

Supporting Information For

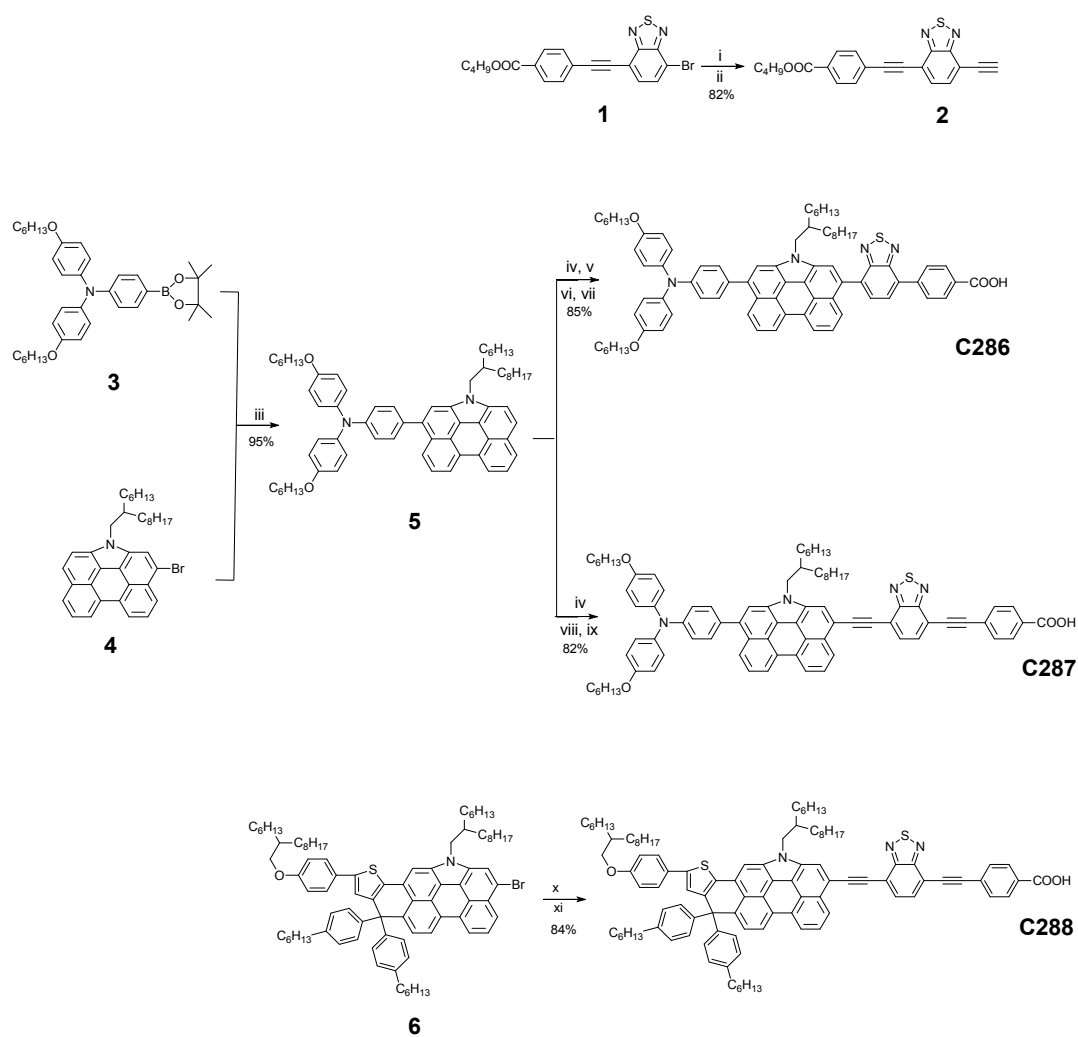
Improving the performance of dye-sensitized solar cells with electron-donor and electron-acceptor characteristic of planar electronic skeletons†

Yameng Ren,^{‡ab} Yang Li,^{‡ab} Shu Chen,^{ab} Jiao Liu,^{ab} Jing Zhang^a and Peng Wang^{*a}

^a State Key Laboratory of Polymer Physics and Chemistry, Changchun Institute of Applied Chemistry, Chinese Academy of Sciences, Changchun, 130022, China. E-mail: peng.wang@ciac.ac.cn; Fax: +86-431-85262953; Tel: +86-431-85262952

^b University of Chinese Academy of Sciences, Beijing, 100049, China

‡ These authors contributed equally to this work.



Scheme S1 Synthetic routes to dyes **C286**, **C287**, and **C288**. Reagents and conditions: (i) (triisopropylsilyl)acetylene, $\text{Pd}(\text{PPh}_3)_2\text{Cl}_2$, PPh_3 , CuI , diisopropylamine, toluene, 80 °C, overnight; (ii) tetra-*n*-butylammonium fluoride, CH_2Cl_2 , RT, 3 h; (iii) $\text{Pd}(\text{OAc})_2$, Sphos, K_3PO_4 , dioxane/ H_2O (v/v, 5/1), reflux, 8 h; (iv) NBS, THF, 0 °C, 0.5 h; (v) *n*-BuLi, THF, -78 °C, 3 h; then Me_3SnCl , -78 °C to RT, 12 h; (vi) butyl 4-(7-bromobenzo[*c*][1,2,5]thiadiazol-4-yl)benzoate, $\text{Pd}_2(\text{dba})_3$, $\text{P}(t\text{-Bu})_3$, CsF, dioxane, reflux, 6 h; (vii) KOH, THF/ H_2O (v/v, 3/1), reflux, 8 h; then phosphoric acid; (viii) **2**, $\text{Pd}_2(\text{dba})_3$, $\text{P}(t\text{-Bu})_3$, Cs_2CO_3 , dioxane, reflux, 5 h; (ix) KOH, THF/ H_2O (v/v, 3/1), reflux, 6 h; then phosphoric acid. (x) **2**, $\text{Pd}_2(\text{dba})_3$, $\text{P}(t\text{-Bu})_3$, Cs_2CO_3 , dioxane, reflux, 5 h; (xi) KOH, THF/ H_2O (v/v, 3/1), reflux, 8 h; then phosphoric acid.

Table S1 Theoretical energy gaps, maximum absorption wavelengths, and transition assignments of **C286**, **C287**, and **C288** ^a

Dye	$\Delta E_{L/H}^{B3LYP}$ [eV]	$\Delta E_{L/H-1}^{B3LYP}$ [eV]	$\Delta E_{L/H-3}^{B3LYP}$ [eV]	$\Delta E_{L+1/H}^{B3LYP}$ [eV]	$\lambda_{ABS,MAX}^{TD-MPW1K}$ [nm]	Transition
C286	2.17	2.55	3.65	/	492	H→L (80.1%); H-1→L (17.3%); H-3→L (2.6%)
C287	1.85	2.21	3.03	2.74	570	H→L (80.0%); H-1→L (14.2%); H-3→L (2.9%); H→L+1 (2.9%)
C288	1.87	2.72	/	2.62	600	H→L (91.0%); H-1→L (3.6%); H→L+1 (5.4%)

^a H and L stand for HOMO and LUMO. Energy gaps $\Delta E_{L/H}^{B3LYP}$, $\Delta E_{L/H-1}^{B3LYP}$, $\Delta E_{L/H-3}^{B3LYP}$, and $\Delta E_{L+1/H}^{B3LYP}$ were computed at the B3LYP/6-311G(d,p) level of theory for a dye molecule in THF. Maximum absorption wavelength ($\lambda_{ABS,MAX}^{TD-MPW1K}$) was calculated at the TD-MPW1K/6-311G(d,p) level of theory for a dye molecule in THF

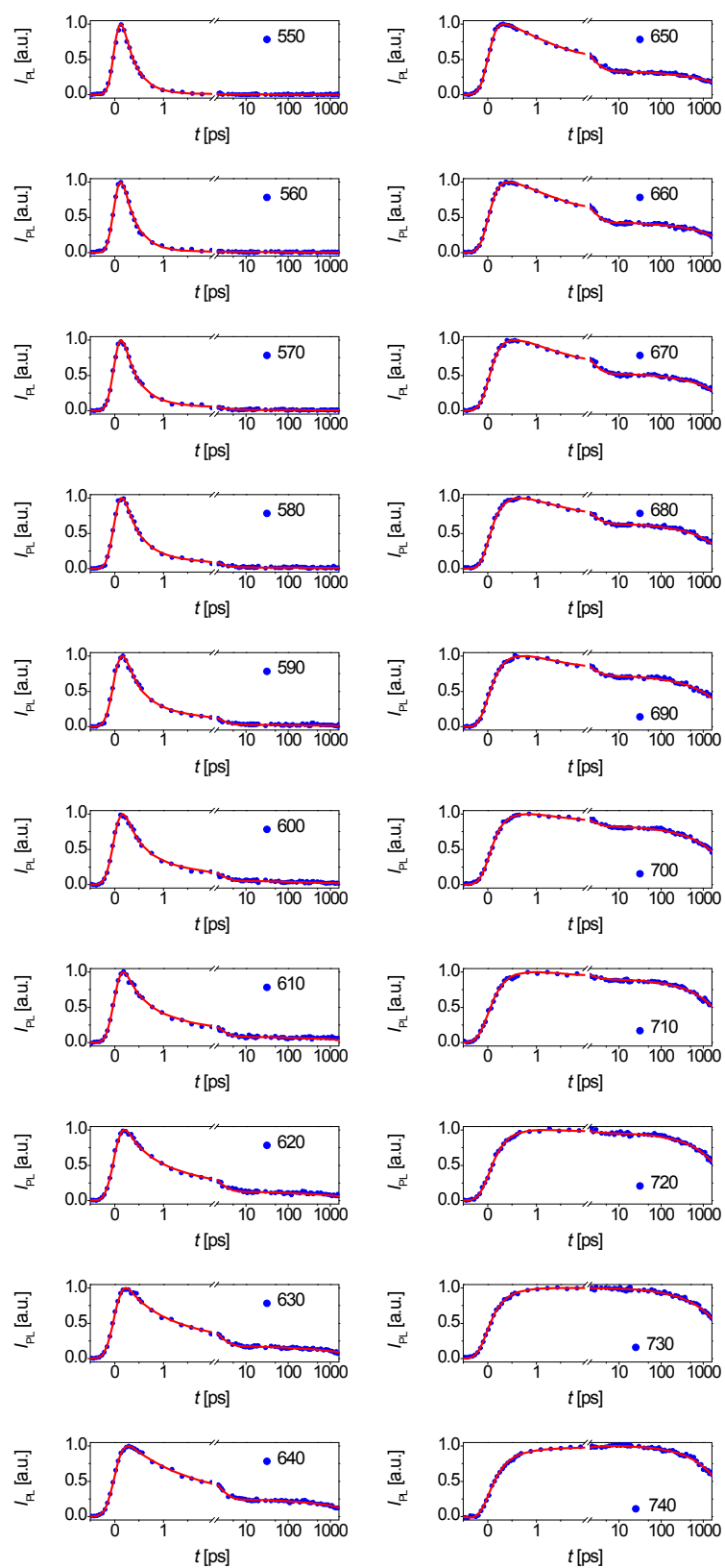


Fig. S1 Up-converted PL traces (blue dots) of **C286** in THF (150 μM) probed at a series of wavelengths. The red solid lines are fittings via eqn. 2. Excitation wavelength: 490 nm; power fluence: 13 $\mu\text{J cm}^{-2}$; gate wavelength: 800 nm.

Table S2 Time constants and amplitudes of up-converted PL traces for **C286** in THF derived from Fig. S1

λ [nm]	A_1	τ_1 [ps]	A_2	τ_2 [ps]	A_3	τ_3 [ps]	A_4	τ_4 [ps]	$\bar{\tau}$ [ps]
550	0.987±0.025	0.27±0.01	0.012±0.001	1.4±0.2	0.001±0.0001	107±3.1	0	3177±51	0.4±0.03
560	0.985±0.025	0.27±0.01	0.012±0.001	1.4±0.2	0.002±0.0001	107±3.1	0.001±0.0001	3177±51	3.7±0.4
570	0.909±0.025	0.27±0.01	0.086±0.001	1.4±0.2	0.002±0.0001	107±3.1	0.003±0.0001	3177±51	10.1±0.5
580	0.846±0.021	0.27±0.01	0.146±0.002	1.4±0.2	0.003±0.0001	107±3.1	0.005±0.0001	3177±51	16.6±0.7
590	0.784±0.021	0.27±0.01	0.203±0.006	1.4±0.2	0.005±0.0001	107±3.1	0.008±0.0001	3177±51	26.4±0.9
600	0.714±0.020	0.27±0.01	0.261±0.010	1.4±0.2	0.01±0.001	107±3.1	0.015±0.001	3177±51	49.3±3.9
610	0.607±0.020	0.27±0.01	0.347±0.011	1.4±0.2	0.011±0.001	107±3.1	0.035±0.001	3177±51	113.0±5.3
620	0.474±0.020	0.27±0.01	0.452±0.015	1.4±0.2	0.015±0.001	107±3.1	0.059±0.002	3177±51	189.8±9.8
630	0.339±0.015	0.27±0.01	0.549±0.015	1.4±0.2	0.018±0.001	107±3.1	0.094±0.002	3177±51	301.4±11.6
640	0.033±0.001	0.27±0.01	0.775±0.015	1.4±0.2	0.023±0.001	107±3.1	0.169±0.005	3177±51	540.5±25.1
650	-0.041±0.001	0.27±0.01	0.752±0.018	1.4±0.2	0.024±0.001	107±3.1	0.224±0.005	3177±51	715.3±27.9
660	-0.065±0.001	0.27±0.01	0.695±0.015	1.4±0.2	0.024±0.001	107±3.1	0.281±0.011	3177±51	896.3±50.2
670	-0.152±0.002	0.27±0.01	0.631±0.015	1.4±0.2	0.031±0.001	107±3.1	0.338±0.011	3177±51	1078.0±53.1
680	-0.181±0.002	0.27±0.01	0.545±0.012	1.4±0.2	0.033±0.001	107±3.1	0.422±0.015	3177±51	1345.0±70.3
690	-0.21±0.011	0.27±0.01	0.487±0.012	1.4±0.2	0.038±0.001	107±3.1	0.475±0.015	3177±51	1513.8±73.1
700	-0.235±0.011	0.27±0.01	0.328±0.011	1.4±0.2	0.042±0.001	107±3.1	0.63±0.015	3177±51	2006.5±80.8
710	-0.26±0.011	0.27±0.01	0.249±0.011	1.4±0.2	0.042±0.001	107±3.1	0.709±0.025	3177±51	2257.3±117.2
720	-0.28±0.012	0.27±0.01	0.127±0.005	1.4±0.2	0.04±0.001	107±3.1	0.833±0.026	3177±51	2650.9±126.7
730	-0.286±0.012	0.27±0.01	0.016±0.001	1.4±0.2	0.039±0.001	107±3.1	0.945±0.026	3177±51	3006.5±132.3
740	-0.3±0.012	0.27±0.01	-0.112±0.005	1.4±0.2	0.038±0.001	107±3.1	0.962±0.027	3177±51	3060.3±136.5

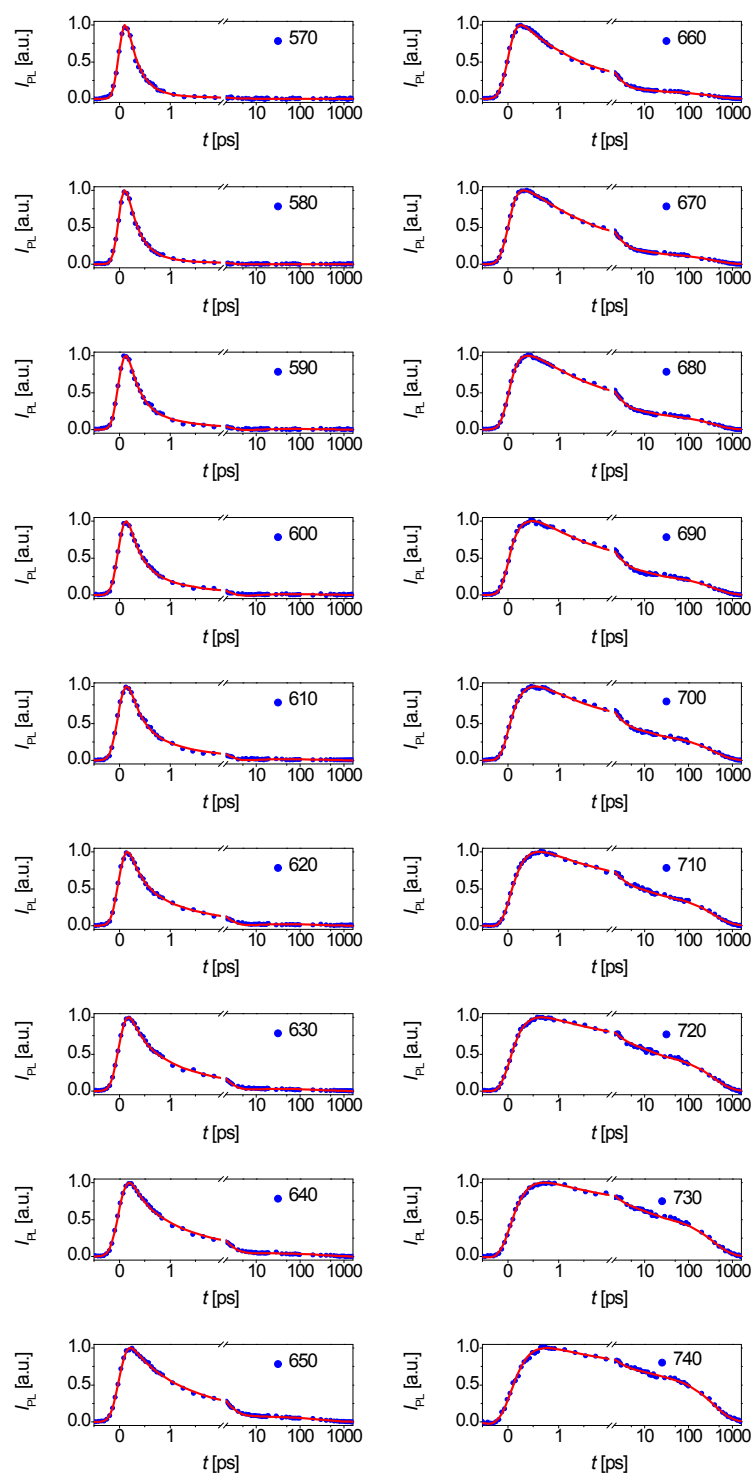


Fig. S2 Up-converted PL traces (blue dots) of **C287** in THF (150 μ M) probed at a series of wavelengths. The red solid lines are fittings via eqn. 2. Excitation wavelength: 490 nm; power fluence: 13 μ J cm⁻²; gate wavelength: 800 nm.

Table S3 Time constants and amplitudes of up-converted PL traces for **C287** in THF derived from Fig. S2

λ [nm]	A_1	τ_1 [ps]	A_2	τ_2 [ps]	A_3	τ_3 [ps]	A_4	τ_4 [ps]	$\bar{\tau}$ [ps]
570	0.966±0.020	0.25±0.02	0.031±0.001	1.2±0.1	0.003±0.0001	10±0.5	0	367±7.5	0.3±0.03
580	0.932±0.025	0.25±0.02	0.06±0.001	1.2±0.1	0.007±0.0001	10±0.5	0.001±0.0001	367±7.5	0.7±0.1
590	0.843±0.025	0.25±0.02	0.146±0.005	1.2±0.1	0.007±0.0002	10±0.5	0.004±0.0002	367±7.5	1.9±0.2
600	0.786±0.022	0.25±0.02	0.201±0.005	1.2±0.1	0.007±0.0002	10±0.5	0.006±0.0002	367±7.5	2.7±0.2
610	0.762±0.022	0.25±0.02	0.223±0.005	1.2±0.1	0.007±0.0002	10±0.5	0.008±0.0005	367±7.5	3.5±0.3
620	0.63±0.021	0.25±0.02	0.35±0.015	1.2±0.1	0.008±0.0002	10±0.5	0.012±0.0005	367±7.5	5.1±0.3
630	0.531±0.015	0.25±0.02	0.442±0.015	1.2±0.1	0.009±0.0002	10±0.5	0.018±0.001	367±7.5	7.4±0.5
640	0.458±0.015	0.25±0.02	0.506±0.015	1.2±0.1	0.011±0.0005	10±0.5	0.025±0.001	367±7.5	10.0±0.6
650	0.197±0.008	0.25±0.02	0.739±0.025	1.2±0.1	0.016±0.001	10±0.5	0.048±0.001	367±7.5	18.7±0.8
660	-0.097±0.002	0.25±0.02	0.877±0.025	1.2±0.1	0.043±0.001	10±0.5	0.08±0.002	367±7.5	30.8±1.5
670	-0.125±0.003	0.25±0.02	0.835±0.027	1.2±0.1	0.066±0.001	10±0.5	0.099±0.002	367±7.5	38.0±1.5
680	-0.145±0.005	0.25±0.02	0.784±0.025	1.2±0.1	0.083±0.001	10±0.5	0.133±0.005	367±7.5	50.6±2.9
690	-0.22±0.005	0.25±0.02	0.724±0.025	1.2±0.1	0.107±0.002	10±0.5	0.169±0.005	367±7.5	64.0±3.1
700	-0.265±0.015	0.25±0.02	0.677±0.025	1.2±0.1	0.109±0.002	10±0.5	0.214±0.015	367±7.5	80.4±7.2
710	-0.295±0.021	0.25±0.02	0.605±0.025	1.2±0.1	0.127±0.009	10±0.5	0.268±0.020	367±7.5	100.4±9.2
720	-0.312±0.021	0.25±0.02	0.495±0.023	1.2±0.1	0.164±0.009	10±0.5	0.341±0.021	367±7.5	127.4±9.8
730	-0.334±0.021	0.25±0.02	0.473±0.020	1.2±0.1	0.149±0.011	10±0.5	0.378±0.021	367±7.5	140.8±10.5
740	-0.36±0.021	0.25±0.02	0.459±0.020	1.2±0.1	0.064±0.002	10±0.5	0.477±0.025	367±7.5	176.2±12.6

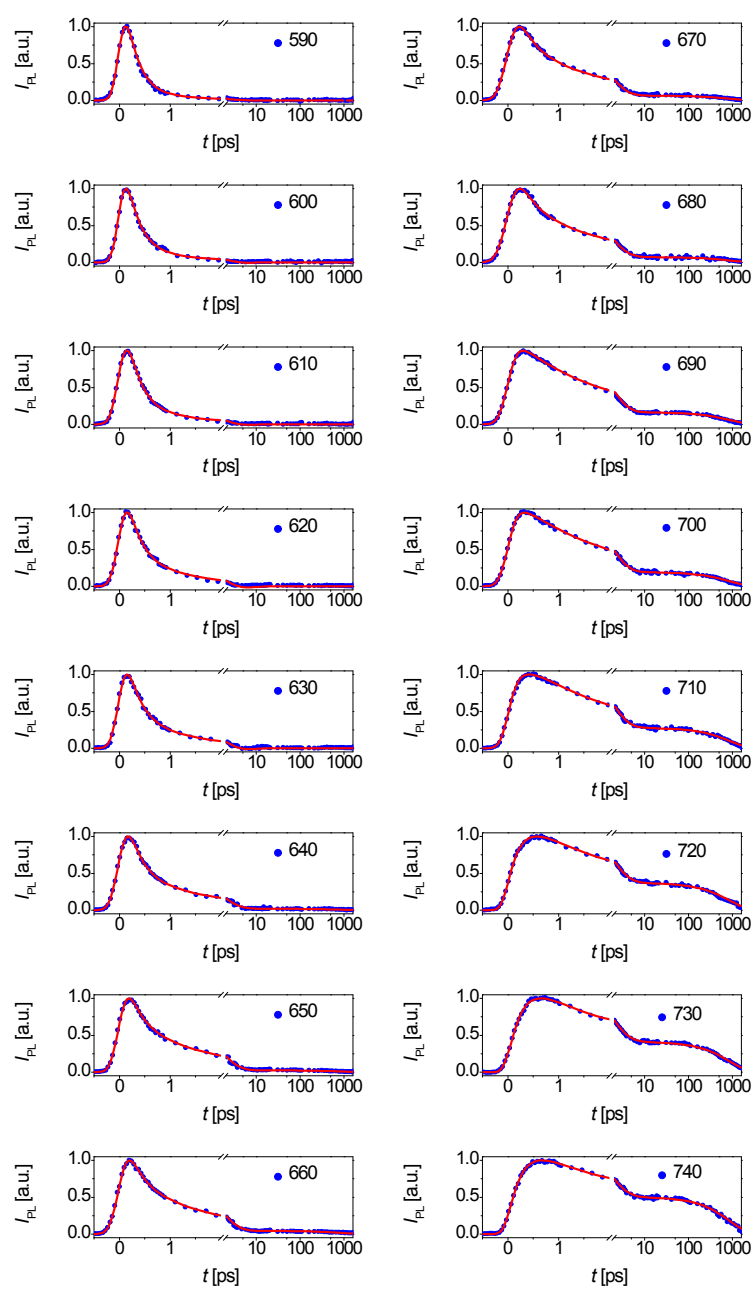


Fig. S3 Up-converted PL traces (blue dots) of **C288** in THF (150 μ M) probed at a series of wavelengths. The red solid lines are fittings via eqn. 2. Excitation wavelength: 490 nm; power fluence: 13 μ J cm⁻²; gate wavelength: 800 nm.

Table S4 Time constants and amplitudes of up-converted PL traces for **C288** in THF derived from Fig. S3

λ [nm]	A_1	τ_1 [ps]	A_2	τ_2 [ps]	A_3	τ_3 [ps]	A_4	τ_4 [ps]	$\bar{\tau}$ [ps]
590	0.961±0.025	0.26±0.01	0.039±0.001	1.5±0.1	0	5±0.3	0	842±9.2	0.3±0.03
600	0.899±0.025	0.26±0.01	0.099±0.002	1.5±0.1	0.002±0.0001	5±0.3	0	842±9.2	0.4±0.02
610	0.877±0.025	0.26±0.01	0.117±0.005	1.5±0.1	0.004±0.0001	5±0.3	0.002±0.0001	842±9.2	2.1±0.2
620	0.772±0.025	0.26±0.01	0.221±0.005	1.5±0.1	0.004±0.0001	5±0.3	0.003±0.0001	842±9.2	3.1±0.1
630	0.757±0.025	0.26±0.01	0.233±0.005	1.5±0.1	0.004±0.0001	5±0.3	0.006±0.0002	842±9.2	5.6±0.3
640	0.74±0.021	0.26±0.01	0.247±0.011	1.5±0.1	0.005±0.0002	5±0.3	0.008±0.0002	842±9.2	7.3±0.3
650	0.584±0.015	0.26±0.01	0.399±0.012	1.5±0.1	0.005±0.0002	5±0.3	0.012±0.0005	842±9.2	10.9±0.6
660	0.560±0.015	0.26±0.01	0.411±0.015	1.5±0.1	0.006±0.0002	5±0.3	0.023±0.001	842±9.2	20.2±1.1
670	0.538±0.015	0.26±0.01	0.422±0.015	1.5±0.1	0.007±0.0002	5±0.3	0.033±0.001	842±9.2	28.6±1.2
680	0.511±0.012	0.26±0.01	0.443±0.015	1.5±0.1	0.01±0.0002	5±0.3	0.036±0.001	842±9.2	31.2±1.2
690	-0.04±0.0001	0.26±0.01	0.86±0.025	1.5±0.1	0.015±0.0005	5±0.3	0.125±0.005	842±9.2	106.6±5.6
700	-0.08±0.0001	0.26±0.01	0.838±0.026	1.5±0.1	0.02±0.0005	5±0.3	0.142±0.005	842±9.2	120.9±5.7
710	-0.12±0.001	0.26±0.01	0.78±0.025	1.5±0.1	0.028±0.001	5±0.3	0.192±0.011	842±9.2	163.0±11.2
720	-0.163±0.005	0.26±0.01	0.72±0.025	1.5±0.1	0.037±0.001	5±0.3	0.243±0.015	842±9.2	205.9±15.0
730	-0.21±0.005	0.26±0.01	0.705±0.025	1.5±0.1	0.035±0.001	5±0.3	0.26±0.015	842±9.2	220.2±15.2
740	-0.256±0.015	0.26±0.01	0.64±0.015	1.5±0.1	0.026±0.001	5±0.3	0.334±0.015	842±9.2	282.3±15.9

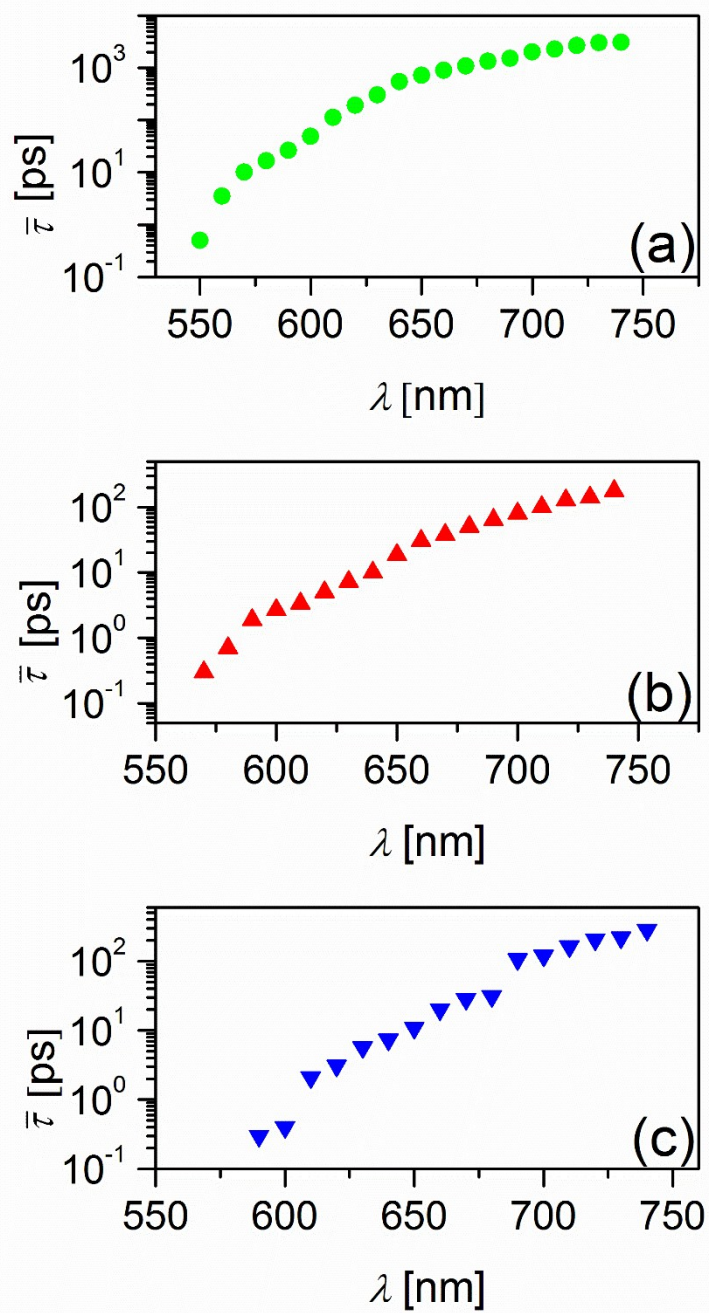


Fig. S4 The average lifetimes ($\bar{\tau}$) at different PL wavelengths for dyes in THF: a) C286, b) C287, and c) C288.

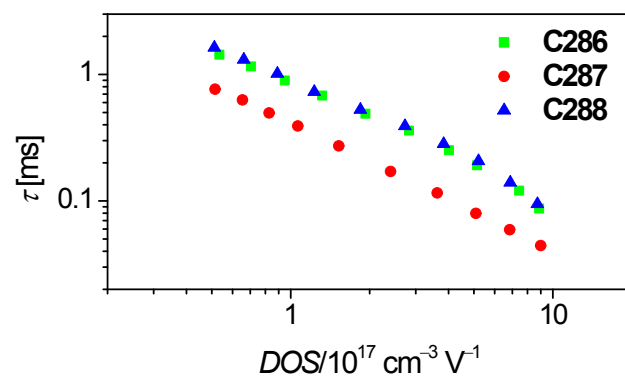


Fig. S5 The electron lifetime as a function of density of states (DOS) derived from IS measurements.

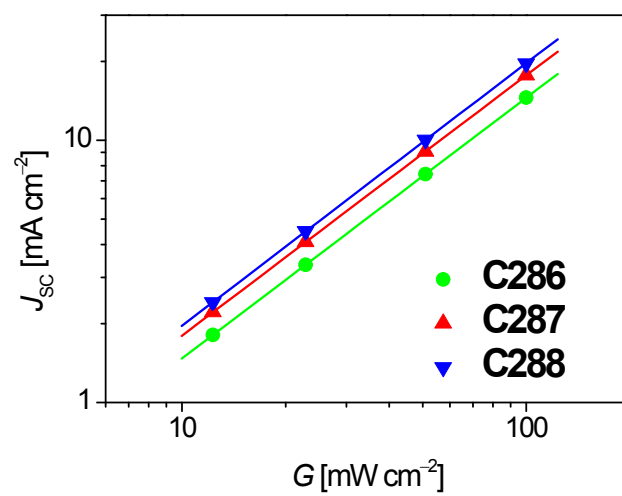


Fig. S6 Plots of short-circuit photocurrent density (J_{sc}) as a function of irradiance (G). A power function $J_{sc} \propto G^\alpha$ was used to fit the experimental data. The obtained α values are 0.994 for **C286**, 0.993 for **C287**, and 1.001 for **C288**, respectively.

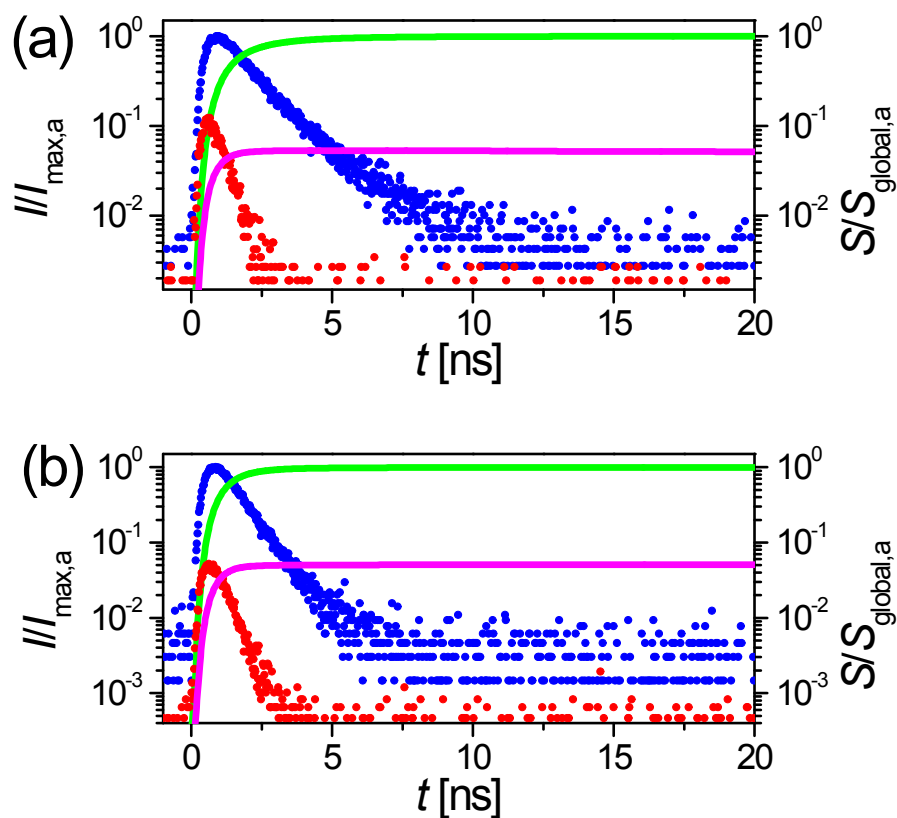


Fig. S7 PL decay traces of dye-grafted alumina (blue line) and titania (red line) films immersed in a cobalt electrolyte: (a) **C287** and (b) **C288**. The PL intensity (I) was corrected in term of the absorbance at 482 nm and further normalized with respect to the PL maximum of a corresponding dye-grafted alumina film ($I_{\max,a}$). The PL integral areas (S) of the alumina (green line) and titania (magenta line) films were normalized with respect to the global PL integral area ($S_{\text{global},a}$) of a corresponding dye-grafted alumina film. Excitation wavelength: 482 nm; probe wavelength: 800 nm.

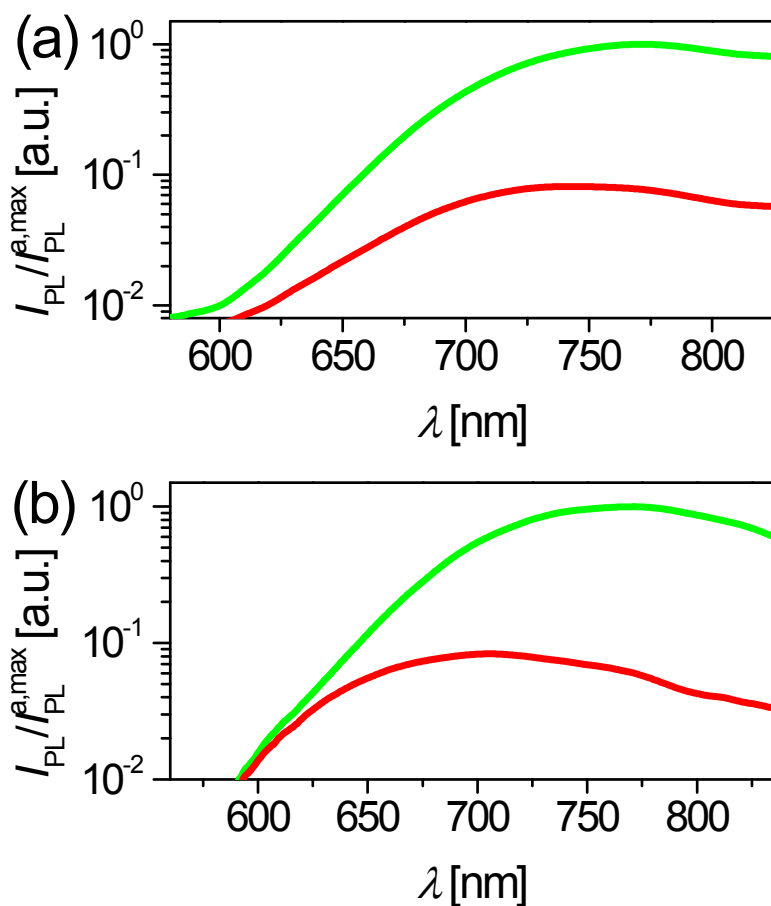


Fig. S8 (a) PL spectra of **C287** grafted on alumina (green line) and titania (red line) films immersed in a cobalt electrolyte using TCSPC technique, Excitation wavelength: 482 nm. The PL intensity was corrected in term of the absorbance at 482 nm and further normalized with respect to the PL maximum of a corresponding dye-grafted alumina film. (b) PL spectra of **C288** grafted on alumina (green line) and titania (red line) films immersed in a cobalt electrolyte using TCSPC technique, Excitation wavelength: 482 nm. The PL intensity was corrected in term of the absorbance at 482 nm and further normalized with respect to the PL maximum of a corresponding dye-grafted alumina film.

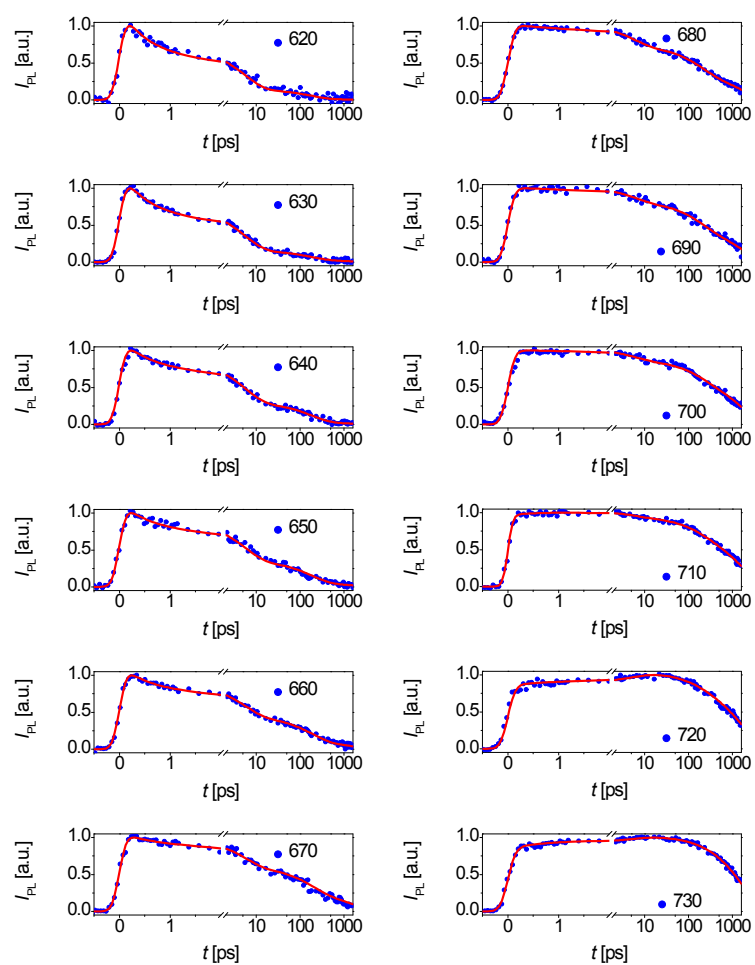


Fig. S9 Up-converted PL traces (blue dots) of **C286** grafted on alumina. The red solid lines are fittings via eqn. 2. Excitation wavelength: 490 nm; power fluence: $13 \mu\text{J cm}^{-2}$; gate wavelength: 800 nm.

Table S5 Time constants and amplitudes of up-converted PL traces for **C286** grafted on alumina derived from Fig. S9

λ [nm]	A_1	τ_1 [ps]	A_2	τ_2 [ps]	A_3	τ_3 [ps]	A_4	τ_4 [ps]	$\bar{\tau}$ [ps]
620	0.48±0.008	0.52±0.03	0.412±0.006	5.8±0.12	0.101±0.002	180±3.2	0.007±0.0001	1710±24.5	32.8±0.1
630	0.447±0.004	0.52±0.03	0.43±0.005	5.8±0.12	0.103±0.001	180±3.2	0.02±0.003	1710±24.5	55.5±3.4
640	0.292±0.009	0.52±0.03	0.46±0.009	5.8±0.12	0.228±0.004	180±3.2	0.02±0.001	1710±24.5	78.1±0.8
650	0.262±0.008	0.52±0.03	0.427±0.012	5.8±0.012	0.254±0.003	180±3.2	0.057±0.003	1710±24.5	145.8±12.3
660	0.255±0.011	0.52±0.03	0.365±0.008	5.8±0.012	0.295±0.003	180±3.2	0.085±0.009	1710±24.5	200.7±16.9
670	0.1±0.004	0.52±0.03	0.346±0.013	5.8±0.012	0.326±0.005	180±3.2	0.228±0.011	1710±24.5	450.6±24.6
680	0.011±0.004	0.52±0.03	0.282±0.011	5.8±0.012	0.364±0.007	180±3.2	0.343±0.02	1710±24.5	653.7±43.9
690	-0.012±0.008	0.52±0.03	0.207±0.004	5.8±0.012	0.35±0.011	180±3.2	0.443±0.031	1710±24.5	821.7±61.4
700	-0.026±0.007	0.52±0.03	0.154±0.013	5.8±0.012	0.256±0.009	180±3.2	0.59±0.015	1710±24.5	1055.9±42
710	-0.062±0.012	0.52±0.03	0.083±0.007	5.8±0.012	0.228±0.012	180±3.2	0.689±0.022	1710±24.5	1219.7±40.2
720	-0.083±0.008	0.52±0.03	-0.134±0.003	5.8±0.012	0.184±0.007	180±3.2	0.816±0.035	1710±24.5	1428.5±82.6
730	-0.111±0.004	0.52±0.03	-0.182±0.008	5.8±0.012	0.063±0.003	180±3.2	0.937±0.08	1710±24.5	1613.6±19.6

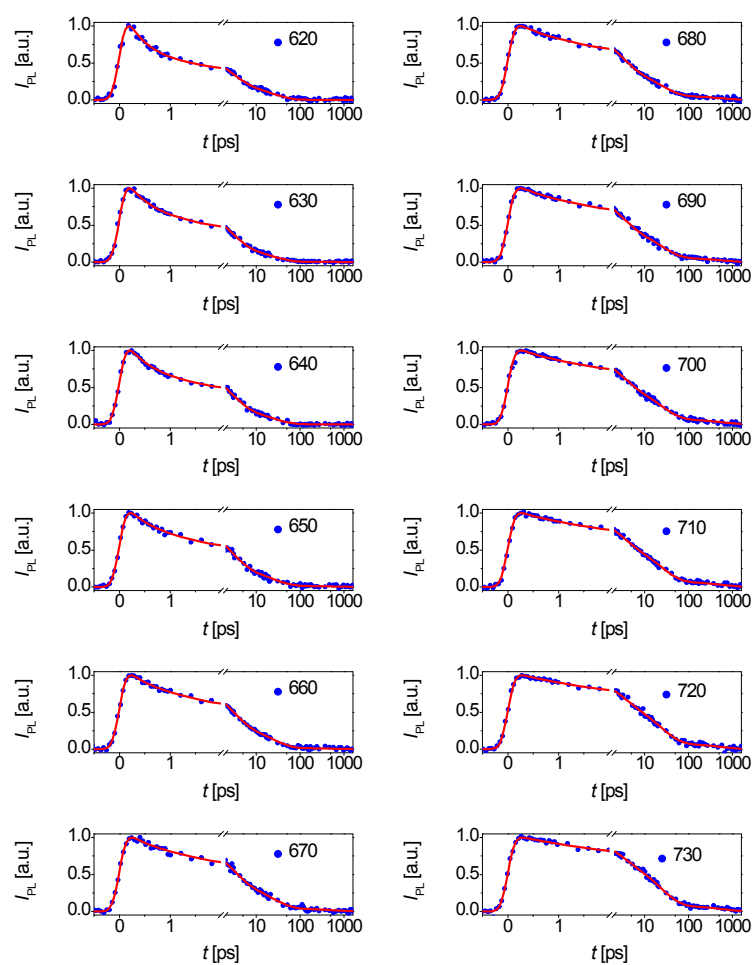


Fig. S10 Up-converted PL traces (blue dots) of **C286** grafted on titania. The red solid lines are fittings via eqn. 2. Excitation wavelength: 490 nm; power fluence: $13 \mu\text{J cm}^{-2}$; gate wavelength: 800 nm.

Table S6 Time constants and amplitudes of up-converted PL traces for **C286** grafted on titania derived from Fig. S10

λ [nm]	A_1	τ_1 [ps]	A_2	τ_2 [ps]	A_3	τ_3 [ps]	A_4	τ_4 [ps]	$\bar{\tau}$ [ps]
620	0.51±0.01	0.38±0.015	0.329±0.007	2.7±0.08	0.16±0.005	24±1.3	0.001±0.0001	520±15.6	5.4±0.7
630	0.379±0.007	0.38±0.015	0.455±0.008	2.7±0.08	0.163±0.007	24±1.3	0.003±0.0001	520±15.6	6.8±0.9
640	0.359±0.006	0.38±0.015	0.468±0.007	2.7±0.08	0.168±0.003	24±1.3	0.0051±0.0002	520±15.6	8.0±0.9
650	0.261±0.009	0.38±0.015	0.52±0.009	2.7±0.08	0.207±0.005	24±1.3	0.0121±0.001	520±15.6	12.7±0.8
660	0.18±0.002	0.38±0.015	0.533±0.008	2.7±0.08	0.274±0.007	24±1.3	0.0131±0.001	520±15.6	14.8±0.6
670	0.117±0.003	0.38±0.015	0.525±0.011	2.7±0.08	0.322±0.004	24±1.3	0.0361±0.002	520±15.6	27.9±0.2
680	0.095±0.004	0.38±0.015	0.514±0.013	2.7±0.08	0.341±0.008	24±1.3	0.051±0.001	520±15.6	35.6±1.1
690	0.077±0.001	0.38±0.015	0.481±0.009	2.7±0.08	0.388±0.010	24±1.3	0.0541±0.003	520±15.6	38.7±0.5
700	0.056±0.002	0.38±0.015	0.429±0.011	2.7±0.08	0.448±0.013	24±1.3	0.0671±0.002	520±15.6	46.8±0.9
710	0.039±0.002	0.38±0.015	0.392±0.007	2.7±0.08	0.5±0.012	24±1.3	0.0691±0.001	520±15.6	49.0±1.0
720	0.02±0.001	0.38±0.015	0.353±0.010	2.7±0.08	0.554±0.015	24±1.3	0.0731±0.003	520±15.6	52.2±1.5
730	0.011±0.001	0.38±0.015	0.311±0.009	2.7±0.08	0.602±0.019	24±1.3	0.0761±0.002	520±15.6	54.8±1.8

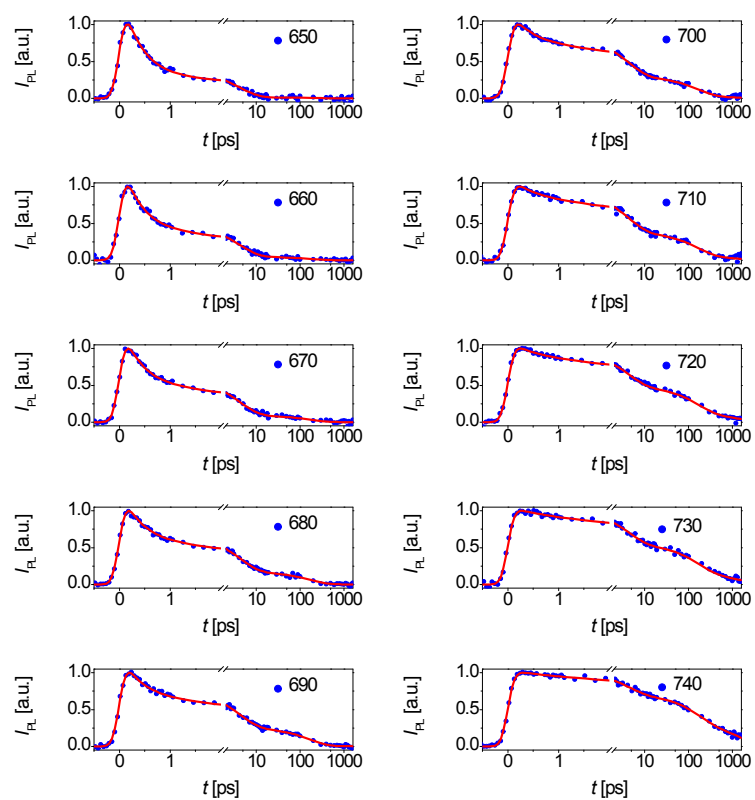


Fig. S11 Up-converted PL traces (blue dots) of **C287** grafted on alumina. The red solid lines are fittings via eqn. 2. Excitation wavelength: 490 nm, power fluence: $13 \mu\text{J cm}^{-2}$, gate wavelength: 800 nm.

Table S7 Time constants and amplitudes of up-converted PL traces for **C287** grafted on alumina derived from Fig. S11

λ [nm]	A_1	τ_1 [ps]	A_2	τ_2 [ps]	A_3	τ_3 [ps]	A_4	τ_4 [ps]	$\bar{\tau}$ [ps]
650	0.77±0.021	0.36±0.018	0.222±0.015	4.3±0.22	0.008±0.001	165±6.25	0	1595±125.1	2.6±0.1
660	0.688±0.013	0.36±0.018	0.281±0.011	4.3±0.22	0.031±0.002	165±6.25	0	1595±125.1	6.6±0.5
670	0.599±0.018	0.36±0.018	0.337±0.009	4.3±0.22	0.064±0.001	165±6.25	0	1595±125.1	12.2±1.1
680	0.517±0.009	0.36±0.018	0.359±0.012	4.3±0.22	0.124±0.008	165±6.25	0	1595±125.1	22.2±0.4
690	0.433±0.011	0.36±0.018	0.375±0.008	4.3±0.22	0.189±0.013	165±6.25	0.003±0.0001	1595±125.1	37.7±2.1
700	0.338±0.007	0.36±0.018	0.427±0.021	4.3±0.22	0.218±0.015	165±6.25	0.017±0.001	1595±125.1	65.0±5.9
710	0.197±0.008	0.36±0.018	0.477±0.018	4.3±0.22	0.283±0.018	165±6.25	0.043±0.002	1595±125.1	117.4±11.6
720	0.143±0.007	0.36±0.018	0.424±0.009	4.3±0.22	0.333±0.011	165±6.25	0.1±0.004	1595±125.1	216.3±21.5
730	0.054±0.011	0.36±0.018	0.416±0.011	4.3±0.22	0.381±0.023	165±6.25	0.149±0.001	1595±125.1	302.3±24.9
740	0.014±0.006	0.36±0.018	0.306±0.008	4.3±0.22	0.375±0.018	165±6.25	0.305±0.005	1595±125.1	549.7±50.8

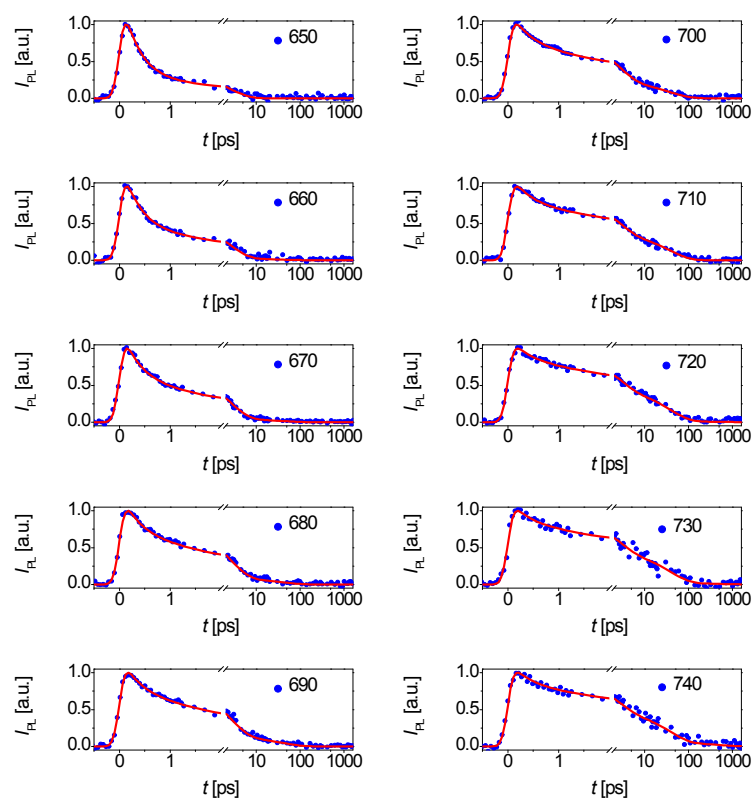


Fig. S12 Up-converted PL traces (blue dots) of **C287** grafted on titania. The red solid lines are fittings via eqn. 2. Excitation wavelength: 490 nm, power fluence: $13 \mu\text{J cm}^{-2}$, gate wavelength: 800 nm.

Table S8 Time constants and amplitudes of up-converted PL traces for **C287** grafted on titania derived from Fig. S12

λ [nm]	A_1	τ_1 [ps]	A_2	τ_2 [ps]	A_3	τ_3 [ps]	A_4	τ_4 [ps]	$\bar{\tau}$ [ps]
650	0.794±0.051	0.32±0.017	0.206±0.008	2.6±0.14	0	39±2.8	0	543±21.2	0.8±0.1
660	0.654±0.032	0.32±0.017	0.331±0.009	2.6±0.14	0.015±0.001	39±2.8	0	543±21.2	1.7±0.1
670	0.536±0.021	0.32±0.017	0.435±0.013	2.6±0.14	0.029±0.001	39±2.8	0	543±21.2	2.4±0.1
680	0.413±0.031	0.32±0.017	0.527±0.008	2.6±0.14	0.06±0.003	39±2.8	0	543±21.2	3.8±0.3
690	0.36±0.015	0.32±0.017	0.54±0.021	2.6±0.14	0.1±0.005	39±2.8	0	543±21.2	5.4±0.5
700	0.354±0.018	0.32±0.017	0.474±0.017	2.6±0.14	0.172±0.01	39±2.8	0	543±21.2	8.1±0.8
710	0.32±0.023	0.32±0.017	0.4±0.013	2.6±0.14	0.28±0.011	39±2.8	0	543±21.2	12.1±1.0
720	0.249±0.014	0.32±0.017	0.395±0.010	2.6±0.14	0.348±0.024	39±2.8	0.008±0.000	543±21.2	19.0±1.1
730	0.244±0.013	0.32±0.017	0.392±0.008	2.6±0.14	0.348±0.019	39±2.8	0.016±0.001	543±21.2	23.4±1.5
740	0.243±0.021	0.32±0.017	0.37±0.011	2.6±0.14	0.347±0.025	39±2.8	0.04±0.002	543±21.2	36.3±2.9

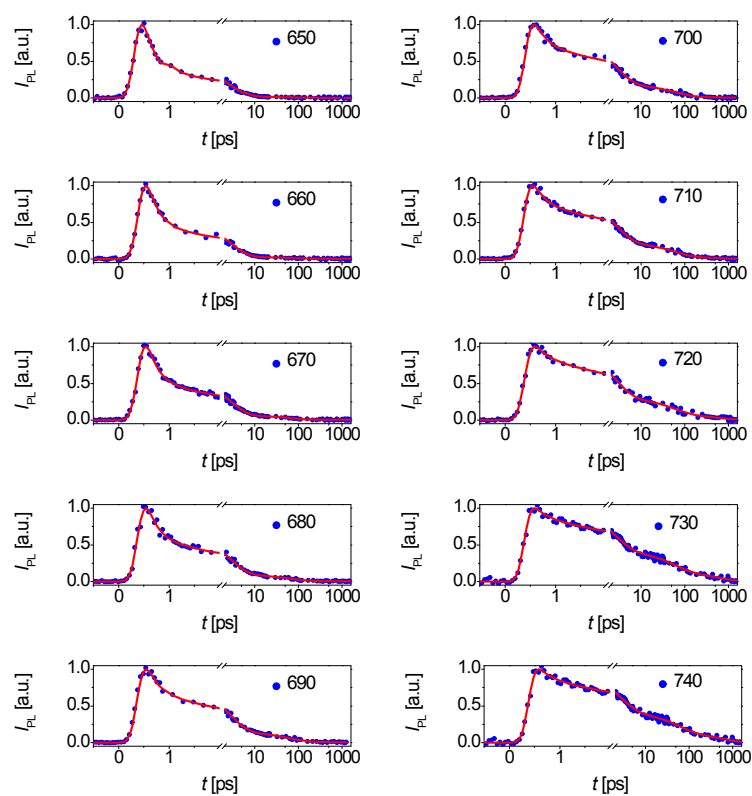


Fig. S13 Up-converted PL traces (blue dots) of **C288** grafted on alumina. The red solid lines are fittings via eqn. 2. Excitation wavelength: 490 nm; power fluence: $13 \mu\text{J cm}^{-2}$; gate wavelength: 800 nm.

Table S9 Time constants and amplitudes of up-converted PL traces for **C288** grafted on alumina derived from Fig. S13

λ [nm]	A_1	τ_1 [ps]	A_2	τ_2 [ps]	A_3	τ_3 [ps]	A_4	τ_4 [ps]	$\bar{\tau}$ [ps]
650	0.826±0.021	0.2±0.001	0.162±0.007	2.5±0.01	0.012±0.0007	60±0.4	0	645±3.5	1.3±0.06
660	0.764±0.021	0.2±0.001	0.214±0.007	2.5±0.01	0.021±0.001	60±0.4	0.001±0.0001	645±3.5	2.6±0.15
670	0.733±0.017	0.2±0.001	0.236±0.011	2.5±0.01	0.028±0.001	60±0.4	0.003±0.0001	645±3.5	4.4±0.13
680	0.682±0.017	0.2±0.001	0.268±0.011	2.5±0.01	0.046±0.001	60±0.4	0.004±0.0001	645±3.5	6.1±0.24
690	0.584±0.015	0.2±0.001	0.337±0.012	2.5±0.01	0.072±0.001	60±0.4	0.007±0.0001	645±3.5	9.8±0.21
700	0.536±0.015	0.2±0.001	0.356±0.012	2.5±0.01	0.098±0.002	60±0.4	0.01±0.0001	645±3.5	13.3±0.32
710	0.494±0.011	0.2±0.001	0.36±0.013	2.5±0.01	0.124±0.002	60±0.4	0.022±0.001	645±3.5	22.6±1.61
720	0.37±0.011	0.2±0.001	0.428±0.013	2.5±0.01	0.151±0.003	60±0.4	0.051±0.001	645±3.5	43.1±1.75
730	0.363±0.010	0.2±0.001	0.426±0.017	2.5±0.01	0.152±0.003	60±0.4	0.059±0.001	645±3.5	48.3±1.79
740	0.328±0.010	0.2±0.001	0.367±0.016	2.5±0.01	0.212±0.007	60±0.4	0.093±0.002	645±3.5	73.7±2.16

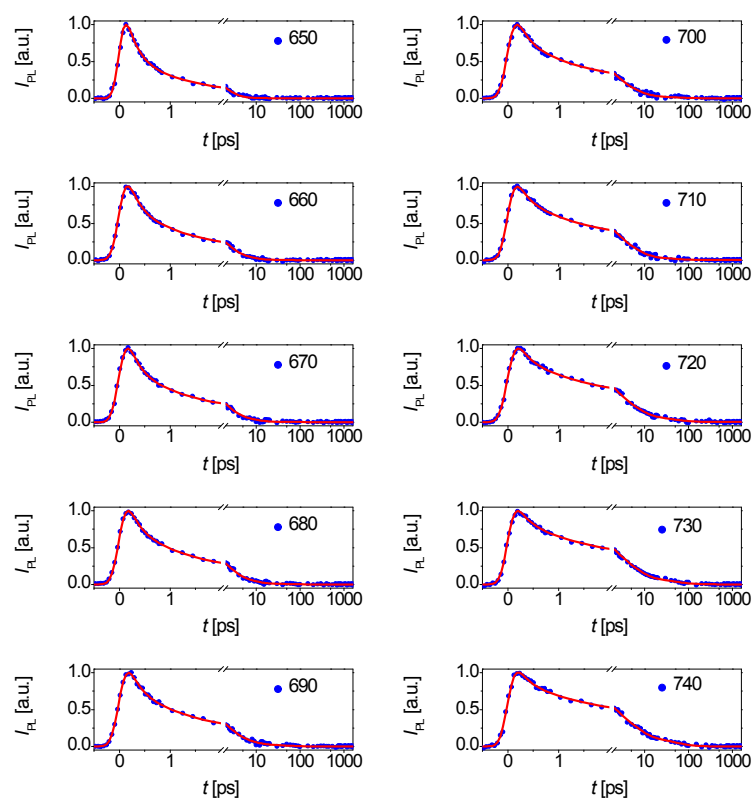


Fig. S14 Up-converted PL traces (blue dots) of **C288** grafted on titania. The red solid lines are fittings via eqn. 2. Excitation wavelength: 490 nm; power fluence: $13 \mu\text{J cm}^{-2}$; gate wavelength: 800 nm.

Table S10 Time constants and amplitudes of up-converted PL traces for **C288** grafted on titania derived from Fig. S14

λ [nm]	A_1	τ_1 [ps]	A_2	τ_2 [ps]	A_3	τ_3 [ps]	A_4	τ_4 [ps]	$\bar{\tau}$ [ps]
650	0.656±0.016	0.22±0.002	0.33±0.006	1.3±0.03	0.014±0.0001	5.2±0.2	0	50±0.4	0.6±0.06
660	0.588±0.016	0.22±0.002	0.331±0.009	1.3±0.03	0.079±0.001	5.2±0.2	0.002±0.0001	50±0.4	1.1±0.02
670	0.575±0.014	0.22±0.002	0.337±0.009	1.3±0.03	0.083±0.001	5.2±0.2	0.005±0.0001	50±0.4	1.2±0.09
680	0.519±0.014	0.22±0.002	0.359±0.011	1.3±0.03	0.115±0.002	5.2±0.2	0.007±0.0001	50±0.4	1.5±0.09
690	0.514±0.013	0.22±0.002	0.352±0.011	1.3±0.03	0.118±0.003	5.2±0.2	0.016±0.001	50±0.4	2.0±0.06
700	0.508±0.013	0.22±0.002	0.312±0.016	1.3±0.03	0.161±0.006	5.2±0.2	0.019±0.001	50±0.4	2.3±0.11
710	0.439±0.016	0.22±0.002	0.3±0.015	1.3±0.03	0.235±0.011	5.2±0.2	0.026±0.001	50±0.4	3.0±0.16
720	0.408±0.015	0.22±0.002	0.277±0.016	1.3±0.03	0.259±0.016	5.2±0.2	0.056±0.001	50±0.4	4.6±0.19
730	0.388±0.016	0.22±0.002	0.262±0.013	1.3±0.03	0.286±0.014	5.2±0.2	0.064±0.001	50±0.4	5.1±0.20
740	0.364±0.014	0.22±0.002	0.236±0.016	1.3±0.03	0.305±0.016	5.2±0.2	0.095±0.001	50±0.4	6.7±0.24

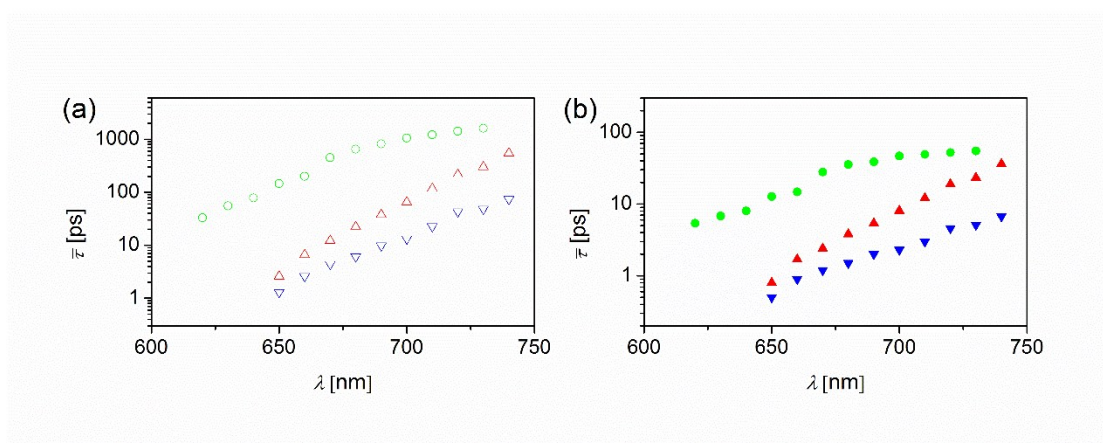


Fig. S15 The average lifetimes ($\bar{\tau}$) at different PL wavelengths for dyes on alumina (panel a): **C286** (green), **C287** (red), and **C288** (blue), and for dyes on titania (panel b): **C286** (green), **C287** (red), and **C288** (blue).

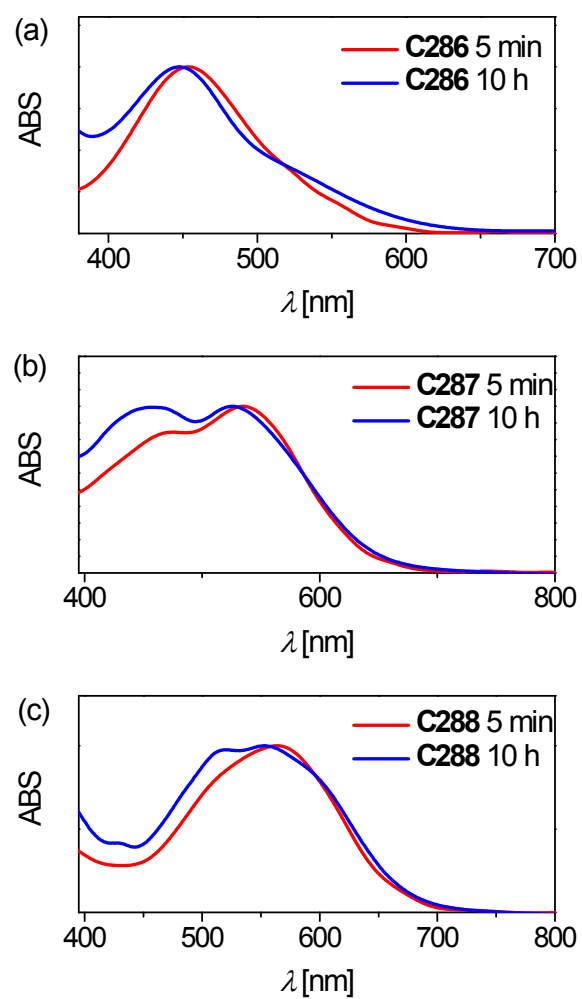


Fig. S16 Normalized absorption spectra of (a) C286, (b) C287, or (c) C288 grated on a titania film with different dyeing times.

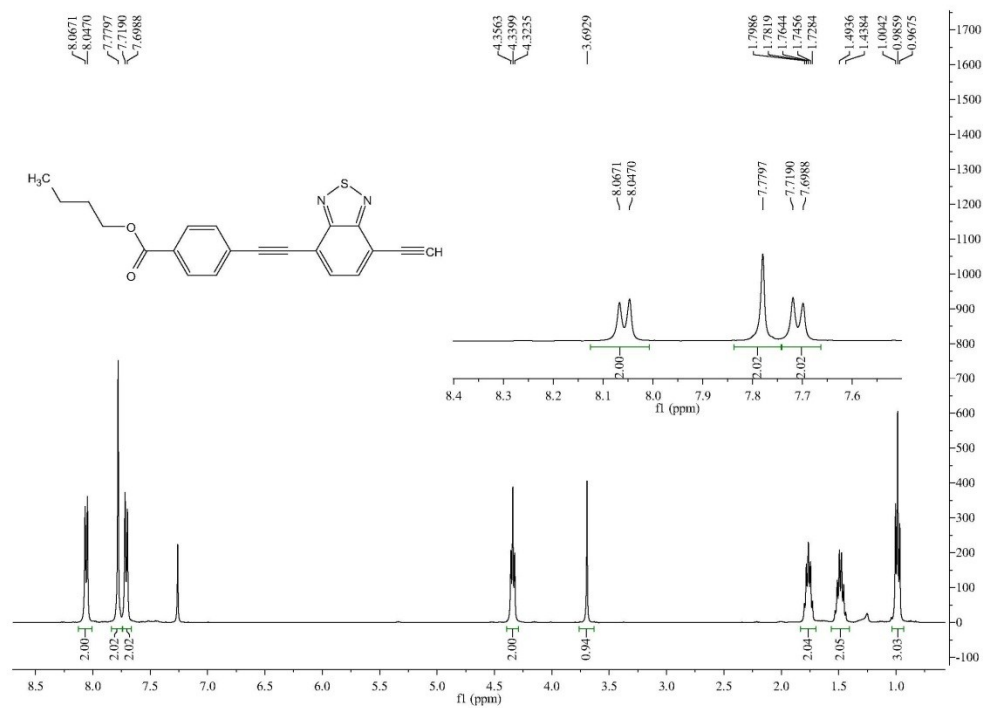


Fig. S17 The ¹H NMR (400 MHz) spectrum of **2** in CDCl₃.

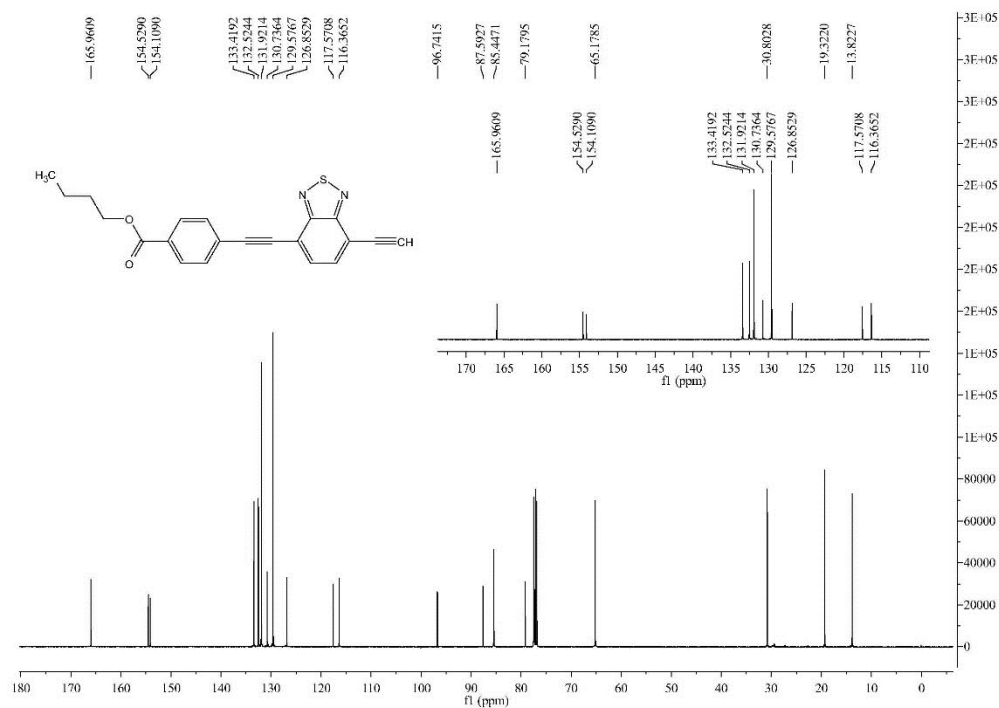


Fig. S18 The ¹³C NMR (100 MHz) spectrum of **2** in CDCl₃.

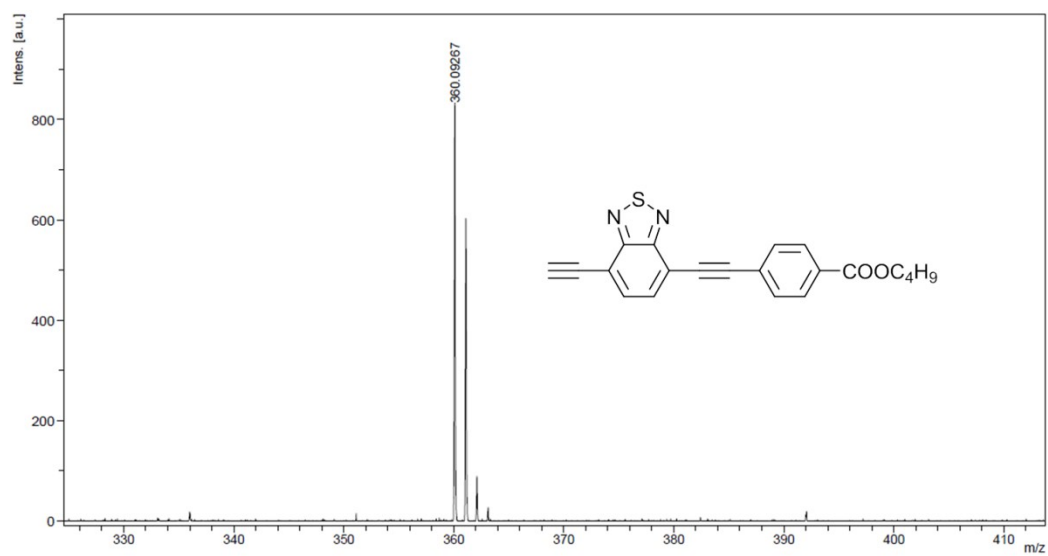


Fig. S19 The high resolution mass spectrum (MALDI-TOF) of **2**.

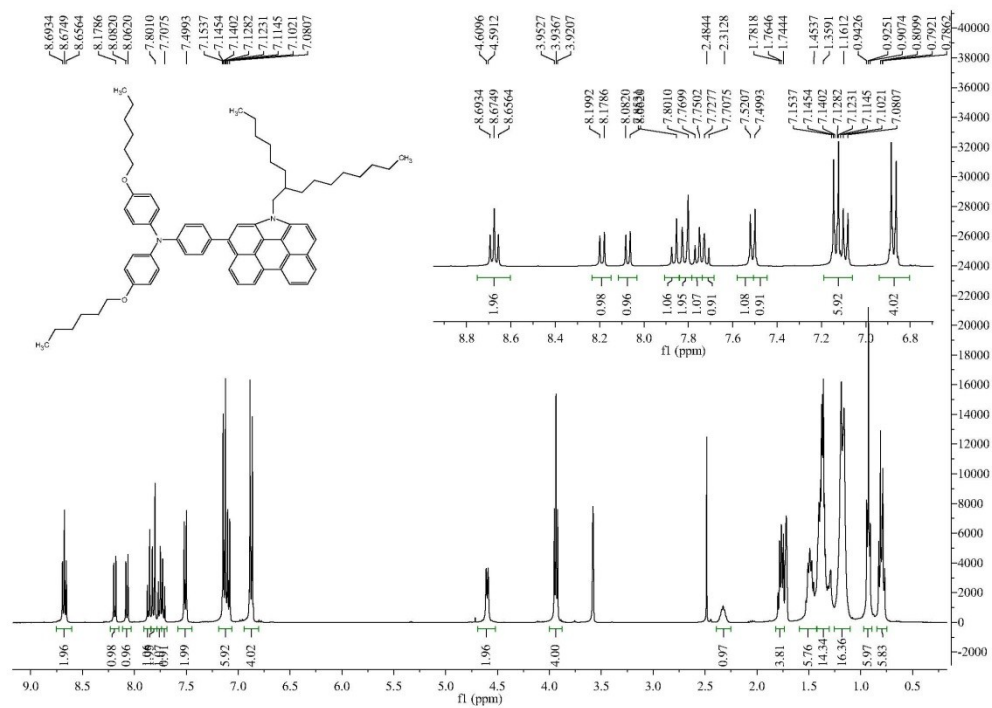


Fig. S20 The ^1H NMR (400 MHz) spectrum of **5** in $\text{THF-}d_8$.

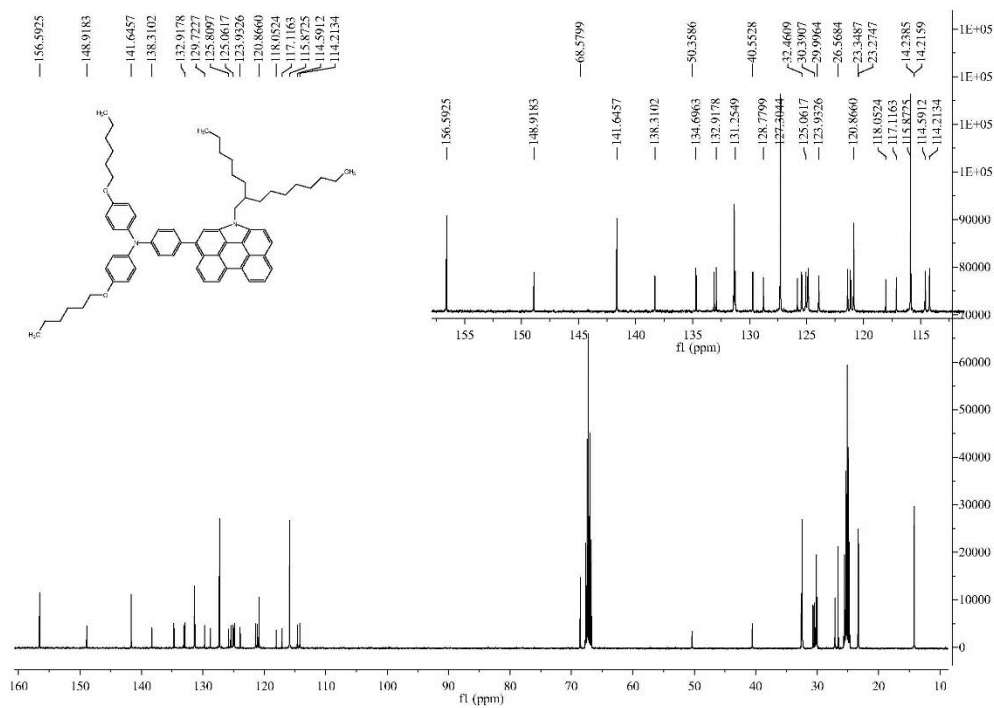


Fig. S21 The ^{13}C NMR (100 MHz) spectrum of **5** in $\text{THF-}d_8$.

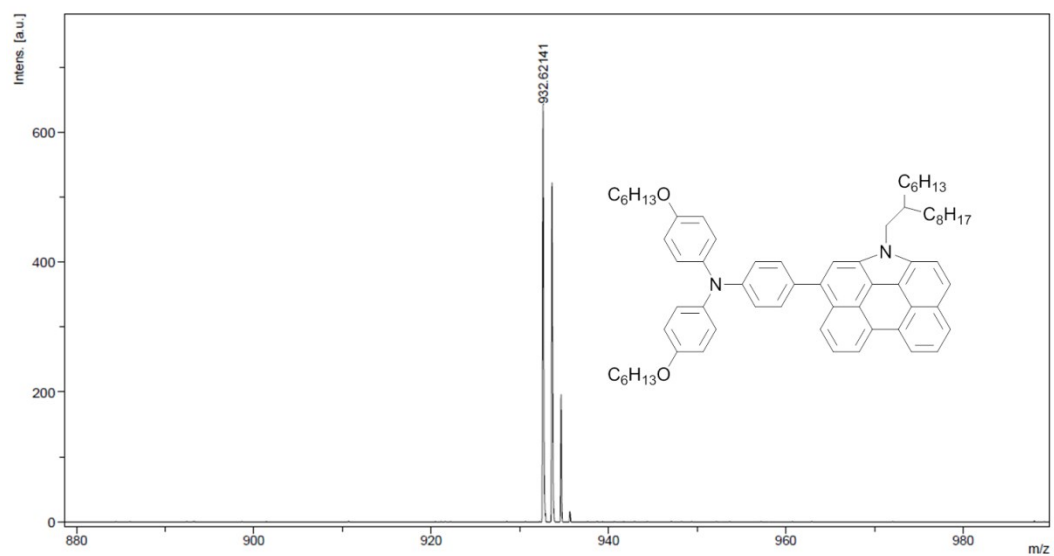


Fig. S22 The high resolution mass spectrum (MALDI-TOF) of **5**.

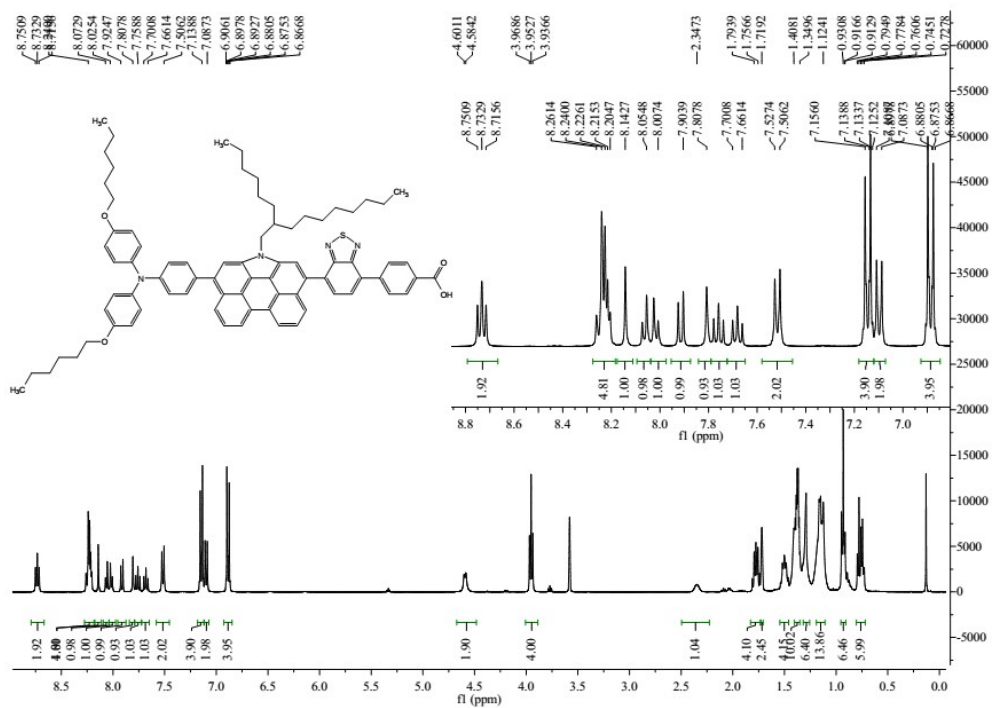


Fig. S23 The ^1H NMR (400 MHz) spectrum of C286 in $\text{THF-}d_8$.

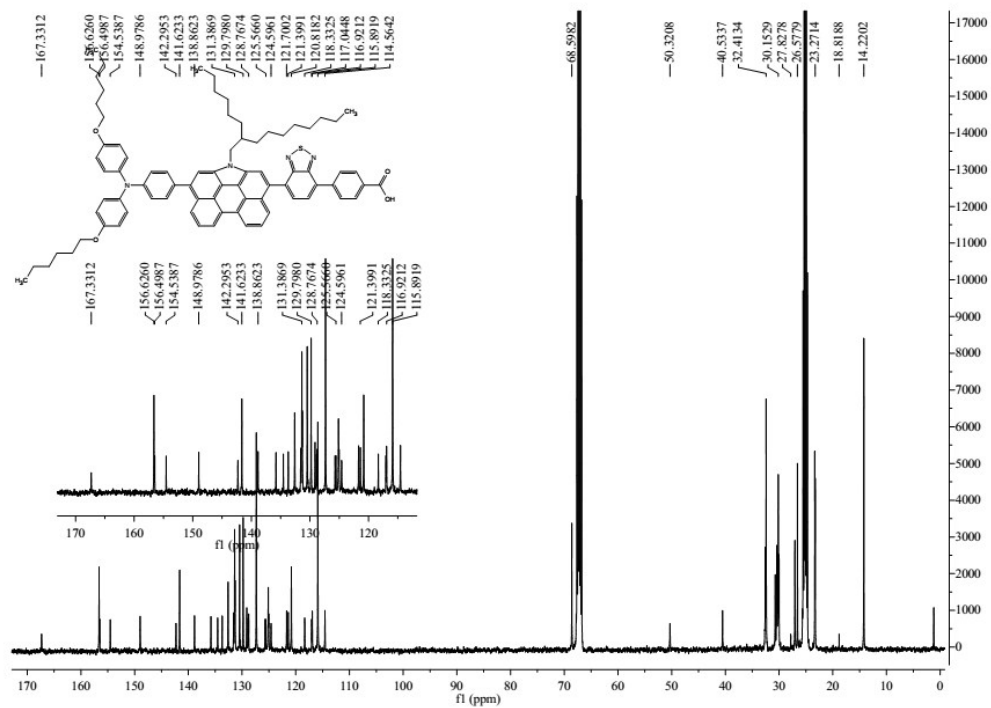
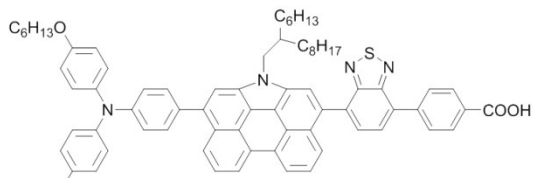
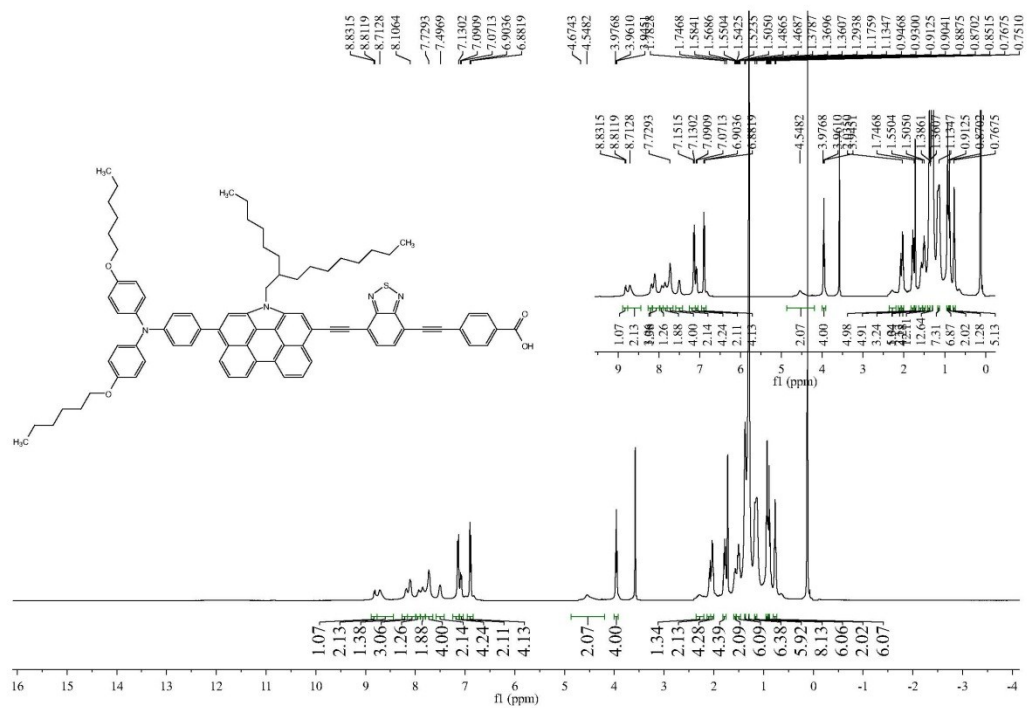


Fig. S24 The ^{13}C NMR (100 MHz) spectrum of C286 in $\text{THF-}d_8$.



S37



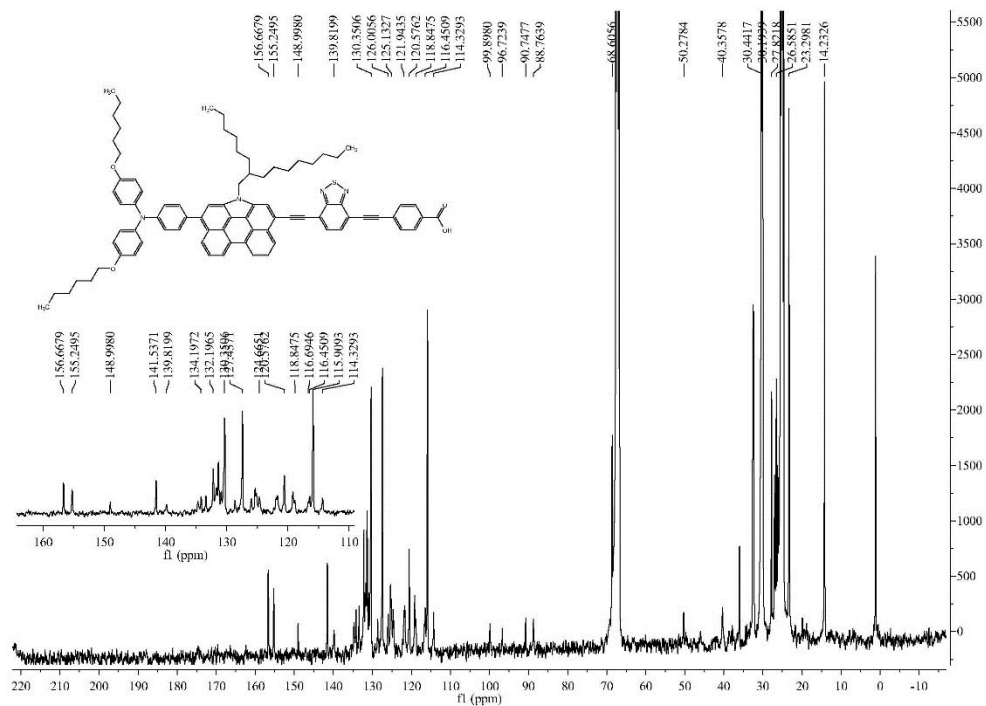


Fig. S27 The ¹³C NMR (100 MHz) spectrum of **C287** in THF-*d*₈.

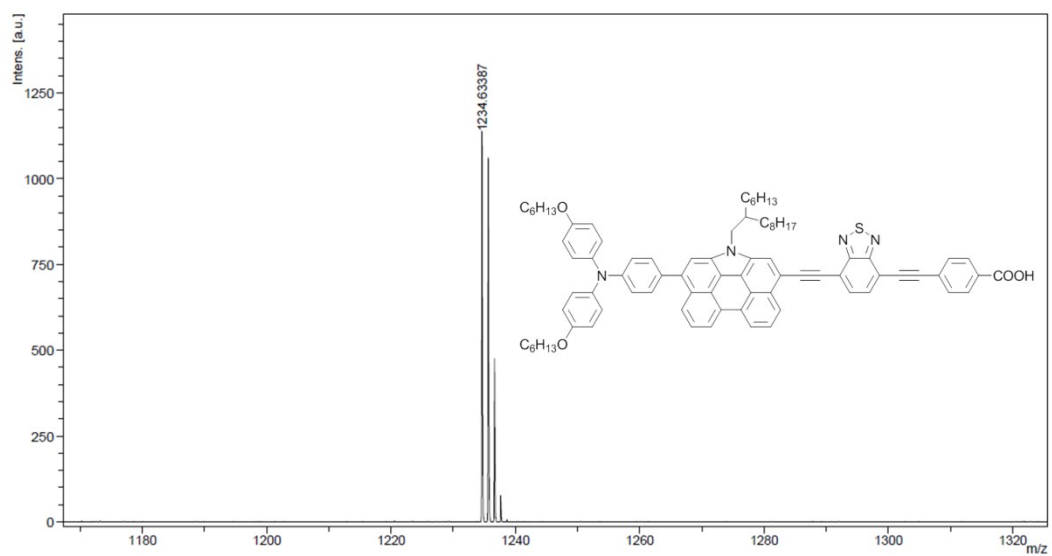


Fig. S28 The high resolution mass spectrum (MALDI-TOF) of **C287**.

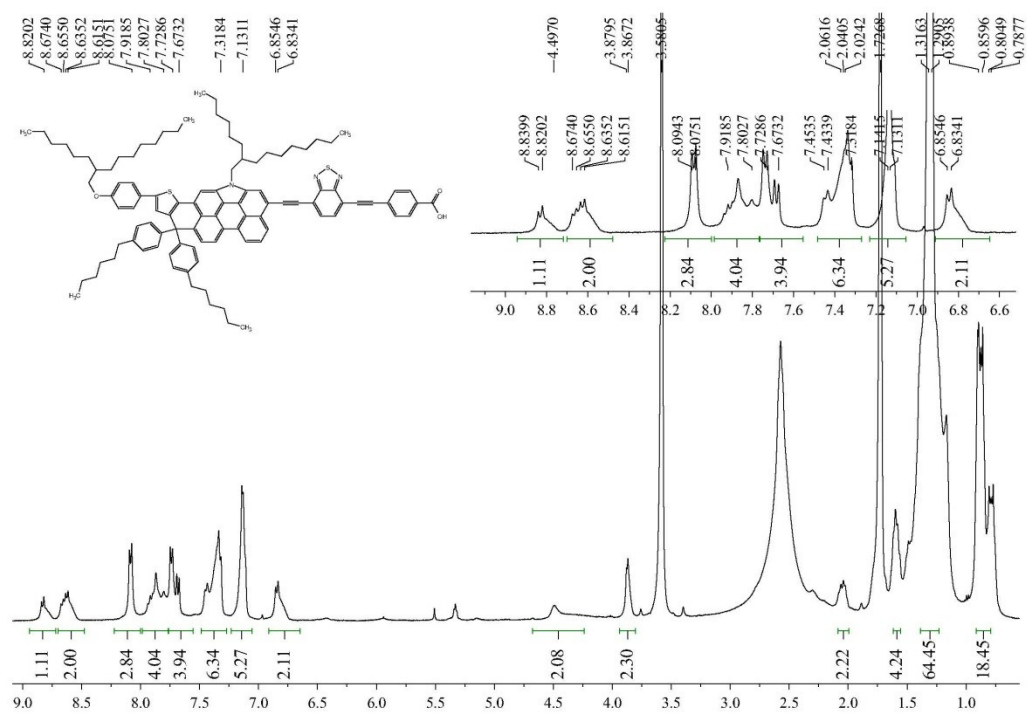


Fig. S29 The ¹H NMR (400 MHz) spectrum of **C288** in THF-*d*₈.

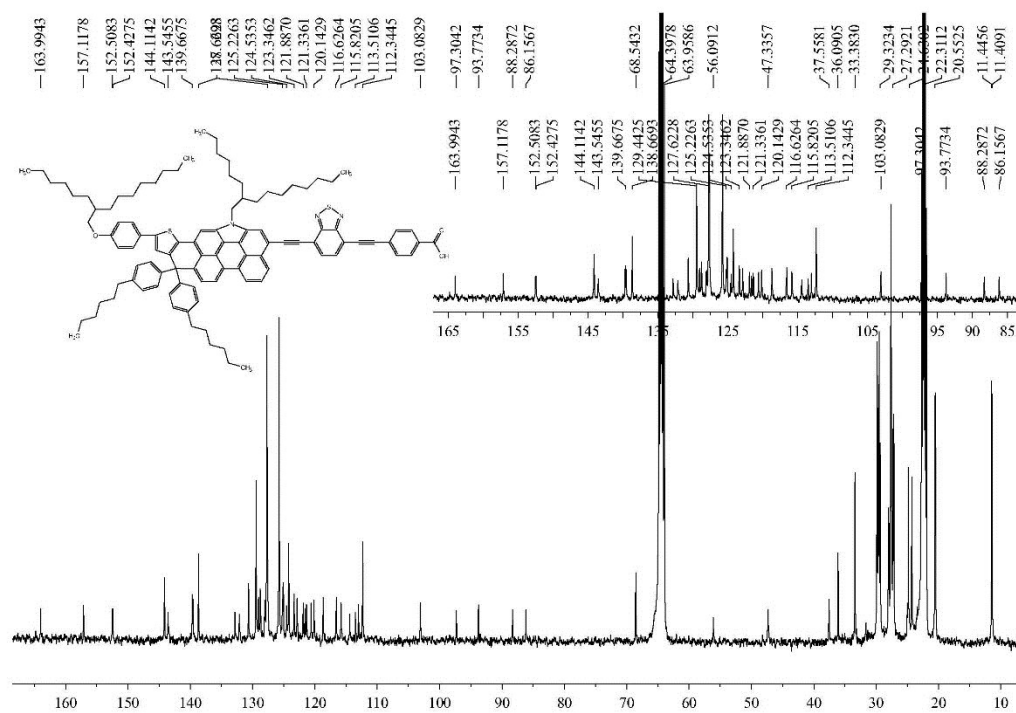


Fig. S30 The ^{13}C NMR (100 MHz) spectrum of **C288** in $\text{THF-}d_8$.

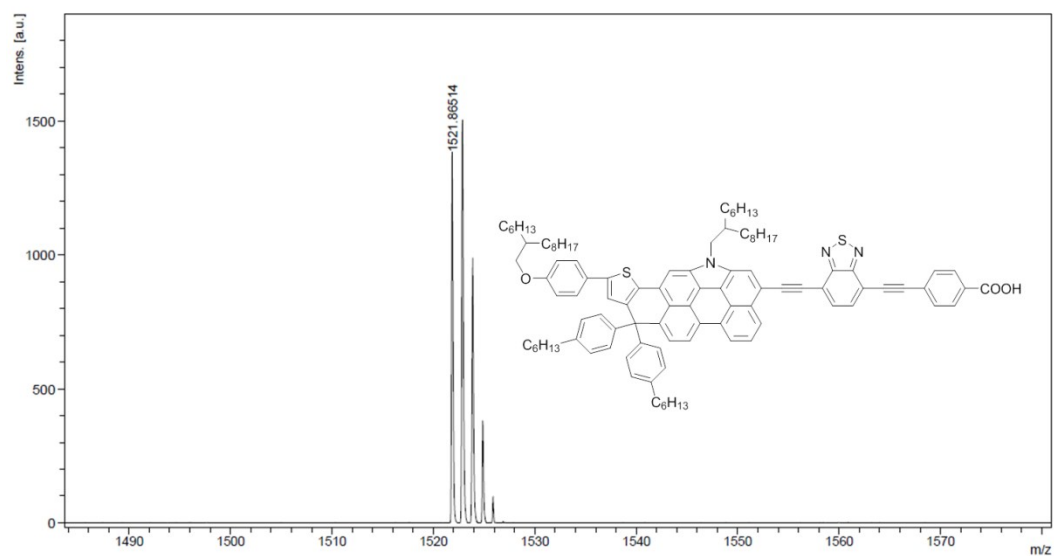


Fig. S31 The high resolution mass spectrum (MALDI-TOF) of **C288**.

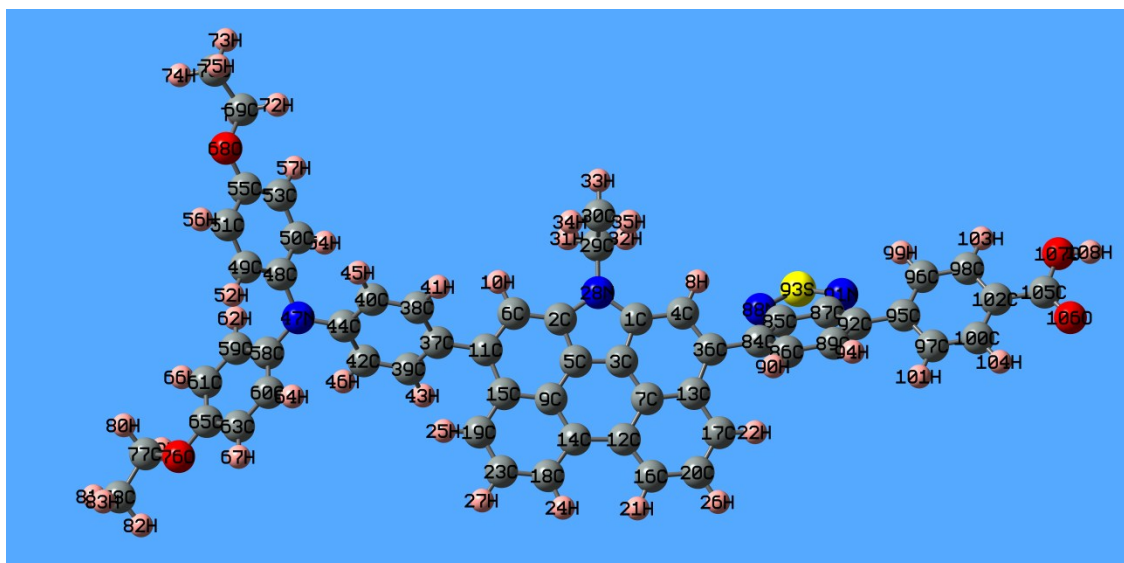


Fig. S32 Geometry of the S_0 state of **C286** in THF optimized at the B3LYP/6-311G(d,p) level of theory.

Table S11. Geometry Parameters and Mulliken Atomic Charges of the S₀ State of **C286** in THF Computed at the B3LYP/6-311G(d,p) Level of Theory

Center number	Atom	Coordinates [Å]			Mulliken atomic charges
		x	y	z	
1	C	-2.45352	0.341297	0.021734	0.256738
2	C	-0.17264	0.33962	-0.06762	0.268425
3	C	-2.01706	-0.92886	-0.32595	-0.1642
4	C	-3.85052	0.517315	0.125271	0.024207
5	C	-0.63584	-0.93062	-0.37389	-0.17072
6	C	1.232807	0.507923	-0.05147	-0.02117
7	C	-2.78397	-2.05523	-0.56781	-0.0235
8	H	-4.29075	1.473277	0.377663	0.109352
9	C	0.109974	-2.05994	-0.66412	-0.01724
10	H	1.693695	1.454988	0.202185	0.109672
11	C	2.059528	-0.58551	-0.33743	-0.01302
12	C	-2.09577	-3.27605	-0.87992	0.048578
13	C	-4.19375	-1.89856	-0.46707	-0.01223
14	C	-0.60097	-3.27414	-0.9456	0.047211
15	C	1.523094	-1.90528	-0.66635	-0.01427
16	C	-2.91354	-4.38479	-1.08479	-0.10647
17	C	-4.95229	-3.07613	-0.66743	-0.10788
18	C	0.196856	-4.37039	-1.26635	-0.10513
19	C	2.260633	-3.05757	-1.02552	-0.10747
20	C	-4.31271	-4.27138	-0.96881	-0.0798
21	H	-2.48968	-5.35337	-1.32301	0.099794
22	H	-6.03073	-3.0623	-0.57851	0.108487
23	C	1.598886	-4.24533	-1.31102	-0.08125
24	H	-0.24563	-5.33245	-1.49719	0.099643
25	H	3.340527	-3.02458	-1.08844	0.109721

26	H	-4.91536	-5.16083	-1.11597	0.106295
27	H	2.18524	-5.11584	-1.58375	0.105722
28	N	-1.30309	1.135686	0.189758	-0.57693
29	C	-1.28914	2.565032	0.494502	-0.0985
30	C	-1.3369	3.452185	-0.75167	-0.28207
31	H	-0.38817	2.770511	1.076504	0.137527
32	H	-2.14002	2.773487	1.146585	0.137758
33	H	-1.3197	4.505185	-0.4591	0.11919
34	H	-0.47798	3.263124	-1.39949	0.117489
35	H	-2.24846	3.272001	-1.32597	0.117477
36	C	-4.69732	-0.56965	-0.12821	0.003007
37	C	3.530278	-0.3652	-0.29706	-0.11838
38	C	4.122932	0.684611	-1.01561	-0.08247
39	C	4.380168	-1.15869	0.489192	-0.08929
40	C	5.489078	0.928166	-0.96357	-0.12046
41	H	3.504176	1.307782	-1.65212	0.102869
42	C	5.745421	-0.9154	0.562933	-0.12017
43	H	3.962067	-1.96133	1.085955	0.109684
44	C	6.332472	0.133402	-0.1675	0.194313
45	H	5.909565	1.734885	-1.55032	0.119547
46	H	6.362636	-1.53526	1.200663	0.120531
47	N	7.716704	0.377359	-0.10421	-0.4974
48	C	8.241775	1.690362	-0.29999	0.06865
49	C	9.299038	1.903996	-1.19655	-0.07939
50	C	7.735902	2.784469	0.40437	-0.06782
51	C	9.831356	3.171121	-1.37574	-0.11085
52	H	9.705884	1.066907	-1.75135	0.11167
53	C	8.250443	4.066895	0.213984	-0.14317
54	H	6.925331	2.638154	1.108343	0.112812

55	C	9.308811	4.268363	-0.6776	0.179842
56	H	10.64939	3.337557	-2.06658	0.109816
57	H	7.829032	4.889593	0.775123	0.125585
58	C	8.632869	-0.67975	0.182752	0.061537
59	C	9.580493	-0.54334	1.197803	-0.07836
60	C	8.618854	-1.86743	-0.564	-0.06296
61	C	10.50274	-1.55491	1.466938	-0.14377
62	H	9.605607	0.36728	1.784613	0.111746
63	C	9.51746	-2.88618	-0.29021	-0.10962
64	H	7.896581	-1.98876	-1.36257	0.112518
65	C	10.47268	-2.74003	0.725995	0.179975
66	H	11.22451	-1.40899	2.25879	0.125457
67	H	9.508564	-3.80433	-0.86561	0.110531
68	O	9.893684	5.47304	-0.93339	-0.37086
69	C	9.410634	6.639156	-0.25019	-0.05021
70	C	10.23192	7.820212	-0.72822	-0.29684
71	H	9.51588	6.501108	0.831877	0.121043
72	H	8.34799	6.783425	-0.47615	0.12059
73	H	9.895119	8.732868	-0.23084	0.117363
74	H	11.28978	7.672544	-0.49997	0.116603
75	H	10.12374	7.954488	-1.80676	0.116617
76	O	11.31744	-3.79409	0.908284	-0.37052
77	C	12.31419	-3.71425	1.938312	-0.05067
78	C	13.10182	-5.00914	1.912608	-0.29679
79	H	11.8273	-3.57074	2.909511	0.121426
80	H	12.96741	-2.85444	1.751483	0.120938
81	H	13.87332	-4.98979	2.686024	0.117465
82	H	12.44713	-5.86329	2.099087	0.116646
83	H	13.58709	-5.14694	0.943858	0.116674

84	C	-6.16094	-0.32667	-0.0799	-0.06118
85	C	-6.79273	0.279331	1.058891	0.120312
86	C	-7.00059	-0.64323	-1.12576	-0.07916
87	C	-8.22327	0.54212	1.077955	0.114
88	N	-6.18028	0.630651	2.194088	-0.48616
89	C	-8.39766	-0.3882	-1.10773	-0.06643
90	H	-6.58056	-1.08284	-2.02227	0.12037
91	N	-8.6402	1.081861	2.227879	-0.5
92	C	-9.05024	0.200311	-0.0452	0.000202
93	S	-7.3251	1.24132	3.190333	0.571272
94	H	-8.96386	-0.64366	-1.99547	0.119295
95	C	-10.5079	0.453921	-0.07601	-0.02413
96	C	-11.0664	1.619072	0.476028	-0.04906
97	C	-11.3706	-0.46689	-0.69689	-0.07857
98	C	-12.4315	1.860562	0.399224	-0.03596
99	H	-10.4257	2.341565	0.961585	0.116552
100	C	-12.7344	-0.22872	-0.77172	-0.04151
101	H	-10.9703	-1.38736	-1.10415	0.118026
102	C	-13.279	0.938674	-0.22602	-0.21308
103	H	-12.8427	2.767861	0.821448	0.116292
104	H	-13.3937	-0.94563	-1.24465	0.112748
105	C	-14.7452	1.150165	-0.32987	0.433375
106	O	-15.5179	0.382316	-0.86175	-0.3699
107	O	-15.1544	2.306389	0.235533	-0.3406
108	H	-16.1151	2.357918	0.118725	0.276329

Table S12. The Bond Lengths of the S₀ State of **C286** in THF Computed at the B3LYP/6-311G(d,p) Level of Theory.

Number	Name	Length[Å]	Number	Name	Length[Å]
R1	R(1,3)	1.3873	R61	R(50,53)	1.3949
R2	R(1,4)	1.4118	R62	R(50,54)	1.0835
R3	R(1,28)	1.4081	R63	R(51,55)	1.4016
R4	R(2,5)	1.3863	R64	R(51,56)	1.0836
R5	R(2,6)	1.4156	R65	R(53,55)	1.3984
R6	R(2,28)	1.4064	R66	R(53,57)	1.0813
R7	R(3,5)	1.3821	R67	R(55,68)	1.3634
R8	R(3,7)	1.384	R68	R(58,59)	1.3953
R9	R(4,8)	1.0823	R69	R(58,60)	1.403
R10	R(4,36)	1.401	R70	R(59,61)	1.3951
R11	R(5,9)	1.3841	R71	R(59,62)	1.0836
R12	R(6,10)	1.0834	R72	R(60,63)	1.3858
R13	R(6,11)	1.4003	R73	R(60,64)	1.0836
R14	R(7,12)	1.4358	R74	R(61,65)	1.398
R15	R(7,13)	1.422	R75	R(61,66)	1.0813
R16	R(9,14)	1.4349	R76	R(63,65)	1.4023
R17	R(9,15)	1.4216	R77	R(63,67)	1.0836
R18	R(11,15)	1.4621	R78	R(65,76)	1.363
R19	R(11,37)	1.4877	R79	R(68,69)	1.4352
R20	R(12,14)	1.4962	R80	R(69,70)	1.5159
R21	R(12,16)	1.3928	R81	R(69,71)	1.0959
R22	R(13,17)	1.415	R82	R(69,72)	1.0959
R23	R(13,36)	1.461	R83	R(70,73)	1.0926
R24	R(14,18)	1.3933	R84	R(70,74)	1.0922
R25	R(15,19)	1.4145	R85	R(70,75)	1.0922
R26	R(16,20)	1.4085	R86	R(76,77)	1.4356

R27	R(16,21)	1.0838	R87	R(77,78)	1.5158
R28	R(17,20)	1.3887	R88	R(77,79)	1.0958
R29	R(17,22)	1.0822	R89	R(77,80)	1.0958
R30	R(18,23)	1.4083	R90	R(78,81)	1.0926
R31	R(18,24)	1.0838	R91	R(78,82)	1.0922
R32	R(19,23)	1.3893	R92	R(78,83)	1.0922
R33	R(19,25)	1.0822	R93	R(84,85)	1.4364
R34	R(20,26)	1.0844	R94	R(84,86)	1.3781
R35	R(23,27)	1.0844	R95	R(85,87)	1.4546
R36	R(28,29)	1.4615	R96	R(85,88)	1.3369
R37	R(29,30)	1.5304	R97	R(86,89)	1.4203
R38	R(29,31)	1.0921	R98	R(86,90)	1.0832
R39	R(29,32)	1.0921	R99	R(87,91)	1.337
R40	R(30,33)	1.093	R100	R(87,92)	1.436
R41	R(30,34)	1.0923	R101	R(88,93)	1.6359
R42	R(30,35)	1.0924	R102	R(89,92)	1.3788
R43	R(36,84)	1.4844	R103	R(89,94)	1.0835
R44	R(37,38)	1.4034	R104	R(91,93)	1.6374
R45	R(37,39)	1.4036	R105	R(92,95)	1.4799
R46	R(38,40)	1.3887	R106	R(95,96)	1.4051
R47	R(38,41)	1.0846	R107	R(95,97)	1.4063
R48	R(39,42)	1.3887	R108	R(96,98)	1.3884
R49	R(39,43)	1.0841	R109	R(96,99)	1.0809
R50	R(40,44)	1.4059	R110	R(97,100)	1.3865
R51	R(40,45)	1.0825	R111	R(97,101)	1.0832
R52	R(42,44)	1.4065	R112	R(98,102)	1.3996
R53	R(42,46)	1.0825	R113	R(98,103)	1.0819
R54	R(44,47)	1.407	R114	R(100,102)	1.399
R55	R(47,48)	1.4276	R115	R(100,104)	1.0827

R56	R(47,58)	1.428	R116	R(102,105)	1.4851
R57	R(48,49)	1.4026	R117	R(105,106)	1.2122
R58	R(48,50)	1.3961	R118	R(105,107)	1.3505
R59	R(49,51)	1.386	R119	R(107,108)	0.9692
R60	R(49,52)	1.0835			

Table S13. The Bond Angles of the S₀ State of **C286** in THF Computed at the B3LYP/6-311G(d,p) Level of Theory.

Number	Name	Angle [°]	Number	Name	Angle [°]
A1	A(3,1,4)	116.3477	A102	A(51,49,52)	119.7277
A2	A(3,1,28)	106.8206	A103	A(48,50,53)	121.1978
A3	A(4,1,28)	136.8301	A104	A(48,50,54)	119.5401
A4	A(5,2,6)	116.3075	A105	A(53,50,54)	119.2612
A5	A(5,2,28)	106.8887	A106	A(49,51,55)	120.5391
A6	A(6,2,28)	136.7744	A107	A(49,51,56)	120.8495
A7	A(1,3,5)	108.9215	A108	A(55,51,56)	118.6063
A8	A(1,3,7)	127.9226	A109	A(50,53,55)	119.9109
A9	A(5,3,7)	123.1415	A110	A(50,53,57)	119.0061
A10	A(1,4,8)	121.985	A111	A(55,53,57)	121.0763
A11	A(1,4,36)	119.2139	A112	A(51,55,53)	119.1404
A12	A(8,4,36)	118.7916	A113	A(51,55,68)	115.9992
A13	A(2,5,3)	108.9711	A114	A(53,55,68)	124.8604
A14	A(2,5,9)	127.8706	A115	A(47,58,59)	120.6327
A15	A(3,5,9)	123.1487	A116	A(47,58,60)	120.8835
A16	A(2,6,10)	121.9367	A117	A(59,58,60)	118.4727
A17	A(2,6,11)	119.4059	A118	A(58,59,61)	121.226
A18	A(10,6,11)	118.6373	A119	A(58,59,62)	119.4618
A19	A(3,7,12)	117.6714	A120	A(61,59,62)	119.311
A20	A(3,7,13)	116.5716	A121	A(58,60,63)	120.7101
A21	A(12,7,13)	125.7521	A122	A(58,60,64)	119.5846
A22	A(5,9,14)	117.6826	A123	A(63,60,64)	119.7052
A23	A(5,9,15)	116.5635	A124	A(59,61,65)	119.8823
A24	A(14,9,15)	125.7519	A125	A(59,61,66)	118.9914
A25	A(6,11,15)	122.2879	A126	A(65,61,66)	121.1224
A26	A(6,11,37)	117.5472	A127	A(60,63,65)	120.5489

A27	A(15,11,37)	120.1649	A128	A(60,63,67)	120.8423
A28	A(7,12,14)	119.1647	A129	A(65,63,67)	118.6012
A29	A(7,12,16)	115.3025	A130	A(61,65,63)	119.1483
A30	A(14,12,16)	125.5292	A131	A(61,65,76)	124.8442
A31	A(7,13,17)	115.4505	A132	A(63,65,76)	116.0072
A32	A(7,13,36)	117.2814	A133	A(55,68,69)	118.962
A33	A(17,13,36)	127.2332	A134	A(68,69,70)	107.4916
A34	A(9,14,12)	119.1734	A135	A(68,69,71)	109.593
A35	A(9,14,18)	115.2926	A136	A(68,69,72)	109.5814
A36	A(12,14,18)	125.5339	A137	A(70,69,71)	110.9455
A37	A(9,15,11)	117.5529	A138	A(70,69,72)	110.9617
A38	A(9,15,19)	115.4736	A139	A(71,69,72)	108.2571
A39	A(11,15,19)	126.9527	A140	A(69,70,73)	109.8914
A40	A(12,16,20)	120.4651	A141	A(69,70,74)	110.7015
A41	A(12,16,21)	120.9387	A142	A(69,70,75)	110.7025
A42	A(20,16,21)	118.5913	A143	A(73,70,74)	108.4428
A43	A(13,17,20)	120.0078	A144	A(73,70,75)	108.4392
A44	A(13,17,22)	120.7937	A145	A(74,70,75)	108.5967
A45	A(20,17,22)	119.1953	A146	A(65,76,77)	118.8989
A46	A(14,18,23)	120.4985	A147	A(76,77,78)	107.5236
A47	A(14,18,24)	120.9091	A148	A(76,77,79)	109.5536
A48	A(23,18,24)	118.589	A149	A(76,77,80)	109.5842
A49	A(15,19,23)	120.0185	A150	A(78,77,79)	110.9626
A50	A(15,19,25)	120.679	A151	A(78,77,80)	110.9541
A51	A(23,19,25)	119.301	A152	A(79,77,80)	108.2516
A52	A(16,20,17)	123.0015	A153	A(77,78,81)	109.8629
A53	A(16,20,26)	118.3474	A154	A(77,78,82)	110.7127
A54	A(17,20,26)	118.65	A155	A(77,78,83)	110.7119
A55	A(18,23,19)	122.9283	A156	A(81,78,82)	108.4359

A56	A(18,23,27)	118.3586	A157	A(81,78,83)	108.4431
A57	A(19,23,27)	118.7128	A158	A(82,78,83)	108.6076
A58	A(1,28,2)	108.3933	A159	A(36,84,85)	121.9064
A59	A(1,28,29)	125.7609	A160	A(36,84,86)	122.5785
A60	A(2,28,29)	125.7368	A161	A(85,84,86)	115.5063
A61	A(28,29,30)	113.3798	A162	A(84,85,87)	121.2771
A62	A(28,29,31)	107.6378	A163	A(84,85,88)	125.6323
A63	A(28,29,32)	107.6821	A164	A(87,85,88)	113.0755
A64	A(30,29,31)	110.5247	A165	A(84,86,89)	123.2616
A65	A(30,29,32)	110.5623	A166	A(84,86,90)	119.0175
A66	A(31,29,32)	106.7775	A167	A(89,86,90)	117.6971
A67	A(29,30,33)	109.8767	A168	A(85,87,91)	113.0102
A68	A(29,30,34)	110.9799	A169	A(85,87,92)	120.8701
A69	A(29,30,35)	111.0092	A170	A(91,87,92)	126.1011
A70	A(33,30,34)	108.2476	A171	A(85,88,93)	107.1353
A71	A(33,30,35)	108.226	A172	A(86,89,92)	123.5029
A72	A(34,30,35)	108.4109	A173	A(86,89,94)	117.4713
A73	A(4,36,13)	122.6397	A174	A(92,89,94)	118.9921
A74	A(4,36,84)	117.5851	A175	A(87,91,93)	107.1219
A75	A(13,36,84)	119.7543	A176	A(87,92,89)	115.5784
A76	A(11,37,38)	120.9545	A177	A(87,92,95)	122.869
A77	A(11,37,39)	122.0107	A178	A(89,92,95)	121.5526
A78	A(38,37,39)	116.9991	A179	A(88,93,91)	99.6569
A79	A(37,38,40)	121.8329	A180	A(92,95,96)	121.6982
A80	A(37,38,41)	119.2976	A181	A(92,95,97)	120.082
A81	A(40,38,41)	118.8468	A182	A(96,95,97)	118.2024
A82	A(37,39,42)	121.7339	A183	A(95,96,98)	120.8843
A83	A(37,39,43)	119.5645	A184	A(95,96,99)	119.6811
A84	A(42,39,43)	118.6623	A185	A(98,96,99)	119.4333

A85	A(38,40,44)	120.8123	A186	A(95,97,100)	120.9833
A86	A(38,40,45)	119.506	A187	A(95,97,101)	119.7118
A87	A(44,40,45)	119.6796	A188	A(100,97,101)	119.2906
A88	A(39,42,44)	120.8907	A189	A(96,98,102)	120.3616
A89	A(39,42,46)	119.4385	A190	A(96,98,103)	119.8652
A90	A(44,42,46)	119.6669	A191	A(102,98,103)	119.7727
A91	A(40,44,42)	117.7236	A192	A(97,100,102)	120.3426
A92	A(40,44,47)	121.1733	A193	A(97,100,104)	120.5836
A93	A(42,44,47)	121.103	A194	A(102,100,104)	119.0717
A94	A(44,47,48)	121.008	A195	A(98,102,100)	119.2233
A95	A(44,47,58)	120.789	A196	A(98,102,105)	122.3607
A96	A(48,47,58)	118.1929	A197	A(100,102,105)	118.4157
A97	A(47,48,49)	120.3311	A198	A(102,105,106)	124.7365
A98	A(47,48,50)	121.2199	A199	A(102,105,107)	113.0636
A99	A(49,48,50)	118.4417	A200	A(106,105,107)	122.1999
A100	A(48,49,51)	120.756	A201	A(105,107,108)	107.1796
A101	A(48,49,52)	119.5157			

Table S14. The Dihedral Angles of the S₀ State of **C286** in THF Computed at the B3LYP/6-311G(d,p) Level of Theory.

Number	Name	Dihedral Angle [°]	Number	Name	Dihedral Angle [°]
D1	D(4,1,3,5)	-179.588	D153	D(40,44,47,58)	-152.531
D2	D(4,1,3,7)	-0.9482	D154	D(42,44,47,48)	-151.422
D3	D(28,1,3,5)	0.0208	D155	D(42,44,47,58)	27.4033
D4	D(28,1,3,7)	178.6601	D156	D(44,47,48,49)	-130.363
D5	D(3,1,4,8)	-179.16	D157	D(44,47,48,50)	50.6316
D6	D(3,1,4,36)	-0.2939	D158	D(58,47,48,49)	50.7819
D7	D(28,1,4,8)	1.388	D159	D(58,47,48,50)	-128.223
D8	D(28,1,4,36)	-179.746	D160	D(44,47,58,59)	-128.19
D9	D(3,1,28,2)	0.4031	D161	D(44,47,58,60)	53.0388
D10	D(3,1,28,29)	176.7764	D162	D(48,47,58,59)	50.6675
D11	D(4,1,28,2)	179.8901	D163	D(48,47,58,60)	-128.104
D12	D(4,1,28,29)	-3.7366	D164	D(47,48,49,51)	-178.845
D13	D(6,2,5,3)	179.0471	D165	D(47,48,49,52)	0.8864
D14	D(6,2,5,9)	0.1575	D166	D(50,48,49,51)	0.1879
D15	D(28,2,5,3)	0.6845	D167	D(50,48,49,52)	179.9191
D16	D(28,2,5,9)	-178.205	D168	D(47,48,50,53)	179.9165
D17	D(5,2,6,10)	-178.342	D169	D(47,48,50,54)	-0.4146
D18	D(5,2,6,11)	0.0025	D170	D(49,48,50,53)	0.8929
D19	D(28,2,6,10)	-0.6301	D171	D(49,48,50,54)	-179.438
D20	D(28,2,6,11)	177.7146	D172	D(48,49,51,55)	-0.9535
D21	D(5,2,28,1)	-0.6694	D173	D(48,49,51,56)	179.8828
D22	D(5,2,28,29)	-177.044	D174	D(52,49,51,55)	179.3159
D23	D(6,2,28,1)	-178.526	D175	D(52,49,51,56)	0.1522
D24	D(6,2,28,29)	5.0995	D176	D(48,50,53,55)	-1.2064
D25	D(1,3,5,2)	-0.4445	D177	D(48,50,53,57)	179.73
D26	D(1,3,5,9)	178.5086	D178	D(54,50,53,55)	179.1238

D27	D(7,3,5,2)	-179.163	D179	D(54,50,53,57)	0.0602
D28	D(7,3,5,9)	-0.2096	D180	D(49,51,55,53)	0.6386
D29	D(1,3,7,12)	-178.363	D181	D(49,51,55,68)	-179.406
D30	D(1,3,7,13)	0.8834	D182	D(56,51,55,53)	179.8208
D31	D(5,3,7,12)	0.1	D183	D(56,51,55,68)	-0.2233
D32	D(5,3,7,13)	179.3461	D184	D(50,53,55,51)	0.4285
D33	D(1,4,36,13)	1.5175	D185	D(50,53,55,68)	-179.523
D34	D(1,4,36,84)	-176.815	D186	D(57,53,55,51)	179.4724
D35	D(8,4,36,13)	-179.58	D187	D(57,53,55,68)	-0.4793
D36	D(8,4,36,84)	2.0874	D188	D(51,55,68,69)	-179.83
D37	D(2,5,9,14)	179.6887	D189	D(53,55,68,69)	0.1231
D38	D(2,5,9,15)	-0.809	D190	D(47,58,59,61)	-178.408
D39	D(3,5,9,14)	0.9429	D191	D(47,58,59,62)	1.2055
D40	D(3,5,9,15)	-179.555	D192	D(60,58,59,61)	0.392
D41	D(2,6,11,15)	0.5245	D193	D(60,58,59,62)	-179.994
D42	D(2,6,11,37)	-179.473	D194	D(47,58,60,63)	179.4192
D43	D(10,6,11,15)	178.924	D195	D(47,58,60,64)	-0.6396
D44	D(10,6,11,37)	-1.073	D196	D(59,58,60,63)	0.6221
D45	D(3,7,12,14)	-0.7233	D197	D(59,58,60,64)	-179.437
D46	D(3,7,12,16)	178.6222	D198	D(58,59,61,65)	-1.013
D47	D(13,7,12,14)	-179.893	D199	D(58,59,61,66)	179.6976
D48	D(13,7,12,16)	-0.547	D200	D(62,59,61,65)	179.3727
D49	D(3,7,13,17)	-177.632	D201	D(62,59,61,66)	0.0833
D50	D(3,7,13,36)	0.3767	D202	D(58,60,63,65)	-1.015
D51	D(12,7,13,17)	1.5452	D203	D(58,60,63,67)	-179.997
D52	D(12,7,13,36)	179.5539	D204	D(64,60,63,65)	179.0438
D53	D(5,9,14,12)	-1.5317	D205	D(64,60,63,67)	0.0614
D54	D(5,9,14,18)	178.342	D206	D(59,61,65,63)	0.6163
D55	D(15,9,14,12)	179.0168	D207	D(59,61,65,76)	-179.578

D56	D(15,9,14,18)	-1.1095	D208	D(66,61,65,63)	179.8902
D57	D(5,9,15,11)	1.2359	D209	D(66,61,65,76)	-0.3044
D58	D(5,9,15,19)	-177.221	D210	D(60,63,65,61)	0.3856
D59	D(14,9,15,11)	-179.307	D211	D(60,63,65,76)	-179.437
D60	D(14,9,15,19)	2.236	D212	D(67,63,65,61)	179.3905
D61	D(6,11,15,9)	-1.1675	D213	D(67,63,65,76)	-0.4317
D62	D(6,11,15,19)	177.0891	D214	D(61,65,76,77)	0.5982
D63	D(37,11,15,9)	178.8295	D215	D(63,65,76,77)	-179.591
D64	D(37,11,15,19)	-2.914	D216	D(55,68,69,70)	-179.785
D65	D(6,11,37,38)	-52.001	D217	D(55,68,69,71)	59.5503
D66	D(6,11,37,39)	125.7614	D218	D(55,68,69,72)	-59.1068
D67	D(15,11,37,38)	128.0019	D219	D(68,69,70,73)	179.9798
D68	D(15,11,37,39)	-54.2357	D220	D(68,69,70,74)	-60.2592
D69	D(7,12,14,9)	1.4598	D221	D(68,69,70,75)	60.2226
D70	D(7,12,14,18)	-178.4	D222	D(71,69,70,73)	-60.2121
D71	D(16,12,14,9)	-177.813	D223	D(71,69,70,74)	59.5489
D72	D(16,12,14,18)	2.3272	D224	D(71,69,70,75)	-179.969
D73	D(7,12,16,20)	-0.6547	D225	D(72,69,70,73)	60.1763
D74	D(7,12,16,21)	-179.835	D226	D(72,69,70,74)	179.9374
D75	D(14,12,16,20)	178.643	D227	D(72,69,70,75)	-59.5809
D76	D(14,12,16,21)	-0.5368	D228	D(65,76,77,78)	-179.91
D77	D(7,13,17,20)	-1.3483	D229	D(65,76,77,79)	59.4082
D78	D(7,13,17,22)	177.9933	D230	D(65,76,77,80)	-59.2201
D79	D(36,13,17,20)	-179.125	D231	D(76,77,78,81)	-179.912
D80	D(36,13,17,22)	0.2162	D232	D(76,77,78,82)	-60.1711
D81	D(7,13,36,4)	-1.5567	D233	D(76,77,78,83)	60.338
D82	D(7,13,36,84)	176.741	D234	D(79,77,78,81)	-60.1225
D83	D(17,13,36,4)	176.1849	D235	D(79,77,78,82)	59.6188
D84	D(17,13,36,84)	-5.5174	D236	D(79,77,78,83)	-179.872

D85	D(9,14,18,23)	-0.5567	D237	D(80,77,78,81)	60.2654
D86	D(9,14,18,24)	-179.868	D238	D(80,77,78,82)	-179.993
D87	D(12,14,18,23)	179.3078	D239	D(80,77,78,83)	-59.4843
D88	D(12,14,18,24)	-0.0037	D240	D(36,84,85,87)	178.4196
D89	D(9,15,19,23)	-1.7044	D241	D(36,84,85,88)	-3.0965
D90	D(9,15,19,25)	177.8437	D242	D(86,84,85,87)	-0.527
D91	D(11,15,19,23)	-179.992	D243	D(86,84,85,88)	177.957
D92	D(11,15,19,25)	-0.4442	D244	D(36,84,86,89)	-178.459
D93	D(12,16,20,17)	0.8102	D245	D(36,84,86,90)	-0.2739
D94	D(12,16,20,26)	-178.797	D246	D(85,84,86,89)	0.4798
D95	D(21,16,20,17)	-179.991	D247	D(85,84,86,90)	178.6648
D96	D(21,16,20,26)	0.4019	D248	D(84,85,87,91)	178.6144
D97	D(13,17,20,16)	0.2697	D249	D(84,85,87,92)	0.0897
D98	D(13,17,20,26)	179.8758	D250	D(88,85,87,91)	-0.0463
D99	D(22,17,20,16)	-179.082	D251	D(88,85,87,92)	-178.571
D100	D(22,17,20,26)	0.5237	D252	D(84,85,88,93)	-178.672
D101	D(14,18,23,19)	1.0015	D253	D(87,85,88,93)	-0.0806
D102	D(14,18,23,27)	-178.803	D254	D(84,86,89,92)	0.0314
D103	D(24,18,23,19)	-179.671	D255	D(84,86,89,94)	177.8959
D104	D(24,18,23,27)	0.5244	D256	D(90,86,89,92)	-178.176
D105	D(15,19,23,18)	0.2164	D257	D(90,86,89,94)	-0.3116
D106	D(15,19,23,27)	-179.98	D258	D(85,87,91,93)	0.1482
D107	D(25,19,23,18)	-179.338	D259	D(92,87,91,93)	178.5809
D108	D(25,19,23,27)	0.4658	D260	D(85,87,92,89)	0.4117
D109	D(1,28,29,30)	-87.8808	D261	D(85,87,92,95)	-179.679
D110	D(1,28,29,31)	149.5533	D262	D(91,87,92,89)	-177.908
D111	D(1,28,29,32)	34.7646	D263	D(91,87,92,95)	2.0019
D112	D(2,28,29,30)	87.8784	D264	D(85,88,93,91)	0.1502
D113	D(2,28,29,31)	-34.6875	D265	D(86,89,92,87)	-0.4828

D114	D(2,28,29,32)	-149.476	D266	D(86,89,92,95)	179.6063
D115	D(28,29,30,33)	-179.764	D267	D(94,89,92,87)	-178.317
D116	D(28,29,30,34)	-60.0786	D268	D(94,89,92,95)	1.7724
D117	D(28,29,30,35)	60.5593	D269	D(87,91,93,88)	-0.1762
D118	D(31,29,30,33)	-58.8113	D270	D(87,92,95,96)	38.2848
D119	D(31,29,30,34)	60.8739	D271	D(87,92,95,97)	-143.259
D120	D(31,29,30,35)	-178.488	D272	D(89,92,95,96)	-141.811
D121	D(32,29,30,33)	59.1991	D273	D(89,92,95,97)	36.6454
D122	D(32,29,30,34)	178.8843	D274	D(92,95,96,98)	177.8816
D123	D(32,29,30,35)	-60.4779	D275	D(92,95,96,99)	-1.7031
D124	D(4,36,84,85)	-53.2999	D276	D(97,95,96,98)	-0.6027
D125	D(4,36,84,86)	125.5717	D277	D(97,95,96,99)	179.8126
D126	D(13,36,84,85)	128.3174	D278	D(92,95,97,100)	-178.057
D127	D(13,36,84,86)	-52.811	D279	D(92,95,97,101)	3.3313
D128	D(11,37,38,40)	178.3014	D280	D(96,95,97,100)	0.4532
D129	D(11,37,38,41)	-3.4529	D281	D(96,95,97,101)	-178.159
D130	D(39,37,38,40)	0.4308	D282	D(95,96,98,102)	0.3666
D131	D(39,37,38,41)	178.6765	D283	D(95,96,98,103)	-179.401
D132	D(11,37,39,42)	-177.461	D284	D(99,96,98,102)	179.9523
D133	D(11,37,39,43)	0.2274	D285	D(99,96,98,103)	0.1843
D134	D(38,37,39,42)	0.3849	D286	D(95,97,100,102)	-0.0662
D135	D(38,37,39,43)	178.0737	D287	D(95,97,100,104)	-179.537
D136	D(37,38,40,44)	-0.8148	D288	D(101,97,100,102)	178.5518
D137	D(37,38,40,45)	178.6558	D289	D(101,97,100,104)	-0.9185
D138	D(41,38,40,44)	-179.068	D290	D(96,98,102,100)	0.0336
D139	D(41,38,40,45)	0.4025	D291	D(96,98,102,105)	179.8227
D140	D(37,39,42,44)	-0.8268	D292	D(103,98,102,100)	179.8018
D141	D(37,39,42,46)	178.4598	D293	D(103,98,102,105)	-0.4091
D142	D(43,39,42,44)	-178.536	D294	D(97,100,102,98)	-0.1826

D143	D(43,39,42,46)	0.7508	D295	D(97,100,102,105)	-179.98
D144	D(38,40,44,42)	0.3666	D296	D(104,100,102,98)	179.2956
D145	D(38,40,44,47)	-179.697	D297	D(104,100,102,105)	-0.5019
D146	D(45,40,44,42)	-179.103	D298	D(98,102,105,106)	179.9419
D147	D(45,40,44,47)	0.8334	D299	D(98,102,105,107)	-0.0174
D148	D(39,42,44,40)	0.4364	D300	D(100,102,105,106)	-0.2673
D149	D(39,42,44,47)	-179.5	D301	D(100,102,105,107)	179.7734
D150	D(46,42,44,40)	-178.849	D302	D(102,105,107,108)	179.9137
D151	D(46,42,44,47)	1.215	D303	D(106,105,107,108)	-0.0468
D152	D(40,44,47,48)	28.6436			

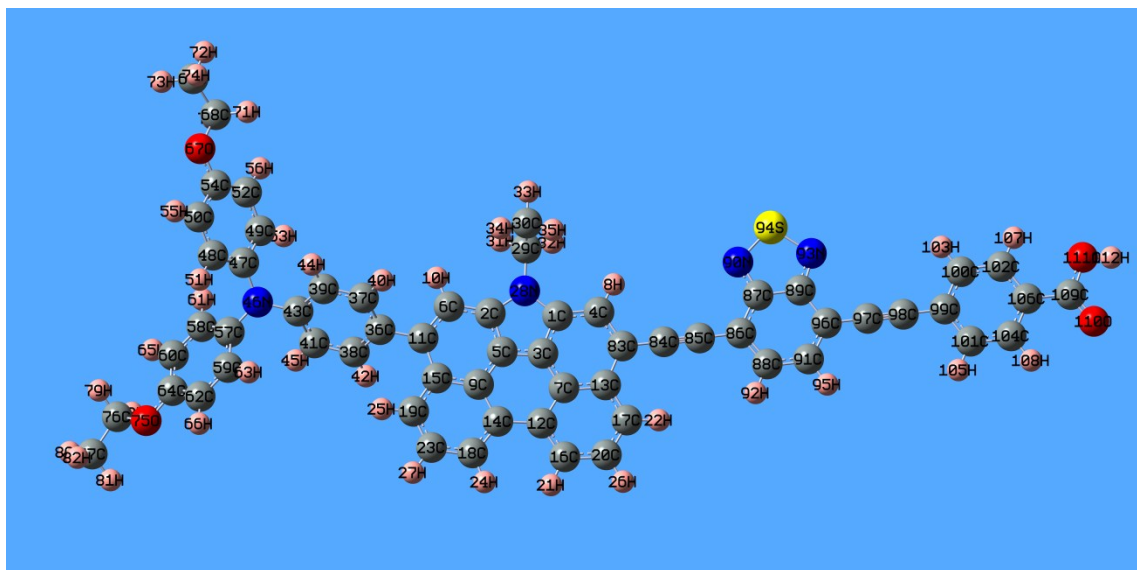


Fig. S33. Geometry of the S_0 state of **C287** in THF optimized at the B3LYP/6-311G(d,p) level of theory.

Table S15. Geometry Parameters and Mulliken Atomic Charges of the S₀ State of **C287** in THF Computed at the B3LYP/6-311G(d,p) Level of Theory

Center number	Atom	Coordinates [Å]			Mulliken atomic charges
		x	y	z	
1	C	-0.96535	0.056644	-0.06566	0.270601
2	C	1.314424	0.142095	-0.09062	0.278689
3	C	-0.46701	-1.20975	-0.35902	-0.11927
4	C	-2.36417	0.182262	-0.00875	0.0303
5	C	0.911219	-1.15611	-0.37077	-0.18915
6	C	2.710349	0.369993	-0.04863	-0.01885
7	C	-1.17709	-2.37314	-0.60492	-0.04098
8	H	-2.86189	1.1189	0.209102	0.114759
9	C	1.709929	-2.25878	-0.62577	-0.0081
10	H	3.125227	1.341262	0.191484	0.112413
11	C	3.587943	-0.69454	-0.28957	-0.00609
12	C	-0.43496	-3.56662	-0.89054	0.053713
13	C	-2.59013	-2.27555	-0.5552	-0.00607
14	C	1.058424	-3.50465	-0.91	0.042632
15	C	3.114398	-2.04353	-0.60254	-0.01744
16	C	-1.20805	-4.70164	-1.13132	-0.09859
17	C	-3.30694	-3.46209	-0.80887	-0.06983
18	C	1.909398	-4.57045	-1.19742	-0.10029
19	C	3.90814	-3.167	-0.92878	-0.10458
20	C	-2.61419	-4.63474	-1.08735	-0.08107
21	H	-0.7421	-5.65405	-1.35523	0.101116
22	H	-4.39022	-3.46458	-0.78795	0.109189
23	C	3.304691	-4.38682	-1.21079	-0.08002
24	H	1.512815	-5.55263	-1.42699	0.101486
25	H	4.986519	-3.08786	-0.97093	0.112017

26	H	-3.17824	-5.54062	-1.27967	0.108311
27	H	3.93399	-5.23456	-1.45784	0.10745
28	N	0.149349	0.899412	0.111592	-0.58085
29	C	0.098785	2.336679	0.376385	-0.10018
30	C	0.071504	3.187141	-0.89543	-0.28129
31	H	0.965745	2.590736	0.989993	0.138921
32	H	-0.78633	2.529146	0.986176	0.13915
33	H	0.035693	4.247161	-0.63172	0.120389
34	H	0.964511	3.015385	-1.50051	0.118039
35	H	-0.80672	2.956107	-1.50245	0.118789
36	C	5.045561	-0.4104	-0.22191	-0.11831
37	C	5.604252	0.662998	-0.93338	-0.08269
38	C	5.914934	-1.16238	0.584208	-0.08976
39	C	6.956484	0.967343	-0.85678	-0.12115
40	H	4.971052	1.255177	-1.58498	0.104468
41	C	7.265943	-0.85788	0.682567	-0.11935
42	H	5.521969	-1.97978	1.177842	0.111246
43	C	7.819659	0.213557	-0.04161	0.19626
44	H	7.351604	1.789549	-1.43952	0.120351
45	H	7.897742	-1.4467	1.335192	0.121206
46	N	9.188974	0.519637	0.046675	-0.49673
47	C	9.658225	1.852415	-0.16057	0.064375
48	C	10.70361	2.104071	-1.06087	-0.07754
49	C	9.105506	2.928671	0.535668	-0.06522
50	C	11.17814	3.39207	-1.25298	-0.11091
51	H	11.14613	1.280746	-1.60894	0.111557
52	C	9.562009	4.231	0.333008	-0.14294
53	H	8.303709	2.75205	1.242791	0.112498
54	C	10.60828	4.471162	-0.56345	0.180462

55	H	11.98654	3.588806	-1.94716	0.110171
56	H	9.106012	5.039112	0.888256	0.125875
57	C	10.14781	-0.49377	0.35165	0.062739
58	C	11.07731	-0.30808	1.375539	-0.07856
59	C	10.19443	-1.68598	-0.38655	-0.06346
60	C	12.04023	-1.27609	1.662274	-0.14379
61	H	11.05554	0.607015	1.955483	0.111875
62	C	11.13408	-2.6619	-0.09553	-0.10947
63	H	9.487444	-1.84459	-1.19223	0.112895
64	C	12.07054	-2.46652	0.929794	0.180126
65	H	12.74609	-1.0932	2.460777	0.125718
66	H	11.1724	-3.58337	-0.66434	0.110674
67	O	11.13801	5.698	-0.832	-0.37055
68	C	10.60597	6.8482	-0.15793	-0.05035
69	C	11.37342	8.059639	-0.64918	-0.29688
70	H	10.71997	6.72472	0.92496	0.121245
71	H	9.53751	6.943875	-0.38206	0.120816
72	H	10.99828	8.96111	-0.1589	0.117504
73	H	12.43739	7.960679	-0.42302	0.116688
74	H	11.25636	8.179271	-1.72851	0.116732
75	O	12.95897	-3.48084	1.128593	-0.37034
76	C	13.94156	-3.34855	2.166754	-0.0508
77	C	14.78646	-4.60707	2.158908	-0.29676
78	H	13.43976	-3.21919	3.132342	0.121471
79	H	14.5574	-2.46188	1.978472	0.121062
80	H	15.54883	-4.54722	2.939266	0.117541
81	H	14.16876	-5.48816	2.346233	0.116675
82	H	15.28669	-4.73047	1.195844	0.11672
83	C	-3.15752	-0.96129	-0.24843	-0.10588

84	C	-4.56245	-0.81831	-0.18923	0.008334
85	C	-5.76973	-0.69157	-0.13768	0.052818
86	C	-7.16696	-0.52754	-0.07319	-0.21905
87	C	-7.7451	0.752492	0.245179	0.154627
88	C	-8.05913	-1.56704	-0.30646	-0.03033
89	C	-9.18025	0.921329	0.312377	0.154876
90	N	-7.06775	1.871485	0.502757	-0.48692
91	C	-9.45879	-1.40076	-0.24075	-0.01968
92	H	-7.66621	-2.54635	-0.54895	0.119799
93	N	-9.55304	2.164559	0.619151	-0.48876
94	S	-8.17814	3.038944	0.805274	0.565941
95	H	-10.0896	-2.25924	-0.43548	0.115033
96	C	-10.0607	-0.187	0.061801	-0.21701
97	C	-11.4627	-0.03008	0.124905	0.140356
98	C	-12.6656	0.110047	0.179671	0.025884
99	C	-14.0724	0.28461	0.246841	-0.17851
100	C	-14.6191	1.547966	0.547414	-0.03321
101	C	-14.9433	-0.79918	0.015067	-0.03598
102	C	-15.9929	1.720488	0.613857	-0.02758
103	H	-13.955	2.384206	0.726299	0.117591
104	C	-16.3147	-0.61952	0.083358	-0.03427
105	H	-14.5309	-1.77319	-0.21639	0.116862
106	C	-16.8523	0.638541	0.382506	-0.20227
107	H	-16.4045	2.693772	0.844909	0.120507
108	H	-16.9879	-1.44868	-0.09344	0.116603
109	C	-18.3306	0.775336	0.442792	0.431247
110	O	-19.1143	-0.12871	0.250047	-0.36757
111	O	-18.7329	2.029311	0.739015	-0.33998
112	H	-19.7019	2.023998	0.756133	0.277791

Table S16. The Bond Lengths of the S₀ State of **C287** in THF Computed at the B3LYP/6-311G(d,p) Level of Theory.

Number	Name	Length[Å]	Number	Name	Length[Å]
R1	R(1,3)	1.3922	R63	R(50,55)	1.0836
R2	R(1,4)	1.4056	R64	R(52,54)	1.3986
R3	R(1,28)	1.4086	R65	R(52,56)	1.0813
R4	R(2,5)	1.3879	R66	R(54,67)	1.363
R5	R(2,6)	1.415	R67	R(57,58)	1.3953
R6	R(2,28)	1.4042	R68	R(57,59)	1.403
R7	R(3,5)	1.3793	R69	R(58,60)	1.3952
R8	R(3,7)	1.385	R70	R(58,61)	1.0836
R9	R(4,8)	1.0828	R71	R(59,62)	1.3857
R10	R(4,83)	1.4123	R72	R(59,63)	1.0836
R11	R(5,9)	1.3852	R73	R(60,64)	1.3981
R12	R(6,10)	1.0831	R74	R(60,65)	1.0813
R13	R(6,11)	1.4005	R75	R(62,64)	1.4023
R14	R(7,12)	1.4341	R76	R(62,66)	1.0836
R15	R(7,13)	1.4173	R77	R(64,75)	1.363
R16	R(9,14)	1.4344	R78	R(67,68)	1.4354
R17	R(9,15)	1.4211	R79	R(68,69)	1.5159
R18	R(11,15)	1.4635	R80	R(68,70)	1.0959
R19	R(11,36)	1.4866	R81	R(68,71)	1.0959
R20	R(12,14)	1.4948	R82	R(69,72)	1.0926
R21	R(12,16)	1.3942	R83	R(69,73)	1.0922
R22	R(13,17)	1.4093	R84	R(69,74)	1.0922
R23	R(13,83)	1.464	R85	R(75,76)	1.4355
R24	R(14,18)	1.3938	R86	R(76,77)	1.5158
R25	R(15,19)	1.4137	R87	R(76,78)	1.0959
R26	R(16,20)	1.4084	R88	R(76,79)	1.0958

R27	R(16,21)	1.0837	R89	R(77,80)	1.0926
R28	R(17,20)	1.3902	R90	R(77,81)	1.0922
R29	R(17,22)	1.0835	R91	R(77,82)	1.0922
R30	R(18,23)	1.4074	R92	R(83,84)	1.4134
R31	R(18,24)	1.0838	R93	R(84,85)	1.215
R32	R(19,23)	1.3898	R94	R(85,86)	1.4083
R33	R(19,25)	1.0821	R95	R(86,87)	1.4402
R34	R(20,26)	1.0843	R96	R(86,88)	1.3896
R35	R(23,27)	1.0843	R97	R(87,89)	1.4466
R36	R(28,29)	1.4623	R98	R(87,90)	1.3332
R37	R(29,30)	1.5302	R99	R(88,91)	1.411
R38	R(29,31)	1.0921	R100	R(88,92)	1.0827
R39	R(29,32)	1.0919	R101	R(89,93)	1.3337
R40	R(30,33)	1.0929	R102	R(89,96)	1.4375
R41	R(30,34)	1.0923	R103	R(90,94)	1.6393
R42	R(30,35)	1.0923	R104	R(91,95)	1.083
R43	R(36,37)	1.4038	R105	R(91,96)	1.3882
R44	R(36,38)	1.404	R106	R(93,94)	1.64
R45	R(37,39)	1.3882	R107	R(96,97)	1.4121
R46	R(37,40)	1.0845	R108	R(97,98)	1.2122
R47	R(38,41)	1.3884	R109	R(98,99)	1.4192
R48	R(38,42)	1.084	R110	R(99,100)	1.409
R49	R(39,43)	1.4063	R111	R(99,101)	1.4095
R50	R(39,44)	1.0825	R112	R(100,102)	1.3862
R51	R(41,43)	1.4068	R113	R(100,103)	1.0827
R52	R(41,45)	1.0825	R114	R(101,104)	1.3848
R53	R(43,46)	1.4059	R115	R(101,105)	1.0827
R54	R(46,47)	1.4281	R116	R(102,106)	1.4009
R55	R(46,57)	1.4281	R117	R(102,107)	1.0817

R56	R(47,48)	1.4024	R118	R(104,106)	1.4004
R57	R(47,49)	1.3959	R119	R(104,108)	1.0826
R58	R(48,50)	1.386	R120	R(106,109)	1.4858
R59	R(48,51)	1.0835	R121	R(109,110)	1.2119
R60	R(49,52)	1.3948	R122	R(109,111)	1.3498
R61	R(49,53)	1.0836	R123	R(111,112)	0.9692
R62	R(50,54)	1.4017			

Table S17. The Bond Angles of the S₀ State of **C287** in THF Computed at the B3LYP/6-311G(d,p) Level of Theory.

Number	Name	Angle [°]	Number	Name	Angle [°]
A1	A(3,1,4)	116.491	A106	A(49,52,54)	119.8879
A2	A(3,1,28)	106.7074	A107	A(49,52,56)	119.0224
A3	A(4,1,28)	136.799	A108	A(54,52,56)	121.0828
A4	A(5,2,6)	116.3092	A109	A(50,54,52)	119.1616
A5	A(5,2,28)	107.0065	A110	A(50,54,67)	115.9769
A6	A(6,2,28)	136.6659	A111	A(52,54,67)	124.8615
A7	A(1,3,5)	108.9103	A112	A(46,57,58)	120.6346
A8	A(1,3,7)	128.1704	A113	A(46,57,59)	120.8611
A9	A(5,3,7)	122.919	A114	A(58,57,59)	118.4927
A10	A(1,4,8)	122.8808	A115	A(57,58,60)	121.2156
A11	A(1,4,83)	118.6725	A116	A(57,58,61)	119.4553
A12	A(8,4,83)	118.4466	A117	A(60,58,61)	119.3281
A13	A(2,5,3)	108.9617	A118	A(57,59,62)	120.6981
A14	A(2,5,9)	127.8945	A119	A(57,59,63)	119.5984
A15	A(3,5,9)	123.1438	A120	A(62,59,63)	119.7035
A16	A(2,6,10)	121.9293	A121	A(58,60,64)	119.8733
A17	A(2,6,11)	119.3824	A122	A(58,60,65)	119.0086
A18	A(10,6,11)	118.6675	A123	A(64,60,65)	121.1142
A19	A(3,7,12)	117.9761	A124	A(59,62,64)	120.5496
A20	A(3,7,13)	116.5574	A125	A(59,62,66)	120.8425
A21	A(12,7,13)	125.4662	A126	A(64,62,66)	118.6
A22	A(5,9,14)	117.7747	A127	A(60,64,62)	119.1592
A23	A(5,9,15)	116.5049	A128	A(60,64,75)	124.8475
A24	A(14,9,15)	125.712	A129	A(62,64,75)	115.993
A25	A(6,11,15)	122.3197	A130	A(54,67,68)	118.99
A26	A(6,11,36)	117.4707	A131	A(67,68,69)	107.4897

A27	A(15,11,36)	120.2093	A132	A(67,68,70)	109.5845
A28	A(7,12,14)	119.0179	A133	A(67,68,71)	109.5902
A29	A(7,12,16)	115.1465	A134	A(69,68,70)	110.954
A30	A(14,12,16)	125.8355	A135	A(69,68,71)	110.9499
A31	A(7,13,17)	116.2841	A136	A(70,68,71)	108.2619
A32	A(7,13,83)	117.1014	A137	A(68,69,72)	109.8839
A33	A(17,13,83)	126.6146	A138	A(68,69,73)	110.7113
A34	A(9,14,12)	119.157	A139	A(68,69,74)	110.7025
A35	A(9,14,18)	115.3234	A140	A(72,69,73)	108.4394
A36	A(12,14,18)	125.5173	A141	A(72,69,74)	108.4374
A37	A(9,15,11)	117.5742	A142	A(73,69,74)	108.5994
A38	A(9,15,19)	115.5151	A143	A(64,75,76)	118.8858
A39	A(11,15,19)	126.8818	A144	A(75,76,77)	107.5329
A40	A(12,16,20)	120.6324	A145	A(75,76,78)	109.5525
A41	A(12,16,21)	120.8469	A146	A(75,76,79)	109.5706
A42	A(20,16,21)	118.5207	A147	A(77,76,78)	110.9645
A43	A(13,17,20)	119.5258	A148	A(77,76,79)	110.9556
A44	A(13,17,22)	120.4642	A149	A(78,76,79)	108.2531
A45	A(20,17,22)	120.01	A150	A(76,77,80)	109.8612
A46	A(14,18,23)	120.4962	A151	A(76,77,81)	110.7105
A47	A(14,18,24)	120.8795	A152	A(76,77,82)	110.7104
A48	A(23,18,24)	118.6199	A153	A(80,77,81)	108.4395
A49	A(15,19,23)	120.0346	A154	A(80,77,82)	108.4447
A50	A(15,19,25)	120.6894	A155	A(81,77,82)	108.6079
A51	A(23,19,25)	119.2737	A156	A(4,83,13)	123.0072
A52	A(16,20,17)	122.945	A157	A(4,83,84)	117.9923
A53	A(16,20,26)	118.3023	A158	A(13,83,84)	119.0004
A54	A(17,20,26)	118.7527	A159	A(85,86,87)	120.792
A55	A(18,23,19)	122.8909	A160	A(85,86,88)	122.8321

A56	A(18,23,27)	118.3947	A161	A(87,86,88)	116.3759
A57	A(19,23,27)	118.7134	A162	A(86,87,89)	120.8146
A58	A(1,28,2)	108.4082	A163	A(86,87,90)	125.7873
A59	A(1,28,29)	125.6941	A164	A(89,87,90)	113.3981
A60	A(2,28,29)	125.7916	A165	A(86,88,91)	122.7446
A61	A(28,29,30)	113.3516	A166	A(86,88,92)	118.7659
A62	A(28,29,31)	107.6339	A167	A(91,88,92)	118.4895
A63	A(28,29,32)	107.6013	A168	A(87,89,93)	113.3775
A64	A(30,29,31)	110.6002	A169	A(87,89,96)	120.6356
A65	A(30,29,32)	110.5935	A170	A(93,89,96)	125.9869
A66	A(31,29,32)	106.7809	A171	A(87,90,94)	106.8138
A67	A(29,30,33)	109.8212	A172	A(88,91,95)	118.424
A68	A(29,30,34)	111.0047	A173	A(88,91,96)	122.9093
A69	A(29,30,35)	111.018	A174	A(95,91,96)	118.6668
A70	A(33,30,34)	108.2381	A175	A(89,93,94)	106.7847
A71	A(33,30,35)	108.2337	A176	A(90,94,93)	99.6259
A72	A(34,30,35)	108.4348	A177	A(89,96,91)	116.52
A73	A(11,36,37)	120.8856	A178	A(89,96,97)	120.9731
A74	A(11,36,38)	122.0678	A179	A(91,96,97)	122.5069
A75	A(37,36,38)	117.0084	A180	A(98,99,100)	120.3322
A76	A(36,37,39)	121.8283	A181	A(98,99,101)	120.6724
A77	A(36,37,40)	119.3189	A182	A(100,99,101)	118.9953
A78	A(39,37,40)	118.8272	A183	A(99,100,102)	120.4217
A79	A(36,38,41)	121.7201	A184	A(99,100,103)	119.3249
A80	A(36,38,42)	119.5944	A185	A(102,100,103)	120.2534
A81	A(41,38,42)	118.6431	A186	A(99,101,104)	120.2673
A82	A(37,39,43)	120.8208	A187	A(99,101,105)	119.4399
A83	A(37,39,44)	119.4982	A188	A(104,101,105)	120.2928
A84	A(43,39,44)	119.6785	A189	A(100,102,106)	120.258

A85	A(38,41,43)	120.9025	A190	A(100,102,107)	119.9525
A86	A(38,41,45)	119.4297	A191	A(106,102,107)	119.7895
A87	A(43,41,45)	119.6636	A192	A(101,104,106)	120.48
A88	A(39,43,41)	117.7122	A193	A(101,104,108)	120.5593
A89	A(39,43,46)	121.1658	A194	A(106,104,108)	118.9606
A90	A(41,43,46)	121.122	A195	A(102,106,104)	119.5777
A91	A(43,46,47)	120.938	A196	A(102,106,109)	122.1739
A92	A(43,46,57)	120.8554	A197	A(104,106,109)	118.2485
A93	A(47,46,57)	118.2061	A198	A(106,109,110)	124.6318
A94	A(46,47,48)	120.3694	A199	A(106,109,111)	113.014
A95	A(46,47,49)	121.1353	A200	A(110,109,111)	122.3543
A96	A(48,47,49)	118.4896	A201	A(109,111,112)	107.2636
A97	A(47,48,50)	120.7274	A202	L(83,84,85,13,-1)	180.1842
A98	A(47,48,51)	119.525	A203	L(84,85,86,87,-1)	179.2726
A99	A(50,48,51)	119.7473	A204	L(96,97,98,91,-1)	180.2573
A100	A(47,49,52)	121.1862	A205	L(97,98,99,100,-1)	179.5549
A101	A(47,49,53)	119.5256	A206	L(83,84,85,13,-2)	180.0176
A102	A(52,49,53)	119.2874	A207	L(84,85,86,87,-2)	180.0512
A103	A(48,50,54)	120.5337	A208	L(96,97,98,91,-2)	180.0676
A104	A(48,50,55)	120.8607	A209	L(97,98,99,100,-2)	180.0524
A105	A(54,50,55)	118.6006			

Table S18. The Dihedral Angles of the S₀ State of **C287** in THF Computed at the B3LYP/6-311G(d,p) Level of Theory.

Number	Name	Dihedral Angle [°]	Number	Name	Dihedral Angle [°]
D1	D(4,1,3,5)	-179.8002	D153	D(43,46,47,49)	51.9698
D2	D(4,1,3,7)	0.0234	D154	D(57,46,47,48)	51.3365
D3	D(28,1,3,5)	-0.2901	D155	D(57,46,47,49)	-127.777
D4	D(28,1,3,7)	179.5335	D156	D(43,46,57,58)	-128.772
D5	D(3,1,4,8)	-179.8899	D157	D(43,46,57,59)	52.4855
D6	D(3,1,4,83)	-0.0182	D158	D(47,46,57,58)	50.9749
D7	D(28,1,4,8)	0.7956	D159	D(47,46,57,59)	-127.767
D8	D(28,1,4,83)	-179.3328	D160	D(46,47,48,50)	-179.038
D9	D(3,1,28,2)	0.6706	D161	D(46,47,48,51)	0.757
D10	D(3,1,28,29)	177.0935	D162	D(49,47,48,50)	0.0992
D11	D(4,1,28,2)	-179.9699	D163	D(49,47,48,51)	179.8938
D12	D(4,1,28,29)	-3.547	D164	D(46,47,49,52)	-179.929
D13	D(6,2,5,3)	179.316	D165	D(46,47,49,53)	-0.262
D14	D(6,2,5,9)	-0.5555	D166	D(48,47,49,52)	0.9409
D15	D(28,2,5,3)	0.6162	D167	D(48,47,49,53)	-179.392
D16	D(28,2,5,9)	-179.2553	D168	D(47,48,50,54)	-0.894
D17	D(5,2,6,10)	-178.1041	D169	D(47,48,50,55)	179.9261
D18	D(5,2,6,11)	0.2139	D170	D(51,48,50,54)	179.3119
D19	D(28,2,6,10)	0.084	D171	D(51,48,50,55)	0.1319
D20	D(28,2,6,11)	178.402	D172	D(47,49,52,54)	-1.1838
D21	D(5,2,28,1)	-0.7944	D173	D(47,49,52,56)	179.7537
D22	D(5,2,28,29)	-177.2129	D174	D(53,49,52,54)	179.1483
D23	D(6,2,28,1)	-179.096	D175	D(53,49,52,56)	0.0858
D24	D(6,2,28,29)	4.4855	D176	D(48,50,54,52)	0.6508
D25	D(1,3,5,2)	-0.204	D177	D(48,50,54,67)	-179.4
D26	D(1,3,5,9)	179.6749	D178	D(55,50,54,52)	179.849

D27	D(7,3,5,2)	179.9612	D179	D(55,50,54,67)	-0.2021
D28	D(7,3,5,9)	-0.1599	D180	D(49,52,54,50)	0.376
D29	D(1,3,7,12)	179.8394	D181	D(49,52,54,67)	-179.568
D30	D(1,3,7,13)	0.03	D182	D(56,52,54,50)	179.4188
D31	D(5,3,7,12)	-0.3594	D183	D(56,52,54,67)	-0.5251
D32	D(5,3,7,13)	179.8312	D184	D(50,54,67,68)	-179.782
D33	D(1,4,83,13)	-0.0388	D185	D(52,54,67,68)	0.1638
D34	D(1,4,83,84)	-179.9229	D186	D(46,57,58,60)	-178.415
D35	D(8,4,83,13)	179.8386	D187	D(46,57,58,61)	1.2181
D36	D(8,4,83,84)	-0.0455	D188	D(59,57,58,60)	0.3565
D37	D(2,5,9,14)	-179.1483	D189	D(59,57,58,61)	179.9896
D38	D(2,5,9,15)	-0.1434	D190	D(46,57,59,62)	179.4121
D39	D(3,5,9,14)	0.9969	D191	D(46,57,59,63)	-0.6202
D40	D(3,5,9,15)	-179.9982	D192	D(58,57,59,62)	0.6436
D41	D(2,6,11,15)	0.7801	D193	D(58,57,59,63)	-179.389
D42	D(2,6,11,36)	-179.4232	D194	D(57,58,60,64)	-0.9848
D43	D(10,6,11,15)	179.1531	D195	D(57,58,60,65)	179.7266
D44	D(10,6,11,36)	-1.0502	D196	D(61,58,60,64)	179.3817
D45	D(3,7,12,14)	0.0204	D197	D(61,58,60,65)	0.093
D46	D(3,7,12,16)	-179.8802	D198	D(57,59,62,64)	-1.0151
D47	D(13,7,12,14)	179.811	D199	D(57,59,62,66)	-179.979
D48	D(13,7,12,16)	-0.0896	D200	D(63,59,62,64)	179.0173
D49	D(3,7,13,17)	179.8786	D201	D(63,59,62,66)	0.0529
D50	D(3,7,13,83)	-0.0826	D202	D(58,60,64,62)	0.6103
D51	D(12,7,13,17)	0.0853	D203	D(58,60,64,75)	-179.604
D52	D(12,7,13,83)	-179.8759	D204	D(65,60,64,62)	179.8836
D53	D(5,9,14,12)	-1.2812	D205	D(65,60,64,75)	-0.3306
D54	D(5,9,14,18)	178.193	D206	D(59,62,64,60)	0.3779
D55	D(15,9,14,12)	179.8155	D207	D(59,62,64,75)	-179.426

D56	D(15,9,14,18)	-0.7103	D208	D(66,62,64,60)	179.3652
D57	D(5,9,15,11)	1.1088	D209	D(66,62,64,75)	-0.4392
D58	D(5,9,15,19)	-177.0699	D210	D(60,64,75,76)	0.4836
D59	D(14,9,15,11)	-179.9755	D211	D(62,64,75,76)	-179.725
D60	D(14,9,15,19)	1.8458	D212	D(54,67,68,69)	-179.821
D61	D(6,11,15,9)	-1.4683	D213	D(54,67,68,70)	59.5101
D62	D(6,11,15,19)	176.4767	D214	D(54,67,68,71)	-59.1529
D63	D(36,11,15,9)	178.7404	D215	D(67,68,69,72)	179.9934
D64	D(36,11,15,19)	-3.3146	D216	D(67,68,69,73)	-60.2485
D65	D(6,11,36,37)	-50.7825	D217	D(67,68,69,74)	60.2432
D66	D(6,11,36,38)	126.9008	D218	D(70,68,69,72)	-60.2051
D67	D(15,11,36,37)	129.0187	D219	D(70,68,69,73)	59.553
D68	D(15,11,36,38)	-53.298	D220	D(70,68,69,74)	-179.955
D69	D(7,12,14,9)	0.8025	D221	D(71,68,69,72)	60.1873
D70	D(7,12,14,18)	-178.6136	D222	D(71,68,69,73)	179.9454
D71	D(16,12,14,9)	-179.3085	D223	D(71,68,69,74)	-59.5629
D72	D(16,12,14,18)	1.2754	D224	D(64,75,76,77)	-179.868
D73	D(7,12,16,20)	0.0236	D225	D(64,75,76,78)	59.4429
D74	D(7,12,16,21)	-179.9171	D226	D(64,75,76,79)	-59.1784
D75	D(14,12,16,20)	-179.8691	D227	D(75,76,77,80)	-179.893
D76	D(14,12,16,21)	0.1902	D228	D(75,76,77,81)	-60.1495
D77	D(7,13,17,20)	-0.0141	D229	D(75,76,77,82)	60.3575
D78	D(7,13,17,22)	179.9848	D230	D(78,76,77,80)	-60.0974
D79	D(83,13,17,20)	179.9428	D231	D(78,76,77,81)	59.6459
D80	D(83,13,17,22)	-0.0583	D232	D(78,76,77,82)	-179.847
D81	D(7,13,83,4)	0.0914	D233	D(79,76,77,80)	60.2948
D82	D(7,13,83,84)	179.9744	D234	D(79,76,77,81)	-179.962
D83	D(17,13,83,4)	-179.8653	D235	D(79,76,77,82)	-59.4549
D84	D(17,13,83,84)	0.0177	D236	D(4,83,86,87)	-0.9614

D85	D(9,14,18,23)	-0.6613	D237	D(4,83,86,88)	179.0974
D86	D(9,14,18,24)	-179.8912	D238	D(13,83,86,87)	179.1418
D87	D(12,14,18,23)	178.7745	D239	D(13,83,86,88)	-0.7995
D88	D(12,14,18,24)	-0.4553	D240	D(85,86,87,89)	-179.961
D89	D(9,15,19,23)	-1.618	D241	D(85,86,87,90)	-0.0228
D90	D(9,15,19,25)	177.8312	D242	D(88,86,87,89)	-0.0009
D91	D(11,15,19,23)	-179.5996	D243	D(88,86,87,90)	179.9373
D92	D(11,15,19,25)	-0.1505	D244	D(85,86,88,91)	179.9701
D93	D(12,16,20,17)	0.0418	D245	D(85,86,88,92)	-0.0309
D94	D(12,16,20,26)	-179.9451	D246	D(87,86,88,91)	0.0108
D95	D(21,16,20,17)	179.9839	D247	D(87,86,88,92)	-179.99
D96	D(21,16,20,26)	-0.0031	D248	D(86,87,89,93)	179.9519
D97	D(13,17,20,16)	-0.0469	D249	D(86,87,89,96)	-0.0238
D98	D(13,17,20,26)	179.94	D250	D(90,87,89,93)	0.0065
D99	D(22,17,20,16)	179.9542	D251	D(90,87,89,96)	-179.969
D100	D(22,17,20,26)	-0.0589	D252	D(86,87,90,94)	-179.932
D101	D(14,18,23,19)	0.8302	D253	D(89,87,90,94)	0.0104
D102	D(14,18,23,27)	-178.8104	D254	D(86,88,91,95)	179.9924
D103	D(24,18,23,19)	-179.9228	D255	D(86,88,91,96)	0.0043
D104	D(24,18,23,27)	0.4366	D256	D(92,88,91,95)	-0.0066
D105	D(15,19,23,18)	0.3965	D257	D(92,88,91,96)	-179.995
D106	D(15,19,23,27)	-179.9639	D258	D(87,89,93,94)	-0.0198
D107	D(25,19,23,18)	-179.0604	D259	D(96,89,93,94)	179.9543
D108	D(25,19,23,27)	0.5792	D260	D(87,89,96,91)	0.0375
D109	D(1,28,29,30)	-88.6598	D261	D(87,89,96,97)	-179.972
D110	D(1,28,29,31)	148.6995	D262	D(93,89,96,91)	-179.935
D111	D(1,28,29,32)	33.9489	D263	D(93,89,96,97)	0.0557
D112	D(2,28,29,30)	87.1549	D264	D(87,90,94,93)	-0.0197
D113	D(2,28,29,31)	-35.4858	D265	D(88,91,96,89)	-0.0284

D114	D(2,28,29,32)	-150.2364	D266	D(88,91,96,97)	179.9811
D115	D(28,29,30,33)	-179.9105	D267	D(95,91,96,89)	179.9836
D116	D(28,29,30,34)	-60.2572	D268	D(95,91,96,97)	-0.0069
D117	D(28,29,30,35)	60.4334	D269	D(89,93,94,90)	0.0233
D118	D(31,29,30,33)	-58.9275	D270	D(89,96,99,100)	0.5827
D119	D(31,29,30,34)	60.7257	D271	D(89,96,99,101)	-179.397
D120	D(31,29,30,35)	-178.5837	D272	D(91,96,99,100)	-179.411
D121	D(32,29,30,33)	59.1537	D273	D(91,96,99,101)	0.6096
D122	D(32,29,30,34)	178.807	D274	D(98,99,100,102)	-179.983
D123	D(32,29,30,35)	-60.5024	D275	D(98,99,100,103)	0.0184
D124	D(11,36,37,39)	178.2846	D276	D(101,99,100,102)	0.0053
D125	D(11,36,37,40)	-3.5739	D277	D(101,99,100,103)	-179.994
D126	D(38,36,37,39)	0.4881	D278	D(98,99,101,104)	179.9704
D127	D(38,36,37,40)	178.6297	D279	D(98,99,101,105)	-0.0065
D128	D(11,36,38,41)	-177.4265	D280	D(100,99,101,104)	-0.0174
D129	D(11,36,38,42)	0.1735	D281	D(100,99,101,105)	-179.994
D130	D(37,36,38,41)	0.3419	D282	D(99,100,102,106)	0.0051
D131	D(37,36,38,42)	177.9419	D283	D(99,100,102,107)	-179.981
D132	D(36,37,39,43)	-0.8392	D284	D(103,100,102,106)	-179.996
D133	D(36,37,39,44)	178.5826	D285	D(103,100,102,107)	0.0181
D134	D(40,37,39,43)	-178.9897	D286	D(99,101,104,106)	0.019
D135	D(40,37,39,44)	0.4322	D287	D(99,101,104,108)	-179.977
D136	D(36,38,41,43)	-0.8308	D288	D(105,101,104,106)	179.9957
D137	D(36,38,41,45)	178.4216	D289	D(105,101,104,108)	-0.0002
D138	D(42,38,41,43)	-178.4529	D290	D(100,102,106,104)	-0.0037
D139	D(42,38,41,45)	0.7995	D291	D(100,102,106,109)	-180
D140	D(37,39,43,41)	0.3428	D292	D(107,102,106,104)	179.9825
D141	D(37,39,43,46)	-179.6717	D293	D(107,102,106,109)	-0.0136
D142	D(44,39,43,41)	-179.078	D294	D(101,104,106,102)	-0.0084

D143	D(44,39,43,46)	0.9075	D295	D(101,104,106,109)	179.9878
D144	D(38,41,43,39)	0.4746	D296	D(108,104,106,102)	179.9876
D145	D(38,41,43,46)	-179.5109	D297	D(108,104,106,109)	-0.0162
D146	D(45,41,43,39)	-178.7761	D298	D(102,106,109,110)	179.9598
D147	D(45,41,43,46)	1.2384	D299	D(102,106,109,111)	-0.0334
D148	D(39,43,46,47)	27.8836	D300	D(104,106,109,110)	-0.0363
D149	D(39,43,46,57)	-152.3761	D301	D(104,106,109,111)	179.9705
D150	D(41,43,46,47)	-152.1314	D302	D(106,109,111,112)	179.9664
D151	D(41,43,46,57)	27.6089	D303	D(110,109,111,112)	-0.0269
D152	D(43,46,47,48)	-128.9165			

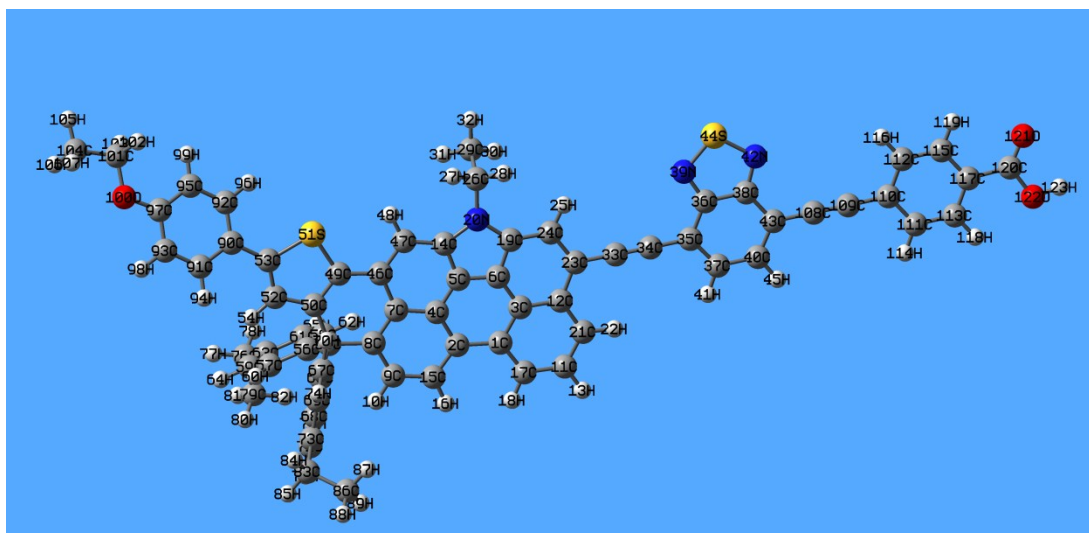


Fig. S34. Geometry of the S₀ state of C288 in THF optimized at the B3LYP/6-311G(d,p) level of theory.

Table S19. Geometry Parameters and Mulliken Atomic Charges of the S₀ State of **C288** in THF Computed at the B3LYP/6-311G(d,p) Level of Theory

Center number	Atom	Coordinates [Å]			Mulliken atomic charges
		x	y	z	
1	C	-0.13058	-2.64474	0.126132	0.038284
2	C	1.34888	-2.45306	0.117259	0.085615
3	C	-0.97887	-1.48899	0.065908	-0.03222
4	C	1.878512	-1.12978	0.042007	-0.01326
5	C	0.98767	-0.06912	-0.0089	-0.17387
6	C	-0.37838	-0.24158	0.003514	-0.13334
7	C	3.253307	-0.79197	0.023179	0.002948
8	C	4.187433	-1.84695	0.083797	-0.09287
9	C	3.683222	-3.14988	0.16452	0.009417
10	H	4.38084	-3.97579	0.219183	0.09723
11	C	-2.20461	-3.91731	0.192372	-0.08161
12	C	-2.39588	-1.50878	0.066965	-0.01021
13	H	-2.68502	-4.88809	0.242856	0.108552
14	C	1.274025	1.289339	-0.07858	0.262924
15	C	2.315225	-3.45957	0.181153	-0.09696
16	H	2.027582	-4.50271	0.245606	0.099689
17	C	-0.79751	-3.86811	0.189786	-0.09651
18	H	-0.24573	-4.79963	0.23826	0.101133
19	C	-0.99121	1.007926	-0.06149	0.270675
20	N	0.043388	1.963057	-0.12138	-0.58348
21	C	-3.00172	-2.77937	0.133164	-0.06929
22	H	-4.08111	-2.87343	0.13804	0.109044
23	C	-3.08188	-0.21659	-1.3E-05	-0.10427
24	C	-2.39557	1.017418	-0.06294	0.030321
25	H	-2.97747	1.929442	-0.10836	0.114895

26	C	-0.13784	3.414226	-0.13918	-0.1015
27	H	0.687817	3.843498	-0.71045	0.13915
28	H	-1.05152	3.62563	-0.69854	0.139912
29	C	-0.2064	4.033969	1.258016	-0.28017
30	H	-1.04244	3.622847	1.828101	0.118961
31	H	0.715153	3.84958	1.814718	0.118187
32	H	-0.3464	5.114807	1.176819	0.120918
33	C	-4.49431	-0.18957	0.000644	0.007411
34	C	-5.70918	-0.16008	0.00132	0.052872
35	C	-7.11612	-0.10695	0.001942	-0.21929
36	C	-7.80609	1.156187	-0.05219	0.154488
37	C	-7.91361	-1.24405	0.053463	-0.03076
38	C	-9.25167	1.211515	-0.05132	0.154828
39	N	-7.23033	2.357252	-0.10722	-0.48706
40	C	-9.32333	-1.18832	0.054103	-0.01994
41	H	-7.4353	-2.21447	0.09505	0.119468
42	N	-9.73363	2.453868	-0.1059	-0.48871
43	C	-10.0312	0.00498	0.003649	-0.21774
44	S	-8.44095	3.461865	-0.15412	0.56573
45	H	-9.8758	-2.11885	0.096301	0.114776
46	C	3.599738	0.623184	-0.04715	0.075415
47	C	2.641681	1.645552	-0.09569	-0.03277
48	H	2.963992	2.678822	-0.14251	0.119627
49	C	5.022682	0.881758	-0.0638	-0.29299
50	C	6.002604	-0.0878	-0.03195	0.035582
51	S	5.724129	2.48509	-0.16233	0.277798
52	C	7.314802	0.463673	-0.07988	0.04384
53	C	7.354692	1.833184	-0.14877	-0.28119
54	H	8.212261	-0.1367	-0.04302	0.106821

55	C	5.711146	-1.59159	0.056523	-0.18708
56	C	6.368591	-2.0806	1.376211	-0.04855
57	C	7.723199	-2.43109	1.442299	-0.08279
58	C	5.647227	-2.07123	2.575699	-0.05331
59	C	8.322335	-2.77394	2.651957	-0.0857
60	H	8.32541	-2.44513	0.542725	0.11573
61	C	6.249229	-2.41334	3.784255	-0.08846
62	H	4.601592	-1.78989	2.57394	0.109338
63	C	7.597707	-2.77598	3.847961	-0.09381
64	H	9.374264	-3.04221	2.6631	0.097986
65	H	5.657264	-2.39298	4.69408	0.09778
66	C	6.256226	-2.30636	-1.21009	-0.04544
67	C	6.266942	-1.64227	-2.4423	-0.05181
68	C	6.653019	-3.64941	-1.19821	-0.08582
69	C	6.66408	-2.28998	-3.60963	-0.08926
70	H	5.963751	-0.60364	-2.49565	0.111358
71	C	7.050371	-4.29427	-2.36707	-0.08522
72	H	6.667705	-4.20459	-0.26907	0.116347
73	C	7.064701	-3.62929	-3.597	-0.09394
74	H	6.665684	-1.73965	-4.54544	0.097429
75	H	7.36118	-5.3333	-2.31698	0.097858
76	C	8.23857	-3.1894	5.153984	-0.1993
77	H	9.296709	-2.91002	5.143268	0.119521
78	H	7.774843	-2.63562	5.976257	0.119817
79	C	8.11695	-4.69846	5.42962	-0.28232
80	H	8.600864	-5.28063	4.64059	0.108046
81	H	8.588845	-4.95886	6.381048	0.111772
82	H	7.068127	-5.00398	5.476324	0.108469
83	C	7.464398	-4.343	-4.86925	-0.19941

84	H	7.915268	-3.62545	-5.56161	0.119319
85	H	8.233999	-5.08711	-4.64129	0.119636
86	C	6.279687	-5.03879	-5.56282	-0.28235
87	H	5.505265	-4.31588	-5.83338	0.10881
88	H	6.606321	-5.54378	-6.47606	0.111599
89	H	5.825821	-5.78589	-4.906	0.108371
90	C	8.525447	2.710301	-0.22142	-0.02375
91	C	9.745996	2.232287	-0.73923	-0.0539
92	C	8.486546	4.040685	0.216804	-0.10499
93	C	10.86494	3.042899	-0.80326	-0.11585
94	H	9.810931	1.217779	-1.11379	0.110492
95	C	9.604039	4.869482	0.149601	-0.14947
96	H	7.571682	4.442527	0.637732	0.11665
97	C	10.80801	4.373041	-0.36051	0.188067
98	H	11.79894	2.671036	-1.20735	0.111527
99	H	9.525418	5.888058	0.503546	0.126717
100	O	11.95903	5.08697	-0.4703	-0.36539
101	C	11.97166	6.46227	-0.05236	-0.05305
102	H	11.22767	7.02518	-0.6266	0.123898
103	H	11.70726	6.524205	1.008982	0.124006
104	C	13.36769	6.998903	-0.29716	-0.29684
105	H	13.42101	8.046688	0.00782	0.118369
106	H	14.105	6.434006	0.277368	0.117636
107	H	13.62631	6.933795	-1.35627	0.117573
108	C	-11.4425	0.051404	0.00519	0.140831
109	C	-12.6539	0.097732	0.006353	0.025947
110	C	-14.0715	0.163507	0.006597	-0.17864
111	C	-14.8454	-1.01314	0.040117	-0.03587
112	C	-14.7265	1.411466	-0.02724	-0.03349

113	C	-16.23	-0.94309	0.039132	-0.0265
114	H	-14.3495	-1.97526	0.066452	0.116393
115	C	-16.1098	1.473822	-0.02743	-0.03532
116	H	-14.1376	2.319624	-0.05316	0.117916
117	C	-16.8739	0.300591	0.00533	-0.20247
118	H	-16.8168	-1.85148	0.064655	0.120218
119	H	-16.6176	2.429583	-0.05324	0.116809
120	C	-18.3545	0.424859	0.002605	0.431158
121	O	-18.9576	1.475712	-0.02276	-0.36744
122	O	-18.9838	-0.76898	0.031324	-0.34015
123	H	-19.9368	-0.59236	0.026616	0.277792

Table S20. The Bond Lengths of the S₀ State of **C288** in THF Computed at the B3LYP/6-311G(d,p) Level of Theory.

Number	Name	Length[Å]	Number	Name	Length[Å]
R1	R(1,2)	1.4919	R69	R(56,57)	1.4008
R2	R(1,3)	1.4349	R70	R(56,58)	1.3997
R3	R(1,17)	1.3948	R71	R(57,59)	1.3928
R4	R(2,4)	1.4273	R72	R(57,60)	1.0826
R5	R(2,15)	1.3968	R73	R(58,61)	1.3929
R6	R(3,6)	1.3858	R74	R(58,62)	1.0828
R7	R(3,12)	1.4171	R75	R(59,63)	1.3984
R8	R(4,5)	1.3861	R76	R(59,64)	1.0857
R9	R(4,7)	1.4158	R77	R(61,63)	1.3978
R10	R(5,6)	1.3769	R78	R(61,65)	1.0856
R11	R(5,14)	1.3901	R79	R(63,76)	1.5124
R12	R(6,19)	1.3932	R80	R(66,67)	1.3998
R13	R(7,8)	1.4104	R81	R(66,68)	1.4005
R14	R(7,46)	1.4586	R82	R(67,69)	1.3928
R15	R(8,9)	1.3994	R83	R(67,70)	1.0833
R16	R(8,55)	1.5452	R84	R(68,71)	1.3928
R17	R(9,10)	1.0825	R85	R(68,72)	1.0825
R18	R(9,15)	1.4027	R86	R(69,73)	1.398
R19	R(11,13)	1.0843	R87	R(69,74)	1.0856
R20	R(11,17)	1.408	R88	R(71,73)	1.3983
R21	R(11,21)	1.3906	R89	R(71,75)	1.0857
R22	R(12,21)	1.4092	R90	R(73,83)	1.5125
R23	R(12,23)	1.4645	R91	R(76,77)	1.0945
R24	R(14,20)	1.4036	R92	R(76,78)	1.0945
R25	R(14,47)	1.4134	R93	R(76,79)	1.5388
R26	R(15,16)	1.084	R94	R(79,80)	1.0935

R27	R(17,18)	1.0838	R95	R(79,81)	1.0935
R28	R(19,20)	1.4093	R96	R(79,82)	1.0934
R29	R(19,24)	1.4044	R97	R(83,84)	1.0943
R30	R(20,26)	1.4625	R98	R(83,85)	1.0945
R31	R(21,22)	1.0835	R99	R(83,86)	1.5391
R32	R(23,24)	1.4134	R100	R(86,87)	1.0934
R33	R(23,33)	1.4127	R101	R(86,88)	1.0935
R34	R(24,25)	1.0828	R102	R(86,89)	1.0934
R35	R(26,27)	1.0919	R103	R(90,91)	1.4094
R36	R(26,28)	1.092	R104	R(90,92)	1.4012
R37	R(26,29)	1.53	R105	R(91,93)	1.3832
R38	R(29,30)	1.0922	R106	R(91,94)	1.0834
R39	R(29,31)	1.0923	R107	R(92,95)	1.3929
R40	R(29,32)	1.0929	R108	R(92,96)	1.0843
R41	R(33,34)	1.2152	R109	R(93,97)	1.403
R42	R(34,35)	1.4079	R110	R(93,98)	1.0835
R43	R(35,36)	1.4403	R111	R(95,97)	1.3986
R44	R(35,37)	1.3898	R112	R(95,99)	1.0812
R45	R(36,38)	1.4466	R113	R(97,100)	1.3589
R46	R(36,39)	1.3331	R114	R(100,101)	1.4375
R47	R(37,40)	1.4108	R115	R(101,102)	1.0955
R48	R(37,41)	1.0827	R116	R(101,103)	1.0955
R49	R(38,42)	1.3337	R117	R(101,104)	1.5155
R50	R(38,43)	1.4375	R118	R(104,105)	1.0926
R51	R(39,44)	1.6395	R119	R(104,106)	1.0922
R52	R(40,43)	1.3884	R120	R(104,107)	1.0922
R53	R(40,45)	1.083	R121	R(108,109)	1.2123
R54	R(42,44)	1.6399	R122	R(109,110)	1.4191
R55	R(43,108)	1.4121	R123	R(110,111)	1.4088

R56	R(46,47)	1.402	R124	R(110,112)	1.4098
R57	R(46,49)	1.4463	R125	R(111,113)	1.3863
R58	R(47,48)	1.0834	R126	R(111,114)	1.0828
R59	R(49,50)	1.3789	R127	R(112,115)	1.3847
R60	R(49,51)	1.7528	R128	R(112,116)	1.0827
R61	R(50,52)	1.4242	R129	R(113,117)	1.4009
R62	R(50,55)	1.5343	R130	R(113,118)	1.0817
R63	R(51,53)	1.7561	R131	R(115,117)	1.4005
R64	R(52,53)	1.3718	R132	R(115,119)	1.0826
R65	R(52,54)	1.0804	R133	R(117,120)	1.4858
R66	R(53,90)	1.4647	R134	R(120,121)	1.2119
R67	R(55,56)	1.5534	R135	R(120,122)	1.3499
R68	R(55,66)	1.5532	R136	R(122,123)	0.9692

Table S21. The Bond Angles of the S₀ State of **C288** in THF Computed at the B3LYP/6-311G(d,p) Level of Theory.

Number	Name	Angle [°]	Number	Name	Angle [°]
A1	A(2,1,3)	118.8509	A119	A(56,57,59)	121.2365
A2	A(2,1,17)	125.9545	A120	A(56,57,60)	120.1295
A3	A(3,1,17)	115.1946	A121	A(59,57,60)	118.6332
A4	A(1,2,4)	119.1709	A122	A(56,58,61)	121.2765
A5	A(1,2,15)	126.3873	A123	A(56,58,62)	119.8683
A6	A(4,2,15)	114.4415	A124	A(61,58,62)	118.8546
A7	A(1,3,6)	118.0815	A125	A(57,59,63)	121.3507
A8	A(1,3,12)	125.4395	A126	A(57,59,64)	119.1146
A9	A(6,3,12)	116.4788	A127	A(63,59,64)	119.5345
A10	A(2,4,5)	118.2226	A128	A(58,61,63)	121.3463
A11	A(2,4,7)	125.6072	A129	A(58,61,65)	119.1362
A12	A(5,4,7)	116.1687	A130	A(63,61,65)	119.5171
A13	A(4,5,6)	122.7819	A131	A(59,63,61)	117.4211
A14	A(4,5,14)	128.1174	A132	A(59,63,76)	121.2913
A15	A(6,5,14)	109.1007	A133	A(61,63,76)	121.2687
A16	A(3,6,5)	122.89	A134	A(55,66,67)	120.1473
A17	A(3,6,19)	128.2267	A135	A(55,66,68)	122.2657
A18	A(5,6,19)	108.8827	A136	A(67,66,68)	117.4033
A19	A(4,7,8)	117.6506	A137	A(66,67,69)	121.287
A20	A(4,7,46)	117.5647	A138	A(66,67,70)	119.74
A21	A(8,7,46)	124.7829	A139	A(69,67,70)	118.9729
A22	A(7,8,9)	117.4047	A140	A(66,68,71)	121.1788
A23	A(7,8,55)	121.9197	A141	A(66,68,72)	120.1964
A24	A(9,8,55)	120.6751	A142	A(71,68,72)	118.6203
A25	A(8,9,10)	118.7561	A143	A(67,69,73)	121.3096
A26	A(8,9,15)	123.8915	A144	A(67,69,74)	119.1519

A27	A(10,9,15)	117.3523	A145	A(73,69,74)	119.5379
A28	A(13,11,17)	118.3043	A146	A(68,71,73)	121.3934
A29	A(13,11,21)	118.7269	A147	A(68,71,75)	119.0813
A30	A(17,11,21)	122.9688	A148	A(73,71,75)	119.524
A31	A(3,12,21)	116.2636	A149	A(69,73,71)	117.4268
A32	A(3,12,23)	117.1301	A150	A(69,73,83)	121.3449
A33	A(21,12,23)	126.6063	A151	A(71,73,83)	121.2101
A34	A(5,14,20)	106.8571	A152	A(63,76,77)	109.3567
A35	A(5,14,47)	116.5029	A153	A(63,76,78)	109.3253
A36	A(20,14,47)	136.6391	A154	A(63,76,79)	112.9081
A37	A(2,15,9)	121.0033	A155	A(77,76,78)	106.7285
A38	A(2,15,16)	120.8357	A156	A(77,76,79)	109.1773
A39	A(9,15,16)	118.1611	A157	A(78,76,79)	109.1558
A40	A(1,17,11)	120.5702	A158	A(76,79,80)	110.9701
A41	A(1,17,18)	120.8291	A159	A(76,79,81)	110.8104
A42	A(11,17,18)	118.6007	A160	A(76,79,82)	110.9449
A43	A(6,19,20)	106.6715	A161	A(80,79,81)	108.0635
A44	A(6,19,24)	116.4852	A162	A(80,79,82)	107.8522
A45	A(20,19,24)	136.8408	A163	A(81,79,82)	108.0741
A46	A(14,20,19)	108.4837	A164	A(73,83,84)	109.3688
A47	A(14,20,26)	125.8211	A165	A(73,83,85)	109.3555
A48	A(19,20,26)	125.5909	A166	A(73,83,86)	112.8901
A49	A(11,21,12)	119.5633	A167	A(84,83,85)	106.7296
A50	A(11,21,22)	119.9871	A168	A(84,83,86)	109.1758
A51	A(12,21,22)	120.4496	A169	A(85,83,86)	109.1329
A52	A(12,23,24)	123.0193	A170	A(83,86,87)	110.9659
A53	A(12,23,33)	119.0243	A171	A(83,86,88)	110.8064
A54	A(24,23,33)	117.9562	A172	A(83,86,89)	110.9595
A55	A(19,24,23)	118.6597	A173	A(87,86,88)	108.0736

A56	A(19,24,25)	122.8966	A174	A(87,86,89)	107.8422
A57	A(23,24,25)	118.4436	A175	A(88,86,89)	108.0672
A58	A(20,26,27)	107.6223	A176	A(53,90,91)	120.4872
A59	A(20,26,28)	107.5782	A177	A(53,90,92)	122.0636
A60	A(20,26,29)	113.35	A178	A(91,90,92)	117.4489
A61	A(27,26,28)	106.7728	A179	A(90,91,93)	121.2525
A62	A(27,26,29)	110.6339	A180	A(90,91,94)	119.7706
A63	A(28,26,29)	110.602	A181	A(93,91,94)	118.9661
A64	A(26,29,30)	111.0059	A182	A(90,92,95)	121.8407
A65	A(26,29,31)	111.0529	A183	A(90,92,96)	119.7823
A66	A(26,29,32)	109.7846	A184	A(95,92,96)	118.3683
A67	A(30,29,31)	108.435	A185	A(91,93,97)	120.5416
A68	A(30,29,32)	108.2386	A186	A(91,93,98)	120.8958
A69	A(31,29,32)	108.2331	A187	A(97,93,98)	118.5576
A70	A(34,35,36)	120.7823	A188	A(92,95,97)	119.802
A71	A(34,35,37)	122.8566	A189	A(92,95,99)	119.1057
A72	A(36,35,37)	116.3611	A190	A(97,95,99)	121.0899
A73	A(35,36,38)	120.8111	A191	A(93,97,95)	119.1118
A74	A(35,36,39)	125.7887	A192	A(93,97,100)	115.99
A75	A(38,36,39)	113.4002	A193	A(95,97,100)	124.8981
A76	A(35,37,40)	122.7556	A194	A(97,100,101)	119.1179
A77	A(35,37,41)	118.7666	A195	A(100,101,102)	109.466
A78	A(40,37,41)	118.4777	A196	A(100,101,103)	109.4902
A79	A(36,38,42)	113.3725	A197	A(100,101,104)	107.4521
A80	A(36,38,43)	120.6506	A198	A(102,101,103)	108.3531
A81	A(42,38,43)	125.9769	A199	A(102,101,104)	111.0366
A82	A(36,39,44)	106.8159	A200	A(103,101,104)	111.0251
A83	A(37,40,43)	122.9145	A201	A(101,104,105)	109.8431
A84	A(37,40,45)	118.4124	A202	A(101,104,106)	110.7169

A85	A(43,40,45)	118.6731	A203	A(101,104,107)	110.7109
A86	A(38,42,44)	106.7933	A204	A(105,104,106)	108.4356
A87	A(38,43,40)	116.5071	A205	A(105,104,107)	108.4395
A88	A(38,43,108)	120.9593	A206	A(106,104,107)	108.6285
A89	A(40,43,108)	122.5336	A207	A(109,110,111)	120.6705
A90	A(39,44,42)	99.6181	A208	A(109,110,112)	120.3425
A91	A(7,46,47)	123.1527	A209	A(111,110,112)	118.987
A92	A(7,46,49)	114.0582	A210	A(110,111,113)	120.4295
A93	A(47,46,49)	122.789	A211	A(110,111,114)	119.412
A94	A(14,47,46)	118.4931	A212	A(113,111,114)	120.1585
A95	A(14,47,48)	121.9224	A213	A(110,112,115)	120.2676
A96	A(46,47,48)	119.5843	A214	A(110,112,116)	119.3579
A97	A(46,49,50)	124.9735	A215	A(115,112,116)	120.3745
A98	A(46,49,51)	123.9095	A216	A(111,113,117)	120.2584
A99	A(50,49,51)	111.1052	A217	A(111,113,118)	119.9549
A100	A(49,50,52)	112.4415	A218	A(117,113,118)	119.7867
A101	A(49,50,55)	123.7444	A219	A(112,115,117)	120.4839
A102	A(52,50,55)	123.8124	A220	A(112,115,119)	120.5529
A103	A(49,51,53)	91.8094	A221	A(117,115,119)	118.9632
A104	A(50,52,53)	114.5224	A222	A(113,117,115)	119.5736
A105	A(50,52,54)	123.3013	A223	A(113,117,120)	122.1608
A106	A(53,52,54)	122.1625	A224	A(115,117,120)	118.2655
A107	A(51,53,52)	110.1199	A225	A(117,120,121)	124.6448
A108	A(51,53,90)	121.2984	A226	A(117,120,122)	112.9908
A109	A(52,53,90)	128.5774	A227	A(121,120,122)	122.3644
A110	A(8,55,50)	110.5057	A228	A(120,122,123)	107.286
A111	A(8,55,56)	110.5077	A229	L(23,33,34,24,-1)	179.7061
A112	A(8,55,66)	106.5237	A230	L(33,34,35,36,-1)	179.2283
A113	A(50,55,56)	106.0891	A231	L(43,108,109,38,-1)	179.6938

A114	A(50,55,66)	109.7157	A232	L(108,109,110,111,-1)	180.4674
A115	A(56,55,66)	113.5417	A233	L(23,33,34,24,-2)	180.0386
A116	A(55,56,57)	121.8799	A234	L(33,34,35,36,-2)	180.0535
A117	A(55,56,58)	120.5178	A235	L(43,108,109,38,-2)	180.0118
A118	A(57,56,58)	117.3626	A236	L(108,109,110,111,-2)	180.0664

Table S22. The Dihedral Angles of the S₀ State of **C288** in THF Computed at the B3LYP/6-311G(d,p) Level of Theory.

Number	Name	Dihedral Angle [°]	Number	Name	Dihedral Angle [°]
D1	D(3,1,2,4)	-0.3366	D177	D(55,50,52,54)	-0.9228
D2	D(3,1,2,15)	179.4255	D178	D(49,50,55,8)	0.7728
D3	D(17,1,2,4)	179.7132	D179	D(49,50,55,56)	-119.039
D4	D(17,1,2,15)	-0.5246	D180	D(49,50,55,66)	117.9399
D5	D(2,1,3,6)	-0.0731	D181	D(52,50,55,8)	-179.736
D6	D(2,1,3,12)	-179.9499	D182	D(52,50,55,56)	60.4526
D7	D(17,1,3,6)	179.8823	D183	D(52,50,55,66)	-62.5685
D8	D(17,1,3,12)	0.0055	D184	D(49,51,53,52)	0.3345
D9	D(2,1,17,11)	179.9466	D185	D(49,51,53,90)	179.6407
D10	D(2,1,17,18)	-0.0518	D186	D(50,52,53,51)	-0.2241
D11	D(3,1,17,11)	-0.0051	D187	D(50,52,53,90)	-179.466
D12	D(3,1,17,18)	179.9965	D188	D(54,52,53,51)	-178.916
D13	D(1,2,4,5)	0.5297	D189	D(54,52,53,90)	1.8428
D14	D(1,2,4,7)	-179.93	D190	D(51,53,90,91)	-154.321
D15	D(15,2,4,5)	-179.26	D191	D(51,53,90,92)	25.8645
D16	D(15,2,4,7)	0.2804	D192	D(52,53,90,91)	24.8456
D17	D(1,2,15,9)	179.987	D193	D(52,53,90,92)	-154.969
D18	D(1,2,15,16)	-0.0485	D194	D(8,55,56,57)	155.9652
D19	D(4,2,15,9)	-0.2411	D195	D(8,55,56,58)	-29.809
D20	D(4,2,15,16)	179.7234	D196	D(50,55,56,57)	-84.2243
D21	D(1,3,6,5)	0.2968	D197	D(50,55,56,58)	90.0015
D22	D(1,3,6,19)	179.978	D198	D(66,55,56,57)	36.3493
D23	D(12,3,6,5)	-179.8154	D199	D(66,55,56,58)	-149.425
D24	D(12,3,6,19)	-0.1341	D200	D(8,55,66,67)	87.1409
D25	D(1,3,12,21)	-0.0016	D201	D(8,55,66,68)	-87.8031
D26	D(1,3,12,23)	179.9841	D202	D(50,55,66,67)	-32.4931

D27	D(6,3,12,21)	-179.8801	D203	D(50,55,66,68)	152.563
D28	D(6,3,12,23)	0.1056	D204	D(56,55,66,67)	-150.999
D29	D(2,4,5,6)	-0.3294	D205	D(56,55,66,68)	34.0573
D30	D(2,4,5,14)	179.6998	D206	D(55,56,57,59)	175.2472
D31	D(7,4,5,6)	-179.9131	D207	D(55,56,57,60)	-5.1068
D32	D(7,4,5,14)	0.1162	D208	D(58,56,57,59)	0.8476
D33	D(2,4,7,8)	-0.0094	D209	D(58,56,57,60)	-179.506
D34	D(2,4,7,46)	-179.5481	D210	D(55,56,58,61)	-175.268
D35	D(5,4,7,8)	179.5393	D211	D(55,56,58,62)	4.4729
D36	D(5,4,7,46)	0.0006	D212	D(57,56,58,61)	-0.7877
D37	D(4,5,6,3)	-0.0982	D213	D(57,56,58,62)	178.9528
D38	D(4,5,6,19)	-179.8335	D214	D(56,57,59,63)	-0.2944
D39	D(14,5,6,3)	179.8775	D215	D(56,57,59,64)	179.8561
D40	D(14,5,6,19)	0.1422	D216	D(60,57,59,63)	-179.946
D41	D(4,5,14,20)	179.4656	D217	D(60,57,59,64)	0.2049
D42	D(4,5,14,47)	-0.2356	D218	D(56,58,61,63)	0.172
D43	D(6,5,14,20)	-0.5084	D219	D(56,58,61,65)	179.9187
D44	D(6,5,14,47)	179.7904	D220	D(62,58,61,63)	-179.571
D45	D(3,6,19,20)	-179.4363	D221	D(62,58,61,65)	0.1757
D46	D(3,6,19,24)	0.0883	D222	D(57,59,63,61)	-0.3391
D47	D(5,6,19,20)	0.2808	D223	D(57,59,63,76)	178.0976
D48	D(5,6,19,24)	179.8054	D224	D(64,59,63,61)	179.5098
D49	D(4,7,8,9)	-0.2962	D225	D(64,59,63,76)	-2.0534
D50	D(4,7,8,55)	179.4238	D226	D(58,61,63,59)	0.3995
D51	D(46,7,8,9)	179.2059	D227	D(58,61,63,76)	-178.038
D52	D(46,7,8,55)	-1.0741	D228	D(65,61,63,59)	-179.346
D53	D(4,7,46,47)	0.0179	D229	D(65,61,63,76)	2.2166
D54	D(4,7,46,49)	-179.9285	D230	D(59,63,76,77)	32.2453
D55	D(8,7,46,47)	-179.4846	D231	D(59,63,76,78)	148.7645

D56	D(8,7,46,49)	0.569	D232	D(59,63,76,79)	-89.5201
D57	D(7,8,9,10)	-179.5729	D233	D(61,63,76,77)	-149.378
D58	D(7,8,9,15)	0.342	D234	D(61,63,76,78)	-32.8589
D59	D(55,8,9,10)	0.7034	D235	D(61,63,76,79)	88.8565
D60	D(55,8,9,15)	-179.3817	D236	D(55,66,67,69)	-175.543
D61	D(7,8,55,50)	0.3828	D237	D(55,66,67,70)	4.5966
D62	D(7,8,55,56)	117.4986	D238	D(68,66,67,69)	-0.3576
D63	D(7,8,55,66)	-118.7373	D239	D(68,66,67,70)	179.7815
D64	D(9,8,55,50)	-179.9061	D240	D(55,66,68,71)	175.4694
D65	D(9,8,55,56)	-62.7904	D241	D(55,66,68,72)	-5.3073
D66	D(9,8,55,66)	60.9737	D242	D(67,66,68,71)	0.3938
D67	D(8,9,15,2)	-0.0592	D243	D(67,66,68,72)	179.6171
D68	D(8,9,15,16)	179.9754	D244	D(66,67,69,73)	0.1417
D69	D(10,9,15,2)	179.8568	D245	D(66,67,69,74)	-179.578
D70	D(10,9,15,16)	-0.1086	D246	D(70,67,69,73)	-179.996
D71	D(13,11,17,1)	179.9984	D247	D(70,67,69,74)	0.2844
D72	D(13,11,17,18)	-0.0031	D248	D(66,68,71,73)	-0.2159
D73	D(21,11,17,1)	0.0012	D249	D(66,68,71,75)	179.3699
D74	D(21,11,17,18)	179.9997	D250	D(72,68,71,73)	-179.451
D75	D(13,11,21,12)	-179.9942	D251	D(72,68,71,75)	0.1347
D76	D(13,11,21,22)	0.0004	D252	D(67,69,73,71)	0.0499
D77	D(17,11,21,12)	0.003	D253	D(67,69,73,83)	178.5134
D78	D(17,11,21,22)	179.9976	D254	D(74,69,73,71)	179.7681
D79	D(3,12,21,11)	-0.0027	D255	D(74,69,73,83)	-1.7685
D80	D(3,12,21,22)	-179.9973	D256	D(68,71,73,69)	-0.0132
D81	D(23,12,21,11)	-179.9869	D257	D(68,71,73,83)	-178.479
D82	D(23,12,21,22)	0.0185	D258	D(75,71,73,69)	-179.597
D83	D(3,12,23,24)	-0.0514	D259	D(75,71,73,83)	1.937
D84	D(3,12,23,33)	-179.9061	D260	D(69,73,83,84)	31.3147

D85	D(21,12,23,24)	179.9327	D261	D(69,73,83,85)	147.8593
D86	D(21,12,23,33)	0.078	D262	D(69,73,83,86)	-90.4452
D87	D(5,14,20,19)	0.6809	D263	D(71,73,83,84)	-150.28
D88	D(5,14,20,26)	177.1253	D264	D(71,73,83,85)	-33.7353
D89	D(47,14,20,19)	-179.7086	D265	D(71,73,83,86)	87.9602
D90	D(47,14,20,26)	-3.2642	D266	D(63,76,79,80)	60.0533
D91	D(5,14,47,46)	0.2301	D267	D(63,76,79,81)	-179.887
D92	D(5,14,47,48)	-179.6215	D268	D(63,76,79,82)	-59.8299
D93	D(20,14,47,46)	-179.3534	D269	D(77,76,79,80)	-61.8132
D94	D(20,14,47,48)	0.795	D270	D(77,76,79,81)	58.2469
D95	D(6,19,20,14)	-0.5955	D271	D(77,76,79,82)	178.3036
D96	D(6,19,20,26)	-177.0502	D272	D(78,76,79,80)	-178.136
D97	D(24,19,20,14)	-179.9734	D273	D(78,76,79,81)	-58.0757
D98	D(24,19,20,26)	3.5719	D274	D(78,76,79,82)	61.9811
D99	D(6,19,24,23)	-0.0183	D275	D(73,83,86,87)	59.9961
D100	D(6,19,24,25)	179.8667	D276	D(73,83,86,88)	-179.937
D101	D(20,19,24,23)	179.3159	D277	D(73,83,86,89)	-59.8814
D102	D(20,19,24,25)	-0.7991	D278	D(84,83,86,87)	-61.8725
D103	D(14,20,26,27)	34.6837	D279	D(84,83,86,88)	58.1949
D104	D(14,20,26,28)	149.4077	D280	D(84,83,86,89)	178.2499
D105	D(14,20,26,29)	-87.9904	D281	D(85,83,86,87)	-178.183
D106	D(19,20,26,27)	-149.4641	D282	D(85,83,86,88)	-58.1154
D107	D(19,20,26,28)	-34.7401	D283	D(85,83,86,89)	61.9397
D108	D(19,20,26,29)	87.8618	D284	D(53,90,91,93)	-179.37
D109	D(12,23,24,19)	0.0059	D285	D(53,90,91,94)	1.8434
D110	D(12,23,24,25)	-179.8843	D286	D(92,90,91,93)	0.4531
D111	D(33,23,24,19)	179.8621	D287	D(92,90,91,94)	-178.334
D112	D(33,23,24,25)	-0.0281	D288	D(53,90,92,95)	179.7855
D113	D(12,23,35,36)	179.4805	D289	D(53,90,92,96)	0.8706

D114	D(12,23,35,37)	-0.4988	D290	D(91,90,92,95)	-0.0342
D115	D(24,23,35,36)	-0.3546	D291	D(91,90,92,96)	-178.949
D116	D(24,23,35,37)	179.666	D292	D(90,91,93,97)	-0.4977
D117	D(20,26,29,30)	-60.115	D293	D(90,91,93,98)	-179.67
D118	D(20,26,29,31)	60.6002	D294	D(94,91,93,97)	178.2988
D119	D(20,26,29,32)	-179.7459	D295	D(94,91,93,98)	-0.8734
D120	D(27,26,29,30)	178.8937	D296	D(90,92,95,97)	-0.3395
D121	D(27,26,29,31)	-60.3911	D297	D(90,92,95,99)	-179.785
D122	D(27,26,29,32)	59.2628	D298	D(96,92,95,97)	178.5902
D123	D(28,26,29,30)	60.7959	D299	D(96,92,95,99)	-0.855
D124	D(28,26,29,31)	-178.4888	D300	D(91,93,97,95)	0.1117
D125	D(28,26,29,32)	-58.835	D301	D(91,93,97,100)	-179.763
D126	D(34,35,36,38)	-179.9878	D302	D(98,93,97,95)	179.303
D127	D(34,35,36,39)	0.0516	D303	D(98,93,97,100)	-0.5718
D128	D(37,35,36,38)	0.0209	D304	D(92,95,97,93)	0.2998
D129	D(37,35,36,39)	-179.9396	D305	D(92,95,97,100)	-179.837
D130	D(34,35,37,40)	179.9939	D306	D(99,95,97,93)	179.7337
D131	D(34,35,37,41)	0.0029	D307	D(99,95,97,100)	-0.4035
D132	D(36,35,37,40)	-0.0151	D308	D(93,97,100,101)	179.2125
D133	D(36,35,37,41)	179.994	D309	D(95,97,100,101)	-0.6541
D134	D(35,36,38,42)	-179.9584	D310	D(97,100,101,102)	-58.9305
D135	D(35,36,38,43)	-0.0015	D311	D(97,100,101,103)	59.713
D136	D(39,36,38,42)	0.0068	D312	D(97,100,101,104)	-179.609
D137	D(39,36,38,43)	179.9637	D313	D(100,101,104,105)	179.9683
D138	D(35,36,39,44)	179.9518	D314	D(100,101,104,106)	-60.301
D139	D(38,36,39,44)	-0.0113	D315	D(100,101,104,107)	60.2364
D140	D(35,37,40,43)	-0.0117	D316	D(102,101,104,105)	60.2865
D141	D(35,37,40,45)	-179.9846	D317	D(102,101,104,106)	-179.983
D142	D(41,37,40,43)	179.9793	D318	D(102,101,104,107)	-59.4454

D143	D(41,37,40,45)	0.0064	D319	D(103,101,104,105)	-60.3272
D144	D(36,38,42,44)	0.0015	D320	D(103,101,104,106)	59.4035
D145	D(43,38,42,44)	-179.9528	D321	D(103,101,104,107)	179.941
D146	D(36,38,43,40)	-0.0241	D322	D(109,110,111,113)	-179.949
D147	D(36,38,43,108)	179.9831	D323	D(109,110,111,114)	0.0342
D148	D(42,38,43,40)	179.927	D324	D(112,110,111,113)	0.0312
D149	D(42,38,43,108)	-0.0657	D325	D(112,110,111,114)	-179.986
D150	D(36,39,44,42)	0.0109	D326	D(109,110,112,115)	179.9771
D151	D(37,40,43,38)	0.0311	D327	D(109,110,112,116)	-0.0162
D152	D(37,40,43,108)	-179.9763	D328	D(111,110,112,115)	-0.0032
D153	D(45,40,43,38)	-179.9961	D329	D(111,110,112,116)	-179.997
D154	D(45,40,43,108)	-0.0035	D330	D(110,111,113,117)	-0.0281
D155	D(38,42,44,39)	-0.0072	D331	D(110,111,113,118)	179.9788
D156	D(38,43,110,111)	179.0455	D332	D(114,111,113,117)	179.9887
D157	D(38,43,110,112)	-0.9103	D333	D(114,111,113,118)	-0.0044
D158	D(40,43,110,111)	-0.9408	D334	D(110,112,115,117)	-0.0279
D159	D(40,43,110,112)	179.1034	D335	D(110,112,115,119)	179.9942
D160	D(7,46,47,14)	-0.1384	D336	D(116,112,115,117)	179.9653
D161	D(7,46,47,48)	179.7168	D337	D(116,112,115,119)	-0.0126
D162	D(49,46,47,14)	179.8034	D338	D(111,113,117,115)	-0.003
D163	D(49,46,47,48)	-0.3414	D339	D(111,113,117,120)	179.9858
D164	D(7,46,49,50)	0.6553	D340	D(118,113,117,115)	179.9901
D165	D(7,46,49,51)	179.2925	D341	D(118,113,117,120)	-0.0211
D166	D(47,46,49,50)	-179.2913	D342	D(112,115,117,113)	0.0312
D167	D(47,46,49,51)	-0.6541	D343	D(112,115,117,120)	-179.958
D168	D(46,49,50,52)	179.0967	D344	D(119,115,117,113)	-179.991
D169	D(46,49,50,55)	-1.3602	D345	D(119,115,117,120)	0.0201
D170	D(51,49,50,52)	0.3091	D346	D(113,117,120,121)	179.8177
D171	D(51,49,50,55)	179.8521	D347	D(113,117,120,122)	-0.1984

D172	D(46,49,51,53)	-179.1724	D348	D(115,117,120,121)	-0.1933
D173	D(50,49,51,53)	-0.3694	D349	D(115,117,120,122)	179.7906
D174	D(49,50,52,53)	-0.0547	D350	D(117,120,122,123)	-179.961
D175	D(49,50,52,54)	178.6198	D351	D(121,120,122,123)	0.0239
D176	D(55,50,52,53)	-179.5974			

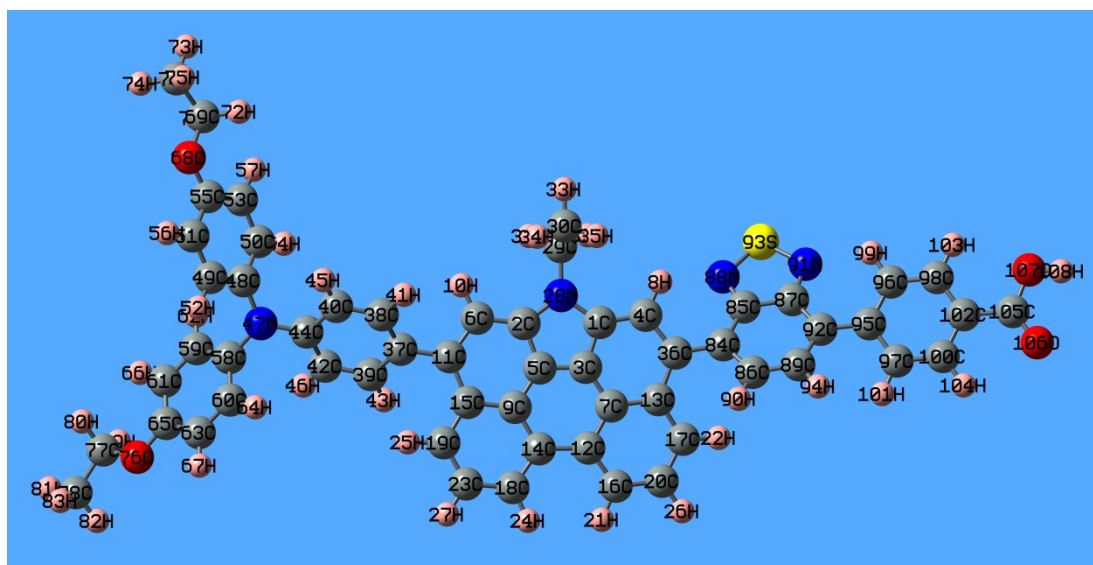


Fig. S35. Geometry of the S_1 state of **C286** in THF optimized at the TD-MPW1K/6-311G(d,p) level of theory.

Table S23. Geometry Parameters and Mulliken Atomic Charges of the S₁ State of **C286** in THF Computed at the TD-MPW1K/6-311G(d,p) Level of Theory

Center number	Atom	Coordinates [Å]			Mulliken atomic charges
		x	y	z	
1	C	-2.41678	0.334781	0.164108	0.278407
2	C	-0.16778	0.329292	-0.02136	0.309026
3	C	-1.99055	-0.95822	-0.1338	-0.23415
4	C	-3.77381	0.529672	0.311109	0.054152
5	C	-0.6387	-0.96385	-0.22857	-0.22408
6	C	1.212449	0.496721	-0.07013	-0.00538
7	C	-2.76011	-2.09287	-0.25674	-0.0192
8	H	-4.20258	1.494496	0.512045	0.147511
9	C	0.095296	-2.10387	-0.46685	-0.01933
10	H	1.680917	1.448457	0.120135	0.133772
11	C	2.031814	-0.61768	-0.30656	0.020309
12	C	-2.08323	-3.31624	-0.48184	0.060383
13	C	-4.14783	-1.92929	-0.08748	-0.04132
14	C	-0.6182	-3.31677	-0.62816	0.067243
15	C	1.492069	-1.94688	-0.5401	-0.02808
16	C	-2.89464	-4.44953	-0.51106	-0.11435
17	C	-4.88551	-3.11333	-0.06307	-0.14756
18	C	0.163434	-4.43102	-0.91979	-0.11148
19	C	2.207648	-3.09999	-0.88322	-0.12961
20	C	-4.25717	-4.3339	-0.2861	-0.07575
21	H	-2.47364	-5.42854	-0.67463	0.113127
22	H	-5.94041	-3.10487	0.15155	0.136717
23	C	1.541252	-4.30248	-1.05747	-0.08075
24	H	-0.2851	-5.4009	-1.06401	0.113556
25	H	3.27397	-3.0676	-1.03123	0.133533

26	H	-4.8566	-5.23033	-0.26845	0.121648
27	H	2.116514	-5.17699	-1.31772	0.120757
28	N	-1.27126	1.125823	0.233529	-0.69968
29	C	-1.2512	2.555564	0.454812	-0.13533
30	C	-1.36338	3.354608	-0.82698	-0.31501
31	H	-0.33059	2.794068	0.980315	0.155966
32	H	-2.06728	2.793269	1.131538	0.156499
33	H	-1.34239	4.417889	-0.60254	0.136414
34	H	-0.5379	3.131457	-1.498	0.133737
35	H	-2.29457	3.134123	-1.34237	0.134279
36	C	-4.65573	-0.57138	0.134297	0.057225
37	C	3.476635	-0.39776	-0.28991	-0.13612
38	C	4.038074	0.720748	-0.91209	-0.10396
39	C	4.350847	-1.25118	0.388453	-0.11829
40	C	5.389862	0.964496	-0.88258	-0.14559
41	H	3.402448	1.39236	-1.46864	0.124161
42	C	5.702858	-1.00738	0.441938	-0.14165
43	H	3.957514	-2.09528	0.932504	0.138026
44	C	6.257488	0.103829	-0.20127	0.239298
45	H	5.787907	1.8203	-1.40238	0.144839
46	H	6.34005	-1.67006	1.004052	0.145987
47	N	7.616938	0.34615	-0.16223	-0.57437
48	C	8.132358	1.651519	-0.34043	0.039715
49	C	9.123332	1.888282	-1.28716	-0.08035
50	C	7.684922	2.707152	0.434672	-0.07015
51	C	9.649904	3.148806	-1.44848	-0.12857
52	H	9.482581	1.072715	-1.89512	0.128963
53	C	8.195486	3.983328	0.26607	-0.15814
54	H	6.924012	2.534647	1.179844	0.131109

55	C	9.188018	4.211077	-0.67692	0.208457
56	H	10.4196	3.338176	-2.17954	0.1286
57	H	7.822233	4.781677	0.884385	0.148327
58	C	8.539419	-0.699	0.076731	0.046156
59	C	9.49389	-0.57692	1.070615	-0.0853
60	C	8.527235	-1.85207	-0.70232	-0.06834
61	C	10.42676	-1.5762	1.292229	-0.16247
62	H	9.515997	0.314468	1.67791	0.13011
63	C	9.438226	-2.85773	-0.47708	-0.1251
64	H	7.796169	-1.95586	-1.48891	0.132008
65	C	10.40032	-2.72916	0.520817	0.20825
66	H	11.15786	-1.44508	2.071501	0.147729
67	H	9.433926	-3.75312	-1.07793	0.129295
68	O	9.756885	5.405514	-0.91159	-0.39607
69	C	9.337186	6.518764	-0.14905	-0.08691
70	C	10.12971	7.710489	-0.60634	-0.33764
71	H	9.507398	6.322745	0.910203	0.137376
72	H	8.269082	6.68277	-0.29655	0.136936
73	H	9.834775	8.590478	-0.04099	0.133138
74	H	11.19289	7.54454	-0.45511	0.132821
75	H	9.955603	7.904939	-1.66116	0.132826
76	O	11.25314	-3.75828	0.658388	-0.39607
77	C	12.24806	-3.68503	1.659394	-0.0871
78	C	13.05557	-4.95035	1.594377	-0.33776
79	H	11.77702	-3.57461	2.636817	0.13754
80	H	12.87904	-2.81249	1.486363	0.137065
81	H	13.83336	-4.93245	2.353101	0.133147
82	H	12.42435	-5.81743	1.76907	0.132804
83	H	13.5268	-5.05481	0.620824	0.132817

84	C	-6.07155	-0.32262	0.123996	-0.02514
85	C	-6.68906	0.687685	0.925609	0.13642
86	C	-6.93509	-1.0175	-0.74364	-0.13468
87	C	-8.12153	0.915271	0.872546	0.15905
88	N	-6.07632	1.454725	1.807047	-0.57122
89	C	-8.2888	-0.78477	-0.80373	-0.0718
90	H	-6.50923	-1.70977	-1.45051	0.157138
91	N	-8.52089	1.844249	1.725241	-0.58607
92	C	-8.95125	0.158241	-0.00504	0.000081
93	S	-7.20603	2.395771	2.520383	0.609202
94	H	-8.85234	-1.32391	-1.54732	0.136424
95	C	-10.3886	0.334815	-0.10404	-0.02399
96	C	-11.029	1.528166	0.265295	-0.07096
97	C	-11.1994	-0.70066	-0.60204	-0.09929
98	C	-12.3898	1.681099	0.126688	-0.03557
99	H	-10.4415	2.337464	0.658963	0.144827
100	C	-12.5574	-0.54869	-0.73223	-0.04376
101	H	-10.759	-1.64957	-0.86027	0.131674
102	C	-13.1732	0.646559	-0.3736	-0.28579
103	H	-12.8533	2.613274	0.405399	0.130511
104	H	-13.1654	-1.35763	-1.10454	0.12818
105	C	-14.6273	0.763527	-0.53206	0.54139
106	O	-15.3416	-0.10413	-0.95989	-0.42206
107	O	-15.1071	1.946586	-0.15241	-0.3756
108	H	-16.0545	1.929318	-0.29283	0.290249

Table S24. The Bond Lengths of the S₁ State of **C286** in THF Computed at the TD-MPW1K/6-311G(d,p) Level of Theory.

Number	Name	Length[Å]	Number	Name	Length[Å]
R1	R(1,3)	1.3937	R61	R(50,53)	1.3848
R2	R(1,4)	1.3788	R62	R(50,54)	1.0789
R3	R(1,28)	1.3938	R63	R(51,55)	1.3918
R4	R(2,5)	1.3917	R64	R(51,56)	1.0783
R5	R(2,6)	1.3912	R65	R(53,55)	1.3879
R6	R(2,28)	1.3846	R66	R(53,57)	1.0766
R7	R(3,5)	1.3552	R67	R(55,68)	1.3436
R8	R(3,7)	1.3765	R68	R(58,59)	1.3834
R9	R(4,8)	1.0748	R69	R(58,60)	1.3916
R10	R(4,36)	1.4217	R70	R(59,61)	1.3849
R11	R(5,9)	1.3766	R71	R(59,62)	1.0788
R12	R(6,10)	1.0777	R72	R(60,63)	1.3755
R13	R(6,11)	1.4033	R73	R(60,64)	1.0789
R14	R(7,12)	1.4161	R74	R(61,65)	1.3875
R15	R(7,13)	1.4075	R75	R(61,66)	1.0766
R16	R(9,14)	1.4164	R76	R(63,65)	1.3921
R17	R(9,15)	1.4075	R77	R(63,67)	1.0783
R18	R(11,15)	1.4535	R78	R(65,76)	1.3436
R19	R(11,37)	1.4616	R79	R(68,69)	1.4131
R20	R(12,14)	1.4723	R80	R(69,70)	1.5025
R21	R(12,16)	1.3941	R81	R(69,71)	1.0906
R22	R(13,17)	1.3953	R82	R(69,72)	1.0906
R23	R(13,36)	1.4666	R83	R(70,73)	1.0867
R24	R(14,18)	1.392	R84	R(70,74)	1.0866
R25	R(15,19)	1.3998	R85	R(70,75)	1.0866
R26	R(16,20)	1.3858	R86	R(76,77)	1.4132

R27	R(16,21)	1.0782	R87	R(77,78)	1.5024
R28	R(17,20)	1.3908	R88	R(77,79)	1.0906
R29	R(17,22)	1.0765	R89	R(77,80)	1.0906
R30	R(18,23)	1.3906	R90	R(78,81)	1.0867
R31	R(18,24)	1.0783	R91	R(78,82)	1.0866
R32	R(19,23)	1.3858	R92	R(78,83)	1.0866
R33	R(19,25)	1.077	R93	R(84,85)	1.4299
R34	R(20,26)	1.0785	R94	R(84,86)	1.4076
R35	R(23,27)	1.0786	R95	R(85,87)	1.4514
R36	R(28,29)	1.4469	R96	R(85,88)	1.3194
R37	R(29,30)	1.5146	R97	R(86,89)	1.3749
R38	R(29,31)	1.0865	R98	R(86,90)	1.0772
R39	R(29,32)	1.0865	R99	R(87,91)	1.3227
R40	R(30,33)	1.0869	R100	R(87,92)	1.4254
R41	R(30,34)	1.087	R101	R(88,93)	1.6342
R42	R(30,35)	1.0869	R102	R(89,92)	1.4021
R43	R(36,84)	1.4375	R103	R(89,94)	1.0776
R44	R(37,38)	1.3976	R104	R(91,93)	1.6326
R45	R(37,39)	1.3974	R105	R(92,95)	1.4515
R46	R(38,40)	1.3739	R106	R(95,96)	1.4038
R47	R(38,41)	1.0793	R107	R(95,97)	1.4063
R48	R(39,42)	1.3749	R108	R(96,98)	1.3763
R49	R(39,43)	1.0785	R109	R(96,99)	1.0748
R50	R(40,44)	1.3992	R110	R(97,100)	1.3727
R51	R(40,45)	1.0775	R111	R(97,101)	1.0775
R52	R(42,44)	1.3986	R112	R(98,102)	1.3908
R53	R(42,46)	1.0776	R113	R(98,103)	1.0777
R54	R(44,47)	1.3814	R114	R(100,102)	1.3915
R55	R(47,48)	1.4147	R115	R(100,104)	1.0782

R56	R(47,58)	1.4144	R116	R(102,105)	1.4674
R57	R(48,49)	1.3908	R117	R(105,106)	1.2026
R58	R(48,50)	1.384	R118	R(105,107)	1.3319
R59	R(49,51)	1.3756	R119	R(107,108)	0.9579
R60	R(49,52)	1.0788			

Table S25. The Bond Angles of the S₁ State of **C286** in THF Computed at the TD-MPW1K/6-311G(d,p) Level of Theory.

Number	Name	Angle [°]	Number	Name	Angle [°]
A1	A(3,1,4)	117.0605	A102	A(51,49,52)	119.9467
A2	A(3,1,28)	106.6087	A103	A(48,50,53)	121.0335
A3	A(4,1,28)	136.3307	A104	A(48,50,54)	119.5297
A4	A(5,2,6)	116.2509	A105	A(53,50,54)	119.4365
A5	A(5,2,28)	106.9939	A106	A(49,51,55)	120.4878
A6	A(6,2,28)	136.7109	A107	A(49,51,56)	120.9093
A7	A(1,3,5)	108.8983	A108	A(55,51,56)	118.5999
A8	A(1,3,7)	127.7979	A109	A(50,53,55)	119.842
A9	A(5,3,7)	123.2311	A110	A(50,53,57)	119.0543
A10	A(1,4,8)	122.6472	A111	A(55,53,57)	121.0969
A11	A(1,4,36)	119.1951	A112	A(51,55,53)	119.2581
A12	A(8,4,36)	118.0995	A113	A(51,55,68)	116.1783
A13	A(2,5,3)	108.8603	A114	A(53,55,68)	124.5635
A14	A(2,5,9)	127.938	A115	A(47,58,59)	120.41
A15	A(3,5,9)	123.1897	A116	A(47,58,60)	120.7962
A16	A(2,6,10)	122.0967	A117	A(59,58,60)	118.774
A17	A(2,6,11)	119.3161	A118	A(58,59,61)	121.0679
A18	A(10,6,11)	118.506	A119	A(58,59,62)	119.4381
A19	A(3,7,12)	117.3273	A120	A(61,59,62)	119.4924
A20	A(3,7,13)	116.401	A121	A(58,60,63)	120.552
A21	A(12,7,13)	126.2104	A122	A(58,60,64)	119.5907
A22	A(5,9,14)	117.4038	A123	A(63,60,64)	119.8573
A23	A(5,9,15)	116.4721	A124	A(59,61,65)	119.8541
A24	A(14,9,15)	126.1208	A125	A(59,61,66)	119.0394
A25	A(6,11,15)	122.4446	A126	A(65,61,66)	121.1043
A26	A(6,11,37)	117.1163	A127	A(60,63,65)	120.5029

A27	A(15,11,37)	120.4326	A128	A(60,63,67)	120.878
A28	A(7,12,14)	119.4531	A129	A(65,63,67)	118.6113
A29	A(7,12,16)	115.302	A130	A(61,65,63)	119.239
A30	A(14,12,16)	125.2233	A131	A(61,65,76)	124.5725
A31	A(7,13,17)	115.1341	A132	A(63,65,76)	116.1882
A32	A(7,13,36)	117.8533	A133	A(55,68,69)	118.7065
A33	A(17,13,36)	126.8676	A134	A(68,69,70)	107.6955
A34	A(9,14,12)	119.3154	A135	A(68,69,71)	109.6428
A35	A(9,14,18)	115.2437	A136	A(68,69,72)	109.6543
A36	A(12,14,18)	125.4409	A137	A(70,69,71)	110.8455
A37	A(9,15,11)	117.5265	A138	A(70,69,72)	110.8633
A38	A(9,15,19)	115.3525	A139	A(71,69,72)	108.1336
A39	A(11,15,19)	127.0764	A140	A(69,70,73)	109.925
A40	A(12,16,20)	120.0674	A141	A(69,70,74)	110.6467
A41	A(12,16,21)	120.9343	A142	A(69,70,75)	110.6631
A42	A(20,16,21)	118.9668	A143	A(73,70,74)	108.4697
A43	A(13,17,20)	120.2045	A144	A(73,70,75)	108.4579
A44	A(13,17,22)	120.9903	A145	A(74,70,75)	108.6143
A45	A(20,17,22)	118.7877	A146	A(65,76,77)	118.6635
A46	A(14,18,23)	120.2062	A147	A(76,77,78)	107.7021
A47	A(14,18,24)	120.9614	A148	A(76,77,79)	109.6324
A48	A(23,18,24)	118.8191	A149	A(76,77,80)	109.6577
A49	A(15,19,23)	119.9869	A150	A(78,77,79)	110.8657
A50	A(15,19,25)	120.9991	A151	A(78,77,80)	110.8528
A51	A(23,19,25)	119.0067	A152	A(79,77,80)	108.1243
A52	A(16,20,17)	122.9183	A153	A(77,78,81)	109.9127
A53	A(16,20,26)	118.6699	A154	A(77,78,82)	110.6612
A54	A(17,20,26)	118.4055	A155	A(77,78,83)	110.659
A55	A(18,23,19)	122.97	A156	A(81,78,82)	108.4616

A56	A(18,23,27)	118.5136	A157	A(81,78,83)	108.4651
A57	A(19,23,27)	118.5153	A158	A(82,78,83)	108.6171
A58	A(1,28,2)	108.6225	A159	A(36,84,85)	122.9275
A59	A(1,28,29)	125.4366	A160	A(36,84,86)	121.5473
A60	A(2,28,29)	125.8432	A161	A(85,84,86)	115.4307
A61	A(28,29,30)	113.0072	A162	A(84,85,87)	121.0986
A62	A(28,29,31)	107.6146	A163	A(84,85,88)	125.7846
A63	A(28,29,32)	107.5199	A164	A(87,85,88)	113.0555
A64	A(30,29,31)	110.8702	A165	A(84,86,89)	123.1899
A65	A(30,29,32)	110.8589	A166	A(84,86,90)	118.6345
A66	A(31,29,32)	106.6871	A167	A(89,86,90)	117.9936
A67	A(29,30,33)	109.871	A168	A(85,87,91)	112.6155
A68	A(29,30,34)	110.9708	A169	A(85,87,92)	120.9134
A69	A(29,30,35)	110.9605	A170	A(91,87,92)	126.4533
A70	A(33,30,34)	108.2791	A171	A(85,88,93)	107.779
A71	A(33,30,35)	108.2345	A172	A(86,89,92)	123.6502
A72	A(34,30,35)	108.4372	A173	A(86,89,94)	117.4125
A73	A(4,36,13)	121.4001	A174	A(92,89,94)	118.8475
A74	A(4,36,84)	118.5423	A175	A(87,91,93)	107.9431
A75	A(13,36,84)	120.0133	A176	A(87,92,89)	115.651
A76	A(11,37,38)	120.8279	A177	A(87,92,95)	123.6283
A77	A(11,37,39)	122.1449	A178	A(89,92,95)	120.7171
A78	A(38,37,39)	116.9713	A179	A(88,93,91)	98.6053
A79	A(37,38,40)	121.8477	A180	A(92,95,96)	122.4959
A80	A(37,38,41)	119.405	A181	A(92,95,97)	120.3657
A81	A(40,38,41)	118.6939	A182	A(96,95,97)	117.1322
A82	A(37,39,42)	121.7214	A183	A(95,96,98)	121.2676
A83	A(37,39,43)	119.65	A184	A(95,96,99)	119.1456
A84	A(42,39,43)	118.5415	A185	A(98,96,99)	119.5862

A85	A(38,40,44)	120.7598	A186	A(95,97,100)	121.4984
A86	A(38,40,45)	119.6048	A187	A(95,97,101)	119.8426
A87	A(44,40,45)	119.6292	A188	A(100,97,101)	118.6293
A88	A(39,42,44)	120.8614	A189	A(96,98,102)	120.6953
A89	A(39,42,46)	119.5212	A190	A(96,98,103)	119.6888
A90	A(44,42,46)	119.6049	A191	A(102,98,103)	119.6156
A91	A(40,44,42)	117.8237	A192	A(97,100,102)	120.5593
A92	A(40,44,47)	121.0703	A193	A(97,100,104)	120.4977
A93	A(42,44,47)	121.1057	A194	A(102,100,104)	118.9401
A94	A(44,47,48)	121.1198	A195	A(98,102,100)	118.8415
A95	A(44,47,58)	121.1313	A196	A(98,102,105)	122.5288
A96	A(48,47,58)	117.7426	A197	A(100,102,105)	118.629
A97	A(47,48,49)	120.1591	A198	A(102,105,106)	124.7194
A98	A(47,48,50)	121.0295	A199	A(102,105,107)	113.394
A99	A(49,48,50)	118.7992	A200	A(106,105,107)	121.8865
A100	A(48,49,51)	120.5685	A201	A(105,107,108)	107.3698
A101	A(48,49,52)	119.4842			

Table S26. The Dihedral Angles of the S₁ State of **C286** in THF Computed at the TD-MPW1K/6-311G(d,p) Level of Theory.

Number	Name	Dihedral Angle [°]	Number	Name	Dihedral Angle [°]
D1	D(4,1,3,5)	-179.426	D153	D(40,44,47,58)	-156.909
D2	D(4,1,3,7)	-2.4793	D154	D(42,44,47,48)	-155.786
D3	D(28,1,3,5)	0.6479	D155	D(42,44,47,58)	23.2766
D4	D(28,1,3,7)	177.5949	D156	D(44,47,48,49)	-127.65
D5	D(3,1,4,8)	-178.138	D157	D(44,47,48,50)	53.6365
D6	D(3,1,4,36)	-0.9671	D158	D(58,47,48,49)	53.2573
D7	D(28,1,4,8)	1.759	D159	D(58,47,48,50)	-125.457
D8	D(28,1,4,36)	178.9299	D160	D(44,47,58,59)	-127.859
D9	D(3,1,28,2)	0.1665	D161	D(44,47,58,60)	53.7796
D10	D(3,1,28,29)	176.7366	D162	D(48,47,58,59)	51.2336
D11	D(4,1,28,2)	-179.738	D163	D(48,47,58,60)	-127.128
D12	D(4,1,28,29)	-3.1678	D164	D(47,48,49,51)	-178.662
D13	D(6,2,5,3)	179.2851	D165	D(47,48,49,52)	1.0577
D14	D(6,2,5,9)	0.5305	D166	D(50,48,49,51)	0.0803
D15	D(28,2,5,3)	1.3009	D167	D(50,48,49,52)	179.7999
D16	D(28,2,5,9)	-177.454	D168	D(47,48,50,53)	179.5875
D17	D(5,2,6,10)	-177.24	D169	D(47,48,50,54)	-0.6249
D18	D(5,2,6,11)	-0.568	D170	D(49,48,50,53)	0.8565
D19	D(28,2,6,10)	-0.0519	D171	D(49,48,50,54)	-179.356
D20	D(28,2,6,11)	176.6199	D172	D(48,49,51,55)	-0.7459
D21	D(5,2,28,1)	-0.8898	D173	D(48,49,51,56)	179.8891
D22	D(5,2,28,29)	-177.442	D174	D(52,49,51,55)	179.5357
D23	D(6,2,28,1)	-178.253	D175	D(52,49,51,56)	0.1707
D24	D(6,2,28,29)	5.1948	D176	D(48,50,53,55)	-1.1241
D25	D(1,3,5,2)	-1.216	D177	D(48,50,53,57)	179.8133
D26	D(1,3,5,9)	177.6103	D178	D(54,50,53,55)	179.0881

D27	D(7,3,5,2)	-178.332	D179	D(54,50,53,57)	0.0255
D28	D(7,3,5,9)	0.4942	D180	D(49,51,55,53)	0.4782
D29	D(1,3,7,12)	-176.004	D181	D(49,51,55,68)	-179.613
D30	D(1,3,7,13)	1.3278	D182	D(56,51,55,53)	179.8576
D31	D(5,3,7,12)	0.5427	D183	D(56,51,55,68)	-0.2337
D32	D(5,3,7,13)	177.8741	D184	D(50,53,55,51)	0.447
D33	D(1,4,36,13)	5.2784	D185	D(50,53,55,68)	-179.453
D34	D(1,4,36,84)	-172.302	D186	D(57,53,55,51)	179.49
D35	D(8,4,36,13)	-177.422	D187	D(57,53,55,68)	-0.4104
D36	D(8,4,36,84)	4.9974	D188	D(51,55,68,69)	-179.391
D37	D(2,5,9,14)	179.1088	D189	D(53,55,68,69)	0.5127
D38	D(2,5,9,15)	-1.5012	D190	D(47,58,59,61)	-178.227
D39	D(3,5,9,14)	0.5171	D191	D(47,58,59,62)	1.3245
D40	D(3,5,9,15)	179.9071	D192	D(60,58,59,61)	0.1673
D41	D(2,6,11,15)	1.6831	D193	D(60,58,59,62)	179.7184
D42	D(2,6,11,37)	-177.396	D194	D(47,58,60,63)	179.1272
D43	D(10,6,11,15)	178.4748	D195	D(47,58,60,64)	-0.8773
D44	D(10,6,11,37)	-0.6041	D196	D(59,58,60,63)	0.7396
D45	D(3,7,12,14)	-2.4816	D197	D(59,58,60,64)	-179.265
D46	D(3,7,12,16)	175.9157	D198	D(58,59,61,65)	-0.8262
D47	D(13,7,12,14)	-179.519	D199	D(58,59,61,66)	179.7139
D48	D(13,7,12,16)	-1.1216	D200	D(62,59,61,65)	179.6229
D49	D(3,7,13,17)	-172.901	D201	D(62,59,61,66)	0.163
D50	D(3,7,13,36)	3.0247	D202	D(58,60,63,65)	-0.9874
D51	D(12,7,13,17)	4.1603	D203	D(58,60,63,67)	-179.962
D52	D(12,7,13,36)	-179.914	D204	D(64,60,63,65)	179.017
D53	D(5,9,14,12)	-2.4528	D205	D(64,60,63,67)	0.0427
D54	D(5,9,14,18)	177.5465	D206	D(59,61,65,63)	0.5787
D55	D(15,9,14,12)	178.2232	D207	D(59,61,65,76)	-179.663

D56	D(15,9,14,18)	-1.7775	D208	D(66,61,65,63)	-179.973
D57	D(5,9,15,11)	2.3869	D209	D(66,61,65,76)	-0.2146
D58	D(5,9,15,19)	-175.357	D210	D(60,63,65,61)	0.3195
D59	D(14,9,15,11)	-178.284	D211	D(60,63,65,76)	-179.459
D60	D(14,9,15,19)	3.9721	D212	D(67,63,65,61)	179.3167
D61	D(6,11,15,9)	-2.6273	D213	D(67,63,65,76)	-0.4614
D62	D(6,11,15,19)	174.8176	D214	D(61,65,76,77)	0.4794
D63	D(37,11,15,9)	176.4219	D215	D(63,65,76,77)	-179.756
D64	D(37,11,15,19)	-6.1333	D216	D(55,68,69,70)	179.7486
D65	D(6,11,37,38)	-42.9365	D217	D(55,68,69,71)	59.0528
D66	D(6,11,37,39)	134.2609	D218	D(55,68,69,72)	-59.5273
D67	D(15,11,37,38)	137.9651	D219	D(68,69,70,73)	-179.987
D68	D(15,11,37,39)	-44.8376	D220	D(68,69,70,74)	-60.2054
D69	D(7,12,14,9)	3.4977	D221	D(68,69,70,75)	60.2363
D70	D(7,12,14,18)	-176.502	D222	D(71,69,70,73)	-60.0494
D71	D(16,12,14,9)	-174.729	D223	D(71,69,70,74)	59.7319
D72	D(16,12,14,18)	5.2723	D224	D(71,69,70,75)	-179.826
D73	D(7,12,16,20)	-1.9698	D225	D(72,69,70,73)	60.0515
D74	D(7,12,16,21)	-179.906	D226	D(72,69,70,74)	179.8328
D75	D(14,12,16,20)	176.3218	D227	D(72,69,70,75)	-59.7255
D76	D(14,12,16,21)	-1.6147	D228	D(65,76,77,78)	-179.913
D77	D(7,13,17,20)	-4.1297	D229	D(65,76,77,79)	59.369
D78	D(7,13,17,22)	174.3286	D230	D(65,76,77,80)	-59.1954
D79	D(36,13,17,20)	-179.626	D231	D(76,77,78,81)	-179.918
D80	D(36,13,17,22)	-1.1681	D232	D(76,77,78,82)	-60.1454
D81	D(7,13,36,4)	-6.3504	D233	D(76,77,78,83)	60.3067
D82	D(7,13,36,84)	171.1951	D234	D(79,77,78,81)	-59.9774
D83	D(17,13,36,4)	169.0383	D235	D(79,77,78,82)	59.7951
D84	D(17,13,36,84)	-13.4163	D236	D(79,77,78,83)	-179.753

D85	D(9,14,18,23)	-1.1556	D237	D(80,77,78,81)	60.1182
D86	D(9,14,18,24)	-179.815	D238	D(80,77,78,82)	179.8908
D87	D(12,14,18,23)	178.8436	D239	D(80,77,78,83)	-59.6572
D88	D(12,14,18,24)	0.1842	D240	D(36,84,85,87)	179.2803
D89	D(9,15,19,23)	-3.2424	D241	D(36,84,85,88)	-3.7701
D90	D(9,15,19,25)	175.7664	D242	D(86,84,85,87)	2.7706
D91	D(11,15,19,23)	179.265	D243	D(86,84,85,88)	179.7201
D92	D(11,15,19,25)	-1.7263	D244	D(36,84,86,89)	-178.441
D93	D(12,16,20,17)	1.8831	D245	D(36,84,86,90)	-3.447
D94	D(12,16,20,26)	-177.195	D246	D(85,84,86,89)	-1.8784
D95	D(21,16,20,17)	179.86	D247	D(85,84,86,90)	173.1154
D96	D(21,16,20,26)	0.7823	D248	D(84,85,87,91)	177.0597
D97	D(13,17,20,16)	1.4022	D249	D(84,85,87,92)	-1.4974
D98	D(13,17,20,26)	-179.518	D250	D(88,85,87,91)	-0.2512
D99	D(22,17,20,16)	-177.09	D251	D(88,85,87,92)	-178.808
D100	D(22,17,20,26)	1.9902	D252	D(84,85,88,93)	-177.198
D101	D(14,18,23,19)	1.7229	D253	D(87,85,88,93)	-0.0362
D102	D(14,18,23,27)	-177.882	D254	D(84,86,89,92)	-0.4426
D103	D(24,18,23,19)	-179.589	D255	D(84,86,89,94)	176.0644
D104	D(24,18,23,27)	0.8058	D256	D(90,86,89,92)	-175.467
D105	D(15,19,23,18)	0.6415	D257	D(90,86,89,94)	1.0404
D106	D(15,19,23,27)	-179.754	D258	D(85,87,91,93)	0.4055
D107	D(25,19,23,18)	-178.387	D259	D(92,87,91,93)	178.8664
D108	D(25,19,23,27)	1.218	D260	D(85,87,92,89)	-0.8148
D109	D(1,28,29,30)	-87.69	D261	D(85,87,92,95)	179.8782
D110	D(1,28,29,31)	149.5653	D262	D(91,87,92,89)	-179.159
D111	D(1,28,29,32)	34.9734	D263	D(91,87,92,95)	1.5342
D112	D(2,28,29,30)	88.2993	D264	D(85,88,93,91)	0.2412
D113	D(2,28,29,31)	-34.4453	D265	D(86,89,92,87)	1.8035

D114	D(2,28,29,32)	-149.037	D266	D(86,89,92,95)	-178.868
D115	D(28,29,30,33)	-179.954	D267	D(94,89,92,87)	-174.656
D116	D(28,29,30,34)	-60.2391	D268	D(94,89,92,95)	4.6724
D117	D(28,29,30,35)	60.393	D269	D(87,91,93,88)	-0.3843
D118	D(31,29,30,33)	-59.0405	D270	D(87,92,95,96)	23.2149
D119	D(31,29,30,34)	60.6744	D271	D(87,92,95,97)	-157.716
D120	D(31,29,30,35)	-178.693	D272	D(89,92,95,96)	-156.058
D121	D(32,29,30,33)	59.2627	D273	D(89,92,95,97)	23.0112
D122	D(32,29,30,34)	178.9777	D274	D(92,95,96,98)	178.2016
D123	D(32,29,30,35)	-60.3902	D275	D(92,95,96,99)	-1.4932
D124	D(4,36,84,85)	-34.3516	D276	D(97,95,96,98)	-0.8965
D125	D(4,36,84,86)	141.9494	D277	D(97,95,96,99)	179.4088
D126	D(13,36,84,85)	148.0332	D278	D(92,95,97,100)	-178.6
D127	D(13,36,84,86)	-35.6657	D279	D(92,95,97,101)	3.4089
D128	D(11,37,38,40)	178.4521	D280	D(96,95,97,100)	0.5182
D129	D(11,37,38,41)	-4.2382	D281	D(96,95,97,101)	-177.473
D130	D(39,37,38,40)	1.1146	D282	D(95,96,98,102)	0.6441
D131	D(39,37,38,41)	178.4244	D283	D(95,96,98,103)	-179.144
D132	D(11,37,39,42)	-177.429	D284	D(99,96,98,102)	-179.662
D133	D(11,37,39,43)	-0.8718	D285	D(99,96,98,103)	0.5497
D134	D(38,37,39,42)	-0.129	D286	D(95,97,100,102)	0.1179
D135	D(38,37,39,43)	176.4278	D287	D(95,97,100,104)	-179.241
D136	D(37,38,40,44)	-1.1269	D288	D(101,97,100,102)	178.1325
D137	D(37,38,40,45)	177.9621	D289	D(101,97,100,104)	-1.2264
D138	D(41,38,40,44)	-178.455	D290	D(96,98,102,100)	0.0191
D139	D(41,38,40,45)	0.6338	D291	D(96,98,102,105)	179.6965
D140	D(37,39,42,44)	-0.8493	D292	D(103,98,102,100)	179.8071
D141	D(37,39,42,46)	177.8635	D293	D(103,98,102,105)	-0.5154
D142	D(43,39,42,44)	-177.443	D294	D(97,100,102,98)	-0.3962

D143	D(43,39,42,46)	1.2697	D295	D(97,100,102,105)	179.9136
D144	D(38,40,44,42)	0.124	D296	D(104,100,102,98)	178.9726
D145	D(38,40,44,47)	-179.696	D297	D(104,100,102,105)	-0.7176
D146	D(45,40,44,42)	-178.965	D298	D(98,102,105,106)	179.9866
D147	D(45,40,44,47)	1.215	D299	D(98,102,105,107)	0.0311
D148	D(39,42,44,40)	0.8456	D300	D(100,102,105,106)	-0.3353
D149	D(39,42,44,47)	-179.334	D301	D(100,102,105,107)	179.7092
D150	D(46,42,44,40)	-177.866	D302	D(102,105,107,108)	179.8891
D151	D(46,42,44,47)	1.9541	D303	D(106,105,107,108)	-0.0678
D152	D(40,44,47,48)	24.0288			

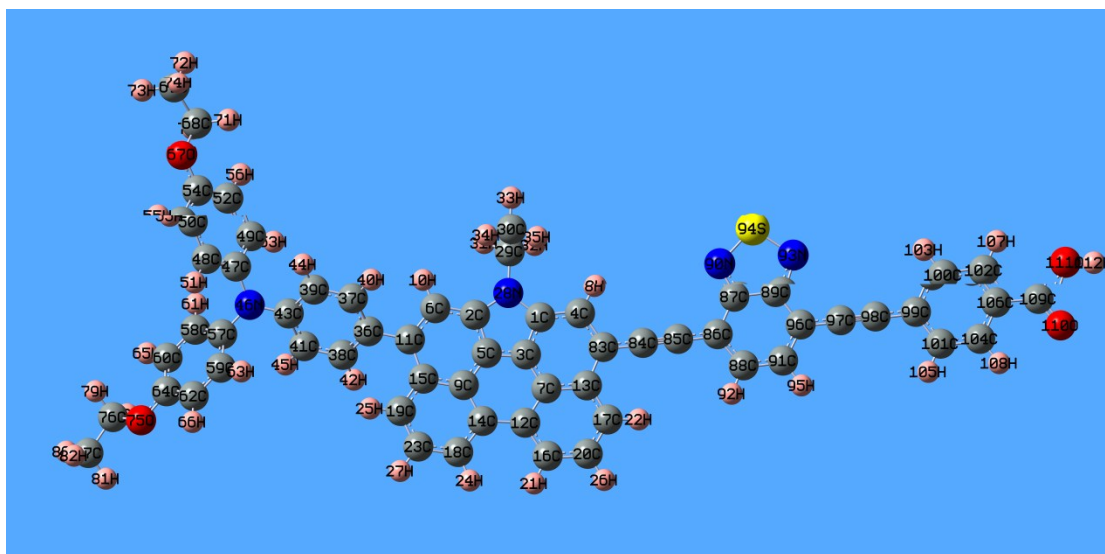


Fig. S36. Geometry of the S_1 state of **C287** in THF optimized at the TD-MPW1K/6-311G(d,p) level of theory.

Table S27. Geometry Parameters and Mulliken Atomic Charges of the S₁ State of **C287** in THF Computed at the TD-MPW1K/6-311G(d,p) Level of Theory

Center number	Atom	Coordinates [Å]			Mulliken atomic charges
		x	y	z	
1	C	-0.95519	0.088308	-0.06281	0.311735
2	C	1.299142	0.169997	-0.12155	0.321335
3	C	-0.45911	-1.19625	-0.29962	-0.15462
4	C	-2.32575	0.225957	-0.00605	0.065866
5	C	0.895061	-1.1443	-0.329	-0.26749
6	C	2.671548	0.399536	-0.11378	-0.0004
7	C	-1.16621	-2.36235	-0.49596	-0.04625
8	H	-2.82351	1.165374	0.167534	0.128076
9	C	1.688009	-2.24923	-0.55306	-0.00217
10	H	3.088324	1.373331	0.085066	0.135397
11	C	3.547963	-0.67761	-0.30937	0.029531
12	C	-0.4335	-3.54774	-0.74386	0.078883
13	C	-2.56411	-2.26082	-0.44462	-0.02356
14	C	1.038363	-3.48711	-0.78507	0.053145
15	C	3.078018	-2.02885	-0.56749	-0.03562
16	C	-1.20603	-4.69025	-0.94011	-0.10485
17	C	-3.27866	-3.43613	-0.64734	-0.06953
18	C	1.880984	-4.55818	-1.06113	-0.10465
19	C	3.860391	-3.1431	-0.89535	-0.12388
20	C	-2.59241	-4.62002	-0.88762	-0.08237
21	H	-0.74242	-5.64406	-1.13487	0.113608
22	H	-4.35693	-3.43462	-0.62104	0.125908
23	C	3.258149	-4.36906	-1.12241	-0.08069
24	H	1.482352	-5.54181	-1.25174	0.115051
25	H	4.929721	-3.05972	-0.99328	0.134921

26	H	-3.16001	-5.52401	-1.04247	0.122284
27	H	3.883219	-5.21272	-1.36937	0.122128
28	N	0.151462	0.924409	0.059591	-0.70315
29	C	0.103385	2.358498	0.248274	-0.13807
30	C	0.037535	3.124916	-1.05646	-0.31377
31	H	0.981245	2.644012	0.82143	0.157184
32	H	-0.75987	2.578434	0.870292	0.157566
33	H	0.002221	4.192587	-0.85609	0.137551
34	H	0.910659	2.922195	-1.67128	0.134316
35	H	-0.85096	2.855195	-1.62144	0.135183
36	C	4.980106	-0.39493	-0.23616	-0.13911
37	C	5.518628	0.742345	-0.84405	-0.10189
38	C	5.861378	-1.2082	0.481325	-0.11717
39	C	6.857552	1.04067	-0.76578	-0.14592
40	H	4.878036	1.384274	-1.42919	0.125037
41	C	7.199197	-0.90914	0.584393	-0.13999
42	H	5.481701	-2.06541	1.014538	0.138388
43	C	7.732764	0.219368	-0.04672	0.238882
44	H	7.240156	1.908548	-1.27701	0.145757
45	H	7.841054	-1.54212	1.174721	0.146737
46	N	9.079761	0.514182	0.039999	-0.57477
47	C	9.552082	1.835341	-0.13874	0.044215
48	C	10.56891	2.097514	-1.05089	-0.08129
49	C	9.033176	2.883928	0.600686	-0.07227
50	C	11.04884	3.376112	-1.215	-0.12877
51	H	10.98459	1.28801	-1.63029	0.129678
52	C	9.496723	4.177361	0.428201	-0.1579
53	H	8.252247	2.69203	1.319919	0.131733
54	C	10.5137	4.430989	-0.48158	0.208612

55	H	11.83747	3.585325	-1.91999	0.128717
56	H	9.067766	4.969424	1.017735	0.148348
57	C	10.03206	-0.49763	0.30344	0.045323
58	C	10.9583	-0.34161	1.319109	-0.08519
59	C	10.07715	-1.65182	-0.47286	-0.06941
60	C	11.91839	-1.30891	1.565225	-0.16206
61	H	10.93599	0.551011	1.924594	0.130056
62	C	11.01533	-2.6261	-0.22357	-0.12473
63	H	9.36908	-1.78159	-1.27646	0.132657
64	C	11.94859	-2.46371	0.796572	0.208208
65	H	12.62578	-1.15208	2.361445	0.148046
66	H	11.0551	-3.52217	-0.82208	0.129352
67	O	11.04037	5.644232	-0.71793	-0.39607
68	C	10.54304	6.752875	0.003547	-0.08679
69	C	11.2995	7.969231	-0.45003	-0.33772
70	H	10.68064	6.5864	1.072533	0.137372
71	H	9.47527	6.866057	-0.1877	0.136948
72	H	10.94441	8.846635	0.083869	0.133198
73	H	12.36233	7.85441	-0.25516	0.13285
74	H	11.15789	8.133728	-1.51477	0.132845
75	O	12.83147	-3.46361	0.957412	-0.39595
76	C	13.80036	-3.35397	1.980437	-0.08727
77	C	14.65001	-4.59246	1.940148	-0.33769
78	H	13.30379	-3.25506	2.94638	0.137594
79	H	14.40624	-2.46192	1.817515	0.13719
80	H	15.4093	-4.54559	2.716186	0.133216
81	H	14.04365	-5.47896	2.105104	0.132823
82	H	15.14647	-4.68577	0.978078	0.132847
83	C	-3.12981	-0.93637	-0.19174	-0.10119

84	C	-4.50094	-0.79572	-0.13518	-0.00911
85	C	-5.71259	-0.65969	-0.08552	0.057703
86	C	-7.07885	-0.49417	-0.02841	-0.2558
87	C	-7.65131	0.794737	0.218933	0.204739
88	C	-7.97446	-1.56978	-0.20876	-0.03413
89	C	-9.08053	0.958713	0.275779	0.207396
90	N	-6.98943	1.913303	0.4123	-0.55234
91	C	-9.33699	-1.40612	-0.15376	-0.01385
92	H	-7.56607	-2.54958	-0.39602	0.134914
93	N	-9.44983	2.201417	0.511114	-0.5567
94	S	-8.09228	3.091214	0.649628	0.591787
95	H	-9.97495	-2.26292	-0.29935	0.128181
96	C	-9.94293	-0.16036	0.085779	-0.25268
97	C	-11.3265	-0.01362	0.137154	0.167941
98	C	-12.5292	0.114783	0.181381	0.02108
99	C	-13.9253	0.27442	0.235891	-0.21444
100	C	-14.4854	1.535478	0.479636	-0.03744
101	C	-14.7787	-0.82175	0.048438	-0.04021
102	C	-15.8506	1.692305	0.534281	-0.025
103	H	-13.834	2.381852	0.624239	0.130567
104	C	-16.1414	-0.65595	0.104544	-0.03317
105	H	-14.3554	-1.79491	-0.13958	0.130075
106	C	-16.6904	0.59876	0.3475	-0.27066
107	H	-16.2739	2.664873	0.722208	0.136756
108	H	-16.8031	-1.49485	-0.03858	0.133946
109	C	-18.1563	0.720634	0.398038	0.536749
110	O	-18.92	-0.19287	0.241917	-0.41727
111	O	-18.5719	1.960699	0.637648	-0.37353
112	H	-19.5297	1.947214	0.652972	0.292426

Table S28. The Bond Lengths of the S₁ State of **C287** in THF Computed at the TD-MPW1K/6-311G(d,p) Level of Theory.

Number	Name	Length[Å]	Number	Name	Length[Å]
R1	R(1,3)	1.3972	R63	R(50,55)	1.0783
R2	R(1,4)	1.3786	R64	R(52,54)	1.3879
R3	R(1,28)	1.3924	R65	R(52,56)	1.0765
R4	R(2,5)	1.3906	R66	R(54,67)	1.3436
R5	R(2,6)	1.3915	R67	R(57,58)	1.3834
R6	R(2,28)	1.3853	R68	R(57,59)	1.3917
R7	R(3,5)	1.3555	R69	R(58,60)	1.3849
R8	R(3,7)	1.3778	R70	R(58,61)	1.0788
R9	R(4,8)	1.0772	R71	R(59,62)	1.3753
R10	R(4,83)	1.4255	R72	R(59,63)	1.0789
R11	R(5,9)	1.3783	R73	R(60,64)	1.3875
R12	R(6,10)	1.0777	R74	R(60,65)	1.0766
R13	R(6,11)	1.4024	R75	R(62,64)	1.3921
R14	R(7,12)	1.4154	R76	R(62,66)	1.0783
R15	R(7,13)	1.4025	R77	R(64,75)	1.3436
R16	R(9,14)	1.4171	R78	R(67,68)	1.4131
R17	R(9,15)	1.4074	R79	R(68,69)	1.5025
R18	R(11,15)	1.4537	R80	R(68,70)	1.0906
R19	R(11,36)	1.4616	R81	R(68,71)	1.0906
R20	R(12,14)	1.4737	R82	R(69,72)	1.0867
R21	R(12,16)	1.3931	R83	R(69,73)	1.0866
R22	R(13,17)	1.3903	R84	R(69,74)	1.0866
R23	R(13,83)	1.4622	R85	R(75,76)	1.4133
R24	R(14,18)	1.3905	R86	R(76,77)	1.5025
R25	R(15,19)	1.4004	R87	R(76,78)	1.0906
R26	R(16,20)	1.3892	R88	R(76,79)	1.0906

R27	R(16,21)	1.0782	R89	R(77,80)	1.0867
R28	R(17,20)	1.3893	R90	R(77,81)	1.0866
R29	R(17,22)	1.0786	R91	R(77,82)	1.0866
R30	R(18,23)	1.3914	R92	R(83,84)	1.3795
R31	R(18,24)	1.0783	R93	R(84,85)	1.2203
R32	R(19,23)	1.3846	R94	R(85,86)	1.3774
R33	R(19,25)	1.077	R95	R(86,87)	1.4318
R34	R(20,26)	1.0786	R96	R(86,88)	1.4112
R35	R(23,27)	1.0786	R97	R(87,89)	1.4397
R36	R(28,29)	1.4472	R98	R(87,90)	1.314
R37	R(29,30)	1.5146	R99	R(88,91)	1.3734
R38	R(29,31)	1.0866	R100	R(88,92)	1.0779
R39	R(29,32)	1.0865	R101	R(89,93)	1.3176
R40	R(30,33)	1.0869	R102	R(89,96)	1.4255
R41	R(30,34)	1.0869	R103	R(90,94)	1.631
R42	R(30,35)	1.0869	R104	R(91,95)	1.0781
R43	R(36,37)	1.3975	R105	R(91,96)	1.4059
R44	R(36,38)	1.3974	R106	R(93,94)	1.6291
R45	R(37,39)	1.374	R107	R(96,97)	1.3923
R46	R(37,40)	1.0793	R108	R(97,98)	1.2103
R47	R(38,41)	1.3747	R109	R(98,99)	1.4062
R48	R(38,42)	1.0786	R110	R(99,100)	1.4012
R49	R(39,43)	1.3991	R111	R(99,101)	1.4018
R50	R(39,44)	1.0775	R112	R(100,102)	1.3753
R51	R(41,43)	1.3988	R113	R(100,103)	1.0778
R52	R(41,45)	1.0776	R114	R(101,104)	1.3739
R53	R(43,46)	1.3816	R115	R(101,105)	1.0778
R54	R(46,47)	1.4144	R116	R(102,106)	1.3914
R55	R(46,57)	1.4142	R117	R(102,107)	1.0772

R56	R(47,48)	1.3909	R118	R(104,106)	1.3909
R57	R(47,49)	1.384	R119	R(104,108)	1.0779
R58	R(48,50)	1.3755	R120	R(106,109)	1.4718
R59	R(48,51)	1.0788	R121	R(109,110)	1.2009
R60	R(49,52)	1.3848	R122	R(109,111)	1.3296
R61	R(49,53)	1.0789	R123	R(111,112)	0.9581
R62	R(50,54)	1.3918			

Table S29. The Bond Angles of the S₁ State of **C287** in THF Computed at the TD-MPW1K/6-311G(d,p) Level of Theory.

Number	Name	Angle [°]	Number	Name	Angle [°]
A1	A(3,1,4)	116.8551	A106	A(49,52,54)	119.8427
A2	A(3,1,28)	106.5454	A107	A(49,52,56)	119.0537
A3	A(4,1,28)	136.5994	A108	A(54,52,56)	121.0971
A4	A(5,2,6)	116.3175	A109	A(50,54,52)	119.2527
A5	A(5,2,28)	107.066	A110	A(50,54,67)	116.1672
A6	A(6,2,28)	136.5964	A111	A(52,54,67)	124.58
A7	A(1,3,5)	108.8527	A112	A(46,57,58)	120.4586
A8	A(1,3,7)	128.3194	A113	A(46,57,59)	120.7477
A9	A(5,3,7)	122.8236	A114	A(58,57,59)	118.7748
A10	A(1,4,8)	123.5785	A115	A(57,58,60)	121.0541
A11	A(1,4,83)	118.293	A116	A(57,58,61)	119.4402
A12	A(8,4,83)	118.1281	A117	A(60,58,61)	119.5045
A13	A(2,5,3)	108.8622	A118	A(57,59,62)	120.5631
A14	A(2,5,9)	127.9332	A119	A(57,59,63)	119.6016
A15	A(3,5,9)	123.1979	A120	A(62,59,63)	119.8353
A16	A(2,6,10)	122.1062	A121	A(58,60,64)	119.8631
A17	A(2,6,11)	119.2686	A122	A(58,60,65)	119.026
A18	A(10,6,11)	118.5594	A123	A(64,60,65)	121.1084
A19	A(3,7,12)	117.9104	A124	A(59,62,64)	120.4968
A20	A(3,7,13)	116.425	A125	A(59,62,66)	120.8789
A21	A(12,7,13)	125.6611	A126	A(64,62,66)	118.6166
A22	A(5,9,14)	117.5892	A127	A(60,64,62)	119.2379
A23	A(5,9,15)	116.3792	A128	A(60,64,75)	124.5665
A24	A(14,9,15)	126.0043	A129	A(62,64,75)	116.1952
A25	A(6,11,15)	122.458	A130	A(54,67,68)	118.7281
A26	A(6,11,36)	117.1823	A131	A(67,68,69)	107.6864

A27	A(15,11,36)	120.3587	A132	A(67,68,70)	109.6501
A28	A(7,12,14)	119.1737	A133	A(67,68,71)	109.6604
A29	A(7,12,16)	115.1157	A134	A(69,68,70)	110.8518
A30	A(14,12,16)	125.7089	A135	A(69,68,71)	110.8523
A31	A(7,13,17)	116.4688	A136	A(70,68,71)	108.1343
A32	A(7,13,83)	117.2261	A137	A(68,69,72)	109.9261
A33	A(17,13,83)	126.3043	A138	A(68,69,73)	110.6563
A34	A(9,14,12)	119.2894	A139	A(68,69,74)	110.655
A35	A(9,14,18)	115.3133	A140	A(72,69,73)	108.4696
A36	A(12,14,18)	125.3876	A141	A(72,69,74)	108.4565
A37	A(9,15,11)	117.5797	A142	A(73,69,74)	108.613
A38	A(9,15,19)	115.4404	A143	A(64,75,76)	118.6475
A39	A(11,15,19)	126.908	A144	A(75,76,77)	107.7181
A40	A(12,16,20)	120.4416	A145	A(75,76,78)	109.6346
A41	A(12,16,21)	120.83	A146	A(75,76,79)	109.6445
A42	A(20,16,21)	118.7284	A147	A(77,76,78)	110.8546
A43	A(13,17,20)	119.4526	A148	A(77,76,79)	110.8587
A44	A(13,17,22)	120.6006	A149	A(78,76,79)	108.1243
A45	A(20,17,22)	119.9467	A150	A(76,77,80)	109.9027
A46	A(14,18,23)	120.2531	A151	A(76,77,81)	110.662
A47	A(14,18,24)	120.9123	A152	A(76,77,82)	110.6648
A48	A(23,18,24)	118.8219	A153	A(80,77,81)	108.4612
A49	A(15,19,23)	119.9915	A154	A(80,77,82)	108.4656
A50	A(15,19,25)	120.9553	A155	A(81,77,82)	108.6203
A51	A(23,19,25)	119.043	A156	A(4,83,13)	122.8793
A52	A(16,20,17)	122.8584	A157	A(4,83,84)	118.1746
A53	A(16,20,26)	118.5158	A158	A(13,83,84)	118.9454
A54	A(17,20,26)	118.6257	A159	A(85,86,87)	120.7899
A55	A(18,23,19)	122.9296	A160	A(85,86,88)	122.1812

A56	A(18,23,27)	118.5108	A161	A(87,86,88)	117.0289
A57	A(19,23,27)	118.5555	A162	A(86,87,89)	120.4134
A58	A(1,28,2)	108.6597	A163	A(86,87,90)	126.1794
A59	A(1,28,29)	125.4563	A164	A(89,87,90)	113.4072
A60	A(2,28,29)	125.746	A165	A(86,88,91)	122.2527
A61	A(28,29,30)	112.9888	A166	A(86,88,92)	118.3314
A62	A(28,29,31)	107.5962	A167	A(91,88,92)	119.416
A63	A(28,29,32)	107.5549	A168	A(87,89,93)	113.1232
A64	A(30,29,31)	110.8886	A169	A(87,89,96)	120.3899
A65	A(30,29,32)	110.8665	A170	A(93,89,96)	126.4869
A66	A(31,29,32)	106.6623	A171	A(87,90,94)	107.1935
A67	A(29,30,33)	109.8568	A172	A(88,91,95)	119.1393
A68	A(29,30,34)	110.9751	A173	A(88,91,96)	122.6841
A69	A(29,30,35)	110.9617	A174	A(95,91,96)	118.1766
A70	A(33,30,34)	108.2756	A175	A(89,93,94)	107.2639
A71	A(33,30,35)	108.2424	A176	A(90,94,93)	99.0121
A72	A(34,30,35)	108.4417	A177	A(89,96,91)	117.2309
A73	A(11,36,37)	120.8763	A178	A(89,96,97)	120.8993
A74	A(11,36,38)	122.0789	A179	A(91,96,97)	121.8698
A75	A(37,36,38)	116.9963	A180	A(98,99,100)	120.3822
A76	A(36,37,39)	121.8326	A181	A(98,99,101)	120.6956
A77	A(36,37,40)	119.4163	A182	A(100,99,101)	118.9222
A78	A(39,37,40)	118.6943	A183	A(99,100,102)	120.4214
A79	A(36,38,41)	121.7088	A184	A(99,100,103)	119.2412
A80	A(36,38,42)	119.628	A185	A(102,100,103)	120.3374
A81	A(41,38,42)	118.5817	A186	A(99,101,104)	120.2672
A82	A(37,39,43)	120.7569	A187	A(99,101,105)	119.3588
A83	A(37,39,44)	119.5966	A188	A(104,101,105)	120.374
A84	A(43,39,44)	119.6394	A189	A(100,102,106)	120.2755

A85	A(38,41,43)	120.8577	A190	A(100,102,107)	119.9949
A86	A(38,41,45)	119.5351	A191	A(106,102,107)	119.7296
A87	A(43,41,45)	119.5967	A192	A(101,104,106)	120.4928
A88	A(39,43,41)	117.8306	A193	A(101,104,108)	120.626
A89	A(39,43,46)	121.1223	A194	A(106,104,108)	118.8812
A90	A(41,43,46)	121.0469	A195	A(102,106,104)	119.6209
A91	A(43,46,47)	121.1287	A196	A(102,106,109)	122.1009
A92	A(43,46,57)	121.0328	A197	A(104,106,109)	118.2781
A93	A(47,46,57)	117.8376	A198	A(106,109,110)	124.4669
A94	A(46,47,48)	120.2024	A199	A(106,109,111)	113.2494
A95	A(46,47,49)	120.9959	A200	A(110,109,111)	122.2837
A96	A(48,47,49)	118.7923	A201	A(109,111,112)	107.5936
A97	A(47,48,50)	120.5642	A202	L(83,84,85,4,-1)	179.4627
A98	A(47,48,51)	119.5023	A203	L(84,85,86,87,-1)	179.4987
A99	A(50,48,51)	119.9331	A204	L(96,97,98,89,-1)	179.9637
A100	A(47,49,52)	121.0381	A205	L(97,98,99,100,-1)	179.5557
A101	A(47,49,53)	119.5238	A206	L(83,84,85,4,-2)	179.7931
A102	A(52,49,53)	119.4375	A207	L(84,85,86,87,-2)	179.9105
A103	A(48,50,54)	120.4978	A208	L(96,97,98,89,-2)	179.9455
A104	A(48,50,55)	120.8991	A209	L(97,98,99,100,-2)	180.0962
A105	A(54,50,55)	118.5996			

Table S30. The Dihedral Angles of the S₁ State of **C287** in THF Computed at the TD-MPW1K/6-311G(d,p) Level of Theory.

Number	Name	Dihedral Angle [°]	Number	Name	Dihedral Angle [°]
D1	D(4,1,3,5)	179.7265	D153	D(43,46,47,49)	53.4912
D2	D(4,1,3,7)	0.467	D154	D(57,46,47,48)	52.0336
D3	D(28,1,3,5)	-0.3715	D155	D(57,46,47,49)	-126.843
D4	D(28,1,3,7)	-179.631	D156	D(43,46,57,58)	-128.676
D5	D(3,1,4,8)	-179.823	D157	D(43,46,57,59)	52.9245
D6	D(3,1,4,83)	-0.0567	D158	D(47,46,57,58)	51.6576
D7	D(28,1,4,8)	0.3139	D159	D(47,46,57,59)	-126.742
D8	D(28,1,4,83)	-179.92	D160	D(46,47,48,50)	-178.94
D9	D(3,1,28,2)	0.9909	D161	D(46,47,48,51)	0.8435
D10	D(3,1,28,29)	176.9134	D162	D(49,47,48,50)	-0.039
D11	D(4,1,28,2)	-179.136	D163	D(49,47,48,51)	179.7444
D12	D(4,1,28,29)	-3.2138	D164	D(46,47,49,52)	179.877
D13	D(6,2,5,3)	179.6332	D165	D(46,47,49,53)	-0.3905
D14	D(6,2,5,9)	-1.2948	D166	D(48,47,49,52)	0.9851
D15	D(28,2,5,3)	0.9949	D167	D(48,47,49,53)	-179.282
D16	D(28,2,5,9)	-179.933	D168	D(47,48,50,54)	-0.7436
D17	D(5,2,6,10)	-177.045	D169	D(47,48,50,55)	179.951
D18	D(5,2,6,11)	-0.038	D170	D(51,48,50,54)	179.474
D19	D(28,2,6,10)	1.0604	D171	D(51,48,50,55)	0.1685
D20	D(28,2,6,11)	178.0674	D172	D(47,49,52,54)	-1.1447
D21	D(5,2,28,1)	-1.2252	D173	D(47,49,52,56)	179.7703
D22	D(5,2,28,29)	-177.133	D174	D(53,49,52,54)	179.1226
D23	D(6,2,28,1)	-179.449	D175	D(53,49,52,56)	0.0376
D24	D(6,2,28,29)	4.6436	D176	D(48,50,54,52)	0.585
D25	D(1,3,5,2)	-0.386	D177	D(48,50,54,67)	-179.516
D26	D(1,3,5,9)	-179.511	D178	D(55,50,54,52)	179.9062

D27	D(7,3,5,2)	178.9226	D179	D(55,50,54,67)	-0.1946
D28	D(7,3,5,9)	-0.2027	D180	D(49,52,54,50)	0.3495
D29	D(1,3,7,12)	178.875	D181	D(49,52,54,67)	-179.541
D30	D(1,3,7,13)	-0.4832	D182	D(56,52,54,50)	179.4155
D31	D(5,3,7,12)	-0.291	D183	D(56,52,54,67)	-0.4747
D32	D(5,3,7,13)	-179.649	D184	D(50,54,67,68)	-179.595
D33	D(1,4,83,13)	-0.2822	D185	D(52,54,67,68)	0.2986
D34	D(1,4,83,84)	-179.965	D186	D(46,57,58,60)	-178.301
D35	D(8,4,83,13)	179.4968	D187	D(46,57,58,61)	1.291
D36	D(8,4,83,84)	-0.1861	D188	D(59,57,58,60)	0.1298
D37	D(2,5,9,14)	-177.824	D189	D(59,57,58,61)	179.7217
D38	D(2,5,9,15)	0.392	D190	D(46,57,59,62)	179.2074
D39	D(3,5,9,14)	1.1263	D191	D(46,57,59,63)	-0.8065
D40	D(3,5,9,15)	179.3426	D192	D(58,57,59,62)	0.7813
D41	D(2,6,11,15)	2.1612	D193	D(58,57,59,63)	-179.233
D42	D(2,6,11,36)	-177.476	D194	D(57,58,60,64)	-0.8177
D43	D(10,6,11,15)	179.2748	D195	D(57,58,60,65)	179.7522
D44	D(10,6,11,36)	-0.3622	D196	D(61,58,60,64)	179.5907
D45	D(3,7,12,14)	-0.16	D197	D(61,58,60,65)	0.1605
D46	D(3,7,12,16)	-179.709	D198	D(57,59,62,64)	-1.0043
D47	D(13,7,12,14)	179.1325	D199	D(57,59,62,66)	-179.976
D48	D(13,7,12,16)	-0.4162	D200	D(63,59,62,64)	179.0096
D49	D(3,7,13,17)	179.7798	D201	D(63,59,62,66)	0.0382
D50	D(3,7,13,83)	0.0972	D202	D(58,60,64,62)	0.5956
D51	D(12,7,13,17)	0.4779	D203	D(58,60,64,75)	-179.64
D52	D(12,7,13,83)	-179.205	D204	D(65,60,64,62)	-179.986
D53	D(5,9,14,12)	-1.5217	D205	D(65,60,64,75)	-0.2218
D54	D(5,9,14,18)	177.4065	D206	D(59,62,64,60)	0.3068
D55	D(15,9,14,12)	-179.546	D207	D(59,62,64,75)	-179.477

D56	D(15,9,14,18)	-0.6182	D208	D(66,62,64,60)	179.3011
D57	D(5,9,15,11)	1.7108	D209	D(66,62,64,75)	-0.4828
D58	D(5,9,15,19)	-175.421	D210	D(60,64,75,76)	0.3786
D59	D(14,9,15,11)	179.7565	D211	D(62,64,75,76)	-179.85
D60	D(14,9,15,19)	2.6244	D212	D(54,67,68,69)	179.9372
D61	D(6,11,15,9)	-3.0345	D213	D(54,67,68,70)	59.235
D62	D(6,11,15,19)	173.7263	D214	D(54,67,68,71)	-59.3539
D63	D(36,11,15,9)	176.5914	D215	D(67,68,69,72)	179.9894
D64	D(36,11,15,19)	-6.6478	D216	D(67,68,69,73)	-60.2226
D65	D(6,11,36,37)	-43.0399	D217	D(67,68,69,74)	60.2184
D66	D(6,11,36,38)	134.3518	D218	D(70,68,69,72)	-60.0665
D67	D(15,11,36,37)	137.315	D219	D(70,68,69,73)	59.7215
D68	D(15,11,36,38)	-45.2933	D220	D(70,68,69,74)	-179.837
D69	D(7,12,14,9)	1.077	D221	D(71,68,69,72)	60.0323
D70	D(7,12,14,18)	-177.735	D222	D(71,68,69,73)	179.8203
D71	D(16,12,14,9)	-179.426	D223	D(71,68,69,74)	-59.7386
D72	D(16,12,14,18)	1.7623	D224	D(64,75,76,77)	-179.966
D73	D(7,12,16,20)	0.045	D225	D(64,75,76,78)	59.3186
D74	D(7,12,16,21)	-179.935	D226	D(64,75,76,79)	-59.2392
D75	D(14,12,16,20)	-179.47	D227	D(75,76,77,80)	-179.937
D76	D(14,12,16,21)	0.5506	D228	D(75,76,77,81)	-60.1709
D77	D(7,13,17,20)	-0.1627	D229	D(75,76,77,82)	60.2895
D78	D(7,13,17,22)	179.9375	D230	D(78,76,77,80)	-59.9903
D79	D(83,13,17,20)	179.4872	D231	D(78,76,77,81)	59.7758
D80	D(83,13,17,22)	-0.4126	D232	D(78,76,77,82)	-179.764
D81	D(7,13,83,4)	0.2618	D233	D(79,76,77,80)	60.1018
D82	D(7,13,83,84)	179.9424	D234	D(79,76,77,81)	179.868
D83	D(17,13,83,4)	-179.386	D235	D(79,76,77,82)	-59.6716
D84	D(17,13,83,84)	0.2949	D236	D(4,83,86,87)	-0.4355

D85	D(9,14,18,23)	-1.3131	D237	D(4,83,86,88)	179.4388
D86	D(9,14,18,24)	179.9971	D238	D(13,83,86,87)	179.9642
D87	D(12,14,18,23)	177.5403	D239	D(13,83,86,88)	-0.1615
D88	D(12,14,18,24)	-1.1495	D240	D(85,86,87,89)	179.945
D89	D(9,15,19,23)	-2.7081	D241	D(85,86,87,90)	-0.0758
D90	D(9,15,19,25)	176.123	D242	D(88,86,87,89)	-0.0166
D91	D(11,15,19,23)	-179.529	D243	D(88,86,87,90)	179.9627
D92	D(11,15,19,25)	-0.6977	D244	D(85,86,88,91)	-179.918
D93	D(12,16,20,17)	0.241	D245	D(85,86,88,92)	0.0542
D94	D(12,16,20,26)	-179.902	D246	D(87,86,88,91)	0.043
D95	D(21,16,20,17)	-179.779	D247	D(87,86,88,92)	-179.985
D96	D(21,16,20,26)	0.0784	D248	D(86,87,89,93)	179.9873
D97	D(13,17,20,16)	-0.1788	D249	D(86,87,89,96)	-0.0312
D98	D(13,17,20,26)	179.9639	D250	D(90,87,89,93)	0.0055
D99	D(22,17,20,16)	179.7216	D251	D(90,87,89,96)	179.987
D100	D(22,17,20,26)	-0.1356	D252	D(86,87,90,94)	-179.977
D101	D(14,18,23,19)	1.1591	D253	D(89,87,90,94)	0.0034
D102	D(14,18,23,27)	-178.09	D254	D(86,88,91,95)	179.9673
D103	D(24,18,23,19)	179.8761	D255	D(86,88,91,96)	-0.0213
D104	D(24,18,23,27)	0.6271	D256	D(92,88,91,95)	-0.0046
D105	D(15,19,23,18)	1.0017	D257	D(92,88,91,96)	-179.993
D106	D(15,19,23,27)	-179.75	D258	D(87,89,93,94)	-0.0114
D107	D(25,19,23,18)	-177.852	D259	D(96,89,93,94)	-179.992
D108	D(25,19,23,27)	1.3971	D260	D(87,89,96,91)	0.0528
D109	D(1,28,29,30)	-87.4795	D261	D(87,89,96,97)	-179.932
D110	D(1,28,29,31)	149.7776	D262	D(93,89,96,91)	-179.968
D111	D(1,28,29,32)	35.2062	D263	D(93,89,96,97)	0.047
D112	D(2,28,29,30)	87.7592	D264	D(87,90,94,93)	-0.0089
D113	D(2,28,29,31)	-34.9837	D265	D(88,91,96,89)	-0.0277

D114	D(2,28,29,32)	-149.555	D266	D(88,91,96,97)	179.9566
D115	D(28,29,30,33)	179.9311	D267	D(95,91,96,89)	179.9836
D116	D(28,29,30,34)	-60.3648	D268	D(95,91,96,97)	-0.032
D117	D(28,29,30,35)	60.2767	D269	D(89,93,94,90)	0.012
D118	D(31,29,30,33)	-59.1788	D270	D(89,96,99,100)	-0.1193
D119	D(31,29,30,34)	60.5254	D271	D(89,96,99,101)	179.9299
D120	D(31,29,30,35)	-178.833	D272	D(91,96,99,100)	179.8976
D121	D(32,29,30,33)	59.1102	D273	D(91,96,99,101)	-0.0532
D122	D(32,29,30,34)	178.8143	D274	D(98,99,100,102)	-179.943
D123	D(32,29,30,35)	-60.5442	D275	D(98,99,100,103)	0.039
D124	D(11,36,37,39)	178.7267	D276	D(101,99,100,102)	0.0345
D125	D(11,36,37,40)	-4.0496	D277	D(101,99,100,103)	-179.984
D126	D(38,36,37,39)	1.207	D278	D(98,99,101,104)	179.95
D127	D(38,36,37,40)	178.4307	D279	D(98,99,101,105)	-0.028
D128	D(11,36,38,41)	-177.658	D280	D(100,99,101,104)	-0.0271
D129	D(11,36,38,42)	-0.9881	D281	D(100,99,101,105)	179.9949
D130	D(37,36,38,41)	-0.1698	D282	D(99,100,102,106)	-0.0145
D131	D(37,36,38,42)	176.4996	D283	D(99,100,102,107)	179.9936
D132	D(36,37,39,43)	-1.1597	D284	D(103,100,102,106)	-179.996
D133	D(36,37,39,44)	177.8699	D285	D(103,100,102,107)	0.0121
D134	D(40,37,39,43)	-178.403	D286	D(99,101,104,106)	-0.0004
D135	D(40,37,39,44)	0.6268	D287	D(99,101,104,108)	-179.989
D136	D(36,38,41,43)	-0.9197	D288	D(105,101,104,106)	179.9775
D137	D(36,38,41,45)	177.8959	D289	D(105,101,104,108)	-0.0112
D138	D(42,38,41,43)	-177.623	D290	D(100,102,106,104)	-0.0134
D139	D(42,38,41,45)	1.1928	D291	D(100,102,106,109)	179.9784
D140	D(37,39,43,41)	0.0459	D292	D(107,102,106,104)	179.9786
D141	D(37,39,43,46)	-179.821	D293	D(107,102,106,109)	-0.0296
D142	D(44,39,43,41)	-178.983	D294	D(101,104,106,102)	0.0208

D143	D(44,39,43,46)	1.15	D295	D(101,104,106,109)	-179.971
D144	D(38,41,43,39)	0.9746	D296	D(108,104,106,102)	-179.99
D145	D(38,41,43,46)	-179.159	D297	D(108,104,106,109)	0.0177
D146	D(45,41,43,39)	-177.84	D298	D(102,106,109,110)	179.9273
D147	D(45,41,43,46)	2.0266	D299	D(102,106,109,111)	-0.0799
D148	D(39,43,46,47)	23.5885	D300	D(104,106,109,110)	-0.0808
D149	D(39,43,46,57)	-156.067	D301	D(104,106,109,111)	179.912
D150	D(41,43,46,47)	-156.274	D302	D(106,109,111,112)	179.9817
D151	D(41,43,46,57)	24.0707	D303	D(110,109,111,112)	-0.0253
D152	D(43,46,47,48)	-127.633			

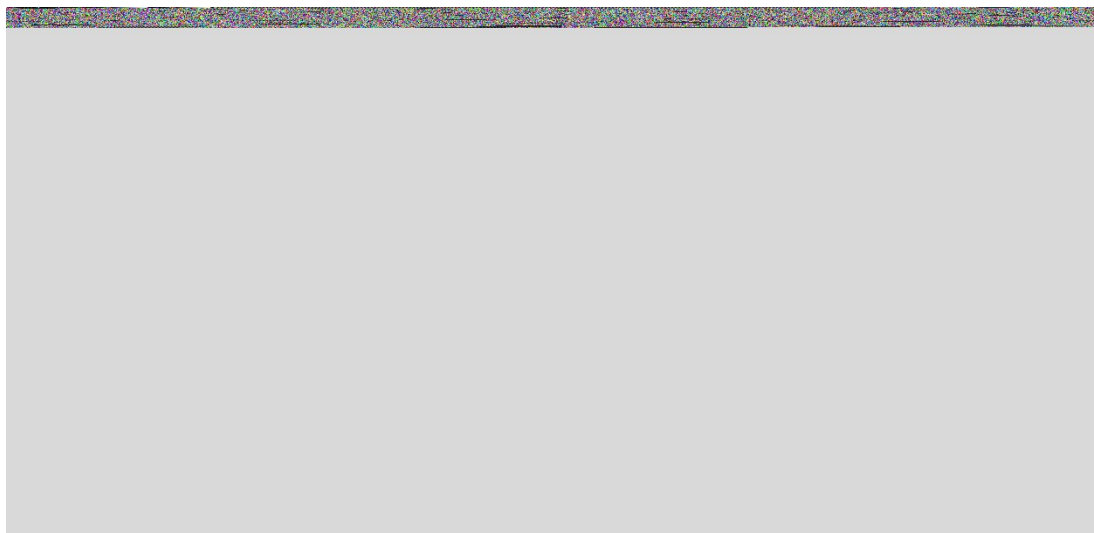


Fig.S37. Geometry of the S_1 state of **C288** in THF optimized at the TD-MPW1K/6-311G(d,p) level of theory.

Table S31. Geometry Parameters and Mulliken Atomic Charges of the S₁ State of **C288** in THF Computed at the TD-MPW1K/6-311G(d,p) Level of Theory

Center number	Atom	Coordinates [Å]			Mulliken atomic charges
		x	y	z	
1	C	-0.09571	-2.67747	0.128593	0.054054
2	C	1.360787	-2.47594	0.118914	0.121945
3	C	-0.94608	-1.54703	0.063885	-0.02836
4	C	1.872611	-1.16467	0.037201	-0.0213
5	C	0.977018	-0.11778	-0.02036	-0.23625
6	C	-0.36263	-0.29923	-0.0065	-0.18308
7	C	3.230339	-0.81222	0.020976	0.018808
8	C	4.166546	-1.84331	0.086866	-0.10889
9	C	3.682109	-3.14911	0.175136	0.016793
10	H	4.391854	-3.95797	0.237025	0.117127
11	C	-2.13561	-3.96698	0.205279	-0.0818
12	C	-2.34857	-1.57837	0.069425	-0.03089
13	H	-2.60935	-4.93435	0.261316	0.12269
14	C	1.250735	1.249882	-0.09125	0.305394
15	C	2.334728	-3.47258	0.191881	-0.09663
16	H	2.057782	-4.51233	0.264267	0.111094
17	C	-0.74838	-3.90728	0.20007	-0.10202
18	H	-0.18804	-4.82717	0.252188	0.113456
19	C	-0.98881	0.949527	-0.07226	0.310307
20	N	0.027902	1.900038	-0.13538	-0.707
21	C	-2.93954	-2.83511	0.142444	-0.07018
22	H	-4.01336	-2.93662	0.150992	0.12383
23	C	-3.04707	-0.29597	0.001014	-0.09507
24	C	-2.36588	0.956028	-0.06736	0.067934
25	H	-2.9578	1.854952	-0.11066	0.128403

26	C	-0.16601	3.334027	-0.14821	-0.13966
27	H	0.652482	3.771227	-0.71339	0.157238
28	H	-1.07468	3.536571	-0.70836	0.158375
29	C	-0.24403	3.932834	1.240846	-0.31251
30	H	-1.07408	3.509757	1.800514	0.135368
31	H	0.672973	3.75089	1.795354	0.134457
32	H	-0.39283	5.007245	1.171503	0.138014
33	C	-4.42679	-0.28234	0.005771	-0.01032
34	C	-5.64582	-0.24519	0.008614	0.057605
35	C	-7.02299	-0.17716	0.011034	-0.25592
36	C	-7.68973	1.089703	-0.0441	0.204247
37	C	-7.83824	-1.3228	0.066313	-0.03544
38	C	-9.12686	1.159392	-0.04165	0.206271
39	N	-7.11125	2.268682	-0.09984	-0.55297
40	C	-9.21331	-1.24808	0.067634	-0.0149
41	H	-7.36267	-2.28915	0.108584	0.133307
42	N	-9.5841	2.394561	-0.09623	-0.55699
43	C	-9.9077	-0.03172	0.01505	-0.253
44	S	-8.29526	3.38435	-0.1462	0.593242
45	H	-9.78595	-2.16062	0.111014	0.127601
46	C	3.55779	0.596178	-0.04863	0.080692
47	C	2.587649	1.615322	-0.10225	-0.00736
48	H	2.904374	2.645132	-0.14691	0.136444
49	C	4.950924	0.874235	-0.05422	-0.31892
50	C	5.940159	-0.08484	-0.0184	0.036862
51	S	5.625554	2.463253	-0.14147	0.342227
52	C	7.227374	0.477599	-0.05527	0.036824
53	C	7.237635	1.844722	-0.11988	-0.3029
54	H	8.130075	-0.10609	-0.01616	0.132305

55	C	5.666066	-1.57366	0.05179	-0.28183
56	C	6.33221	-2.07287	1.341015	-0.06305
57	C	7.677369	-2.4195	1.380381	-0.0994
58	C	5.627506	-2.07816	2.537606	-0.05349
59	C	8.286803	-2.7744	2.569553	-0.08935
60	H	8.262333	-2.42171	0.474304	0.139204
61	C	6.240567	-2.43325	3.725168	-0.09652
62	H	4.585703	-1.79853	2.549246	0.130069
63	C	7.580441	-2.79188	3.764579	-0.13291
64	H	9.333725	-3.04128	2.566003	0.113062
65	H	5.664196	-2.42672	4.638916	0.112932
66	C	6.196266	-2.25436	-1.21883	-0.05535
67	C	6.193635	-1.56926	-2.42681	-0.04968
68	C	6.595131	-3.58552	-1.23004	-0.10337
69	C	6.583223	-2.18925	-3.59994	-0.09779
70	H	5.886821	-0.53518	-2.45609	0.132954
71	C	6.98515	-4.20134	-2.40469	-0.08859
72	H	6.619377	-4.15206	-0.31288	0.139991
73	C	6.98767	-3.51646	-3.61236	-0.13305
74	H	6.576499	-1.62603	-4.52183	0.112157
75	H	7.300419	-5.2344	-2.37782	0.112994
76	C	8.231857	-3.22148	5.045108	-0.23567
77	H	9.282857	-2.93757	5.027702	0.140265
78	H	7.77565	-2.68823	5.877547	0.140367
79	C	8.116217	-4.72167	5.280531	-0.31482
80	H	8.58991	-5.27899	4.475084	0.125128
81	H	8.595281	-5.00592	6.214796	0.128374
82	H	7.07331	-5.02769	5.329006	0.125638
83	C	7.37678	-4.19933	-4.88958	-0.23582

84	H	7.807564	-3.46872	-5.5721	0.139698
85	H	8.153754	-4.93383	-4.6836	0.140431
86	C	6.196174	-4.88711	-5.56257	-0.31482
87	H	5.415346	-4.16944	-5.80519	0.126011
88	H	6.505174	-5.3745	-6.48459	0.128138
89	H	5.763232	-5.64251	-4.91016	0.125484
90	C	8.384928	2.732159	-0.177	-0.04008
91	C	9.636976	2.252218	-0.57621	-0.05035
92	C	8.286473	4.078594	0.157544	-0.12733
93	C	10.72974	3.080002	-0.6295	-0.13692
94	H	9.750304	1.220084	-0.8667	0.126491
95	C	9.378391	4.923408	0.102954	-0.17219
96	H	7.340903	4.484176	0.484373	0.13334
97	C	10.61417	4.427238	-0.29142	0.218244
98	H	11.69185	2.708255	-0.9434	0.129151
99	H	9.255525	5.957402	0.375454	0.14817
100	O	11.73356	5.155711	-0.378	-0.39091
101	C	11.67944	6.534201	-0.06162	-0.0896
102	H	10.96098	7.029975	-0.7147	0.140028
103	H	11.34673	6.659039	0.969004	0.139998
104	C	13.05797	7.09956	-0.25268	-0.33769
105	H	13.05751	8.160705	-0.01853	0.13401
106	H	13.76999	6.603149	0.400933	0.133715
107	H	13.38459	6.974177	-1.28136	0.133655
108	C	-11.301	0.027952	0.016993	0.167952
109	C	-12.5087	0.089608	0.017911	0.022174
110	C	-13.9134	0.179468	0.017305	-0.21349
111	C	-14.7052	-0.9747	0.059656	-0.04142
112	C	-14.5411	1.431708	-0.02645	-0.03602

113	C	-16.0776	-0.87815	0.05757	-0.0233
114	H	-14.2292	-1.94104	0.093631	0.129606
115	C	-15.9124	1.519228	-0.02771	-0.03474
116	H	-13.9367	2.32348	-0.05902	0.13095
117	C	-16.6926	0.368726	0.013829	-0.27083
118	H	-16.6803	-1.77036	0.089837	0.136483
119	H	-16.4012	2.479348	-0.06116	0.134146
120	C	-18.1572	0.518699	0.009487	0.536777
121	O	-18.732	1.572233	-0.02527	-0.4169
122	O	-18.8034	-0.64257	0.048066	-0.37355
123	H	-19.7424	-0.45232	0.041356	0.292474

Table S32. The Bond Lengths of the S₁ State of **C288** in THF Computed at the TD-MPW1K/6-311G(d,p) Level of Theory.

Number	Name	Length[Å]	Number	Name	Length[Å]
R1	R(1,2)	1.4704	R69	R(56,57)	1.3897
R2	R(1,3)	1.4161	R70	R(56,58)	1.3887
R3	R(1,17)	1.3941	R71	R(57,59)	1.3826
R4	R(2,4)	1.41	R72	R(57,60)	1.0785
R5	R(2,15)	1.3954	R73	R(58,61)	1.3828
R6	R(3,6)	1.3793	R74	R(58,62)	1.0787
R7	R(3,12)	1.4028	R75	R(59,63)	1.3883
R8	R(4,5)	1.3789	R76	R(59,64)	1.0804
R9	R(4,7)	1.4028	R77	R(61,63)	1.3876
R10	R(5,6)	1.3519	R78	R(61,65)	1.0804
R11	R(5,14)	1.3966	R79	R(63,76)	1.4996
R12	R(6,19)	1.3985	R80	R(66,67)	1.3887
R13	R(7,8)	1.3943	R81	R(66,68)	1.3897
R14	R(7,46)	1.4476	R82	R(67,69)	1.3829
R15	R(8,9)	1.3956	R83	R(67,70)	1.079
R16	R(8,55)	1.524	R84	R(68,71)	1.3824
R17	R(9,10)	1.0779	R85	R(68,72)	1.0783
R18	R(9,15)	1.3858	R86	R(69,73)	1.3875
R19	R(11,13)	1.0786	R87	R(69,74)	1.0804
R20	R(11,17)	1.3885	R88	R(71,73)	1.3884
R21	R(11,21)	1.3897	R89	R(71,75)	1.0804
R22	R(12,21)	1.3907	R90	R(73,83)	1.4997
R23	R(12,23)	1.4619	R91	R(76,77)	1.0888
R24	R(14,20)	1.3856	R92	R(76,78)	1.0888
R25	R(14,47)	1.386	R93	R(76,79)	1.5229
R26	R(15,16)	1.0784	R94	R(79,80)	1.088

R27	R(17,18)	1.0784	R95	R(79,81)	1.0877
R28	R(19,20)	1.3933	R96	R(79,82)	1.088
R29	R(19,24)	1.3771	R97	R(83,84)	1.0887
R30	R(20,26)	1.4471	R98	R(83,85)	1.0889
R31	R(21,22)	1.0786	R99	R(83,86)	1.5231
R32	R(23,24)	1.4269	R100	R(86,87)	1.0879
R33	R(23,33)	1.3798	R101	R(86,88)	1.0877
R34	R(24,25)	1.0772	R102	R(86,89)	1.088
R35	R(26,27)	1.0865	R103	R(90,91)	1.399
R36	R(26,28)	1.0865	R104	R(90,92)	1.3909
R37	R(26,29)	1.5146	R105	R(91,93)	1.3719
R38	R(29,30)	1.0868	R106	R(91,94)	1.0782
R39	R(29,31)	1.087	R107	R(92,95)	1.3817
R40	R(29,32)	1.0869	R108	R(92,96)	1.0795
R41	R(33,34)	1.2196	R109	R(93,97)	1.3938
R42	R(34,35)	1.3789	R110	R(93,98)	1.0781
R43	R(35,36)	1.4327	R111	R(95,97)	1.3888
R44	R(35,37)	1.4072	R112	R(95,99)	1.0763
R45	R(36,38)	1.4388	R113	R(97,100)	1.3384
R46	R(36,39)	1.3144	R114	R(100,101)	1.4154
R47	R(37,40)	1.3771	R115	R(101,102)	1.0902
R48	R(37,41)	1.0779	R116	R(101,103)	1.0902
R49	R(38,42)	1.3182	R117	R(101,104)	1.5022
R50	R(38,43)	1.4254	R118	R(104,105)	1.0867
R51	R(39,44)	1.6275	R119	R(104,106)	1.0866
R52	R(40,43)	1.4016	R120	R(104,107)	1.0865
R53	R(40,45)	1.0782	R121	R(108,109)	1.2092
R54	R(42,44)	1.6258	R122	R(109,110)	1.4077
R55	R(43,108)	1.3946	R123	R(110,111)	1.4003

R56	R(46,47)	1.4081	R124	R(110,112)	1.4014
R57	R(46,49)	1.4206	R125	R(111,113)	1.3757
R58	R(47,48)	1.0783	R126	R(111,114)	1.0778
R59	R(49,50)	1.3783	R127	R(112,115)	1.374
R60	R(49,51)	1.7285	R128	R(112,116)	1.0778
R61	R(50,52)	1.4052	R129	R(113,117)	1.391
R62	R(50,55)	1.5155	R130	R(113,118)	1.0772
R63	R(51,53)	1.7268	R131	R(115,117)	1.3907
R64	R(52,53)	1.3687	R132	R(115,119)	1.0779
R65	R(52,54)	1.0757	R133	R(117,120)	1.4722
R66	R(53,90)	1.4516	R134	R(120,121)	1.2007
R67	R(55,56)	1.5346	R135	R(120,122)	1.3295
R68	R(55,66)	1.5359	R136	R(122,123)	0.9581

Table S33. The Bond Angles of the S₁ State of **C288** in THF Computed at the TD-MPW1K/6-311G(d,p) Level of Theory.

Number	Name	Angle [°]	Number	Name	Angle [°]
A1	A(2,1,3)	19.0211	A119	A(56,57,59)	121.0026
A2	A(2,1,17)	125.8015	A120	A(56,57,60)	120.1144
A3	A(3,1,17)	115.1773	A121	A(59,57,60)	118.8816
A4	A(1,2,4)	119.1702	A122	A(56,58,61)	121.0639
A5	A(1,2,15)	126.3791	A123	A(56,58,62)	119.8936
A6	A(4,2,15)	114.4496	A124	A(61,58,62)	119.0421
A7	A(1,3,6)	118.0673	A125	A(57,59,63)	121.2877
A8	A(1,3,12)	125.6163	A126	A(57,59,64)	119.1907
A9	A(6,3,12)	116.316	A127	A(63,59,64)	119.5216
A10	A(2,4,5)	118.211	A128	A(58,61,63)	121.2548
A11	A(2,4,7)	125.8495	A129	A(58,61,65)	119.2272
A12	A(5,4,7)	115.9366	A130	A(63,61,65)	119.5175
A13	A(4,5,6)	122.7692	A131	A(59,63,61)	117.6197
A14	A(4,5,14)	128.1937	A132	A(59,63,76)	121.1745
A15	A(6,5,14)	109.036	A133	A(61,63,76)	121.1823
A16	A(3,6,5)	122.7594	A134	A(55,66,67)	120.0207
A17	A(3,6,19)	128.3747	A135	A(55,66,68)	122.0251
A18	A(5,6,19)	108.8658	A136	A(67,66,68)	117.7803
A19	A(4,7,8)	117.6153	A137	A(66,67,69)	121.0768
A20	A(4,7,46)	117.6404	A138	A(66,67,70)	119.7963
A21	A(8,7,46)	124.7408	A139	A(69,67,70)	119.1265
A22	A(7,8,9)	117.5074	A140	A(66,68,71)	120.966
A23	A(7,8,55)	121.9217	A141	A(66,68,72)	120.1898
A24	A(9,8,55)	120.5685	A142	A(71,68,72)	118.8375
A25	A(8,9,10)	118.5035	A143	A(67,69,73)	121.2356
A26	A(8,9,15)	123.8269	A144	A(67,69,74)	119.236

A27	A(10,9,15)	117.6693	A145	A(73,69,74)	119.5277
A28	A(13,11,17)	118.5259	A146	A(68,71,73)	121.3238
A29	A(13,11,21)	118.6032	A147	A(68,71,75)	119.1514
A30	A(17,11,21)	122.8709	A148	A(73,71,75)	119.5233
A31	A(3,12,21)	116.4385	A149	A(69,73,71)	117.6159
A32	A(3,12,23)	117.2517	A150	A(69,73,83)	121.2525
A33	A(21,12,23)	126.3097	A151	A(71,73,83)	121.1095
A34	A(5,14,20)	106.7472	A152	A(63,76,77)	109.3276
A35	A(5,14,47)	116.5934	A153	A(63,76,78)	109.303
A36	A(20,14,47)	136.6593	A154	A(63,76,79)	112.4094
A37	A(2,15,9)	120.7489	A155	A(77,76,78)	106.7965
A38	A(2,15,16)	120.8557	A156	A(77,76,79)	109.428
A39	A(9,15,16)	118.3953	A157	A(78,76,79)	109.4172
A40	A(1,17,11)	120.3878	A158	A(76,79,80)	110.9219
A41	A(1,17,18)	120.7784	A159	A(76,79,81)	110.9011
A42	A(11,17,18)	118.8338	A160	A(76,79,82)	110.901
A43	A(6,19,20)	106.5325	A161	A(80,79,81)	108.0735
A44	A(6,19,24)	116.8588	A162	A(80,79,82)	107.8334
A45	A(20,19,24)	136.6076	A163	A(81,79,82)	108.0839
A46	A(14,20,19)	108.8112	A164	A(73,83,84)	109.331
A47	A(14,20,26)	125.6971	A165	A(73,83,85)	109.3415
A48	A(19,20,26)	125.3565	A166	A(73,83,86)	112.3843
A49	A(11,21,12)	119.5091	A167	A(84,83,85)	106.7943
A50	A(11,21,22)	119.926	A168	A(84,83,86)	109.4364
A51	A(12,21,22)	120.5648	A169	A(85,83,86)	109.3954
A52	A(12,23,24)	122.9438	A170	A(83,86,87)	110.9147
A53	A(12,23,33)	119.0963	A171	A(83,86,88)	110.8968
A54	A(24,23,33)	117.9597	A172	A(83,86,89)	110.9178
A55	A(19,24,23)	118.2548	A173	A(87,86,88)	108.0851

A56	A(19,24,25)	123.5934	A174	A(87,86,89)	107.8269
A57	A(23,24,25)	118.1516	A175	A(88,86,89)	108.0734
A58	A(20,26,27)	107.6027	A176	A(53,90,91)	120.586
A59	A(20,26,28)	107.5398	A177	A(53,90,92)	121.7637
A60	A(20,26,29)	112.9879	A178	A(91,90,92)	117.6503
A61	A(27,26,28)	106.6681	A179	A(90,91,93)	121.1259
A62	A(27,26,29)	110.902	A180	A(90,91,94)	119.9557
A63	A(28,26,29)	110.8569	A181	A(93,91,94)	118.9081
A64	A(26,29,30)	110.9589	A182	A(90,92,95)	121.7674
A65	A(26,29,31)	110.9908	A183	A(90,92,96)	119.902
A66	A(26,29,32)	109.8374	A184	A(95,92,96)	118.3242
A67	A(30,29,31)	108.4488	A185	A(91,93,97)	120.5141
A68	A(30,29,32)	108.246	A186	A(91,93,98)	120.9346
A69	A(31,29,32)	108.2714	A187	A(97,93,98)	118.5477
A70	A(34,35,36)	120.5561	A188	A(92,95,97)	119.7342
A71	A(34,35,37)	122.5841	A189	A(92,95,99)	119.1554
A72	A(36,35,37)	116.8598	A190	A(97,95,99)	121.1088
A73	A(35,36,38)	120.5042	A191	A(93,97,95)	119.2072
A74	A(35,36,39)	126.1545	A192	A(93,97,100)	116.1729
A75	A(38,36,39)	113.3413	A193	A(95,97,100)	124.6199
A76	A(35,37,40)	122.3001	A194	A(97,100,101)	118.9261
A77	A(35,37,41)	118.4131	A195	A(100,101,102)	109.5241
A78	A(40,37,41)	119.2868	A196	A(100,101,103)	109.5436
A79	A(36,38,42)	113.0643	A197	A(100,101,104)	107.6399
A80	A(36,38,43)	120.4483	A198	A(102,101,103)	108.2481
A81	A(42,38,43)	126.4874	A199	A(102,101,104)	110.943
A82	A(36,39,44)	107.2118	A200	A(103,101,104)	110.9297
A83	A(37,40,43)	122.803	A201	A(101,104,105)	109.86
A84	A(37,40,45)	118.9757	A202	A(101,104,106)	110.6652

A85	A(43,40,45)	118.2213	A203	A(101,104,107)	110.6616
A86	A(38,42,44)	107.2623	A204	A(105,104,106)	108.4689
A87	A(38,43,40)	117.0846	A205	A(105,104,107)	108.4706
A88	A(38,43,108)	120.7708	A206	A(106,104,107)	108.6513
A89	A(40,43,108)	122.1446	A207	A(109,110,111)	120.775
A90	A(39,44,42)	99.1202	A208	A(109,110,112)	120.2663
A91	A(7,46,47)	123.3771	A209	A(111,110,112)	118.9587
A92	A(7,46,49)	114.3578	A210	A(110,111,113)	120.4086
A93	A(47,46,49)	122.2648	A211	A(110,111,114)	119.3554
A94	A(14,47,46)	118.2578	A212	A(113,111,114)	120.236
A95	A(14,47,48)	122.3738	A213	A(110,112,115)	120.2593
A96	A(46,47,48)	119.3682	A214	A(110,112,116)	119.284
A97	A(46,49,50)	124.5786	A215	A(115,112,116)	120.4568
A98	A(46,49,51)	124.2551	A216	A(111,113,117)	120.2649
A99	A(50,49,51)	111.1542	A217	A(111,113,118)	119.9995
A100	A(49,50,52)	112.2258	A218	A(117,113,118)	119.7356
A101	A(49,50,55)	123.7109	A219	A(112,115,117)	120.4747
A102	A(52,50,55)	124.0633	A220	A(112,115,119)	120.6197
A103	A(49,51,53)	91.974	A221	A(117,115,119)	118.9056
A104	A(50,52,53)	114.0732	A222	A(113,117,115)	119.6338
A105	A(50,52,54)	123.407	A223	A(113,117,120)	122.089
A106	A(53,52,54)	122.5085	A224	A(115,117,120)	118.2773
A107	A(51,53,52)	110.5715	A225	A(117,120,121)	124.4562
A108	A(51,53,90)	121.2241	A226	A(117,120,122)	113.233
A109	A(52,53,90)	128.2026	A227	A(121,120,122)	122.3108
A110	A(8,55,50)	110.6618	A228	A(120,122,123)	107.6212
A111	A(8,55,56)	110.5008	A229	L(23,33,34,24,-1)	178.8184
A112	A(8,55,66)	106.2777	A230	L(33,34,35,36,-1)	178.9169
A113	A(50,55,56)	106.2588	A231	L(43,108,109,38,-1)	179.5287

A114	A(50,55,66)	109.5514	A232	L(108,109,110,112,-1)	179.2606
A115	A(56,55,66)	113.6396	A233	L(23,33,34,24,-2)	179.9964
A116	A(55,56,57)	121.6761	A234	L(33,34,35,36,-2)	180.0316
A117	A(55,56,58)	120.3211	A235	L(43,108,109,38,-2)	179.9707
A118	A(57,56,58)	117.7651	A236	L(108,109,110,112,-2)	179.918

Table S34. The Dihedral Angles of the S₁ State of **C288** in THF Computed at the TD-MPW1K/6-311G(d,p) Level of Theory.

Number	Name	Dihedral Angle [°]	Number	Name	Dihedral Angle [°]
D1	D(3,1,2,4)	-0.3896	D177	D(55,50,52,54)	-1.3024
D2	D(3,1,2,15)	179.2026	D178	D(49,50,55,8)	-0.4288
D3	D(17,1,2,4)	179.7573	D179	D(49,50,55,56)	-120.42
D4	D(17,1,2,15)	-0.6505	D180	D(49,50,55,66)	116.4312
D5	D(2,1,3,6)	0.0336	D181	D(52,50,55,8)	179.6115
D6	D(2,1,3,12)	-179.73	D182	D(52,50,55,56)	59.6203
D7	D(17,1,3,6)	179.902	D183	D(52,50,55,66)	-63.5285
D8	D(17,1,3,12)	0.1388	D184	D(49,51,53,52)	0.2992
D9	D(2,1,17,11)	179.8194	D185	D(49,51,53,90)	179.8472
D10	D(2,1,17,18)	-0.1807	D186	D(50,52,53,51)	-0.189
D11	D(3,1,17,11)	-0.0387	D187	D(50,52,53,90)	-179.697
D12	D(3,1,17,18)	179.9613	D188	D(54,52,53,51)	-179.003
D13	D(1,2,4,5)	0.4896	D189	D(54,52,53,90)	1.4895
D14	D(1,2,4,7)	179.8396	D190	D(51,53,90,91)	-159.828
D15	D(15,2,4,5)	-179.15	D191	D(51,53,90,92)	20.116
D16	D(15,2,4,7)	0.2004	D192	D(52,53,90,91)	19.6337
D17	D(1,2,15,9)	-179.912	D193	D(52,53,90,92)	-160.423
D18	D(1,2,15,16)	-0.0143	D194	D(8,55,56,57)	155.2227
D19	D(4,2,15,9)	-0.3033	D195	D(8,55,56,58)	-30.5045
D20	D(4,2,15,16)	179.5945	D196	D(50,55,56,57)	-84.6815
D21	D(1,3,6,5)	0.2257	D197	D(50,55,56,58)	89.5913
D22	D(1,3,6,19)	-179.713	D198	D(66,55,56,57)	35.8612
D23	D(12,3,6,5)	-179.989	D199	D(66,55,56,58)	-149.866
D24	D(12,3,6,19)	0.0723	D200	D(8,55,66,67)	87.6009
D25	D(1,3,12,21)	-0.1356	D201	D(8,55,66,68)	-87.4984
D26	D(1,3,12,23)	179.7494	D202	D(50,55,66,67)	-31.988

D27	D(6,3,12,21)	-179.902	D203	D(50,55,66,68)	152.9126
D28	D(6,3,12,23)	-0.0174	D204	D(56,55,66,67)	-150.658
D29	D(2,4,5,6)	-0.2472	D205	D(56,55,66,68)	34.2423
D30	D(2,4,5,14)	179.3329	D206	D(55,56,57,59)	175.2485
D31	D(7,4,5,6)	-179.662	D207	D(55,56,57,60)	-5.1868
D32	D(7,4,5,14)	-0.0813	D208	D(58,56,57,59)	0.8351
D33	D(2,4,7,8)	0.2156	D209	D(58,56,57,60)	-179.6
D34	D(2,4,7,46)	-179.144	D210	D(55,56,58,61)	-175.306
D35	D(5,4,7,8)	179.5788	D211	D(55,56,58,62)	4.471
D36	D(5,4,7,46)	0.2194	D212	D(57,56,58,61)	-0.813
D37	D(4,5,6,3)	-0.124	D213	D(57,56,58,62)	178.9635
D38	D(4,5,6,19)	179.8251	D214	D(56,57,59,63)	-0.2703
D39	D(14,5,6,3)	-179.775	D215	D(56,57,59,64)	179.8332
D40	D(14,5,6,19)	0.1742	D216	D(60,57,59,63)	-179.84
D41	D(4,5,14,20)	179.7244	D217	D(60,57,59,64)	0.2632
D42	D(4,5,14,47)	-0.1927	D218	D(56,58,61,63)	0.2248
D43	D(6,5,14,20)	-0.6491	D219	D(56,58,61,65)	179.9778
D44	D(6,5,14,47)	179.4338	D220	D(62,58,61,63)	-179.554
D45	D(3,6,19,20)	-179.688	D221	D(62,58,61,65)	0.1994
D46	D(3,6,19,24)	-0.0032	D222	D(57,59,63,61)	-0.3329
D47	D(5,6,19,20)	0.367	D223	D(57,59,63,76)	177.9213
D48	D(5,6,19,24)	-179.949	D224	D(64,59,63,61)	179.5632
D49	D(4,7,8,9)	-0.5126	D225	D(64,59,63,76)	-2.1825
D50	D(4,7,8,55)	178.9214	D226	D(58,61,63,59)	0.3555
D51	D(46,7,8,9)	178.7968	D227	D(58,61,63,76)	-177.899
D52	D(46,7,8,55)	-1.7692	D228	D(65,61,63,59)	-179.397
D53	D(4,7,46,47)	-0.1033	D229	D(65,61,63,76)	2.3492
D54	D(4,7,46,49)	179.6946	D230	D(59,63,76,77)	32.6886
D55	D(8,7,46,47)	-179.413	D231	D(59,63,76,78)	149.2603

D56	D(8,7,46,49)	0.3854	D232	D(59,63,76,79)	-89.0411
D57	D(7,8,9,10)	-179.389	D233	D(61,63,76,77)	-149.12
D58	D(7,8,9,15)	0.4304	D234	D(61,63,76,78)	-32.5477
D59	D(55,8,9,10)	1.1693	D235	D(61,63,76,79)	89.1509
D60	D(55,8,9,15)	-179.012	D236	D(55,66,67,69)	-175.708
D61	D(7,8,55,50)	1.6759	D237	D(55,66,67,70)	4.504
D62	D(7,8,55,56)	119.0924	D238	D(68,66,67,69)	-0.4035
D63	D(7,8,55,66)	-117.187	D239	D(68,66,67,70)	179.8084
D64	D(9,8,55,50)	-178.907	D240	D(55,66,68,71)	175.6725
D65	D(9,8,55,56)	-61.4906	D241	D(55,66,68,72)	-5.2854
D66	D(9,8,55,66)	62.2305	D242	D(67,66,68,71)	0.4682
D67	D(8,9,15,2)	-0.0004	D243	D(67,66,68,72)	179.5103
D68	D(8,9,15,16)	-179.901	D244	D(66,67,69,73)	0.1183
D69	D(10,9,15,2)	179.8199	D245	D(66,67,69,74)	-179.564
D70	D(10,9,15,16)	-0.0803	D246	D(70,67,69,73)	179.9078
D71	D(13,11,17,1)	179.9917	D247	D(70,67,69,74)	0.2255
D72	D(13,11,17,18)	-0.0083	D248	D(66,68,71,73)	-0.2504
D73	D(21,11,17,1)	-0.0562	D249	D(66,68,71,75)	179.3128
D74	D(21,11,17,18)	179.9438	D250	D(72,68,71,73)	-179.305
D75	D(13,11,21,12)	-179.987	D251	D(72,68,71,75)	0.2579
D76	D(13,11,21,22)	0.0373	D252	D(67,69,73,71)	0.1115
D77	D(17,11,21,12)	0.0607	D253	D(67,69,73,83)	178.4203
D78	D(17,11,21,22)	-179.915	D254	D(74,69,73,71)	179.7929
D79	D(3,12,21,11)	0.0308	D255	D(74,69,73,83)	-1.8983
D80	D(3,12,21,22)	-179.994	D256	D(68,71,73,69)	-0.0461
D81	D(23,12,21,11)	-179.842	D257	D(68,71,73,83)	-178.358
D82	D(23,12,21,22)	0.133	D258	D(75,71,73,69)	-179.608
D83	D(3,12,23,24)	-0.1015	D259	D(75,71,73,83)	2.0809
D84	D(3,12,23,33)	-179.917	D260	D(69,73,83,84)	30.8281

D85	D(21,12,23,24)	179.7707	D261	D(69,73,83,85)	147.421
D86	D(21,12,23,33)	-0.045	D262	D(69,73,83,86)	-90.8978
D87	D(5,14,20,19)	0.8771	D263	D(71,73,83,84)	-150.922
D88	D(5,14,20,26)	176.824	D264	D(71,73,83,85)	-34.3292
D89	D(47,14,20,19)	-179.231	D265	D(71,73,83,86)	87.352
D90	D(47,14,20,26)	-3.2841	D266	D(63,76,79,80)	59.9494
D91	D(5,14,47,46)	0.3037	D267	D(63,76,79,81)	-179.95
D92	D(5,14,47,48)	-179.496	D268	D(63,76,79,82)	-59.8493
D93	D(20,14,47,46)	-179.581	D269	D(77,76,79,80)	-61.7231
D94	D(20,14,47,48)	0.6197	D270	D(77,76,79,81)	58.3779
D95	D(6,19,20,14)	-0.7733	D271	D(77,76,79,82)	178.4782
D96	D(6,19,20,26)	-176.737	D272	D(78,76,79,80)	-178.417
D97	D(24,19,20,14)	179.6365	D273	D(78,76,79,81)	-58.3161
D98	D(24,19,20,26)	3.6724	D274	D(78,76,79,82)	61.7842
D99	D(6,19,24,23)	-0.1159	D275	D(73,83,86,87)	59.9429
D100	D(6,19,24,25)	179.7764	D276	D(73,83,86,88)	-179.949
D101	D(20,19,24,23)	179.4437	D277	D(73,83,86,89)	-59.854
D102	D(20,19,24,25)	-0.6639	D278	D(84,83,86,87)	-61.723
D103	D(14,20,26,27)	34.7662	D279	D(84,83,86,88)	58.3849
D104	D(14,20,26,28)	149.3401	D280	D(84,83,86,89)	178.4801
D105	D(14,20,26,29)	-87.9976	D281	D(85,83,86,87)	-178.407
D106	D(19,20,26,27)	-149.939	D282	D(85,83,86,88)	-58.2988
D107	D(19,20,26,28)	-35.3655	D283	D(85,83,86,89)	61.7964
D108	D(19,20,26,29)	87.2968	D284	D(53,90,91,93)	-179.76
D109	D(12,23,24,19)	0.1718	D285	D(53,90,91,94)	1.4228
D110	D(12,23,24,25)	-179.727	D286	D(92,90,91,93)	0.2943
D111	D(33,23,24,19)	179.9895	D287	D(92,90,91,94)	-178.523
D112	D(33,23,24,25)	0.0912	D288	D(53,90,92,95)	-179.987
D113	D(12,23,35,36)	179.4246	D289	D(53,90,92,96)	0.9481

D114	D(12,23,35,37)	-0.5794	D290	D(91,90,92,95)	-0.0421
D115	D(24,23,35,36)	-0.3907	D291	D(91,90,92,96)	-179.107
D116	D(24,23,35,37)	179.6054	D292	D(90,91,93,97)	-0.3272
D117	D(20,26,29,30)	-60.167	D293	D(90,91,93,98)	-179.621
D118	D(20,26,29,31)	60.4921	D294	D(94,91,93,97)	178.5024
D119	D(20,26,29,32)	-179.812	D295	D(94,91,93,98)	-0.7918
D120	D(27,26,29,30)	178.9254	D296	D(90,92,95,97)	-0.1765
D121	D(27,26,29,31)	-60.4155	D297	D(90,92,95,99)	-179.725
D122	D(27,26,29,32)	59.2809	D298	D(96,92,95,97)	178.9022
D123	D(28,26,29,30)	60.6268	D299	D(96,92,95,99)	-0.6458
D124	D(28,26,29,31)	-178.714	D300	D(91,93,97,95)	0.1007
D125	D(28,26,29,32)	-59.0178	D301	D(91,93,97,100)	-179.805
D126	D(34,35,36,38)	179.9933	D302	D(98,93,97,95)	179.4115
D127	D(34,35,36,39)	-0.0199	D303	D(98,93,97,100)	-0.4939
D128	D(37,35,36,38)	0.0054	D304	D(92,95,97,93)	0.1476
D129	D(37,35,36,39)	179.9921	D305	D(92,95,97,100)	-179.956
D130	D(34,35,37,40)	-179.961	D306	D(99,95,97,93)	179.6866
D131	D(34,35,37,41)	0.0179	D307	D(99,95,97,100)	-0.4165
D132	D(36,35,37,40)	0.0264	D308	D(93,97,100,101)	179.3434
D133	D(36,35,37,41)	-179.994	D309	D(95,97,100,101)	-0.5562
D134	D(35,36,38,42)	-179.997	D310	D(97,100,101,102)	-58.8615
D135	D(35,36,38,43)	-0.0293	D311	D(97,100,101,103)	59.7206
D136	D(39,36,38,42)	0.0152	D312	D(97,100,101,104)	-179.573
D137	D(39,36,38,43)	179.9823	D313	D(100,101,104,105)	-179.998
D138	D(35,36,39,44)	-180.001	D314	D(100,101,104,106)	-60.2472
D139	D(38,36,39,44)	-0.0131	D315	D(100,101,104,107)	60.2522
D140	D(35,37,40,43)	-0.0352	D316	D(102,101,104,105)	60.1875
D141	D(35,37,40,45)	179.9765	D317	D(102,101,104,106)	179.9378
D142	D(41,37,40,43)	179.9857	D318	D(102,101,104,107)	-59.5628

D143	D(41,37,40,45)	-0.0026	D319	D(103,101,104,105)	-60.1666
D144	D(36,38,42,44)	-0.0091	D320	D(103,101,104,106)	59.5838
D145	D(43,38,42,44)	-179.974	D321	D(103,101,104,107)	-179.917
D146	D(36,38,43,40)	0.0216	D322	D(109,110,111,113)	-179.943
D147	D(36,38,43,108)	-179.963	D323	D(109,110,111,114)	0.037
D148	D(42,38,43,40)	179.984	D324	D(112,110,111,113)	0.0323
D149	D(42,38,43,108)	-0.0004	D325	D(112,110,111,114)	-179.988
D150	D(36,39,44,42)	0.007	D326	D(109,110,112,115)	179.9672
D151	D(37,40,43,38)	0.01	D327	D(109,110,112,116)	-0.0331
D152	D(37,40,43,108)	179.9941	D328	D(111,110,112,115)	-0.0081
D153	D(45,40,43,38)	179.9983	D329	D(111,110,112,116)	179.9915
D154	D(45,40,43,108)	-0.0175	D330	D(110,111,113,117)	-0.0248
D155	D(38,42,44,39)	0.0014	D331	D(110,111,113,118)	179.9716
D156	D(38,43,110,111)	179.3917	D332	D(114,111,113,117)	179.9954
D157	D(38,43,110,112)	-0.5431	D333	D(114,111,113,118)	-0.0081
D158	D(40,43,110,111)	-0.565	D334	D(110,112,115,117)	-0.0235
D159	D(40,43,110,112)	179.5001	D335	D(110,112,115,119)	179.9949
D160	D(7,46,47,14)	-0.1728	D336	D(116,112,115,117)	179.9768
D161	D(7,46,47,48)	179.633	D337	D(116,112,115,119)	-0.0047
D162	D(49,46,47,14)	-179.955	D338	D(111,113,117,115)	-0.007
D163	D(49,46,47,48)	-0.1492	D339	D(111,113,117,120)	179.9795
D164	D(7,46,49,50)	0.9588	D340	D(118,113,117,115)	179.9966
D165	D(7,46,49,51)	179.5759	D341	D(118,113,117,120)	-0.017
D166	D(47,46,49,50)	-179.241	D342	D(112,115,117,113)	0.0313
D167	D(47,46,49,51)	-0.6237	D343	D(112,115,117,120)	-179.956
D168	D(46,49,50,52)	179.067	D344	D(119,115,117,113)	-179.987
D169	D(46,49,50,55)	-0.8969	D345	D(119,115,117,120)	0.0262
D170	D(51,49,50,52)	0.2926	D346	D(113,117,120,121)	179.875
D171	D(51,49,50,55)	-179.671	D347	D(113,117,120,122)	-0.139

D172	D(46,49,51,53)	-179.119	D348	D(115,117,120,121)	-0.1384
D173	D(50,49,51,53)	-0.3395	D349	D(115,117,120,122)	179.8476
D174	D(49,50,52,53)	-0.0675	D350	D(117,120,122,123)	-179.949
D175	D(49,50,52,54)	178.7339	D351	D(121,120,122,123)	0.038
D176	D(55,50,52,53)	179.8963			