Supplementary Information for

Effective Synthesis, Development and Application of a Highly Fluorescent Cyanine Dye for Antibody Conjugation and Microscopy Imaging

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Experimental Methods

All chemical reagents and solvents were purchased from Merck/Sigma Aldrich, ThermoFisher, or VWR International and used as received. NMR solvents were purchased from Eurisotop. Trastuzumab antibody was from Genentech Inc.

Reactions were monitored by LC-MS (Shimazu MS2020, Supelco Ascentis, 2.0 × 50 mm, 2.1 μm C18 column; using injection volume of 1 μl; a linear gradient of 5–98% MeCN/H_2O, with a constant 0.1% v/v TFA additive. Each run was 6 min in duration, at a flow rate of 0.8 ml min^{-1}; ESI, and the positive ion mode was also used. Reaction products were purified by gradient-elution preparative HPLC (HPLC Gilson 333 instrument, with UV detection at 220 nm) on a Phenomenex Gemini C18, 250×50.00 mm; 10 μm particle size, 110A column, using 0.2% v/v TFA in water and acetonitrile as the mobile phase components.

^{1}H NMR and ^{13}C NMR spectra were recorded in DMSO-d_6 solution at room temperature, on a Varian Unity Inova 600 spectrometer (at 600 MHz and 141 MHz for ^{1}H and ^{13}C/APT NMR spectra, respectively), and on a Varian Unity Inova 400 spectrometer (at 400 MHz and 101 MHz for ^{1}H and ^{13}C NMR spectra, respectively). All chemical shifts are quoted in parts per million (ppm), measured from the center of the signal except in the case of multiplets, which are quoted as a range. ^{1}H NMR and ^{13}C chemical shifts are referenced to the residual solvent peak of $(CD_3)_2SO$ (^{1}H referenced to 2.50 ppm and ^{13}C referenced to 39.52 ppm) or to TMS as the internal standard. Coupling constants are given with an accuracy of 0.1 Hz. Splitting patterns are abbreviated as follows: singlet (s), doublet (d), triplet (t), quartet (q), multiplet (m), broad singlet (bs) and combinations thereof. Assignment of spectra was aided by 2D NMR spectroscopy (^{1}H-^{13}C HSQC and HMBC).

High-resolution mass spectrometry (HRMS) analysis was performed on a Sciex TripleTOF 5600+ high-resolution tandem mass spectrometer equipped with DuoSpray ion source. Electrospray ionization was applied in the positive ion detection mode. Samples were dissolved in acetonitrile and flow-injected into 50% acetonitrile in water, at a flow rate of 0.2 mL/min. The resolution of the mass spectrometer was 35 000.

Computational Methods

All theoretical computations were carried out with the Gaussian16 program package (G16)[1], using standard convergence criteria for the gradients of the root mean square (RMS) Force, Maximum Force, RMS displacement, and maximum displacement vectors (3.0×10^{-4}, 4.5 ×

10^{-4}, 1.2×10^{-3} and 1.8×10^{-3}). Optimization and frequency calculations were carried out with the B3LYP method[2] using the 6-31G(d,p) basis set. The vibrational frequencies were computed at the same levels of theory, to confirm that all structures resided at minima on their potential energy hypersurfaces. Thermodynamic functions electronic energy (U), enthalpy (H), Gibbs' free energy (G) and entropy (S) were computed at 298.15 K. Reported values were obtained by using the Polarizable Continuum Model (PCM) using the integral equation formalism variant (IEFPCM) to model the solvent effect, using the default settings of G16 (ε = 78.3553 for water)[3,4]. To predict the wavelengths of the probes reliably, the vertical excitation was modelled by the TDB3LYP/6-31G(d,p) level of theory. The wavelengths of fluorescence emission was modelled by using geometry optimization obtained at the TD-B3LYP/6-31G(d,p) level of theory. The aromaticity[5] and olefinicity[6] values for the ground, excited and triplet states were calculated according to previous publications and described in the subsequent section. The Nucleus-Independent Chemical Shifts (NICS, given in ppm) were calculated by a method described elsewhere[7].

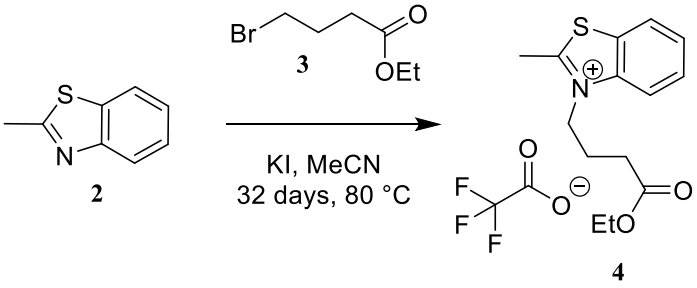
Fluorescent dye – antibody conjugates

Table S1. A collectioFluorescent antibody conjugates with different fluorescent dyes

Reference	mAb	Dye	Conjgation method	λ_{exc} [nm]	λ_{em} [nm]
Clin Cancer Res **2007,** *13*(10), 2936-2945	Trastuzumab	BODIPY-FL	Free amino-group coupling by acid	500	509
Clin Cancer Res **2007,** *13*(10), 2936-2945	Trastuzumab	Oregon Green 488	Free amino-group coupling by NHS ester	496	524
EJSO **2010**, *36*, 6-15	Cetuximab	Oregon Green 488	Free amino-group coupling by NHS ester	496	524
Clin Cancer Res **2007,** *13*(10), 2936-2945	Trastuzumab	FITC	Free amino-group coupling by ITC	495	525
Clin Cancer Res **2007,** *13*(10), 2936-2945	Trastuzumab	Rhodamine 6G	Free amino-group coupling by NHS ester	525	548
Chem Comm **2021**, *57*, 9760-9763	Rituximab	Cy3	Click reaction on modified Tyr	554	568
Chem Comm **2021**, *57*, 9760-9763	Rituximab	TAMRA	Click reaction on modified Tyr	552	578
Chem Comm **2021**, *57*, 9760-9763	Rituximab	ATTO590	Click reaction on modified Tyr	592	622
Eur J Med Chem **2023**, *252*, 115298	Trastuzumab	Cy5	Free amino-group coupling by NHS ester	649	667
Breast Cancer Res. 2012, 14, R61	Panitumumab	Alexa680	Free amino-group coupling by NHS ester	684	702
Eur Radiol **2004**, *14*, 1124–1129	Trastuzumab	Cy5.5	Free amino-group coupling by NHS ester	683	703
Mol Imaging **2021**, Article ID 5540569	Trastuzumab	IRDye800	Free amino-group coupling by NHS ester	775	792
Chin J Cancer Res **2016,** *28*(3):362-369	Trastuzumab	IRDye800	Free amino-group coupling by NHS ester	775	792
J. Nucl. Med. **2007**, *48* (9), 1501-1510	Trastuzumab	IRDye800	Free amino-group coupling by NHS ester	775	792
Breast Cancer Res. 2012, 14, R61	Trastuzumab	ICG	Free amino-group coupling by NHS ester	789	814

Synthesis of cyanine with azide functional group

*Synthesis of thiazole **2**.*



Scheme S1. The synthesis of thiazole **4.**

2-Methylbenzothiazole (**2**) (1.7 mL, 2.0 g, 13 mmol, 1.0 equiv.), ethyl 4-bromobutyrate (**3**) (2.3 mL, 3.1 g, 16 mmol, 1.3 equiv.) and potassium-iodide (1.1 g, 7.0 mmol, 0.5 equiv.) were dissolved in acetonitrile (8 mL), and the white, opaque mixture was stirred for 32 days at 80 °C. The reaction was monitored with HPLC-MS. After 11 days additional ethyl 4-bromobutyrate (**3**) (1. mL, 7.0 mmol, 0.5 equiv.) was added. The white precipitate was filtered off then the residual brown solution was evaporated, resulting 4.7 g of crude product (brown solid). 0.9 g of the crude product was purified by preparative HPLC (0.2% TFA in water–acetonitrile, using the gradient method). After purification, the pure product was lyophilized, resulting 0.528 g of 3-(4-ethoxy-4-oxobutyl)-2-methylbenzo[d]thiazol-3-ium TFA salt (**4**, yield: 78% (calc. for the portion), HPLC purity: 96%) as a brown oil.

*Spectroscopic data of **4***

^{1}H NMR (400 MHz, DMSO-*d6*) δ = 8.44 (dd, J = 8.2, 1.2 Hz, 1H, H_{10}), 8.37 (d, J = 8.5 Hz, 1H, H_7), 7.91 (ddd, J = 8.5, 7.2, 1.3 Hz, 1H, H_8), 7.85 – 7.76 (m, 1H, H_9), 4.77 – 4.68 (m, 2H, H_{11}), 4.04 (q, J = 7.1 Hz, 2H, H_{18}), 3.21 (s, 3H, H_1), 2.60 (t, J = 7.1 Hz, 2H, H_{13}), 2.10 (tq, J = 7.4, 5.1, 3.2 Hz, 2H, H_{12}), 1.16 (t, J = 7.1 Hz, 3H, H_{17}). ^{13}C NMR (101 MHz, DMSO-*d6*) δ = 177.6, 172.3, 140.9, 129.5, 129.2, 128.1, 124.7, 116.7, 60.2, 48.27, 30.1, 22.9, 16.8, 14.1.

HRMS (ESI/Q-TOF) *m*/*z*: $[M]^+$ Calc. for $C_{14}H_{18}NO_2S^+$ 264.1053; found 264.1048.

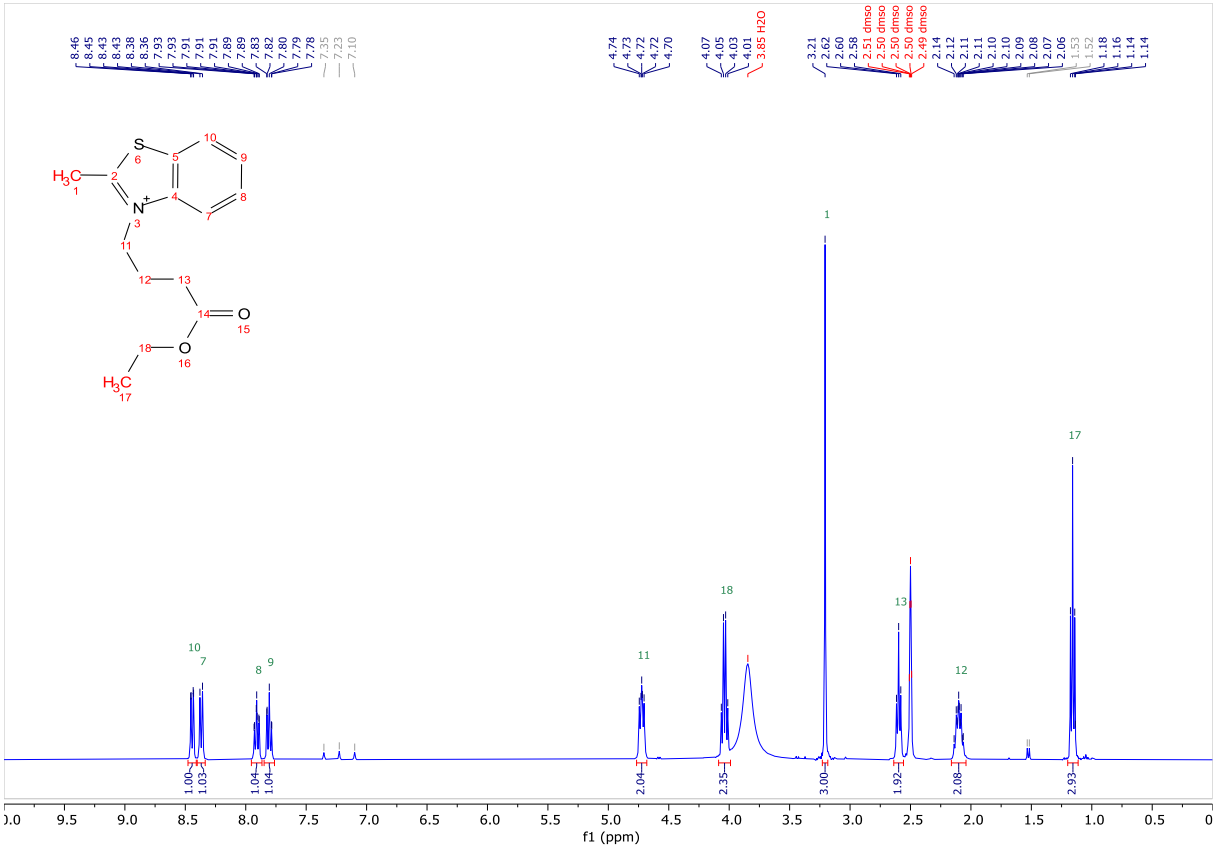


Figure S1. ^{1}H NMR spectrum of **4** recorded at 400 MHz in DMSO-d_6.

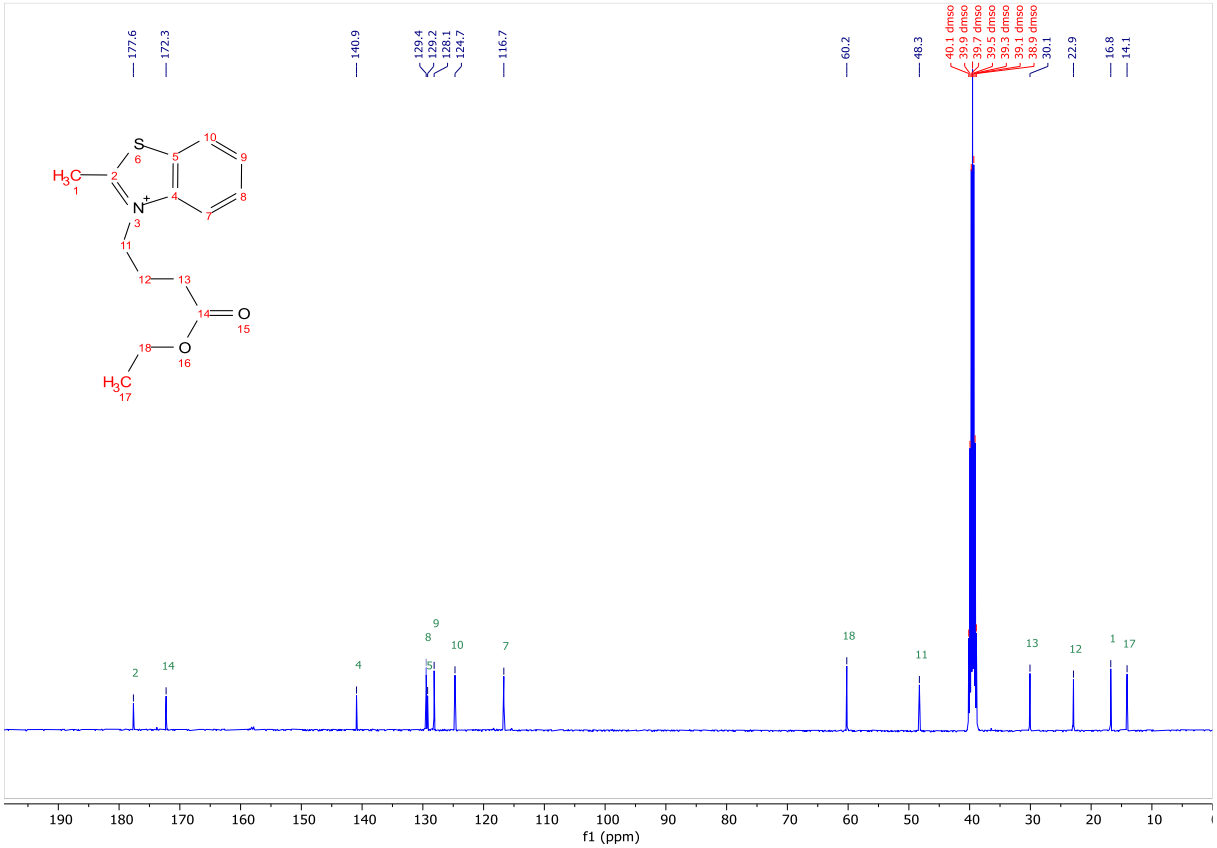


Figure S2. ^{13}C NMR spectrum of **4** recorded at 101 MHz in DMSO-d_6.

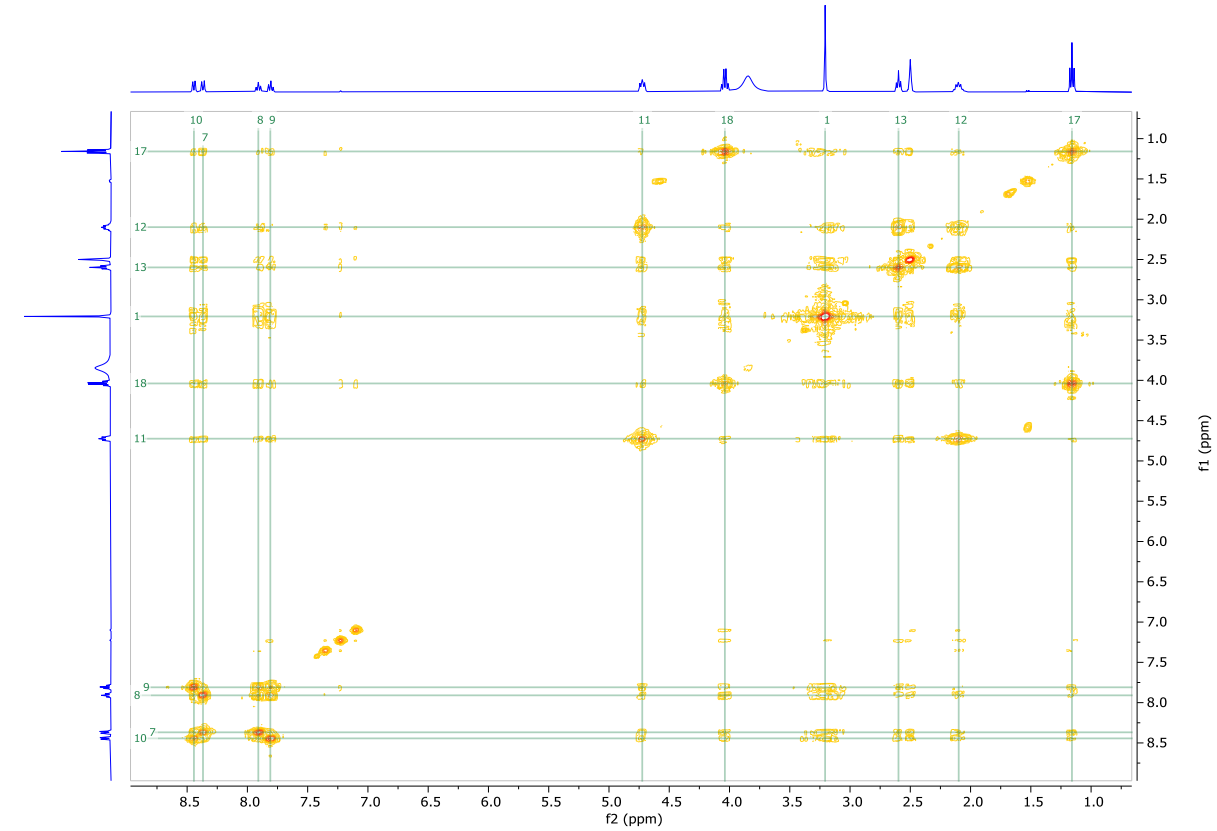


Figure S3. COSY spectrum of **4** recorded at 400 MHz in DMSO-d_6.

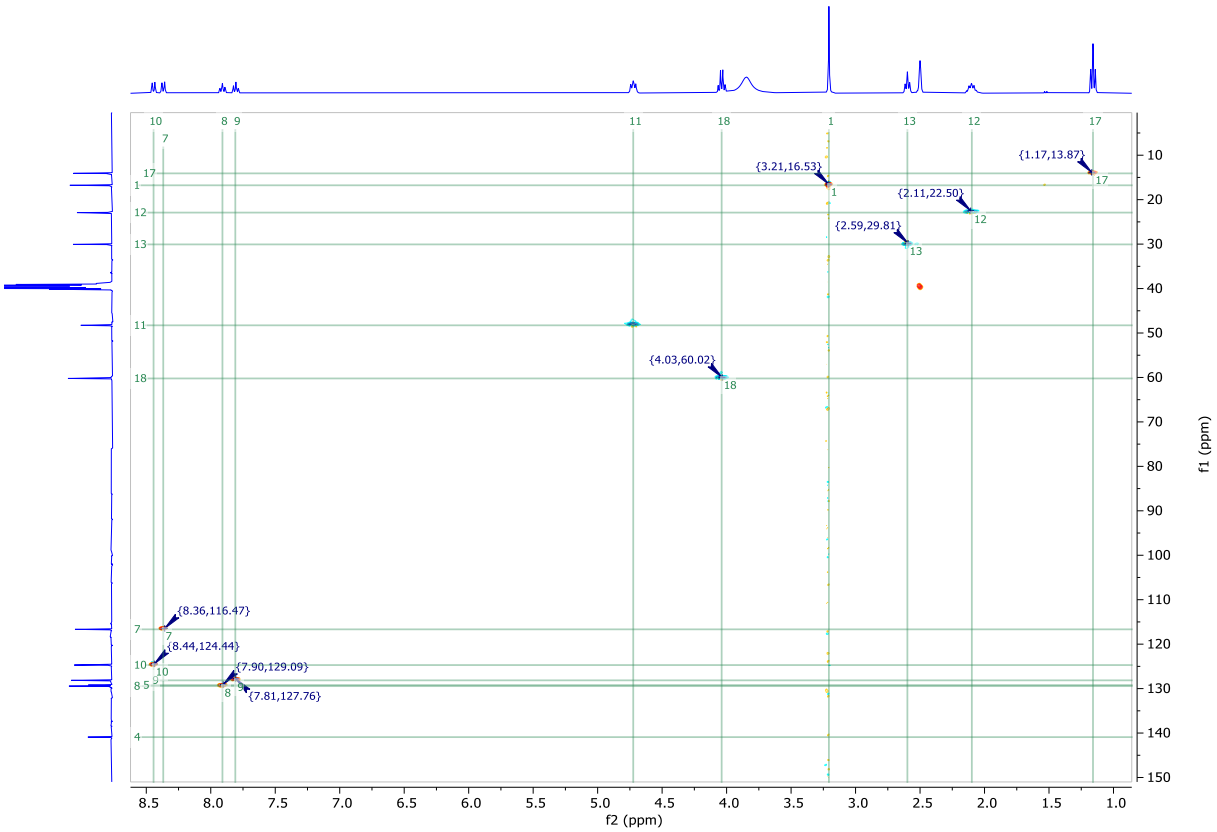


Figure S4. HSQC spectrum of **4** recorded at 400 MHz and 101 MHz in DMSO-d_6.

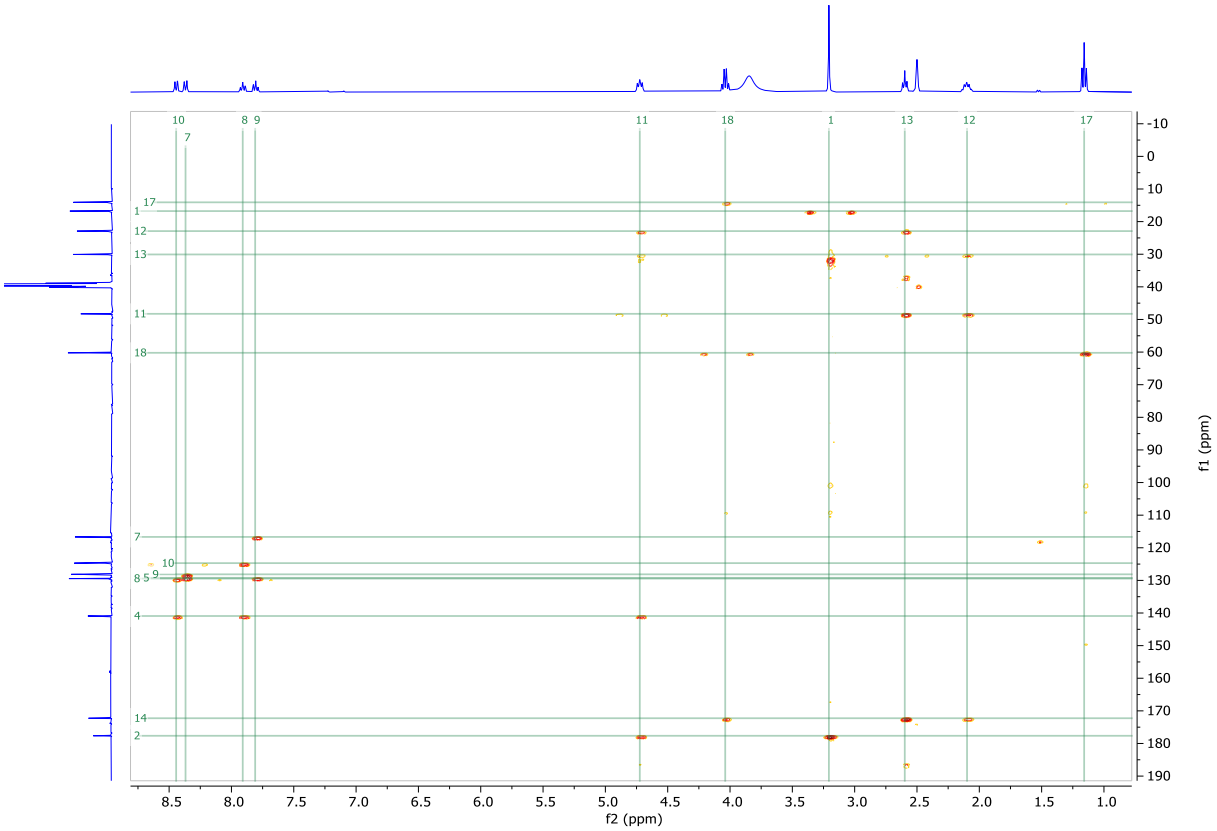


Figure S5. HMBC spectrum of **4** recorded at 400 MHz and 101 MHz in DMSO-d_6.

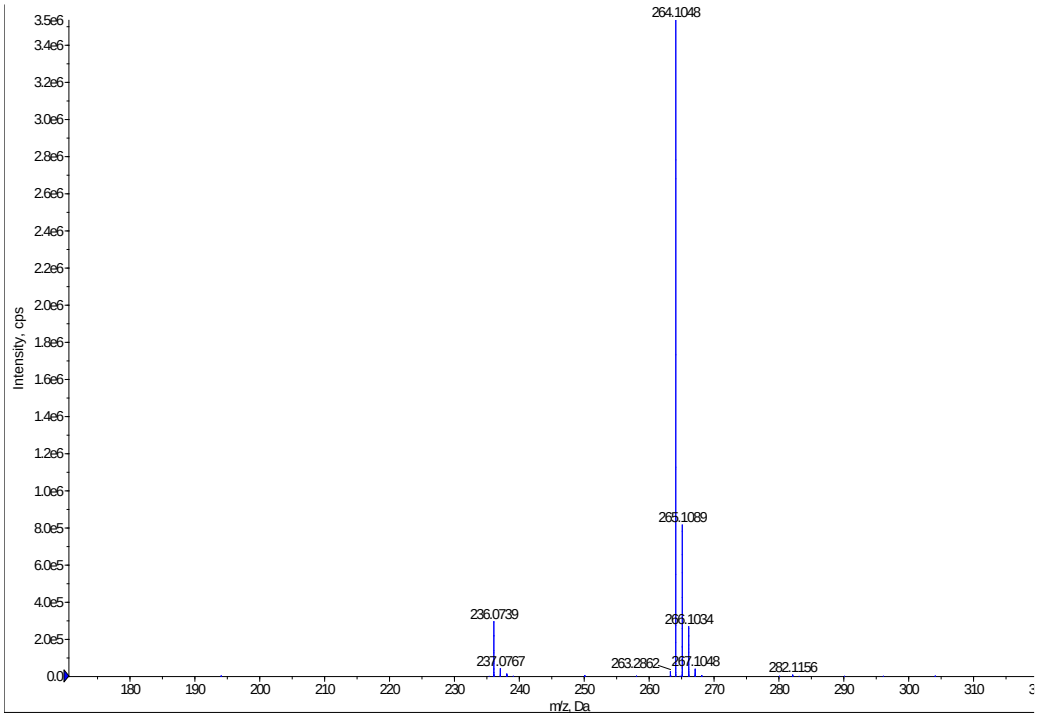
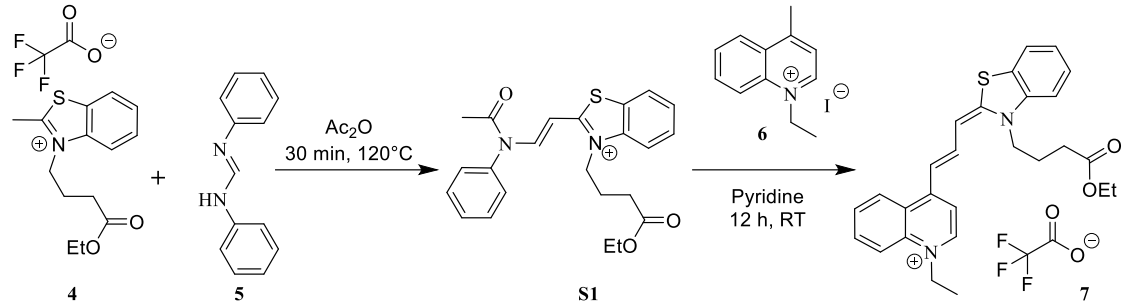


Figure S6. HRMS spectrum of **4**.

*Synthesis of cyanine ester **7**.*



Scheme S2. The synthesis of cyanine ester **7**.

A solution of indolium salt (**4**, 240 mg, 0.69 mmol, 1.0 equiv.) and *N*,*N*-diphenylformamidine (**5**, 164 mg, 0.83 mmol, 1.2 equiv.) in acetic anhydride (3 mL) was heated in an oil bath at 120 °C for 30 minutes. The pink solution turned to brown after 30 minutes. After the indolium salt was converted to the intermediate **S1** (monitored with HPLC-MS) the reaction mixture was cooled to room temperature. 1-ethyl-4-methylquinolin-1-ium iodide (**6**, 292 mg; 0.97 mmol, 1.4 equiv.) in dry pyridine (2 mL) was added. The solution turned deep red. The mixture was stirred at room temperature for 12 hours. The mixture was cooled down using an icy water bath, and 2 mL MeOH was added to the reaction mixture to quench the acetic anhydride. The solvent was removed under reduced pressure. The crude product was purified by preparative HPLC (0.2% TFA in water–acetonitrile, using the gradient elution). After purification, the pure product was lyophilized, resulting 80 mg TFA salt of the cyanine ester (**7**, yield: 16%, HPLC purity: 76%) as a blue powder.

*Spectroscopic data of **7***

^{1}H NMR (600 MHz, DMSO-*d6*) δ = 8.46 – 8.41 (m, 2H, H_{22}, H_{23}), 8.12 (t, J = 12.8 Hz, 1H, H_{16}), 8.08 (d, J = 8.7 Hz, 1H, H_{27}), 7.95 (ddd, J = 8.6, 6.9, 1.3 Hz, 1H, H_{26}), 7.84 (ddd, J = 10.2, 7.1, 3.3 Hz, 2H, H_7, H_{10}), 7.70 (ddd, J = 8.2, 6.9, 1.0 Hz, 1H, H_{25}), 7.57 (d, J = 8.2 Hz, 1H, H_{24}), 7.46 (ddd, J = 8.4, 7.3, 1.3 Hz, 1H, H_8), 7.31 – 7.25 (m, 1H, H_9), 7.05 (d, J = 13.3 Hz, 1H, H_{17}), 6.51 (d, J = 12.2 Hz, 1H, H_1), 4.59 (q, J = 7.1 Hz, 2H, H_{28}), 4.24 (t, J = 7.7 Hz, 2H, H_{11}), 4.06 (q, J = 7.1 Hz, 2H, H_{32}), 2.54 (t, J = 7.2 Hz, 2H, H_{13}), 1.98 (p, J = 7.3 Hz, 2H, H_{12}), 1.45 (t, J = 7.2 Hz, 3H, H_{29}), 1.17 (t, J = 7.1 Hz, 3H, H_{31}).^{13}C NMR (151 MHz, DMSO-*d6*) δ = 172.3, 160.9, 150.4, 143.8, 142.3, 141.4, 137.7, 133.5, 127.6, 126.7, 125.2, 124.7, 124.3, 124.1, 122.6, 117.8, 112.2, 110.0, 109.4, 98.3, 60.1, 49.4, 44.7, 30.3, 22.1, 14.7, 14.1.

HRMS (ESI/Q-TOF) *m*/*z*: $[M]^+$ Calc. for $C_{27}H_{29}N_2O_2S^+$ 445.1949; found 445.1954.

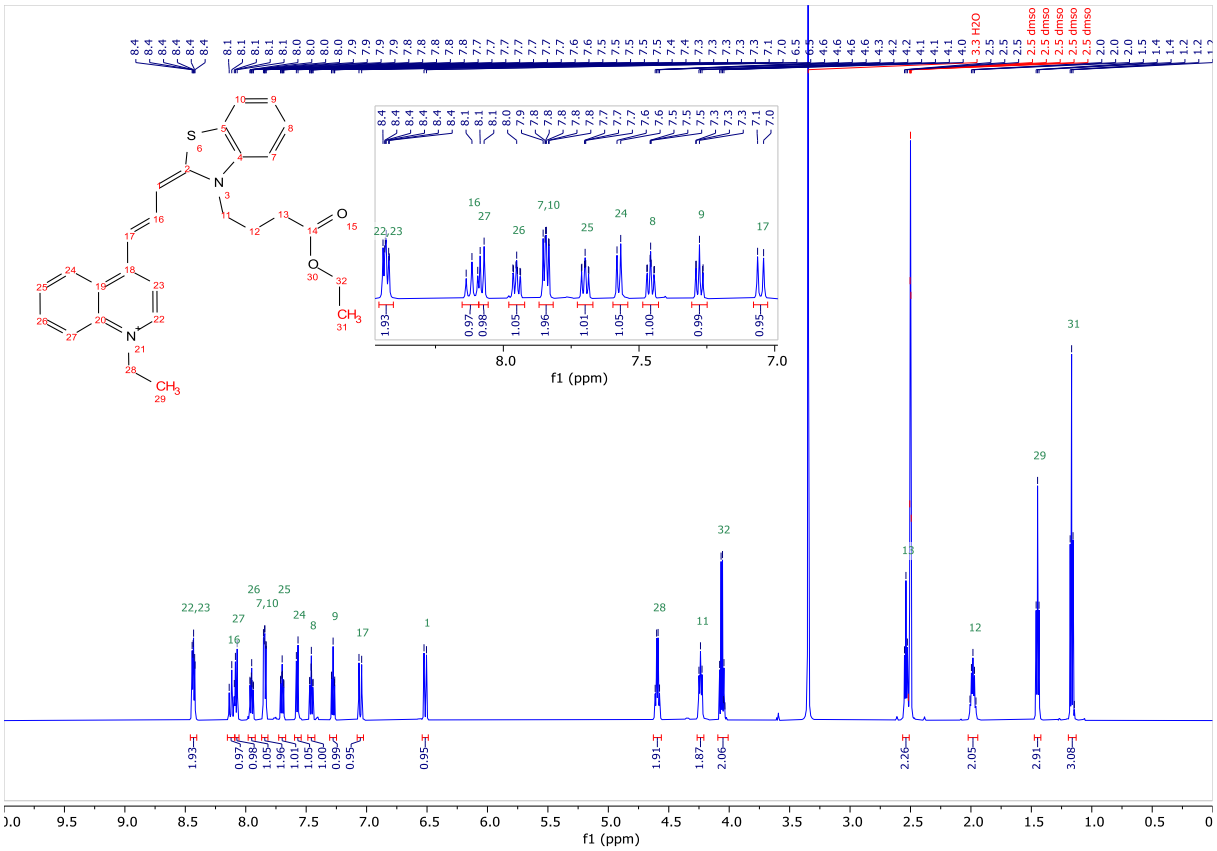


Figure S7. ^{1}H NMR spectrum of **7** recorded at 600 MHz in DMSO-d_6.

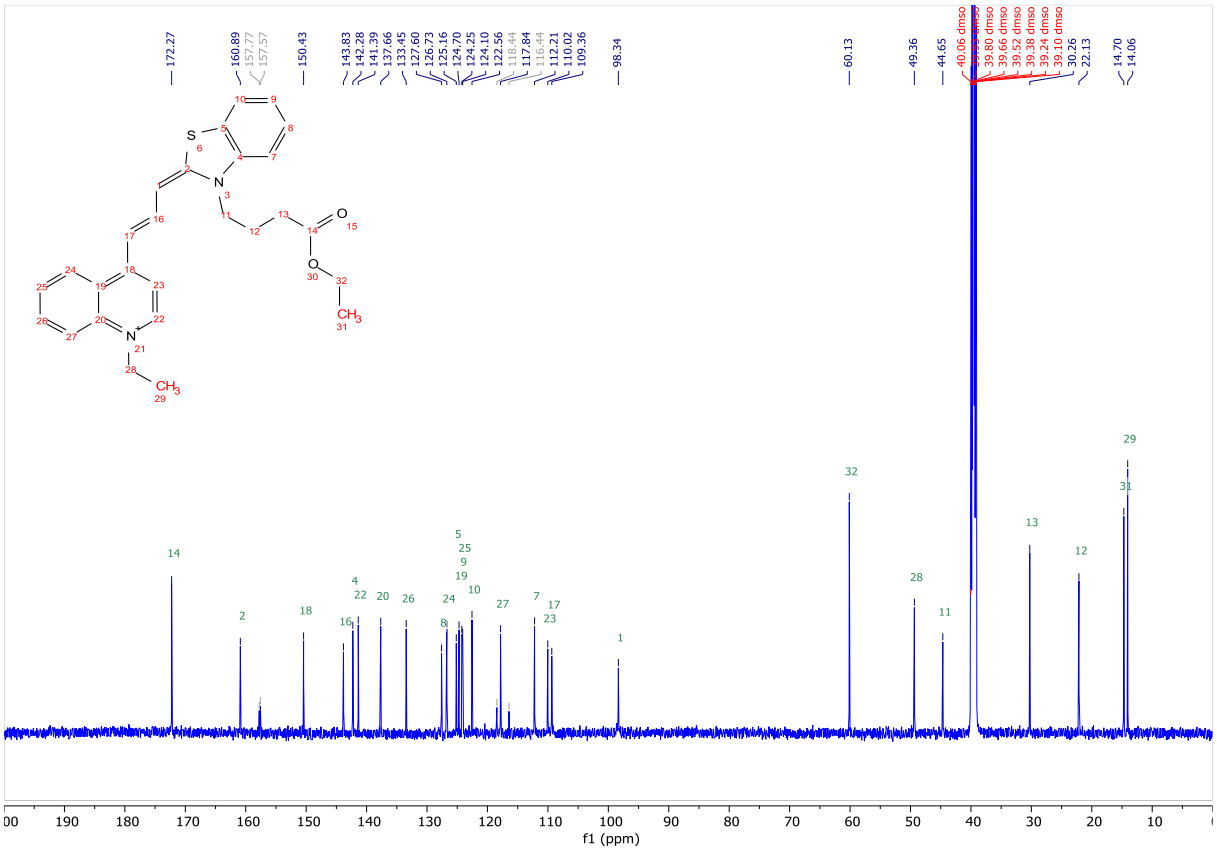


Figure S8. ^{13}C NMR spectrum of **7** recorded at 151 MHz in DMSO-d_6.

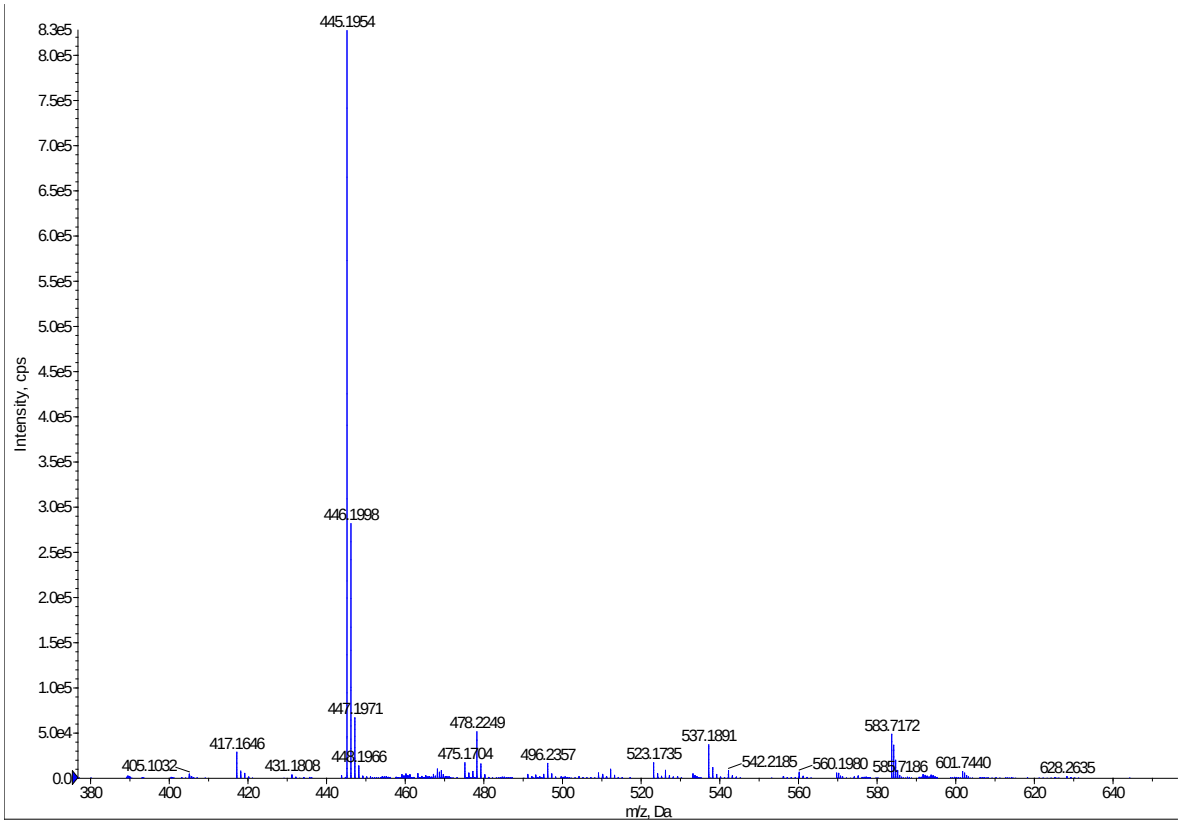
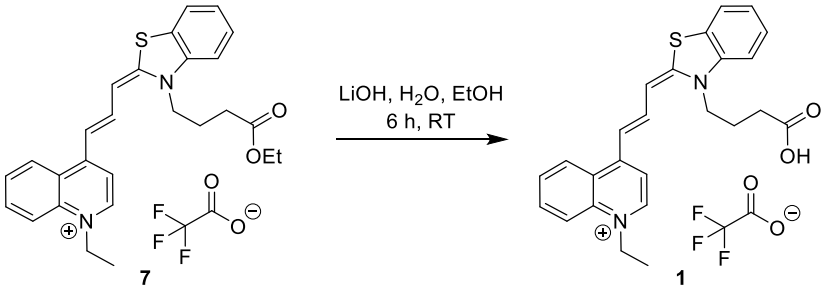


Figure S9. HRMS spectrum of **7**.

*Synthesis of cyanine carboxylic acid **1**.*



Scheme S3. The synthesis of cyanine carboxylic acid **1**.

The TFA salt of cyanine ester **6** (62 mg, 0.11 mmol, 1.0 equiv.) was dissolved in EtOH (1 mL). LiOH (5 mg, 0.22 mmol, 2.0 equiv.) dissolved in a drop of water was added. The solution was stirred at room temperature. After 2 hours, 4 mg LiOH (0.18 mmol, 1.6 equiv.) was added and stirred for an additional 2 hours, then 10 mg LiOH (0.44 mmol, 4.0 equiv.) was added to the mixture and stirred for an additional 2 hours. The solution was neutralized with 4 droplets of 1 M HCl solution, then the solvent was removed under reduced pressure. The crude product was purified by preparative HPLC (0.2% TFA in water–acetonitrile, using gradient elution).

After purification, the pure product was lyophilized, resulting in 40 mg of the cyanine carboxylic acid TFA salt **1** (yield: 85%, HPLC purity: 98%) as a blue powder.

HRMS (ESI/Q-TOF) *m/z*: $[M]^+$ Calc. for $C_{25}H_{25}N_2O_2S^+$ 417.1636; found 417.1651.

*Spectroscopic data of **1***

^{1}H NMR (600 MHz, DMSO-*d6*) δ = 8.46 (dd, J = 7.4, 2.9 Hz, 2H, H_{23}, H_{24}), 8.16 (t, J = 12.8 Hz, 1H, H_{17}), 8.10 (d, J = 8.8 Hz, 1H, H_{28}), 7.97 (ddd, J = 8.6, 6.8, 1.4 Hz, 1H, H_{27}), 7.89 (dd, J = 7.5, 5.6 Hz, 2H, H_7, H_{10}), 7.72 (t, J = 7.7 Hz, 1H, H_{26}), 7.62 (d, J = 8.2 Hz, 1H, H_{25}), 7.53 – 7.47 (m, 1H, H_8), 7.31 (t, J = 7.6 Hz, 1H, H_9), 7.08 (d, J = 13.3 Hz, 1H, H_{18}), 6.56 (d, J = 12.2 Hz, 1H, H_1), 4.61 (q, J = 7.2 Hz, 2H, H_{29}), 4.25 (t, J = 7.8 Hz, 2H, H_{11}), 2.47 (t, J = 7.2 Hz, 2H, H_{13}), 1.95 (p, J = 7.3 Hz, 2H, H_{12}), 1.45 (t, J = 7.2 Hz, 3H, H_{30}). ^{13}C NMR (151 MHz, DMSO-*d6*) δ = 173.8, 160.9, 150.5, 144.0, 142.3, 141.4, 137.7, 133.5, 127.7, 126.8, 125.2, 124.8, 124.3, 124.2, 122.7, 117.8, 112.3, 110.1, 109.4, 98.6, 49.4, 44.8, 30.3, 22.2, 14.7.

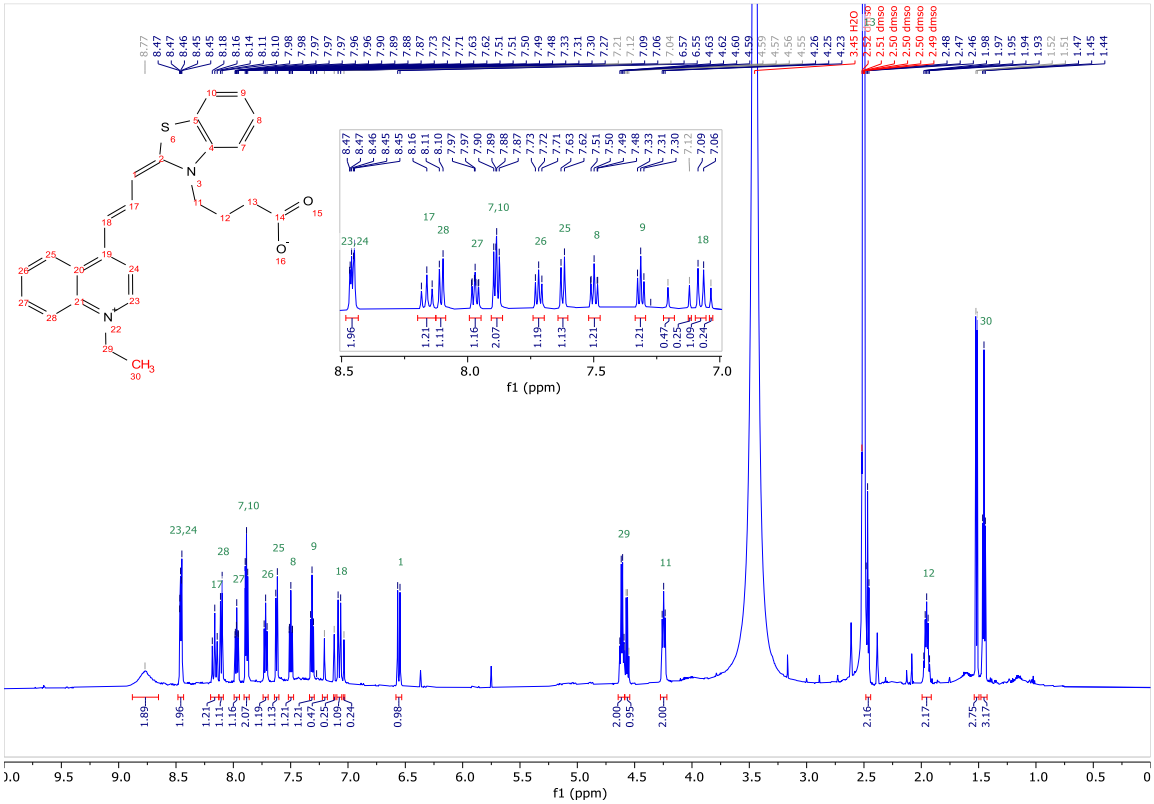


Figure S10. ^{1}H NMR spectrum of **1** recorded at 600 MHz in DMSO-d_6.

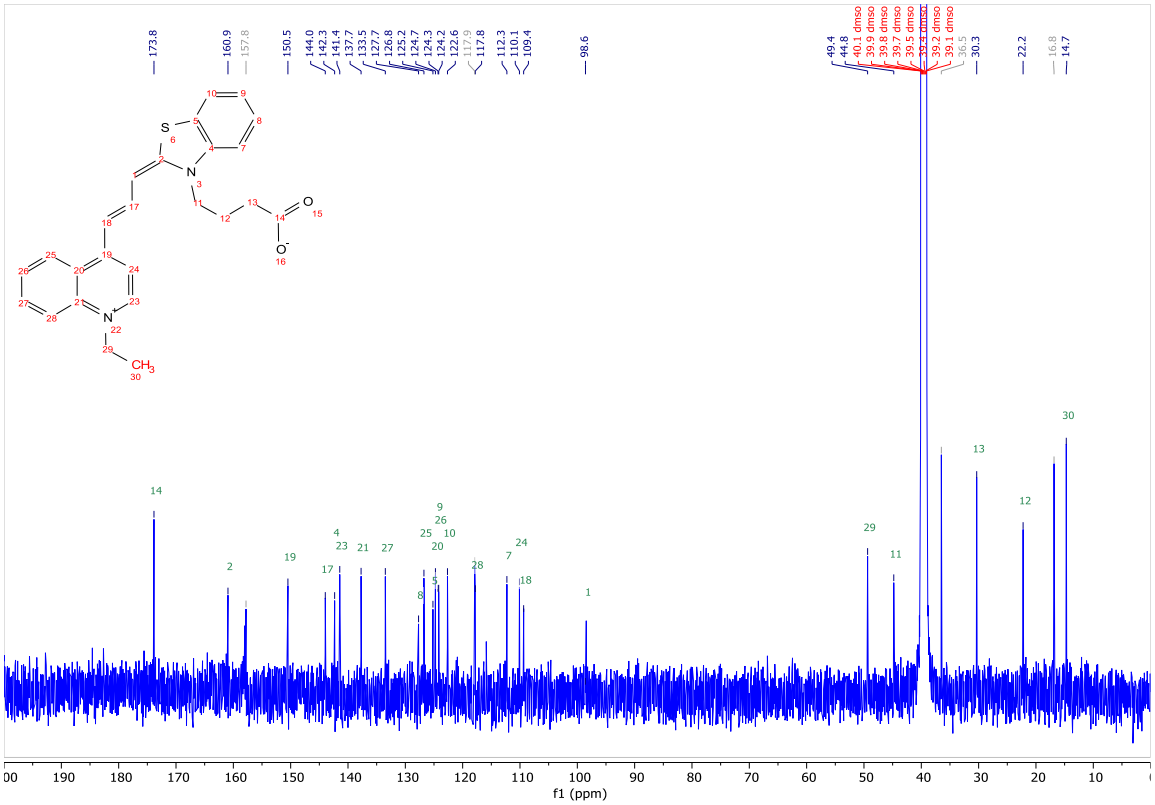


Figure S11. ^{13}C NMR spectrum of **1** recorded at 151 MHz in DMSO-d_6.

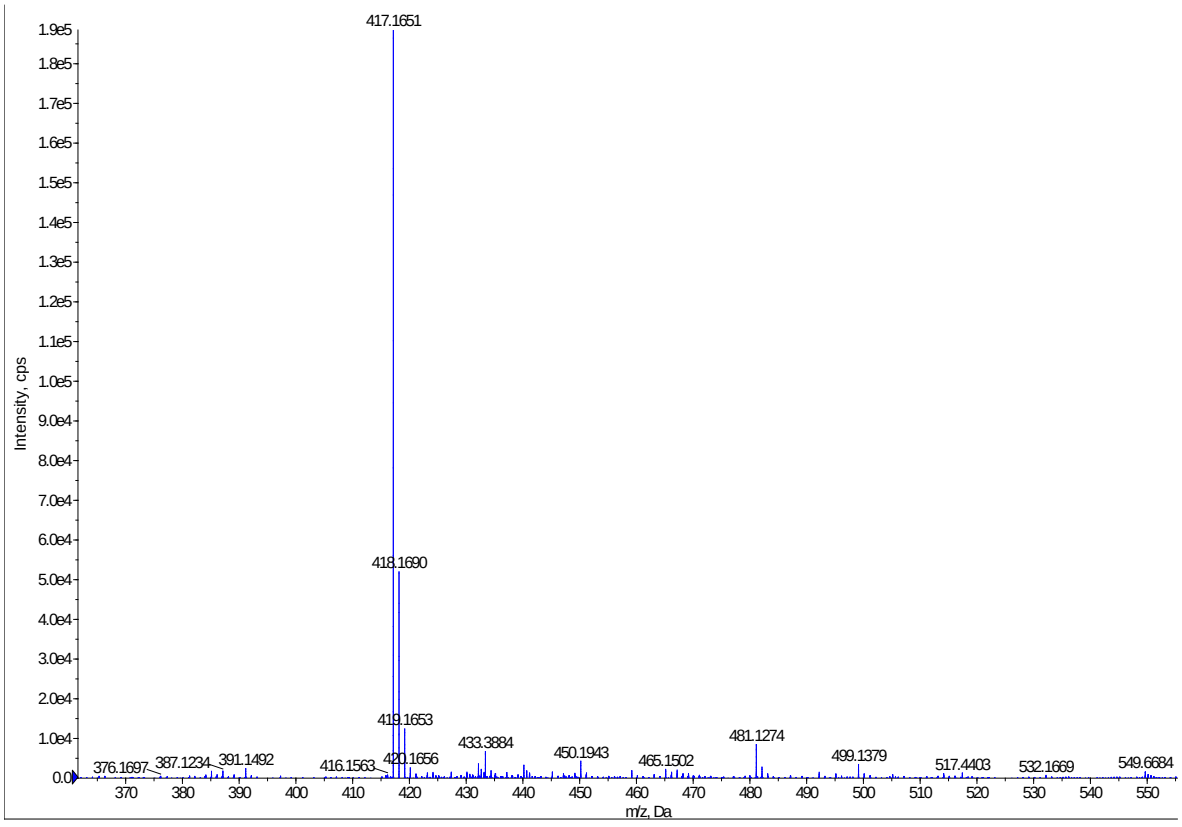
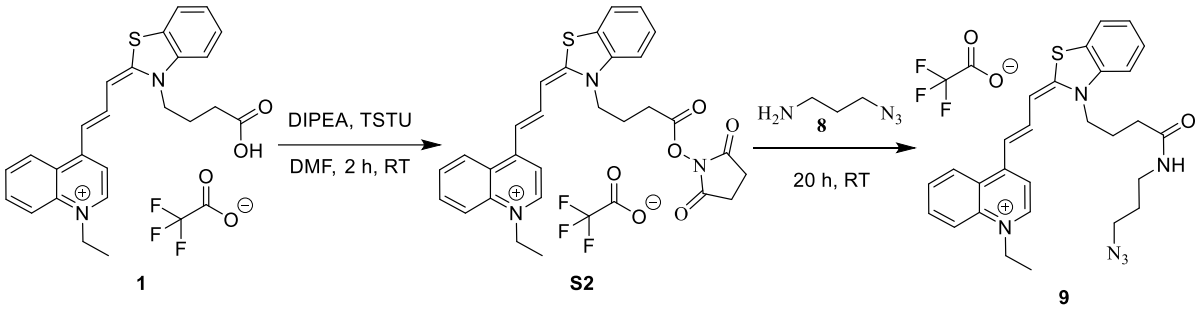


Figure S12. HRMS spectrum of **1**.

*Synthesis of cyanine dye with azide function (**9**)*



Scheme S4. The synthesis of cyanine dye with azide group (**9)**

The cyanine carboxylic acid TFA salt (**1**, 50 mg, 0.09 mmol, 1.0 equiv.) was dissolved in 1 mL dry DMF, then 0.31 ml DIPEA (233 mg, 1.8 mmol, 19 equiv.) was added to the solution. After cooling the mixture to 0 °C, a solution of 54 mg N,N,N′,N′-tetramethyl-O-(N-succinimidyl)uronium tetrafluoroborate, (TSTU, 0.18 mmol, 1.9 equiv.) in 1 mL of DMS was added, then the mixture was stirred for 2 hours at room temperature. The reaction was monitored with HPLC-MS, and after total conversion, 3-azidopropylamine (**8**, 120 mg, 1.2 mmol, 12.8 equiv.) was added to the mixture, and stirred at room temperature overnight. Due to the low conversion, additional 3-azidopropylamine (**8**) (120 mg, 1.2 mmol, 12.8 equiv.) was added to the solution, and after 30 minutes the solvent was evaporated under reduced pressure, resulting in a dark blue solid. The crude product was purified by preparative HPLC (0.2% TFA in water–acetonitrile, using the gradient elution). After purification, the pure product was lyophilized, resulting 23 mg of cyanine dye azide TFA salt **9** (yield: 40%, HPLC purity: >95%).

*Spectroscopic data of **9***

^{1}H NMR (400 MHz, Methanol-d_4) δ = 8.54 (s, 1H), 8.50 (d, J = 8.5 Hz, 1H), 8.21 (d, J = 7.0 Hz, 1H), 8.19 (t, J = 12.8 Hz, 1H), 8.00 (d, J = 8.7 Hz, 1H), 7.98 – 7.89 (m, 1H), 7.71 – 7.64 (m, 3H), 7.50 – 7.43 (m, 2H), 7.28 (ddd, J = 8.2, 6.6, 1.6 Hz, 1H), 7.08 (d, J = 13.4 Hz, 1H), 6.50 (d, J = 12.3 Hz, 1H), 4.57 (q, J = 7.2 Hz, 2H), 4.27 (t, J = 7.8 Hz, 2H), 3.36 (t, J = 6.7 Hz, 2H), 3.30 (t, J = 7.0 Hz, 2H), 2.43 (t, J = 6.7 Hz, 2H), 2.12 (p, J = 6.8 Hz, 2H), 1.77 (p, J = 6.8 Hz, 2H), 1.56 (t, J = 7.2 Hz, 3H). ^{13}C NMR (101 MHz, Methanol-d_4) δ = 173.4, 162.3, 152.0, 144.3, 141.9, 141.7, 138.4, 133.6, 127. 8, 126.8, 125.6, 125.4, 125.1, 124.4, 122.3, 117.4, 112.2, 109.6, 109.4, 98.4, 49.9, 49.0, 45.2, 36.8, 31.5, 28.6, 22.7, 13.9.

HRMS (ESI/Q-TOF) *m/z*: $[M]^+$ Calc. for $C_{28}H_{31}N_6OS^+$ 499.2275; found 499.2278

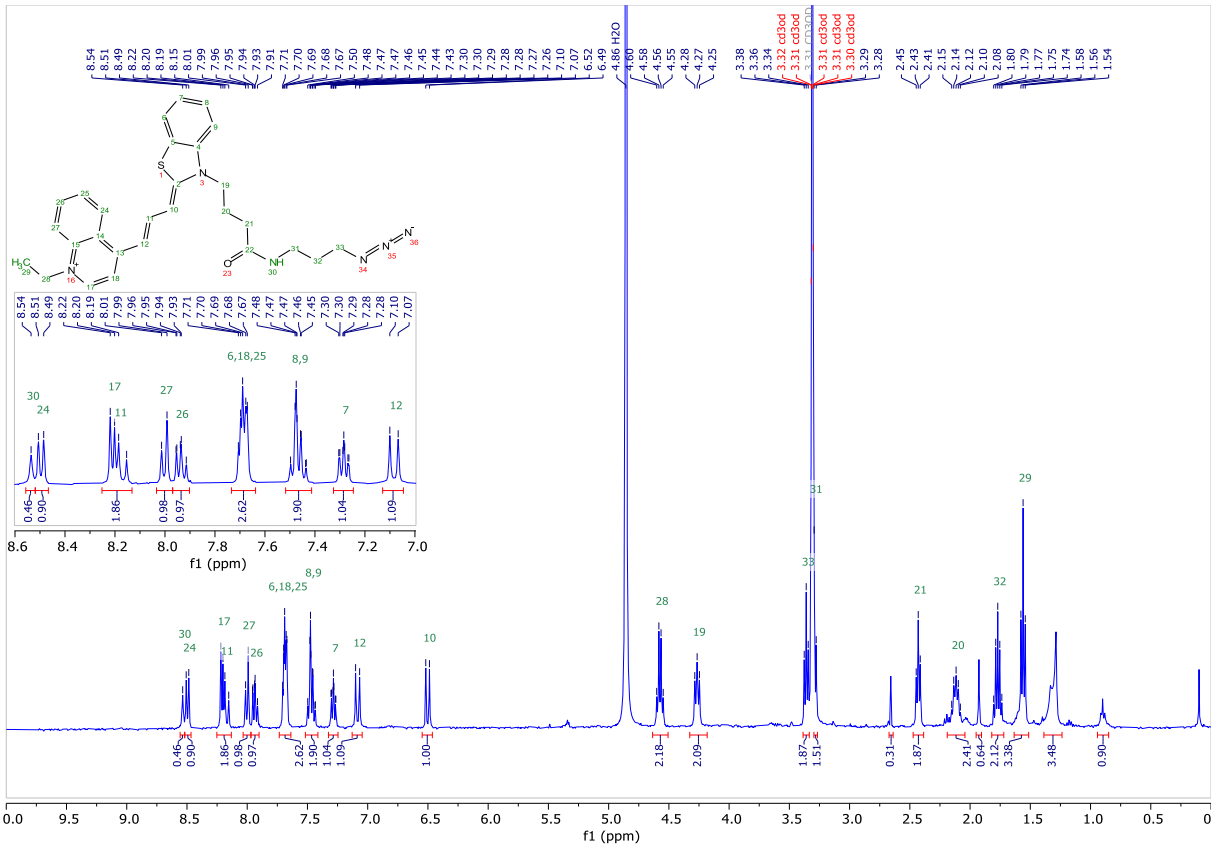


Figure S13. ^{1}H NMR spectrum of **9** recorded at 400 MHz in methanol-d_4.

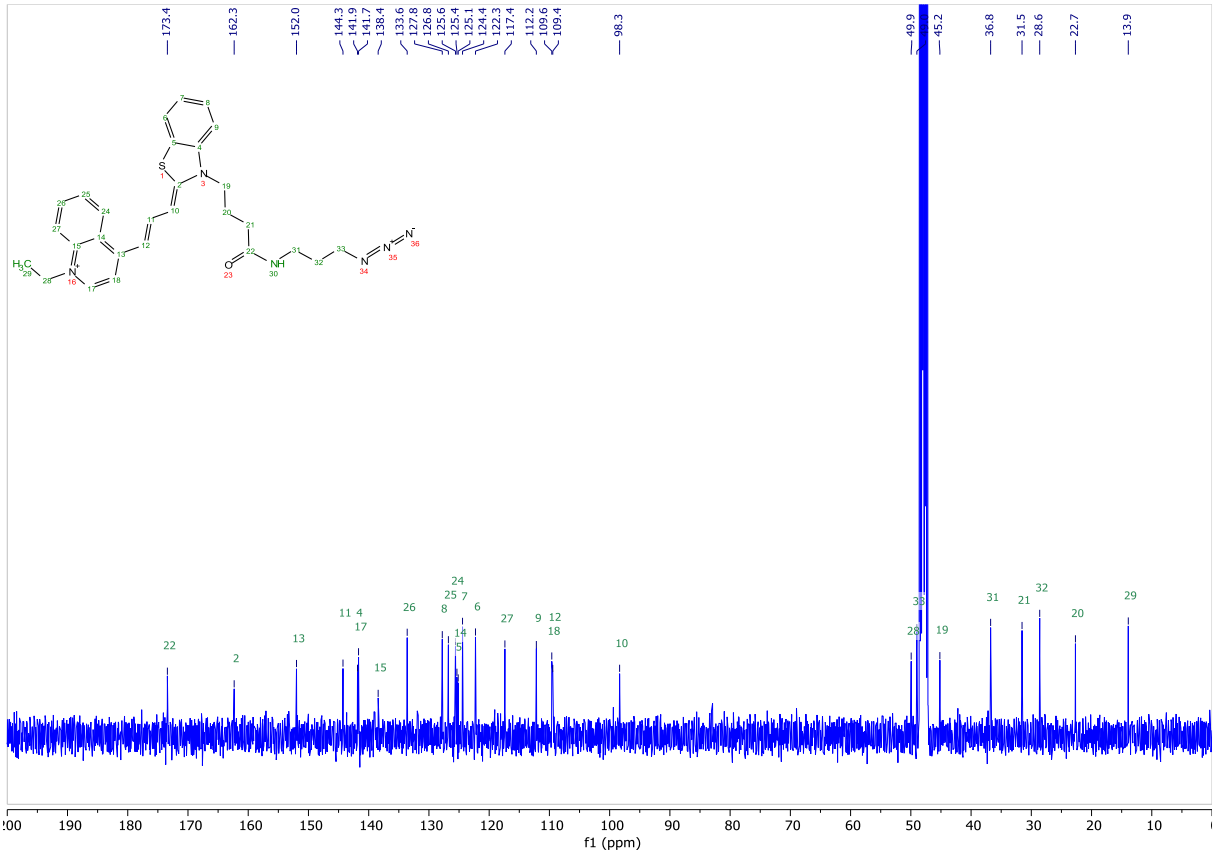


Figure S14. ^{13}C NMR spectrum of **9** recorded at 101 MHz in methanol-d_4.

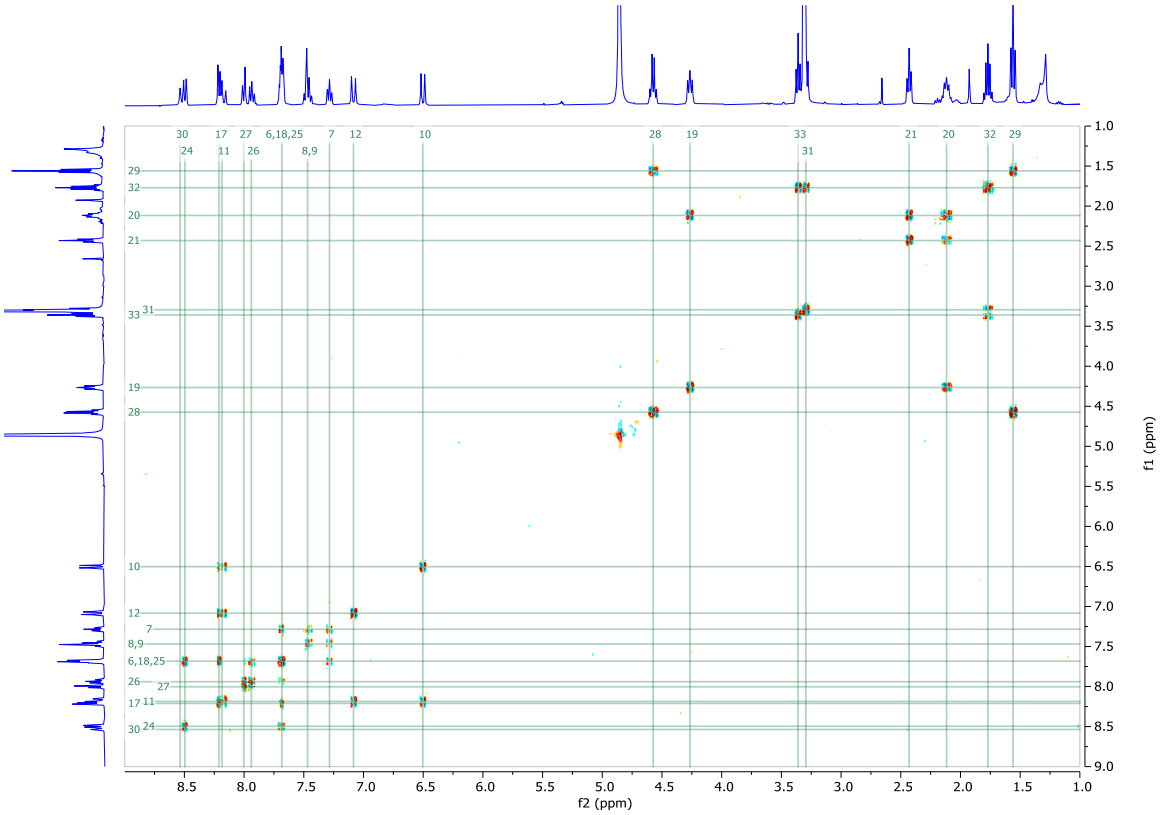


Figure S15. COSY spectrum of **9** recorded at 400 MHz in methanol-d_4.

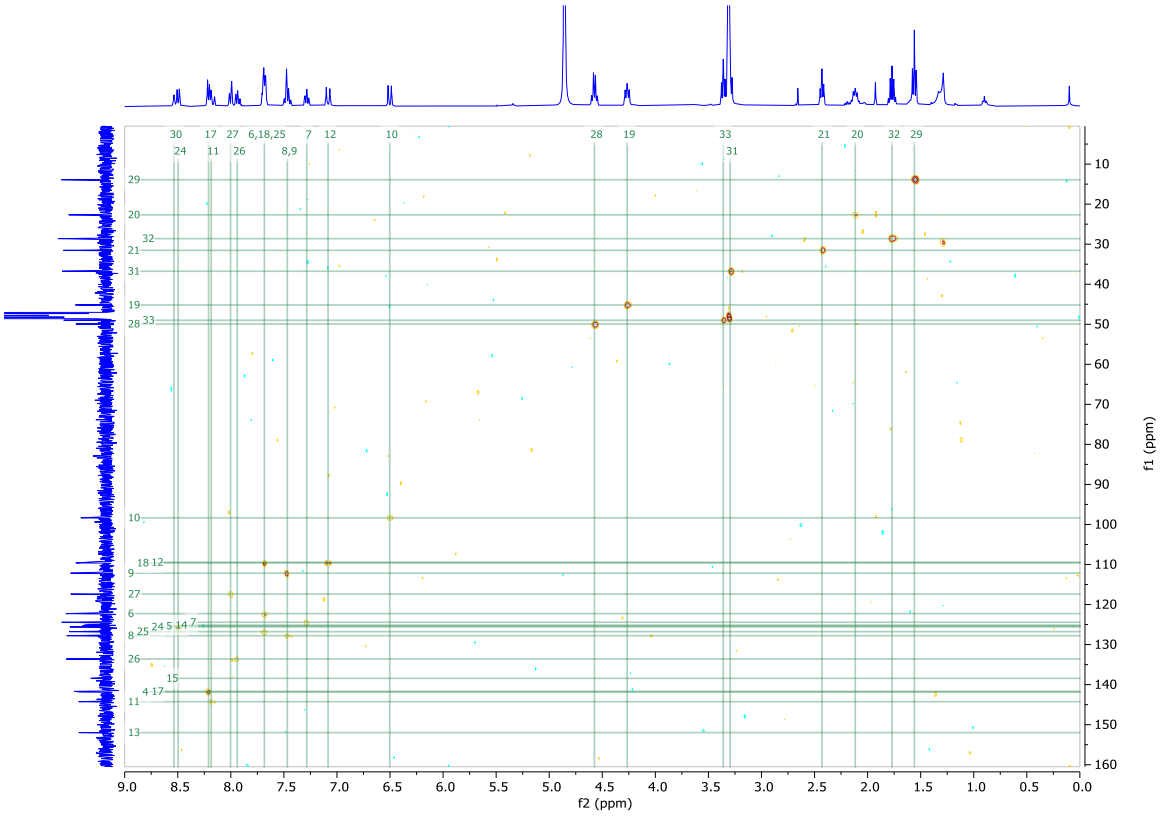


Figure S16. HSQC spectrum of **9** recorded at 400 MHz and 101 MHz in methanol-d_4.

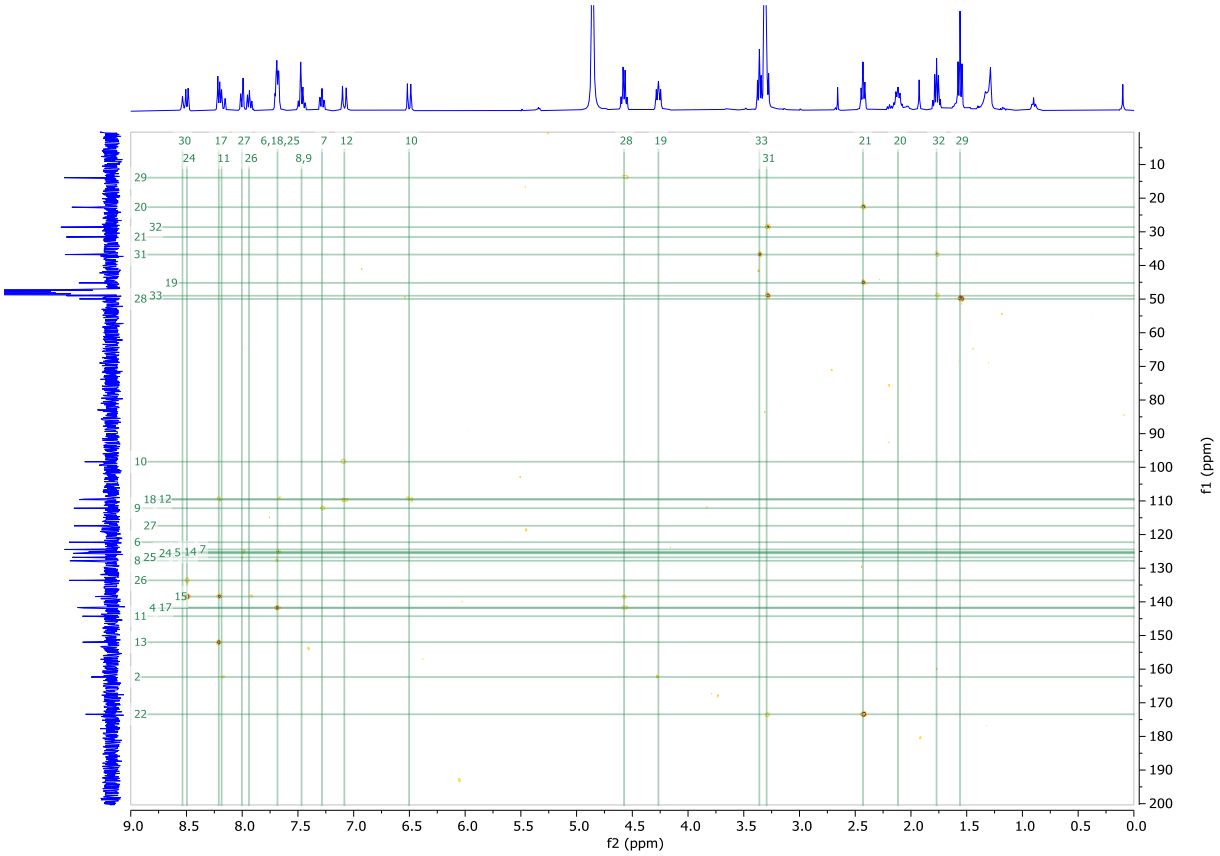


Figure S17. HMBC spectrum of **9** recorded at 400 MHz and 101 MHz in methanol-d_4.

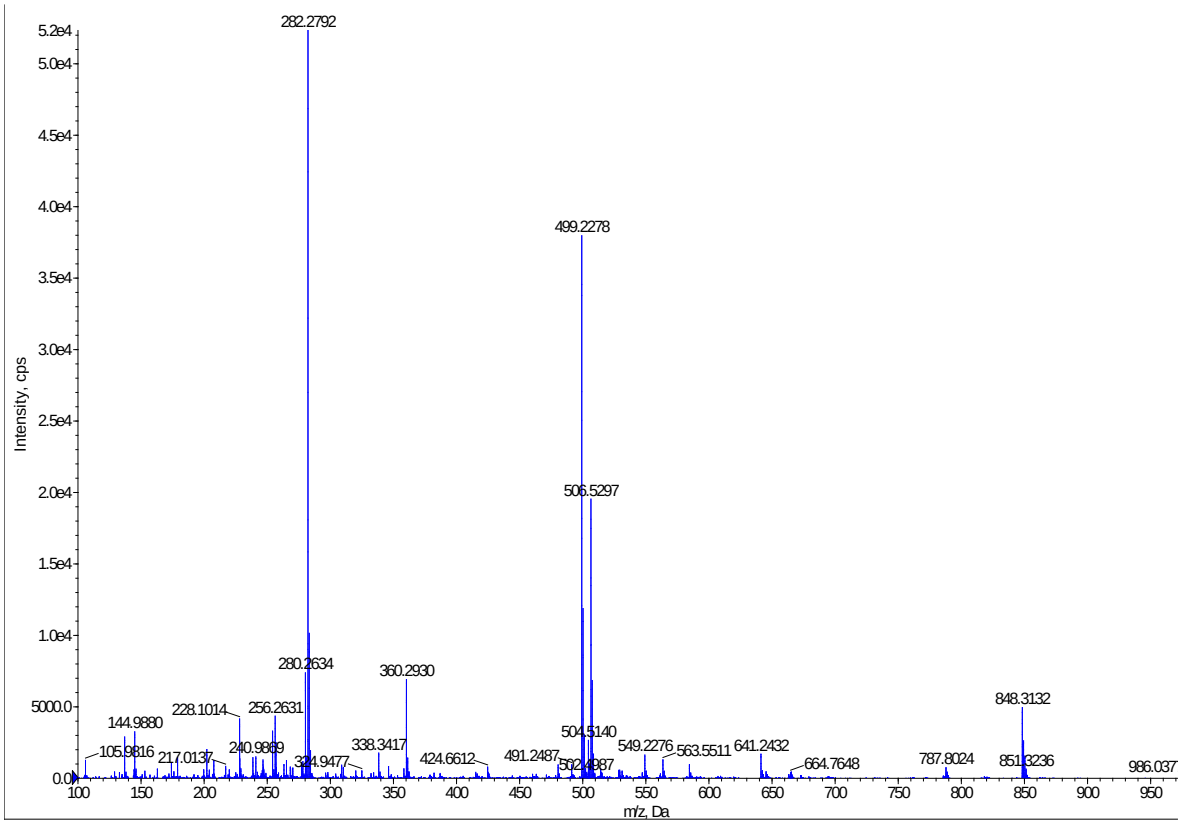


Figure S18. HRMS spectrum of **9**.

SDS-PAGE and densitometry

Non-reducing glycine-SDS-PAGE at 10% acrylamide was performed following standard lab procedures. A 4% stacking gel was used and a broad-range MW marker (4.6–300 kDa, ProSieve QuadColor Protein Marker, Lonza) was co-run to estimate protein weights. Samples (10 µL at 5 µM) were mixed with loading buffer (3 µL, composition for 6×SDS: 1 g SDS, 3 mL glycerol, 6 mL 0.5 M Tris buffer pH = 6.8; 2 mg Coomassie Blue R250 in 10 mL), and heated at 65 °C for 5 minutes. Samples were subsequently loaded into the wells at a volume of 13 µL. All gels were run at constant 200 mA for 45 minutes. Gels were stained using a Coomassie stain (0.12 g Coomassie Blue G-250, 0.10 g Coomassie Blue R-250, 500 mL MeOH, 400 mL distilled water, 100 mL acetic acid), after washing it was rested at room temperature for 16 h in a water-ethanol mixture. Then the gels were imaged using a HP DeskjetJ1350? scanner at 600 dpi. Images were saved under default brightness, contrast, and gamma settings. Densitometry was performed using ImageJ[8]. Background subtraction was achieved using the built-in plugin with a rolling ball radius of 30°, sliding paraboloid, and smoothing. Brightness and contrast settings were auto-adjusted within the software.

Photophysical measurements

Absorbance measurements were carried out on a Jasco V-750 Spectrophotometer (in a quartz standard cell cuvette with a 1 cm path length, 1 nm bandwidth, 400 nm/min recording speed) operating at 21 °C. The absorbance spectra was measured from 220 nm to 750 nm. The UV/Vis absorbance measurements of the trastuzumab conjugate were carried out on SpectraMax iD5 Multi-Mode Microplate Reader (Molecular Devices; San Jose, CA). Before the measurements were taken, buffer exchange was performed six times on each sample with Sartorius Vivaspin 500 10000 MWCO at 15000 g for 10 minutes. Sample buffer was used as blank for baseline correction with extinction coefficients; ε_{280}= 232,677 $M^{-1}cm^{-1}$ and ε_{627}= 0 $M^{-1}cm^{-1}$ for trastuzumab (in equation T); ε_{280}= 16,381 $M^{-1}cm^{-1}$for ε_{627}= 35,488 $M^{-1}cm^{-1}$ for 4-((1*E*,3*Z*)-3-(3-(4-((3-azidopropyl)amino)-4-oxobutyl)benzo[*d*]thiazol-2(3*H*)-ylidene)prop-1-en-1-yl)-1-ethylquinolin-1-ium (**9**) measured in water/BBS. FAR values were calculated from Lambert-Beer equation for absorbance at 280 and 627 nm.

$$A_{280nm} = \varepsilon_{9,280nm} \cdot l \cdot c_9 + \varepsilon_{T,280nm} \cdot l \cdot c_T$$
$$A_{627nm} = \varepsilon_{9,543nm} \cdot l \cdot c_9 + \varepsilon_{T,627nm} \cdot l \cdot c_T$$

The fluorescence measurements were carried out on a Jasco FP8300 spectrofluorometer, in a quartz standard cell cuvette with a 1 cm light path length. The widths of the excitation slit and the emission slit were both set to 2.5 nm with the scanning speed of 1000 nm/min. Pure solvents were used as blank correction. 1 μM HEPES pH=7.4 buffer was used as solvent if not otherwise mentioned. The absorbance spectra were measured from 250 nm to 700 nm. The excitement spectra were recorded between 250 nm and 700 nm. To measure the emission spectra, the sample irradiated at the excitation maximum, and the respective emission spectrum was recorded from a wavelength 10 nm greater than that of the excitation maximum up to 800 nm. The quantum yields were determined by recording the fluorescence spectra of a series of concentrations. The gradient of the integrated fluorescence intensities was plotted against absorbance at the excitation wavelength and was used for the calculation of the quantum yields as follows:

$$\Phi_x = \Phi_{St} \cdot \left(\frac{Grad_x}{Grad_{St}}\right) \cdot \left(\frac{\eta_x^2}{\eta_{St}^2}\right)$$

Compound **9** was excited at 555 nm and Cresyl violet was used as a reference (Φ_F^{MeOH}=0.54). During the computations we used refraction coefficient values from the literature[9].

The solvent screen measurement was carried out with 5 μM solutions of the cyanine (**9**) in acetonitrile, 1,4-dioxane, HEPES buffer, dichloromethane, tetrahydrofuran, ethanol, and ethyl acetate.

The photostability measurement was carried out with 5 μM solutions of compound **9** in HEPES. We used a 7 W, 630 nm emitting diode, and measured the emission spectra every 5 minutes for 10 minutes. During the photostability measurements the solutions were excited at 627 nm. As a reference Cyanine5 dye was used with the same conditions. For the emission spectra recording the solution was excited at 647 nm.

Trastuzumab reconjugation with DBPD-CO

The reconjugation was carried out by procedure described in detail elsewhere[10] The resulting T-CO conjugate (**10**) was buffer-exchanged twice using a Vivaspin500 10 kDa MWCO membrane filter. At the last step the retentate was further purified to remove the small molecular reactants with ZebaSpin 7 kDa MWCO columns. The conjugate was investigated with UV/Vis absorbance measurement and non-reducing SDS-PAGE (see for example at Figure S23). The DAR was calculated from the absorbance spectra and it is resulted DAR=4.

*The Click reaction between compound **9** and the T-CO conjugate (**10**), and the resulting fluorescent conjugate (**11**)*

To 13 µL of T-CO (**10**, 0.00078 µmol, c=59.77 µM) solution 0.39 µL 20 mM **9** cyanine azide (0.0078 µmol, 10 equiv.) was added. The reaction mixture was gently shaken overnight. The solution was filtered twice using a Vivaspin500 10 kDa MWCO membrane filter to remove the buffer. At the last step the retentate was further purified to remove the small molecular reactants with ZebaSpin 7 kDa MWCO columns. The conjugate **(11)** was investigated with UV/Vis absorbance measurements (Table S2) and non-reducing SDS-PAGE. The average FAR determined from UV gives cca. 4.

$$A_{280nm} = \varepsilon_{9,280nm} \cdot l \cdot c_9 + \varepsilon_{T,280nm} \cdot l \cdot c_T$$

$$A_{627nm} = \varepsilon_{9,543nm} \cdot l \cdot c_9 + \varepsilon_{T,627nm} \cdot l \cdot c_T$$

$$0.039 = 16381 M^{-1}cm^{-1} \cdot 0.05cm \cdot c_9 + 232677 M^{-1}cm^{-1} \cdot 0.05cm \cdot c_T$$

$$0.018 = 35488 M^{-1}cm^{-1} \cdot 0.05cm \cdot c_9 + 0 M^{-1}cm^{-1} \cdot 0.05cm \cdot c_T$$

$$c_T = 2.6\mu M; c_9 = 10.4\mu M; FAR = \frac{c_9}{c_T} = 4.0$$

Cell lines and culture conditions applied in this studies

MCF-7 (HER2- human breast adenocarcinoma) and NCI-N87-GFP (HER2+ human gastric carcinoma) cell lines were cultured in sterile culture flasks at 37 °C in a humidified atmosphere with 5% CO_2 in an incubator. The cells were cultured in DMEM-F12 (Dulbecco's Modified Eagle's Medium, Nutrient Mixture F12; Gibco, Waltham, Massachusetts, USA), supplemented with 10% FBS (Fetal Bovine Serum; Euroclone, Pero, Italy), 100 units/mL penicillin, 100 mg/mL streptomycin, and 0.25 µg/mL amphotericin B (Lonza, Basel, Switzerland).

All precedures with these cell lines were carried out in a laminar flow biosafety cabinet.

Flow cytometry

Samples were analyzed with an Attune NxT flow cytometer (ThermoFisher Scientific). Trastuzumab fluorescence (BL1-H) was measured at 488 nm for the excitation and 530/30 nm for the emission spectra, **11** fluorescence (RL1-H) was measured at 633 nm for the excitation and for the 650/16 nm emission spectra. Spectral analysis was performed using the Attune NxT 3.1.2 software.

*Preparing labelled cells with trastuzumab – cyanine conjugate (**11**) for FACS*

Human breast cancer cell lines NCI-N87 GFP (HER2 positive) and MCF-7 (HER2 negative) were applied. The cells were cultured in DMEM-F12 medium (Gibco) supplemented with 10% foetal bovine serum (EuroClone), 100 units/mL penicillin, 100 mg/mL streptomycin, and 0.25 μg/mL amphotericin B (Lonza). Both cell lines were maintained at 37 °C in a humidified incubator with 5% CO_2.

Cultured cells were harvested using 0.25% trypsin in 2.21 mM EDTA (Corning) and washed with fluorescence activated cell sorting (FACS) buffer (pH=7.4 PBS buffer containing 1% FBS). Cells were put 1.5 mL microtubes and stained with 10 μg/mL of the trastuzumab conjugate (**11**) (the antibody was diluted in 3% bovine serum albumin in PBS). The cells were incubated in 200 μL staining volume for 30 minutes at room temperature, then washed three times in 200 μL FACS buffer. Finally, cells were suspended in 500 μL FACS buffer, and the samples underwent FACS analysis.

Immunocytochemistry

Glass coverslips were sterilized in 90% ethanol, and after drying they were placed in 6-well cell culture plates (Starstedt, Nümbrech, Germany). Cells were suspended using 0.25% trypsin in 2.21 mM EDTA (Corning, Manassas, VA, USA) and washed with PBS (Gibco, Waltham, Massachusetts USA, supplemented with 1% FBS). Approximately 200 000 cells were placed in each well in 1mL of culture medium. After 24 hours of incubation at 37 °C, the cells were washed 3 times with PBS (Gibco, Waltham, Massachusetts, USA) and then fixed in 4% paraformaldehyde (Thermo Scientific, Waltham, Massachusetts, USA) for 10 minutes. After three PBS washes, the non-specific protein binding sites were blocked by incubating the samples in BSA (Sigma, St. Louis, Missouri, USA) for 30 minutes. The cells were incubated with the dye-conjugated primary antibody (**11**) at 20 μg/mL concentration for 1 hour. After three PBS washes the samples were mounted with Vectashield-DAPI (for nucleus staining, Vector, Newark, California, USA). The samples were investigated with both a Zeiss LSM 710 Zeiss LSM 710 confocal microscope (Zeiss, Jena, Germany).

Photophysical results

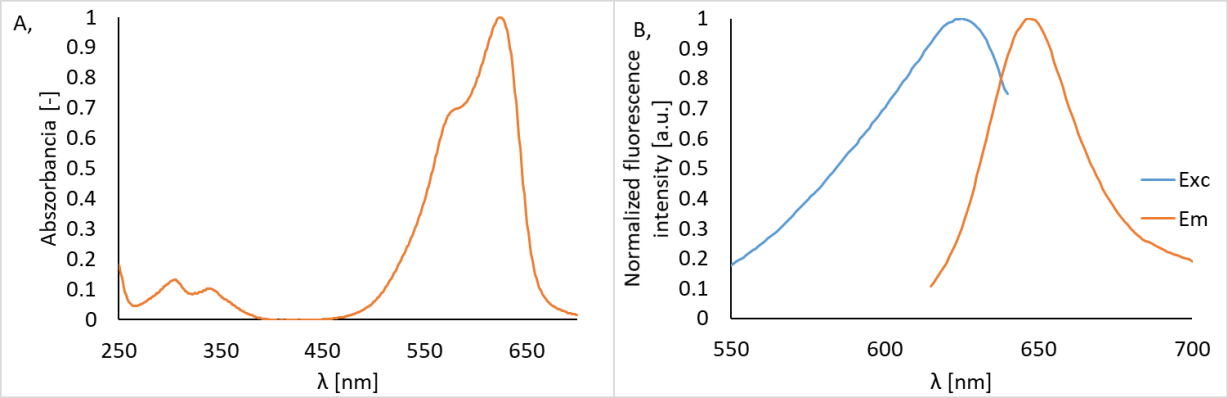


Figure S19. (A) Normalized absorption (B) excitation (orange) and fluorescence emission spectra (blue) (B) of **9** in HEPES buffer (c= 5 μM, pH = 7.4).

*Photostability measurement of **9** dye*

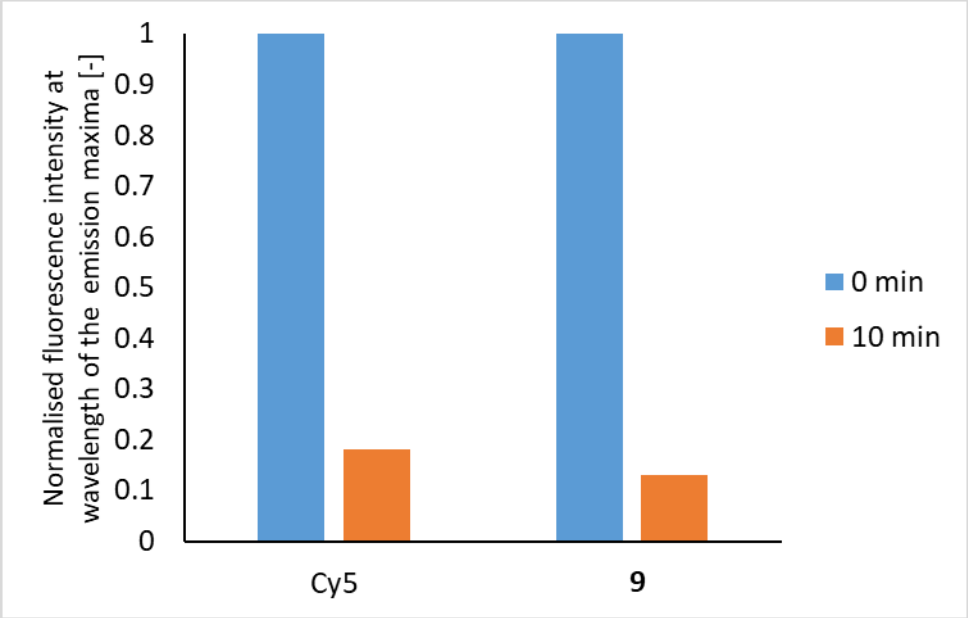


Figure S20. Change in emission intensity after 10 minutes in the case of Cyanine5 and **9** cyanine. Both was exctited at 630 nm in pH=7.4 HEPES buffer (c= 5 μM).

*Solvent dependence of **9** cyanine derivative*

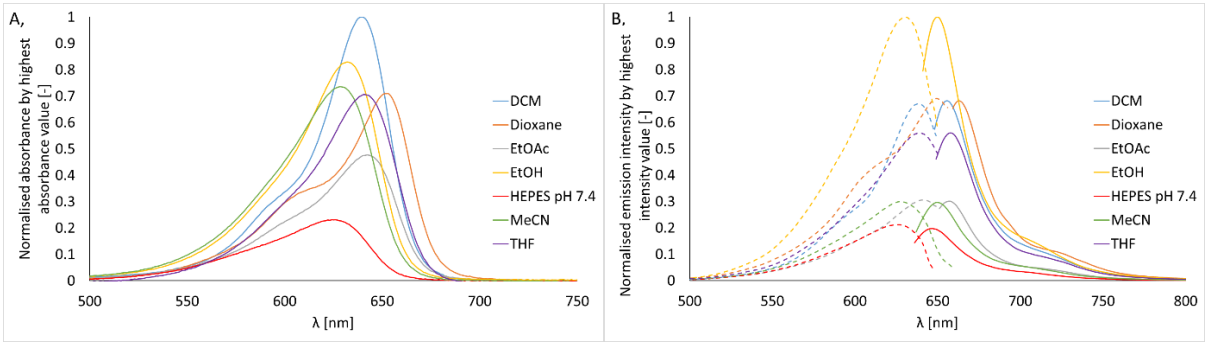


Figure S21. Normalized (A) UV-Vis absorption spectra, (B) excitation (dotted line) and fluorescence emission (solid line) spectra at c = 5.0 µM concentration of **9** in different solvents. Excitations were executed at or near the wavelength position of absorption maxima.

*The pH dependent of absorption and emission spectra of **9***

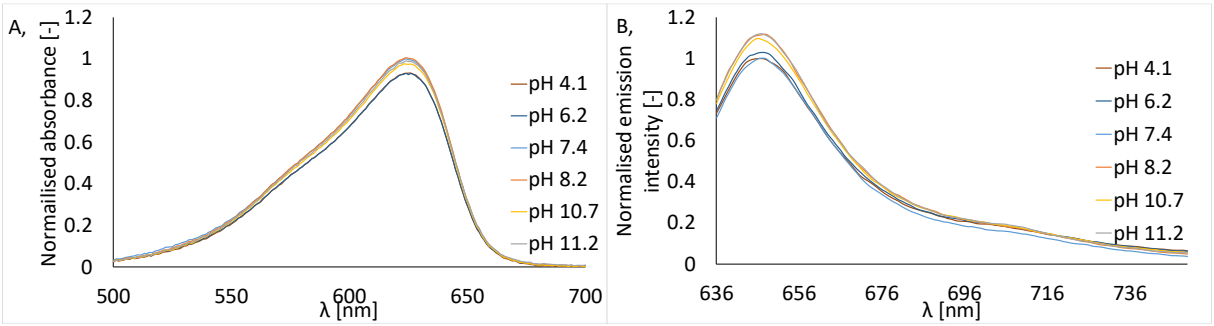


Figure S22. (A) pH-dependent UV-Vis absorption spectra of **9** in HEPES buffer (c= 5 µM), normalized to absorbance at pH=7.4. The numbers placed at the spectra denote the wavelength of absorption maxima. (B) Fluorescence emission spectra of **9** in HEPES buffer (c= 5 µM) at different pH values. Excitation was performed at or near the wavelength position of absorption maxima in the spectra recorded at the same pH values.

*Absorbance measurement of cyanine-trastuzumab conjugate (**11**)*

Table S2. Average calculated FAR value from measured absorbance values

Experiment	Measured Values				
	$A_{280\ nm}$	$A_{627\ nm}$	c_9	c_T	FAR
1	0.030	0.016	1.9	9.0	4.7
2	0.48	0.021	3.3	11.8	3.6
AVG					4.2

*SDS-PAGE results of **11** conjugate*

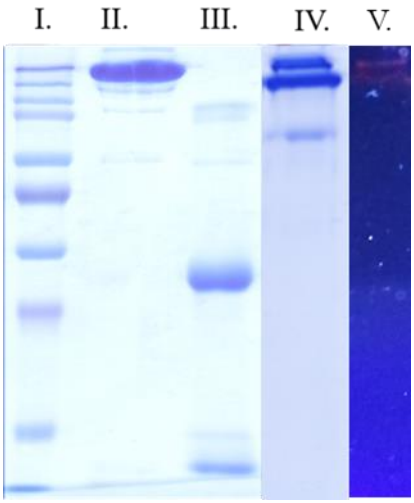


Figure S23. SDS-PAGE in non-reducing, denaturating gel. I-IV. Coomassie stained gel, V. Fluorescence of gel (λ_{exc}: 366 nm). I. molecular weight protein marker, II. native trastuzumab, III. Reduced trastuzumab, IV. **11** (fully reconjugated antibody 90%, misbridged half antibody 10%), V. **11** under 366 nm light.

*Flow cytometry measurements of cells without or treated with **11** antibody conjugate*

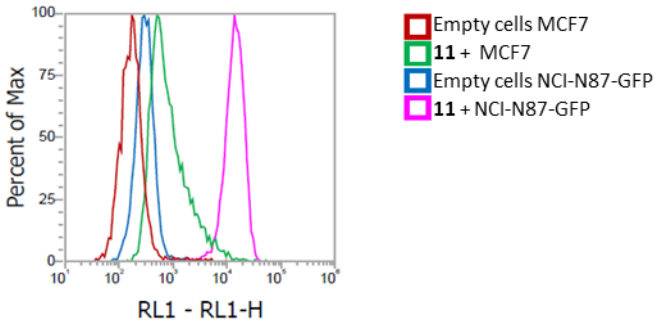


Figure S24. Results of the flow cytometry measurement. Red line: untreated MCF-7 cell line (Her2-); green line: trastuzumab-cyanine conjugate (**11**) treated MCF-7 cell line (Her2-); blue line: untreated NCI-N87-GFP cell line (Her2+); pink line: trastuzumab-cyanine conjugate (**11**) treated NCI-N87-GFP cell line (Her2+)

Raw computational data

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

Number	Filename	E	ZPE	U	H	G	S
	002aaa_mol_b3lyp631dp_PCMw.log	-1358.58311524	-1358.204382	-1358.182325	-1358.181381	-1358.258138	161.549
	002aba_mol_TD_b3lyp631dp_PCMw_opt.log	-1358.58095709	-1358.130776	-1358.108423	-1358.107479	-1358.184683	162.489
	002aca_mol_b3lyp631dp_PCMw_opt_TRIPLET.log	-1358.53039291	-1358.153725	-1358.131361	-1358.130417	-1358.208920	165.224
	002baa_mol_TD_B3LYP631dp_PCMw_opt_rot.log	-1358.55476917	-1358.136688	-1358.114727	-1358.113783	-1358.189609	159.591

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

Number	Filename	E	ZPE	U	H	G	S
	002gdb_mol_b3lyp631dp_+1H2_ARA_PCMw.log	-1359.71941410	-1359.319348	-1359.296676	-1359.295732	-1359.373627	163.942
	002geb_mol_b3lyp631dp_+5H2_ARA_PCMw.log	-1363.36955790	-1362.897124	-1362.873046	-1362.872102	-1362.953704	171.746
	002gfb_mol_b3lyp631dp_+6H2_ARA_PCMw.log	-1364.60707466	-1364.110264	-1364.086079	-1364.085135	-1364.166681	171.627
	002haa_mol_b3lyp631dp_+1H2_ARBb_PCMw.log	-1359.73145182	-1359.330501	-1359.307986	-1359.307041	-1359.384569	163.171
	002hba_mol_b3lyp631dp_+3H2_ARBb_PCMw.log	-1362.15479041	-1361.705371	-1361.682175	-1361.681231	-1361.759340	164.394
	002hca_mol_b3lyp631dp_+4H2_ARBb_PCMw.log	-1363.38459174	-1362.910609	-1362.887280	-1362.886336	-1362.965017	165.599
	002daa_mol_b3lyp631dp_+1H2_OL_PCMw.log	-1359.78358699	-1359.381527	-1359.359038	-1359.358094	-1359.436007	163.982
	002dba_mol_b3lyp631dp_+1H2_OL2_PCMw.log	-1359.77342070	-1359.371325	-1359.348948	-1359.348003	-1359.426036	164.234
	002dca_mol_b3lyp631dp_+1H2_OL3_PCMw.log	-1359.75899240	-1359.357922	-1359.335339	-1359.334395	-1359.412870	165.165
	002dda_mol_b3lyp631dp_+1H2_OL4_PCMw.log	-1359.77236548	-1359.370587	-1359.348085	-1359.347141	-1359.425714	165.370
	002dea_mol_b3lyp631dp_+1H2_OL5_PCMw.log	-1359.77604126	-1359.374292	-1359.351776	-1359.350832	-1359.428307	163.060
	002eaa_mol_b3lyp631dp_+2H2_OL_PCMw.log	-1361.00218861	-1360.576188	-1360.553480	-1360.552536	-1360.630831	164.785

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

Number	Filename	E	ZPE	U	H	G	S
	002haa_mol_TDb3lyp631dp_+1H2_ARBb_PCMw_opt.log	-1359.72903875	-1359.248778	-1359.225936	-1359.224991	-1359.303057	164.302
	002gdb_mol_TDb3lyp631dp_+1H2_ARA_PCMw_opt.log	-1359.71747555	-1359.244909	-1359.221865	-1359.220921	-1359.299903	166.232
	002fad_mol_TDb3lyp631dp_+1H2_AR_PCMw_opt_rot.log	-1359.71908349	-1359.298201	-1359.275478	-1359.274534	-1359.352869	164.871
	002fae_mol_TDb3lyp631dp_+1H2_AR_PCMw_opt_rot_1.log	-1359.69975008	-1359.259239	-1359.236723	-1359.235779	-1359.312847	162.204
	002gde_mol_TDb3lyp631dp_+1H2_ARA_PCMw_opt_rot1.log	-1359.67678887	-1359.251063	-1359.228522	-1359.227577	-1359.305111	163.184
	002dab_mol_TDb3lyp631dp_+1H2_OL_PCMw_opt.log	-1359.77545807	-1359.332034	-1359.309467	-1359.308523	-1359.386057	163.186
	002dbb_mol_TDb3lyp631dp_+1H2_OL2_PCMw_opt.log	-1359.76339533	-1359.323732	-1359.300970	-1359.300026	-1359.378821	165.838
	002dcb_mol_TDb3lyp631dp_+1H2_OL3_PCMw_opt.log	-1359.74781295	-1359.308813	-1359.286051	-1359.285106	-1359.363776	165.573
	002ddb_mol_TDb3lyp631dp_+1H2_OL4_PCMw_opt.log	-1359.74370350	-1359.315208	-1359.292526	-1359.291582	-1359.370337	165.756
	002deb_mol_TDb3lyp631dp_+1H2_OL5_PCMw_opt.log	-1359.76945454	-1359.310973	-1359.288194	-1359.287250	-1359.365334	164.340

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

Number	Filename	E	ZPE	U	H	G	S
	002hac_mol_TDb3lyp631dp_+1H2_ARBb_PCMw_opt_TRIPLET.log	-1359.67471110	-1359.275997	-1359.253129	-1359.252185	-1359.331134	166.161
	002gdc_mol_TDb3lyp631dp_+1H2_ARA_PCMw_opt_TRIPLET.log	-1359.66999705	-1359.271695	-1359.248711	-1359.247767	-1359.327601	168.026
	002dac_mol_b3lyp631dp_+1H2_OL_PCMw_triplet.log	-1359.72745045	-1359.328552	-1359.305763	-1359.304819	-1359.384457	167.613
	002dbc_mol_b3lyp631dp_+1H2_OL2_PCMw_triplet.log	-1359.72100428	-1359.321729	-1359.299014	-1359.298070	-1359.377177	166.495
	002dcc_mol_b3lyp631dp_+1H2_OL3_PCMw_triplet.log	-1359.70689076	-1359.308569	-1359.285619	-1359.284675	-1359.365143	169.359
	002ddc_mol_b3lyp631dp_+1H2_OL4_PCMw_triplet.log	-1359.71385220	-1359.314163	-1359.291197	-1359.290253	-1359.371761	171.548
	002dec_mol_b3lyp631dp_+1H2_OL5_PCMw_triplet.log	-1359.72845502	-1359.328640	-1359.305778	-1359.304834	-1359.384340	167.335

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

Number	Filename	E	ZPE	U	H	G	S
	H2	-1.17867441	-1.168517	-1.166156	-1.165212	-1.180005	31.134
	000baa_benzene_b3lyp631dp_PCMw.log	-232.26074862	-232.160178	-232.155795	-232.154850	-232.187640	69.012
	000ba_benzene_+1H2_b3lyp631dp_PCMw.log	-233.43269415	-233.310409	-233.305209	-233.304265	-233.338686	72.445
	000ca_benzene_+2H2_b3lyp631dp_PCMw.log	-234.66359619	-234.517431	-234.511914	-234.510970	-234.546076	73.886
	000da_benzene_+3H2_b3lyp631dp_PCMw.log	-235.89731046	-235.727125	-235.721399	-235.720455	-235.755914	74.631
	001aaa_cyclobutadine_b3lyp631dp_PCMw.log	-154.68443666	-154.623272	-154.619489	-154.618545	-154.648576	63.207
	001baa_cyclobutene_b3lyp631dp_PCMw.log	-155.98312337	-155.896616	-155.892795	-155.891851	-155.922231	63.940
	001caa_cyclobutane_b3lyp631dp_PCMw.log	-157.22469628	-157.113944	-157.109795	-157.108851	-157.140101	65.771

The coordinates of all computed geometries are the following:

002aaa_mol_b3lyp631dp_PCMw.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.998031	2.114930	-0.093920
2	6	0	5.944338	0.735984	-0.157904
3	6	0	4.700243	0.067741	-0.170627
4	6	0	3.484941	0.819159	-0.108433
5	6	0	3.592736	2.230047	-0.046423
6	6	0	4.815197	2.870510	-0.039049
7	1	0	6.963409	2.610072	-0.086516
8	1	0	6.868537	0.176442	-0.195844
9	6	0	2.196177	0.136223	-0.113060
10	1	0	2.694649	2.831981	-0.006287
11	1	0	4.860214	3.953146	0.008989
12	6	0	2.251664	-1.276509	-0.196704
13	6	0	3.445245	-1.945418	-0.259609
14	1	0	1.350823	-1.874689	-0.211210
15	1	0	3.477900	-3.026087	-0.320120
16	6	0	5.871451	-2.156515	-0.268066
17	6	0	6.465416	-2.373267	1.123464
18	1	0	6.589429	-1.698119	-0.949637
19	1	0	5.586021	-3.111218	-0.711889
20	1	0	7.354866	-3.003821	1.039288
21	1	0	6.757906	-1.431340	1.593771
22	1	0	5.747247	-2.877024	1.776086
23	7	0	4.646485	-1.321677	-0.249013
24	6	0	0.971402	0.849011	-0.035145
25	6	0	-0.293958	0.284560	-0.050894
26	1	0	1.010824	1.928751	0.046932
27	1	0	-0.383580	-0.796145	-0.138347
28	6	0	-1.481760	1.022695	0.039250
29	1	0	-1.409805	2.100711	0.132347
30	6	0	-2.755140	0.460482	0.019612
31	6	0	-4.820695	-0.973537	-0.058436
32	6	0	-5.088439	0.399253	0.077730
33	6	0	-5.844348	-1.915129	-0.117992
34	6	0	-6.411313	0.846383	0.157031
35	6	0	-7.162076	-1.463353	-0.038722
36	1	0	-5.621064	-2.971110	-0.223056
37	6	0	-7.436358	-0.097024	0.097287
38	1	0	-6.649281	1.897636	0.262909
39	1	0	-7.976595	-2.178398	-0.082874
40	1	0	-8.465332	0.241529	0.158155
41	7	0	-3.918936	1.169351	0.117399
42	16	0	-3.083960	-1.266921	-0.135296
43	6	0	-3.906650	2.626611	0.258809
44	1	0	-3.372963	2.910694	1.168861
45	1	0	-3.422255	3.083942	-0.607129
46	1	0	-4.927072	2.993022	0.322422

002aba_mol_b3lyp631dp_PCMw_SCAN_1.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.056221	-2.883264	0.383511
2	6	0	4.881265	-1.793931	0.181914

3	6	0	4.355057	-0.483027	0.185633
4	6	0	2.943857	-0.277426	0.332613
5	6	0	2.153678	-1.422227	0.596380
6	6	0	2.685777	-2.696289	0.621031
7	1	0	4.481690	-3.881248	0.385753
8	1	0	5.939777	-1.958610	0.037470
9	6	0	2.397191	1.073223	0.246173
10	1	0	1.109372	-1.299583	0.836371
11	1	0	2.046091	-3.545514	0.835338
12	6	0	3.360889	2.113820	0.275128
13	6	0	4.703581	1.863965	0.173188
14	1	0	3.037736	3.147175	0.311851
15	1	0	5.426493	2.669334	0.142748
16	6	0	6.665087	0.456201	-0.151774
17	6	0	7.007910	0.165239	-1.612440
18	1	0	7.039663	-0.320994	0.516250
19	1	0	7.126906	1.391471	0.167051
20	1	0	8.093083	0.077344	-1.714623
21	1	0	6.556010	-0.766761	-1.960445
22	1	0	6.665677	0.977685	-2.258980
23	7	0	5.208764	0.612045	0.077651
24	6	0	1.039493	1.486957	0.168524
25	6	0	-0.148063	0.773770	0.102740
26	1	0	0.919293	2.568263	0.210183
27	1	0	-0.128247	-0.302303	-0.027840
28	6	0	-1.408974	1.387396	0.129142
29	1	0	-1.452719	2.464264	0.249657
30	6	0	-2.615301	0.701218	0.021680
31	6	0	-4.517644	-0.930385	-0.199227
32	6	0	-4.929981	0.405660	-0.057539
33	6	0	-5.436107	-1.967997	-0.333311
34	6	0	-6.293629	0.716787	-0.047875
35	6	0	-6.795029	-1.651651	-0.323537
36	1	0	-5.102256	-2.994073	-0.442509
37	6	0	-7.213097	-0.322796	-0.181927
38	1	0	-6.642072	1.736563	0.060418
39	1	0	-7.529538	-2.443195	-0.426538
40	1	0	-8.272794	-0.090183	-0.175542
41	7	0	-3.848644	1.287823	0.061270
42	16	0	-2.758472	-1.046460	-0.180491
43	6	0	-3.992348	2.735949	0.220955
44	1	0	-3.550270	3.055328	1.167783
45	1	0	-3.501684	3.255114	-0.605657
46	1	0	-5.046506	2.997042	0.220787

002aba_mol_TD_b3lyp631dp_PCMw_opt.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.952936	2.176988	-0.262247
2	6	0	5.938419	0.786886	-0.235626
3	6	0	4.720232	0.083870	-0.182516
4	6	0	3.474435	0.804048	-0.133996
5	6	0	3.541249	2.216761	-0.182173
6	6	0	4.751091	2.893177	-0.241498
7	1	0	6.903281	2.698802	-0.303725
8	1	0	6.879256	0.254559	-0.255388
9	6	0	2.227325	0.073432	-0.051141
10	1	0	2.625126	2.793469	-0.183852
11	1	0	4.760311	3.977833	-0.273961
12	6	0	2.306677	-1.341021	-0.059377
13	6	0	3.513244	-1.986412	-0.121880
14	1	0	1.415494	-1.951343	0.009516

15	1	0	3.586043	-3.066149	-0.120225
16	6	0	5.945287	-2.103895	-0.206426
17	6	0	6.589580	-2.242377	1.174703
18	1	0	6.630388	-1.651544	-0.926163
19	1	0	5.682278	-3.087004	-0.600453
20	1	0	7.497981	-2.845535	1.089374
21	1	0	6.861590	-1.271184	1.595160
22	1	0	5.908640	-2.741516	1.869519
23	7	0	4.698715	-1.310683	-0.185015
24	6	0	0.959401	0.746980	0.057629
25	6	0	-0.292634	0.170987	-0.039737
26	1	0	0.979124	1.815190	0.249115
27	1	0	-0.385346	-0.888785	-0.260915
28	6	0	-1.483311	0.928284	0.130519
29	1	0	-1.377172	1.988697	0.336657
30	6	0	-2.768381	0.417089	0.057650
31	6	0	-4.856474	-0.956210	-0.143722
32	6	0	-5.097444	0.417185	0.111809
33	6	0	-5.901119	-1.866923	-0.282990
34	6	0	-6.419890	0.878191	0.232668
35	6	0	-7.207715	-1.396974	-0.163578
36	1	0	-5.698852	-2.914037	-0.478839
37	6	0	-7.455962	-0.037252	0.092372
38	1	0	-6.638523	1.919546	0.432788
39	1	0	-8.037707	-2.087235	-0.268261
40	1	0	-8.479509	0.310549	0.184434
41	7	0	-3.931338	1.151474	0.212608
42	16	0	-3.136881	-1.283600	-0.246298
43	6	0	-3.882709	2.591592	0.462716
44	1	0	-3.380439	2.791851	1.412814
45	1	0	-3.345833	3.092051	-0.346947
46	1	0	-4.893094	2.987408	0.508014

002abb_mol_b3lyp631dp_PCMw_SCAN_2_f.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.941586	-2.841077	-0.620216
2	6	0	-4.781040	-1.806222	-0.254178
3	6	0	-4.302240	-0.478524	-0.203979
4	6	0	-2.919076	-0.208252	-0.460690
5	6	0	-2.119158	-1.291520	-0.898516
6	6	0	-2.608950	-2.580479	-0.976221
7	1	0	-4.331270	-3.852728	-0.662655
8	1	0	-5.814487	-2.025843	-0.025105
9	6	0	-2.410508	1.150449	-0.319121
10	1	0	-1.109723	-1.098715	-1.230631
11	1	0	-1.968755	-3.383317	-1.325399
12	6	0	-3.401191	2.157605	-0.204095
13	6	0	-4.720490	1.849419	0.000549
14	1	0	-3.113166	3.202031	-0.196159
15	1	0	-5.462770	2.622498	0.154029
16	6	0	-6.594493	0.348865	0.419303
17	6	0	-6.778815	-0.047907	1.883503
18	1	0	-7.008836	-0.398609	-0.258982
19	1	0	-7.116348	1.283623	0.210746
20	1	0	-7.844660	-0.185155	2.085790
21	1	0	-6.263675	-0.981768	2.121461
22	1	0	-6.400256	0.734692	2.546451
23	7	0	-5.174178	0.575064	0.060221
24	6	0	-1.056881	1.580878	-0.306968
25	6	0	0.116423	0.850910	-0.196377
26	1	0	-0.935965	2.660805	-0.371230

27	1	0	0.061292	-0.216910	-0.009883
28	6	0	1.392651	1.431718	-0.237674
29	1	0	1.465127	2.498526	-0.418635
30	6	0	2.578606	0.723983	-0.066996
31	6	0	4.432953	-0.938288	0.292661
32	6	0	4.883038	0.375059	0.074389
33	6	0	5.320996	-1.988210	0.509749
34	6	0	6.254372	0.650325	0.073135
35	6	0	6.687872	-1.707839	0.506640
36	1	0	4.957951	-2.996390	0.676951
37	6	0	7.143474	-0.401632	0.290286
38	1	0	6.631501	1.652267	-0.091033
39	1	0	7.399106	-2.509646	0.673697
40	1	0	8.208877	-0.196649	0.290743
41	7	0	3.827907	1.274829	-0.122725
42	16	0	2.671813	-1.010472	0.248991
43	6	0	4.012549	2.705362	-0.372848
44	1	0	3.566433	2.978452	-1.331977
45	1	0	3.549544	3.290116	0.425729
46	1	0	5.073948	2.933276	-0.404259

002aca_mol_b3lyp631dp_PCMw_opt_TRIPLET.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.942658	2.213903	-0.105324
2	6	0	5.939777	0.826894	-0.166413
3	6	0	4.728667	0.110734	-0.175021
4	6	0	3.478179	0.809073	-0.110971
5	6	0	3.531045	2.219072	-0.052573
6	6	0	4.732022	2.912536	-0.049734
7	1	0	6.887617	2.746691	-0.100343
8	1	0	6.885858	0.304597	-0.204031
9	6	0	2.229451	0.056150	-0.110465
10	1	0	2.610347	2.787574	-0.009507
11	1	0	4.727021	3.996653	-0.003319
12	6	0	2.338047	-1.360282	-0.183342
13	6	0	3.552747	-1.983250	-0.248247
14	1	0	1.455929	-1.986906	-0.189994
15	1	0	3.641314	-3.060272	-0.303467
16	6	0	5.989653	-2.063450	-0.278606
17	6	0	6.600021	-2.260788	1.110311
18	1	0	6.686384	-1.569018	-0.957863
19	1	0	5.750725	-3.029378	-0.726604
20	1	0	7.517809	-2.848783	1.020946
21	1	0	6.848812	-1.307914	1.583865
22	1	0	5.907781	-2.800198	1.762628
23	7	0	4.731941	-1.289372	-0.251579
24	6	0	0.960238	0.690440	-0.037355
25	6	0	-0.299479	0.085803	-0.042418
26	1	0	0.950356	1.773994	0.032287
27	1	0	-0.389879	-0.993586	-0.113348
28	6	0	-1.469107	0.862959	0.042700
29	1	0	-1.350869	1.939905	0.116068
30	6	0	-2.775174	0.371413	0.036428
31	6	0	-4.891635	-0.960021	-0.048180
32	6	0	-5.100964	0.430989	0.075902
33	6	0	-5.958256	-1.854564	-0.114225
34	6	0	-6.409068	0.936816	0.130384
35	6	0	-7.252649	-1.342882	-0.056330
36	1	0	-5.781223	-2.920063	-0.209322
37	6	0	-7.468800	0.039401	0.064084
38	1	0	-6.601826	1.998720	0.218541

39	1	0	-8.098865	-2.019444	-0.106227
40	1	0	-8.483434	0.421018	0.105188
41	7	0	-3.911370	1.145717	0.129121
42	16	0	-3.176928	-1.337032	-0.102171
43	6	0	-3.834072	2.601696	0.264433
44	1	0	-3.217395	2.861626	1.127194
45	1	0	-3.408359	3.043463	-0.639794
46	1	0	-4.831068	3.003561	0.418789

002baa_mol_TD_B3LYP631dp_PCMw_opt_rot.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.736704	2.695517	-0.738810
2	6	0	5.201370	1.376318	-0.790442
3	6	0	4.411378	0.316388	-0.325084
4	6	0	3.111501	0.588080	0.222341
5	6	0	2.679492	1.933148	0.258339
6	6	0	3.475948	2.973222	-0.214958
7	1	0	5.370030	3.495525	-1.107806
8	1	0	6.187488	1.187961	-1.193836
9	6	0	2.307866	-0.499533	0.711021
10	1	0	1.697846	2.151529	0.664656
11	1	0	3.111834	3.994909	-0.171100
12	6	0	2.836323	-1.804892	0.651262
13	6	0	4.073873	-2.040040	0.115632
14	1	0	2.263823	-2.647516	1.021513
15	1	0	4.499585	-3.030973	0.043891
16	6	0	6.188654	-1.352999	-0.903797
17	6	0	7.303770	-1.167739	0.128119
18	1	0	6.378654	-0.759651	-1.801583
19	1	0	6.146917	-2.395689	-1.226581
20	1	0	8.266759	-1.441285	-0.313151
21	1	0	7.367101	-0.131561	0.470799
22	1	0	7.131087	-1.806714	0.999105
23	7	0	4.855674	-1.013779	-0.387575
24	6	0	0.980978	-0.259518	1.314786
25	6	0	-0.194374	-0.289250	0.615502
26	1	0	0.924294	-0.056083	2.387220
27	1	0	-0.154699	-0.487443	-0.453378
28	6	0	-1.446464	-0.078182	1.234491
29	1	0	-1.458933	0.118429	2.300317
30	6	0	-2.675709	-0.104336	0.564351
31	6	0	-4.583334	-0.236892	-1.031504
32	6	0	-4.971864	0.037855	0.295351
33	6	0	-5.521780	-0.346460	-2.058920
34	6	0	-6.326865	0.212226	0.611041
35	6	0	-6.862538	-0.174020	-1.736045
36	1	0	-5.211388	-0.558834	-3.075411
37	6	0	-7.256158	0.102777	-0.414266
38	1	0	-6.652576	0.427713	1.620540
39	1	0	-7.613516	-0.253623	-2.514175
40	1	0	-8.308188	0.234723	-0.187026
41	7	0	-3.880622	0.101035	1.160982
42	16	0	-2.845577	-0.403560	-1.151142
43	6	0	-3.994651	0.368860	2.602028
44	1	0	-3.547824	-0.451900	3.164501
45	1	0	-3.495507	1.308401	2.844292
46	1	0	-5.043636	0.445089	2.869006

002bba_mol_TD_b3lyp631dp_PCMw_SCAN_1.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.192685	-2.899882	0.232737
2	6	0	4.988103	-1.765548	0.126745
3	6	0	4.415406	-0.478806	0.170070
4	6	0	2.983196	-0.328530	0.266543
5	6	0	2.226780	-1.513143	0.416178
6	6	0	2.811011	-2.773318	0.399712
7	1	0	4.656146	-3.880428	0.200209
8	1	0	6.057019	-1.886269	0.020380
9	6	0	2.406300	1.002571	0.228781
10	1	0	1.165655	-1.445562	0.593589
11	1	0	2.189552	-3.654781	0.518685
12	6	0	3.317745	2.087649	0.277590
13	6	0	4.673719	1.901297	0.228504
14	1	0	2.944743	3.104540	0.321978
15	1	0	5.371404	2.727843	0.247863
16	6	0	6.692188	0.557299	-0.000771
17	6	0	7.137707	0.351648	-1.450102
18	1	0	7.052320	-0.242789	0.648872
19	1	0	7.103494	1.488798	0.391523
20	1	0	8.229543	0.298961	-1.486781
21	1	0	6.736129	-0.573329	-1.871119
22	1	0	6.811520	1.186878	-2.075747
23	7	0	5.224118	0.654067	0.140685
24	6	0	1.012817	1.370922	0.167225
25	6	0	-0.161185	0.644662	0.090219
26	1	0	0.868423	2.449271	0.221710
27	1	0	-0.156711	-0.430002	-0.033128
28	6	0	-1.425038	1.300848	0.097981
29	1	0	-1.427385	2.383109	0.181859
30	6	0	-2.650253	0.662937	0.018026
31	6	0	-4.588030	-0.921819	-0.135001
32	6	0	-4.968444	0.441755	-0.058223
33	6	0	-5.534729	-1.939640	-0.224386
34	6	0	-6.332142	0.782653	-0.067051
35	6	0	-6.883347	-1.588353	-0.235049
36	1	0	-5.227048	-2.977790	-0.283327
37	6	0	-7.269759	-0.239079	-0.156203
38	1	0	-6.656494	1.813817	-0.004007
39	1	0	-7.638940	-2.363396	-0.303575
40	1	0	-8.324374	0.015559	-0.163480
41	7	0	-3.883077	1.293046	0.019527
42	16	0	-2.842965	-1.089749	-0.099069
43	6	0	-3.982195	2.749639	0.102354
44	1	0	-3.585641	3.101358	1.058701
45	1	0	-3.421329	3.207210	-0.716257
46	1	0	-5.023092	3.048618	0.020402

002bbb_mol_TD_b3lyp631dp_PCMw_SCAN_2_f.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.394012	2.578843	1.237236
2	6	0	4.998035	1.556878	0.495807
3	6	0	4.233058	0.522195	-0.059459
4	6	0	2.812272	0.499551	0.150848
5	6	0	2.240789	1.548860	0.905494
6	6	0	3.015573	2.575903	1.439455
7	1	0	5.011501	3.368252	1.652961

8	1	0	6.071229	1.577753	0.360154
9	6	0	2.032093	-0.573121	-0.403366
10	1	0	1.168986	1.543693	1.071947
11	1	0	2.542551	3.366398	2.013649
12	6	0	2.692619	-1.566032	-1.154717
13	6	0	4.047234	-1.520008	-1.346191
14	1	0	2.135064	-2.385425	-1.593520
15	1	0	4.581884	-2.270186	-1.911641
16	6	0	6.273684	-0.553523	-1.038370
17	6	0	7.033674	-1.173619	0.136546
18	1	0	6.636877	0.453897	-1.256231
19	1	0	6.438258	-1.142584	-1.943308
20	1	0	8.105167	-1.192721	-0.083514
21	1	0	6.884308	-0.604614	1.057999
22	1	0	6.700144	-2.200878	0.310388
23	7	0	4.820983	-0.496326	-0.825977
24	6	0	0.563310	-0.616294	-0.239062
25	6	0	-0.055781	-1.314086	0.763287
26	1	0	-0.037016	-0.100884	-0.989488
27	1	0	0.586468	-1.867047	1.443818
28	6	0	-1.441210	-1.457187	1.029825
29	1	0	-1.690398	-2.182155	1.794686
30	6	0	-2.539249	-0.781697	0.470248
31	6	0	-4.193393	0.737073	-0.618743
32	6	0	-4.782281	-0.276757	0.161180
33	6	0	-4.967668	1.679291	-1.297898
34	6	0	-6.177679	-0.352262	0.284013
35	6	0	-6.349254	1.592955	-1.176351
36	1	0	-4.503111	2.453554	-1.897111
37	6	0	-6.943431	0.587952	-0.390950
38	1	0	-6.654562	-1.111062	0.890996
39	1	0	-6.976341	2.312274	-1.691277
40	1	0	-8.023638	0.545555	-0.306548
41	7	0	-3.832379	-1.115629	0.740351
42	16	0	-2.449018	0.616539	-0.574196
43	6	0	-4.193759	-2.271544	1.574799
44	1	0	-3.576476	-3.125808	1.301159
45	1	0	-4.060473	-2.030262	2.631319
46	1	0	-5.232258	-2.528916	1.388287

002cba_mol_b3lyp631dp_PCMw_TRIPLET_SCAN_1_f.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.123486	-2.832350	-0.636032
2	6	0	-4.904035	-1.751159	-0.244958
3	6	0	-4.362299	-0.453406	-0.198334
4	6	0	-2.976206	-0.244509	-0.503848
5	6	0	-2.236098	-1.363222	-0.939848
6	6	0	-2.790482	-2.635250	-1.005160
7	1	0	-4.563232	-3.823731	-0.666302
8	1	0	-5.939768	-1.922873	0.013880
9	6	0	-2.415073	1.097148	-0.405686
10	1	0	-1.215313	-1.222320	-1.267379
11	1	0	-2.185664	-3.469669	-1.344783
12	6	0	-3.337170	2.154018	-0.174883
13	6	0	-4.658099	1.915607	0.087261
14	1	0	-2.989304	3.180958	-0.159955
15	1	0	-5.358772	2.713358	0.293595
16	6	0	-6.585437	0.479431	0.513394
17	6	0	-6.751775	0.071103	1.978257
18	1	0	-7.054361	-0.240992	-0.159672
19	1	0	-7.072722	1.438723	0.331573

20	1	0	-7.816776	-0.022498	2.208832
21	1	0	-6.270868	-0.887300	2.189322
22	1	0	-6.320834	0.827010	2.640457
23	7	0	-5.172009	0.644460	0.120373
24	6	0	-1.036628	1.455884	-0.440252
25	6	0	0.119251	0.694632	-0.257142
26	1	0	-0.867385	2.526509	-0.556888
27	1	0	0.052881	-0.361097	-0.022488
28	6	0	1.389079	1.301095	-0.319499
29	1	0	1.427129	2.366617	-0.525530
30	6	0	2.608081	0.647329	-0.134434
31	6	0	4.496901	-0.931093	0.311468
32	6	0	4.911145	0.397899	0.076018
33	6	0	5.415791	-1.943525	0.582155
34	6	0	6.275685	0.722555	0.123366
35	6	0	6.768305	-1.612616	0.620566
36	1	0	5.082980	-2.960156	0.759374
37	6	0	7.187251	-0.291376	0.394428
38	1	0	6.621714	1.735726	-0.039071
39	1	0	7.502255	-2.383196	0.829938
40	1	0	8.244340	-0.050943	0.433545
41	7	0	3.844943	1.249904	-0.183694
42	16	0	2.749430	-1.072358	0.212398
43	6	0	3.992035	2.678655	-0.471064
44	1	0	3.435291	2.931267	-1.374937
45	1	0	3.625924	3.275436	0.368126
46	1	0	5.040649	2.905252	-0.641380

002cbb_mol_b3lyp631dp_PCMw_TRIPLET_SCAN_2.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.237615	2.962941	-0.093762
2	6	0	4.909419	1.749899	-0.159121
3	6	0	4.199241	0.535341	-0.174951
4	6	0	2.766288	0.536272	-0.115319
5	6	0	2.127808	1.794229	-0.048050
6	6	0	2.840062	2.984122	-0.038831
7	1	0	4.804144	3.887979	-0.083305
8	1	0	5.990122	1.753413	-0.193917
9	6	0	2.041082	-0.728949	-0.123581
10	1	0	1.047367	1.845407	-0.000217
11	1	0	2.308329	3.928541	0.013692
12	6	0	2.826879	-1.912769	-0.190547
13	6	0	4.191425	-1.864949	-0.252057
14	1	0	2.363705	-2.890197	-0.205977
15	1	0	4.792788	-2.762592	-0.309217
16	6	0	6.359315	-0.750662	-0.280325
17	6	0	6.988032	-0.635756	1.109604
18	1	0	6.727730	0.024652	-0.954303
19	1	0	6.619659	-1.707942	-0.734961
20	1	0	8.075862	-0.703510	1.019775
21	1	0	6.742763	0.314955	1.589242
22	1	0	6.644852	-1.447651	1.756696
23	7	0	4.883563	-0.685555	-0.253142
24	6	0	0.620401	-0.788683	-0.072708
25	6	0	-0.167956	-1.943322	-0.051220
26	1	0	0.107572	0.164535	-0.050019
27	1	0	0.328154	-2.907163	-0.061703
28	6	0	-1.575755	-2.034751	-0.019598
29	1	0	-1.948868	-3.053253	-0.011198
30	6	0	-2.582328	-1.061909	0.003283
31	6	0	-4.085325	0.949255	0.032729

32	6	0	-4.781073	-0.277956	0.047621
33	6	0	-4.755029	2.170961	0.045600
34	6	0	-6.185145	-0.279836	0.075565
35	6	0	-6.147776	2.157778	0.073676
36	1	0	-4.203968	3.104662	0.033941
37	6	0	-6.849044	0.941310	0.088258
38	1	0	-6.750421	-1.203130	0.086914
39	1	0	-6.692377	3.095646	0.084162
40	1	0	-7.933603	0.948898	0.109809
41	7	0	-3.929678	-1.374393	0.031676
42	16	0	-2.350937	0.682421	-0.002614
43	6	0	-4.398119	-2.762233	0.039785
44	1	0	-4.064921	-3.276452	-0.864434
45	1	0	-4.017945	-3.281727	0.922035
46	1	0	-5.483245	-2.776188	0.068774

002daa_mol_b3lyp631dp_+1H2_OL_PCMw.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.184459	2.300232	-1.361824
2	6	0	5.452383	0.988466	-1.030813
3	6	0	4.447318	0.194583	-0.434543
4	6	0	3.155217	0.750285	-0.171696
5	6	0	2.927170	2.105267	-0.531083
6	6	0	3.916663	2.864886	-1.112170
7	1	0	5.963082	2.900924	-1.819368
8	1	0	6.434878	0.584351	-1.229327
9	6	0	2.137725	-0.056812	0.435098
10	1	0	1.956204	2.545129	-0.343294
11	1	0	3.723197	3.898033	-1.378808
12	6	0	2.461117	-1.367183	0.748186
13	6	0	3.728390	-1.870444	0.471474
14	1	0	1.746520	-2.036303	1.206649
15	1	0	3.988509	-2.894674	0.707327
16	6	0	6.019094	-1.766013	-0.324813
17	6	0	7.025482	-1.422140	0.770527
18	1	0	6.364181	-1.466808	-1.314296
19	1	0	5.841057	-2.840596	-0.361853
20	1	0	7.969591	-1.925868	0.547331
21	1	0	7.217087	-0.348628	0.832062
22	1	0	6.672219	-1.769215	1.744812
23	7	0	4.686842	-1.132712	-0.096764
24	6	0	0.767394	0.514698	0.709908
25	6	0	-0.265554	-0.439800	1.342379
26	1	0	0.886455	1.391778	1.358941
27	1	0	0.129118	-0.816548	2.294706
28	6	0	-1.586561	0.237722	1.586616
29	1	0	-1.637771	0.930807	2.420001
30	6	0	-2.689397	0.056292	0.831128
31	6	0	-4.508038	-0.702888	-0.783886
32	6	0	-4.943434	0.249334	0.158508
33	6	0	-5.371857	-1.243893	-1.727098
34	6	0	-6.283745	0.650383	0.156107
35	6	0	-6.709891	-0.830429	-1.731290
36	1	0	-5.015579	-1.975059	-2.445784
37	6	0	-7.152801	0.105676	-0.795102
38	1	0	-6.656113	1.366367	0.879592
39	1	0	-7.398315	-1.243423	-2.461195
40	1	0	-8.192106	0.419508	-0.795253
41	7	0	-3.926926	0.684942	1.004368
42	16	0	-2.782944	-1.059149	-0.574164
43	6	0	-4.098374	1.674530	2.054384

44	1	0	-4.072856	1.211889	3.047895
45	1	0	-3.299162	2.419468	1.994480
46	1	0	-5.050342	2.185951	1.926754
47	1	0	0.360630	0.901797	-0.232491
48	1	0	-0.399356	-1.314610	0.694534

002dab_mol_TDb3lyp631dp_+1H2_OL_PCMw_opt.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.392786	2.299462	-1.247650
2	6	0	5.595840	0.957211	-0.905191
3	6	0	4.543929	0.173018	-0.410948
4	6	0	3.241664	0.753226	-0.233972
5	6	0	3.080443	2.110646	-0.593996
6	6	0	4.135098	2.874516	-1.094365
7	1	0	6.225099	2.881618	-1.629620
8	1	0	6.584331	0.534077	-1.025310
9	6	0	2.160772	-0.043909	0.292921
10	1	0	2.107301	2.572576	-0.478176
11	1	0	3.969452	3.914356	-1.358547
12	6	0	2.439931	-1.383174	0.613739
13	6	0	3.686123	-1.924519	0.429972
14	1	0	1.674979	-2.036163	1.015320
15	1	0	3.916999	-2.953280	0.666885
16	6	0	6.043096	-1.826316	-0.219350
17	6	0	6.973482	-1.557212	0.965912
18	1	0	6.500838	-1.508984	-1.159773
19	1	0	5.858977	-2.899016	-0.313432
20	1	0	7.928483	-2.068820	0.813369
21	1	0	7.173582	-0.489119	1.085741
22	1	0	6.529572	-1.928312	1.894418
23	7	0	4.731652	-1.179491	-0.090021
24	6	0	0.804614	0.589128	0.479453
25	6	0	-0.269674	-0.339146	1.087964
26	1	0	0.893829	1.481695	1.116604
27	1	0	0.083165	-0.709621	2.060060
28	6	0	-1.549028	0.383643	1.325812
29	1	0	-1.526043	1.210724	2.026516
30	6	0	-2.748666	0.093341	0.714986
31	6	0	-4.634025	-0.786269	-0.654997
32	6	0	-4.993787	0.300565	0.176296
33	6	0	-5.566404	-1.401068	-1.494266
34	6	0	-6.311493	0.788143	0.166966
35	6	0	-6.864841	-0.911443	-1.492908
36	1	0	-5.279510	-2.233685	-2.125524
37	6	0	-7.228884	0.173305	-0.669028
38	1	0	-6.611849	1.621564	0.788326
39	1	0	-7.609107	-1.368742	-2.134940
40	1	0	-8.249879	0.537305	-0.689142
41	7	0	-3.928074	0.762864	0.930854
42	16	0	-2.949225	-1.193394	-0.465090
43	6	0	-4.013489	1.882176	1.878202
44	1	0	-3.638452	1.565215	2.851616
45	1	0	-3.431095	2.727089	1.506797
46	1	0	-5.050998	2.181741	1.986489
47	1	0	0.427647	0.960807	-0.484173
48	1	0	-0.419707	-1.214274	0.448800

002dac_mol_b3lyp631dp_+1H2_OL_PCMw_triplet.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.529068	2.248788	-1.187761
2	6	0	5.688189	0.899082	-0.849212
3	6	0	4.604130	0.139191	-0.386482
4	6	0	3.312938	0.754490	-0.239270
5	6	0	3.197604	2.118322	-0.590977
6	6	0	4.284228	2.857556	-1.060516
7	1	0	6.386354	2.810796	-1.545342
8	1	0	6.668364	0.450915	-0.947725
9	6	0	2.196612	-0.016807	0.255809
10	1	0	2.234675	2.606347	-0.492892
11	1	0	4.153322	3.903832	-1.320173
12	6	0	2.431223	-1.365845	0.575055
13	6	0	3.667935	-1.939552	0.419923
14	1	0	1.636745	-1.999840	0.951369
15	1	0	3.865383	-2.976727	0.654984
16	6	0	6.046375	-1.896492	-0.159813
17	6	0	6.949740	-1.652750	1.052353
18	1	0	6.540120	-1.589313	-1.085763
19	1	0	5.839465	-2.964654	-0.261466
20	1	0	7.895870	-2.187684	0.925037
21	1	0	7.172982	-0.590168	1.180215
22	1	0	6.471187	-2.014603	1.967217
23	7	0	4.748039	-1.218257	-0.067603
24	6	0	0.851243	0.651376	0.414250
25	6	0	-0.275270	-0.263667	0.942402
26	1	0	0.940993	1.513704	1.092098
27	1	0	0.025277	-0.674616	1.917151
28	6	0	-1.542217	0.492877	1.148571
29	1	0	-1.494556	1.361560	1.797699
30	6	0	-2.764960	0.172930	0.591415
31	6	0	-4.719654	-0.825237	-0.587568
32	6	0	-5.037793	0.331280	0.165132
33	6	0	-5.697076	-1.515739	-1.307568
34	6	0	-6.362040	0.801922	0.209644
35	6	0	-6.999744	-1.037130	-1.260641
36	1	0	-5.442569	-2.398594	-1.882195
37	6	0	-7.324369	0.109286	-0.506373
38	1	0	-6.634197	1.674393	0.789507
39	1	0	-7.778861	-1.554318	-1.809648
40	1	0	-8.351057	0.457401	-0.482806
41	7	0	-3.930232	0.870548	0.795092
42	16	0	-3.023347	-1.208699	-0.462100
43	6	0	-3.973454	2.077041	1.632945
44	1	0	-3.870309	1.804055	2.685175
45	1	0	-3.170174	2.752191	1.338288
46	1	0	-4.921397	2.583708	1.479664
47	1	0	0.526631	1.074090	-0.547638
48	1	0	-0.421603	-1.114857	0.270519

002dba_mol_b3lyp631dp_+1H2_OL2_PCMw.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.648160	1.795000	1.461715
2	6	0	5.721847	0.649898	0.696645
3	6	0	4.558329	0.136069	0.081778
4	6	0	3.299835	0.794887	0.266739
5	6	0	3.278327	1.979069	1.050506
6	6	0	4.422702	2.469188	1.636777

7	1	0	6.548813	2.180318	1.927360
8	1	0	6.676070	0.157138	0.576419
9	6	0	2.117744	0.260415	-0.350599
10	1	0	2.346694	2.514490	1.177799
11	1	0	4.383565	3.375852	2.230238
12	6	0	2.262535	-0.884225	-1.132340
13	6	0	3.503590	-1.476447	-1.297483
14	1	0	1.409558	-1.357093	-1.600639
15	1	0	3.622387	-2.369416	-1.897887
16	6	0	5.885818	-1.753639	-0.911466
17	6	0	6.199263	-2.687120	0.255838
18	1	0	6.680246	-1.028174	-1.085388
19	1	0	5.764909	-2.318609	-1.835582
20	1	0	7.133917	-3.212355	0.042442
21	1	0	6.319535	-2.143846	1.195811
22	1	0	5.408109	-3.430489	0.382282
23	7	0	4.613535	-1.001063	-0.714795
24	6	0	0.805352	0.875084	-0.147722
25	6	0	-0.217308	0.786921	-1.017452
26	1	0	0.661056	1.449577	0.761501
27	1	0	-0.087301	0.253174	-1.957846
28	6	0	-1.557884	1.419054	-0.800891
29	1	0	-1.713634	2.169149	-1.587902
30	6	0	-2.709643	0.400468	-0.890253
31	6	0	-4.335790	-0.872398	0.667294
32	6	0	-4.935107	0.182640	-0.047690
33	6	0	-5.087462	-1.755765	1.429229
34	6	0	-6.325778	0.324476	-0.009521
35	6	0	-6.480209	-1.597119	1.477014
36	1	0	-4.604555	-2.562745	1.971519
37	6	0	-7.085831	-0.566946	0.759313
38	1	0	-6.818695	1.113661	-0.565799
39	1	0	-7.080461	-2.284019	2.064904
40	1	0	-8.165194	-0.451005	0.784375
41	7	0	-4.030218	1.019039	-0.715474
42	16	0	-2.567467	-0.855663	0.474378
43	6	0	-4.518179	1.797153	-1.850862
44	1	0	-3.726737	2.450526	-2.219770
45	1	0	-4.863230	1.159997	-2.679078
46	1	0	-5.342869	2.437911	-1.532448
47	1	0	-1.604379	1.932898	0.163100
48	1	0	-2.653410	-0.132166	-1.852990

002dbb_mol_TDb3lyp631dp_+1H2_OL2_PCMw_opt.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.905647	-2.621636	1.020641
2	6	0	5.311632	-1.420838	0.445531
3	6	0	4.403249	-0.364324	0.258781
4	6	0	3.033572	-0.517106	0.658300
5	6	0	2.665610	-1.759467	1.224708
6	6	0	3.575729	-2.791646	1.410310
7	1	0	5.627647	-3.420571	1.153804
8	1	0	6.342875	-1.314525	0.136888
9	6	0	2.091322	0.574847	0.463836
10	1	0	1.636432	-1.922120	1.519756
11	1	0	3.247031	-3.727738	1.850311
12	6	0	2.605891	1.750719	-0.150562
13	6	0	3.914009	1.858391	-0.514161
14	1	0	1.967252	2.608971	-0.317060
15	1	0	4.313116	2.756819	-0.966183
16	6	0	6.203188	1.047168	-0.780894

17	6	0	6.469752	0.452670	-2.165585
18	1	0	6.889886	0.639846	-0.035259
19	1	0	6.373206	2.125783	-0.798202
20	1	0	7.506840	0.644930	-2.455996
21	1	0	6.306114	-0.628025	-2.179809
22	1	0	5.813716	0.908619	-2.912803
23	7	0	4.822706	0.844281	-0.314232
24	6	0	0.713489	0.478844	0.863727
25	6	0	-0.289167	1.355413	0.588913
26	1	0	0.435209	-0.391104	1.452681
27	1	0	-0.104677	2.251623	0.000857
28	6	0	-1.682149	1.205501	1.147262
29	1	0	-1.886547	1.992076	1.889333
30	6	0	-2.748262	1.318813	0.051964
31	6	0	-4.099035	-0.637353	-0.929074
32	6	0	-4.812960	0.117697	0.059760
33	6	0	-4.687309	-1.748535	-1.539665
34	6	0	-6.126772	-0.262037	0.428059
35	6	0	-5.975119	-2.102437	-1.168013
36	1	0	-4.145659	-2.315185	-2.287387
37	6	0	-6.684545	-1.361424	-0.187807
38	1	0	-6.669346	0.289893	1.184486
39	1	0	-6.449754	-2.959260	-1.631637
40	1	0	-7.686902	-1.671312	0.084421
41	7	0	-4.119439	1.166207	0.547120
42	16	0	-2.517710	0.005186	-1.234609
43	6	0	-4.667117	2.139275	1.491884
44	1	0	-4.058599	3.041869	1.464452
45	1	0	-5.687464	2.396406	1.203302
46	1	0	-4.664248	1.733744	2.507293
47	1	0	-1.797208	0.244202	1.657558
48	1	0	-2.672372	2.283454	-0.464753

002dbc_mol_b3lyp631dp_+1H2_OL2_PCMw_triplet.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.781741	-2.664782	0.994458
2	6	0	5.228842	-1.467094	0.442396
3	6	0	4.355393	-0.380191	0.263891
4	6	0	2.976830	-0.499063	0.645233
5	6	0	2.568468	-1.735791	1.193621
6	6	0	3.444631	-2.799429	1.371606
7	1	0	5.478548	-3.487239	1.121222
8	1	0	6.266248	-1.386865	0.145955
9	6	0	2.064823	0.623527	0.452125
10	1	0	1.533560	-1.870279	1.484075
11	1	0	3.083436	-3.730435	1.797332
12	6	0	2.626633	1.795779	-0.134547
13	6	0	3.941794	1.870352	-0.476341
14	1	0	2.015173	2.673548	-0.304069
15	1	0	4.373559	2.763184	-0.910677
16	6	0	6.210077	0.993496	-0.729419
17	6	0	6.476981	0.414589	-2.121244
18	1	0	6.876754	0.553283	0.016321
19	1	0	6.413313	2.066775	-0.726886
20	1	0	7.523435	0.579295	-2.395250
21	1	0	6.280335	-0.660149	-2.156277
22	1	0	5.845417	0.903137	-2.869009
23	7	0	4.819648	0.825379	-0.281435
24	6	0	0.682537	0.562980	0.829659
25	6	0	-0.278060	1.511807	0.628178
26	1	0	0.355054	-0.335442	1.346469

27	1	0	-0.051435	2.441369	0.111154
28	6	0	-1.688755	1.362705	1.117329
29	1	0	-1.974797	2.223656	1.736497
30	6	0	-2.700997	1.307563	-0.057859
31	6	0	-4.034054	-0.748109	-0.834130
32	6	0	-4.786189	0.142109	0.000842
33	6	0	-4.610893	-1.923476	-1.321200
34	6	0	-6.124762	-0.167395	0.347883
35	6	0	-5.925206	-2.206687	-0.975914
36	1	0	-4.042379	-2.595378	-1.953495
37	6	0	-6.671861	-1.332216	-0.144868
38	1	0	-6.696859	0.491001	0.989230
39	1	0	-6.391010	-3.113583	-1.345312
40	1	0	-7.694302	-1.589021	0.108971
41	7	0	-4.097487	1.241505	0.372600
42	16	0	-2.417637	-0.180348	-1.114412
43	6	0	-4.665058	2.337023	1.159626
44	1	0	-4.063281	3.232093	1.008423
45	1	0	-5.682894	2.538231	0.823566
46	1	0	-4.674103	2.080109	2.223021
47	1	0	-1.809195	0.461938	1.726498
48	1	0	-2.575006	2.191974	-0.693270

002dca_mol_b3lyp631dp_+1H2_OL3_PCMw.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	6.262729	1.309013	0.700892
2	6	0	5.785265	0.100305	0.201964
3	6	0	4.454194	-0.020954	-0.247098
4	6	0	3.592956	1.101292	-0.146094
5	6	0	4.109745	2.307099	0.338066
6	6	0	5.432580	2.429560	0.760223
7	1	0	7.293735	1.371552	1.036581
8	1	0	6.456910	-0.747627	0.158254
9	6	0	2.116919	1.005443	-0.500713
10	1	0	3.446836	3.167762	0.393117
11	1	0	5.804381	3.377006	1.136961
12	6	0	1.871151	-0.180172	-1.389232
13	6	0	2.744822	-1.196993	-1.458403
14	1	0	0.942776	-0.247723	-1.945101
15	1	0	2.537329	-2.082601	-2.049668
16	6	0	4.804451	-2.419340	-0.885578
17	6	0	4.840256	-3.197623	0.432671
18	1	0	5.818007	-2.160011	-1.209139
19	1	0	4.385854	-3.050058	-1.673523
20	1	0	5.463530	-4.090799	0.323195
21	1	0	5.253532	-2.593359	1.245076
22	1	0	3.833216	-3.513719	0.720705
23	7	0	3.984293	-1.206150	-0.828315
24	6	0	1.248299	0.930391	0.823274
25	6	0	-0.209919	1.025047	0.554579
26	1	0	1.491312	0.004056	1.351777
27	1	0	-0.563257	1.985787	0.179586
28	6	0	-1.083030	0.005576	0.713002
29	1	0	-0.718162	-0.943642	1.087340
30	6	0	-2.487318	0.096827	0.409060
31	6	0	-4.780232	0.714249	-0.345799
32	6	0	-4.703502	-0.540840	0.276383
33	6	0	-5.990902	1.212456	-0.828323
34	6	0	-5.843282	-1.338530	0.425350
35	6	0	-7.123859	0.418778	-0.675642
36	1	0	-6.044937	2.183241	-1.307272

37	6	0	-7.048357	-0.840655	-0.057785
38	1	0	-5.795759	-2.313336	0.894662
39	1	0	-8.078710	0.779614	-1.042259
40	1	0	-7.945980	-1.440387	0.045097
41	7	0	-3.399218	-0.844864	0.695062
42	16	0	-3.195573	1.460969	-0.406449
43	6	0	-3.117060	-2.112120	1.389510
44	1	0	-3.128700	-2.933465	0.670576
45	1	0	-2.151834	-2.063813	1.882496
46	1	0	-3.884598	-2.268037	2.147083
47	1	0	1.816750	1.932724	-1.007173
48	1	0	1.545977	1.775574	1.455744

002dcb_mol_TDb3lyp631dp_+1H2_OL3_PCMw_opt.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	6.258924	-1.149597	-1.051496
2	6	0	5.829422	-0.018453	-0.373179
3	6	0	4.542630	0.013320	0.197618
4	6	0	3.676741	-1.100925	0.069685
5	6	0	4.144516	-2.229875	-0.604599
6	6	0	5.420619	-2.263319	-1.162401
7	1	0	7.252382	-1.165401	-1.485275
8	1	0	6.498579	0.825836	-0.286304
9	6	0	2.266823	-1.068857	0.611024
10	1	0	3.497126	-3.096579	-0.689534
11	1	0	5.761433	-3.153431	-1.679831
12	6	0	2.031885	0.100943	1.500376
13	6	0	2.917473	1.137145	1.582451
14	1	0	1.118767	0.156386	2.075665
15	1	0	2.709087	2.014862	2.179217
16	6	0	4.937544	2.366569	1.013111
17	6	0	4.817978	3.232471	-0.242493
18	1	0	5.968417	2.071954	1.208882
19	1	0	4.590900	2.914398	1.888824
20	1	0	5.432079	4.126462	-0.108992
21	1	0	5.164832	2.707102	-1.135026
22	1	0	3.782520	3.544097	-0.400360
23	7	0	4.110336	1.139462	0.928881
24	6	0	1.211900	-1.073376	-0.543610
25	6	0	-0.203212	-0.968147	-0.042143
26	1	0	1.437177	-0.239108	-1.216805
27	1	0	-0.473636	-1.590895	0.808332
28	6	0	-1.173110	-0.235312	-0.694010
29	1	0	-0.864042	0.366643	-1.544808
30	6	0	-2.530798	-0.185320	-0.361659
31	6	0	-4.856982	-0.475119	0.571198
32	6	0	-4.783518	0.446956	-0.490999
33	6	0	-6.062062	-0.768462	1.199299
34	6	0	-5.952092	1.075104	-0.940132
35	6	0	-7.223720	-0.130286	0.752931
36	1	0	-6.098662	-1.480028	2.017558
37	6	0	-7.161008	0.778645	-0.307262
38	1	0	-5.932132	1.774431	-1.767474
39	1	0	-8.173317	-0.347282	1.230365
40	1	0	-8.067099	1.265161	-0.654157
41	7	0	-3.487891	0.615479	-0.972547
42	16	0	-3.260016	-1.148613	0.936544
43	6	0	-3.132845	1.526531	-2.052746
44	1	0	-2.252225	2.108647	-1.771285
45	1	0	-2.920771	0.981263	-2.978030
46	1	0	-3.952844	2.219020	-2.229001

47	1	0	2.095327	-1.981394	1.202568
48	1	0	1.366601	-1.992732	-1.129342

002dcc_mol_b3lyp631dp_+1H2_OL3_PCMw_triplet.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	6.289604	-1.389128	-0.704842
2	6	0	5.880445	-0.173077	-0.185012
3	6	0	4.546571	-0.002686	0.247990
4	6	0	3.614748	-1.071019	0.130680
5	6	0	4.068567	-2.289188	-0.380354
6	6	0	5.386904	-2.457055	-0.795240
7	1	0	7.315890	-1.510610	-1.033089
8	1	0	6.595599	0.634202	-0.112925
9	6	0	2.169863	-0.905782	0.524667
10	1	0	3.374903	-3.120917	-0.449965
11	1	0	5.712880	-3.414104	-1.188199
12	6	0	1.914792	0.384623	1.202471
13	6	0	2.860088	1.360580	1.299000
14	1	0	0.920875	0.583759	1.585279
15	1	0	2.649179	2.317625	1.758007
16	6	0	5.044446	2.370967	0.921114
17	6	0	5.125420	3.152797	-0.391697
18	1	0	6.022334	2.014505	1.244841
19	1	0	4.653778	3.002125	1.719296
20	1	0	5.794366	4.005330	-0.248676
21	1	0	5.517784	2.540087	-1.206424
22	1	0	4.141177	3.530025	-0.680082
23	7	0	4.132822	1.204067	0.824311
24	6	0	1.187431	-1.057915	-0.722438
25	6	0	-0.255043	-1.124697	-0.339021
26	1	0	1.376792	-0.224594	-1.406533
27	1	0	-0.568057	-1.996600	0.233288
28	6	0	-1.181142	-0.157084	-0.690351
29	1	0	-0.822964	0.699203	-1.257162
30	6	0	-2.545956	-0.175863	-0.393330
31	6	0	-4.898888	-0.642415	0.396238
32	6	0	-4.771275	0.563398	-0.324791
33	6	0	-6.121178	-1.059573	0.909587
34	6	0	-5.903256	1.365120	-0.525382
35	6	0	-7.247105	-0.255385	0.702352
36	1	0	-6.198150	-1.991260	1.460607
37	6	0	-7.129701	0.942875	-0.008058
38	1	0	-5.841059	2.300205	-1.069382
39	1	0	-8.209357	-0.565261	1.096173
40	1	0	-8.005681	1.564651	-0.164400
41	7	0	-3.471708	0.799383	-0.758276
42	16	0	-3.339965	-1.473174	0.524344
43	6	0	-3.059047	1.965993	-1.526473
44	1	0	-2.350070	2.574656	-0.955980
45	1	0	-2.587559	1.656116	-2.463901
46	1	0	-3.927580	2.574916	-1.764572
47	1	0	1.888913	-1.724500	1.204828
48	1	0	1.499938	-1.975859	-1.235440

002dda_mol_b3lyp631dp_+1H2_OL4_PCMw.log

Standard orientation:

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

1	6	0	6.173621	1.715822	0.442880
2	6	0	5.899787	0.380497	0.181487
3	6	0	4.593009	-0.045927	-0.135196
4	6	0	3.532669	0.907069	-0.174842
5	6	0	3.856340	2.249502	0.093695
6	6	0	5.147000	2.662438	0.397600
7	1	0	7.189663	2.014228	0.682404
8	1	0	6.709846	-0.335363	0.226587
9	6	0	2.139935	0.486802	-0.493797
10	1	0	3.071413	2.996107	0.061428
11	1	0	5.350492	3.709366	0.598582
12	6	0	1.998924	-0.935943	-0.752254
13	6	0	3.050425	-1.783739	-0.705318
14	1	0	1.029427	-1.355046	-0.989907
15	1	0	2.928547	-2.843048	-0.899819
16	6	0	5.382259	-2.424872	-0.330795
17	6	0	5.659073	-2.902994	1.096869
18	1	0	6.293291	-2.048729	-0.803354
19	1	0	5.045926	-3.263668	-0.944678
20	1	0	6.435679	-3.673963	1.085658
21	1	0	6.000173	-2.085621	1.737796
22	1	0	4.756264	-3.332138	1.541436
23	7	0	4.338856	-1.393118	-0.416870
24	6	0	1.090422	1.354242	-0.543212
25	6	0	-0.333349	0.986616	-0.865322
26	1	0	1.247304	2.403553	-0.317600
27	1	0	-0.380091	0.105481	-1.514404
28	6	0	-1.167734	0.719703	0.409959
29	1	0	-1.118245	1.596450	1.067152
30	6	0	-2.611030	0.400208	0.165542
31	6	0	-4.863533	-0.091841	-0.753064
32	6	0	-4.801720	-0.119103	0.647517
33	6	0	-6.057622	-0.347715	-1.430516
34	6	0	-5.935177	-0.404597	1.415729
35	6	0	-7.184233	-0.631055	-0.665957
36	1	0	-6.101933	-0.326202	-2.513164
37	6	0	-7.121948	-0.658753	0.738490
38	1	0	-5.894586	-0.428453	2.497827
39	1	0	-8.126393	-0.834230	-1.163316
40	1	0	-8.017075	-0.883189	1.308071
41	7	0	-3.509944	0.166144	1.118933
42	16	0	-3.287429	0.291912	-1.417328
43	6	0	-3.220554	0.188028	2.562262
44	1	0	-3.409051	-0.803466	2.976566
45	1	0	-2.182648	0.459450	2.726950
46	1	0	-3.869076	0.923274	3.040384
47	1	0	-0.798559	1.811200	-1.419530
48	1	0	-0.723279	-0.114082	0.967178

002ddb_mol_TDb3lyp631dp_+1H2_OL4_PCMw_opt.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-6.135369	-1.715907	0.410578
2	6	0	-5.865043	-0.364123	0.340927
3	6	0	-4.572852	0.083344	-0.008467
4	6	0	-3.536519	-0.858596	-0.282026
5	6	0	-3.860544	-2.231145	-0.206058
6	6	0	-5.129268	-2.656728	0.132986
7	1	0	-7.132541	-2.046951	0.678792
8	1	0	-6.654037	0.341363	0.558221
9	6	0	-2.197730	-0.383226	-0.633374

10	1	0	-3.105071	-2.974709	-0.423668
11	1	0	-5.347892	-3.717571	0.182543
12	6	0	-2.028359	1.022463	-0.709035
13	6	0	-3.068739	1.880992	-0.437788
14	1	0	-1.074974	1.458503	-0.968209
15	1	0	-2.936434	2.953562	-0.485943
16	6	0	-5.327875	2.476146	0.226117
17	6	0	-5.470541	2.709537	1.729303
18	1	0	-6.266692	2.169165	-0.234349
19	1	0	-5.014260	3.391444	-0.275663
20	1	0	-6.228073	3.479847	1.894963
21	1	0	-5.780879	1.804951	2.257154
22	1	0	-4.526870	3.056159	2.158378
23	7	0	-4.298950	1.451706	-0.095630
24	6	0	-1.128912	-1.251628	-0.861880
25	6	0	0.263088	-0.873619	-1.231153
26	1	0	-1.293391	-2.313853	-0.726557
27	1	0	0.313057	0.128779	-1.663631
28	6	0	1.231077	-0.973183	-0.020001
29	1	0	1.166100	-1.982322	0.398148
30	6	0	2.652316	-0.682486	-0.405622
31	6	0	4.669644	0.869973	-0.284816
32	6	0	4.838337	-0.339893	0.416946
33	6	0	5.688237	1.812871	-0.359147
34	6	0	6.054531	-0.601912	1.064363
35	6	0	6.902411	1.545254	0.285900
36	1	0	5.544073	2.738297	-0.907043
37	6	0	7.074946	0.349695	0.988066
38	1	0	6.201044	-1.519418	1.622230
39	1	0	7.707270	2.271019	0.237941
40	1	0	8.017403	0.150551	1.488623
41	7	0	3.724075	-1.162547	0.369280
42	16	0	3.054402	0.949191	-1.010061
43	6	0	3.747642	-2.509098	0.927388
44	1	0	3.604602	-2.497703	2.012644
45	1	0	2.961646	-3.107541	0.469796
46	1	0	4.705307	-2.985741	0.702290
47	1	0	0.614670	-1.569726	-2.001983
48	1	0	0.876764	-0.291664	0.771521

002ddc_mol_b3lyp631dp_+1H2_OL4_PCMw_triplet.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-6.102487	-1.803221	0.421006
2	6	0	-5.884390	-0.442697	0.341658
3	6	0	-4.607864	0.052119	-0.004660
4	6	0	-3.532037	-0.853478	-0.266954
5	6	0	-3.805148	-2.237202	-0.178376
6	6	0	-5.058735	-2.707468	0.157935
7	1	0	-7.087716	-2.170394	0.686987
8	1	0	-6.701360	0.233281	0.549722
9	6	0	-2.214090	-0.329661	-0.615217
10	1	0	-3.020389	-2.953911	-0.381520
11	1	0	-5.236750	-3.775533	0.217628
12	6	0	-2.093234	1.078768	-0.687218
13	6	0	-3.166869	1.900602	-0.428557
14	1	0	-1.152632	1.548593	-0.937630
15	1	0	-3.074764	2.977723	-0.478615
16	6	0	-5.454663	2.414471	0.204110
17	6	0	-5.615355	2.660457	1.703657
18	1	0	-6.378079	2.065992	-0.258225
19	1	0	-5.172247	3.334749	-0.307365

20	1	0	-6.401971	3.404366	1.854696
21	1	0	-5.895784	1.751490	2.240634
22	1	0	-4.687996	3.047271	2.133870
23	7	0	-4.384456	1.425601	-0.098531
24	6	0	-1.113299	-1.166207	-0.857826
25	6	0	0.267958	-0.748571	-1.230917
26	1	0	-1.244867	-2.235984	-0.736981
27	1	0	0.307486	0.285886	-1.580977
28	6	0	1.262204	-0.945788	-0.052743
29	1	0	1.186091	-1.979406	0.299317
30	6	0	2.686265	-0.660147	-0.452401
31	6	0	4.704713	0.894896	-0.242921
32	6	0	4.869895	-0.349677	0.401710
33	6	0	5.723800	1.838500	-0.266540
34	6	0	6.084588	-0.644118	1.038551
35	6	0	6.936063	1.539163	0.371126
36	1	0	5.583857	2.789449	-0.770572
37	6	0	7.105935	0.310525	1.013972
38	1	0	6.229273	-1.589840	1.548262
39	1	0	7.741217	2.266584	0.361814
40	1	0	8.046956	0.086182	1.507079
41	7	0	3.759200	-1.169575	0.310458
42	16	0	3.096441	1.003415	-0.979796
43	6	0	3.804793	-2.551342	0.773997
44	1	0	3.753620	-2.608752	1.866562
45	1	0	2.969722	-3.107377	0.351438
46	1	0	4.731690	-3.028523	0.439978
47	1	0	0.605174	-1.380593	-2.062057
48	1	0	0.944952	-0.307629	0.788863

002dea_mol_b3lyp631dp_+1H2_OL5_PCMw.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.950032	2.134458	-0.259774
2	6	0	5.902460	0.753260	-0.253760
3	6	0	4.665802	0.056470	-0.214844
4	6	0	3.449349	0.832822	-0.189154
5	6	0	3.556234	2.247817	-0.196915
6	6	0	4.771003	2.900045	-0.228271
7	1	0	6.917300	2.627566	-0.286508
8	1	0	6.832679	0.201703	-0.264341
9	6	0	2.157870	0.173311	-0.230926
10	1	0	2.649532	2.840738	-0.214887
11	1	0	4.814305	3.983550	-0.243738
12	6	0	2.206528	-1.293417	-0.586823
13	6	0	3.365806	-1.973529	0.127402
14	1	0	1.284050	-1.816559	-0.334905
15	1	0	3.431816	-3.017155	-0.188083
16	6	0	5.841831	-2.127063	-0.040628
17	6	0	6.367402	-2.208777	1.397635
18	1	0	6.613755	-1.745549	-0.713507
19	1	0	5.595147	-3.129251	-0.402138
20	1	0	7.259690	-2.841436	1.431420
21	1	0	6.635252	-1.220690	1.782256
22	1	0	5.619146	-2.644454	2.066392
23	7	0	4.629658	-1.315637	-0.197050
24	6	0	0.967208	0.840617	-0.005806
25	6	0	-0.322630	0.276387	-0.095116
26	1	0	1.001939	1.889314	0.272115
27	1	0	-0.411225	-0.774752	-0.356819
28	6	0	-1.480701	0.994479	0.128168
29	1	0	-1.400199	2.045819	0.380607

30	6	0	-2.778549	0.445729	0.053472
31	6	0	-4.849940	-0.939398	-0.162891
32	6	0	-5.099097	0.405965	0.156468
33	6	0	-5.887016	-1.857272	-0.319232
34	6	0	-6.412789	0.854704	0.331750
35	6	0	-7.192875	-1.404007	-0.146793
36	1	0	-5.680654	-2.892443	-0.566389
37	6	0	-7.447809	-0.063112	0.175773
38	1	0	-6.633490	1.883923	0.585369
39	1	0	-8.018579	-2.097769	-0.262265
40	1	0	-8.470992	0.271345	0.308988
41	7	0	-3.915848	1.151368	0.261149
42	16	0	-3.123375	-1.232110	-0.313350
43	6	0	-3.887767	2.586504	0.573850
44	1	0	-3.418364	2.748781	1.546115
45	1	0	-3.336526	3.121612	-0.200827
46	1	0	-4.904414	2.966446	0.601661
47	1	0	3.193772	-1.966149	1.215270
48	1	0	2.349277	-1.386893	-1.672390

002deb_mol_TDb3lyp631dp_+1H2_OL5_PCMw_opt.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.958836	2.186768	-0.107395
2	6	0	5.895881	0.806303	0.064579
3	6	0	4.674286	0.107696	-0.091481
4	6	0	3.470495	0.845291	-0.394236
5	6	0	3.584729	2.213402	-0.596638
6	6	0	4.808264	2.895083	-0.444455
7	1	0	6.905425	2.699041	0.024155
8	1	0	6.793877	0.275715	0.350303
9	6	0	2.181170	0.129964	-0.516655
10	1	0	2.705248	2.774461	-0.892599
11	1	0	4.845263	3.968782	-0.593530
12	6	0	2.315784	-1.317443	-0.881435
13	6	0	3.341185	-1.967975	0.063712
14	1	0	1.375480	-1.862152	-0.784202
15	1	0	3.525720	-3.007715	-0.213181
16	6	0	5.826178	-2.084052	0.193142
17	6	0	6.184401	-2.329765	1.665922
18	1	0	6.653493	-1.611916	-0.337773
19	1	0	5.629627	-3.036822	-0.305174
20	1	0	7.076294	-2.960419	1.715257
21	1	0	6.393920	-1.390937	2.185205
22	1	0	5.372715	-2.842245	2.188580
23	7	0	4.621859	-1.263063	0.025198
24	6	0	0.997109	0.745302	-0.195096
25	6	0	-0.310162	0.194864	-0.285665
26	1	0	1.050753	1.767016	0.177381
27	1	0	-0.428776	-0.805479	-0.693225
28	6	0	-1.444595	0.896532	0.109013
29	1	0	-1.309465	1.894824	0.514155
30	6	0	-2.755789	0.416880	0.032892
31	6	0	-4.892687	-0.874498	-0.249955
32	6	0	-5.076268	0.417947	0.281468
33	6	0	-5.966147	-1.732810	-0.469318
34	6	0	-6.366353	0.856716	0.608449
35	6	0	-7.248615	-1.286420	-0.146296
36	1	0	-5.807030	-2.723955	-0.879965
37	6	0	-7.438918	-0.005171	0.387360
38	1	0	-6.539261	1.839698	1.029037
39	1	0	-8.099973	-1.938720	-0.308535

40	1	0	-8.440369	0.328767	0.638333
41	7	0	-3.877850	1.115556	0.415119
42	16	0	-3.186371	-1.187574	-0.560907
43	6	0	-3.781671	2.481155	0.928582
44	1	0	-3.279671	2.491237	1.900008
45	1	0	-3.224983	3.103759	0.224731
46	1	0	-4.778990	2.897544	1.040440
47	1	0	2.945079	-1.958659	1.087472
48	1	0	2.666819	-1.442706	-1.913549

002dec_mol_b3lyp631dp_+1H2_OL5_PCMw_triplet.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.889021	2.237570	-0.325303
2	6	0	5.893862	0.860215	-0.332810
3	6	0	4.686973	0.121458	-0.194820
4	6	0	3.414559	0.832553	-0.094608
5	6	0	3.480885	2.253012	-0.073117
6	6	0	4.670853	2.939752	-0.182623
7	1	0	6.824296	2.779582	-0.415025
8	1	0	6.838624	0.339840	-0.409679
9	6	0	2.177816	0.105851	-0.093421
10	1	0	2.564223	2.824284	-0.000550
11	1	0	4.669017	4.024803	-0.172605
12	6	0	2.252372	-1.387507	-0.296829
13	6	0	3.513208	-1.957643	0.333428
14	1	0	1.395616	-1.892018	0.157094
15	1	0	3.630779	-3.012171	0.079616
16	6	0	5.937941	-2.030271	-0.262032
17	6	0	6.672796	-2.221992	1.070385
18	1	0	6.584943	-1.558947	-1.003304
19	1	0	5.648146	-3.001313	-0.671527
20	1	0	7.566468	-2.830528	0.905556
21	1	0	6.981729	-1.263897	1.496668
22	1	0	6.041040	-2.736801	1.799404
23	7	0	4.703701	-1.242976	-0.141483
24	6	0	0.932007	0.747266	0.033700
25	6	0	-0.329885	0.156586	-0.054727
26	1	0	0.929201	1.816044	0.228610
27	1	0	-0.414023	-0.904245	-0.271661
28	6	0	-1.508606	0.908776	0.120408
29	1	0	-1.402266	1.967778	0.335043
30	6	0	-2.802699	0.404904	0.045713
31	6	0	-4.903714	-0.948929	-0.152358
32	6	0	-5.132301	0.417771	0.112799
33	6	0	-5.956417	-1.850769	-0.290531
34	6	0	-6.445773	0.890512	0.246774
35	6	0	-7.258582	-1.371487	-0.158372
36	1	0	-5.764125	-2.898232	-0.494751
37	6	0	-7.493835	-0.014169	0.108121
38	1	0	-6.653049	1.932542	0.456080
39	1	0	-8.094226	-2.055211	-0.261588
40	1	0	-8.513020	0.343250	0.210475
41	7	0	-3.951726	1.146947	0.210654
42	16	0	-3.182218	-1.289017	-0.267659
43	6	0	-3.894581	2.586304	0.469192
44	1	0	-3.405993	2.778961	1.427515
45	1	0	-3.343895	3.086444	-0.330567
46	1	0	-4.902719	2.989182	0.500500
47	1	0	3.460435	-1.879283	1.428137
48	1	0	2.235061	-1.632167	-1.368900

002eaa_mol_b3lyp631dp_+2H2_OL_PCMw.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	6.026743	2.050575	0.764733
2	6	0	6.029097	0.762452	0.272087
3	6	0	4.807083	0.129705	-0.047336
4	6	0	3.569274	0.822520	0.141196
5	6	0	3.618115	2.147062	0.651535
6	6	0	4.817101	2.749212	0.957444
7	1	0	6.970543	2.527651	1.005715
8	1	0	6.971309	0.250310	0.138113
9	6	0	2.331502	0.177542	-0.184129
10	1	0	2.694233	2.690736	0.801293
11	1	0	4.833577	3.761358	1.346252
12	6	0	2.391798	-1.114555	-0.679218
13	6	0	3.616875	-1.751747	-0.850424
14	1	0	1.500590	-1.663640	-0.949213
15	1	0	3.674343	-2.760722	-1.238441
16	6	0	6.032388	-1.956481	-0.735710
17	6	0	6.523196	-2.583083	0.567212
18	1	0	6.776756	-1.301000	-1.187133
19	1	0	5.799077	-2.726763	-1.470477
20	1	0	7.429791	-3.157024	0.358469
21	1	0	6.761400	-1.830467	1.322033
22	1	0	5.772231	-3.262848	0.977671
23	7	0	4.779818	-1.165928	-0.551069
24	6	0	1.019214	0.898209	0.010524
25	6	0	-0.247636	0.128858	-0.379339
26	1	0	0.950347	1.197548	1.064650
27	1	0	-0.309403	-0.797690	0.204184
28	6	0	-1.505779	0.974561	-0.140137
29	1	0	-1.406464	1.914807	-0.695848
30	6	0	-2.794881	0.284516	-0.591379
31	6	0	-4.852507	-0.932752	0.415773
32	6	0	-5.128489	0.365612	-0.055534
33	6	0	-5.862249	-1.782882	0.844284
34	6	0	-6.458380	0.794670	-0.119643
35	6	0	-7.191969	-1.338882	0.794860
36	1	0	-5.626126	-2.780093	1.202749
37	6	0	-7.478901	-0.062741	0.313042
38	1	0	-6.705634	1.780317	-0.497329
39	1	0	-7.991604	-1.995544	1.122277
40	1	0	-8.508711	0.277885	0.261133
41	7	0	-3.993974	1.115766	-0.387565
42	16	0	-3.105342	-1.262926	0.401800
43	6	0	-4.156558	2.227051	-1.320973
44	1	0	-3.207583	2.749830	-1.442343
45	1	0	-4.505646	1.896480	-2.311122
46	1	0	-4.872957	2.946727	-0.918987
47	1	0	1.060850	1.836416	-0.557930
48	1	0	-0.200611	-0.158923	-1.436760
49	1	0	-1.599934	1.235640	0.919604
50	1	0	-2.706040	-0.009563	-1.650131

002faa_mol_b3lyp631dp_+1H2_AR_PCMw.log

Standard orientation:

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

1	6	0	6.096309	2.100816	-0.048332
2	6	0	6.033937	0.721970	-0.125316
3	6	0	4.786919	0.060272	-0.155388
4	6	0	3.576060	0.818041	-0.097557
5	6	0	3.692060	2.226378	-0.021083
6	6	0	4.918203	2.861897	0.003209
7	1	0	7.064875	2.589522	-0.027546
8	1	0	6.955200	0.157121	-0.159651
9	6	0	2.278662	0.143262	-0.119776
10	1	0	2.796506	2.832533	0.018186
11	1	0	4.967661	3.943880	0.062445
12	6	0	2.331078	-1.273898	-0.212951
13	6	0	3.519406	-1.946574	-0.270900
14	1	0	1.427215	-1.867184	-0.241802
15	1	0	3.547919	-3.026931	-0.340433
16	6	0	5.946301	-2.169654	-0.262723
17	6	0	6.528714	-2.405353	1.130931
18	1	0	6.674489	-1.709965	-0.932969
19	1	0	5.660502	-3.118737	-0.718801
20	1	0	7.415844	-3.039576	1.048288
21	1	0	6.821766	-1.469882	1.613802
22	1	0	5.802575	-2.911977	1.772592
23	7	0	4.727681	-1.329186	-0.246754
24	6	0	1.063246	0.858002	-0.051796
25	6	0	-0.212395	0.298407	-0.073843
26	1	0	1.104724	1.938214	0.027066
27	1	0	-0.305181	-0.782757	-0.154773
28	6	0	-1.390854	1.038219	0.002610
29	1	0	-1.317325	2.117229	0.085675
30	6	0	-2.677318	0.483362	-0.029977
31	6	0	-4.758387	-0.907659	-0.117265
32	6	0	-5.002241	0.423649	0.011345
33	6	0	-5.858562	-1.913039	-0.300075
34	6	0	-6.368997	0.938000	0.032116
35	6	0	-7.142953	-1.408840	0.391719
36	1	0	-6.036845	-2.054062	-1.376284
37	6	0	-7.382962	0.068671	0.183466
38	1	0	-6.555543	1.998394	-0.091312
39	1	0	-7.999205	-1.989118	0.036560
40	1	0	-8.405504	0.433237	0.207540
41	7	0	-3.836144	1.195571	0.077389
42	16	0	-3.042234	-1.226352	-0.200519
43	6	0	-3.821299	2.645705	0.289032
44	1	0	-3.186212	2.886816	1.143887
45	1	0	-3.446480	3.157484	-0.600712
46	1	0	-4.830020	2.988390	0.501069
47	1	0	-5.577050	-2.890111	0.101848
48	1	0	-7.074487	-1.595386	1.474513

002faa_mol_TDb3lyp631dp_+1H2_AR_PCMw_opt.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	6.038706	2.137369	-0.392993
2	6	0	6.014073	0.749074	-0.304063
3	6	0	4.792519	0.059823	-0.191404
4	6	0	3.554456	0.792285	-0.144827
5	6	0	3.630525	2.202291	-0.259627
6	6	0	4.843581	2.864601	-0.377279
7	1	0	6.992079	2.648044	-0.480309
8	1	0	6.950180	0.208245	-0.322855
9	6	0	2.304605	0.081401	-0.000648
10	1	0	2.717067	2.783305	-0.269433

11	1	0	4.860862	3.946556	-0.460480
12	6	0	2.369279	-1.331200	0.048126
13	6	0	3.567407	-1.992800	-0.015661
14	1	0	1.472965	-1.925644	0.172072
15	1	0	3.629499	-3.072189	0.032663
16	6	0	5.996740	-2.139351	-0.143121
17	6	0	6.667472	-2.221136	1.229735
18	1	0	6.672083	-1.727641	-0.895882
19	1	0	5.717330	-3.137014	-0.486368
20	1	0	7.569229	-2.835665	1.155216
21	1	0	6.955582	-1.234289	1.600153
22	1	0	5.996320	-2.681709	1.959941
23	7	0	4.758443	-1.334019	-0.133970
24	6	0	1.043509	0.777073	0.115959
25	6	0	-0.207803	0.224500	-0.009443
26	1	0	1.083213	1.838885	0.340587
27	1	0	-0.307658	-0.825196	-0.275190
28	6	0	-1.406185	0.980927	0.186969
29	1	0	-1.299705	2.028928	0.449627
30	6	0	-2.680069	0.478853	0.066178
31	6	0	-4.763411	-0.870819	-0.263326
32	6	0	-5.006868	0.443866	0.072061
33	6	0	-5.862252	-1.824418	-0.614493
34	6	0	-6.368869	0.939015	0.163999
35	6	0	-7.167783	-1.431693	0.108121
36	1	0	-6.015879	-1.796421	-1.704447
37	6	0	-7.389069	0.057217	0.158106
38	1	0	-6.557614	2.003531	0.234173
39	1	0	-8.015826	-1.926695	-0.372955
40	1	0	-8.408447	0.421373	0.243497
41	7	0	-3.860953	1.187813	0.269930
42	16	0	-3.061505	-1.199052	-0.371561
43	6	0	-3.825059	2.580672	0.706299
44	1	0	-3.227708	2.667476	1.618230
45	1	0	-3.388740	3.213886	-0.071908
46	1	0	-4.833722	2.923886	0.919153
47	1	0	-5.587747	-2.853811	-0.367779
48	1	0	-7.144734	-1.804883	1.143523

002fac_mol_TDb3lyp631dp_+1H2_AR_PCMw_opt_TRIPLET.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	6.034598	2.198369	-0.049709
2	6	0	6.024083	0.810962	-0.127335
3	6	0	4.810589	0.100224	-0.157030
4	6	0	3.562691	0.804661	-0.096298
5	6	0	3.623882	2.214413	-0.020059
6	6	0	4.828088	2.902810	0.002521
7	1	0	6.982935	2.725093	-0.028818
8	1	0	6.967905	0.283950	-0.161250
9	6	0	2.308912	0.061529	-0.115825
10	1	0	2.705356	2.786623	0.021770
11	1	0	4.827732	3.986428	0.062250
12	6	0	2.411221	-1.354612	-0.202817
13	6	0	3.620799	-1.984411	-0.265009
14	1	0	1.524821	-1.975380	-0.224460
15	1	0	3.703207	-3.061445	-0.332145
16	6	0	6.059428	-2.078840	-0.276300
17	6	0	6.658175	-2.299312	1.114407
18	1	0	6.767209	-1.581377	-0.942491
19	1	0	5.820272	-3.038120	-0.739046
20	1	0	7.574397	-2.890254	1.026396

21	1	0	6.906673	-1.354092	1.603478
22	1	0	5.957655	-2.844013	1.753593
23	7	0	4.807908	-1.298690	-0.251804
24	6	0	1.039403	0.708028	-0.049535
25	6	0	-0.214699	0.117793	-0.068671
26	1	0	1.040170	1.791417	0.025981
27	1	0	-0.314164	-0.961047	-0.143785
28	6	0	-1.394492	0.901986	0.007176
29	1	0	-1.272202	1.978573	0.084476
30	6	0	-2.689376	0.416937	-0.017098
31	6	0	-4.804501	-0.901124	-0.110342
32	6	0	-5.008647	0.459058	0.001132
33	6	0	-5.936669	-1.866595	-0.288133
34	6	0	-6.358628	1.004712	0.019454
35	6	0	-7.215803	-1.319539	0.379209
36	1	0	-6.108469	-2.008488	-1.365319
37	6	0	-7.397237	0.163365	0.176695
38	1	0	-6.517451	2.069801	-0.097271
39	1	0	-8.085522	-1.863453	0.000627
40	1	0	-8.406158	0.563737	0.207797
41	7	0	-3.843247	1.185386	0.069221
42	16	0	-3.114735	-1.290190	-0.162158
43	6	0	-3.771163	2.637027	0.249779
44	1	0	-3.142011	2.867721	1.111866
45	1	0	-3.356346	3.109013	-0.644179
46	1	0	-4.767008	3.029374	0.433720
47	1	0	-5.686779	-2.849413	0.120200
48	1	0	-7.183020	-1.513134	1.461950

002fad_mol_TDb3lyp631dp_+1H2_AR_PCMw_opt_rot.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.881367	-0.225733	2.769720
2	6	0	5.266625	-0.315530	1.436094
3	6	0	4.371541	0.007425	0.400858
4	6	0	3.035429	0.425299	0.712658
5	6	0	2.690045	0.499676	2.081357
6	6	0	3.586645	0.185632	3.093585
7	1	0	5.592226	-0.480061	3.549008
8	1	0	6.271197	-0.643467	1.205551
9	6	0	2.102947	0.747211	-0.360291
10	1	0	1.691391	0.812297	2.360479
11	1	0	3.275568	0.257761	4.130808
12	6	0	2.604909	0.628472	-1.688122
13	6	0	3.883441	0.234783	-1.940488
14	1	0	1.975654	0.857140	-2.538789
15	1	0	4.268248	0.146501	-2.948090
16	6	0	6.118351	-0.536013	-1.321882
17	6	0	6.251080	-2.060593	-1.327398
18	1	0	6.854380	-0.075719	-0.658489
19	1	0	6.315009	-0.140171	-2.320364
20	1	0	7.264581	-2.341077	-1.628896
21	1	0	6.058956	-2.486844	-0.339353
22	1	0	5.546352	-2.505771	-2.035732
23	7	0	4.776227	-0.068850	-0.939080
24	6	0	0.752516	1.151736	-0.105112
25	6	0	-0.214436	1.441531	-1.025029
26	1	0	0.450421	1.230413	0.934858
27	1	0	-0.010668	1.409276	-2.093713
28	6	0	-1.575808	1.866440	-0.642558
29	1	0	-1.802937	2.925999	-0.537245
30	6	0	-2.588460	0.975907	-0.447308

31	6	0	-4.030382	-1.037175	-0.237878
32	6	0	-4.704804	0.152459	-0.000572
33	6	0	-4.736672	-2.356811	-0.254172
34	6	0	-6.123422	0.150155	0.314004
35	6	0	-5.968503	-2.325607	0.673586
36	1	0	-5.054369	-2.558023	-1.286815
37	6	0	-6.717255	-1.020312	0.615689
38	1	0	-6.684505	1.075812	0.308779
39	1	0	-6.634387	-3.154778	0.420995
40	1	0	-7.771673	-1.027191	0.873992
41	7	0	-3.903989	1.259256	-0.103640
42	16	0	-2.369672	-0.768440	-0.605560
43	6	0	-4.340192	2.639658	0.130089
44	1	0	-3.653846	3.119942	0.828329
45	1	0	-4.357055	3.191735	-0.811749
46	1	0	-5.334257	2.636195	0.567563
47	1	0	-4.062697	-3.168029	0.030184
48	1	0	-5.658290	-2.491409	1.715701

002fae_mol_TDb3lyp631dp_+1H2_AR_PCMw_opt_rot_1.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.785795	2.475646	-1.311344
2	6	0	5.248322	1.174942	-1.081014
3	6	0	4.460964	0.242704	-0.391875
4	6	0	3.165549	0.629965	0.092941
5	6	0	2.735467	1.952537	-0.158064
6	6	0	3.529777	2.863758	-0.850094
7	1	0	5.417171	3.175426	-1.848873
8	1	0	6.230937	0.901270	-1.441808
9	6	0	2.364992	-0.325497	0.808874
10	1	0	1.757781	2.257882	0.198854
11	1	0	3.167516	3.872063	-1.024404
12	6	0	2.890142	-1.614969	1.028598
13	6	0	4.123975	-1.962498	0.548607
14	1	0	2.319309	-2.356739	1.575177
15	1	0	4.547914	-2.946736	0.689766
16	6	0	6.232823	-1.516089	-0.608260
17	6	0	7.356729	-1.110909	0.348510
18	1	0	6.414612	-1.133826	-1.615744
19	1	0	6.189097	-2.604038	-0.694747
20	1	0	8.315916	-1.474674	-0.031645
21	1	0	7.421868	-0.025035	0.456792
22	1	0	7.193124	-1.544726	1.339307
23	7	0	4.903600	-1.070575	-0.167970
24	6	0	1.045436	0.043150	1.359450
25	6	0	-0.142440	-0.124738	0.688673
26	1	0	0.998502	0.467046	2.365574
27	1	0	-0.115324	-0.536745	-0.316920
28	6	0	-1.377780	0.221164	1.261669
29	1	0	-1.371234	0.646673	2.257480
30	6	0	-2.625778	0.028853	0.626510
31	6	0	-4.493937	-0.209435	-1.066496
32	6	0	-4.953955	-0.137955	0.377443
33	6	0	-5.497143	-0.972818	-1.887373
34	6	0	-6.302245	0.532842	0.435571
35	6	0	-6.792679	-0.730561	-1.612435
36	1	0	-5.181607	-1.584047	-2.725069
37	6	0	-7.178356	0.177461	-0.523274
38	1	0	-6.587597	1.159483	1.272300
39	1	0	-7.575627	-1.175647	-2.218282
40	1	0	-8.199869	0.542738	-0.491550

41	7	0	-3.805177	0.437780	1.110183
42	16	0	-2.769132	-0.840071	-0.907358
43	6	0	-4.014502	1.135230	2.378996
44	1	0	-4.439136	0.447072	3.115418
45	1	0	-3.078515	1.538732	2.753922
46	1	0	-4.703620	1.964538	2.216392
47	1	0	-4.399774	0.812049	-1.465638
48	1	0	-5.071223	-1.168759	0.762255

002fba_mol_b3lyp631dp_+2H2_ARB_PCMw.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	6.135828	2.097191	-0.225617
2	6	0	6.073661	0.717228	-0.230092
3	6	0	4.825989	0.056588	-0.191226
4	6	0	3.616137	0.817262	-0.139148
5	6	0	3.732535	2.228927	-0.138762
6	6	0	4.958193	2.861688	-0.180739
7	1	0	7.103769	2.586370	-0.256987
8	1	0	6.993842	0.150818	-0.261210
9	6	0	2.323673	0.143057	-0.091209
10	1	0	2.838443	2.837213	-0.107035
11	1	0	5.009903	3.945092	-0.178953
12	6	0	2.370405	-1.272273	-0.111814
13	6	0	3.559154	-1.950452	-0.168050
14	1	0	1.466120	-1.864680	-0.082571
15	1	0	3.585296	-3.032901	-0.181486
16	6	0	5.983438	-2.176925	-0.216420
17	6	0	6.605680	-2.337059	1.170375
18	1	0	6.689293	-1.752949	-0.932169
19	1	0	5.683423	-3.148088	-0.612323
20	1	0	7.488462	-2.978041	1.095167
21	1	0	6.915191	-1.377911	1.592504
22	1	0	5.898100	-2.805702	1.859682
23	7	0	4.763542	-1.334408	-0.208442
24	6	0	1.104177	0.866281	-0.026846
25	6	0	-0.163502	0.307981	0.004494
26	1	0	1.150664	1.948486	0.002365
27	1	0	-0.263180	-0.774500	-0.030410
28	6	0	-1.347968	1.053832	0.087709
29	1	0	-1.268938	2.133245	0.161238
30	6	0	-2.623612	0.493773	0.072025
31	6	0	-4.668610	-1.013491	0.321130
32	6	0	-4.980562	0.413808	-0.113063
33	6	0	-5.711110	-1.967795	-0.182540
34	6	0	-6.331404	0.822179	0.464951
35	6	0	-6.960600	-1.527680	-0.371572
36	6	0	-7.409197	-0.100269	-0.157488
37	1	0	-6.315853	0.719145	1.555669
38	1	0	-7.724457	-2.227289	-0.704205
39	1	0	-8.304999	-0.091895	0.474486
40	7	0	-3.776912	1.176284	0.274179
41	16	0	-2.925071	-1.230116	-0.264546
42	6	0	-3.795012	2.628589	0.420820
43	1	0	-3.051757	2.933672	1.159605
44	1	0	-3.586218	3.133917	-0.529733
45	1	0	-4.774822	2.938257	0.779725
46	1	0	-5.453053	-3.012708	-0.325728
47	1	0	-4.606293	-1.054152	1.415418
48	1	0	-5.055079	0.436173	-1.211977
49	1	0	-6.574520	1.863064	0.234610
50	1	0	-7.732367	0.309445	-1.124601

002fda_mol_b3lyp631dp_+3H2_ARB_PCMw.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	6.228928	2.073203	-0.146725
2	6	0	6.154386	0.694137	-0.178595
3	6	0	4.900466	0.044347	-0.169097
4	6	0	3.696911	0.814993	-0.118584
5	6	0	3.826023	2.225129	-0.088716
6	6	0	5.057767	2.847452	-0.102323
7	1	0	7.201577	2.553906	-0.155769
8	1	0	7.069850	0.119968	-0.208206
9	6	0	2.397443	0.152037	-0.100632
10	1	0	2.937036	2.840796	-0.055696
11	1	0	5.119063	3.930100	-0.078340
12	6	0	2.432289	-1.263492	-0.146137
13	6	0	3.615370	-1.951131	-0.199767
14	1	0	1.522523	-1.848143	-0.140989
15	1	0	3.631996	-3.033358	-0.233500
16	6	0	6.038019	-2.198941	-0.222011
17	6	0	6.638928	-2.393699	1.169782
18	1	0	6.757963	-1.766985	-0.918686
19	1	0	5.734985	-3.158901	-0.642265
20	1	0	7.517781	-3.039966	1.093650
21	1	0	6.949608	-1.446185	1.616657
22	1	0	5.917917	-2.871230	1.838796
23	7	0	4.825951	-1.345515	-0.213583
24	6	0	1.184037	0.884568	-0.041252
25	6	0	-0.088998	0.336128	-0.027899
26	1	0	1.238832	1.966043	-0.000763
27	1	0	-0.196042	-0.745346	-0.071142
28	6	0	-1.268340	1.089518	0.047106
29	1	0	-1.182665	2.168071	0.124659
30	6	0	-2.548047	0.536540	0.017586
31	6	0	-4.613904	-0.966494	0.206861
32	6	0	-4.913139	0.478877	-0.183437
33	6	0	-5.641570	-1.928577	-0.377321
34	6	0	-6.241200	0.912124	0.438114
35	6	0	-7.026922	-1.524759	0.171105
36	1	0	-5.629908	-1.869769	-1.472240
37	6	0	-7.346119	-0.038780	-0.072308
38	1	0	-6.171027	0.873722	1.532068
39	1	0	-7.798550	-2.150502	-0.289341
40	1	0	-8.294830	0.221529	0.407663
41	7	0	-3.697649	1.225777	0.204850
42	16	0	-2.855674	-1.183648	-0.315290
43	6	0	-3.704580	2.678316	0.353418
44	1	0	-2.966315	2.976747	1.099848
45	1	0	-3.481733	3.182247	-0.594684
46	1	0	-4.685055	2.996565	0.702247
47	1	0	-5.409131	-2.961523	-0.100923
48	1	0	-7.055591	-1.732176	1.248606
49	1	0	-4.617004	-1.046146	1.299744
50	1	0	-5.008729	0.538528	-1.280095
51	1	0	-6.492133	1.939773	0.157762
52	1	0	-7.484237	0.129793	-1.148298

002gdb_mol_b3lyp631dp_+1H2_ARA_PCMw.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.936905	2.124401	-0.250060
2	6	0	5.927642	0.782166	-0.283334
3	6	0	4.616494	0.062768	-0.525331
4	6	0	3.469454	0.791562	0.204779
5	6	0	3.507926	2.258052	-0.187439
6	6	0	4.687216	2.873403	-0.371914
7	1	0	6.873553	2.666101	-0.159288
8	1	0	6.854510	0.224440	-0.244064
9	6	0	2.133098	0.072009	0.025435
10	1	0	2.583642	2.818475	-0.257375
11	1	0	4.727618	3.935110	-0.596352
12	6	0	2.221221	-1.324358	-0.121098
13	6	0	3.443048	-1.981259	-0.107059
14	1	0	1.335091	-1.945669	-0.129319
15	1	0	3.470552	-3.064672	-0.038738
16	6	0	5.868047	-2.173706	-0.178548
17	6	0	6.540283	-2.240207	1.194013
18	1	0	6.544175	-1.764853	-0.933527
19	1	0	5.602609	-3.179676	-0.513075
20	1	0	7.449979	-2.844702	1.128707
21	1	0	6.813235	-1.247137	1.560306
22	1	0	5.871335	-2.701861	1.925920
23	7	0	4.630528	-1.374208	-0.176825
24	6	0	0.930601	0.781862	0.152809
25	6	0	-0.351456	0.234589	0.050838
26	1	0	0.981835	1.845425	0.359516
27	1	0	-0.441858	-0.829122	-0.159998
28	6	0	-1.522990	0.971385	0.190656
29	1	0	-1.443074	2.032877	0.397415
30	6	0	-2.810364	0.429103	0.087283
31	6	0	-4.885584	-0.960869	-0.153303
32	6	0	-5.139822	0.398344	0.095577
33	6	0	-5.919680	-1.880493	-0.311208
34	6	0	-6.457806	0.856325	0.195628
35	6	0	-7.231332	-1.417847	-0.213691
36	1	0	-5.707838	-2.926388	-0.503289
37	6	0	-7.491835	-0.064259	0.037806
38	1	0	-6.684159	1.896653	0.393562
39	1	0	-8.054246	-2.114465	-0.332437
40	1	0	-8.517655	0.280376	0.113631
41	7	0	-3.959951	1.145528	0.216620
42	16	0	-3.153295	-1.268656	-0.220585
43	6	0	-3.935483	2.590482	0.465510
44	1	0	-3.487072	2.797583	1.439765
45	1	0	-3.364225	3.091978	-0.318013
46	1	0	-4.951058	2.974860	0.454417
47	1	0	3.691132	0.739023	1.289512
48	1	0	4.397087	0.114199	-1.610578

002gdb_mol_TDb3lyp631dp_+1H2_ARA_PCMw_opt.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.924173	2.144214	-0.312961
2	6	0	5.928871	0.802058	-0.375325
3	6	0	4.616000	0.068492	-0.544908
4	6	0	3.491625	0.778656	0.256741
5	6	0	3.503696	2.256282	-0.083772
6	6	0	4.665477	2.886333	-0.324649
7	1	0	6.860504	2.692918	-0.275936

8	1	0	6.865144	0.260040	-0.415066
9	6	0	2.162222	0.054997	0.083412
10	1	0	2.577235	2.817469	-0.062337
11	1	0	4.687071	3.956343	-0.508483
12	6	0	2.258721	-1.355125	-0.035073
13	6	0	3.484682	-2.008544	-0.076703
14	1	0	1.373059	-1.978176	-0.021284
15	1	0	3.534988	-3.090545	-0.012353
16	6	0	5.911685	-2.138188	-0.201540
17	6	0	6.595872	-2.152623	1.170386
18	1	0	6.577927	-1.736677	-0.969295
19	1	0	5.665205	-3.159353	-0.503795
20	1	0	7.514862	-2.743927	1.111945
21	1	0	6.855547	-1.144540	1.503334
22	1	0	5.939984	-2.604325	1.919794
23	7	0	4.660785	-1.368606	-0.212409
24	6	0	0.929913	0.718694	0.161389
25	6	0	-0.348923	0.141097	0.030053
26	1	0	0.940571	1.787464	0.353071
27	1	0	-0.436051	-0.919586	-0.186779
28	6	0	-1.520128	0.899187	0.166226
29	1	0	-1.414061	1.961194	0.366071
30	6	0	-2.819536	0.397378	0.072778
31	6	0	-4.917734	-0.955596	-0.147024
32	6	0	-5.148109	0.422212	0.084651
33	6	0	-5.968975	-1.857380	-0.291447
34	6	0	-6.466576	0.898524	0.177781
35	6	0	-7.273303	-1.372661	-0.200719
36	1	0	-5.774335	-2.909328	-0.468871
37	6	0	-7.510975	-0.008176	0.032480
38	1	0	-6.677498	1.944580	0.361554
39	1	0	-8.108363	-2.056210	-0.309770
40	1	0	-8.531955	0.352160	0.103362
41	7	0	-3.973212	1.145945	0.194073
42	16	0	-3.197500	-1.300574	-0.213591
43	6	0	-3.916076	2.589115	0.425972
44	1	0	-3.458913	2.798696	1.396784
45	1	0	-3.333498	3.069799	-0.363501
46	1	0	-4.921840	2.999109	0.413399
47	1	0	3.775942	0.689413	1.323945
48	1	0	4.339845	0.127622	-1.616462

002gdc_mol_TDb3lyp631dp_+1H2_ARA_PCMw_opt_TRIPLET.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.897645	2.186431	-0.287960
2	6	0	5.927473	0.844260	-0.328213
3	6	0	4.629370	0.089580	-0.529420
4	6	0	3.483746	0.782984	0.246609
5	6	0	3.471026	2.253663	-0.128072
6	6	0	4.624980	2.903373	-0.352328
7	1	0	6.821806	2.753509	-0.228688
8	1	0	6.872805	0.316747	-0.326143
9	6	0	2.172140	0.025447	0.074336
10	1	0	2.532012	2.794581	-0.142238
11	1	0	4.630199	3.969223	-0.560067
12	6	0	2.293557	-1.373586	-0.023360
13	6	0	3.530936	-2.013792	-0.055957
14	1	0	1.417372	-2.010647	-0.011628
15	1	0	3.598616	-3.093342	0.013547
16	6	0	5.957611	-2.105056	-0.216291
17	6	0	6.650948	-2.149714	1.148139

18	1	0	6.607249	-1.668295	-0.978156
19	1	0	5.722178	-3.118770	-0.549228
20	1	0	7.580014	-2.721431	1.065895
21	1	0	6.893922	-1.148069	1.511747
22	1	0	6.009759	-2.636978	1.887911
23	7	0	4.694271	-1.350240	-0.189759
24	6	0	0.915411	0.658516	0.156124
25	6	0	-0.352866	0.078900	0.015580
26	1	0	0.913037	1.726415	0.360793
27	1	0	-0.443962	-0.978712	-0.213326
28	6	0	-1.520093	0.848018	0.163282
29	1	0	-1.400252	1.906408	0.375215
30	6	0	-2.824973	0.368139	0.067312
31	6	0	-4.944333	-0.949822	-0.154281
32	6	0	-5.153789	0.424061	0.091852
33	6	0	-6.010270	-1.834821	-0.300947
34	6	0	-6.461608	0.920206	0.199435
35	6	0	-7.305951	-1.331968	-0.196353
36	1	0	-5.832721	-2.887691	-0.490314
37	6	0	-7.522233	0.032076	0.052316
38	1	0	-6.654332	1.967495	0.396105
39	1	0	-8.151472	-2.002294	-0.306640
40	1	0	-8.536742	0.407608	0.134308
41	7	0	-3.963963	1.134230	0.200621
42	16	0	-3.227546	-1.321455	-0.234884
43	6	0	-3.887576	2.575083	0.445038
44	1	0	-3.448568	2.770904	1.426619
45	1	0	-3.282568	3.051216	-0.329400
46	1	0	-4.886204	3.001137	0.412921
47	1	0	3.761826	0.727174	1.318008
48	1	0	4.377705	0.137297	-1.606146

002gdd_mol_TDb3lyp631dp_+1H2_ARA_PCMw_opt_rot.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.897976	2.186560	-0.285452
2	6	0	5.927697	0.844404	-0.326269
3	6	0	4.629613	0.090015	-0.528904
4	6	0	3.483685	0.783111	0.246960
5	6	0	3.471275	2.253939	-0.127149
6	6	0	4.625423	2.903637	-0.350482
7	1	0	6.822127	2.753543	-0.225088
8	1	0	6.872946	0.316748	-0.323413
9	6	0	2.172102	0.025709	0.074093
10	1	0	2.532330	2.794959	-0.141650
11	1	0	4.630863	3.969560	-0.557832
12	6	0	2.293473	-1.373316	-0.024039
13	6	0	3.530824	-2.013556	-0.056816
14	1	0	1.417267	-2.010354	-0.012684
15	1	0	3.598449	-3.093150	0.012066
16	6	0	5.957434	-2.105061	-0.217773
17	6	0	6.650683	-2.151766	1.146618
18	1	0	6.607168	-1.667239	-0.978938
19	1	0	5.721875	-3.118240	-0.552261
20	1	0	7.579637	-2.723563	1.063653
21	1	0	6.893835	-1.150662	1.511611
22	1	0	6.009369	-2.639906	1.885706
23	7	0	4.694220	-1.350016	-0.190210
24	6	0	0.915357	0.658772	0.155648
25	6	0	-0.352904	0.079107	0.015061
26	1	0	0.912931	1.726706	0.360103
27	1	0	-0.443965	-0.978582	-0.213507

28	6	0	-1.520153	0.848257	0.162358
29	1	0	-1.400310	1.906694	0.374074
30	6	0	-2.825032	0.368348	0.066482
31	6	0	-4.944310	-0.950014	-0.153546
32	6	0	-5.153833	0.424059	0.091403
33	6	0	-6.010201	-1.835259	-0.299100
34	6	0	-6.461661	0.920157	0.199162
35	6	0	-7.305894	-1.332442	-0.194474
36	1	0	-5.832601	-2.888270	-0.487620
37	6	0	-7.522240	0.031785	0.053175
38	1	0	-6.654400	1.967553	0.395231
39	1	0	-8.151387	-2.002950	-0.303878
40	1	0	-8.536762	0.407251	0.135319
41	7	0	-3.964057	1.134522	0.198923
42	16	0	-3.227500	-1.321532	-0.234239
43	6	0	-3.887959	2.575608	0.442005
44	1	0	-3.453510	2.772548	1.425412
45	1	0	-3.279014	3.050296	-0.330190
46	1	0	-4.886147	3.002265	0.404264
47	1	0	3.761414	0.726871	1.318430
48	1	0	4.378614	0.138567	-1.605746

002gde_mol_TDb3lyp631dp_+1H2_ARA_PCMw_opt_rot1.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.865843	2.285021	-1.539924
2	6	0	5.285003	1.048758	-1.219735
3	6	0	4.530387	0.263354	-0.166975
4	6	0	3.013212	0.519360	-0.318908
5	6	0	2.758432	2.014202	-0.356616
6	6	0	3.639522	2.832085	-0.956098
7	1	0	5.437800	2.898449	-2.230448
8	1	0	6.206289	0.658021	-1.635604
9	6	0	2.239383	-0.256065	0.733441
10	1	0	1.817355	2.394249	0.029636
11	1	0	3.440063	3.895876	-1.049197
12	6	0	2.772626	-1.468908	1.135992
13	6	0	3.992791	-1.938781	0.651918
14	1	0	2.222567	-2.111314	1.815848
15	1	0	4.348917	-2.930820	0.895015
16	6	0	6.177728	-1.665446	-0.361993
17	6	0	7.159834	-1.230211	0.730575
18	1	0	6.533634	-1.346563	-1.344610
19	1	0	6.123380	-2.756970	-0.400137
20	1	0	8.144484	-1.669329	0.543666
21	1	0	7.279231	-0.142970	0.759533
22	1	0	6.817064	-1.563328	1.715226
23	7	0	4.801629	-1.186930	-0.172752
24	6	0	0.929227	0.220034	1.215170
25	6	0	-0.261770	-0.064330	0.602742
26	1	0	0.891365	0.842888	2.113123
27	1	0	-0.248240	-0.682102	-0.292678
28	6	0	-1.497663	0.406414	1.099007
29	1	0	-1.484273	1.018745	1.993391
30	6	0	-2.742027	0.132363	0.518880
31	6	0	-4.690049	-0.627882	-0.835523
32	6	0	-5.044452	0.177772	0.265566
33	6	0	-5.654655	-1.144321	-1.702049
34	6	0	-6.391616	0.475819	0.515750
35	6	0	-6.987159	-0.841930	-1.447176
36	1	0	-5.370280	-1.762046	-2.545843
37	6	0	-7.347145	-0.040758	-0.348662

38	1	0	-6.691726	1.088003	1.356497
39	1	0	-7.757684	-1.230118	-2.103976
40	1	0	-8.393475	0.180076	-0.168963
41	7	0	-3.931245	0.589212	0.997044
42	16	0	-2.955651	-0.849240	-0.914408
43	6	0	-4.008600	1.442008	2.191794
44	1	0	-3.662706	0.887941	3.065908
45	1	0	-3.399079	2.334561	2.045924
46	1	0	-5.038784	1.745333	2.347894
47	1	0	4.819634	0.667220	0.823882
48	1	0	2.729081	0.124709	-1.316667

002geb_mol_b3lyp631dp_+5H2_ARA_PCMw.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.777846	2.923527	-0.618970
2	6	0	5.388508	1.625225	-0.068866
3	6	0	4.403102	0.475834	-0.053148
4	6	0	3.075047	0.595851	-0.219241
5	6	0	2.475039	1.958580	-0.518982
6	6	0	3.359009	3.133550	-0.100706
7	1	0	5.430183	3.760849	-0.352343
8	1	0	6.260008	1.383695	-0.681374
9	6	0	2.071887	-0.558521	-0.180912
10	1	0	2.268543	2.005750	-1.598667
11	1	0	3.370644	3.212985	0.993894
12	6	0	2.726971	-1.854074	0.321299
13	6	0	4.132854	-2.017267	-0.215087
14	1	0	2.752365	-1.862450	1.418032
15	1	0	4.169579	-1.986786	-1.306439
16	6	0	6.446513	-1.057186	-0.204709
17	6	0	7.054164	-2.398339	0.183127
18	1	0	7.019214	-0.255834	0.255286
19	1	0	6.433585	-0.909714	-1.285989
20	1	0	8.123444	-2.347554	-0.038253
21	1	0	6.950030	-2.597088	1.254224
22	1	0	6.641941	-3.237412	-0.379331
23	7	0	5.005970	-0.881447	0.270191
24	6	0	0.844390	-0.249469	0.643558
25	6	0	-0.419481	-0.299511	0.174095
26	1	0	1.019670	-0.016075	1.694427
27	1	0	-0.556169	-0.541407	-0.881421
28	6	0	-1.609456	-0.059534	0.953887
29	1	0	-1.479311	0.180611	2.004222
30	6	0	-2.878147	-0.108870	0.458842
31	6	0	-5.016854	-0.290057	-0.899127
32	6	0	-5.228621	0.030620	0.455148
33	6	0	-6.073066	-0.425530	-1.791542
34	6	0	-6.534614	0.223562	0.917866
35	6	0	-7.377327	-0.234089	-1.321991
36	1	0	-5.887936	-0.673893	-2.831543
37	6	0	-7.596948	0.087286	0.019471
38	1	0	-6.733367	0.477061	1.952488
39	1	0	-8.214705	-0.335290	-2.004401
40	1	0	-8.609878	0.237226	0.379763
41	7	0	-4.042831	0.115887	1.184378
42	16	0	-3.288872	-0.476247	-1.242331
43	6	0	-3.969063	0.424609	2.604882
44	1	0	-3.445652	-0.374431	3.139233
45	1	0	-3.435630	1.366853	2.768321
46	1	0	-4.971808	0.515046	3.015184
47	1	0	4.582676	-2.944393	0.133843

48	1	0	2.132701	-2.719744	0.017011
49	1	0	1.746804	-0.712193	-1.220983
50	1	0	1.499028	2.018388	-0.029612
51	1	0	2.939352	4.069059	-0.484641
52	1	0	4.757047	2.871738	-1.714522
53	1	0	5.765621	1.788459	0.951481
54	1	0	5.041477	-0.951764	1.294070

002gfa_mol_b3lyp631dp_+6H2_ARA_PCMw.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	6.395838	0.330401	0.543824
2	6	0	5.194957	-0.525250	0.998335
3	6	0	4.124657	-0.458894	-0.092104
4	6	0	3.637409	0.990762	-0.289471
5	6	0	4.825351	1.833060	-0.787359
6	6	0	5.993574	1.774777	0.209880
7	1	0	7.158307	0.319207	1.329176
8	1	0	5.530281	-1.551804	1.168767
9	6	0	2.353500	1.078677	-1.182470
10	1	0	5.148271	1.469676	-1.772728
11	1	0	5.697029	2.289572	1.133467
12	6	0	2.251078	-0.180651	-2.061863
13	6	0	2.170315	-1.471618	-1.233249
14	1	0	1.376885	-0.138304	-2.717106
15	1	0	2.647793	-2.305551	-1.750070
16	6	0	3.097967	-2.707776	0.727984
17	6	0	3.011918	-2.701223	2.247649
18	1	0	4.056594	-3.075517	0.358901
19	1	0	2.314764	-3.346502	0.316864
20	1	0	3.129963	-3.729240	2.600134
21	1	0	3.786869	-2.094094	2.716653
22	1	0	2.033215	-2.346237	2.584952
23	7	0	2.884345	-1.336613	0.107999
24	6	0	1.125081	1.350400	-0.336140
25	6	0	-0.120168	0.853259	-0.509146
26	1	0	1.275942	2.076246	0.464049
27	1	0	-0.297206	0.149829	-1.322433
28	6	0	-1.263378	1.201323	0.299646
29	1	0	-1.109993	1.919704	1.098422
30	6	0	-2.516427	0.694725	0.122658
31	6	0	-4.647212	-0.488161	-0.592205
32	6	0	-4.819175	0.382603	0.500332
33	6	0	-5.706452	-1.215903	-1.120324
34	6	0	-6.088488	0.524506	1.070928
35	6	0	-6.973264	-1.071055	-0.543952
36	1	0	-5.552706	-1.882044	-1.963059
37	6	0	-7.153796	-0.207910	0.539360
38	1	0	-6.257166	1.188971	1.910170
39	1	0	-7.812589	-1.630862	-0.943014
40	1	0	-8.138351	-0.096969	0.982790
41	7	0	-3.636106	1.015953	0.881022
42	16	0	-2.961604	-0.493019	-1.137360
43	6	0	-3.525956	1.964806	1.979516
44	1	0	-2.788711	1.616547	2.709703
45	1	0	-3.219126	2.948534	1.609399
46	1	0	-4.486659	2.063816	2.478635
47	1	0	1.145357	-1.754329	-0.994066
48	1	0	3.121835	-0.219810	-2.721996
49	1	0	2.494371	1.935564	-1.857059
50	1	0	3.375528	1.369409	0.708214
51	1	0	4.496892	2.868943	-0.925522

52	1	0	6.856616	2.318895	-0.188759
53	1	0	6.848720	-0.138687	-0.339472
54	1	0	4.799252	-0.138184	1.944356
55	1	0	4.566747	-0.842656	-1.017634
56	1	0	2.245314	-0.816352	0.721901

002gfb_mol_b3lyp631dp_+6H2_ARA_PCMw.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.712707	2.961566	-0.554313
2	6	0	5.349163	1.622149	-0.147033
3	6	0	4.383366	0.451458	-0.390634
4	6	0	3.032323	0.663407	0.331627
5	6	0	2.427142	2.012035	-0.106429
6	6	0	3.371326	3.190322	0.145159
7	1	0	5.417532	3.767934	-0.326976
8	1	0	6.270443	1.493638	-0.718410
9	6	0	2.042756	-0.510073	0.106363
10	1	0	2.179624	1.959578	-1.176233
11	1	0	3.533674	3.307174	1.225128
12	6	0	2.726961	-1.835702	0.486984
13	6	0	4.053542	-2.037651	-0.227405
14	1	0	2.883179	-1.878150	1.572759
15	1	0	3.932496	-2.084478	-1.312756
16	6	0	6.373686	-1.145135	-0.582922
17	6	0	7.029463	-2.441714	-0.126006
18	1	0	7.000935	-0.303866	-0.299292
19	1	0	6.224788	-1.120101	-1.664527
20	1	0	8.058606	-2.436568	-0.494550
21	1	0	7.071160	-2.510609	0.965313
22	1	0	6.543401	-3.334314	-0.522803
23	7	0	5.008337	-0.891659	0.039260
24	6	0	0.763579	-0.337294	0.881397
25	6	0	-0.469833	-0.317666	0.335062
26	1	0	0.867625	-0.249749	1.964492
27	1	0	-0.543702	-0.409970	-0.749991
28	6	0	-1.705709	-0.185730	1.069859
29	1	0	-1.637907	-0.097183	2.149486
30	6	0	-2.943144	-0.163537	0.501155
31	6	0	-5.001284	-0.171450	-0.988428
32	6	0	-5.292103	-0.038375	0.382716
33	6	0	-6.004823	-0.195049	-1.948905
34	6	0	-6.624998	0.073227	0.792763
35	6	0	-7.336172	-0.083010	-1.532334
36	1	0	-5.759302	-0.298230	-3.000862
37	6	0	-7.634272	0.049328	-0.174246
38	1	0	-6.884791	0.176943	1.839699
39	1	0	-8.133031	-0.099340	-2.268472
40	1	0	-8.667991	0.136042	0.145570
41	7	0	-4.149857	-0.036447	1.182262
42	16	0	-3.253971	-0.294660	-1.255622
43	6	0	-4.157957	0.088454	2.632119
44	1	0	-3.702345	-0.793088	3.094767
45	1	0	-3.599644	0.977614	2.942640
46	1	0	-5.180872	0.178419	2.989189
47	1	0	4.540525	-2.950842	0.109480
48	1	0	2.082135	-2.682215	0.232482
49	1	0	1.800975	-0.545040	-0.965660
50	1	0	3.243346	0.725511	1.411176
51	1	0	1.480936	2.152560	0.423431
52	1	0	2.913372	4.120867	-0.207740
53	1	0	4.564619	2.971026	-1.642182

54	1	0	5.622264	1.652525	0.916244
55	1	0	4.210811	0.332045	-1.466443
56	1	0	5.147000	-0.844181	1.055056

002haa_mol_b3lyp631dp_+1H2_ARBb_PCMw.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	6.062990	2.091978	-0.157010
2	6	0	5.998338	0.712559	-0.183575
3	6	0	4.748769	0.054409	-0.169364
4	6	0	3.539769	0.816968	-0.119573
5	6	0	3.658967	2.228448	-0.095593
6	6	0	4.886328	2.858506	-0.113685
7	1	0	7.032127	2.579579	-0.169603
8	1	0	6.917707	0.144730	-0.212728
9	6	0	2.246588	0.144811	-0.096843
10	1	0	2.765995	2.838301	-0.064059
11	1	0	4.940575	3.941592	-0.094241
12	6	0	2.289692	-1.269108	-0.137780
13	6	0	3.477981	-1.949612	-0.190943
14	1	0	1.383927	-1.859840	-0.128183
15	1	0	3.501605	-3.031787	-0.220556
16	6	0	5.901687	-2.181168	-0.215856
17	6	0	6.506171	-2.365274	1.175731
18	1	0	6.616711	-1.746780	-0.915941
19	1	0	5.604218	-3.144830	-0.631398
20	1	0	7.389004	-3.006147	1.100553
21	1	0	6.811612	-1.413770	1.617640
22	1	0	5.789591	-2.844528	1.848209
23	7	0	4.683222	-1.335781	-0.208450
24	6	0	1.026282	0.870594	-0.036298
25	6	0	-0.240754	0.314466	-0.022800
26	1	0	1.074864	1.952233	0.005302
27	1	0	-0.341389	-0.767497	-0.069047
28	6	0	-1.426538	1.062251	0.056749
29	1	0	-1.346495	2.140621	0.142502
30	6	0	-2.699833	0.503897	0.028713
31	6	0	-4.743597	-1.001458	0.233720
32	6	0	-5.051323	0.428981	-0.178388
33	6	0	-5.807735	-1.927306	-0.290838
34	6	0	-6.400320	0.802575	0.387431
35	6	0	-7.075138	-1.478627	-0.212987
36	1	0	-5.565273	-2.936721	-0.604207
37	6	0	-7.364815	-0.133862	0.303356
38	1	0	-6.611017	1.806556	0.738271
39	1	0	-7.905739	-2.119270	-0.493321
40	1	0	-8.381945	0.097525	0.604462
41	7	0	-3.856228	1.192106	0.214003
42	16	0	-2.999644	-1.220718	-0.307603
43	6	0	-3.865165	2.651629	0.279291
44	1	0	-3.182044	2.990958	1.060441
45	1	0	-3.569956	3.098207	-0.677490
46	1	0	-4.865586	2.994336	0.534912
47	1	0	-5.131160	0.463828	-1.282688
48	1	0	-4.732046	-1.054028	1.333198

002haa_mol_TDb3lyp631dp_+1H2_ARBb_PCMw_opt.log

Standard orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	5.994280	2.159556	-0.443255
2	6	0	5.983595	0.771302	-0.341195
3	6	0	4.769280	0.073926	-0.204035
4	6	0	3.524801	0.798172	-0.146522
5	6	0	3.585710	2.205647	-0.276044
6	6	0	4.793725	2.876371	-0.416649
7	1	0	6.941569	2.677822	-0.548590
8	1	0	6.923918	0.238533	-0.369357
9	6	0	2.286347	0.073896	0.022797
10	1	0	2.667961	2.779951	-0.278447
11	1	0	4.800831	3.957663	-0.508434
12	6	0	2.359411	-1.338042	0.086699
13	6	0	3.563414	-1.990406	0.013307
14	1	0	1.469230	-1.937375	0.228840
15	1	0	3.637436	-3.068316	0.069603
16	6	0	5.989424	-2.114463	-0.162873
17	6	0	6.684877	-2.186080	1.198503
18	1	0	6.646759	-1.698276	-0.928738
19	1	0	5.711283	-3.115155	-0.497825
20	1	0	7.590740	-2.792159	1.107422
21	1	0	6.970206	-1.195644	1.561151
22	1	0	6.031914	-2.652008	1.941505
23	7	0	4.744519	-1.318238	-0.132509
24	6	0	1.020090	0.756631	0.152311
25	6	0	-0.236820	0.185747	0.037787
26	1	0	1.048487	1.817722	0.380780
27	1	0	-0.328247	-0.863902	-0.227803
28	6	0	-1.420240	0.931875	0.252686
29	1	0	-1.311648	1.978225	0.519682
30	6	0	-2.719376	0.426253	0.140998
31	6	0	-4.810864	-1.013872	0.118403
32	6	0	-5.056519	0.465843	-0.135032
33	6	0	-5.879643	-1.836560	-0.548987
34	6	0	-6.417849	0.820560	0.411737
35	6	0	-7.134413	-1.354694	-0.469905
36	1	0	-5.653822	-2.811455	-0.966593
37	6	0	-7.404966	-0.066898	0.184235
38	1	0	-6.612134	1.786452	0.864122
39	1	0	-7.971422	-1.929529	-0.854321
40	1	0	-8.426611	0.164604	0.469430
41	7	0	-3.859381	1.138181	0.387219
42	16	0	-3.052318	-1.233746	-0.379879
43	6	0	-3.825312	2.582368	0.591502
44	1	0	-3.143722	2.826614	1.409058
45	1	0	-3.503802	3.110224	-0.315671
46	1	0	-4.818758	2.928931	0.868811
47	1	0	-5.083731	0.629959	-1.232490
48	1	0	-4.839027	-1.195337	1.204155

002hac_mol_TDb3lyp631dp_+1H2_ARBb_PCMw_opt_TRIPLET.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	6.016271	2.196731	-0.086995
2	6	0	6.001676	0.810350	-0.156488
3	6	0	4.784135	0.105359	-0.167660
4	6	0	3.539523	0.813739	-0.098888
5	6	0	3.604012	2.222099	-0.030123
6	6	0	4.811412	2.904784	-0.024744
7	1	0	6.965475	2.721713	-0.079842
8	1	0	6.943164	0.280265	-0.198144

9	6	0	2.285303	0.069560	-0.102319
10	1	0	2.688541	2.798331	0.020642
11	1	0	4.815732	3.988499	0.029596
12	6	0	2.381678	-1.348027	-0.177930
13	6	0	3.591823	-1.980720	-0.247234
14	1	0	1.494486	-1.967189	-0.187540
15	1	0	3.672178	-3.058016	-0.307057
16	6	0	6.027005	-2.079167	-0.285142
17	6	0	6.636752	-2.290018	1.102039
18	1	0	6.725970	-1.585188	-0.962124
19	1	0	5.779106	-3.039926	-0.739054
20	1	0	7.549212	-2.885250	1.007065
21	1	0	6.894352	-1.342344	1.581140
22	1	0	5.940823	-2.827852	1.751617
23	7	0	4.775002	-1.294743	-0.250510
24	6	0	1.021861	0.710695	-0.033390
25	6	0	-0.247188	0.110561	-0.025025
26	1	0	1.016902	1.795217	0.020361
27	1	0	-0.344160	-0.969258	-0.068201
28	6	0	-1.407089	0.894211	0.045921
29	1	0	-1.282614	1.971219	0.105001
30	6	0	-2.722843	0.403757	0.035681
31	6	0	-4.836907	-0.972516	0.300569
32	6	0	-5.064720	0.444080	-0.204727
33	6	0	-5.936763	-1.875959	-0.187626
34	6	0	-6.405948	0.919491	0.298207
35	6	0	-7.180912	-1.361422	-0.170083
36	1	0	-5.738226	-2.914351	-0.428714
37	6	0	-7.413520	0.027218	0.250293
38	1	0	-6.574291	1.954085	0.574632
39	1	0	-8.036696	-1.977432	-0.428793
40	1	0	-8.424192	0.327842	0.508789
41	7	0	-3.842279	1.174185	0.165513
42	16	0	-3.096089	-1.316350	-0.188709
43	6	0	-3.784579	2.633238	0.124383
44	1	0	-3.055758	2.996667	0.850519
45	1	0	-3.515153	2.995300	-0.874872
46	1	0	-4.756846	3.037986	0.397420
47	1	0	-5.111400	0.414699	-1.311875
48	1	0	-4.844135	-0.957780	1.401436

002had_mol_TDb3lyp631dp_+1H2_ARBb_PCMw_opt_rot.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.055949	-1.859908	1.949951
2	6	0	-5.370708	-0.794551	1.113786
3	6	0	-4.416675	-0.264801	0.226369
4	6	0	-3.093383	-0.815231	0.185389
5	6	0	-2.822068	-1.899482	1.050518
6	6	0	-3.775385	-2.417004	1.916168
7	1	0	-5.810988	-2.250263	2.624378
8	1	0	-6.366250	-0.374252	1.158706
9	6	0	-2.099979	-0.256863	-0.724196
10	1	0	-1.838057	-2.351575	1.042946
11	1	0	-3.520967	-3.250526	2.562857
12	6	0	-2.532444	0.825226	-1.543188
13	6	0	-3.802246	1.312040	-1.477107
14	1	0	-1.854166	1.294485	-2.244298
15	1	0	-4.133280	2.134665	-2.097454
16	6	0	-6.078816	1.430150	-0.599114
17	6	0	-6.238296	2.454445	0.526476
18	1	0	-6.839991	0.649159	-0.536445

19	1	0	-6.214996	1.914762	-1.568071
20	1	0	-7.240127	2.892003	0.486049
21	1	0	-6.104590	1.998383	1.510830
22	1	0	-5.506786	3.260689	0.419980
23	7	0	-4.750591	0.795546	-0.627373
24	6	0	-0.761702	-0.757250	-0.792726
25	6	0	0.239532	-0.327100	-1.618346
26	1	0	-0.501147	-1.560960	-0.111341
27	1	0	0.078464	0.448149	-2.365849
28	6	0	1.575244	-0.936431	-1.630665
29	1	0	1.770670	-1.792026	-2.272078
30	6	0	2.644424	-0.417645	-0.885480
31	6	0	4.039109	0.662035	0.924503
32	6	0	4.839054	0.062975	-0.217002
33	6	0	4.814332	1.788731	1.551362
34	6	0	6.160983	-0.435589	0.306547
35	6	0	6.138722	1.591264	1.692808
36	1	0	4.304418	2.650772	1.966054
37	6	0	6.777725	0.364024	1.197305
38	1	0	6.635720	-1.318927	-0.104093
39	1	0	6.751258	2.321511	2.212132
40	1	0	7.774884	0.120897	1.550120
41	7	0	3.909380	-0.869287	-0.887567
42	16	0	2.390861	0.985969	0.155882
43	6	0	4.427607	-1.978478	-1.686336
44	1	0	3.621091	-2.499416	-2.193215
45	1	0	5.131926	-1.591751	-2.427433
46	1	0	4.941954	-2.680648	-1.028066
47	1	0	5.043705	0.858107	-0.959749
48	1	0	3.857472	-0.115876	1.682369

002hba_mol_b3lyp631dp_+3H2_ARBb_PCMw.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	6.287160	1.694817	0.094643
2	6	0	6.019683	0.336161	0.065012
3	6	0	4.696544	-0.138030	-0.062799
4	6	0	3.616529	0.791557	-0.152959
5	6	0	3.938022	2.165414	-0.119237
6	6	0	5.240564	2.620337	0.000756
7	1	0	7.313678	2.033604	0.192601
8	1	0	6.843443	-0.360207	0.144309
9	6	0	2.224139	0.319051	-0.277155
10	1	0	3.142464	2.896650	-0.190018
11	1	0	5.444344	3.685805	0.023249
12	6	0	2.080384	-1.110071	-0.308902
13	6	0	3.149642	-1.943587	-0.224734
14	1	0	1.104462	-1.566054	-0.408605
15	1	0	3.025628	-3.019516	-0.251241
16	6	0	5.510669	-2.515848	0.029146
17	6	0	5.925372	-2.768621	1.479834
18	1	0	6.362414	-2.207191	-0.580939
19	1	0	5.130816	-3.436853	-0.417510
20	1	0	6.711453	-3.528989	1.508402
21	1	0	6.309892	-1.863088	1.956171
22	1	0	5.076156	-3.130738	2.066408
23	7	0	4.440971	-1.510009	-0.107827
24	6	0	1.145842	1.190084	-0.356492
25	6	0	-0.220640	0.811174	-0.469377
26	1	0	1.330966	2.258459	-0.328765
27	1	0	-0.459842	-0.250486	-0.490481
28	6	0	-1.264419	1.687132	-0.563384

29	1	0	-1.071780	2.756691	-0.575214
30	6	0	-2.689602	1.297641	-0.648817
31	6	0	-4.497026	-0.541232	-0.628090
32	6	0	-4.552003	0.147779	0.517663
33	6	0	-5.530115	-1.555883	-1.031742
34	6	0	-5.606154	0.010149	1.575458
35	6	0	-6.378676	-1.979511	0.180025
36	1	0	-5.036660	-2.425208	-1.480472
37	6	0	-6.813409	-0.765823	1.011284
38	1	0	-5.186429	-0.510970	2.448415
39	1	0	-7.254844	-2.535237	-0.167572
40	1	0	-7.408503	-0.090831	0.384562
41	7	0	-3.345912	0.993692	0.745867
42	16	0	-3.071469	-0.218972	-1.632733
43	6	0	-3.571521	2.260045	1.514977
44	1	0	-2.623049	2.793309	1.562570
45	1	0	-4.321886	2.854718	0.995607
46	1	0	-3.907330	2.012317	2.520066
47	1	0	-5.937913	0.991746	1.931022
48	1	0	-7.453796	-1.079207	1.840860
49	1	0	-5.794021	-2.662999	0.807722
50	1	0	-6.160744	-1.121677	-1.818663
51	1	0	-2.656708	0.439854	1.272519
52	1	0	-3.310053	2.107463	-1.038213

002hca_mol_b3lyp631dp_+4H2_ARBb_PCMw.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	6.310738	1.654388	0.209200
2	6	0	6.026140	0.301441	0.123043
3	6	0	4.699876	-0.149650	-0.048095
4	6	0	3.633901	0.797326	-0.123372
5	6	0	3.972459	2.164154	-0.031160
6	6	0	5.278321	2.596805	0.130592
7	1	0	7.339472	1.975036	0.339770
8	1	0	6.839074	-0.408651	0.192191
9	6	0	2.237508	0.349020	-0.291702
10	1	0	3.187638	2.908136	-0.088280
11	1	0	5.495120	3.657847	0.197555
12	6	0	2.075890	-1.076979	-0.374835
13	6	0	3.132263	-1.927168	-0.302764
14	1	0	1.095814	-1.515454	-0.506809
15	1	0	2.994897	-2.999779	-0.369542
16	6	0	5.481744	-2.540033	-0.035581
17	6	0	5.865689	-2.858858	1.410570
18	1	0	6.348747	-2.217658	-0.616399
19	1	0	5.099226	-3.436633	-0.527490
20	1	0	6.640585	-3.631091	1.422235
21	1	0	6.253207	-1.979358	1.931210
22	1	0	5.000417	-3.232489	1.965631
23	7	0	4.427727	-1.515502	-0.149911
24	6	0	1.172756	1.235945	-0.363013
25	6	0	-0.196820	0.877875	-0.515326
26	1	0	1.370939	2.300393	-0.296728
27	1	0	-0.450867	-0.178394	-0.578021
28	6	0	-1.228422	1.766481	-0.603440
29	1	0	-1.024008	2.834302	-0.584108
30	6	0	-2.660619	1.394412	-0.714205
31	6	0	-4.191233	-0.837347	-0.459087
32	6	0	-4.600881	0.336603	0.425915
33	6	0	-5.434017	-1.546198	-1.000651
34	6	0	-5.357881	-0.146869	1.661746

35	6	0	-6.273023	-2.046011	0.192735
36	1	0	-5.142731	-2.384777	-1.640135
37	6	0	-6.608328	-0.918797	1.184515
38	1	0	-4.714371	-0.800306	2.263618
39	1	0	-7.197753	-2.501503	-0.176081
40	1	0	-7.299934	-0.210206	0.711223
41	7	0	-3.327768	1.111712	0.679064
42	16	0	-3.038427	-0.126652	-1.716772
43	6	0	-3.503992	2.371320	1.467080
44	1	0	-2.540017	2.874964	1.521571
45	1	0	-4.235353	3.000482	0.960215
46	1	0	-3.847996	2.120288	2.468729
47	1	0	-5.231997	1.024916	-0.146923
48	1	0	-3.615419	-1.552749	0.138909
49	1	0	-5.661763	0.693913	2.291713
50	1	0	-7.127428	-1.326962	2.057063
51	1	0	-5.718104	-2.837274	0.712958
52	1	0	-6.015159	-0.850546	-1.617858
53	1	0	-2.669019	0.514965	1.191451
54	1	0	-3.250504	2.224401	-1.106381

003aaa_Me_benztiazol_B3LYP631dp_PCMw_opt.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.214380	-0.199092	-0.000013
2	1	0	3.587873	0.320104	-0.887917
3	6	0	1.724879	-0.229559	-0.000008
4	6	0	-0.680520	-0.829806	0.000009
5	6	0	-0.437162	0.552109	-0.000008
6	6	0	-1.982172	-1.335323	0.000016
7	6	0	-1.490681	1.471843	-0.000019
8	6	0	-3.028966	-0.419666	0.000006
9	1	0	-2.167464	-2.403155	0.000039
10	6	0	-2.784806	0.965061	-0.000017
11	1	0	-1.309593	2.539845	-0.000008
12	1	0	-4.051163	-0.782148	0.000019
13	1	0	-3.621921	1.654382	-0.000023
14	7	0	0.937503	0.841523	-0.000012
15	16	0	0.839096	-1.704489	-0.000002
16	6	0	1.423939	2.230672	0.000029
17	1	0	2.509627	2.239302	0.000054
18	1	0	1.055104	2.734711	-0.894307
19	1	0	1.055065	2.734662	0.894380
20	1	0	3.613171	-1.213339	-0.000423
21	1	0	3.587895	0.319366	0.888318

003aba_Me_benztiazol_1H2Ar_B3LYP631dp_PCMw_opt.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.234446	-0.196586	-0.046734
2	1	0	3.572667	0.239810	-0.992382
3	6	0	1.744387	-0.216168	-0.003841
4	6	0	-0.682784	-0.802774	-0.348003
5	6	0	-0.440975	0.542202	0.308616
6	6	0	-2.022201	-1.338223	0.078715
7	6	0	-1.526424	1.497287	-0.113697
8	6	0	-3.020300	-0.435914	0.137272

9	1	0	-2.184262	-2.402090	0.206318
10	6	0	-2.772714	0.987358	-0.135355
11	1	0	-1.326598	2.551838	-0.263975
12	1	0	-4.035946	-0.754156	0.349985
13	1	0	-3.623031	1.631625	-0.334416
14	7	0	0.984654	0.853135	0.027397
15	16	0	0.877297	-1.724194	0.025142
16	6	0	1.461723	2.239144	0.044992
17	1	0	2.544706	2.265437	-0.038794
18	1	0	1.022196	2.777237	-0.796534
19	1	0	1.154943	2.709952	0.982204
20	1	0	3.630821	-1.209027	0.023026
21	1	0	3.637205	0.402994	0.774166
22	1	0	-0.496440	0.421603	1.406376
23	1	0	-0.676540	-0.678022	-1.441815

003aca_Me_benztiazol_3H2Ar_B3LYP631dp_PCMw_opt.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.307152	-0.229372	0.303573
2	1	0	-3.865054	0.686944	0.095864
3	6	0	-1.922526	-0.181042	-0.314746
4	6	0	0.545221	-0.797906	-0.065462
5	6	0	0.390063	0.522979	0.070379
6	6	0	1.887946	-1.466552	-0.154715
7	6	0	1.490976	1.533536	0.182521
8	6	0	2.997755	-0.520520	0.336588
9	1	0	1.878056	-2.390380	0.434015
10	6	0	2.827788	0.890196	-0.240903
11	1	0	1.294098	2.406163	-0.449231
12	1	0	2.972657	-0.474235	1.431992
13	1	0	3.648825	1.537239	0.080556
14	7	0	-1.041687	0.922933	0.271402
15	16	0	-0.960935	-1.733453	-0.074347
16	6	0	-1.402721	2.275751	-0.279923
17	1	0	-1.175376	2.285775	-1.344706
18	1	0	-2.463585	2.446877	-0.108986
19	1	0	-0.822932	3.031731	0.245084
20	1	0	-3.261989	-0.391568	1.383600
21	1	0	-3.862420	-1.057012	-0.144104
22	1	0	1.550500	1.902315	1.216825
23	1	0	2.867171	0.842072	-1.335614
24	1	0	3.972484	-0.930330	0.055598
25	1	0	2.061148	-1.767511	-1.196108
26	1	0	-1.210741	0.954721	1.286736
27	1	0	-1.960176	0.029480	-1.385640

003ada_Me_benztiazol_4H2Ar_B3LYP631dp_PCMw_opt.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.248253	-0.263325	0.530243
2	1	0	-3.841589	0.650469	0.435435
3	6	0	-1.976566	-0.190638	-0.297829
4	6	0	0.562699	-0.848182	0.301370
5	6	0	0.371997	0.575679	-0.207149
6	6	0	1.881428	-1.422227	-0.221578
7	6	0	1.457912	1.505025	0.329931

8	6	0	3.036136	-0.520184	0.258037
9	1	0	2.017943	-2.444609	0.142636
10	6	0	2.825742	0.952726	-0.130488
11	1	0	1.328150	2.523961	-0.044877
12	1	0	3.126212	-0.602208	1.348649
13	1	0	3.618671	1.572850	0.298052
14	7	0	-1.058161	0.944344	0.162860
15	16	0	-0.965739	-1.746518	-0.212791
16	6	0	-1.496853	2.278837	-0.370214
17	1	0	-1.360362	2.279607	-1.450807
18	1	0	-2.544032	2.433096	-0.118635
19	1	0	-0.892101	3.056410	0.091885
20	1	0	-3.027215	-0.448248	1.584813
21	1	0	-3.858913	-1.090557	0.161565
22	1	0	0.382938	0.580324	-1.301853
23	1	0	0.592002	-0.840782	1.396665
24	1	0	1.412656	1.542041	1.425259
25	1	0	2.898991	1.058014	-1.220310
26	1	0	3.979184	-0.882760	-0.163286
27	1	0	1.854467	-1.465228	-1.316880
28	1	0	-1.115112	0.984025	1.187185
29	1	0	-2.198401	0.021218	-1.344791

003baa_mol_b3lyp631dp_PCMw.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.260720	2.758048	-0.107932
2	6	0	0.687008	1.762771	-0.227697
3	6	0	0.291983	0.407425	-0.177565
4	6	0	-1.087623	0.071421	-0.000298
5	6	0	-2.026637	1.129772	0.118044
6	6	0	-1.625016	2.444799	0.066054
7	1	0	0.053454	3.795399	-0.149185
8	1	0	1.724778	2.035261	-0.357459
9	6	0	-1.485591	-1.300718	0.050736
10	1	0	-3.074511	0.890529	0.249473
11	1	0	-2.354934	3.241497	0.157633
12	6	0	-0.500200	-2.265549	-0.080043
13	6	0	0.829826	-1.898356	-0.255319
14	1	0	-0.742199	-3.320687	-0.053146
15	1	0	1.609044	-2.642418	-0.361516
16	6	0	2.677720	-0.335116	-0.456408
17	6	0	3.354970	-0.023359	0.876112
18	1	0	2.784356	0.476914	-1.175440
19	1	0	3.114662	-1.223114	-0.912881
20	1	0	4.416760	0.160861	0.692905
21	1	0	2.932610	0.862543	1.355447
22	1	0	3.266204	-0.867801	1.564391
23	7	0	1.220327	-0.619891	-0.303406
24	6	0	-2.920490	-1.698241	0.237082
25	1	0	-3.544138	-1.299799	-0.569815
26	1	0	-3.023755	-2.783800	0.248165
27	1	0	-3.316002	-1.303536	1.178669

003bba_mol_1H2Ar_b3lyp631dp_PCMw.log

Standard orientation:

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

1	6	0	-0.151563	2.765219	-0.105704
2	6	0	0.745624	1.787584	-0.311852
3	6	0	0.240884	0.380824	-0.537084
4	6	0	-0.992739	0.087359	0.328967
5	6	0	-2.003619	1.206833	0.172198
6	6	0	-1.580287	2.467853	-0.006385
7	1	0	0.176421	3.797469	-0.034602
8	1	0	1.793613	2.020691	-0.446869
9	6	0	-1.494388	-1.321678	0.076643
10	1	0	-3.056207	0.984184	0.302094
11	1	0	-2.291246	3.286785	-0.051108
12	6	0	-0.570555	-2.266319	-0.242724
13	6	0	0.816474	-1.929733	-0.290505
14	1	0	-0.836990	-3.310739	-0.350135
15	1	0	1.563205	-2.717887	-0.265596
16	6	0	2.713911	-0.426548	-0.362176
17	6	0	3.245410	-0.016757	1.010907
18	1	0	2.897627	0.340091	-1.116732
19	1	0	3.202692	-1.339538	-0.705760
20	1	0	4.317073	0.183424	0.927971
21	1	0	2.755804	0.884149	1.387493
22	1	0	3.098614	-0.821300	1.736106
23	7	0	1.256745	-0.702198	-0.346454
24	6	0	-2.928900	-1.663123	0.297713
25	1	0	-3.560646	-1.144480	-0.433585
26	1	0	-3.102944	-2.736362	0.211646
27	1	0	-3.257719	-1.326374	1.288113
28	1	0	-0.678934	0.094590	1.393939
29	1	0	-0.059088	0.291609	-1.597785

003bca_mol_5H2Ar_b3lyp631dp_PCMw.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.381555	2.751510	-0.515446
2	6	0	-0.757968	1.735959	-0.352972
3	6	0	-0.243780	0.342962	-0.070778
4	6	0	1.039586	0.021278	0.163905
5	6	0	2.061242	1.125741	0.362312
6	6	0	1.451910	2.516545	0.548854
7	1	0	0.828972	2.644884	-1.511216
8	1	0	-1.428928	2.070196	0.447971
9	6	0	1.570607	-1.402162	0.257906
10	1	0	2.682463	0.858367	1.226727
11	1	0	2.238494	3.275327	0.489038
12	6	0	0.533171	-2.402191	-0.258342
13	6	0	-0.831188	-2.086533	0.309685
14	1	0	0.499100	-2.384750	-1.354985
15	1	0	-0.807276	-2.048082	1.401243
16	6	0	-2.602464	-0.376013	0.610984
17	6	0	-3.694163	0.204673	-0.274534
18	1	0	-2.315834	0.283854	1.429329
19	1	0	-2.945412	-1.315896	1.042819
20	1	0	-4.594818	0.319817	0.334581
21	1	0	-3.441104	1.181982	-0.686208
22	1	0	-3.937739	-0.475203	-1.096916
23	7	0	-1.307398	-0.722178	-0.149199
24	6	0	2.907510	-1.592007	-0.482513
25	1	0	3.708325	-0.985807	-0.054288
26	1	0	3.213183	-2.640432	-0.414862
27	1	0	2.810527	-1.336393	-1.542931
28	1	0	2.741302	1.133968	-0.499244
29	1	0	1.002930	2.597046	1.547012

30	1	0	-0.029085	3.763759	-0.454672
31	1	0	-1.358929	1.717648	-1.270938
32	1	0	-1.596621	-2.797885	-0.003182
33	1	0	0.801872	-3.421399	0.034907
34	1	0	1.751748	-1.609394	1.323661
35	1	0	-1.567486	-0.814942	-1.137816

003bda_mol_6H2Ar_b3lyp631dp_PCMw.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.549449	2.428236	-0.590027
2	6	0	0.078598	2.033030	-0.340427
3	6	0	-0.060882	0.611146	0.261452
4	6	0	1.101656	-0.304143	-0.177335
5	6	0	2.429186	0.275338	0.388234
6	6	0	2.454466	1.816461	0.480541
7	1	0	1.870023	2.083186	-1.579953
8	1	0	-0.377113	2.758486	0.338816
9	6	0	0.914558	-1.782834	0.224854
10	1	0	2.614209	-0.158062	1.378224
11	1	0	3.481714	2.179232	0.375955
12	6	0	-0.463411	-2.281103	-0.223299
13	6	0	-1.584348	-1.413520	0.322046
14	1	0	-0.519147	-2.317695	-1.319349
15	1	0	-1.589889	-1.396898	1.414891
16	6	0	-2.580014	0.887133	0.379355
17	6	0	-3.937075	0.465928	-0.168169
18	1	0	-2.358523	1.907389	0.074228
19	1	0	-2.542626	0.836125	1.469577
20	1	0	-4.665359	1.225098	0.128517
21	1	0	-3.933316	0.421235	-1.261602
22	1	0	-4.281357	-0.491464	0.226577
23	7	0	-1.429576	0.025946	-0.121389
24	6	0	2.024208	-2.683811	-0.332321
25	1	0	3.008663	-2.404871	0.051329
26	1	0	1.843222	-3.727052	-0.054554
27	1	0	2.059355	-2.629774	-1.426704
28	1	0	1.146624	-0.262588	-1.275680
29	1	0	-0.091906	0.656840	1.355093
30	1	0	3.243524	-0.064558	-0.258077
31	1	0	2.110705	2.144197	1.469768
32	1	0	1.627123	3.519515	-0.600079
33	1	0	-0.473611	2.089104	-1.286389
34	1	0	-2.557753	-1.753598	-0.028002
35	1	0	-0.635575	-3.302811	0.130790
36	1	0	0.946250	-1.834929	1.323358
37	1	0	-1.476558	0.031104	-1.146448

010aaa_intermed_TD_b3lyp631dp_opt_S0_opt_2.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.494377	-0.670901	-0.588871
2	6	0	-4.600696	0.714327	-0.366997
3	6	0	-3.512532	1.443358	0.162065
4	6	0	-2.308407	0.769102	0.404964
5	6	0	-2.189459	-0.613147	0.149954
6	6	0	-3.278026	-1.347636	-0.349018

7	6	0	-3.167572	-2.822785	-0.674449
8	1	0	-2.139332	-3.176006	-0.659507
9	1	0	-3.718729	-3.429175	0.054078
10	1	0	-3.589788	-3.035976	-1.660856
11	6	0	-5.696807	-1.443053	-1.092290
12	1	0	-5.773165	-1.407113	-2.187464
13	1	0	-5.651920	-2.494570	-0.807491
14	1	0	-6.628866	-1.039148	-0.691830
15	6	0	-5.897996	1.427378	-0.688217
16	1	0	-6.363866	1.022257	-1.589328
17	1	0	-6.628412	1.326421	0.125779
18	1	0	-5.746098	2.494047	-0.854265
19	6	0	-3.683358	2.910534	0.500813
20	1	0	-3.735925	3.526957	-0.404402
21	1	0	-4.607248	3.076705	1.062545
22	1	0	-2.858964	3.295752	1.097858
23	6	0	-0.885158	-1.299425	0.416653
24	8	0	-0.744590	-2.347747	1.000554
25	8	0	0.134928	-0.578613	-0.152016
26	6	0	-1.146018	1.468763	1.048762
27	8	0	-0.636482	1.130580	2.095348
28	8	0	-0.704121	2.536131	0.339620
29	1	0	0.028240	2.913162	0.858315
30	6	0	1.488790	-0.812663	0.025771
31	6	0	2.284172	0.232115	-0.443300
32	6	0	2.053827	-1.971288	0.585361
33	6	0	3.667087	0.123064	-0.345822
34	1	0	1.828648	1.115602	-0.873763
35	6	0	3.436835	-2.053165	0.671183
36	1	0	1.421416	-2.767721	0.943919
37	6	0	4.272319	-1.020299	0.213391
38	1	0	3.890625	-2.940220	1.103973
39	6	0	5.810930	1.177546	-0.763487
40	6	0	5.710184	-1.046065	0.275214
41	6	0	6.440601	-0.005923	-0.187456
42	1	0	6.199031	-1.918288	0.702036
43	1	0	7.523138	0.009526	-0.156515
44	8	0	4.411697	1.167512	-0.809913
45	8	0	6.379216	2.150733	-1.197146

010aaa_intermed_TD_b3lyp631dp_opt_S0_opt_3.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.381692	-1.071046	0.297567
2	6	0	-4.740500	0.244967	-0.047503
3	6	0	-3.757128	1.250423	-0.175332
4	6	0	-2.407865	0.892811	-0.022865
5	6	0	-2.047839	-0.433647	0.294957
6	6	0	-3.024658	-1.426453	0.463297
7	6	0	-2.653666	-2.861582	0.776351
8	1	0	-1.580754	-3.032919	0.727827
9	1	0	-2.969864	-3.137412	1.788981
10	1	0	-3.143475	-3.552847	0.083466
11	6	0	-5.464847	-2.111612	0.495201
12	1	0	-5.816261	-2.516556	-0.463255
13	1	0	-5.118191	-2.954015	1.093019
14	1	0	-6.335526	-1.689833	1.003117
15	6	0	-6.198513	0.590596	-0.271535
16	1	0	-6.747301	-0.248688	-0.703041
17	1	0	-6.702571	0.857681	0.667193
18	1	0	-6.314610	1.435825	-0.951096
19	6	0	-4.188203	2.684053	-0.412163

20	1	0	-4.485240	2.846968	-1.455194
21	1	0	-5.046570	2.938460	0.215478
22	1	0	-3.394829	3.395813	-0.195110
23	6	0	-0.599806	-0.790886	0.454135
24	8	0	-0.101474	-1.331036	1.408357
25	8	0	0.096424	-0.484968	-0.697508
26	6	0	-1.303625	1.901487	-0.096764
27	8	0	-0.404836	1.995228	0.715601
28	8	0	-1.376005	2.711610	-1.177980
29	1	0	-0.613352	3.312015	-1.108480
30	6	0	1.482502	-0.603250	-0.702376
31	6	0	2.263886	0.124062	0.187209
32	6	0	2.044594	-1.417072	-1.693665
33	6	0	3.649836	0.018115	0.076035
34	1	0	1.817066	0.762004	0.938761
35	6	0	3.424287	-1.505290	-1.789730
36	1	0	1.391066	-1.959014	-2.367485
37	6	0	4.254860	-0.792841	-0.906062
38	1	0	3.879112	-2.131003	-2.552147
39	6	0	5.797791	0.732339	0.949521
40	6	0	5.693947	-0.833343	-0.939207
41	6	0	6.426621	-0.113028	-0.060520
42	1	0	6.181104	-1.455578	-1.685944
43	1	0	7.509720	-0.119652	-0.056282
44	8	0	4.399579	0.742823	0.955531
45	8	0	6.370137	1.413334	1.766112

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