-0.517921
6	-1.312085	0.091343	-0.559121
6	0.049169	1.836934	-0.308736
6	0.968669	0.938238	-0.818876
6	0.317829	3.233658	0.086609
6	-0.248463	3.739722	1.268790
6	1.118299	4.077224	-0.700101
6	0.001565	5.052545	1.665679
1	-0.877063	3.093628	1.872300
6	1.368037	5.391615	-0.300103
1	1.517889	3.719564	-1.643577
6	0.814768	5.881353	0.885238
1	-0.435919	5.429219	2.585102
1	1.984581	6.033896	-0.921070
6	-9.062712	-1.937887	0.640460
7	-10.162253	-2.288540	0.792902
6	-2.450672	-2.045920	-0.973013
7	-2.314785	-3.137754	-1.353876
16	0.193107	-0.582793	-1.153254
7	-1.224884	1.334916	-0.161429
1	1.008265	6.903495	1.195259
6	2.429698	1.118503	-1.043139
1	2.699131	1.119593	-2.103164
1	2.774281	2.050815	-0.594233
8	3.116144	0.003597	-0.403799
6	4.448065	-0.029174	-0.549217
8	5.094385	0.800808	-1.159300
6	5.032990	-1.238049	0.149562
1	4.749398	-1.197822	1.207468
1	4.569309	-2.138343	-0.270091
7	6.468578	-1.237951	-0.024481
1	6.877369	-0.485493	-0.562814
6	7.314062	-2.169398	0.480656
8	8.531296	-2.163033	0.328899
8	6.640005	-3.115243	1.179574
6	7.449120	-4.155271	1.762341
1	7.987073	-4.699983	0.984068
1	8.161596	-3.730307	2.472096
1	6.746102	-4.812024	2.272714

Mol6a-B_s0_dmso.out

6	-7.336475	-0.191517	0.788865
6	-6.022951	0.214525	0.600789
6	-5.046750	-0.667361	0.085490
6	-5.436679	-1.985659	-0.237626
6	-6.747272	-2.401777	-0.053394
6	-7.704054	-1.507344	0.460649
1	-8.073490	0.497233	1.185074

1	-5.739215	1.230510	0.854369
1	-4.723160	-2.694228	-0.633449
1	-7.035874	-3.415891	-0.304524
6	-3.705698	-0.127905	-0.066327
1	-3.594439	0.907668	0.241584
6	-2.552290	-0.689833	-0.528744
6	-1.310767	0.096026	-0.569668
6	0.052478	1.839562	-0.311725
6	0.970481	0.943943	-0.828946
6	0.322166	3.234568	0.090261
6	-0.231216	3.731612	1.282643
6	1.110332	4.085290	-0.701469
6	0.018625	5.043484	1.684040
1	-0.848820	3.080092	1.891775
6	1.359976	5.398563	-0.296828
1	1.500945	3.733767	-1.650934
6	0.819052	5.879903	0.898012
1	-0.408680	5.413052	2.611077
1	1.966917	6.046397	-0.921448
6	-9.055597	-1.940250	0.649817
7	-10.154702	-2.292359	0.803676
6	-2.450626	-2.037465	-0.995419
7	-2.313099	-3.125652	-1.386226
16	0.192558	-0.574184	-1.171622
7	-1.222138	1.337810	-0.165629
1	1.012427	6.901070	1.211330
6	2.431094	1.123853	-1.054525
1	2.700799	1.105705	-2.113815
1	2.773517	2.063572	-0.620189
8	3.118373	0.020917	-0.392875
6	4.445726	-0.030966	-0.553638
8	5.095903	0.775384	-1.192886
6	5.026046	-1.228035	0.168820
1	4.763130	-1.152839	1.229930
1	4.544387	-2.132921	-0.218311
7	6.459095	-1.252904	-0.030219
1	6.867490	-0.518026	-0.592682
6	7.298885	-2.184151	0.479280
8	8.515861	-2.196407	0.303299
8	6.629478	-3.104999	1.210319
6	7.431841	-4.146987	1.801157
1	7.940535	-4.721526	1.024704
1	8.165984	-3.719247	2.486562
1	6.727636	-4.777326	2.341755

Mol6a-B_s0_h2o.out

6	-7.335803	-0.193576	0.789328
6	-6.022403	0.212966	0.601426
6	-5.046003	-0.668326	0.085480
6	-5.435529	-1.986560	-0.238392
6	-6.745967	-2.403216	-0.054311
6	-7.702954	-1.509324	0.460319
1	-8.072956	0.494741	1.186018
1	-5.738983	1.228860	0.855679
1	-4.721845	-2.694701	-0.634667
1	-7.034244	-3.417285	-0.305968
6	-3.705119	-0.128374	-0.066060
1	-3.594197	0.906975	0.242697
6	-2.551576	-0.689511	-0.529112
6	-1.310319	0.096816	-0.569686
6	0.052287	1.840826	-0.311312
6	0.970891	0.945359	-0.827638
6	0.321282	3.236076	0.090348
6	-0.232693	3.733323	1.282384
6	1.109367	4.086823	-0.701462
6	0.016454	5.045473	1.683375
1	-0.850154	3.081781	1.891647
6	1.358318	5.400365	-0.297220
1	1.500496	3.735069	-1.650627
6	0.816780	5.881942	0.897269
1	-0.411279	5.415196	2.610152
1	1.965209	6.048210	-0.921875
6	-9.054332	-1.942787	0.649234
7	-10.153325	-2.295390	0.802857
6	-2.449476	-2.036734	-0.996846
7	-2.311414	-3.124521	-1.388589
16	0.193642	-0.573117	-1.170375
7	-1.222326	1.338768	-0.165995

1	1.009616	6.903309	1.210268
6	2.431543	1.125695	-1.052536
1	2.701744	1.107218	-2.111669
1	2.773457	2.065623	-0.618260
8	3.118777	0.023156	-0.390052
6	4.445759	-0.030369	-0.552384
8	5.096168	0.774576	-1.193275
6	5.025650	-1.227391	0.170497
1	4.764029	-1.151042	1.231822
1	4.542771	-2.132099	-0.215494
7	6.458513	-1.253811	-0.030049
1	6.866865	-0.520060	-0.594015
6	7.297771	-2.186015	0.478314
8	8.514587	-2.199844	0.300271
8	6.628582	-3.105730	1.210720
6	7.430499	-4.148632	1.800698
1	7.936743	-4.724484	1.023613
1	8.166519	-3.721605	2.484531
1	6.726331	-4.777527	2.342992

Mol6a-B_s0_meoh.out

6	-7.336948	-0.191907	0.787635
6	-6.023445	0.214314	0.599830
6	-5.046840	-0.667614	0.085372
6	-5.436397	-1.986181	-0.237105
6	-6.746988	-2.402443	-0.053122
6	-7.704189	-1.507978	0.460046
1	-8.074285	0.496883	1.183192
1	-5.740014	1.230508	0.852965
1	-4.722564	-2.694830	-0.632235
1	-7.035286	-3.416774	-0.303737
6	-3.705798	-0.128034	-0.066154
1	-3.594666	0.907645	0.241477
6	-2.552228	-0.689982	-0.528115
6	-1.310791	0.096000	-0.568864
6	0.052123	1.839814	-0.311276
6	0.970474	0.943953	-0.827489
6	0.321528	3.235048	0.090056
6	-0.232837	3.732824	1.281648
6	1.110416	4.085243	-0.701500
6	0.016807	5.044882	1.682496
1	-0.851107	3.081699	1.890522
6	1.359852	5.398712	-0.297419
1	1.501740	3.733139	-1.650462
6	0.817981	5.880760	0.896684
1	-0.411259	5.415048	2.608945
1	1.967352	6.046155	-0.921902
6	-9.055730	-1.941059	0.648934
7	-10.154824	-2.293263	0.802567
6	-2.450374	-2.037669	-0.994631
7	-2.312819	-3.125894	-1.385310
16	0.192952	-0.574511	-1.169569
7	-1.222491	1.338000	-0.165492
1	1.011184	6.902086	1.209583
6	2.431112	1.124083	-1.052755
1	2.700964	1.107180	-2.112055
1	2.773480	2.063369	-0.617403
8	3.118385	0.020444	-0.392394
6	4.445915	-0.030724	-0.552922
8	5.095835	0.776775	-1.190858
6	5.026456	-1.228754	0.167781
1	4.762164	-1.156167	1.228722
1	4.545937	-2.133234	-0.221836
7	6.459726	-1.251924	-0.029523
1	6.867977	-0.516826	-0.591800
6	7.299754	-2.183711	0.478922
8	8.516639	-2.195402	0.303496
8	6.630187	-3.105763	1.208547
6	7.433038	-4.147867	1.798445
1	7.942515	-4.721073	1.021522
1	8.166723	-3.720418	2.484532
1	6.729059	-4.779325	2.338056

Mol6a-C_s0_acn.out

6	-6.102589	-3.118623	-0.587335
6	-4.882132	-2.462359	-0.658193
6	-4.715403	-1.159857	-0.136640

6	-5.824865	-0.533858	0.472435
6	-7.049030	-1.182457	0.550075
6	-7.195377	-2.477059	0.019574
1	-6.214186	-4.116845	-0.994194
1	-4.039228	-2.960165	-1.126097
1	-5.740514	0.458112	0.891927
1	-7.893644	-0.692967	1.021002
6	-3.390609	-0.574264	-0.272105
1	-2.668249	-1.250116	-0.721826
6	-2.905197	0.656984	0.054137
6	-1.507101	1.043031	-0.165124
6	0.282282	2.376855	-0.200791
6	0.884446	1.221798	-0.658554
6	0.936883	3.683013	0.011715
6	0.631198	4.431841	1.161099
6	1.851165	4.204632	-0.917726
6	1.245361	5.663408	1.385545
1	-0.082823	4.037088	1.876068
6	2.466093	5.437834	-0.689927
1	2.057363	3.665671	-1.836745
6	2.168665	6.168306	0.463195
1	1.005711	6.228621	2.280888
1	3.167064	5.830854	-1.419586
6	-8.460453	-3.142550	0.100506
7	-9.489257	-3.683774	0.165942
6	-3.707546	1.694946	0.630596
7	-4.346045	2.547796	1.098463
16	-0.286648	-0.064291	-0.765148
7	-1.061990	2.249809	0.081712
1	2.645643	7.127464	0.638819
6	2.313332	0.981643	-1.001781
1	2.468914	0.825601	-2.072733
1	2.930959	1.819107	-0.675334
8	2.739353	-0.222627	-0.301374
6	3.993053	-0.629262	-0.535632
8	4.776889	-0.057605	-1.270505
6	4.299835	-1.893174	0.237287
1	4.137443	-1.699277	1.303814
1	3.581017	-2.665955	-0.059488
7	5.659557	-2.298316	-0.029717
1	6.211851	-1.735091	-0.663316
6	6.192741	-3.400938	0.542415
8	5.597114	-4.142919	1.320547
8	7.474555	-3.582729	0.144846
6	8.144370	-4.735352	0.692924
1	8.192676	-4.667194	1.781618
1	7.626617	-5.651773	0.402292
1	9.145880	-4.713271	0.266191

Mol6a-C_s0_chl.out

6	-6.022900	-3.187129	-0.524125
6	-4.811238	-2.514508	-0.589347
6	-4.681716	-1.183086	-0.134316
6	-5.822488	-0.543961	0.398621
6	-7.038458	-1.208963	0.468681
6	-7.147110	-2.533185	0.007412
1	-6.105313	-4.208072	-0.878504
1	-3.944676	-3.022802	-0.999923
1	-5.768974	0.472204	0.761488
1	-7.907478	-0.708240	0.879820
6	-3.362276	-0.582489	-0.256887
1	-2.621281	-1.259853	-0.673454
6	-2.898956	0.662220	0.049497
6	-1.501866	1.059939	-0.153081
6	0.273133	2.412215	-0.187266
6	0.898047	1.252004	-0.600809
6	0.907044	3.730405	0.006334
6	0.520115	4.528868	1.096278
6	1.880960	4.216013	-0.881152
6	1.115299	5.771506	1.307080
1	-0.245354	4.164133	1.772535
6	2.476389	5.460793	-0.666950
1	2.148557	3.641509	-1.762037
6	2.099622	6.239334	0.429753
1	0.811505	6.375647	2.156332
1	3.223790	5.825469	-1.364590
6	-8.404005	-3.215431	0.079788
7	-9.425323	-3.771072	0.137733

6	-3.725966	1.699668	0.591738
7	-4.391627	2.544669	1.034706
16	-0.255466	-0.050640	-0.698280
7	-1.074827	2.275713	0.071373
1	2.561282	7.207832	0.594828
6	2.336454	1.022753	-0.913407
1	2.527225	0.938170	-1.987492
1	2.947858	1.833607	-0.514366
8	2.732597	-0.227700	-0.284685
6	4.001436	-0.611243	-0.486646
8	4.812654	0.016771	-1.139536
6	4.281625	-1.925365	0.208146
1	4.065383	-1.810415	1.276889
1	3.584567	-2.680094	-0.175150
7	5.655254	-2.303046	-0.021446
1	6.237453	-1.686119	-0.572688
6	6.166174	-3.444424	0.496859
8	5.535104	-4.245397	1.179541
8	7.471076	-3.586462	0.159987
6	8.118424	-4.771202	0.662119
1	8.102748	-4.781335	1.753986
1	7.625382	-5.667390	0.279689
1	9.142548	-4.713961	0.296168

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6	-6.107195	-3.115056	-0.590221
6	-4.886265	-2.459709	-0.661483
6	-4.717574	-1.158631	-0.137044
6	-5.825448	-0.533165	0.475442
6	-7.050056	-1.180827	0.553558
6	-7.198378	-2.473984	0.020082
1	-6.220307	-4.112190	-0.999313
1	-4.044572	-2.957103	-1.131980
1	-5.739538	0.457672	0.897299
1	-7.893396	-0.691733	1.027170
6	-3.392455	-0.573879	-0.273024
1	-2.671180	-1.249516	-0.724769
6	-2.905763	0.656411	0.054885
6	-1.507566	1.041791	-0.165093
6	0.282518	2.374660	-0.201169
6	0.883536	1.219752	-0.660777
6	0.938198	3.680248	0.011812
6	0.636504	4.426990	1.163601
6	1.849577	4.203303	-0.919664
6	1.251668	5.658046	1.388282
1	-0.075066	4.031011	1.880354
6	2.465532	5.435968	-0.691630
1	2.052741	3.665794	-1.840208
6	2.172024	6.164430	0.463785
1	1.015190	6.221630	2.285494
1	3.164256	5.830131	-1.422823
6	-8.463994	-3.138410	0.101379
7	-9.493291	-3.678674	0.167120
6	-3.706682	1.694192	0.633610
7	-4.343719	2.547207	1.103199
16	-0.288424	-0.065510	-0.767433
7	-1.061530	2.248158	0.082543
1	2.649819	7.123145	0.639601
6	2.311864	0.979038	-1.005815
1	2.465439	0.819913	-2.076577
1	2.929874	1.817529	-0.682831
8	2.739446	-0.223192	-0.302675
6	3.992658	-0.630341	-0.538076
8	4.775411	-0.060314	-1.275440
6	4.300650	-1.892708	0.236919
1	4.139258	-1.697016	1.303239
1	3.581826	-2.666200	-0.058014
7	5.660353	-2.297746	-0.030536
1	6.211114	-1.736625	-0.667330
6	6.195177	-3.398147	0.544198
8	5.601303	-4.137954	1.325879
8	7.476378	-3.580484	0.145094
6	8.147981	-4.731162	0.695174
1	8.198977	-4.659496	1.783524
1	7.629858	-5.648641	0.408610
1	9.148439	-4.710075	0.265948

Mol6a-C_s0_h2o.out

6	-6.110566	-3.112435	-0.593249
6	-4.889242	-2.457814	-0.664540
6	-4.718902	-1.158192	-0.137022
6	-5.825379	-0.533565	0.478858
6	-7.050329	-1.180500	0.557107
6	-7.200345	-2.472108	0.020352
1	-6.225004	-4.108396	-1.004798
1	-4.048573	-2.954553	-1.137519
1	-5.738088	0.455975	0.903472
1	-7.892561	-0.692083	1.033377
6	-3.393552	-0.574080	-0.273346
1	-2.672911	-1.249735	-0.726049
6	-2.906106	0.655739	0.055261
6	-1.507843	1.040701	-0.164918
6	0.282567	2.373145	-0.201228
6	0.883007	1.218337	-0.661719
6	0.938774	3.678486	0.011881
6	0.640257	4.423662	1.165515
6	1.847537	4.202815	-0.921441
6	1.255852	5.654559	1.390072
1	-0.068997	4.026558	1.883968
6	2.463966	5.435286	-0.693524
1	2.048342	3.666326	-1.843101
6	2.173534	6.162271	0.463622
1	1.021906	6.216900	2.288728
1	3.160695	5.830428	-1.426089
6	-8.466355	-3.135750	0.101714
7	-9.496038	-3.675290	0.167539
6	-3.706384	1.693660	0.634575
7	-4.342600	2.547149	1.104456
16	-0.289372	-0.066561	-0.768386
7	-1.061382	2.246919	0.083147
1	2.651723	7.120804	0.639348
6	2.311037	0.977589	-1.007821
1	2.463434	0.816259	-2.078387
1	2.929027	1.816985	-0.687192
8	2.739936	-0.223037	-0.302555
6	3.992756	-0.630515	-0.538830
8	4.774641	-0.061811	-1.278218
6	4.301732	-1.891666	0.237770
1	4.141430	-1.694324	1.303934
1	3.582710	-2.665642	-0.055380
7	5.661241	-2.296912	-0.030453
1	6.210876	-1.737112	-0.669399
6	6.197020	-3.396273	0.545084
8	5.604463	-4.135007	1.328937
8	7.477595	-3.579238	0.144310
6	8.150214	-4.728874	0.695384
1	8.202069	-4.655756	1.783585
1	7.632425	-5.647005	0.410316
1	9.150337	-4.707847	0.265393

Mol6a-C_s0_meoh.out

6	-6.100556	-3.120411	-0.585004
6	-4.880357	-2.463695	-0.656083
6	-4.714652	-1.160146	-0.136821
6	-5.824972	-0.533469	0.469987
6	-7.048905	-1.182508	0.547790
6	-7.194183	-2.478221	0.019719
1	-6.211323	-4.119473	-0.990033
1	-4.036817	-2.962005	-1.122316
1	-5.741497	0.459419	0.887481
1	-7.894180	-0.692481	1.016971
6	-3.390000	-0.574204	-0.272224
1	-2.667209	-1.250177	-0.721078
6	-2.905100	0.657415	0.053380
6	-1.507008	1.043684	-0.165476
6	0.282187	2.377758	-0.200707
6	0.884764	1.222626	-0.657780
6	0.936530	3.684021	0.011856
6	0.629341	4.433495	1.160417
6	1.852081	4.205095	-0.916642
6	1.243323	5.665110	1.385045
1	-0.085767	4.039214	1.874551
6	2.466813	5.438354	-0.688661
1	2.059412	3.665706	-1.835154
6	2.167923	6.169436	0.463691

1	1.002485	6.230831	2.279747
1	3.168770	5.830952	-1.417601
6	-8.459006	-3.144173	0.100843
7	-9.487593	-3.685787	0.166410
6	-3.708021	1.695440	0.628939
7	-4.347135	2.548183	1.096148
16	-0.286063	-0.063677	-0.764523
7	-1.062193	2.250580	0.081164
1	2.644755	7.128642	0.639457
6	2.313834	0.982585	-1.000396
1	2.470079	0.827975	-2.071475
1	2.931447	1.819487	-0.672463
8	2.739103	-0.222699	-0.301382
6	3.993096	-0.628970	-0.534931
8	4.777554	-0.056346	-1.268353
6	4.299228	-1.893753	0.236816
1	4.135951	-1.701022	1.303429
1	3.580629	-2.666214	-0.061334
7	5.659139	-2.298634	-0.029536
1	6.212119	-1.734530	-0.661747
6	6.191677	-3.402086	0.541701
8	5.595177	-4.145018	1.318214
8	7.473879	-3.583428	0.145206
6	8.143017	-4.736832	0.692400
1	8.190065	-4.670253	1.781250
1	7.625531	-5.652821	0.399910
1	9.145010	-4.714202	0.266826

Mol6a-D_s0_acn.out

6	-7.421117	-0.178530	0.793110
6	-6.104797	0.215211	0.598543
6	-5.133123	-0.683798	0.104707
6	-5.530915	-2.006188	-0.190932
6	-6.844483	-2.409940	-0.000453
6	-7.796473	-1.498793	0.492660
1	-8.154452	0.523231	1.173004
1	-5.815178	1.234684	0.830588
1	-4.821361	-2.727430	-0.570647
1	-7.139120	-3.427278	-0.230662
6	-3.788149	-0.156562	-0.055305
1	-3.672361	0.886750	0.223405
6	-2.635369	-0.738637	-0.493718
6	-1.388861	0.038295	-0.550038
6	-0.017775	1.782089	-0.340464
6	0.900986	0.861945	-0.811203
6	0.256135	3.189883	0.010639
6	-0.310503	3.737201	1.174394
6	1.061964	4.003352	-0.802216
6	-0.056641	5.062071	1.527628
1	-0.941557	3.114382	1.799535
6	1.315598	5.329764	-0.445808
1	1.463418	3.612073	-1.731417
6	0.761206	5.861378	0.721201
1	-0.494379	5.470744	2.433131
1	1.936236	5.948381	-1.086393
6	-9.151060	-1.919110	0.688363
7	-10.252645	-2.260935	0.847553
6	-2.538786	-2.100448	-0.918442
7	-2.405236	-3.200846	-1.274915
16	0.117824	-0.663413	-1.106277
7	-1.297387	1.293941	-0.192148
1	0.957639	6.892722	0.997024
6	2.365383	1.025859	-1.024856
1	2.646746	0.979698	-2.080359
1	2.709297	1.974151	-0.610710
8	3.037596	-0.064711	-0.329022
6	4.368597	-0.116416	-0.457826
8	5.031523	0.681709	-1.094374
6	4.934354	-1.299924	0.296256
1	4.641740	-1.215339	1.349279
1	4.470422	-2.214399	-0.091431
7	6.369616	-1.322656	0.141951
1	6.802808	-0.597810	-0.415428
6	7.127530	-2.281210	0.719946
8	6.689379	-3.198495	1.410896
8	8.439478	-2.098439	0.437359
6	9.344271	-3.065922	1.005301
1	9.285063	-3.049870	2.095479

1	9.112637	-4.067406	0.637057
1	10.335139	-2.759133	0.674099

Mol6a-D_s0_acn_scan.out

6	-6.561514	-0.969736	1.887894
6	-5.312347	-0.447581	1.586201
6	-4.816138	-0.453967	0.263181
6	-5.603882	-1.039249	-0.752542
6	-6.848644	-1.575805	-0.458371
6	-7.336086	-1.535587	0.861127
1	-6.935981	-0.948653	2.904447
1	-4.708514	-0.018682	2.378617
1	-5.249577	-1.086791	-1.772533
1	-7.445235	-2.027535	-1.242222
6	-3.505065	0.130918	0.066613
1	-2.955193	0.339652	0.979714
6	-2.836084	0.483512	-1.073010
6	-1.484813	1.032100	-0.975197
6	0.361173	1.746595	0.037979
6	0.757890	1.957138	-1.307731
6	1.159804	2.031423	1.232222
6	1.074405	1.156050	2.332353
6	1.996225	3.158592	1.308862
6	1.842586	1.387830	3.470465
1	0.420598	0.293091	2.274757
6	2.752668	3.391121	2.455668
1	2.023155	3.871542	0.493182
6	2.684286	2.504339	3.534213
1	1.784169	0.701265	4.308781
1	3.387604	4.269329	2.510247
6	-8.625851	-2.082023	1.161392
7	-9.674840	-2.523066	1.406091
6	-3.380039	0.378291	-2.390550
7	-3.779022	0.325454	-3.482655
16	-0.559571	1.485067	-2.372743
7	-0.876557	1.220772	0.186681
1	3.278516	2.685769	4.424081
6	2.020152	2.267670	-1.807716
1	2.146042	2.502716	-2.855903
1	2.817390	2.548972	-1.133369
8	2.950880	0.305743	-2.147193
6	3.953441	0.139811	-1.363780
8	4.468342	0.981340	-0.605185
6	4.546080	-1.276969	-1.438504
1	3.739917	-2.010430	-1.349438
1	4.994074	-1.405483	-2.432090
7	5.524827	-1.449726	-0.386687
1	5.783673	-0.617593	0.129696
6	6.068528	-2.643992	-0.084856
8	5.818660	-3.702761	-0.661947
8	6.938819	-2.536368	0.954220
6	7.573909	-3.758898	1.371374
1	6.830936	-4.472954	1.733518
1	8.137007	-4.201722	0.547132
1	8.245982	-3.470738	2.178384

Mol6a-D_s0_chl.out

6	-7.459353	-0.161944	0.652570
6	-6.139659	0.231421	0.482182
6	-5.139962	-0.690633	0.099284
6	-5.513074	-2.037422	-0.103888
6	-6.829752	-2.440863	0.065623
6	-7.810789	-1.506245	0.443828
1	-8.214965	0.558116	0.944740
1	-5.869155	1.269683	0.644289
1	-4.780617	-2.778165	-0.391830
1	-7.104945	-3.477453	-0.091609
6	-3.794060	-0.161892	-0.048249
1	-3.688073	0.891913	0.193037
6	-2.630443	-0.753606	-0.442528
6	-1.386497	0.026920	-0.498971
6	-0.026480	1.781191	-0.311743
6	0.899468	0.857643	-0.762349
6	0.238637	3.195423	0.017963
6	-0.349774	3.762386	1.161077
6	1.057879	3.996089	-0.793940
6	-0.103546	5.093123	1.495713

1	-0.992375	3.149228	1.783848
6	1.303785	5.328587	-0.456292
1	1.475294	3.590284	-1.709835
6	0.728061	5.879338	0.690945
1	-0.558292	5.516990	2.385741
1	1.934923	5.936992	-1.096427
6	-9.168628	-1.926411	0.617756
7	-10.272759	-2.267087	0.759355
6	-2.522934	-2.126185	-0.828889
7	-2.383999	-3.235151	-1.155203
16	0.127223	-0.677213	-1.034106
7	-1.303593	1.288228	-0.160639
1	0.918453	6.915549	0.952397
6	2.363223	1.029016	-0.977037
1	2.641269	1.009991	-2.034778
1	2.706241	1.969382	-0.543594
8	3.041605	-0.074795	-0.312298
6	4.374635	-0.110780	-0.445574
8	5.025638	0.709421	-1.064609
6	4.954911	-1.305845	0.278135
1	4.665841	-1.250697	1.334322
1	4.498129	-2.216833	-0.126618
7	6.389000	-1.309526	0.116637
1	6.812299	-0.567715	-0.425565
6	7.158858	-2.272185	0.675761
8	6.733240	-3.205361	1.349298
8	8.468603	-2.068143	0.391881
6	9.381726	-3.038488	0.938521
1	9.320969	-3.048476	2.028779
1	9.158823	-4.034265	0.549586
1	10.369982	-2.715189	0.614603

Mol6a-D_s0_chl_scan.out

6	-6.145692	-1.443870	1.781315
6	-4.920171	-0.842276	1.535533
6	-4.559028	-0.417115	0.236576
6	-5.475079	-0.620473	-0.819796
6	-6.702009	-1.221792	-0.583074
6	-7.043598	-1.635294	0.717754
1	-6.411395	-1.765173	2.781568
1	-4.225360	-0.694265	2.355543
1	-5.237007	-0.313681	-1.828341
1	-7.399158	-1.374906	-1.398535
6	-3.255292	0.199970	0.101253
1	-2.675202	0.253679	1.017827
6	-2.617805	0.735361	-0.984902
6	-1.276809	1.292605	-0.831463
6	0.576994	1.887120	0.243134
6	0.934749	2.312305	-1.070428
6	1.397227	2.034741	1.442015
6	1.365415	1.024466	2.421471
6	2.199987	3.170979	1.648298
6	2.151854	1.133136	3.563583
1	0.742990	0.151656	2.260412
6	2.975300	3.280260	2.800460
1	2.182351	3.985588	0.933119
6	2.960582	2.259428	3.754763
1	2.139049	0.340220	4.304310
1	3.584072	4.164623	2.957087
6	-8.312517	-2.255356	0.958209
7	-9.343247	-2.758550	1.154750
6	-3.176971	0.797508	-2.299144
7	-3.587914	0.876440	-3.385129
16	-0.411576	1.998437	-2.161696
7	-0.640207	1.307907	0.332683
1	3.570078	2.344071	4.648848
6	2.175900	2.712125	-1.531756
1	2.309033	3.085560	-2.537781
1	2.997673	2.809183	-0.836580
8	3.122354	0.772027	-2.371379
6	3.687752	0.211009	-1.370993
8	3.844022	0.685164	-0.228594
6	4.205014	-1.208702	-1.669285
1	3.368572	-1.819134	-2.026600
1	4.935278	-1.154592	-2.484210
7	4.792650	-1.772212	-0.472479
1	4.794064	-1.174682	0.346142
6	5.349742	-2.997720	-0.441287

8	5.413416	-3.776129	-1.391167
8	5.841717	-3.278962	0.798165
6	6.461052	-4.568518	0.940230
1	5.743902	-5.365958	0.731882
1	7.314737	-4.662114	0.265130
1	6.790904	-4.616343	1.977558

Mol6a-D_s0_dmso.out

6	-7.420723	-0.180239	0.792767
6	-6.104499	0.213976	0.598447
6	-5.132516	-0.684610	0.104454
6	-5.529853	-2.007023	-0.191688
6	-6.843293	-2.411276	-0.001442
6	-7.795587	-1.500543	0.491878
1	-8.154292	0.521204	1.172781
1	-5.815252	1.233471	0.830825
1	-4.820067	-2.727910	-0.571631
1	-7.137580	-3.428631	-0.232007
6	-3.787702	-0.156893	-0.055321
1	-3.672404	0.886457	0.223428
6	-2.634602	-0.738507	-0.493515
6	-1.388386	0.038926	-0.549761
6	-0.017938	1.783249	-0.340093
6	0.901272	0.863367	-0.810406
6	0.255363	3.191200	0.010849
6	-0.311806	3.738535	1.174366
6	1.061150	4.004805	-0.801920
6	-0.058540	5.063572	1.527431
1	-0.942755	3.115603	1.799505
6	1.314199	5.331386	-0.445665
1	1.463064	3.613503	-1.730911
6	0.759261	5.863034	0.721081
1	-0.496681	5.472243	2.432739
1	1.934830	5.950090	-1.086171
6	-9.150040	-1.921377	0.687311
7	-10.251515	-2.263697	0.846269
6	-2.537300	-2.100377	-0.917859
7	-2.403002	-3.200788	-1.274027
16	0.118702	-0.662310	-1.105466
7	-1.297467	1.294690	-0.192121
1	0.955249	6.894498	0.996773
6	2.365675	1.027658	-1.023697
1	2.647307	0.981243	-2.079098
1	2.709250	1.976108	-0.609643
8	3.037894	-0.062619	-0.327308
6	4.368684	-0.115486	-0.457160
8	5.031862	0.681683	-1.094689
6	4.933983	-1.299067	0.297162
1	4.641978	-1.213755	1.350282
1	4.469203	-2.213318	-0.090022
7	6.369181	-1.322982	0.142180
1	6.802660	-0.598732	-0.415763
6	7.126570	-2.282248	0.719513
8	6.687951	-3.199206	1.410778
8	8.438468	-2.100809	0.436092
6	9.342930	-3.069035	1.003411
1	9.284891	-3.052561	2.093647
1	9.110017	-4.070389	0.635623
1	10.333745	-2.763275	0.671124

Mol6a-D_s0_dmso_scan.out

6	-6.348845	-1.289731	1.879319
6	-5.114207	-0.726400	1.591175
6	-4.726098	-0.453937	0.259593
6	-5.621778	-0.772971	-0.785380
6	-6.857274	-1.337700	-0.507117
6	-7.226110	-1.597194	0.825893
1	-6.635694	-1.492023	2.904439
1	-4.435000	-0.488634	2.402840
1	-5.361047	-0.586814	-1.817416
1	-7.539000	-1.580319	-1.313717
6	-3.415459	0.137213	0.081323
1	-2.847817	0.277548	0.996283
6	-2.759488	0.557804	-1.043773
6	-1.414599	1.116458	-0.929068
6	0.430911	1.805078	0.101102
6	0.807926	2.091185	-1.239308

6	1.247315	2.055603	1.289954
6	1.235475	1.116907	2.338259
6	2.025427	3.220354	1.413369
6	2.018140	1.324064	3.470908
1	0.628716	0.223288	2.242929
6	2.796372	3.428325	2.555871
1	1.994251	3.979139	0.639445
6	2.801950	2.478475	3.581400
1	2.018322	0.587236	4.267579
1	3.384994	4.335070	2.648805
6	-8.503628	-2.179872	1.109320
7	-9.541563	-2.653062	1.339687
6	-3.301341	0.496568	-2.364465
7	-3.686666	0.473917	-3.441807
16	-0.521142	1.669825	-2.311714
7	-0.794096	1.250479	0.236066
1	3.406433	2.641060	4.468062
6	2.062366	2.443266	-1.719953
1	2.203080	2.732664	-2.752329
1	2.862427	2.649656	-1.022891
8	2.996201	0.503954	-2.254939
6	3.779024	0.150942	-1.303193
8	4.116481	0.830008	-0.315369
6	4.322006	-1.280422	-1.456898
1	3.473557	-1.969444	-1.528663
1	4.875673	-1.347613	-2.400097
7	5.166440	-1.603768	-0.326585
1	5.300573	-0.866781	0.355888
6	5.836148	-2.767553	-0.224974
8	5.775891	-3.694964	-1.033095
8	6.595212	-2.797364	0.902662
6	7.346011	-4.005695	1.122536
1	6.676391	-4.864714	1.203558
1	8.057347	-4.169127	0.310023
1	7.874504	-3.848023	2.061738

Mol6a-D_s0_h2o_expl-1.out

6	7.769729	1.089800	-0.640920
6	6.410254	1.228156	-0.400980
6	5.612356	0.120510	-0.036077
6	6.227372	-1.145360	0.078799
6	7.585505	-1.295349	-0.160311
6	8.361955	-0.178499	-0.520310
1	8.370116	1.948082	-0.918625
1	5.949225	2.205847	-0.492593
1	5.655136	-2.020413	0.351082
1	8.049300	-2.270755	-0.071512
6	4.203733	0.398364	0.189340
1	3.927992	1.433029	0.017720
6	3.173545	-0.406433	0.580016
6	1.813683	0.125333	0.740222
6	0.158036	1.620364	0.796197
6	-0.571787	0.496985	1.134225
6	-0.382703	2.984704	0.611009
6	-0.126171	3.670850	-0.587040
6	-1.140058	3.609976	1.612305
6	-0.628009	4.958112	-0.782450
1	0.455895	3.186800	-1.364988
6	-1.642747	4.897298	1.413404
1	-1.313593	3.101479	2.555219
6	-1.390083	5.572991	0.216182
1	-0.427801	5.477935	-1.714045
1	-2.223028	5.374260	2.196856
6	9.762510	-0.335801	-0.765540
7	10.900859	-0.463493	-0.964972
6	3.323281	-1.800883	0.855011
7	3.392397	-2.937656	1.089168
16	0.467021	-0.896376	1.168543
7	1.496069	1.392821	0.577212
1	-1.780896	6.574058	0.063654
6	-2.046127	0.382353	1.291690
1	-2.333531	-0.541671	1.791598
1	-2.475170	1.241543	1.803121
8	-2.607016	0.336966	-0.067665
6	-3.912677	0.532204	-0.202388
8	-4.682802	0.734575	0.726177
6	-4.336030	0.502768	-1.666697
1	-4.272403	1.523480	-2.052709

1	-3.640089	-0.107549	-2.241381
7	-5.695342	0.036205	-1.832286
1	-6.430545	0.734171	-1.718292
6	-5.995366	-1.250645	-1.576604
8	-5.154576	-2.140871	-1.370629
8	-7.319892	-1.489057	-1.585654
6	-7.731540	-2.873441	-1.427089
1	-7.199129	-3.503626	-2.138697
1	-7.541274	-3.201937	-0.404606
1	-8.799554	-2.874186	-1.634659
1	-5.062721	-0.356543	2.313854
8	-5.276397	-1.078572	2.926644
1	-5.185488	-1.884442	2.382418
1	-6.384409	1.786252	0.243585
8	-7.068127	2.133659	-0.354525
1	-7.877819	1.620918	-0.148752
1	-1.011140	0.227188	-1.680803
8	-0.795866	-0.368965	-2.411079
1	-1.320988	-1.170818	-2.216380
1	-5.057606	-3.001480	0.254484
8	-4.848912	-3.276756	1.170591
1	-5.230326	-4.156569	1.292133
1	-3.384713	-2.446079	-1.731989
8	-2.417754	-2.604056	-1.754507
1	-2.285148	-3.397452	-2.291091
1	3.767809	-4.841070	1.496028
8	3.931790	-5.784509	1.673497
1	4.792629	-5.816081	2.110797
1	12.828469	-0.636974	-1.314698
8	13.779766	-0.771009	-1.480706
1	14.130441	0.105548	-1.685150
1	-8.684772	-0.369752	-0.654538
8	-9.133648	0.283093	-0.090898
1	-9.982957	0.461645	-0.517205
1	2.562631	2.956740	0.449117
8	3.194825	3.706123	0.389462
1	2.666957	4.457092	0.087854
1	-1.990174	-2.778079	0.119257
8	-2.029053	-2.837457	1.092533
1	-2.962195	-3.065164	1.265494

Mol6a-D_s0_h2o.out

6	-7.420145	-0.181875	0.793076
6	-6.104135	0.212943	0.598464
6	-5.131991	-0.685102	0.103814
6	-5.528883	-2.007540	-0.192781
6	-6.842095	-2.412415	-0.002292
6	-7.794528	-1.502223	0.491766
1	-8.153826	0.519143	1.173637
1	-5.815243	1.232453	0.831164
1	-4.818974	-2.727979	-0.573320
1	-7.136040	-3.429776	-0.233236
6	-3.787379	-0.156823	-0.056008
1	-3.672572	0.886541	0.222848
6	-2.634015	-0.737980	-0.494103
6	-1.388002	0.039831	-0.550125
6	-0.017957	1.784461	-0.339936
6	0.901569	0.864839	-0.810095
6	0.254930	3.192446	0.011202
6	-0.312674	3.739617	1.174609
6	1.060777	4.006254	-0.801329
6	-0.059820	5.064721	1.527785
1	-0.943578	3.116538	1.799653
6	1.313419	5.332897	-0.444948
1	1.463089	3.615066	-1.730189
6	0.758021	5.864404	0.721661
1	-0.498289	5.473252	2.432996
1	1.934114	5.951743	-1.085252
6	-9.148720	-1.923707	0.687546
7	-10.249995	-2.266571	0.846798
6	-2.536069	-2.099829	-0.918362
7	-2.401032	-3.200186	-1.274432
16	0.119405	-0.660944	-1.105581
7	-1.297446	1.295582	-0.192358
1	0.953707	6.895902	0.997440
6	2.365997	1.029455	-1.022993
1	2.647825	0.983537	-2.078340
1	2.709433	1.977667	-0.608293

8	3.038036	-0.061213	-0.326916
6	4.368666	-0.114815	-0.456919
8	5.032381	0.682028	-1.094382
6	4.933262	-1.298885	0.297181
1	4.641973	-1.213010	1.350451
1	4.467368	-2.212664	-0.089723
7	6.368372	-1.324326	0.141433
1	6.802400	-0.600196	-0.416247
6	7.125148	-2.283638	0.719286
8	6.685835	-3.199973	1.411134
8	8.437105	-2.103407	0.435760
6	9.341127	-3.071897	1.003505
1	9.283093	-3.054914	2.093724
1	9.107794	-4.073265	0.635997
1	10.332080	-2.766747	0.671111

Mol6a-D_s0_h2o_scan.out

6	-7.375678	0.174924	1.114489
6	-6.051015	0.468027	0.822291
6	-5.201741	-0.488606	0.222853
6	-5.727627	-1.766601	-0.067217
6	-7.049604	-2.070647	0.223877
6	-7.880807	-1.101104	0.813973
1	-8.015719	0.920512	1.571493
1	-5.660311	1.452639	1.056494
1	-5.110506	-2.532168	-0.515405
1	-7.443031	-3.055213	-0.000757
6	-3.836434	-0.066076	-0.040183
1	-3.590507	0.930255	0.315272
6	-2.802097	-0.698186	-0.665119
6	-1.497889	-0.033921	-0.789232
6	0.049451	1.550179	-0.556510
6	0.804012	0.635004	-1.276401
6	0.509035	2.864935	-0.065258
6	0.220221	3.247672	1.255184
6	1.214769	3.750247	-0.895590
6	0.650886	4.481968	1.741261
1	-0.333488	2.569020	1.895385
6	1.643959	4.985608	-0.406425
1	1.399024	3.488783	-1.932588
6	1.367831	5.352537	0.913419
1	0.428906	4.763766	2.765803
1	2.183341	5.663713	-1.060121
6	-9.245531	-1.418456	1.111746
7	-10.372345	-1.680477	1.357156
6	-2.891805	-2.004703	-1.239847
7	-2.910651	-3.077904	-1.734874
16	-0.160883	-0.768417	-1.642326
7	-1.236357	1.151295	-0.289173
1	1.701518	6.313374	1.292538
6	2.227986	0.685700	-1.612985
1	2.506441	0.263613	-2.574576
1	2.690929	1.650685	-1.440997
8	2.972423	-0.318468	-0.523778
6	4.291396	-0.342334	-0.637936
8	4.947538	0.298175	-1.447116
6	4.909186	-1.284478	0.382873
1	4.607636	-0.961312	1.385603
1	4.493503	-2.286810	0.229430
7	6.345913	-1.276510	0.232070
1	6.742267	-0.685604	-0.487695
6	7.147347	-2.031527	1.014005
8	6.754302	-2.779446	1.907749
8	8.450814	-1.858086	0.685373
6	9.399994	-2.617939	1.458748
1	9.337550	-2.346421	2.514590
1	9.219242	-3.688376	1.341032
1	10.375742	-2.351364	1.055532

Mol6a-D_s0_meoh_expl-1.out

6	-7.915448	0.651363	0.408633
6	-6.579686	1.001020	0.271897
6	-5.549000	0.060921	0.495600
6	-5.902177	-1.250029	0.883219
6	-7.234309	-1.609237	1.026520
6	-8.245684	-0.661443	0.785095
1	-8.696908	1.380419	0.229638

1	-6.318453	2.014184	-0.014819
1	-5.145779	-1.994553	1.085240
1	-7.496991	-2.617313	1.325188
6	-4.193204	0.546662	0.300135
1	-4.132907	1.611659	0.097766
6	-2.995507	-0.107334	0.299873
6	-1.738309	0.613538	0.064731
6	-0.347633	2.335328	-0.233900
6	0.549997	1.307708	-0.441015
6	-0.044162	3.780523	-0.275655
6	-0.439064	4.602447	0.791652
6	0.619629	4.349599	-1.373018
6	-0.165326	5.969386	0.764023
1	-0.953884	4.165568	1.640860
6	0.895696	5.717834	-1.396207
1	0.897377	3.728151	-2.218257
6	0.504817	6.529996	-0.328596
1	-0.472272	6.596175	1.595271
1	1.408325	6.147601	-2.250737
6	-9.618835	-1.035592	0.930177
7	-10.735226	-1.338391	1.047488
6	-2.872276	-1.518344	0.483104
7	-2.737096	-2.667416	0.613108
16	-0.247438	-0.228931	-0.275529
7	-1.629830	1.924090	0.055405
1	0.717243	7.594238	-0.348498
6	2.006786	1.400652	-0.699752
1	2.321146	0.798485	-1.550925
1	2.309280	2.435230	-0.845544
8	2.699002	0.872533	0.484373
6	4.000704	0.623865	0.359375
8	4.658552	0.907796	-0.632104
6	4.572682	-0.048146	1.601810
1	4.794739	0.731576	2.335678
1	3.821253	-0.709914	2.033344
7	5.783797	-0.779872	1.310840
1	6.633859	-0.230329	1.158555
6	5.704573	-1.966585	0.674217
8	4.649656	-2.578170	0.454134
8	6.915942	-2.429027	0.318976
6	6.951153	-3.656331	-0.452585
1	6.569617	-4.485746	0.143280
1	6.362591	-3.535047	-1.362688
1	8.001525	-3.805805	-0.692368
1	4.474437	2.408895	-1.847359
8	4.346885	3.268018	-2.283177
1	6.654148	1.183329	-0.446224
8	7.502114	1.099971	0.022666
1	1.800502	1.448092	2.210111
8	1.462274	1.714694	3.077796
1	4.181661	-4.390972	0.447809
8	3.916038	-5.323243	0.357026
1	3.256195	-2.043178	-0.582822
8	2.618780	-1.741907	-1.259650
1	-3.390638	-3.914328	-0.895616
8	-3.793370	-4.171489	-1.741278
1	-12.639587	-1.809383	1.121382
8	-13.587601	-2.026658	1.078674
1	8.494667	-1.886152	1.389638
8	9.064501	-1.555751	2.101440
1	-2.956203	3.282098	0.109269
8	-3.708892	3.898407	-0.011277
1	1.229385	-2.902242	-1.268758
8	0.487007	-3.540479	-1.317820
6	-14.007968	-1.895740	-0.279074
1	-15.072129	-2.141098	-0.317384
1	-13.872759	-0.871204	-0.650156
1	-13.467123	-2.584917	-0.940994
6	-4.201155	-2.977083	-2.410027
1	-4.596860	-3.272094	-3.384326
1	-4.989706	-2.450250	-1.857606
1	-3.358146	-2.292446	-2.566971
6	-3.501728	4.592383	-1.241284
1	-4.367240	5.238769	-1.405557
1	-2.597958	5.213845	-1.205428
1	-3.418316	3.897881	-2.087720
6	-0.286160	-3.243026	-2.477491
1	0.287177	-3.401139	-3.401428
1	-1.149922	-3.911958	-2.480869

1	-0.652876	-2.207996	-2.467378
6	0.157649	1.155072	3.248144
1	-0.568373	1.605166	2.561244
1	0.160099	0.068241	3.102677
1	-0.153776	1.371163	4.272298
6	3.291705	-1.742556	-2.527189
1	4.156885	-1.071479	-2.507303
1	3.618605	-2.751292	-2.802428
1	2.577905	-1.383177	-3.270872
6	3.603463	-5.559515	-1.017198
1	2.756819	-4.947552	-1.350933
1	4.466318	-5.364797	-1.667939
1	3.330862	-6.613462	-1.112437
6	4.539327	4.292621	-1.305886
1	3.793493	4.235716	-0.501807
1	5.542143	4.247995	-0.863339
1	4.420206	5.251625	-1.814328
6	8.474124	0.543659	-0.873105
1	8.145727	-0.426316	-1.263636
1	8.676085	1.222656	-1.708995
1	9.390896	0.400750	-0.298728
6	8.526102	-2.023072	3.341314
1	7.499942	-1.666171	3.493719
1	8.534936	-3.118762	3.399316
1	9.158494	-1.625251	4.138005

Mol6a-D_s0_meoh.out

6	-7.421458	-0.178182	0.792071
6	-6.105080	0.215469	0.597702
6	-5.133228	-0.683802	0.104701
6	-5.530902	-2.006384	-0.190236
6	-6.844527	-2.410040	0.000066
6	-7.796713	-1.498627	0.492296
1	-8.154935	0.523795	1.171296
1	-5.815571	1.235091	0.829243
1	-4.821202	-2.727850	-0.569257
1	-7.139057	-3.427533	-0.229596
6	-3.788211	-0.156638	-0.055224
1	-3.672468	0.886792	0.223072
6	-2.635340	-0.738866	-0.493186
6	-1.388846	0.038086	-0.549545
6	-0.017818	1.781965	-0.340250
6	0.900944	0.861779	-0.810927
6	0.256014	3.189799	0.010682
6	-0.310979	3.737311	1.174182
6	1.062113	4.003148	-0.802015
6	-0.057184	5.062207	1.527316
1	-0.942264	3.114584	1.799177
6	1.315681	5.329598	-0.445706
1	1.463810	3.611785	-1.731076
6	0.760952	5.861382	0.721054
1	-0.495205	5.471017	2.432620
1	1.936530	5.948105	-1.086193
6	-9.151365	-1.918844	0.687787
7	-10.252999	-2.260579	0.846805
6	-2.538670	-2.100813	-0.917463
7	-2.405094	-3.201327	-1.273565
16	0.117854	-0.663654	-1.105760
7	-1.297406	1.293763	-0.191807
1	0.957330	6.892756	0.996802
6	2.365335	1.025713	-1.024642
1	2.646662	0.979855	-2.080175
1	2.709309	1.973880	-0.610254
8	3.037593	-0.065061	-0.329176
6	4.368601	-0.116717	-0.458217
8	5.031370	0.681562	-1.094710
6	4.934513	-1.300394	0.295477
1	4.642084	-1.216153	1.348576
1	4.470539	-2.214793	-0.092365
7	6.369750	-1.322996	0.140932
1	6.802800	-0.598010	-0.416374
6	7.127936	-2.280938	0.719653
8	6.690037	-3.197962	1.411063
8	8.439871	-2.097804	0.437111
6	9.344940	-3.064650	1.005686
1	9.285581	-3.048047	2.095847
1	9.113681	-4.066420	0.637975
1	10.335734	-2.757671	0.674425

Mol6a-D_s0_meoh_scan.out

6	-6.292433	1.858789	-1.510159
6	-5.071749	1.219265	-1.352658
6	-4.764004	0.509806	-0.169189
6	-5.730293	0.456817	0.860600
6	-6.953822	1.091647	0.711342
6	-7.238889	1.795869	-0.473560
1	-6.516710	2.401290	-2.420760
1	-4.338810	1.265414	-2.150941
1	-5.535507	-0.078664	1.778826
1	-7.690966	1.046880	1.504351
6	-3.457842	-0.111918	-0.118499
1	-2.855703	0.015119	-1.013077
6	-2.836536	-0.833835	0.865707
6	-1.486247	-1.336994	0.642063
6	0.388900	-1.705912	-0.492861
6	0.738411	-2.353886	0.733207
6	1.237369	-1.616376	-1.678407
6	1.216838	-0.435390	-2.445205
6	2.055926	-2.688429	-2.079190
6	2.030546	-0.318047	-3.567975
1	0.579690	0.385769	-2.136632
6	2.856058	-2.569520	-3.213491
1	2.031502	-3.624619	-1.533232
6	2.853003	-1.383395	-3.953318
1	2.025181	0.601712	-4.143628
1	3.475021	-3.404633	-3.524144
6	-8.502791	2.452162	-0.623959
7	-9.511519	2.976405	-0.744393
6	-3.417521	-1.135786	2.136402
7	-3.842136	-1.410127	3.184531
16	-0.629613	-2.253814	1.840677
7	-0.832013	-1.136821	-0.498580
1	3.481656	-1.291978	-4.833288
6	1.979429	-2.802688	1.127279
1	2.123216	-3.303973	2.075098
1	2.812239	-2.772434	0.437469
8	2.955892	-0.919234	2.156203
6	3.796313	-0.447603	1.321121
8	4.171010	-0.967226	0.247137
6	4.378358	0.920828	1.725108
1	3.551137	1.629273	1.844876
1	4.864409	0.821758	2.701907
7	5.314060	1.373917	0.717447
1	5.440072	0.760313	-0.079331
6	5.964045	2.549409	0.797259
8	5.858416	3.359882	1.718928
8	6.769266	2.738872	-0.282923
6	7.518000	3.967911	-0.297496
1	6.845801	4.828424	-0.275760
1	8.199381	4.012709	0.555075
1	8.080369	3.950328	-1.230156

Mol6a-D_s1r_acn.out

6	-7.421515	-0.348242	0.346024
6	-6.136671	0.113842	0.239320
6	-5.029596	-0.773765	0.017796
6	-5.327167	-2.173447	-0.084775
6	-6.616910	-2.631690	0.023484
6	-7.682197	-1.733297	0.238821
1	-8.240411	0.342160	0.512566
1	-5.939598	1.177485	0.322066
1	-4.534731	-2.889745	-0.248550
1	-6.821810	-3.693318	-0.056624
6	-3.755157	-0.207386	-0.074458
1	-3.693664	0.868914	0.039445
6	-2.484660	-0.815939	-0.295312
6	-1.338414	0.005673	-0.309797
6	-0.134181	1.871575	-0.203329
6	0.909164	0.951696	-0.418954
6	0.027057	3.315924	-0.003313
6	-0.862835	3.981720	0.852448
6	1.027256	4.052290	-0.651214
6	-0.737382	5.345857	1.072630
1	-1.641769	3.413061	1.346843
6	1.144771	5.419638	-0.433480

1	1.692033	3.575412	-1.361627
6	0.268487	6.068829	0.432720
1	-1.424457	5.847694	1.745553
1	1.917031	5.979884	-0.949280
6	-9.013967	-2.219820	0.347979
7	-10.102585	-2.615717	0.437465
6	-2.274520	-2.201479	-0.514509
7	-2.035772	-3.323865	-0.701497
16	0.297738	-0.636587	-0.553012
7	-1.365110	1.326994	-0.139847
1	0.364858	7.135733	0.603976
6	2.371041	1.216371	-0.498559
1	2.677308	1.492669	-1.513715
1	2.660913	2.022756	0.178965
8	3.046972	0.005451	-0.130874
6	4.379795	0.019535	-0.228376
8	5.019386	0.981704	-0.589044
6	4.962546	-1.310497	0.167398
1	4.640654	-1.541354	1.188222
1	4.537913	-2.081754	-0.484319
7	6.396250	-1.249437	0.061900
1	6.822107	-0.391401	-0.261624
6	7.165659	-2.304394	0.395383
8	6.735501	-3.376644	0.800633
8	8.471201	-2.030208	0.226368
6	9.381702	-3.088200	0.554269
1	9.284944	-3.361906	1.605827
1	9.193552	-3.960983	-0.072601
1	10.373511	-2.686942	0.357081

Mol6a-D_s1r_chl.out

6	-7.425894	-0.345263	0.341808
6	-6.138617	0.114415	0.248001
6	-5.034570	-0.773384	0.025974
6	-5.333774	-2.169668	-0.092757
6	-6.626374	-2.625829	0.002389
6	-7.690110	-1.727907	0.219497
1	-8.244652	0.345142	0.509382
1	-5.939059	1.176864	0.342058
1	-4.541458	-2.885733	-0.259510
1	-6.833685	-3.686034	-0.090178
6	-3.754037	-0.210434	-0.054094
1	-3.689279	0.865477	0.063207
6	-2.488835	-0.822646	-0.268253
6	-1.340274	0.001585	-0.284884
6	-0.133724	1.866691	-0.194778
6	0.907972	0.944997	-0.407190
6	0.026614	3.310708	-0.004648
6	-0.879735	3.985247	0.827596
6	1.040785	4.041990	-0.637989
6	-0.754948	5.349890	1.041700
1	-1.670658	3.420878	1.307311
6	1.157037	5.409801	-0.426937
1	1.716842	3.560016	-1.334172
6	0.265513	6.066305	0.418121
1	-1.454573	5.857908	1.696801
1	1.939823	5.965556	-0.931625
6	-9.025224	-2.211029	0.314862
7	-10.115827	-2.602610	0.392984
6	-2.277743	-2.209622	-0.477031
7	-2.036607	-3.332822	-0.655352
16	0.295793	-0.645795	-0.525277
7	-1.366343	1.321447	-0.122517
1	0.361103	7.134046	0.584489
6	2.370100	1.207410	-0.491502
1	2.675003	1.483869	-1.507304
1	2.663520	2.015333	0.182893
8	3.047958	-0.001890	-0.124812
6	4.382022	0.016096	-0.233450
8	5.012050	0.978549	-0.607692
6	4.974133	-1.307424	0.168694
1	4.666527	-1.530114	1.195955
1	4.542865	-2.089096	-0.466435
7	6.405482	-1.242989	0.043332
1	6.825837	-0.388417	-0.295552
6	7.179773	-2.293745	0.387102
8	6.754547	-3.356588	0.814925
8	8.483573	-2.020537	0.197562

6	9.394583	-3.074923	0.532459
1	9.307664	-3.332525	1.589006
1	9.196222	-3.957981	-0.076757
1	10.385276	-2.679488	0.317732

Mol6a-D_s1r_dmso.out

6	-7.421360	-0.348558	0.345657
6	-6.136623	0.113671	0.238523
6	-5.029350	-0.773901	0.017299
6	-5.326765	-2.173747	-0.084432
6	-6.616381	-2.632122	0.024264
6	-7.681809	-1.733735	0.239251
1	-8.240317	0.341826	0.511959
1	-5.939721	1.177381	0.320684
1	-4.534259	-2.890039	-0.247842
1	-6.821116	-3.693830	-0.055181
6	-3.755172	-0.207332	-0.075352
1	-3.693886	0.869003	0.038267
6	-2.484401	-0.815715	-0.296174
6	-1.338277	0.005834	-0.310498
6	-0.134236	1.871832	-0.203424
6	0.909247	0.952053	-0.418969
6	0.026906	3.316235	-0.003218
6	-0.862358	3.981692	0.853430
6	1.026410	4.052841	-0.651857
6	-0.737042	5.345857	1.073651
1	-1.640695	3.412828	1.348544
6	1.143810	5.420217	-0.434061
1	1.690753	3.576159	-1.362807
6	0.268107	6.069130	0.432930
1	-1.423631	5.847453	1.747250
1	1.915544	5.980668	-0.950426
6	-9.013423	-2.220456	0.348924
7	-10.101944	-2.616576	0.438819
6	-2.274219	-2.201211	-0.515617
7	-2.035503	-3.323587	-0.702729
16	0.297942	-0.636166	-0.553574
7	-1.365079	1.327228	-0.140379
1	0.364383	7.136037	0.604219
6	2.371108	1.216884	-0.498270
1	2.677519	1.493007	-1.513415
1	2.660732	2.023331	0.179279
8	3.046989	0.005991	-0.130279
6	4.379724	0.019775	-0.227777
8	5.019673	0.981780	-0.588337
6	4.962127	-1.310469	0.167875
1	4.640052	-1.541338	1.188631
1	4.537431	-2.081430	-0.484138
7	6.395880	-1.249691	0.062574
1	6.821870	-0.391617	-0.260705
6	7.165182	-2.304793	0.395476
8	6.734960	-3.377333	0.800188
8	8.470725	-2.030674	0.226654
6	9.381305	-3.088797	0.554020
1	9.284632	-3.362972	1.605462
1	9.193235	-3.961253	-0.073324
1	10.373084	-2.687395	0.357013

Mol6a-D_s1r_h2o.out

6	-7.421238	-0.348765	0.344977
6	-6.136657	0.113638	0.237065
6	-5.029107	-0.773953	0.016588
6	-5.326288	-2.174066	-0.083442
6	-6.615728	-2.632597	0.026023
6	-7.681355	-1.734151	0.240188
1	-8.240293	0.341645	0.510670
1	-5.940013	1.177479	0.317981
1	-4.533681	-2.890402	-0.246091
1	-6.820223	-3.694445	-0.052112
6	-3.755286	-0.207153	-0.076907
1	-3.694276	0.869259	0.036046
6	-2.484196	-0.815365	-0.297703
6	-1.338181	0.006038	-0.311834
6	-0.134308	1.872094	-0.203803
6	0.909324	0.952406	-0.419141
6	0.026809	3.316535	-0.003137
6	-0.861546	3.981482	0.854798

6	1.025449	4.053459	-0.652666
6	-0.736284	5.345642	1.075272
1	-1.639134	3.412337	1.350788
6	1.142817	5.420831	-0.434593
1	1.689159	3.577057	-1.364393
6	0.267957	6.069317	0.433563
1	-1.422167	5.846883	1.749855
1	1.913888	5.981568	-0.951636
6	-9.012760	-2.221105	0.350688
7	-10.101145	-2.617510	0.441259
6	-2.274011	-2.200807	-0.517536
7	-2.035373	-3.323115	-0.705181
16	0.298094	-0.635687	-0.554654
7	-1.365078	1.327536	-0.141439
1	0.364202	7.136196	0.605054
6	2.371164	1.217417	-0.498010
1	2.677752	1.493465	-1.513108
1	2.660480	2.023849	0.179682
8	3.046965	0.006488	-0.129833
6	4.379606	0.020009	-0.226974
8	5.020034	0.981950	-0.586979
6	4.961567	-1.310572	0.168294
1	4.639126	-1.541691	1.188871
1	4.536922	-2.081027	-0.484327
7	6.395399	-1.250051	0.063494
1	6.821554	-0.391847	-0.259254
6	7.164589	-2.305305	0.395693
8	6.734302	-3.378298	0.799511
8	8.470144	-2.031131	0.227426
6	9.380861	-3.089379	0.554162
1	9.284067	-3.364336	1.605386
1	9.193143	-3.961332	-0.073981
1	10.372606	-2.687654	0.357696

Mol6a-D_s1r_meoh.out

6	-7.421570	-0.348205	0.345957
6	-6.136690	0.113851	0.239448
6	-5.029654	-0.773759	0.017957
6	-5.327233	-2.173398	-0.084788
6	-6.617017	-2.631617	0.023277
6	-7.682290	-1.733230	0.238581
1	-8.240473	0.342199	0.512468
1	-5.939585	1.177481	0.322323
1	-4.534790	-2.889694	-0.248555
1	-6.821945	-3.693231	-0.056971
6	-3.755126	-0.207419	-0.074143
1	-3.693592	0.868876	0.039800
6	-2.484713	-0.816015	-0.294945
6	-1.338435	0.005644	-0.309433
6	-0.134158	1.871529	-0.203164
6	0.909149	0.951636	-0.418866
6	0.027075	3.315866	-0.003273
6	-0.863068	3.981795	0.852139
6	1.027496	4.052158	-0.650939
6	-0.737609	5.345933	1.072255
1	-1.642198	3.413205	1.346296
6	1.145009	5.419506	-0.433281
1	1.692437	3.575212	-1.361154
6	0.268498	6.068805	0.432609
1	-1.424878	5.847860	1.744911
1	1.917439	5.979682	-0.948903
6	-9.014110	-2.219711	0.347524
7	-10.102758	-2.615546	0.436838
6	-2.274563	-2.201556	-0.514112
7	-2.035809	-3.323953	-0.701019
16	0.297706	-0.636687	-0.552708
7	-1.365110	1.326926	-0.139517
1	0.364870	7.135717	0.603811
6	2.371034	1.216257	-0.498584
1	2.677267	1.492538	-1.513757
1	2.660991	2.022669	0.178872
8	3.046982	0.005357	-0.130899
6	4.379823	0.019455	-0.228642
8	5.019279	0.981594	-0.589592
6	4.962688	-1.310478	0.167269
1	4.641009	-1.541184	1.188195
1	4.537928	-2.081903	-0.484175
7	6.396361	-1.249409	0.061480

1	6.822162	-0.391502	-0.262452
6	7.165805	-2.304262	0.395348
8	6.735678	-3.376265	0.801171
8	8.471335	-2.030171	0.225972
6	9.381798	-3.088074	0.554223
1	9.285177	-3.361292	1.605920
1	9.193454	-3.961152	-0.072180
1	10.373610	-2.686989	0.356675

Mol7_s0r_DMSO.out

C	-7.27018400	0.19270000	0.91526400
C	-5.94487300	0.51759600	0.69289700
C	-5.02990600	-0.41938400	0.14858300
C	-5.52230900	-1.70659200	-0.15938600
C	-6.85171900	-2.04569800	0.05968200
C	-7.73727000	-1.09594900	0.59963800
H	-7.96322000	0.91555600	1.33156400
H	-5.59428500	1.51499700	0.94042000
H	-4.86803300	-2.46090400	-0.57487700
H	-7.18886900	-3.04343800	-0.18959200
C	-3.67154500	0.02807900	-0.04133300
H	-3.48397200	1.05272400	0.26827300
C	-2.56156300	-0.59859500	-0.54375000
C	-1.27982200	0.11316100	-0.61527300
C	0.20018000	1.76817700	-0.39592700
C	1.04457400	0.82608600	-0.94929500
C	0.56626400	3.14199900	0.00642900
C	0.11317600	3.64757500	1.23675800
C	1.34639600	3.96511800	-0.82158300
C	0.45358100	4.93888200	1.63897300
H	-0.49874100	3.01836300	1.87449000
C	1.68721200	5.25766800	-0.41641400
H	1.66010900	3.60836600	-1.79733600
C	1.24592300	5.74663500	0.81578600
H	0.10291700	5.31453400	2.59531800
H	2.28701200	5.88420500	-1.06913000
C	-2.55797900	-1.94182200	-1.02253400
N	-2.50494800	-3.03433800	-1.42588300
S	0.16172500	-0.64283700	-1.27216100
N	-1.09920400	1.34518200	-0.20868300
H	1.50984600	6.75179400	1.12949100
C	2.50646900	0.91051300	-1.20757700
H	2.76219500	0.76041900	-2.25953700
H	2.90045100	1.87311600	-0.88255800
O	3.15637100	-0.14548400	-0.43235900
C	4.48490900	-0.23308100	-0.55177300
O	5.16767400	0.50383700	-1.24029400
C	5.02553100	-1.37246100	0.28528400
H	4.72768900	-1.21293200	1.32790600
H	4.54870800	-2.30306500	-0.04427700
N	6.46142600	-1.42888800	0.14475400
H	6.90882200	-0.75673600	-0.46505900
C	7.20110700	-2.34917100	0.80248800
O	6.74518300	-3.20246100	1.56093100
O	8.51756900	-2.20851500	0.51630000
C	9.40404100	-3.14073100	1.16619300
H	9.33820200	-3.03708600	2.25116500
H	9.15969200	-4.16490900	0.87702300
H	10.40153100	-2.87575700	0.81915900
O	-9.04635400	-1.32985900	0.84886800
C	-9.58614600	-2.62500400	0.55170800
H	-10.63728700	-2.57457800	0.83155700
H	-9.49766000	-2.84752100	-0.51615600
H	-9.08344300	-3.39979000	1.13884300

Mol7_s1r_DMSO.out

C	-7.34488285	-0.09504394	0.34301746
C	-6.05013217	0.35481599	0.23751486
C	-4.94812214	-0.54223311	0.01662887
C	-5.27037468	-1.93534725	-0.08704066
C	-6.57557290	-2.39021532	0.02036856
C	-7.62811333	-1.47847784	0.23560400
H	-8.16699463	0.59330136	0.50919287
H	-5.84508498	1.41794631	0.32197419
H	-4.48635519	-2.66201451	-0.25114752
H	-6.77217759	-3.45187664	-0.06328854
C	-3.65218505	0.00659937	-0.07434835

H	-3.57060867	1.08127158	0.04239504
C	-2.39311679	-0.63876880	-0.29981384
C	-1.21637423	0.16178642	-0.30642220
C	0.07406576	1.98675365	-0.19116634
C	1.08878219	1.03355143	-0.41336046
C	0.27548015	3.42100867	0.00600457
C	-0.64668476	4.13433696	0.80392449
C	1.34351595	4.12480383	-0.58855570
C	-0.48258160	5.49725942	1.02649432
H	-1.47473656	3.59709346	1.25120838
C	1.49746737	5.49138132	-0.36952077
H	2.02629218	3.62291784	-1.26333660
C	0.59202287	6.18149513	0.44444856
H	-1.19030696	6.02947468	1.65392867
H	2.31712430	6.02119464	-0.84361437
C	-2.21078983	-2.01949279	-0.53083146
N	-1.98294833	-3.15304231	-0.72956450
S	0.41501678	-0.55014590	-0.56441410
N	-1.19080068	1.47862919	-0.12572775
H	0.71782841	7.24557903	0.61668253
C	2.56176558	1.24007873	-0.49247457
H	2.89139962	1.46102663	-1.51483602
H	2.88156380	2.05775124	0.15759798
O	3.20055555	0.01308761	-0.06650435
C	4.53288204	-0.04572144	-0.21590114
O	5.21251920	0.85894252	-0.66020894
C	5.06170157	-1.38556437	0.24242986
H	4.77374130	-1.53473256	1.28964359
H	4.56679807	-2.17219482	-0.33909996
N	6.49483262	-1.41711180	0.07258354
H	6.95256512	-0.59818461	-0.30606660
C	7.21978588	-2.50912621	0.40505449
O	6.74966851	-3.54593314	0.86800891
O	8.53655191	-2.31003861	0.16046718
C	9.40777981	-3.41411773	0.47640664
H	9.34636085	-3.65684234	1.53915754
H	9.14429769	-4.29058554	-0.11913844
H	10.40891067	-3.06937410	0.22248570
O	-8.93032382	-1.82308442	0.35239606
C	-9.29448137	-3.20617277	0.25615989
H	-10.37597097	-3.23367093	0.37946295
H	-9.02092425	-3.61128547	-0.72341705
H	-8.81436626	-3.78910966	1.04880232

Mol8_s0r_DMSO.out

C	-6.63135200	0.39402200	0.60611500
C	-5.28653500	0.70576000	0.44075700
C	-4.36143600	-0.24883500	-0.03623600
C	-4.83799700	-1.54145700	-0.34523300
C	-6.18011900	-1.86380700	-0.18393500
C	-7.06557600	-0.89309100	0.29038900
H	-7.32748200	1.13853400	0.97344000
H	-4.94174700	1.70555200	0.68507400
H	-4.16853300	-2.30657300	-0.71291300
H	-6.53335000	-2.85947700	-0.42452600
C	-2.98503200	0.18993700	-0.16609800
H	-2.80705600	1.22165500	0.12355900
C	-1.86168000	-0.46037900	-0.58882200
C	-0.56843600	0.23721300	-0.61530000
C	0.91075100	1.88581600	-0.36323500
C	1.77224300	0.92099700	-0.84930300
C	1.26907200	3.26591900	0.02163900
C	0.73636100	3.81632800	1.19992600
C	2.12103800	4.05103700	-0.77183900
C	1.06845100	5.11434400	1.58657000
H	0.06937300	3.21626800	1.80985400
C	2.45308700	5.35057500	-0.38205100
H	2.49807700	3.66087400	-1.71168900
C	1.93203200	5.88416200	0.79935500
H	0.65595000	5.52488800	2.50303600
H	3.10893200	5.94755600	-1.00795500
C	-1.84375700	-1.82049600	-1.02496400
N	-1.77371900	-2.92445900	-1.39012400
S	0.89523600	-0.54706900	-1.17880500
N	-0.39916600	1.47686900	-0.23101200
H	2.18949600	6.89463500	1.10106200
C	3.24448500	0.99463100	-1.05250100
H	3.53192900	0.91502300	-2.10422500
H	3.64119900	1.92672300	-0.64932900
O	3.84842400	-0.12248700	-0.33371200

C	5.17396900	-0.25502300	-0.45549500
O	5.88590800	0.49049500	-1.10329000
C	5.66681300	-1.45590700	0.32228800
H	5.37648600	-1.33497900	1.37234100
H	5.15142400	-2.34860900	-0.05084300
N	7.09879200	-1.56542700	0.17451400
H	7.57489200	-0.87817600	-0.39537100
C	7.79809200	-2.55479600	0.77364200
O	7.30574400	-3.43144900	1.48086900
O	9.11918100	-2.45426900	0.49218700
C	9.96478200	-3.46201000	1.08096900
H	9.90478400	-3.42181200	2.17048900
H	9.67565900	-4.45506900	0.73092100
H	10.97250600	-3.22008200	0.74691600
Br	-8.90249400	-1.33916200	0.50911800

Mol8_s0r_DMSO.out
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C	-6.64484600	0.33254600	0.26950600
C	-5.33097800	0.71054900	0.15834300
C	-4.28455600	-0.24603400	-0.07030900
C	-4.67685200	-1.62146400	-0.17447600
C	-5.99660900	-1.99506500	-0.06311300
C	-6.98079600	-1.02536600	0.15745400
H	-7.41721600	1.07276600	0.44170600
H	-5.06671400	1.75953600	0.24357500
H	-3.93532400	-2.38986300	-0.34116700
H	-6.27313300	-3.03978500	-0.14427100
C	-2.97402800	0.23216500	-0.16296200
H	-2.83265700	1.29892300	-0.03564700
C	-1.75106800	-0.47112400	-0.40474100
C	-0.54187800	0.25091700	-0.40095400
C	0.81547600	2.00556400	-0.23036600
C	1.77639100	1.02246400	-0.49268400
C	1.09984000	3.42784400	0.01589800
C	0.34492000	4.11604800	0.97468100
C	2.09047200	4.11660500	-0.69318400
C	0.59403600	5.45690800	1.23475100
H	-0.42873900	3.58434300	1.51690800
C	2.33372100	5.46114100	-0.43433100
H	2.64940300	3.61939200	-1.47819800
C	1.59142200	6.13285100	0.53324400
H	0.01028000	5.97670800	1.98714800
H	3.09860500	5.98574600	-0.99683800
C	-1.65339100	-1.85873000	-0.67608000
N	-1.50217700	-2.98917000	-0.90646600
S	1.03235500	-0.50964000	-0.69440200
N	-0.45882900	1.56531100	-0.17666100
H	1.78452200	7.18102400	0.73604800
C	3.25316900	1.17409400	-0.58255400
H	3.58745100	1.33535800	-1.61308800
H	3.59790700	2.01139600	0.02714100
O	3.84322900	-0.04751500	-0.10175500
C	5.16653700	-0.15736500	-0.23277500
O	5.87501500	0.70312800	-0.70680200
C	5.65094700	-1.48506400	0.28680700
H	5.35695300	-1.57422900	1.33804000
H	5.13391100	-2.28128100	-0.25891600
N	7.07819700	-1.56594200	0.12187900
H	7.56320000	-0.77706300	-0.28405500
C	7.76247500	-2.66682800	0.48927900
O	7.25633200	-3.66644800	0.98333200
O	9.07767800	-2.52978300	0.24411500
C	9.90134100	-3.64977500	0.59462300
H	9.83136200	-3.85475500	1.66377900
H	9.60300200	-4.53385900	0.02932000
H	10.91521000	-3.35628800	0.33090700
Br	-8.77738700	-1.54821600	0.30712300