Electronic Supplementary Information (40 pages)

# Photodimerization and complexation dynamics of courmarins in the presence of cucurbit[8]urils.

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## Contents

## 1. General methods

Coumarin derivatives were purchased from Alfa Aesar® and were used as received without further purification, unless otherwise stated. 7-methyl, 4,6-dimethyl and 4,7-dimethy coumarin derivatives were synthesized according to literature procedure. [1] 7-acetoxy , 7-acetoxy-4-methyl, and 7-methoxy-4-methyl coumarin derivatives were synthesized from the corresponding hydroxycoumarins via acetylation or methylation. [1]Cucurbit[8]uril (CB[8]) was synthesized using previously reported procedures.[2] Ethyl acetate, for the extraction process was used as received without further purification. HPLC grade methanol and water was used as the solvent for carrying out photoreactions. $^{1}$H NMR and $^{13}$C NMR spectra were obtained on Varian 400 MHz or 500 MHz spectrometer. Coupling constants (*J*) were reported in hertz (Hz). Standard abbreviations indicating multiplicity were used as follows: s (singlet), br (broad), d (doublet), t (triplet), q (quartet), m (multiplet). Electrospray ionization spectra were recorded on a Broker BioTof mass spectrometer in positive (ESI+) ion mode. Absorbance measurements were performed using Shimadzu UV-2501PC UV-Vis recording spectrophotometer. All computations were done using Gaussian 03 package at RB3LYP/6-31g(d,p) level.

## 2. Absorbance measurements to identify the stoichiometry of coumarin@CB[8] complex.

**Table S1:** Concentration to identify the stoichiometric ratio of the host-guest complex

| Concentration | | CB[8] : Coumarin |
|---|---|---|
| CB[8] (M) | Coumarin (M) | |
| $1.33 \times 10^{-04}$ | $3.33 \times 10^{-05}$ | 4:1 |
| $1.17 \times 10^{-04}$ | $3.33 \times 10^{-05}$ | 3.5:1 |
| $1.00 \times 10^{-04}$ | $3.33 \times 10^{-05}$ | 3:1 |
| $6.67 \times 10^{-05}$ | $3.33 \times 10^{-05}$ | 2:1 |
| $5.00 \times 10^{-05}$ | $3.33 \times 10^{-05}$ | 1.5:1 |
| $3.33 \times 10^{-05}$ | $3.33 \times 10^{-05}$ | 1:1 |
| $2.53 \times 10^{-05}$ | $3.33 \times 10^{-05}$ | 1:1.5 |
| $1.67 \times 10^{-05}$ | $3.33 \times 10^{-05}$ | 1:2 |
| $1.40 \times 10^{-05}$ | $3.33 \times 10^{-05}$ | 1:2.4 |
| $1.20 \times 10^{-05}$ | $3.33 \times 10^{-05}$ | 1:2.7 |
| $1.00 \times 10^{-05}$ | $3.33 \times 10^{-05}$ | 1:3 |
| $8.67 \times 10^{-06}$ | $3.33 \times 10^{-05}$ | 1:3.8 |
| $6.67 \times 10^{-06}$ | $3.33 \times 10^{-05}$ | 1:5 |
| $3.33 \times 10^{-06}$ | $3.33 \times 10^{-05}$ | 1:10 |

In two separate 5 mL volumetric flasks, 0.012 M solutions were prepared by dissolving coumarins derivatives (10.5mg) and CB[8] (79.7mg) in water. Appropriate amounts of these stock solutions were mixed separately to get various ratios of CB[8] : coumarin with a total

concentration listed in table 1. The absorbance was recorded at various mol fractions listed in table S1 and the normalized corrected absorbance was plotted against the wavelength for various host-guest ratio in table S1. A Job plot (Figures S1-S8) with varying mole fractions gave the host-guest complex ratio of various coumarin derivatives with CB[8].

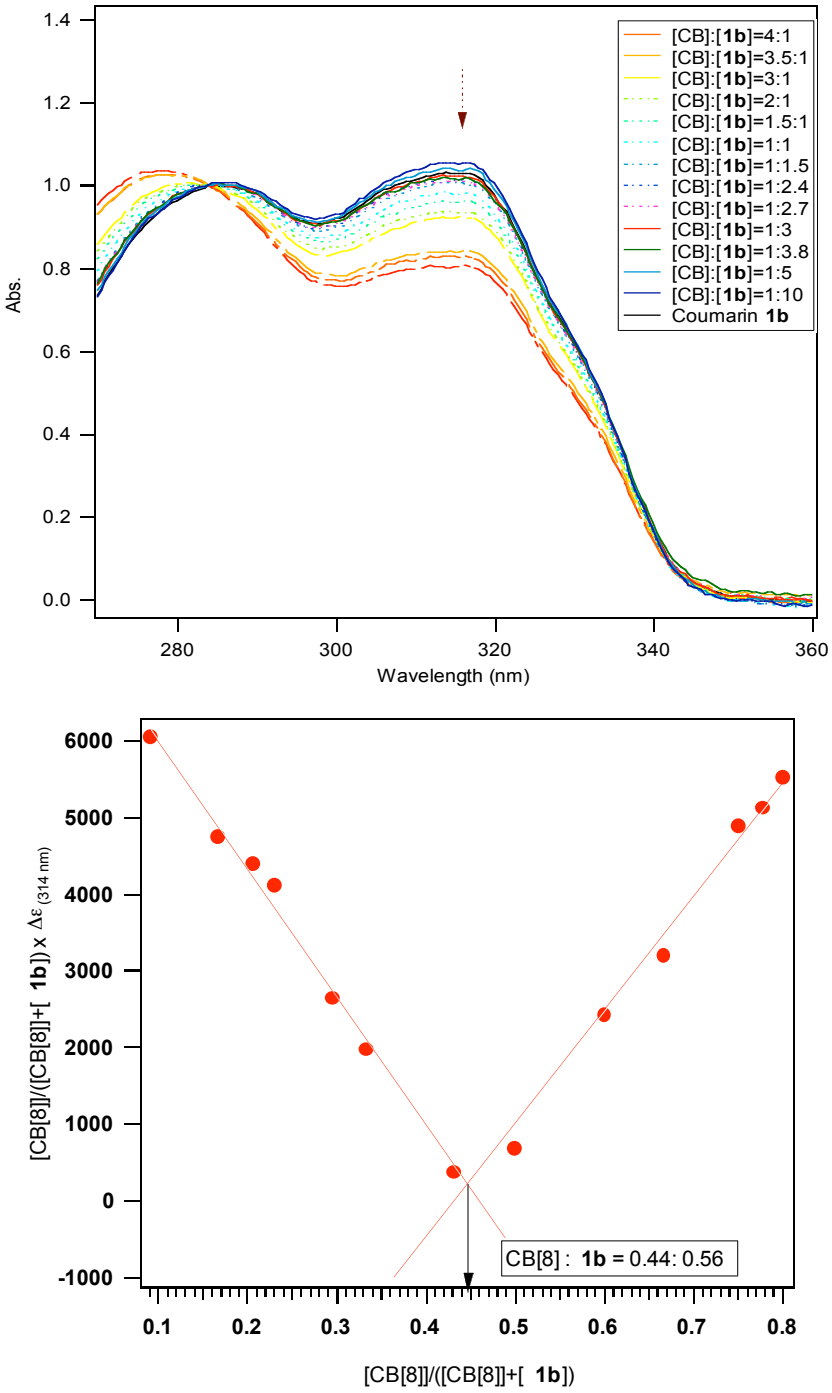



**Figure S1:** Absorbance measurements to determine Host : Guest ratio of **1b** presence of CB[8].

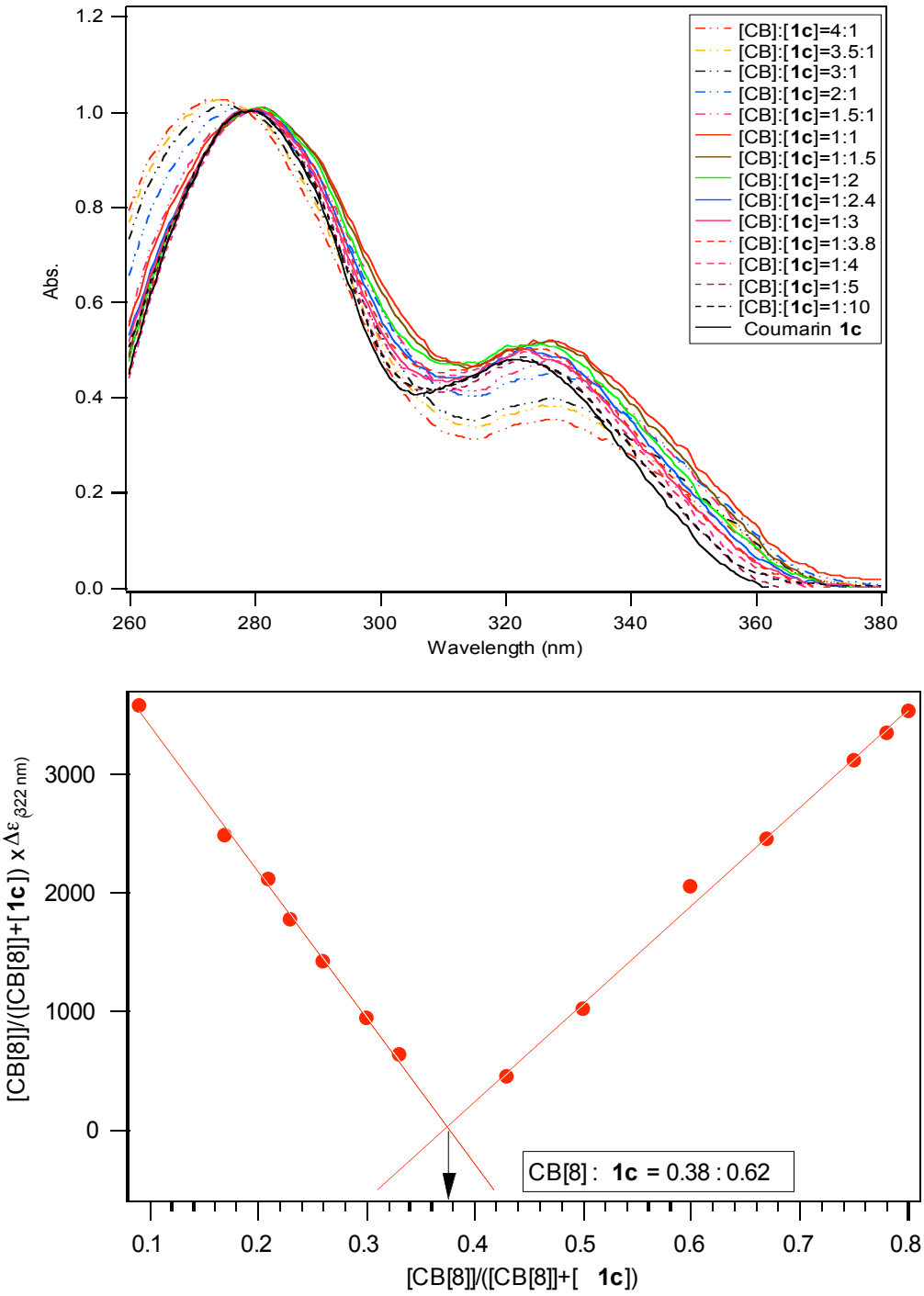



**Figure S2:** Absorbance measurements to determine Host : Guest ratio of **1c** presence of CB[8].

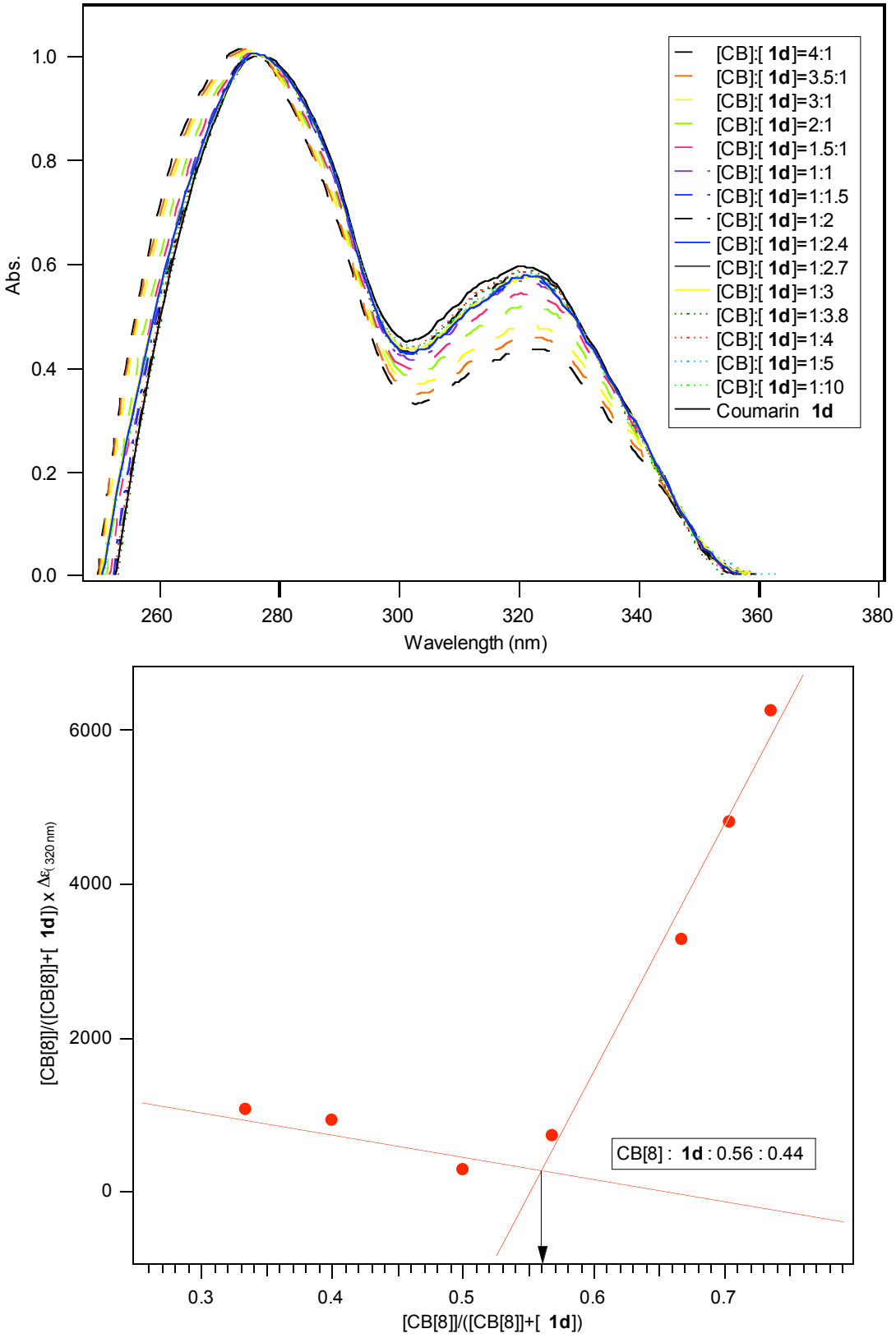



**Figure S3:** Absorbance measurements to determine Host : Guest ratio of **1d** presence of CB[8].

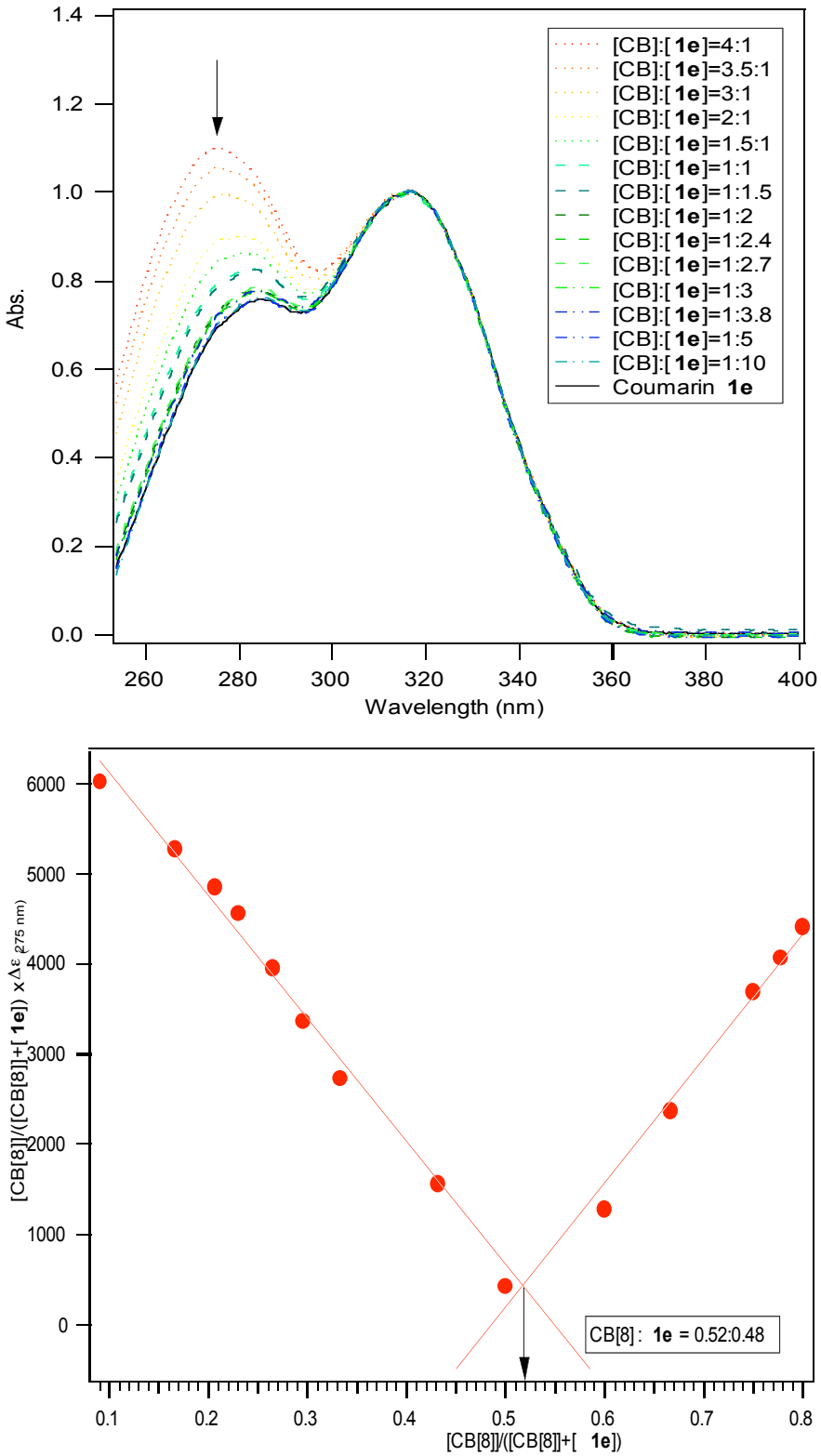



**Figure S4:** Absorbance measurements to determine Host : Guest ratio of **1e** presence of CB[8].

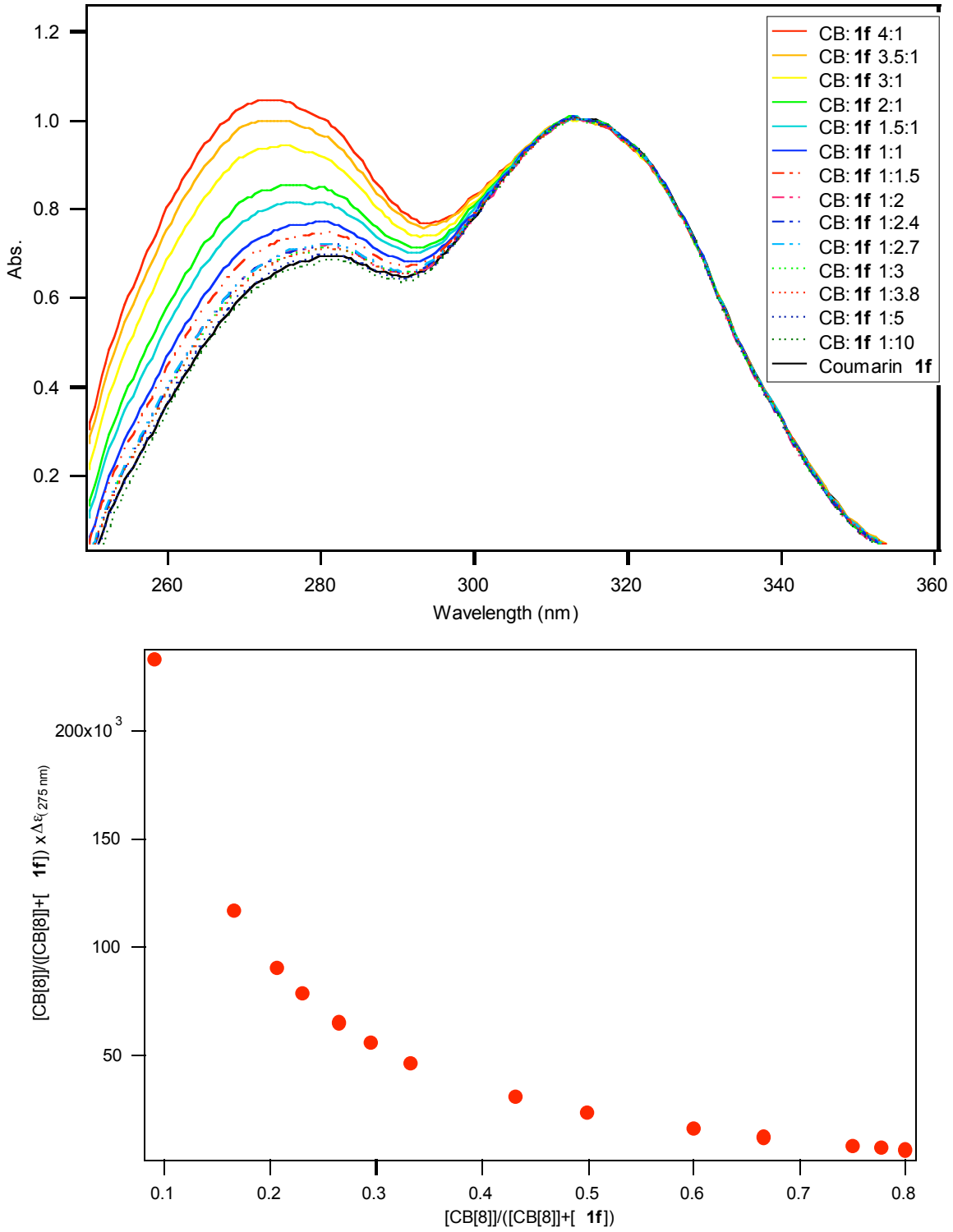
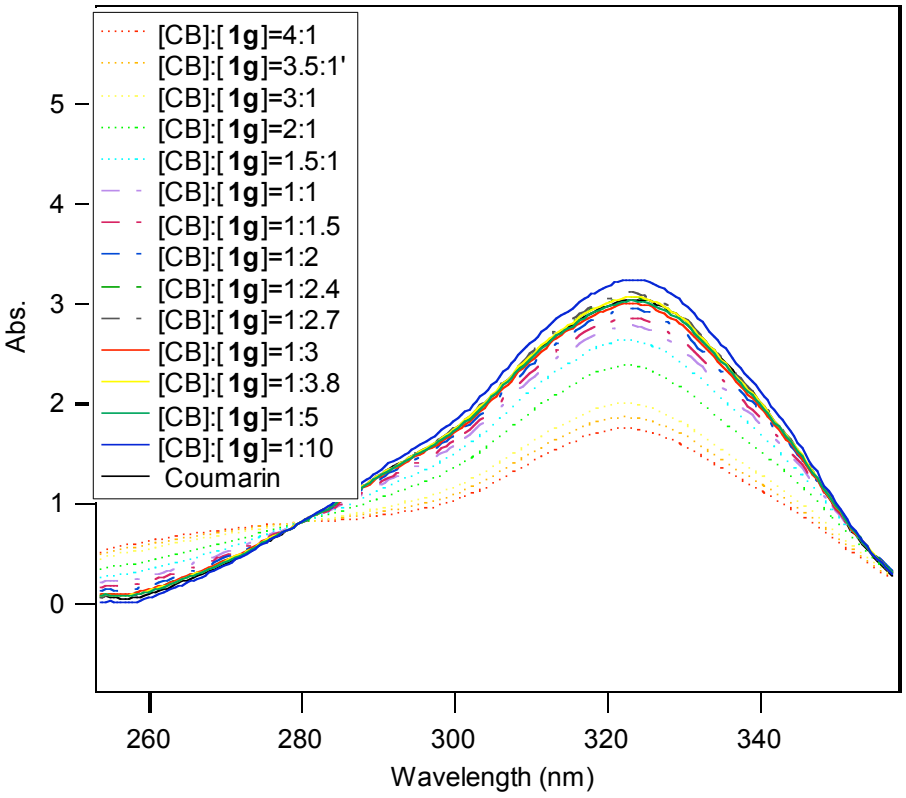



**Figure S5:** Absorbance measurements to determine Host : Guest ratio of **1f** presence of CB[8].



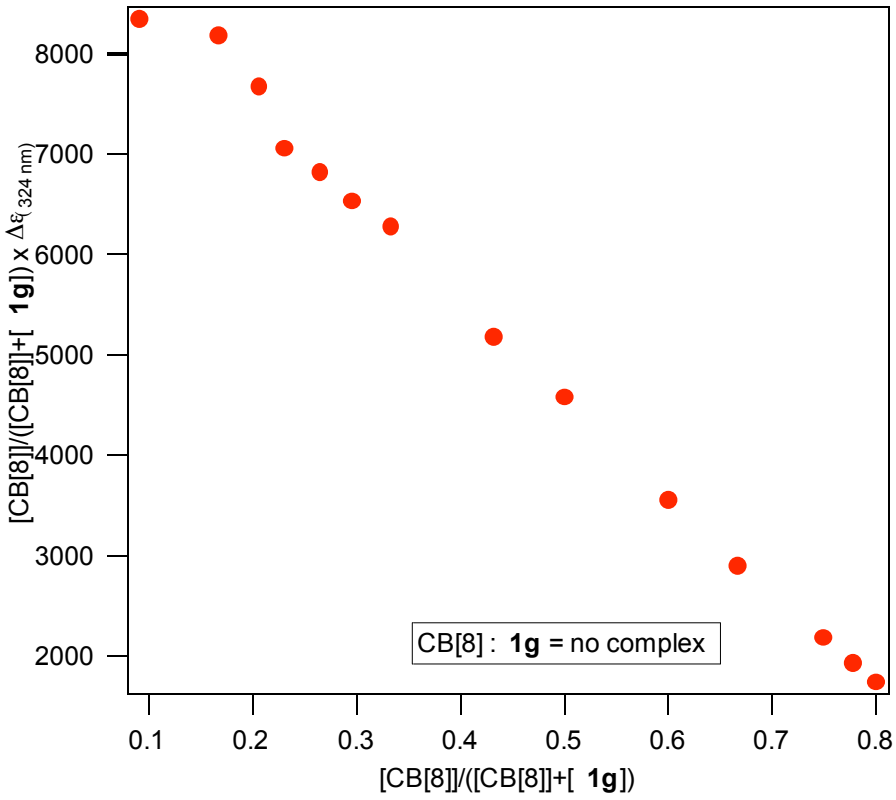




**Figure S6:** Absorbance measurements to determine Host : Guest ratio of **1g** presence of CB[8].

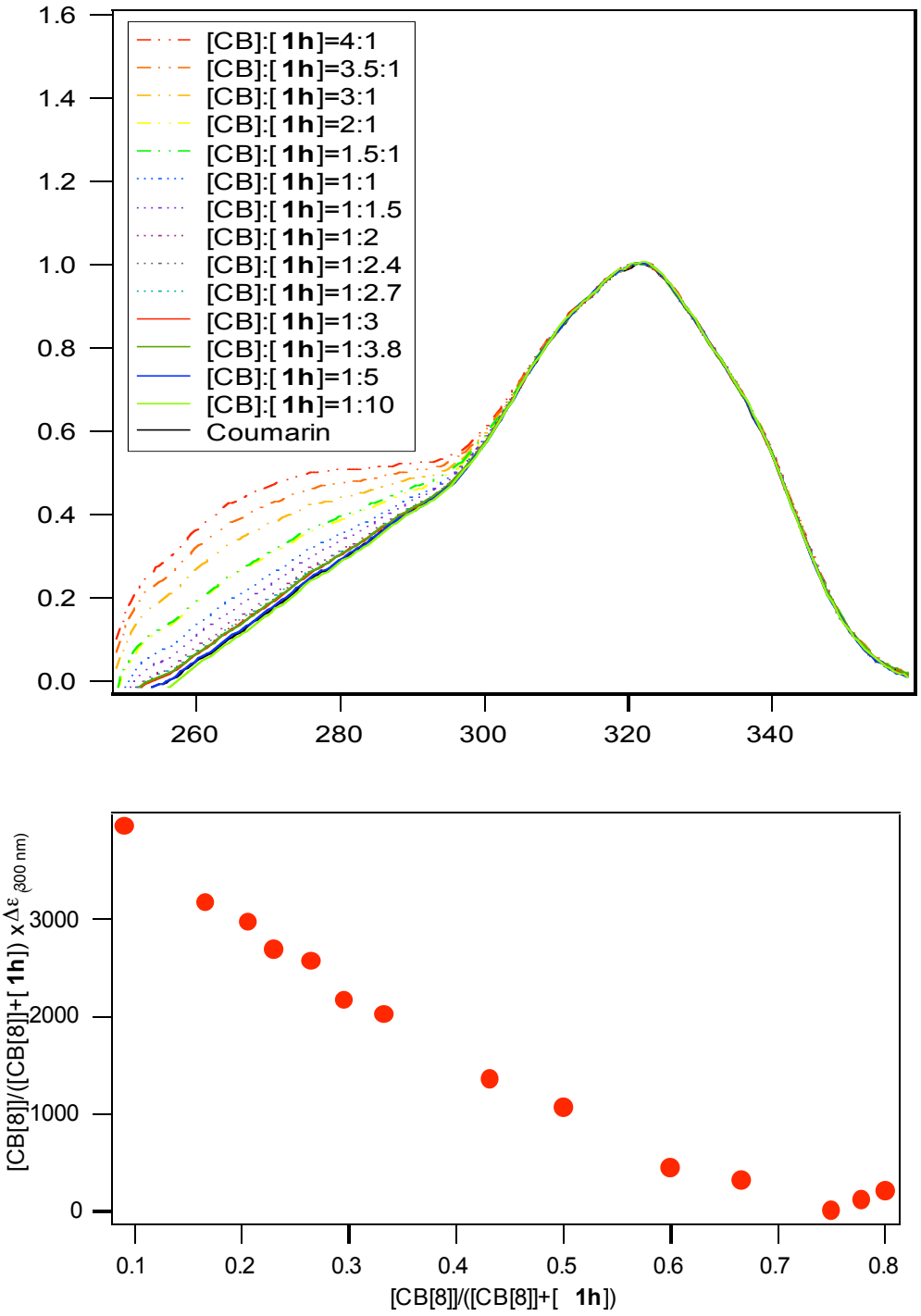



**Figure S7:** Absorbance measurements to determine Host : Guest ratio of **1h** presence of CB[8].

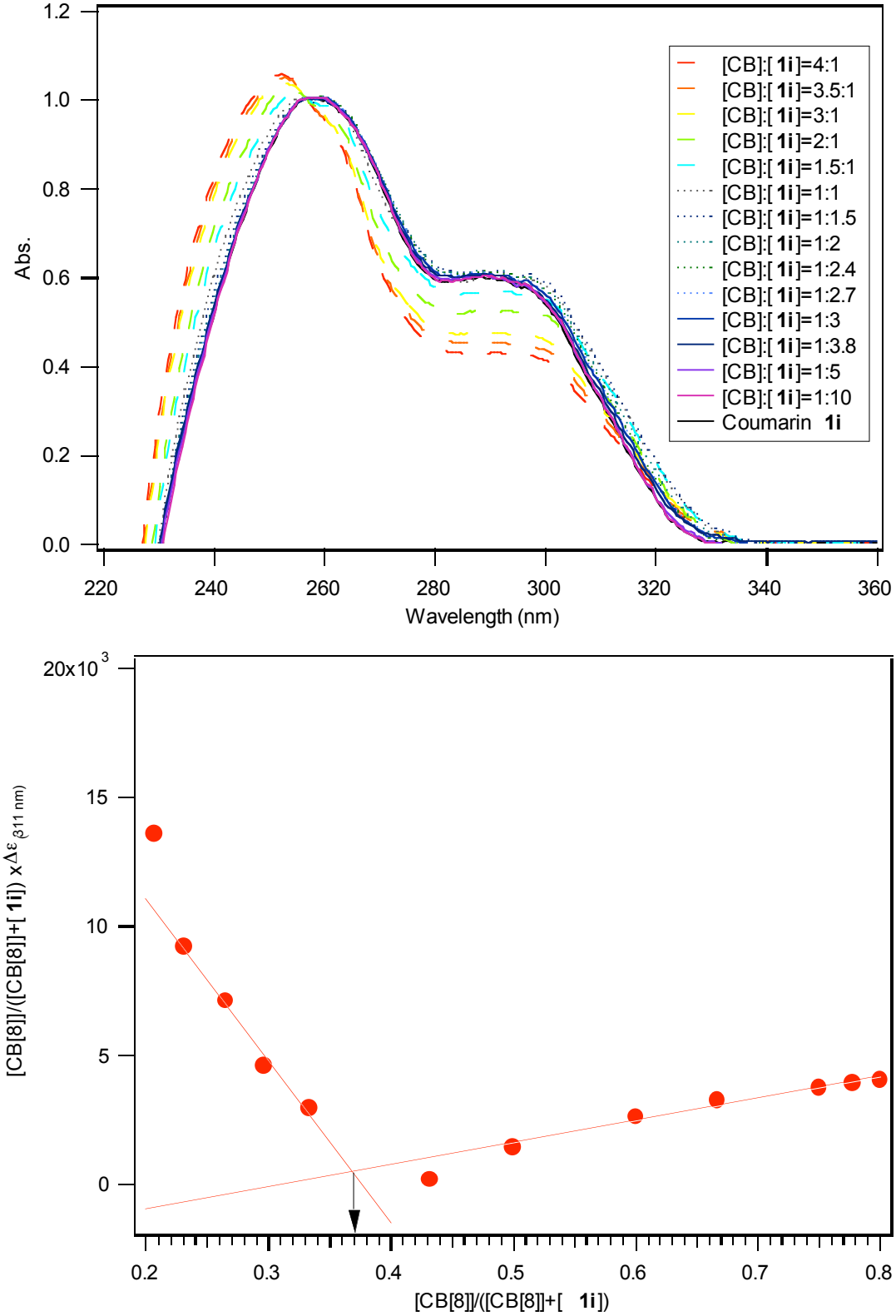



**Figure S8:** Absorbance measurements to determine Host : Guest ratio of **1i** presence of CB[8].

### 3. $^{1}$H NMR spectroscopy to characterize 1a@CB[8] complex.

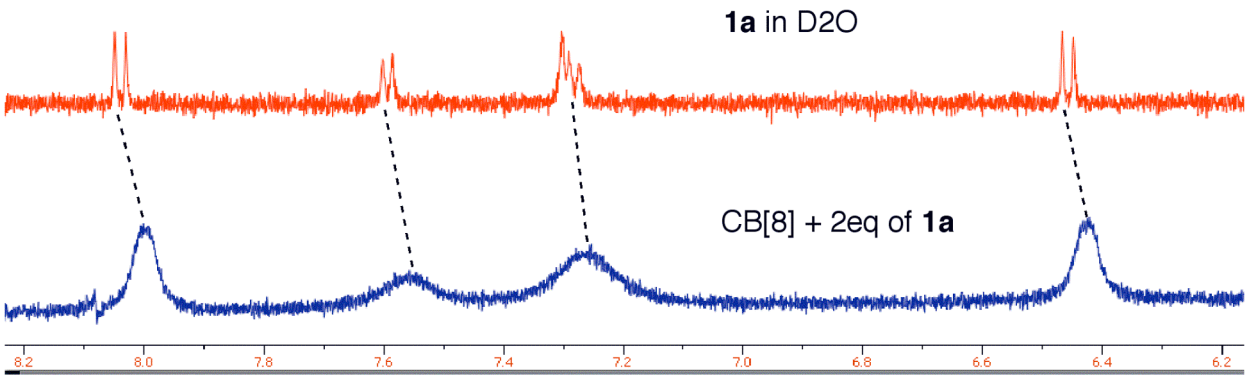



**Figure S9:** 1H NMR spectra of **1a** in water (top) and 1:2 host : guest ratio of **1b**@CB[8]

### 4. Direct photoirradiation of coumarin derivatives in solution without CB[8]

In $CDCl_3$: Coumarin derivatives (0.08 M) were irradiated with 450 W medium pressure Hg-lamp (Pyrex cut off) for the specific time in $CDCl_3$. Product distribution was analyzed by $^{1}$H-NMR spectroscopy.

In methanol: Coumarin derivatives (0.003 M) were irradiated in methanol using 450 W medium pressure Hg-lamp (Pyrex cut off) for the specific time. The solvent was removed from the photolysate and product distribution was analyzed by $^{1}$H-NMR spectroscopy in $CDCl_3$. Similar procedure was followed for irradiation in benzene.

In water: coumarin derivatives (0.2 mM) were irradiated using 450 W medium pressure Hg-lamp (Pyrex cutoff) for the specific time. The product was extracted with ethyl acetate (150 ml). Organic layer was dried over anhydrous sodium sulfate and solvent was removed in vacuuo. Without further purification product distribution was analyzed by $^{1}$H-NMR spectroscopy in $CDCl_3$.

### 5. Photoirradiation of coumarin derivatives in solution within CB[8]

In a typical experiment, coumarin derivatives (0.2 mM, 2eq) and CB[8] (26.4mg, 0.1mM, 1eq) was suspended in 200 mL of water. The mixture was sonicated for 2-3 hours at 60°C to obtain a clear homogeneous solution. The aqueous solution thus obtained was irradiated with 450 W medium pressure Hg-lamp (Pyrex cut off) for specific time. After photoirradiation,

ammonium chloride (100 mg) was added followed by 150 ml of ethyl acetate to the reaction mixture and stirred for 1 hour at room temperature. Organic layer was separated, washed with sodium bicarbonate solution and dried over anhydrous sodium sulfate. Solvent was removed under reduced pressure and residue was re-dissolved in chloroform (2 mL). The solution was passed through a silica plug and chloroform was removed under high vacuum to obtain light yellow solid. Without further purification, the product distribution was analyzed by $^1$H-NMR spectroscopy.

## 6. Characterization of photodimers of various coumarin derivatives (1a-1h) by $^1$H-NMR spectroscopy

*In $CDCl_3$:*

i) **1a**: $^1$H-NMR (500 MHz, $CDCl_3$, δ ppm): 2.37 (s, 3H, *anti*-HH), 3.78 (d, 1H, J = 8 Hz, *anti*-HH), 3.88 (d, 1H, *J* = 8 Hz, *anti*-HH), 6.67-7.05 (m, aromatic protons)**.**

ii) **1b:** $^1$H-NMR (500 MHz, $CDCl_3$, δ ppm): 1.25 (s, 3H, *anti*-HH), 2.37 (s, 3H, *anti*-HH), 3.38 (s, 1H, *anti*-HH), 6.91 (s, 1H, *anti*-HH), 7.02 (t, 2H, *J* = 8 Hz, *anti*-HH)**.**

iii) **1c:** $^1$H-NMR (500 MHz, $CDCl_3$, δ ppm): 2.35 (s, 3H, *anti*-HH), 3.78 (d, *J* = 7.5 Hz, 1H, *anti*-HH), 3.89 (d, *J* = 7.5 Hz, 1H, *anti*-HH), 6.95 (s, 1H ), 7.00 (d, 1H, *J*=8.5Hz), 7.12 (d, 1H, *J*=8Hz)

iv) **1d:** $^1$H-NMR (500 MHz, $CDCl_3$, δ ppm): 1.26 (s, 3H, *anti*-HH), 2.37 (s, 3H, *anti*-HH), 3.37 (s, 1H, *anti*-HH), 6.91 (s, 1H, *anti*-HH), 7.00 (d, 1H, *J* = 10.5 Hz, *anti*-HH)**,** 7.11 (d, 1H, *J* = 10.5 Hz, *anti*-HH)**.**

v) **1e:** $^1$H-NMR (500 MHz, $CDCl_3$, δ ppm): 2.32 (s, 3H, *anti*-HH), 3.88 (d, 1H, *J* = 8 Hz, *anti*-HH), 3.92 (d, 1H, *J* = 8 Hz, *anti*-HH), 6.90 (d, 1H, *J* = 2 Hz, *anti*-HH), 6.92 (d, 1H, *J* = 2 Hz, *anti*-HH), 6.94 (d, 1H, *J* = 2 Hz, *anti*-HH).

vi) **1f:** $^1$H-NMR (500 MHz, $CDCl_3$, δ ppm): 1.30 (s, 3H, *anti*-HH), 2.32 (s, 3H, *anti*-HH), 3.44 (s, 1H, *anti*-HH), 3.48 (s, 1H, *anti*-HT), 6.63-6.83(m, aromatic protons, *anti*-HT), 6.90 (d, 1H, *J* = 2 Hz, *anti*-HH), 6.99 (d, 1H, *J* = 2 Hz, *anti*-HH), 7.00 (d, 1H, *J* = 2 Hz, *anti*-HH).

vii) **1g:** $^1$H-NMR (500 MHz, $CDCl_3$, δ ppm): 3.71 (s, 3H, *syn*-HT), 3.74 (s, 3H, *syn*-HH), 4.00 (dd, *J* = 10 Hz, *syn*-HH), 4.06 (dd, *J* = 10 Hz, *syn* -HH), 4.17 (dd, *J* = 9 Hz, *syn* -HT), 4.24 (dd, *J* = 9 Hz, *syn*-HT), 6.19 (d, 1H, *J* = 2.5 Hz, *syn*-HT), 6.43 (m, 1H,

*syn*-HH), 6.68 (d, 1H, *J* = 8.5 Hz, *syn*-HT), 6.82 (d, 1H, *J* = 8.5 Hz, *syn*-HH), 7.03 (d, 1H, *J* = 8.5 Hz, *syn*-HT), 7.36 (d, 1H, *J* = 8.5 Hz, *syn*-HH)

viii) **1h:** $^1$H-NMR (500 MHz, $CDCl_3$, δ ppm): 124 (s, 3H, *anti*-HH), 1.67 (s, 3H, *syn*-HH), 3.41 (s, 1H, *anti*-HH), 3.66 (s, 1H, *syn*-HH), 6.05 (d, 1H, *J* = 2.5 Hz, *syn*-HH), 6.62-6.65(m, aromatic protons, *anti*-HH), 7.05 (d, 1H, *J* = 9 Hz, *anti*-HH), 7.09 (d, 1H, *J* = 8.5 Hz, *syn*-HH), 7.35 (s, 1H, *syn*-HH).

*In methanol*

i) **1b**: $^1$H-NMR (500 MHz, $CDCl_3$, δ ppm): 1.25 (s, 3H, *anti*-HH), 2.37 (s, 3H, *anti*-HH), 2.42 (s, 3H, *syn*-HH), 3.38 (s, 1H, *anti*-HH), 3.60 (s, 1H, *syn*-HH), 6.61-7.06 (m, aromatic protons)

ii) **1c**: $^1$H-NMR (500 MHz, $CDCl_3$, δ ppm): 2.35 (s, 3H, *anti*-HH), 3.78 (d, *J* = 7.5 Hz, 1H, *anti*-HH), 3.89 (d, *J* = 7.5 Hz, 1H, *anti*-HH), 6.95 (s, 1H ), 7.00 (d, 1H, *J*=8.5Hz), 7.0 (d, 1H, *J*=8Hz)

iii) **1d:** $^1$H-NMR (500 MHz, $CDCl_3$, δ ppm): 1.26 (s, 6H, *anti*-HH/HT), 1.64 (s, 3H, *syn*-HT), 2.23 (s, 3H, *anti*-HT), 2.37 (s, 3H, *anti*-HH), 2.60 (s, 3H, *syn*-HT), 3.37 (s, 1H, *anti*-HH), 3.42 (s, 1H, *anti*-HT), 3.47 (s, 1H, *syn*-HT), 6.80-7.16 (m, aromatic protons)

iv) **1f:** $^1$H-NMR (500 MHz, $CDCl_3$, δ ppm): 1.30 (s, 6H, *anti*-HH/ *anti*-HT), 1.66 (s, 3H, *syn*-HH), 1.72 (s, 3H, *syn*-HT), 2.25 (s, 3H, *anti*-HH), 2.31 (s, 3H, *anti*-HT), 2.33 (s, 3H, *syn*-HH), 2.35(s, 3H, *syn*-HT), 3.44 (s, 1H, *anti*-HH), 3.49 (s, 1H, *anti*-HT), 3.65 (s, 1H, *syn*-HH), 3.77 (s, 1H, *syn*-HT), 6.63-7.03 (m, aromatic protons)

v) **1g:** $^1$H-NMR (500 MHz, $CDCl_3$, δ ppm): 3.71 (s, 3H, *syn*-HT), 3.74 (s, 3H, *syn*-HH), 4.00 (dd, *J* = 10 Hz, *syn*-HH), 4.06 (dd, *J* = 10 Hz, *syn* -HH), 4.17 (dd, *J* = 9 Hz, *syn* -HT), 4.24 (dd, *J* = 9 Hz, *syn*-HT), 6.19 (d, 1H, *J* = 2.5 Hz, *syn*-HT), 6.43 (m, 1H, *syn*-HH), 6.68 (d, 1H, *J* = 8.5 Hz, *syn*-HT), 6.82 (d, 1H, *J* = 8.5 Hz, *syn*-HH), 7.03 (d, 1H, *J* = 8.5 Hz, *syn*-HT), 7.36 (d, 1H, *J* = 8.5 Hz, *syn*-HH)

vi) **1h:** $^1$H-NMR (500 MHz, $CDCl_3$, δ ppm): 1.24 (s, 3H, *anti*-HH), 1.67 (s, 3H, *syn*-HH), 3.41 (s, 1H, *anti*-HH), 3.66 (s, 1H, *syn*-HH), 6.05 (d, 1H, *J* = 2.5 Hz, *syn*-HH), 6.62-6.65(m, aromatic protons, *anti*-HH), 7.05 (d, 1H, *J* = 9 Hz, *anti*-HH), 7.09 (d, 1H, *J* = 8.5 Hz, *syn*-HH), 7.35 (s, 1H, *syn*-HH).

*In water*

i) **1a:** $^{1}$H-NMR (500 MHz, $CDCl_3$, δ ppm): 2.22 (s, 3H, *syn*-HT), 2.26 (s, 3H, *syn*-HH), 2.37 (s, 3H, *anti*-HH), 3.78 (d, 1H, J = 8 Hz, *anti*-HH), 3.88 (d, 1H, *J* = 8 Hz, *anti*-HH), 3.98 (dd, 1H, J = 7 Hz, *syn*-HH), 4.11(dd, 1H, *J* = 7 Hz, *syn*-HH), 4.18 (dd, 1H, J = 8 Hz, *syn*-HT), 4.25 (dd, 1H, *J* = 8 Hz, *syn*-HT), 6.65-7.02 (m, aromatic protons)**.**

ii) **1b:** $^{1}$H-NMR (500 MHz, $CDCl_3$, δ ppm): 1.25 (s, 3H, *anti*-HH), 2.37 (s, 3H, *anti*-HH), 2.42 (s, 3H, *syn*-HH), 3.38 (s, 1H, *anti*-HH), 3.60 (s, 1H, *syn*-HH), 6.61-7.06 (m, aromatic protons)

iii) **1c:** $^{1}$H-NMR (500 MHz, $CDCl_3$, δ ppm): 2.13 (s, 3H, *syn*-HH), 4.02 (dd, *J* = 8 Hz, 1H, *syn*-HH), 4.12 (dd, *J* = 8 Hz, 1H, *syn* -HH), 6.57 (s, 1H ), 6.75 (d, 1H, *J* = 8.5 Hz), 6.98 (d, 1H, *J* = 8 Hz)

iv) **1d:** $^{1}$H-NMR (500 MHz, $CDCl_3$, δ ppm): 1.26 (s, 3H, *anti*-HH), 1.64 (s, 3H, *syn*-HH), 2.37 (s, 3H, *anti*-HH), 2.63 (s, 3H, *syn*-HH), 3.37 (s, 1H, *anti*-HH), 3.61 (s, 1H, *syn*-HH), 6.51-7.12 (m, aromatic protons)

v) **1e:** $^{1}$H-NMR (500 MHz, $CDCl_3$, δ ppm): 2.24 (s, 3H, *syn*-HH), 2.26 (d, 1H, *J* = 8 Hz, *syn*-HT), 4.04 (dd, 1H, *J* = 9.5 Hz, *syn*-HH), 4.17 (dd, 1H, *J* = 9.5Hz, *syn*-HH), 4.22 (dd, 1H, *J* = 7.5 Hz, *syn*-HH), 4.29 (dd, 1H, *J* = 7.5Hz, *syn*-HH), 6.45-6.88(m, aromatic protons, *syn*-isomer)

vi) **1f:** $^{1}$H-NMR (500 MHz, $CDCl_3$, δ ppm): 1.30 (s, 3H, *anti*-HH/HT), 1.63 (s, 3H, *syn*-HH), 2.23 (s, 3H, *anti*-HT), 2.26 (s, 3H, *syn*-HH), 2.32 (s, 3H, *anti*-HH), 3.44 (s, 1H, *anti*-HH), 3.48 (s, 1H, *anti*-HT), 3.47 (s, 1H, *syn*-HH), 6.32-7.00 (m, aromatic protons), 7.13-7.17 (m, aromatic protons)

vii) **1g:** $^{1}$H-NMR (400 MHz, $CDCl_3$, δ ppm): 3.71 (s, 3H, *syn*-HT), 4.17 (dd, 1H, *J* = 9 Hz, *syn* -HT), 4.24 (dd, 1H, *J* = 9 Hz, *syn*-HT), 6.19 (d, 1H, *J* = 2.5 Hz, *syn*-HT), 6.68 (d, 1H, *J* = 8.5 Hz, *syn*-HT), 7.03 (d, 1H, *J* = 8.5 Hz, *syn*-HT)

viii) **1h:** $^{1}$H-NMR (500 MHz, $CDCl_3$, δ ppm): 1.24 (s, 3H, *anti*-HH/HT), 1.67 (s, 3H, *syn*-HH), 3.41 (s, 1H, *anti*-HH), 3.66 (s, 1H, *syn*-HH), 3.84 (s, 1H, *anti*-HT), 6.05 (d, 1H, *J* = 2.5 Hz, *syn*-HH), 6.62-7.05(m, aromatic protons, *anti*-HH/HT), 7.09 (d, 1H, *J* = 8.5 Hz, *syn*-HH), 7.35 (s, 1H, *syn*-HH)

ix) **1i:** $^1$H-NMR (500 MHz, $CDCl_3$, δ ppm): 4.07(dd, 1H, *J* = 9.5 Hz, *syn* -HH), 4.20 (dd, 1H, *J* = 9.5 Hz, *syn* -HH), 4.26 (dd, 1H, *J* = 10.5 Hz, *syn* -HT), 4.30 (dd, 1H, *J* = 10.5 Hz, *syn* -HT), 6.58-7.21(m, aromatic protons)

*In CB[8] / Water*

i) **1a:** $^1$H-NMR (500 MHz, $CDCl_3$, δ ppm): 2.26 (s, 3H, *syn*-HH), 3.88 (d, 1H, *J* = 8 Hz, *anti*-HH), 3.98 (dd, 1H, J = 7 Hz, *syn*-HH), 4.11(dd, 1H, *J* = 7 Hz, *syn*-HH), 6.65-7.02 (m, aromatic protons)

ii) **1b:** $^1$H-NMR (500 MHz, $CDCl_3$, δ ppm): 1.25 (s, 3H, *anti*-HH), 2.37 (s, 3H, *anti*-HH), 2.42 (s, 3H, *syn*-HH), 3.38 (s, 1H, *anti*-HH), 3.60 (s, 1H, *syn*-HH), 6.61-7.06 (m, aromatic protons)

iii) **1c:** $^1$H-NMR (500 MHz, $CDCl_3$, δ ppm): 2.13 (s, 3H, *syn*-HH), 2.27 (s, 3H, *syn*-HT), 4.02 (dd, *J* = 8 Hz, *syn*-HH), 4.12 (dd, *J* = 8 Hz, *syn* -HH), 4.19 (dd, *J* = 8 Hz, *syn* -HT), 4.24 (dd, *J* = 8 Hz, *syn*-HT), 6.50 (d, 1H, *J* = 9.5 Hz, *syn*-HT), 6.57 (s, 1H, *syn*-HH ), 6.75 (d, 1H, *J* = 8.5 Hz, *syn*-HH), 6.90 (d, 1H, *J* = 7 Hz, *syn*-HT), 6.98 (d, 1H, *J* = 10 Hz, *syn*-HH), 7.03 (d, 1H, *J* = 8.5 Hz, *syn*-HT)

iv) **1d:** $^1$H-NMR (500 MHz, $CDCl_3$, δ ppm): 1.26 (s, 3H, *anti*-HH), 1.64 (s, 3H, *syn*-HH), 2.37 (s, 3H, *anti*-HH), 2.63 (s, 3H, *syn*-HH), 3.37 (s, 1H, *anti*-HH), 3.61 (s, 1H, *syn*-HH), 6.51-7.12 (m, aromatic protons)

v) **1e: :** $^1$H-NMR (500 MHz, $CDCl_3$, δ ppm): 2.24 (s, 3H, *syn*-HH), 2.26 (d, 1H, *J* = 8 Hz, *syn*-HT), 4.04 (dd, 1H, *J* = 9.5 Hz, *syn*-HH), 4.17 (dd, 1H, *J* = 9.5Hz, *syn*-HH), 4.22 (dd, 1H, *J* = 7.5 Hz, *syn*-HH), 4.29 (dd, 1H, *J* = 7.5Hz, *syn*-HH), 6.45-6.88(m, aromatic protons, *syn*-isomer)

vi) **1f:** $^1$H-NMR (500 MHz, $CDCl_3$, δ ppm): 1.30 (s, 3H, *anti*-HH/HT), 1.63 (s, 3H, *syn*-HH), 2.23 (s, 3H, *anti*-HT), 2.26 (s, 3H, *syn*-HH), 2.32 (s, 3H, *anti*-HH), 3.44 (s, 1H, *anti*-HH), 3.48 (s, 1H, *anti*-HT), 3.47 (s, 1H, *syn*-HH), 6.32-7.00 (m, aromatic protons), 7.13-7.17 (m, aromatic protons)

vii) **1g:** $^1$H-NMR (400 MHz, $CDCl_3$, δ ppm): 3.71 (s, 3H, *syn*-HT), 4.17 (dd, 1H, *J* = 9 Hz, *syn* -HT), 4.24 (dd, 1H, *J* = 9 Hz, *syn*-HT), 6.19 (d, 1H, *J* = 2.5 Hz, *syn*-HT), 6.68 (d, 1H, *J* = 8.5 Hz, *syn*-HT), 7.03 (d, 1H, *J* = 8.5 Hz, *syn*-HT)

viii) **1h:** $^{1}$H-NMR (500 MHz, $CDCl_3$, δ ppm): 1.24 (s, 3H, *anti*-HH/HT), 1.67 (s, 3H, *syn*-HH), 3.41 (s, 1H, *anti*-HH), 3.66 (s, 1H, *syn*-HH), 3.84 (s, 1H, *anti*-HT), 6.05 (d, 1H, $J$ = 2.5 Hz, *syn*-HH), 6.62-7.05(m, aromatic protons, *anti*-HH/HT), 7.09 (d, 1H, $J$ = 8.5 Hz, *syn*-HH), 7.35 (s, 1H, *syn*-HH)

ix) **1i:** $^{1}$H-NMR (500 MHz, $CDCl_3$, δ ppm): 4.07(dd, 1H, $J$ = 9.5 Hz, *syn* -HH), 4.20 (dd, 1H, $J$ = 9.5 Hz, *syn* -HH), 4.26 (dd, 1H, $J$ = 10.5 Hz, *syn* -HT), 4.30 (dd, 1H, $J$ = 10.5 Hz, *syn* -HT), 6.58-7.21(m, aromatic protons)

## 7. Effective volume and Geometric parameters for adducts 2-5 of coumarin derivatives optimized data at RB3LYP/6-31g(d,p) level. The frequency calculations were performed at the same level and were positive for all vibrations.

Optimized geometric parameters for *anti*-HT dimer of **1a**

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 4.465708 | 1.438410 | -0.153782 |
| 2 | 6 | 0 | 3.096493 | 1.515462 | -0.380246 |
| 3 | 6 | 0 | 2.292637 | 0.367114 | -0.373605 |
| 4 | 6 | 0 | 2.916022 | -0.855116 | -0.123687 |
| 5 | 6 | 0 | 4.290157 | -0.945786 | 0.100226 |
| 6 | 6 | 0 | 5.085245 | 0.201131 | 0.088257 |
| 7 | 1 | 0 | 5.063898 | 2.345320 | -0.167201 |
| 8 | 1 | 0 | 2.623337 | 2.477539 | -0.559402 |
| 9 | 6 | 0 | 0.816705 | 0.432446 | -0.625902 |
| 10 | 1 | 0 | 4.719308 | -1.925494 | 0.284316 |
| 11 | 6 | 0 | 0.086876 | -0.936092 | -0.572059 |
| 12 | 6 | 0 | -0.810797 | -0.423705 | 0.615999 |
| 13 | 6 | 0 | -2.288666 | -0.364482 | 0.374568 |
| 14 | 6 | 0 | -0.085869 | 0.947085 | 0.557128 |
| 15 | 6 | 0 | -2.917295 | 0.854607 | 0.122589 |
| 16 | 6 | 0 | -3.089135 | -1.515126 | 0.392691 |
| 17 | 6 | 0 | -4.293319 | 0.940315 | -0.091644 |
| 18 | 6 | 0 | -4.460101 | -1.443078 | 0.175667 |
| 19 | 1 | 0 | -2.611870 | -2.475049 | 0.572367 |
| 20 | 6 | 0 | -5.084997 | -0.208716 | -0.067804 |
| 21 | 1 | 0 | -4.726557 | 1.917790 | -0.277972 |
| 22 | 1 | 0 | -5.055502 | -2.351668 | 0.197483 |
| 23 | 6 | 0 | 0.880739 | -2.175467 | -0.235683 |
| 24 | 6 | 0 | -0.884760 | 2.180839 | 0.211441 |
| 25 | 8 | 0 | 2.231883 | -2.069291 | -0.070560 |
| 26 | 8 | 0 | 0.362792 | -3.255451 | -0.087322 |
| 27 | 8 | 0 | -0.370036 | 3.260327 | 0.049004 |
| 28 | 8 | 0 | -2.236722 | 2.070224 | 0.056804 |
| 29 | 6 | 0 | -6.572656 | -0.131214 | -0.314769 |
| 30 | 1 | 0 | -6.833754 | -0.560307 | -1.289445 |
| 31 | 1 | 0 | -7.130422 | -0.691353 | 0.442943 |
| 32 | 1 | 0 | -6.928092 | 0.902229 | -0.301326 |
| 33 | 6 | 0 | 6.570492 | 0.118003 | 0.347654 |
| 34 | 1 | 0 | 7.135169 | 0.699434 | -0.388441 |
| 35 | 1 | 0 | 6.821325 | 0.519833 | 1.336623 |
| 36 | 1 | 0 | 6.927098 | -0.914443 | 0.309399 |
| 37 | 1 | 0 | -0.499247 | -1.171442 | -1.463313 |
| 38 | 1 | 0 | 0.622046 | 0.983093 | -1.551081 |
| 39 | 1 | 0 | 0.495918 | 1.190737 | 1.449073 |
| 40 | 1 | 0 | -0.606867 | -0.972465 | 1.540326 |

Optimized geometric parameters for *anti*-HH dimer of **1a**

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 1.382850 | 2.041694 | -1.110222 |
| 2 | 6 | 0 | 0.231507 | 1.137672 | -0.752113 |
| 3 | 6 | 0 | 0.471130 | -0.391757 | -0.629912 |
| 4 | 6 | 0 | 1.910686 | -0.703077 | -0.316589 |
| 5 | 6 | 0 | 2.321799 | -1.983987 | 0.078341 |
| 6 | 1 | 0 | 1.578416 | -2.774806 | 0.145463 |
| 7 | 6 | 0 | 3.649378 | -2.263809 | 0.380012 |
| 8 | 6 | 0 | 4.628060 | -1.259619 | 0.302099 |
| 9 | 6 | 0 | 4.231809 | 0.016974 | -0.096670 |
| 10 | 1 | 0 | 4.949429 | 0.826404 | -0.184581 |
| 11 | 6 | 0 | 2.895898 | 0.283710 | -0.401868 |
| 12 | 8 | 0 | 2.643347 | 1.585191 | -0.822051 |
| 13 | 8 | 0 | 1.259205 | 3.134377 | -1.598981 |
| 14 | 6 | 0 | -1.382742 | 2.041704 | 1.110202 |
| 15 | 6 | 0 | -0.231441 | 1.137643 | 0.752048 |
| 16 | 1 | 0 | 0.598678 | 1.383205 | 1.415658 |
| 17 | 6 | 0 | -0.471131 | -0.391769 | 0.629768 |
| 18 | 6 | 0 | -1.910708 | -0.703004 | 0.316469 |
| 19 | 6 | 0 | -2.321881 | -1.983886 | -0.078609 |
| 20 | 1 | 0 | -1.578501 | -2.774692 | -0.145911 |
| 21 | 6 | 0 | -3.649443 | -2.263630 | -0.380273 |
| 22 | 6 | 0 | -4.628124 | -1.259402 | -0.302156 |
| 23 | 6 | 0 | -4.231817 | 0.017118 | 0.096658 |
| 24 | 1 | 0 | -4.949395 | 0.826576 | 0.184596 |
| 25 | 6 | 0 | -2.895856 | 0.283789 | 0.401855 |
| 26 | 8 | 0 | -2.643265 | 1.585252 | 0.822067 |
| 27 | 8 | 0 | -1.259039 | 3.134373 | 1.598980 |
| 28 | 1 | 0 | -3.932967 | -3.269006 | -0.679063 |
| 29 | 1 | 0 | 3.932876 | -3.269241 | 0.678618 |
| 30 | 1 | 0 | -0.598601 | 1.383302 | -1.415712 |
| 31 | 6 | 0 | -6.066698 | -1.550936 | -0.655647 |
| 32 | 1 | 0 | -6.734476 | -0.761953 | -0.300499 |
| 33 | 1 | 0 | -6.197106 | -1.630939 | -1.741594 |
| 34 | 1 | 0 | -6.398830 | -2.498835 | -0.220322 |
| 35 | 6 | 0 | 6.066514 | -1.550873 | 0.656295 |
| 36 | 1 | 0 | 6.735547 | -0.767008 | 0.292232 |
| 37 | 1 | 0 | 6.198403 | -1.619960 | 1.742836 |
| 38 | 1 | 0 | 6.395819 | -2.503891 | 0.230202 |
| 39 | 1 | 0 | -0.109306 | -0.995057 | 1.468516 |
| 40 | 1 | 0 | 0.109292 | -0.994983 | -1.468697 |

Optimized geometric parameters for *syn*-HT dimer of **1a**

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -3.254429 | 1.005021 | -0.901749 |
| 2 | 6 | 0 | -2.630354 | -0.234297 | -0.978261 |
| 3 | 6 | 0 | -1.768033 | -0.682918 | 0.034228 |
| 4 | 6 | 0 | -1.577525 | 0.159990 | 1.131046 |
| 5 | 6 | 0 | -2.199576 | 1.405695 | 1.218411 |
| 6 | 6 | 0 | -3.046449 | 1.847594 | 0.201876 |
| 7 | 1 | 0 | -3.910105 | 1.324661 | -1.706835 |
| 8 | 1 | 0 | -2.795145 | -0.868169 | -1.844280 |
| 9 | 6 | 0 | -1.103241 | -2.031950 | -0.023064 |
| 10 | 1 | 0 | -2.008420 | 2.014864 | 2.095957 |
| 11 | 6 | 0 | -0.044886 | -2.228019 | 1.094397 |
| 12 | 6 | 0 | 1.108792 | -2.029199 | 0.033774 |
| 13 | 6 | 0 | 1.770094 | -0.678725 | -0.030308 |
| 14 | 6 | 0 | 0.050978 | -2.233776 | -1.082610 |
| 15 | 6 | 0 | 1.578568 | 0.157587 | -1.132531 |
| 16 | 6 | 0 | 2.633596 | -0.224344 | 0.977971 |
| 17 | 6 | 0 | 2.200900 | 1.402000 | -1.228562 |
| 18 | 6 | 0 | 3.258448 | 1.014489 | 0.892737 |
| 19 | 1 | 0 | 2.802587 | -0.854604 | 1.845812 |
| 20 | 6 | 0 | 3.047435 | 1.851114 | -0.214237 |
| 21 | 1 | 0 | 2.012058 | 2.004146 | -2.111504 |
| 22 | 1 | 0 | 3.918793 | 1.336985 | 1.692792 |
| 23 | 6 | 0 | -0.050770 | -1.317489 | 2.295680 |
| 24 | 6 | 0 | 0.055347 | -1.330124 | -2.289063 |
| 25 | 8 | 0 | -0.783490 | -0.169620 | 2.226626 |
| 26 | 8 | 0 | 0.581800 | -1.542720 | 3.298728 |
| 27 | 8 | 0 | -0.576710 | -1.562265 | -3.290883 |
| 28 | 8 | 0 | 0.786167 | -0.180710 | -2.226668 |
| 29 | 6 | 0 | 3.705440 | 3.207358 | -0.296957 |
| 30 | 1 | 0 | 3.204228 | 3.928110 | 0.360356 |
| 31 | 1 | 0 | 4.753366 | 3.160653 | 0.015833 |
| 32 | 1 | 0 | 3.671820 | 3.608563 | -1.313255 |
| 33 | 6 | 0 | -3.731168 | 3.190431 | 0.288733 |
| 34 | 1 | 0 | -3.537871 | 3.791726 | -0.606192 |
| 35 | 1 | 0 | -4.818271 | 3.075405 | 0.370064 |
| 36 | 1 | 0 | -3.390118 | 3.759148 | 1.157436 |
| 37 | 1 | 0 | -1.860991 | -2.819145 | -0.080046 |
| 38 | 1 | 0 | -0.022294 | -3.250161 | 1.476544 |
| 39 | 1 | 0 | 1.868471 | -2.814203 | 0.094842 |
| 40 | 1 | 0 | 0.030750 | -3.258098 | -1.459033 |

Optimized geometric parameters for *syn*-HH dimer of **1a**:

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -3.897411 | -0.159595 | -1.056380 |
| 2 | 6 | 0 | -2.727327 | -0.748039 | -1.528621 |
| 3 | 6 | 0 | -1.650807 | -1.016606 | -0.675308 |
| 4 | 6 | 0 | -1.805158 | -0.690205 | 0.674502 |
| 5 | 6 | 0 | -2.972272 | -0.107375 | 1.162499 |
| 6 | 6 | 0 | -4.034995 | 0.173531 | 0.299467 |
| 7 | 1 | 0 | -4.716555 | 0.035419 | -1.742831 |
| 8 | 6 | 0 | -0.383794 | -1.668700 | -1.123926 |
| 9 | 1 | 0 | -3.033530 | 0.118908 | 2.222240 |
| 10 | 6 | 0 | 0.346230 | -1.595192 | 1.351520 |
| 11 | 6 | 0 | 0.475349 | -2.286749 | 0.004815 |
| 12 | 6 | 0 | 0.895361 | -0.854984 | -1.588477 |
| 13 | 6 | 0 | 1.069166 | 0.525876 | -1.013505 |
| 14 | 6 | 0 | 1.751108 | -1.897990 | -0.813933 |
| 15 | 6 | 0 | 2.130929 | 0.808866 | -0.145427 |
| 16 | 6 | 0 | 0.218294 | 1.589203 | -1.348499 |
| 17 | 6 | 0 | 3.005872 | -1.447396 | -0.103219 |
| 18 | 6 | 0 | 2.324832 | 2.084246 | 0.385177 |
| 19 | 6 | 0 | 0.406879 | 2.865359 | -0.829771 |
| 20 | 1 | 0 | -0.606580 | 1.404977 | -2.030030 |
| 21 | 6 | 0 | 1.463134 | 3.130718 | 0.055011 |
| 22 | 1 | 0 | 3.166502 | 2.236941 | 1.053026 |
| 23 | 1 | 0 | -0.271256 | 3.665439 | -1.113186 |
| 24 | 8 | 0 | 1.187307 | -1.660953 | 2.210648 |
| 25 | 8 | 0 | -0.812107 | -0.916288 | 1.620189 |
| 26 | 8 | 0 | 3.094217 | -0.121816 | 0.220721 |
| 27 | 8 | 0 | 3.926920 | -2.176330 | 0.158028 |
| 28 | 1 | 0 | -2.643467 | -1.014510 | -2.579515 |
| 29 | 1 | 0 | 1.036739 | -0.841228 | -2.674337 |
| 30 | 1 | 0 | -0.595162 | -2.420658 | -1.890834 |
| 31 | 1 | 0 | 2.037893 | -2.744005 | -1.440438 |
| 32 | 1 | 0 | 0.356441 | -3.358059 | 0.195419 |
| 33 | 6 | 0 | 1.651834 | 4.504203 | 0.652508 |
| 34 | 1 | 0 | 1.060476 | 4.617641 | 1.569378 |
| 35 | 1 | 0 | 2.697583 | 4.687341 | 0.914399 |
| 36 | 1 | 0 | 1.331168 | 5.287826 | -0.040365 |
| 37 | 6 | 0 | -5.289992 | 0.836670 | 0.814326 |
| 38 | 1 | 0 | -5.468176 | 0.595679 | 1.866030 |
| 39 | 1 | 0 | -5.217756 | 1.928586 | 0.737479 |
| 40 | 1 | 0 | -6.168396 | 0.527761 | 0.240322 |

Optimized geometric parameters for *anti*-HT dimer of **1b**:

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -3.283437 | -0.903322 | -0.184015 |
| 2 | 1 | 0 | -2.989424 | -1.945350 | -0.283419 |
| 3 | 6 | 0 | -4.613276 | -0.592928 | 0.105965 |
| 4 | 6 | 0 | -4.955109 | 0.760094 | 0.260698 |
| 5 | 6 | 0 | -3.995857 | 1.757861 | 0.142659 |
| 6 | 1 | 0 | -4.244133 | 2.805185 | 0.276932 |
| 7 | 6 | 0 | -2.674445 | 1.413208 | -0.145028 |
| 8 | 6 | 0 | -2.295955 | 0.082928 | -0.328485 |
| 9 | 6 | 0 | -0.440394 | 2.325625 | -0.346049 |
| 10 | 8 | 0 | 0.269289 | 3.301261 | -0.285423 |
| 11 | 8 | 0 | -1.787923 | 2.487521 | -0.209725 |
| 12 | 6 | 0 | 0.103306 | 0.937530 | -0.567283 |
| 13 | 1 | 0 | 0.758573 | 1.015661 | -1.437888 |
| 14 | 6 | 0 | 4.613279 | 0.592889 | -0.106040 |
| 15 | 6 | 0 | 3.283452 | 0.903308 | 0.183961 |
| 16 | 1 | 0 | 2.989458 | 1.945340 | 0.283383 |
| 17 | 6 | 0 | 2.295958 | -0.082926 | 0.328464 |
| 18 | 6 | 0 | 2.674420 | -1.413215 | 0.145034 |
| 19 | 6 | 0 | 3.995827 | -1.757892 | -0.142660 |
| 20 | 1 | 0 | 4.244090 | -2.805226 | -0.276889 |
| 21 | 6 | 0 | 4.955091 | -0.760145 | -0.260736 |
| 22 | 6 | 0 | 0.865713 | 0.277954 | 0.655976 |
| 23 | 6 | 0 | 0.440359 | -2.325591 | 0.346156 |
| 24 | 8 | 0 | -0.269335 | -3.301219 | 0.285575 |
| 25 | 8 | 0 | 1.787886 | -2.487512 | 0.209783 |
| 26 | 6 | 0 | -0.103302 | -0.937480 | 0.567351 |
| 27 | 1 | 0 | -0.758593 | -1.015558 | 1.437942 |
| 28 | 6 | 0 | -5.658647 | -1.675398 | 0.235588 |
| 29 | 1 | 0 | -6.295099 | -1.513305 | 1.111700 |
| 30 | 1 | 0 | -6.317277 | -1.699143 | -0.641127 |
| 31 | 1 | 0 | -5.200440 | -2.663387 | 0.329898 |
| 32 | 6 | 0 | 5.658646 | 1.675344 | -0.235827 |
| 33 | 1 | 0 | 6.318271 | 1.698188 | 0.640158 |
| 34 | 1 | 0 | 6.294085 | 1.513983 | -1.112815 |
| 35 | 1 | 0 | 5.200461 | 2.663476 | -0.328728 |
| 36 | 1 | 0 | -5.982077 | 1.033736 | 0.487538 |
| 37 | 1 | 0 | 5.982056 | -1.033810 | -0.487559 |
| 38 | 6 | 0 | -0.865691 | -0.277918 | -0.655941 |
| 39 | 6 | 0 | 0.761372 | 1.034423 | 1.986310 |
| 40 | 1 | 0 | 1.174775 | 0.424624 | 2.795709 |
| 41 | 1 | 0 | 1.306135 | 1.980683 | 1.953916 |
| 42 | 1 | 0 | -0.283047 | 1.258392 | 2.229373 |
| 43 | 6 | 0 | -0.761260 | -1.034395 | -1.986260 |
| 44 | 1 | 0 | -1.305981 | -1.980679 | -1.953879 |
| 45 | 1 | 0 | -1.174659 | -0.424627 | -2.795684 |
| 46 | 1 | 0 | 0.283180 | -1.258318 | -2.229277 |

Optimized geometric parameters for *anti*-HH dimer of **1b**:

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 1.821972 | -0.453465 | 0.437092 |
| 2 | 6 | 0 | 1.966325 | -1.823192 | 0.700964 |
| 3 | 6 | 0 | 3.187310 | -2.474899 | 0.551942 |
| 4 | 6 | 0 | 4.328393 | -1.774953 | 0.135820 |
| 5 | 6 | 0 | 4.199079 | -0.410742 | -0.133070 |
| 6 | 6 | 0 | 2.967374 | 0.226163 | 0.008441 |
| 7 | 1 | 0 | 1.103538 | -2.390218 | 1.036964 |
| 8 | 1 | 0 | 3.257763 | -3.537116 | 0.769139 |
| 9 | 1 | 0 | 5.047981 | 0.180838 | -0.461203 |
| 10 | 6 | 0 | 0.521269 | 0.287541 | 0.617289 |
| 11 | 6 | 0 | 0.640010 | 1.831615 | 0.439869 |
| 12 | 1 | 0 | 0.549945 | 2.419763 | 1.359161 |
| 13 | 6 | 0 | 1.857384 | 2.366483 | -0.283934 |
| 14 | 8 | 0 | 2.971977 | 1.573280 | -0.339344 |
| 15 | 8 | 0 | 1.906779 | 3.462080 | -0.780799 |
| 16 | 6 | 0 | -0.139480 | -0.055055 | 1.960629 |
| 17 | 1 | 0 | -0.447173 | -1.102535 | 2.005892 |
| 18 | 1 | 0 | 0.562097 | 0.132871 | 2.779174 |
| 19 | 1 | 0 | -1.032738 | 0.550360 | 2.139433 |
| 20 | 6 | 0 | 5.652507 | -2.476634 | -0.047924 |
| 21 | 1 | 0 | 5.755021 | -2.863173 | -1.069433 |
| 22 | 1 | 0 | 6.492774 | -1.799534 | 0.129478 |
| 23 | 1 | 0 | 5.750525 | -3.327057 | 0.632970 |
| 24 | 8 | 0 | -1.906915 | 3.462635 | 0.779179 |
| 25 | 6 | 0 | -1.857359 | 2.366545 | 0.283402 |
| 26 | 6 | 0 | -0.640024 | 1.831421 | -0.440177 |
| 27 | 8 | 0 | -2.971601 | 1.572996 | 0.340284 |
| 28 | 6 | 0 | -0.521062 | 0.287207 | -0.616766 |
| 29 | 1 | 0 | -0.549730 | 2.419246 | -1.359676 |
| 30 | 6 | 0 | -2.967269 | 0.226037 | -0.008033 |
| 31 | 6 | 0 | -1.821875 | -0.453734 | -0.436612 |
| 32 | 6 | 0 | 0.140127 | -0.056100 | -1.959691 |
| 33 | 6 | 0 | -4.199118 | -0.410638 | 0.133235 |
| 34 | 6 | 0 | -1.966551 | -1.823370 | -0.700868 |
| 35 | 1 | 0 | 0.448833 | -1.103276 | -2.003709 |
| 36 | 1 | 0 | -0.561485 | 0.130347 | -2.778544 |
| 37 | 1 | 0 | 1.032934 | 0.549823 | -2.139089 |
| 38 | 6 | 0 | -4.328705 | -1.774737 | -0.136047 |
| 39 | 1 | 0 | -5.047872 | 0.181045 | 0.461560 |
| 40 | 6 | 0 | -3.187711 | -2.474819 | -0.552170 |
| 41 | 1 | 0 | -1.103900 | -2.390561 | -1.036897 |
| 42 | 6 | 0 | -5.652964 | -2.476234 | 0.047394 |
| 43 | 1 | 0 | -3.258412 | -3.536965 | -0.769642 |
| 44 | 1 | 0 | -5.755837 | -2.862644 | 1.068916 |
| 45 | 1 | 0 | -6.493104 | -1.799059 | -0.130334 |
| 46 | 1 | 0 | -5.750872 | -3.326716 | -0.633440 |

Optimized geometric parameters for *syn*-HT dimer of **1b**:

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 1.684439 | -0.382422 | -0.018777 |
| 2 | 6 | 0 | 2.449972 | 0.156309 | 1.027334 |
| 3 | 6 | 0 | 3.003379 | 1.429231 | 0.944735 |
| 4 | 6 | 0 | 2.822415 | 2.218926 | -0.200536 |
| 5 | 6 | 0 | 2.066931 | 1.692437 | -1.248532 |
| 6 | 6 | 0 | 1.514363 | 0.415404 | -1.153833 |
| 7 | 1 | 0 | 2.595651 | -0.428999 | 1.929787 |
| 8 | 1 | 0 | 3.580568 | 1.815971 | 1.779896 |
| 9 | 1 | 0 | 1.891899 | 2.260320 | -2.156687 |
| 10 | 6 | 0 | 1.113377 | -1.785313 | 0.036889 |
| 11 | 6 | 0 | 0.056146 | -1.999909 | -1.083545 |
| 12 | 1 | 0 | 0.038553 | -3.037608 | -1.425614 |
| 13 | 6 | 0 | 0.083855 | -1.146266 | -2.322143 |
| 14 | 8 | 0 | 0.802858 | 0.011668 | -2.279892 |
| 15 | 8 | 0 | -0.508606 | -1.424730 | -3.337128 |
| 16 | 6 | 0 | 2.227360 | -2.834432 | 0.109552 |
| 17 | 1 | 0 | 1.810834 | -3.847378 | 0.097026 |
| 18 | 1 | 0 | 2.910443 | -2.732493 | -0.740074 |
| 19 | 1 | 0 | 2.811805 | -2.720831 | 1.027387 |
| 20 | 6 | 0 | 3.444200 | 3.590761 | -0.304481 |
| 21 | 1 | 0 | 4.513390 | 3.522324 | -0.539299 |
| 22 | 1 | 0 | 2.972131 | 4.186385 | -1.090248 |
| 23 | 1 | 0 | 3.355385 | 4.139362 | 0.638415 |
| 24 | 8 | 0 | 0.507960 | -1.425824 | 3.336898 |
| 25 | 6 | 0 | -0.056872 | -2.000163 | 1.083113 |
| 26 | 8 | 0 | -0.802865 | 0.011378 | 2.279959 |
| 27 | 6 | 0 | -1.114045 | -1.784901 | -0.037260 |
| 28 | 1 | 0 | -0.039667 | -3.037957 | 1.424915 |
| 29 | 6 | 0 | -1.514160 | 0.415606 | 1.153952 |
| 30 | 6 | 0 | -1.684521 | -0.381791 | 0.018768 |
| 31 | 6 | 0 | -2.228418 | -2.833577 | -0.110187 |
| 32 | 6 | 0 | -2.066514 | 1.692817 | 1.249077 |
| 33 | 6 | 0 | -2.450121 | 0.157442 | -1.027178 |
| 34 | 1 | 0 | -2.911446 | -2.731612 | 0.739482 |
| 35 | 1 | 0 | -2.812844 | -2.719515 | -1.027977 |
| 36 | 1 | 0 | -1.812278 | -3.846685 | -0.097936 |
| 37 | 6 | 0 | -2.821868 | 2.219769 | 0.201373 |
| 38 | 1 | 0 | -1.891453 | 2.260322 | 2.157449 |
| 39 | 6 | 0 | -3.003268 | 1.430338 | -0.944154 |
| 40 | 1 | 0 | -2.596163 | -0.427704 | -1.929677 |
| 41 | 6 | 0 | -3.442034 | 3.592394 | 0.304586 |
| 42 | 1 | 0 | -3.580701 | 1.817325 | -1.779049 |
| 43 | 1 | 0 | -3.324387 | 4.152269 | -0.628623 |
| 44 | 1 | 0 | -4.517757 | 3.524956 | 0.507342 |
| 45 | 1 | 0 | -2.990524 | 4.176714 | 1.110584 |
| 46 | 6 | 0 | -0.084318 | -1.146845 | 2.321950 |

Optimized geometric parameters for *syn*-HH dimer of **1b**:

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 3.792918 | -0.371087 | 0.879471 |
| 2 | 6 | 0 | 2.595647 | -1.012717 | 1.185212 |
| 3 | 6 | 0 | 1.533897 | -1.073195 | 0.271600 |
| 4 | 6 | 0 | 1.742127 | -0.463815 | -0.970178 |
| 5 | 6 | 0 | 2.937944 | 0.173910 | -1.293678 |
| 6 | 6 | 0 | 3.985374 | 0.230079 | -0.371882 |
| 7 | 1 | 0 | 4.588386 | -0.340674 | 1.618824 |
| 8 | 6 | 0 | 0.227979 | -1.772969 | 0.557426 |
| 9 | 1 | 0 | 3.028567 | 0.625149 | -2.276735 |
| 10 | 6 | 0 | -0.431978 | -1.047922 | -1.871063 |
| 11 | 6 | 0 | -0.660731 | -1.985760 | -0.702470 |
| 12 | 6 | 0 | -1.002004 | -0.944495 | 1.196431 |
| 13 | 6 | 0 | -0.972140 | 0.541711 | 0.884107 |
| 14 | 6 | 0 | -1.920620 | -1.665512 | 0.163413 |
| 15 | 6 | 0 | -1.952248 | 1.130324 | 0.074098 |
| 16 | 6 | 0 | -0.017870 | 1.405986 | 1.443553 |
| 17 | 6 | 0 | -3.093971 | -0.932591 | -0.439539 |
| 18 | 6 | 0 | -1.963109 | 2.499666 | -0.195373 |
| 19 | 6 | 0 | -0.024070 | 2.772372 | 1.188448 |
| 20 | 1 | 0 | 0.749293 | 0.993238 | 2.090054 |
| 21 | 6 | 0 | -0.996339 | 3.341674 | 0.352574 |
| 22 | 1 | 0 | -2.750143 | 2.885926 | -0.834992 |
| 23 | 1 | 0 | 0.734425 | 3.405108 | 1.640888 |
| 24 | 8 | 0 | -1.244066 | -0.874201 | -2.743799 |
| 25 | 8 | 0 | 0.779450 | -0.424677 | -1.970432 |
| 26 | 8 | 0 | -3.011934 | 0.430529 | -0.486070 |
| 27 | 8 | 0 | -4.091030 | -1.473839 | -0.841774 |
| 28 | 1 | 0 | 2.481885 | -1.473510 | 2.161672 |
| 29 | 6 | 0 | 5.293448 | 0.893509 | -0.729584 |
| 30 | 1 | 0 | 5.965529 | 0.191239 | -1.237947 |
| 31 | 1 | 0 | 5.141065 | 1.741829 | -1.403103 |
| 32 | 1 | 0 | 5.813711 | 1.255217 | 0.161835 |
| 33 | 6 | 0 | -0.985713 | 4.817754 | 0.036896 |
| 34 | 1 | 0 | -0.334434 | 5.030838 | -0.819662 |
| 35 | 1 | 0 | -1.985635 | 5.181283 | -0.215422 |
| 36 | 1 | 0 | -0.612566 | 5.403353 | 0.882452 |
| 37 | 6 | 0 | -1.327970 | -1.173709 | 2.675538 |
| 38 | 1 | 0 | -0.556446 | -0.743993 | 3.322591 |
| 39 | 1 | 0 | -2.275004 | -0.686198 | 2.929282 |
| 40 | 1 | 0 | -1.422131 | -2.236154 | 2.914994 |
| 41 | 1 | 0 | 0.871592 | -2.981343 | 2.275717 |
| 42 | 6 | 0 | 0.465705 | -3.115025 | 1.269573 |
| 43 | 1 | 0 | -0.456690 | -3.694950 | 1.363818 |
| 44 | 1 | 0 | 1.180282 | -3.714177 | 0.697073 |
| 45 | 1 | 0 | -0.652723 | -2.997054 | -1.123664 |
| 46 | 1 | 0 | -2.325995 | -2.596746 | 0.561485 |

Optimized geometric parameters for *anti*-HT dimer of **1c**:

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.038130 | 0.006547 | 0.014054 |
| 2 | 1 | 0 | 0.055981 | 0.005757 | 1.004673 |
| 3 | 6 | 0 | 1.232596 | 0.008892 | -0.704237 |
| 4 | 6 | 0 | 1.201626 | -0.029461 | -2.098000 |
| 5 | 6 | 0 | -0.012453 | 0.007027 | -2.780297 |
| 6 | 1 | 0 | -0.033639 | 0.027354 | -3.769545 |
| 7 | 6 | 0 | -1.207853 | 0.015627 | -2.048296 |
| 8 | 6 | 0 | -1.184835 | 0.004965 | -0.659630 |
| 9 | 6 | 0 | -3.649732 | -0.190203 | -2.076063 |
| 10 | 8 | 0 | -4.664976 | -0.050630 | -2.711403 |
| 11 | 8 | 0 | -2.453633 | -0.010979 | -2.712187 |
| 12 | 6 | 0 | -3.652085 | -0.330044 | -0.594669 |
| 13 | 1 | 0 | -4.384827 | 0.305943 | -0.276029 |
| 14 | 6 | 0 | -7.529410 | -1.615508 | 1.220670 |
| 15 | 6 | 0 | -6.353389 | -1.665606 | 0.488794 |
| 16 | 1 | 0 | -6.401859 | -1.687727 | -0.500544 |
| 17 | 6 | 0 | -5.103157 | -1.681535 | 1.106415 |
| 18 | 6 | 0 | -5.071188 | -1.485048 | 2.481425 |
| 19 | 6 | 0 | -6.245914 | -1.546432 | 3.240059 |
| 20 | 1 | 0 | -6.190871 | -1.623306 | 4.225805 |
| 21 | 6 | 0 | -7.484227 | -1.500990 | 2.608734 |
| 22 | 6 | 0 | -3.855043 | -1.666041 | 0.258308 |
| 23 | 6 | 0 | -2.648282 | -1.228710 | 2.514802 |
| 24 | 8 | 0 | -1.673981 | -1.109412 | 3.221549 |
| 25 | 8 | 0 | -3.846925 | -1.371028 | 3.143966 |
| 26 | 6 | 0 | -2.575429 | -1.226951 | 1.032081 |
| 27 | 1 | 0 | -1.820557 | -1.867574 | 0.771115 |
| 28 | 6 | 0 | 2.576702 | 0.050159 | 0.035437 |
| 29 | 1 | 0 | 3.180418 | -0.794290 | -0.257154 |
| 30 | 1 | 0 | 3.099960 | 0.960756 | -0.210475 |
| 31 | 1 | 0 | 2.409148 | 0.014182 | 1.099620 |
| 32 | 6 | 0 | -8.883058 | -1.684233 | 0.499690 |
| 33 | 1 | 0 | -9.440495 | -2.536594 | 0.854465 |
| 34 | 1 | 0 | -9.448040 | -0.786308 | 0.695037 |
| 35 | 1 | 0 | -8.727204 | -1.780041 | -0.562561 |
| 36 | 1 | 0 | 2.099771 | 0.058588 | -2.683789 |
| 37 | 1 | 0 | -8.399775 | -1.432071 | 3.168937 |
| 38 | 1 | 0 | -3.796088 | -2.587181 | -0.298888 |
| 39 | 6 | 0 | -2.454576 | 0.010215 | 0.170989 |
| 40 | 1 | 0 | -2.454359 | 0.986774 | 0.630965 |

Optimized geometric parameters for *syn*-HT dimer of **1c**:

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.022307 | -0.012330 | 0.017742 |
| 2 | 6 | 0 | 0.026563 | 0.001361 | 1.523366 |
| 3 | 6 | 0 | 2.449471 | 0.023986 | 1.467751 |
| 4 | 6 | 0 | 3.580934 | -0.096460 | 2.270282 |
| 5 | 6 | 0 | 4.848646 | -0.062730 | 1.689331 |
| 6 | 6 | 0 | 4.995681 | 0.092755 | 0.306388 |
| 7 | 6 | 0 | 3.843618 | 0.214353 | -0.472205 |
| 8 | 6 | 0 | 2.554876 | 0.171894 | 0.082176 |
| 9 | 6 | 0 | 1.316189 | 0.347833 | -0.761943 |
| 10 | 6 | 0 | -0.035500 | -1.404623 | -0.726453 |
| 11 | 6 | 0 | 2.076116 | -1.677738 | -2.298805 |
| 12 | 6 | 0 | 1.685270 | -3.231991 | -0.480668 |
| 13 | 6 | 0 | 2.207235 | -4.357799 | 0.150910 |
| 14 | 6 | 0 | 1.575955 | -4.871238 | 1.283866 |
| 15 | 6 | 0 | 0.420770 | -4.266848 | 1.792390 |
| 16 | 6 | 0 | -0.081198 | -3.141736 | 1.136352 |
| 17 | 6 | 0 | 0.538794 | -2.595208 | 0.001924 |
| 18 | 6 | 0 | 0.960036 | -0.819582 | -1.764912 |
| 19 | 8 | 0 | 1.235221 | 0.011957 | 2.153928 |
| 20 | 8 | 0 | -0.980031 | -0.006016 | 2.190315 |
| 21 | 8 | 0 | 2.373739 | -2.823656 | -1.622885 |
| 22 | 8 | 0 | 2.718563 | -1.395809 | -3.281599 |
| 23 | 1 | 0 | -0.828901 | 0.596316 | -0.296301 |
| 24 | 1 | 0 | 3.454334 | -0.209518 | 3.341061 |
| 25 | 1 | 0 | 3.945599 | 0.331713 | -1.547411 |
| 26 | 1 | 0 | 3.098664 | -4.821216 | -0.256489 |
| 27 | 1 | 0 | -0.975326 | -2.662023 | 1.524485 |
| 28 | 1 | 0 | 0.447404 | -0.400230 | -2.633806 |
| 29 | 1 | 0 | -1.026986 | -1.643458 | -1.115023 |
| 30 | 1 | 0 | 1.317785 | 1.332797 | -1.231962 |
| 31 | 1 | 0 | 5.719782 | -0.155972 | 2.330625 |
| 32 | 1 | 0 | 1.995658 | -5.750951 | 1.762182 |
| 33 | 6 | 0 | -0.262660 | -4.811620 | 3.038956 |
| 34 | 1 | 0 | -0.181700 | -5.900140 | 3.076070 |
| 35 | 1 | 0 | 0.203468 | -4.402668 | 3.940097 |
| 36 | 1 | 0 | -1.319686 | -4.539463 | 3.048791 |
| 37 | 6 | 0 | 6.375864 | 0.112319 | -0.335872 |
| 38 | 1 | 0 | 7.100024 | 0.592556 | 0.325763 |
| 39 | 1 | 0 | 6.718628 | -0.906916 | -0.536481 |
| 40 | 1 | 0 | 6.352771 | 0.656265 | -1.281951 |

Optimized geometric parameters for *anti*-HH dimer of **1c**:

| -Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.026134 | -0.040871 | -0.019009 |
| 2 | 6 | 0 | -0.048424 | -0.005254 | 1.485834 |
| 3 | 6 | 0 | 1.292735 | 0.010914 | 2.271293 |
| 4 | 6 | 0 | 2.399440 | 0.615531 | 1.443757 |
| 5 | 6 | 0 | 3.638679 | 0.949372 | 2.008312 |
| 6 | 1 | 0 | 3.792114 | 0.767294 | 3.070411 |
| 7 | 6 | 0 | 4.676977 | 1.511130 | 1.264449 |
| 8 | 6 | 0 | 4.462401 | 1.742702 | -0.099342 |
| 9 | 6 | 0 | 3.244728 | 1.411198 | -0.693842 |
| 10 | 1 | 0 | 3.071153 | 1.572670 | -1.751785 |
| 11 | 6 | 0 | 2.228293 | 0.847283 | 0.074774 |
| 12 | 8 | 0 | 1.071388 | 0.513864 | -0.626374 |
| 13 | 8 | 0 | -0.914834 | -0.478597 | -0.702381 |
| 14 | 6 | 0 | -1.848856 | 1.583888 | 2.522863 |
| 15 | 6 | 0 | -0.405827 | 1.364297 | 2.154414 |
| 16 | 1 | 0 | -0.090588 | 2.198236 | 1.525230 |
| 17 | 6 | 0 | 0.628246 | 1.040535 | 3.268785 |
| 18 | 6 | 0 | -0.035966 | 0.378654 | 4.450272 |
| 19 | 6 | 0 | 0.713963 | -0.212895 | 5.476647 |
| 20 | 1 | 0 | 1.799914 | -0.191363 | 5.405810 |
| 21 | 6 | 0 | 0.123069 | -0.832719 | 6.578330 |
| 22 | 6 | 0 | -1.274600 | -0.855581 | 6.652499 |
| 23 | 6 | 0 | -2.049392 | -0.265863 | 5.653450 |
| 24 | 1 | 0 | -3.132280 | -0.264756 | 5.706344 |
| 25 | 6 | 0 | -1.429743 | 0.349562 | 4.567588 |
| 26 | 8 | 0 | -2.294564 | 0.944751 | 3.651598 |
| 27 | 8 | 0 | -2.624586 | 2.237234 | 1.874966 |
| 28 | 1 | 0 | -0.721055 | -0.792897 | 1.829178 |
| 29 | 1 | 0 | 5.241684 | 2.181215 | -0.714492 |
| 30 | 1 | 0 | 1.602579 | -0.942692 | 2.702573 |
| 31 | 1 | 0 | 1.258096 | 1.872437 | 3.589088 |
| 32 | 1 | 0 | -1.775607 | -1.330296 | 7.490116 |
| 33 | 6 | 0 | 6.001228 | 1.870389 | 1.925943 |
| 34 | 1 | 0 | 5.888125 | 2.755032 | 2.558862 |
| 35 | 1 | 0 | 6.354984 | 1.047327 | 2.551199 |
| 36 | 1 | 0 | 6.759873 | 2.083103 | 1.171277 |
| 37 | 6 | 0 | 0.980588 | -1.473502 | 7.662027 |
| 38 | 1 | 0 | 1.454518 | -2.385717 | 7.289063 |
| 39 | 1 | 0 | 1.767947 | -0.788415 | 7.985174 |
| 40 | 1 | 0 | 0.370329 | -1.733102 | 8.528305 |

Optimized geometric parameters for *syn*-HH dimer of **1c**:

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.010187 | 0.006693 | 0.010829 |
| 2 | 6 | 0 | -0.007866 | 0.005033 | 1.522545 |
| 3 | 6 | 0 | 2.418464 | 0.023462 | 1.547417 |
| 4 | 6 | 0 | 3.516900 | 0.162660 | 2.387706 |
| 5 | 6 | 0 | 4.792657 | 0.175207 | 1.834612 |
| 6 | 6 | 0 | 4.980488 | 0.063549 | 0.451005 |
| 7 | 6 | 0 | 3.846663 | -0.044823 | -0.361552 |
| 8 | 6 | 0 | 2.553778 | -0.073095 | 0.164931 |
| 9 | 6 | 0 | 1.339819 | -0.236367 | -0.697338 |
| 10 | 6 | 0 | 6.365587 | 0.081301 | -0.149211 |
| 11 | 6 | 0 | -0.590940 | -1.298743 | -0.659167 |
| 12 | 6 | 0 | -1.386670 | -2.222686 | 0.212334 |
| 13 | 6 | 0 | 0.649556 | -3.423343 | 0.745253 |
| 14 | 6 | 0 | 1.173054 | -4.433212 | 1.547136 |
| 15 | 6 | 0 | 2.487554 | -4.844059 | 1.361881 |
| 16 | 6 | 0 | 3.285223 | -4.270483 | 0.369042 |
| 17 | 6 | 0 | 2.726756 | -3.264139 | -0.420456 |
| 18 | 6 | 0 | 1.411702 | -2.812828 | -0.248246 |
| 19 | 6 | 0 | 0.849304 | -1.699261 | -1.080292 |
| 20 | 6 | 0 | 4.714103 | -4.724820 | 0.136762 |
| 21 | 8 | 0 | 1.176372 | 0.007959 | 2.188633 |
| 22 | 8 | 0 | -1.026304 | 0.013384 | 2.169897 |
| 23 | 8 | 0 | -0.697213 | -3.127861 | 0.972550 |
| 24 | 8 | 0 | -2.587186 | -2.195408 | 0.304578 |
| 25 | 1 | 0 | -0.555501 | 0.875718 | -0.243486 |
| 26 | 1 | 0 | 3.369324 | 0.259992 | 3.423593 |
| 27 | 1 | 0 | 5.640456 | 0.342465 | 2.444622 |
| 28 | 1 | 0 | 3.976074 | -0.062440 | -1.410527 |
| 29 | 1 | 0 | 1.444322 | 0.333172 | -1.579560 |
| 30 | 1 | 0 | 7.101441 | 0.425052 | 0.521539 |
| 31 | 1 | 0 | 6.360963 | 0.597583 | -1.071342 |
| 32 | 1 | 0 | 6.669872 | -0.895190 | -0.420229 |
| 33 | 1 | 0 | -1.181399 | -1.023800 | -1.506475 |
| 34 | 1 | 0 | 0.539404 | -4.871046 | 2.272788 |
| 35 | 1 | 0 | 2.891686 | -5.590526 | 1.985477 |
| 36 | 1 | 0 | 3.299348 | -2.843410 | -1.206681 |
| 37 | 1 | 0 | 0.966459 | -1.874126 | -2.119166 |
| 38 | 1 | 0 | 5.363295 | -3.903382 | 0.086576 |
| 39 | 1 | 0 | 5.022076 | -5.197584 | 1.041505 |
| 40 | 1 | 0 | 4.808860 | -5.453627 | -0.595801 |

Optimized geometric parameters for *syn*-HH dimer of **1d**:

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 3.766500 | -0.547408 | 0.051600 |
| 2 | 6 | 0 | 2.592003 | -0.968740 | 0.679695 |
| 3 | 6 | 0 | 1.367837 | -1.084078 | 0.002510 |
| 4 | 6 | 0 | 1.358620 | -0.765950 | -1.357775 |
| 5 | 6 | 0 | 2.514149 | -0.349890 | -2.018964 |
| 6 | 6 | 0 | 3.707163 | -0.240376 | -1.316059 |
| 7 | 1 | 0 | 2.630595 | -1.214745 | 1.737014 |
| 8 | 6 | 0 | 0.098218 | -1.558568 | 0.668540 |
| 9 | 1 | 0 | 2.452630 | -0.116329 | -3.076358 |
| 10 | 1 | 0 | 4.604268 | 0.085386 | -1.835830 |
| 11 | 6 | 0 | -0.988087 | -1.263769 | -1.697248 |
| 12 | 6 | 0 | -1.039565 | -1.918052 | -0.331085 |
| 13 | 1 | 0 | -1.187481 | -2.987648 | -0.516263 |
| 14 | 1 | 0 | -2.755652 | 3.043072 | -1.132689 |
| 15 | 6 | 0 | -1.891011 | 2.692845 | -0.579778 |
| 16 | 6 | 0 | -1.928583 | 1.410559 | -0.029511 |
| 17 | 6 | 0 | -0.768704 | 3.489196 | -0.398306 |
| 18 | 6 | 0 | -0.844759 | 0.895997 | 0.692923 |
| 19 | 6 | 0 | 0.332831 | 3.023894 | 0.335246 |
| 20 | 1 | 0 | -0.749046 | 4.488007 | -0.826004 |
| 21 | 6 | 0 | -0.914851 | -0.485599 | 1.323497 |
| 22 | 6 | 0 | -3.290871 | -0.572513 | 0.137573 |
| 23 | 6 | 0 | -2.072265 | -1.293372 | 0.659792 |
| 24 | 1 | 0 | -2.451285 | -2.075131 | 1.319389 |
| 25 | 1 | 0 | 1.113412 | 1.362773 | 1.436466 |
| 26 | 6 | 0 | 0.266605 | 1.735844 | 0.868748 |
| 27 | 8 | 0 | -3.127114 | 0.735829 | -0.217582 |
| 28 | 8 | 0 | 0.219018 | -0.815043 | -2.150399 |
| 29 | 8 | 0 | -1.947020 | -1.176985 | -2.421461 |
| 30 | 8 | 0 | -4.382992 | -1.071864 | 0.053203 |
| 31 | 6 | 0 | 0.374439 | -2.749748 | 1.601590 |
| 32 | 1 | 0 | 0.912329 | -3.529639 | 1.054107 |
| 33 | 1 | 0 | 0.982364 | -2.466103 | 2.464558 |
| 34 | 1 | 0 | -0.551299 | -3.188179 | 1.984324 |
| 35 | 6 | 0 | 5.066596 | -0.438486 | 0.813209 |
| 36 | 1 | 0 | 4.920866 | -0.618506 | 1.881780 |
| 37 | 1 | 0 | 5.803129 | -1.165878 | 0.452272 |
| 38 | 1 | 0 | 5.515079 | 0.554668 | 0.699595 |
| 39 | 6 | 0 | 1.562800 | 3.881482 | 0.516864 |
| 40 | 1 | 0 | 2.210714 | 3.839358 | -0.367303 |
| 41 | 1 | 0 | 1.298228 | 4.931911 | 0.674225 |
| 42 | 1 | 0 | 2.158039 | 3.551926 | 1.373211 |
| 43 | 6 | 0 | -0.952180 | -0.372302 | 2.850593 |
| 44 | 1 | 0 | -0.037895 | 0.089389 | 3.236986 |
| 45 | 1 | 0 | -1.791570 | 0.260698 | 3.156647 |
| 46 | 1 | 0 | -1.073866 | -1.346326 | 3.331858 |

Optimized geometric parameters for *syn*-HT dimer of **1d**:

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 3.163764 | -1.579256 | 0.258407 |
| 2 | 6 | 0 | 2.657854 | -0.304700 | -0.010826 |
| 3 | 6 | 0 | 1.550206 | 0.224862 | 0.667717 |
| 4 | 6 | 0 | 0.954127 | -0.568820 | 1.652150 |
| 5 | 6 | 0 | 1.435162 | -1.843833 | 1.944861 |
| 6 | 6 | 0 | 2.531540 | -2.341794 | 1.250508 |
| 7 | 1 | 0 | 3.127138 | 0.293249 | -0.786657 |
| 8 | 6 | 0 | 1.041551 | 1.627517 | 0.395650 |
| 9 | 1 | 0 | 0.935591 | -2.424906 | 2.712382 |
| 10 | 1 | 0 | 2.899251 | -3.338191 | 1.480253 |
| 11 | 6 | 0 | -0.366575 | 1.841343 | 1.020613 |
| 12 | 6 | 0 | -1.041512 | 1.627129 | -0.396696 |
| 13 | 6 | 0 | -1.550284 | 0.224442 | -0.667937 |
| 14 | 6 | 0 | 0.366548 | 1.840709 | -1.021748 |
| 15 | 6 | 0 | -0.954077 | -0.569948 | -1.651769 |
| 16 | 6 | 0 | -2.658034 | -0.304590 | 0.010783 |
| 17 | 6 | 0 | -1.435065 | -1.845138 | -1.943635 |
| 18 | 6 | 0 | -3.163947 | -1.579347 | -0.257641 |
| 19 | 1 | 0 | -3.127420 | 0.293914 | 0.786128 |
| 20 | 6 | 0 | -2.531570 | -2.342592 | -1.249068 |
| 21 | 1 | 0 | -0.935423 | -2.426796 | -2.710666 |
| 22 | 1 | 0 | -2.899258 | -3.339149 | -1.478157 |
| 23 | 8 | 0 | 0.136091 | -0.166408 | -2.418234 |
| 24 | 8 | 0 | -0.135928 | -0.164787 | 2.418489 |
| 25 | 6 | 0 | 4.369530 | -2.106704 | -0.482603 |
| 26 | 1 | 0 | 4.449720 | -1.664011 | -1.479307 |
| 27 | 1 | 0 | 5.298641 | -1.877216 | 0.054007 |
| 28 | 1 | 0 | 4.322347 | -3.193712 | -0.597901 |
| 29 | 6 | 0 | -4.369820 | -2.106239 | 0.483581 |
| 30 | 1 | 0 | -4.449950 | -1.663072 | 1.480083 |
| 31 | 1 | 0 | -5.298888 | -1.876836 | -0.053140 |
| 32 | 1 | 0 | -4.322813 | -3.193198 | 0.599390 |
| 33 | 6 | 0 | 2.095484 | 2.677746 | 0.761004 |
| 34 | 1 | 0 | 2.397029 | 2.573554 | 1.808418 |
| 35 | 1 | 0 | 2.989495 | 2.567625 | 0.140269 |
| 36 | 1 | 0 | 1.704275 | 3.690279 | 0.614716 |
| 37 | 6 | 0 | -2.095404 | 2.677334 | -0.762502 |
| 38 | 1 | 0 | -2.397254 | 2.572572 | -1.809782 |
| 39 | 1 | 0 | -2.989256 | 2.567765 | -0.141448 |
| 40 | 1 | 0 | -1.703856 | 3.689814 | -0.616914 |
| 41 | 1 | 0 | -0.514345 | 2.879363 | 1.328565 |
| 42 | 1 | 0 | 0.514206 | 2.878514 | -1.330437 |
| 43 | 6 | 0 | 0.818603 | 0.988060 | -2.176431 |
| 44 | 6 | 0 | -0.818475 | 0.989514 | 2.175975 |
| 45 | 8 | 0 | -1.758255 | 1.268832 | 2.881842 |
| 46 | 8 | 0 | 1.758485 | 1.266897 | -2.882368 |

Optimized geometric parameters for *anti*-HT dimer of **1d**:

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 4.954845 | -0.760407 | -0.261651 |
| 2 | 6 | 0 | 3.995470 | -1.758025 | -0.143442 |
| 3 | 6 | 0 | 2.674214 | -1.413187 | 0.144772 |
| 4 | 6 | 0 | 2.295998 | -0.082880 | 0.328557 |
| 5 | 6 | 0 | 3.283617 | 0.903227 | 0.183931 |
| 6 | 6 | 0 | 4.613293 | 0.592652 | -0.106552 |
| 7 | 1 | 0 | 5.981690 | -1.034171 | -0.488901 |
| 8 | 1 | 0 | 4.243523 | -2.805373 | -0.277936 |
| 9 | 6 | 0 | 0.865858 | 0.278161 | 0.656331 |
| 10 | 1 | 0 | 2.989832 | 1.945288 | 0.283629 |
| 11 | 6 | 0 | -0.103303 | -0.937182 | 0.567938 |
| 12 | 6 | 0 | 0.440161 | -2.325392 | 0.346985 |
| 13 | 1 | 0 | -0.758666 | -1.014958 | 1.438498 |
| 14 | 6 | 0 | -0.440494 | 2.325773 | -0.345427 |
| 15 | 6 | 0 | 0.103359 | 0.937773 | -0.566797 |
| 16 | 6 | 0 | -0.865521 | -0.277768 | -0.655587 |
| 17 | 1 | 0 | 0.758555 | 1.016088 | -1.437450 |
| 18 | 6 | 0 | -2.674560 | 1.413209 | -0.145343 |
| 19 | 6 | 0 | -2.295899 | 0.082930 | -0.328579 |
| 20 | 6 | 0 | -3.996067 | 1.757747 | 0.142011 |
| 21 | 6 | 0 | -3.283313 | -0.903397 | -0.184243 |
| 22 | 6 | 0 | -4.955253 | 0.759889 | 0.259918 |
| 23 | 1 | 0 | -4.244494 | 2.805051 | 0.276157 |
| 24 | 6 | 0 | -4.613262 | -0.593104 | 0.105380 |
| 25 | 1 | 0 | -2.989171 | -1.945407 | -0.283453 |
| 26 | 1 | 0 | -5.982293 | 1.033454 | 0.486520 |
| 27 | 8 | 0 | -1.788129 | 2.487590 | -0.209961 |
| 28 | 8 | 0 | 1.787578 | -2.487390 | 0.209722 |
| 29 | 8 | 0 | 0.269130 | 3.301406 | -0.284159 |
| 30 | 8 | 0 | -0.269609 | -3.301013 | 0.287096 |
| 31 | 6 | 0 | -5.658540 | -1.675688 | 0.234766 |
| 32 | 1 | 0 | -5.200253 | -2.663631 | 0.329175 |
| 33 | 1 | 0 | -6.295226 | -1.513670 | 1.110716 |
| 34 | 1 | 0 | -6.316942 | -1.699497 | -0.642122 |
| 35 | 6 | 0 | 5.658830 | 1.674929 | -0.236476 |
| 36 | 1 | 0 | 6.293031 | 1.514402 | -1.114517 |
| 37 | 1 | 0 | 5.200854 | 2.663316 | -0.327579 |
| 38 | 1 | 0 | 6.319657 | 1.696470 | 0.638634 |
| 39 | 6 | 0 | -0.760469 | -1.034445 | -1.985752 |
| 40 | 1 | 0 | 0.284095 | -1.258291 | -2.228304 |
| 41 | 1 | 0 | -1.305098 | -1.980791 | -1.953401 |
| 42 | 1 | 0 | -1.173623 | -0.424896 | -2.795467 |
| 43 | 6 | 0 | 0.761684 | 1.034719 | 1.986638 |
| 44 | 1 | 0 | 1.306475 | 1.980958 | 1.954139 |
| 45 | 1 | 0 | -0.282710 | 1.258748 | 2.229748 |
| 46 | 1 | 0 | 1.175106 | 0.424951 | 2.796049 |

Optimized geometric parameters for *anti*-HT dimer of **1g**:

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 4.373047 | 1.695051 | 0.227556 |
| 2 | 6 | 0 | 3.001341 | 1.690135 | 0.421775 |
| 3 | 6 | 0 | 2.258625 | 0.497882 | 0.414828 |
| 4 | 6 | 0 | 2.956080 | -0.687848 | 0.197120 |
| 5 | 6 | 0 | 4.339226 | -0.718914 | 0.002248 |
| 6 | 6 | 0 | 5.051773 | 0.481749 | 0.019235 |
| 7 | 1 | 0 | 4.943236 | 2.617183 | 0.233028 |
| 8 | 1 | 0 | 2.473130 | 2.627705 | 0.573338 |
| 9 | 6 | 0 | 0.776237 | 0.485023 | 0.629077 |
| 10 | 1 | 0 | 4.812103 | -1.678594 | -0.158836 |
| 11 | 6 | 0 | 0.127081 | -0.923880 | 0.585990 |
| 12 | 6 | 0 | -0.775894 | -0.484389 | -0.628291 |
| 13 | 6 | 0 | -2.258366 | -0.497641 | -0.414701 |
| 14 | 6 | 0 | -0.127049 | 0.924637 | -0.584908 |
| 15 | 6 | 0 | -2.956140 | 0.687895 | -0.196942 |
| 16 | 6 | 0 | -3.000849 | -1.690035 | -0.422311 |
| 17 | 6 | 0 | -4.339378 | 0.718649 | -0.002695 |
| 18 | 6 | 0 | -4.372641 | -1.695260 | -0.228715 |
| 19 | 1 | 0 | -2.472393 | -2.627466 | -0.573863 |
| 20 | 6 | 0 | -5.051688 | -0.482143 | -0.020369 |
| 21 | 1 | 0 | -4.812511 | 1.678191 | 0.158474 |
| 22 | 1 | 0 | -4.942656 | -2.617497 | -0.234695 |
| 23 | 6 | 0 | 0.996991 | -2.119937 | 0.285952 |
| 24 | 6 | 0 | -0.997257 | 2.120354 | -0.284346 |
| 25 | 8 | 0 | 2.344572 | -1.939493 | 0.145560 |
| 26 | 8 | 0 | 0.547067 | -3.230622 | 0.144036 |
| 27 | 8 | 0 | -0.547504 | 3.230974 | -0.141387 |
| 28 | 8 | 0 | -2.344875 | 1.939634 | -0.144682 |
| 29 | 1 | 0 | 0.524580 | 1.039718 | 1.538123 |
| 30 | 1 | 0 | -0.461872 | -1.178165 | 1.470155 |
| 31 | 1 | 0 | -0.523678 | -1.038931 | -1.537275 |
| 32 | 1 | 0 | 0.461604 | 1.179415 | -1.469141 |
| 33 | 8 | 0 | -6.397713 | -0.578649 | 0.156234 |
| 34 | 8 | 0 | 6.397739 | 0.577963 | -0.158020 |
| 35 | 6 | 0 | -7.136595 | 0.614684 | 0.377416 |
| 36 | 1 | 0 | -8.176487 | 0.306566 | 0.491420 |
| 37 | 1 | 0 | -6.809109 | 1.128163 | 1.289961 |
| 38 | 1 | 0 | -7.054441 | 1.303671 | -0.472425 |
| 39 | 6 | 0 | 7.136326 | -0.615553 | -0.379217 |
| 40 | 1 | 0 | 6.808310 | -1.129242 | -1.291453 |
| 41 | 1 | 0 | 8.176212 | -0.307637 | -0.493818 |
| 42 | 1 | 0 | 7.054477 | -1.304282 | 0.470862 |

Optimized geometric parameters for *anti*-HH dimer of **1g**:

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 3.154148 | -2.083735 | -0.767626 |
| 2 | 6 | 0 | 1.962577 | -1.373918 | -0.921980 |
| 3 | 6 | 0 | 1.801178 | -0.077301 | -0.430369 |
| 4 | 6 | 0 | 2.899442 | 0.501081 | 0.222359 |
| 5 | 6 | 0 | 4.100686 | -0.172327 | 0.387384 |
| 6 | 6 | 0 | 4.231149 | -1.476286 | -0.107668 |
| 7 | 1 | 0 | 3.233551 | -3.087704 | -1.164971 |
| 8 | 6 | 0 | 0.545861 | 0.716221 | -0.574363 |
| 9 | 1 | 0 | 4.931458 | 0.304049 | 0.893854 |
| 10 | 6 | 0 | 1.803464 | 2.641180 | 0.602869 |
| 11 | 6 | 0 | 0.692073 | 2.244549 | -0.353285 |
| 12 | 6 | 0 | -0.545798 | 0.716105 | 0.574213 |
| 13 | 6 | 0 | -1.801122 | -0.077387 | 0.430233 |
| 14 | 6 | 0 | -0.692043 | 2.244481 | 0.353395 |
| 15 | 6 | 0 | -2.899387 | 0.501044 | -0.222448 |
| 16 | 6 | 0 | -1.962582 | -1.373978 | 0.921892 |
| 17 | 6 | 0 | -1.803398 | 2.641181 | -0.602802 |
| 18 | 6 | 0 | -4.100683 | -0.172282 | -0.387400 |
| 19 | 6 | 0 | -3.154205 | -2.083724 | 0.767604 |
| 20 | 1 | 0 | -1.132056 | -1.842956 | 1.442984 |
| 21 | 6 | 0 | -4.231202 | -1.476227 | 0.107684 |
| 22 | 1 | 0 | -4.931448 | 0.304140 | -0.893838 |
| 23 | 1 | 0 | -3.233644 | -3.087681 | 1.164973 |
| 24 | 8 | 0 | 1.815375 | 3.680716 | 1.209886 |
| 25 | 8 | 0 | 2.856773 | 1.779121 | 0.769152 |
| 26 | 8 | 0 | -2.856631 | 1.779060 | -0.769292 |
| 27 | 8 | 0 | -1.815343 | 3.680780 | -1.209704 |
| 28 | 1 | 0 | 1.132040 | -1.842855 | -1.443093 |
| 29 | 8 | 0 | -5.443164 | -2.061287 | -0.100543 |
| 30 | 8 | 0 | 5.443070 | -2.061412 | 0.100612 |
| 31 | 6 | 0 | 5.645021 | -3.382660 | -0.380052 |
| 32 | 1 | 0 | 5.536622 | -3.437158 | -1.470456 |
| 33 | 1 | 0 | 6.667212 | -3.647311 | -0.107216 |
| 34 | 1 | 0 | 4.951126 | -4.092895 | 0.086787 |
| 35 | 6 | 0 | -5.645182 | -3.382508 | 0.380168 |
| 36 | 1 | 0 | -5.536717 | -3.436985 | 1.470566 |
| 37 | 1 | 0 | -6.667409 | -3.647091 | 0.107402 |
| 38 | 1 | 0 | -4.951370 | -4.092808 | -0.086698 |
| 39 | 1 | 0 | -0.057719 | 0.508436 | 1.531798 |
| 40 | 1 | 0 | -0.771872 | 2.886505 | 1.235790 |
| 41 | 1 | 0 | 0.057816 | 0.508699 | -1.532008 |
| 42 | 1 | 0 | 0.771789 | 2.886723 | -1.235594 |

Optimized geometric parameters for *syn*-HH dimer of **1g**:

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.726694 | -2.550946 | 0.028614 |
| 2 | 6 | 0 | 0.603994 | -1.840621 | 1.365707 |
| 3 | 6 | 0 | -1.561100 | -0.962329 | 0.698895 |
| 4 | 6 | 0 | -2.721002 | -0.381872 | 1.191096 |
| 5 | 6 | 0 | -3.787049 | -0.128132 | 0.319266 |
| 6 | 6 | 0 | -3.678304 | -0.471593 | -1.035602 |
| 7 | 6 | 0 | -2.499394 | -1.060837 | -1.494183 |
| 8 | 6 | 0 | -1.414493 | -1.309819 | -0.651342 |
| 9 | 6 | 0 | -0.145052 | -1.954514 | -1.101975 |
| 10 | 6 | 0 | 1.993445 | -2.164352 | -0.804824 |
| 11 | 6 | 0 | 3.252154 | -1.698998 | -0.111392 |
| 12 | 6 | 0 | 2.368367 | 0.553077 | -0.169516 |
| 13 | 6 | 0 | 2.561880 | 1.827668 | 0.347571 |
| 14 | 6 | 0 | 1.678025 | 2.856064 | 0.007010 |
| 15 | 6 | 0 | 0.605040 | 2.593389 | -0.856365 |
| 16 | 6 | 0 | 0.434105 | 1.302981 | -1.353626 |
| 17 | 6 | 0 | 1.294987 | 0.250646 | -1.024256 |
| 18 | 6 | 0 | 1.125180 | -1.136244 | -1.584777 |
| 19 | 8 | 0 | -0.558124 | -1.166767 | 1.636462 |
| 20 | 8 | 0 | 1.452560 | -1.886590 | 2.218369 |
| 21 | 8 | 0 | 3.339151 | -0.368623 | 0.195125 |
| 22 | 8 | 0 | 4.179166 | -2.420135 | 0.150117 |
| 23 | 1 | 0 | 0.616541 | -3.620133 | 0.235872 |
| 24 | 1 | 0 | -2.802681 | -0.127062 | 2.240848 |
| 25 | 1 | 0 | -2.422813 | -1.338621 | -2.542599 |
| 26 | 1 | 0 | 2.279648 | -3.016435 | -1.423378 |
| 27 | 1 | 0 | 3.398723 | 2.022767 | 1.007059 |
| 28 | 1 | 0 | -0.400850 | 1.105891 | -2.018873 |
| 29 | 1 | 0 | -4.493031 | -0.295868 | -1.726629 |
| 30 | 1 | 0 | -0.091548 | 3.371783 | -1.141055 |
| 31 | 8 | 0 | 1.949465 | 4.071133 | 0.558715 |
| 32 | 8 | 0 | -4.882787 | 0.446809 | 0.887858 |
| 33 | 6 | 0 | 1.083602 | 5.155666 | 0.258257 |
| 34 | 1 | 0 | 1.478454 | 6.013814 | 0.803415 |
| 35 | 1 | 0 | 1.076707 | 5.382450 | -0.815369 |
| 36 | 1 | 0 | 0.057095 | 4.957430 | 0.590982 |
| 37 | 6 | 0 | -6.006170 | 0.719850 | 0.062802 |
| 38 | 1 | 0 | -6.416790 | -0.197280 | -0.377641 |
| 39 | 1 | 0 | -6.754391 | 1.170635 | 0.715739 |
| 40 | 1 | 0 | -5.756306 | 1.424512 | -0.740296 |
| 41 | 1 | 0 | -0.353506 | -2.718782 | -1.857652 |
| 42 | 1 | 0 | 1.259841 | -1.136216 | -2.671765 |

Optimized geometric parameters for *syn*-HT dimer of **1g**:

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.032497 | -2.536685 | -1.087814 |
| 2 | 6 | 0 | -0.118183 | -1.638494 | -2.294134 |
| 3 | 6 | 0 | 1.480240 | -0.141145 | -1.259566 |
| 4 | 6 | 0 | 2.079248 | 1.102446 | -1.406087 |
| 5 | 6 | 0 | 2.989394 | 1.549712 | -0.442216 |
| 6 | 6 | 0 | 3.291879 | 0.736419 | 0.658433 |
| 7 | 6 | 0 | 2.674346 | -0.507575 | 0.775858 |
| 8 | 6 | 0 | 1.751598 | -0.975359 | -0.166012 |
| 9 | 6 | 0 | 1.105364 | -2.330042 | -0.053379 |
| 10 | 6 | 0 | -1.105357 | -2.330042 | 0.053391 |
| 11 | 6 | 0 | 0.118192 | -1.638476 | 2.294140 |
| 12 | 6 | 0 | -1.480237 | -0.141139 | 1.259565 |
| 13 | 6 | 0 | -2.079250 | 1.102450 | 1.406081 |
| 14 | 6 | 0 | -2.989400 | 1.549707 | 0.442209 |
| 15 | 6 | 0 | -3.291885 | 0.736407 | -0.658434 |
| 16 | 6 | 0 | -2.674348 | -0.507585 | -0.775853 |
| 17 | 6 | 0 | -1.751594 | -0.975360 | 0.166016 |
| 18 | 6 | 0 | 0.032504 | -2.536677 | 1.087827 |
| 19 | 8 | 0 | 0.616990 | -0.489905 | -2.293565 |
| 20 | 8 | 0 | -0.825398 | -1.872555 | -3.244140 |
| 21 | 8 | 0 | -0.616985 | -0.489890 | 2.293565 |
| 22 | 8 | 0 | 0.825410 | -1.872530 | 3.244145 |
| 23 | 1 | 0 | -0.081386 | -3.562711 | -1.457151 |
| 24 | 1 | 0 | 1.845191 | 1.721177 | -2.263880 |
| 25 | 1 | 0 | 2.904793 | -1.129626 | 1.635364 |
| 26 | 1 | 0 | -1.845193 | 1.721187 | 2.263870 |
| 27 | 1 | 0 | -2.904796 | -1.129642 | -1.635355 |
| 28 | 1 | 0 | 0.081395 | -3.562700 | 1.457172 |
| 29 | 1 | 0 | 3.993702 | 1.055758 | 1.418278 |
| 30 | 1 | 0 | -3.993712 | 1.055739 | -1.418279 |
| 31 | 8 | 0 | -3.525091 | 2.780739 | 0.668613 |
| 32 | 8 | 0 | 3.525079 | 2.780745 | -0.668625 |
| 33 | 6 | 0 | 4.450761 | 3.296572 | 0.277804 |
| 34 | 1 | 0 | 5.343279 | 2.663420 | 0.356483 |
| 35 | 1 | 0 | 4.740293 | 4.280506 | -0.093019 |
| 36 | 1 | 0 | 3.996139 | 3.403460 | 1.270376 |
| 37 | 6 | 0 | -4.450774 | 3.296559 | -0.277819 |
| 38 | 1 | 0 | -5.343291 | 2.663405 | -0.356494 |
| 39 | 1 | 0 | -4.740307 | 4.280495 | 0.092999 |
| 40 | 1 | 0 | -3.996152 | 3.403442 | -1.270391 |
| 41 | 1 | 0 | 1.869245 | -3.113444 | -0.050973 |
| 42 | 1 | 0 | -1.869237 | -3.113446 | 0.050992 |

Optimized geometric parameters for *anti*-HT dimer of **1h**:

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.758186 | -0.353401 | -0.663440 |
| 2 | 6 | 0 | -3.039617 | -1.409939 | -0.280297 |
| 3 | 1 | 0 | -2.561364 | -2.384198 | -0.330787 |
| 4 | 6 | 0 | -4.414646 | -1.341542 | -0.062813 |
| 5 | 1 | 0 | -4.985302 | -2.256530 | 0.033975 |
| 6 | 6 | 0 | -5.030984 | -0.085465 | 0.029252 |
| 7 | 6 | 0 | -4.257754 | 1.075014 | -0.078692 |
| 8 | 1 | 0 | -4.722313 | 2.049821 | 0.008458 |
| 9 | 6 | 0 | -2.888535 | 0.971083 | -0.290174 |
| 10 | 6 | 0 | -2.244598 | -0.266663 | -0.412478 |
| 11 | 8 | 0 | -6.362995 | 0.113266 | 0.232473 |
| 12 | 6 | 0 | -0.440859 | -1.120735 | -1.953291 |
| 13 | 1 | 0 | -0.792727 | -2.153896 | -1.901289 |
| 14 | 1 | 0 | 0.638106 | -1.143924 | -2.142181 |
| 15 | 1 | 0 | -0.924290 | -0.633151 | -2.805561 |
| 16 | 6 | 0 | -0.861250 | 2.289502 | -0.432809 |
| 17 | 8 | 0 | -0.358171 | 3.385864 | -0.376578 |
| 18 | 8 | 0 | -2.221200 | 2.191575 | -0.351143 |
| 19 | 6 | 0 | -0.049290 | 1.030286 | -0.588861 |
| 20 | 1 | 0 | 0.610619 | 1.212393 | -1.440177 |
| 21 | 6 | 0 | 4.429858 | 1.522621 | 0.017510 |
| 22 | 1 | 0 | 5.042032 | 2.409000 | -0.105377 |
| 23 | 6 | 0 | 3.067288 | 1.611243 | 0.251557 |
| 24 | 1 | 0 | 2.595837 | 2.589006 | 0.296804 |
| 25 | 6 | 0 | 2.263204 | 0.468752 | 0.410717 |
| 26 | 6 | 0 | 2.894911 | -0.767823 | 0.296939 |
| 27 | 6 | 0 | 4.267952 | -0.893346 | 0.066499 |
| 28 | 1 | 0 | 4.683877 | -1.889457 | -0.007314 |
| 29 | 6 | 0 | 5.041663 | 0.260238 | -0.067520 |
| 30 | 6 | 0 | 0.781532 | 0.569997 | 0.682239 |
| 31 | 8 | 0 | 6.384222 | 0.263230 | -0.291996 |
| 32 | 6 | 0 | 0.490424 | 1.341558 | 1.975486 |
| 33 | 1 | 0 | -0.585452 | 1.375836 | 2.179875 |
| 34 | 1 | 0 | 0.851178 | 2.371163 | 1.917117 |
| 35 | 1 | 0 | 0.981428 | 0.849913 | 2.821127 |
| 36 | 6 | 0 | 0.864428 | -2.075624 | 0.476710 |
| 37 | 8 | 0 | 0.355671 | -3.170424 | 0.440455 |
| 38 | 8 | 0 | 2.224574 | -1.986396 | 0.383669 |
| 39 | 6 | 0 | 0.062471 | -0.808407 | 0.616153 |
| 40 | 1 | 0 | -0.604834 | -0.975640 | 1.464640 |
| 41 | 6 | 0 | 7.053019 | -0.986494 | -0.389984 |
| 42 | 1 | 0 | 6.958188 | -1.567762 | 0.535574 |
| 43 | 1 | 0 | 6.673321 | -1.582405 | -1.229349 |
| 44 | 1 | 0 | 8.104045 | -0.751712 | -0.561895 |
| 45 | 6 | 0 | -7.201932 | -1.025807 | 0.360786 |
| 46 | 1 | 0 | -8.210499 | -0.638941 | 0.511124 |
| 47 | 1 | 0 | -7.184057 | -1.645304 | -0.544568 |
| 48 | 1 | 0 | -6.919191 | -1.641429 | 1.223831 |

Optimized geometric parameters for *anti*-HH dimer of **1h**:

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 1.299822 | 2.324870 | -1.161276 |
| 2 | 6 | 0 | 0.193841 | 1.389474 | -0.757315 |
| 3 | 6 | 0 | 0.455882 | -0.143314 | -0.669303 |
| 4 | 6 | 0 | 1.925760 | -0.399558 | -0.391342 |
| 5 | 6 | 0 | 2.412808 | -1.673006 | -0.072721 |
| 6 | 1 | 0 | 1.712133 | -2.500154 | -0.008628 |
| 7 | 6 | 0 | 3.759882 | -1.928228 | 0.176730 |
| 8 | 6 | 0 | 4.679252 | -0.872727 | 0.101642 |
| 9 | 6 | 0 | 4.231359 | 0.407577 | -0.235222 |
| 10 | 1 | 0 | 4.935153 | 1.226849 | -0.319633 |
| 11 | 6 | 0 | 2.881107 | 0.625740 | -0.483491 |
| 12 | 8 | 0 | 2.577838 | 1.925795 | -0.866035 |
| 13 | 8 | 0 | 1.131457 | 3.398299 | -1.678876 |
| 14 | 6 | 0 | -1.299832 | 2.324841 | 1.161346 |
| 15 | 6 | 0 | -0.193845 | 1.389463 | 0.757359 |
| 16 | 1 | 0 | 0.672007 | 1.618083 | 1.381433 |
| 17 | 6 | 0 | -0.455883 | -0.143325 | 0.669324 |
| 18 | 6 | 0 | -1.925761 | -0.399568 | 0.391359 |
| 19 | 6 | 0 | -2.412811 | -1.673019 | 0.072751 |
| 20 | 1 | 0 | -1.712141 | -2.500171 | 0.008681 |
| 21 | 6 | 0 | -3.759883 | -1.928236 | -0.176717 |
| 22 | 6 | 0 | -4.679248 | -0.872729 | -0.101662 |
| 23 | 6 | 0 | -4.231353 | 0.407578 | 0.235189 |
| 24 | 1 | 0 | -4.935144 | 1.226855 | 0.319578 |
| 25 | 6 | 0 | -2.881104 | 0.625736 | 0.483480 |
| 26 | 8 | 0 | -2.577838 | 1.925791 | 0.866027 |
| 27 | 8 | 0 | -1.131469 | 3.398318 | 1.678846 |
| 28 | 1 | 0 | -4.075967 | -2.933705 | -0.424127 |
| 29 | 1 | 0 | 4.075964 | -2.933695 | 0.424151 |
| 30 | 8 | 0 | -6.016667 | -0.989262 | -0.327083 |
| 31 | 8 | 0 | 6.016674 | -0.989263 | 0.327045 |
| 32 | 6 | 0 | 0.006676 | -0.941574 | 1.891860 |
| 33 | 1 | 0 | -0.101113 | -2.020005 | 1.739101 |
| 34 | 1 | 0 | 1.051373 | -0.736839 | 2.135608 |
| 35 | 1 | 0 | -0.609037 | -0.672305 | 2.756735 |
| 36 | 1 | 0 | -0.672011 | 1.618097 | -1.381389 |
| 37 | 6 | 0 | -0.006672 | -0.941547 | -1.891852 |
| 38 | 1 | 0 | 0.101117 | -2.019980 | -1.739108 |
| 39 | 1 | 0 | -1.051367 | -0.736808 | -2.135604 |
| 40 | 1 | 0 | 0.609046 | -0.672265 | -2.756719 |
| 41 | 6 | 0 | -6.535787 | -2.269321 | -0.658169 |
| 42 | 1 | 0 | -6.361249 | -2.996368 | 0.144772 |
| 43 | 1 | 0 | -7.609481 | -2.131621 | -0.790453 |
| 44 | 1 | 0 | -6.103489 | -2.652117 | -1.591172 |
| 45 | 6 | 0 | 6.535793 | -2.269322 | 0.658134 |
| 46 | 1 | 0 | 6.361234 | -2.996377 | -0.144795 |
| 47 | 1 | 0 | 7.609490 | -2.131626 | 0.790395 |
| 48 | 1 | 0 | 6.103512 | -2.652105 | 1.591150 |

Optimized geometric parameters for *syn*-HH dimer of **1h**:

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -1.059963 | -2.198835 | -0.620205 |
| 2 | 6 | 0 | -0.787878 | -1.329826 | -1.831580 |
| 3 | 6 | 0 | 1.435033 | -0.854136 | -0.989663 |
| 4 | 6 | 0 | 2.661083 | -0.320662 | -1.362545 |
| 5 | 6 | 0 | 3.718562 | -0.309050 | -0.447153 |
| 6 | 6 | 0 | 3.528920 | -0.841531 | 0.834590 |
| 7 | 6 | 0 | 2.285717 | -1.378367 | 1.171261 |
| 8 | 6 | 0 | 1.205196 | -1.398275 | 0.283220 |
| 9 | 6 | 0 | -0.141410 | -1.989100 | 0.618527 |
| 10 | 6 | 0 | -2.282986 | -1.754716 | 0.243941 |
| 11 | 6 | 0 | -3.416228 | -0.976886 | -0.378282 |
| 12 | 6 | 0 | -2.138378 | 1.031520 | 0.015104 |
| 13 | 6 | 0 | -2.069688 | 2.377401 | -0.323869 |
| 14 | 6 | 0 | -1.030182 | 3.167272 | 0.173540 |
| 15 | 6 | 0 | -0.067740 | 2.593885 | 1.015960 |
| 16 | 6 | 0 | -0.160571 | 1.239875 | 1.330529 |
| 17 | 6 | 0 | -1.178952 | 0.415024 | 0.837333 |
| 18 | 6 | 0 | -1.302703 | -1.047289 | 1.228363 |
| 19 | 8 | 0 | 0.460103 | -0.790975 | -1.974343 |
| 20 | 8 | 0 | -1.599683 | -1.140575 | -2.701007 |
| 21 | 8 | 0 | -3.249962 | 0.374995 | -0.491472 |
| 22 | 8 | 0 | -4.452260 | -1.470929 | -0.740588 |
| 23 | 1 | 0 | -1.125433 | -3.225889 | -0.995750 |
| 24 | 1 | 0 | 2.795895 | 0.086012 | -2.357567 |
| 25 | 1 | 0 | 2.160235 | -1.793400 | 2.166490 |
| 26 | 1 | 0 | -2.741889 | -2.637361 | 0.691620 |
| 27 | 1 | 0 | -2.826617 | 2.810876 | -0.966070 |
| 28 | 1 | 0 | 0.594769 | 0.809000 | 1.979015 |
| 29 | 1 | 0 | 4.328754 | -0.850158 | 1.564421 |
| 30 | 1 | 0 | 0.746155 | 3.180975 | 1.422389 |
| 31 | 8 | 0 | -1.046333 | 4.473473 | -0.210929 |
| 32 | 8 | 0 | 4.881903 | 0.236358 | -0.898910 |
| 33 | 6 | 0 | 0.010103 | -3.308849 | 1.393237 |
| 34 | 1 | 0 | 0.669624 | -3.986290 | 0.842431 |
| 35 | 1 | 0 | 0.440965 | -3.155700 | 2.386327 |
| 36 | 1 | 0 | -0.950236 | -3.813898 | 1.529437 |
| 37 | 6 | 0 | -1.622042 | -1.178759 | 2.720829 |
| 38 | 1 | 0 | -1.790469 | -2.217542 | 3.017504 |
| 39 | 1 | 0 | -0.811403 | -0.774239 | 3.335816 |
| 40 | 1 | 0 | -2.526805 | -0.610312 | 2.960076 |
| 41 | 6 | 0 | -0.010256 | 5.325147 | 0.255154 |
| 42 | 1 | 0 | -0.213208 | 6.306634 | -0.175026 |
| 43 | 1 | 0 | -0.012342 | 5.403894 | 1.349703 |
| 44 | 1 | 0 | 0.976605 | 4.981262 | -0.079000 |
| 45 | 6 | 0 | 5.997140 | 0.265765 | -0.020236 |
| 46 | 1 | 0 | 6.302426 | -0.744514 | 0.279736 |
| 47 | 1 | 0 | 6.807413 | 0.734102 | -0.580189 |
| 48 | 1 | 0 | 5.788755 | 0.860142 | 0.878316 |

Optimized geometric parameters for *syn*-HT dimer of **1h**:

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.035854 | -2.312812 | -1.083804 |
| 2 | 6 | 0 | -0.115968 | -1.460815 | -2.320630 |
| 3 | 6 | 0 | 1.408877 | 0.105383 | -1.286590 |
| 4 | 6 | 0 | 1.946398 | 1.376666 | -1.435779 |
| 5 | 6 | 0 | 2.785326 | 1.895044 | -0.443944 |
| 6 | 6 | 0 | 3.075232 | 1.125052 | 0.690014 |
| 7 | 6 | 0 | 2.521846 | -0.148922 | 0.808173 |
| 8 | 6 | 0 | 1.673562 | -0.692242 | -0.163534 |
| 9 | 6 | 0 | 1.113251 | -2.096264 | -0.058021 |
| 10 | 6 | 0 | -1.113267 | -2.096254 | 0.058001 |
| 11 | 6 | 0 | 0.115954 | -1.460836 | 2.320617 |
| 12 | 6 | 0 | -1.408882 | 0.105382 | 1.286593 |
| 13 | 6 | 0 | -1.946393 | 1.376667 | 1.435795 |
| 14 | 6 | 0 | -2.785305 | 1.895066 | 0.443959 |
| 15 | 6 | 0 | -3.075206 | 1.125094 | -0.690013 |
| 16 | 6 | 0 | -2.521831 | -0.148884 | -0.808184 |
| 17 | 6 | 0 | -1.673562 | -0.692226 | 0.163524 |
| 18 | 6 | 0 | 0.035836 | -2.312821 | 1.083783 |
| 19 | 8 | 0 | 0.608019 | -0.305189 | -2.346801 |
| 20 | 8 | 0 | -0.799269 | -1.737445 | -3.277527 |
| 21 | 8 | 0 | -0.608038 | -0.305214 | 2.346806 |
| 22 | 8 | 0 | 0.799203 | -1.737512 | 3.277538 |
| 23 | 1 | 0 | -0.080828 | -3.350972 | -1.422087 |
| 24 | 1 | 0 | 1.716495 | 1.963122 | -2.317067 |
| 25 | 1 | 0 | 2.746286 | -0.731666 | 1.695928 |
| 26 | 1 | 0 | -1.716493 | 1.963108 | 2.317094 |
| 27 | 1 | 0 | -2.746267 | -0.731613 | -1.695951 |
| 28 | 1 | 0 | 0.080802 | -3.350983 | 1.422058 |
| 29 | 1 | 0 | 3.717984 | 1.500036 | 1.476252 |
| 30 | 1 | 0 | -3.717947 | 1.500095 | -1.476253 |
| 31 | 8 | 0 | -3.264236 | 3.148465 | 0.675752 |
| 32 | 8 | 0 | 3.264264 | 3.148441 | -0.675723 |
| 33 | 6 | 0 | 2.229000 | -3.145624 | -0.081907 |
| 34 | 1 | 0 | 1.814061 | -4.159158 | -0.059303 |
| 35 | 1 | 0 | 2.835763 | -3.042032 | -0.987433 |
| 36 | 1 | 0 | 2.890883 | -3.032554 | 0.781925 |
| 37 | 6 | 0 | -2.229027 | -3.145603 | 0.081881 |
| 38 | 1 | 0 | -1.814098 | -4.159141 | 0.059267 |
| 39 | 1 | 0 | -2.835787 | -3.042012 | 0.987409 |
| 40 | 1 | 0 | -2.890910 | -3.032518 | -0.781949 |
| 41 | 6 | 0 | 4.112898 | 3.735607 | 0.300813 |
| 42 | 1 | 0 | 5.033574 | 3.154890 | 0.438238 |
| 43 | 1 | 0 | 4.366755 | 4.725547 | -0.080110 |
| 44 | 1 | 0 | 3.604961 | 3.839472 | 1.267551 |
| 45 | 6 | 0 | -4.112837 | 3.735661 | -0.300796 |
| 46 | 1 | 0 | -5.033523 | 3.154967 | -0.438245 |
| 47 | 1 | 0 | -4.366678 | 4.725603 | 0.080133 |
| 48 | 1 | 0 | -3.604878 | 3.839525 | -1.267522 |

## 8. References

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