Electronic Supplementary Material (ESI) for New Journal of Chemistry.


# Synthesis, characterization, and optoelectronic properties of phenothiazine-based organic co-poly-ynes

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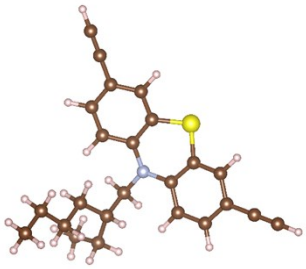


**Figure S1** Optimized structure of the precursor PTZ moiety **4**.

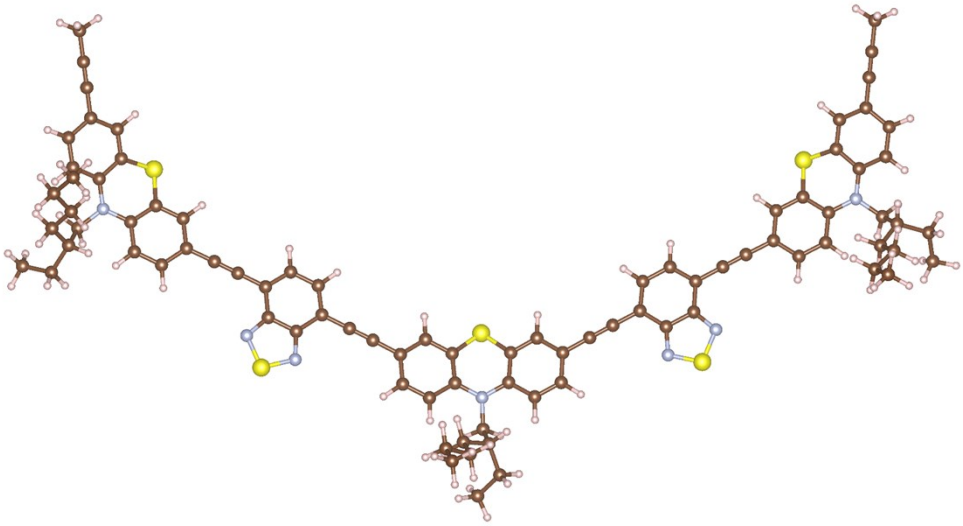


**Figure S2** Optimized structure of the model compound **M1**.

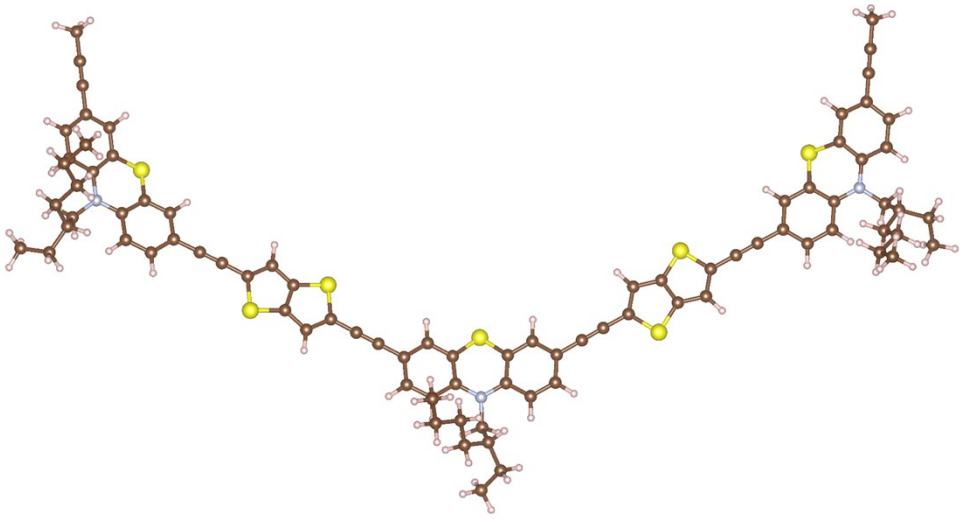


**Figure S3** Optimized structure of the model compound **M2**.

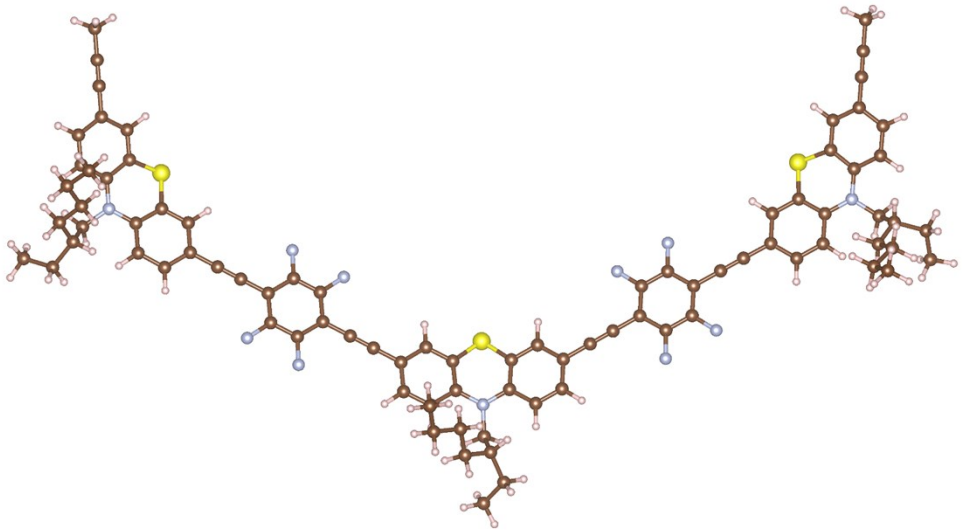


**Figure S4** Optimized structure of the model compound **M3**.

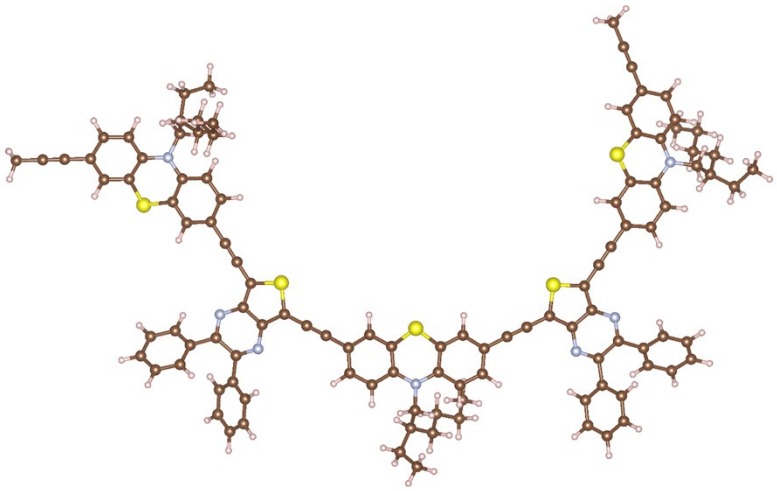


**Figure S5** Optimized structure of the model compound **M4**.

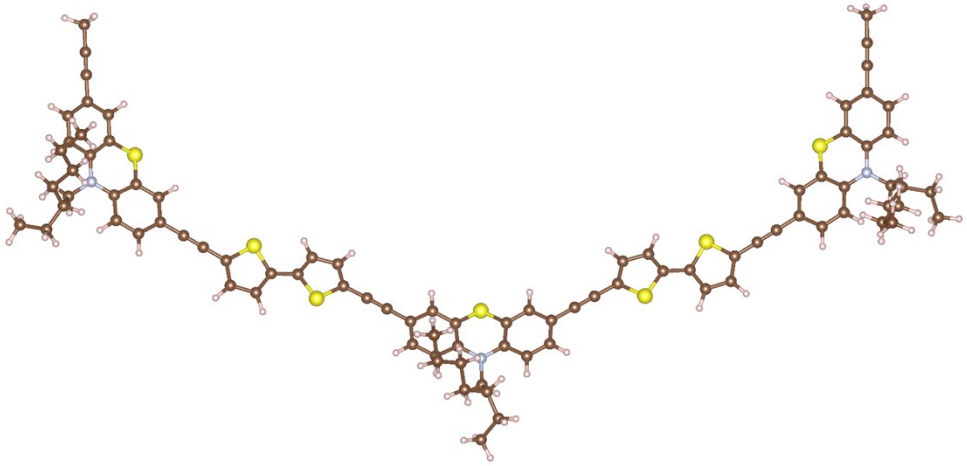


**Figure S6** Optimized structure of the model compound **M5**.

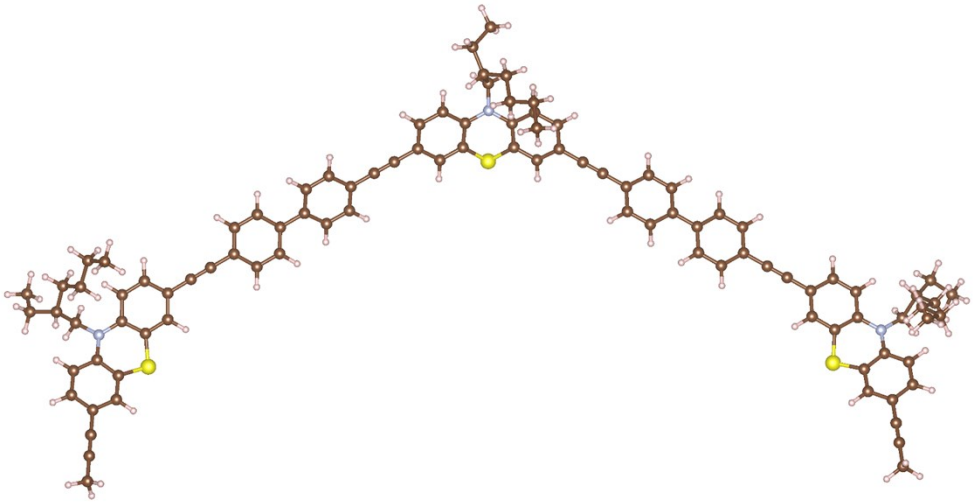


**Figure S7** Optimized structure of the model compound **M6**.

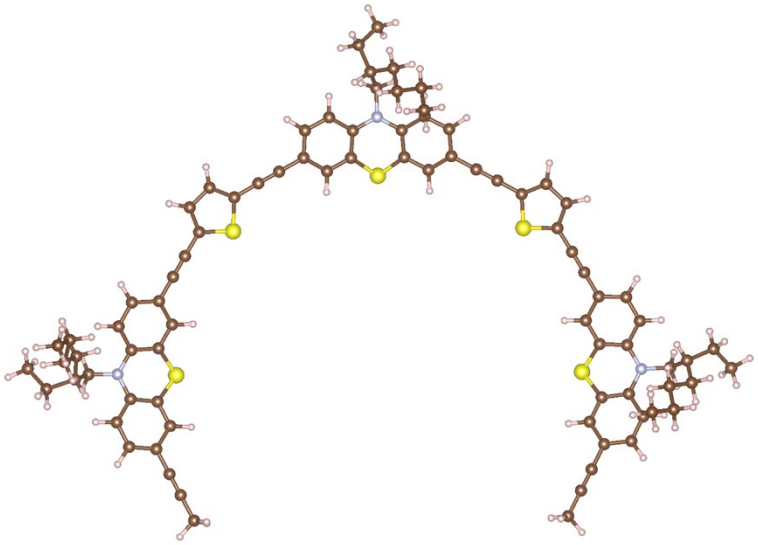
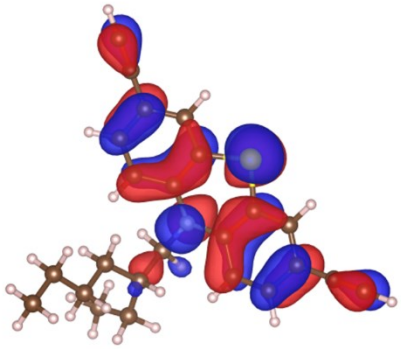


**Figure S8** Optimized structure of the model compound **M7**.

(a) HOMO



(b) LUMO

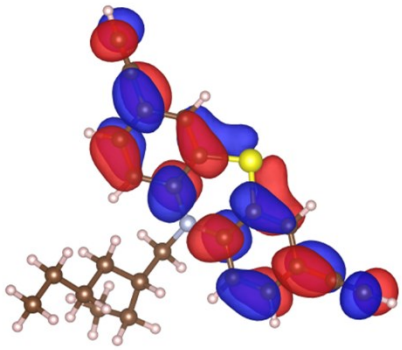


**Figure S9** Highest-occupied molecular orbital (HOMO; a) and lowest-unoccupied molecular orbital (LUMO; b) of the precursor PTZ moiety **4**. The isosurfaces are drawn to a contour value of 2.5 $\times$ $10^{-2}$ *e* $bohr^{-3}$.

(a) HOMO

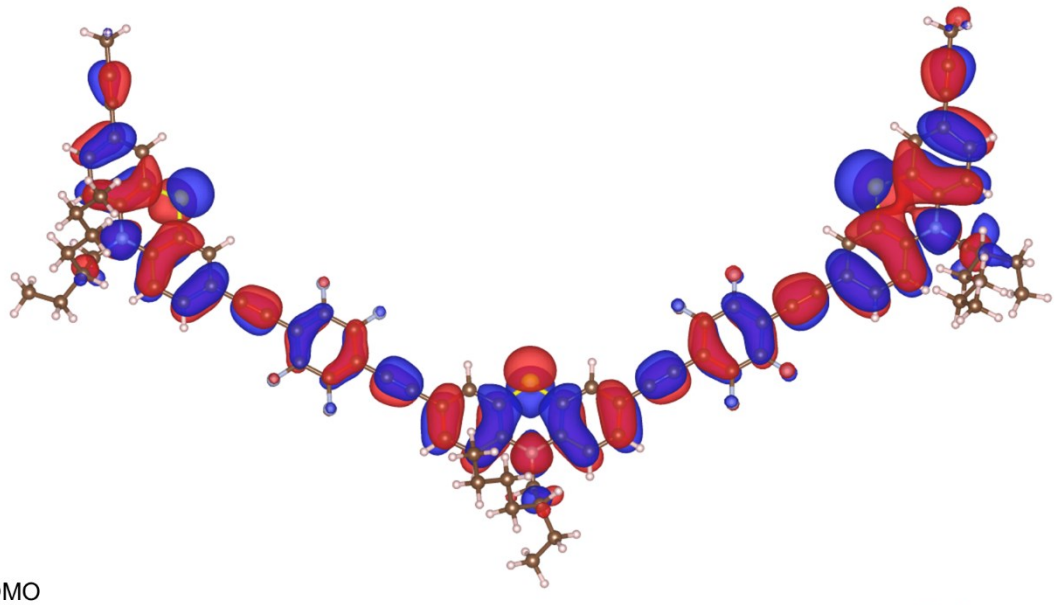
(b) LUMO

**Figure S10** Highest-occupied molecular orbital (HOMO; a) and lowest-unoccupied molecular orbital (LUMO; b) of the model compound **M1**. The isosurfaces are drawn to a contour value of $10^{-2}$ *e* $bohr^{-3}$.

(a) HOMO

(b) LUMO

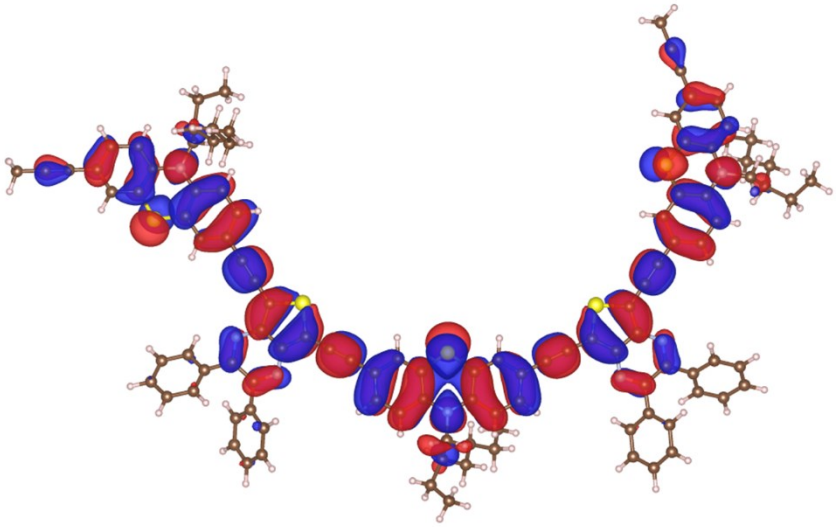
**Figure S11** Highest-occupied molecular orbital (HOMO; a) and lowest-unoccupied molecular orbital (LUMO; b) of the model compound **M2**. The isosurfaces are drawn to a contour value of $10^{-2}$ *e* $bohr^{-3}$.



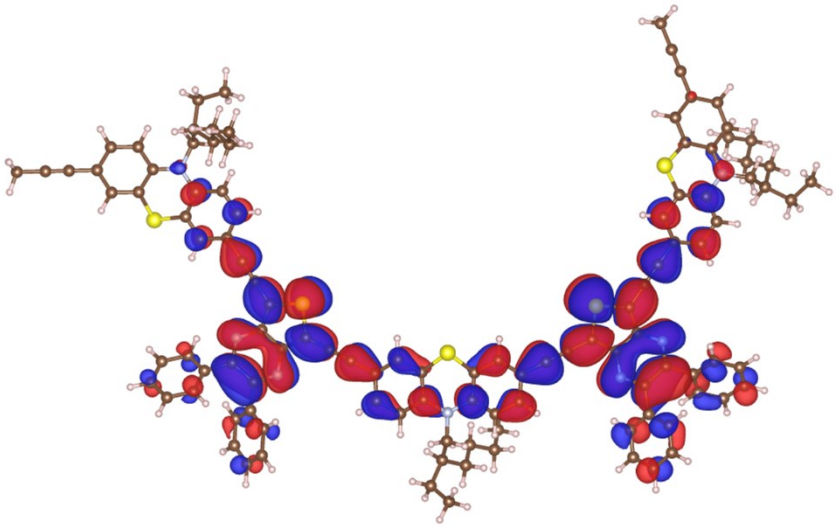
(a) HOMO

(b) LUMO

**Figure S12** Highest-occupied molecular orbital (HOMO; a) and lowest-unoccupied molecular orbital (LUMO; b) of the model compound **M3**. The isosurfaces are drawn to a contour value of $10^{-2}$ *e* $bohr^{-3}$.

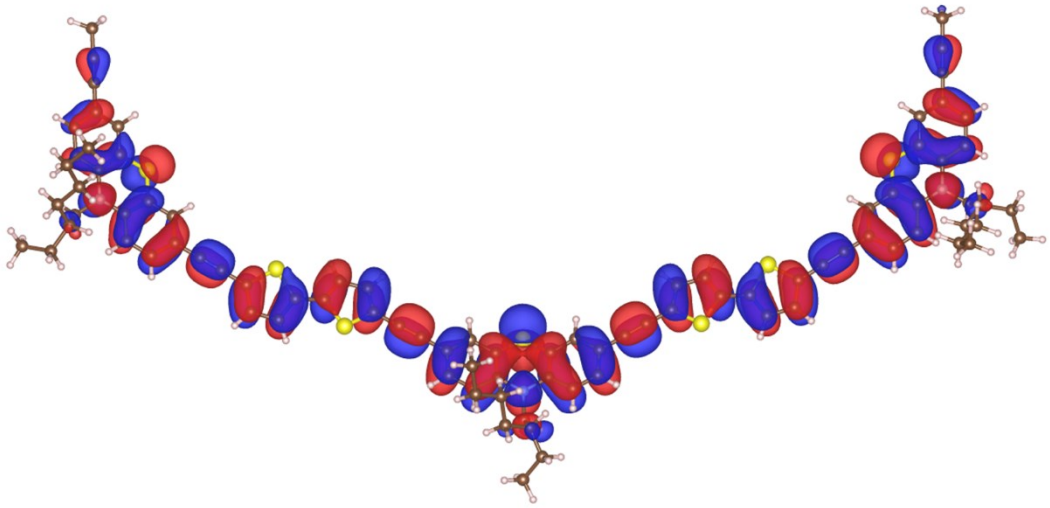


(a) HOMO

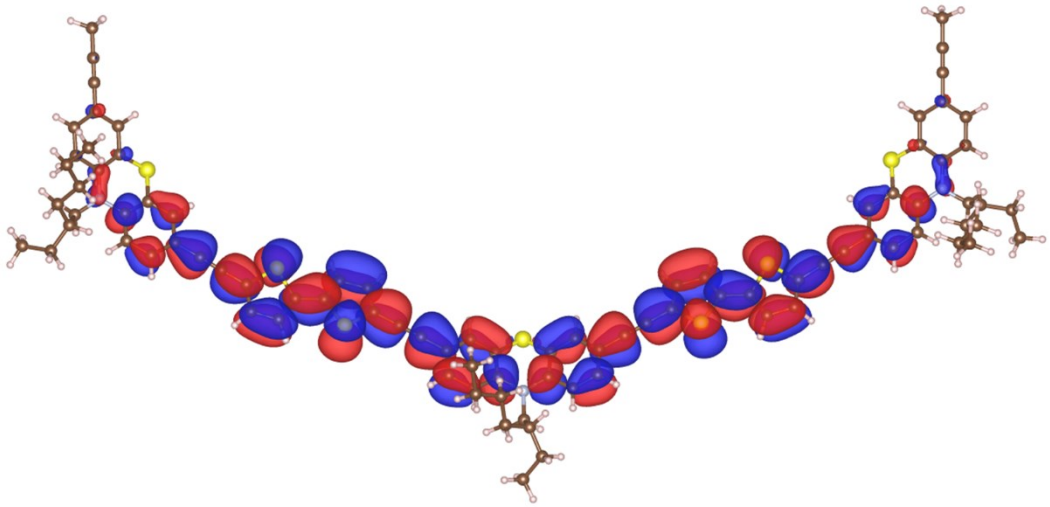


(b) LUMO

**Figure S13** Highest-occupied molecular orbital (HOMO; a) and lowest-unoccupied molecular orbital (LUMO; b) of the model compound **M4**. The isosurfaces are drawn to a contour value of $10^{-2}$ *e* $bohr^{-3}$.



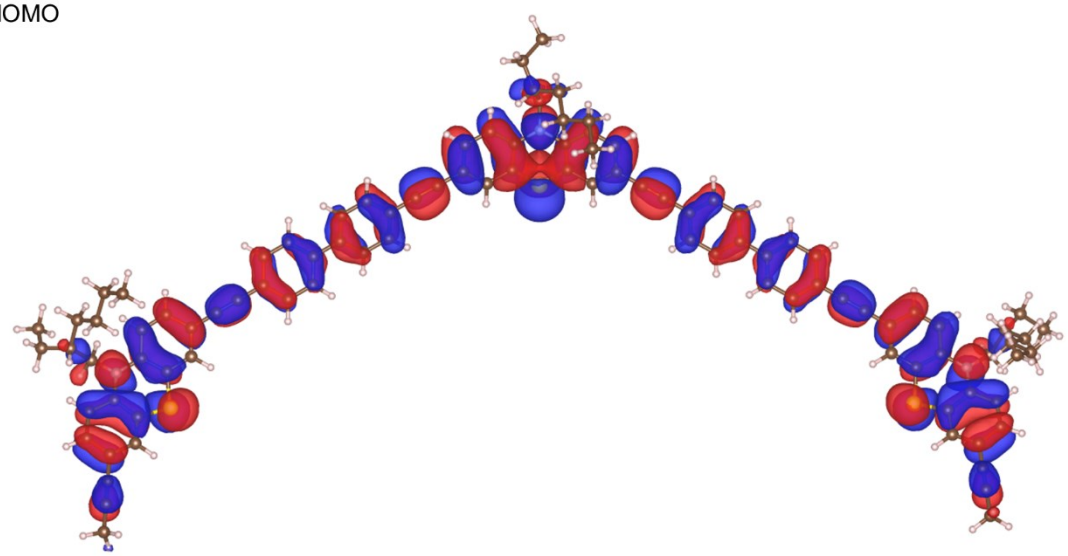
(a) HOMO



(b) LUMO

**Figure S14** Highest-occupied molecular orbital (HOMO; a) and lowest-unoccupied molecular orbital (LUMO; b) of the model compound **M5**. The isosurfaces are drawn to a contour value of $10^{-2}$ *e* $bohr^{-3}$.

(a) HOMO



(b) LUMO

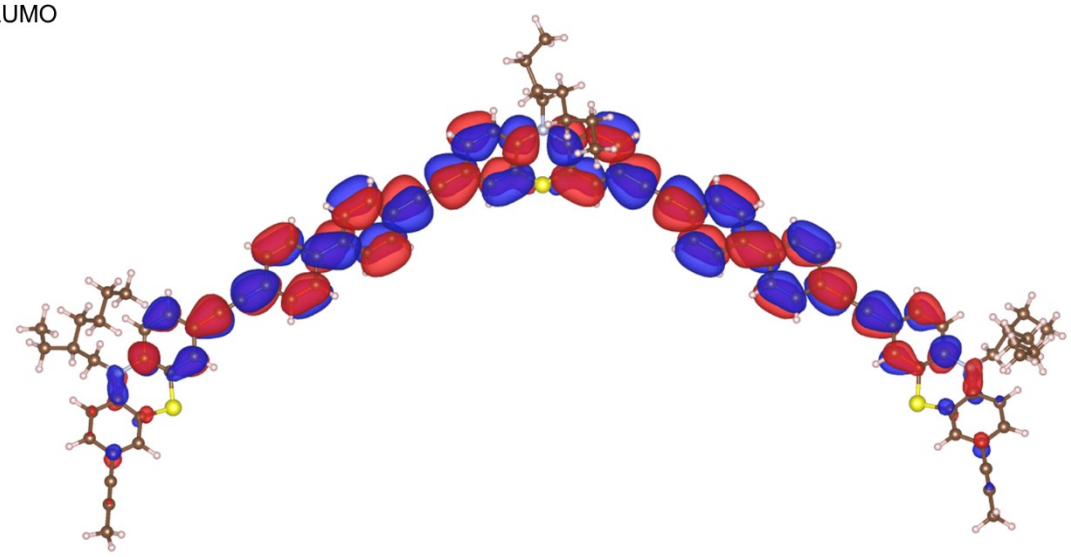
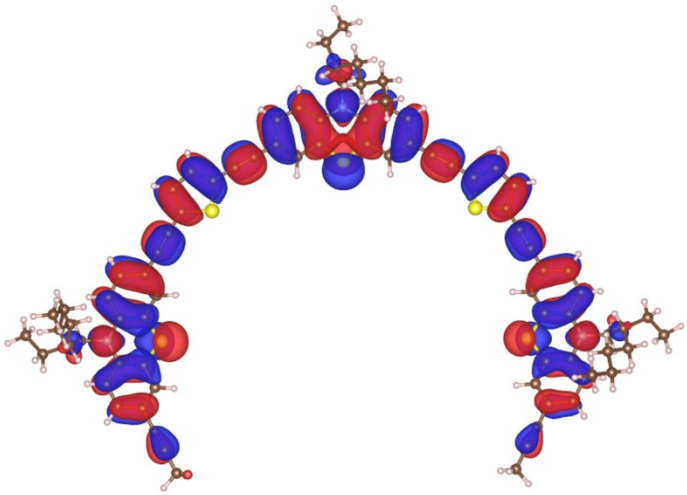


**Figure S15** Highest-occupied molecular orbital (HOMO; a) and lowest-unoccupied molecular orbital (LUMO; b) of the model compound **M6**. The isosurfaces are drawn to a contour value of $10^{-2}$ *e* $bohr^{-3}$.

(a) HOMO



(b) LUMO

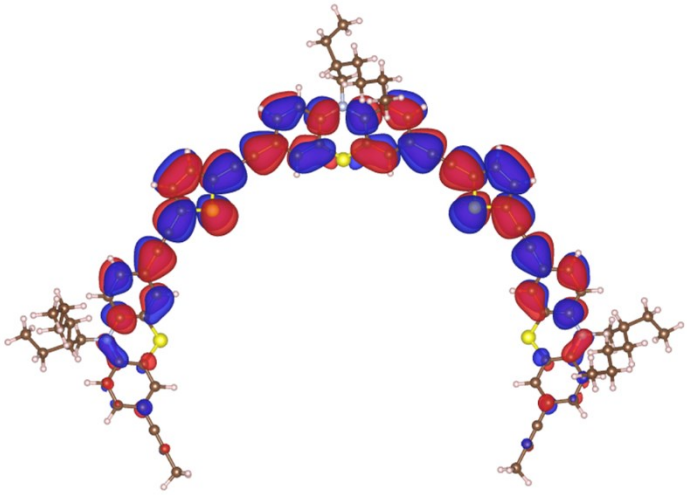


**Figure S16** Highest-occupied molecular orbital (HOMO; a) and lowest-unoccupied molecular orbital (LUMO; b) of the model compound **M7**. The isosurfaces are drawn to a contour value of $10^{-2}$ *e* $bohr^{-3}$.

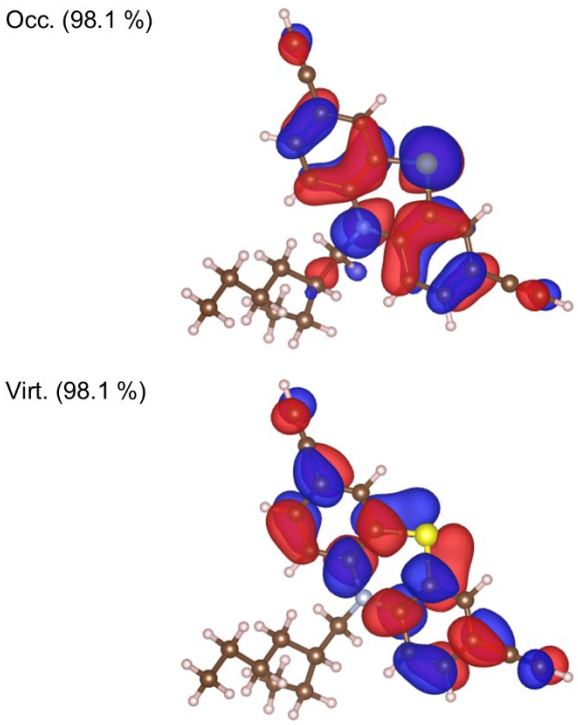



**Figure S17** Natural transition orbitals of the $S_1$ excited state in the precursor PTZ moiety **4** (*E* = 3.56 eV, *λ* = 348 nm, *f* = 0.135). Occupied particle and virtual hole states with % contributions to the transition > 10 % are shown. The isosurfaces are drawn to a contour value of 2.5 × $10^{-2}$ *e* $bohr^{-3}$.

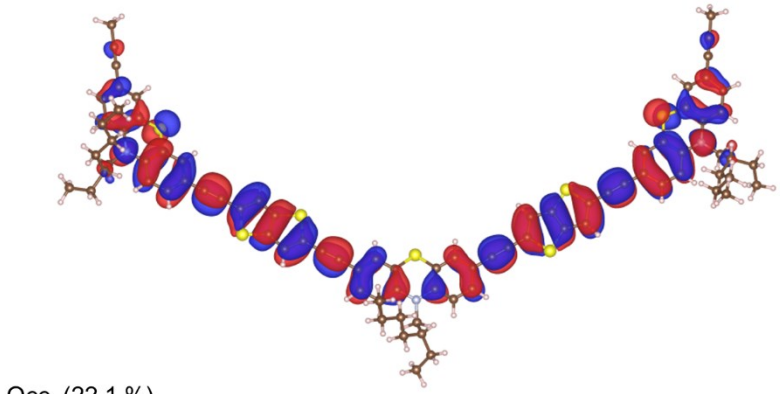
Occ. (28.5 %)

Occ. (64.3 %)

Virt. (64.3 %)

Virt. (28.5 %)

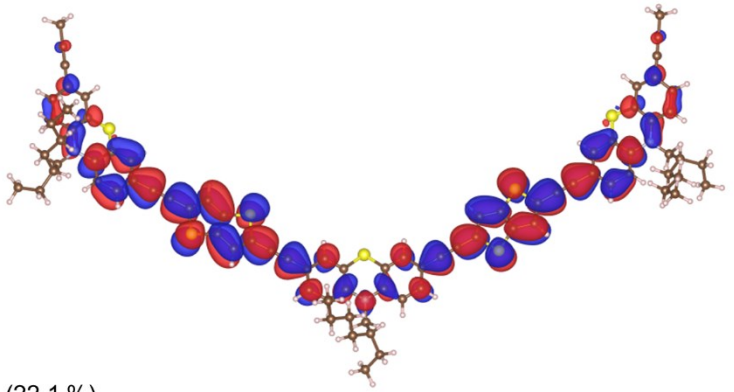
**Figure S18** Natural transition orbitals of the $S_1$ excited state in the model compound **M1** ($E$ = 2.68 eV, $\lambda$ = 462 nm, $f$ = 2.712). Occupied particle and virtual hole states with % contributions to the transition > 10 % are shown. The isosurfaces are drawn to a contour value of 2.5 $\times$ $10^{-2}$ $e$ bohr$^{-3}$.



Occ. (22.1 %)

Occ. (62.0 %)

Virt. (62.0 %)



Virt. (22.1 %)

**Figure S19** Natural transition orbitals of the $S_1$ excited state in the model compound **M2** ($E$ = 3.03 eV, $\lambda$ = 410 nm, $f$ = 3.681). Occupied particle and virtual hole states with % contributions to the transition > 10 % are shown. The isosurfaces are drawn to a contour value of 2.5 $\times$ $10^{-2}$ $e$ bohr$^{-3}$.

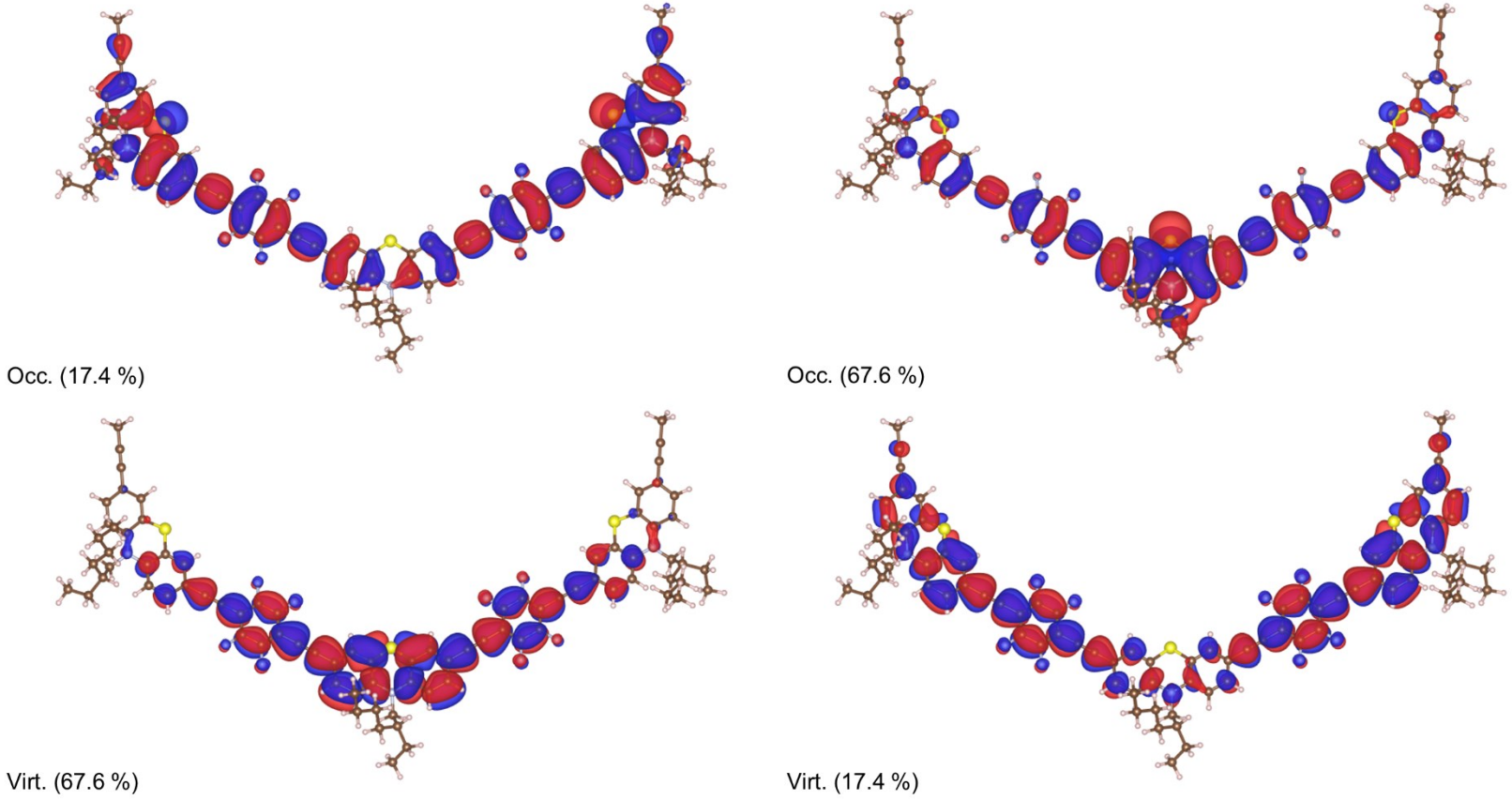
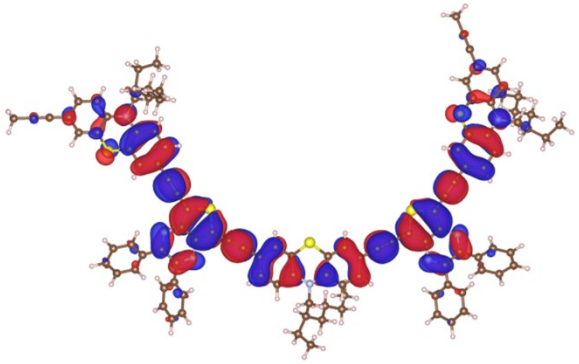
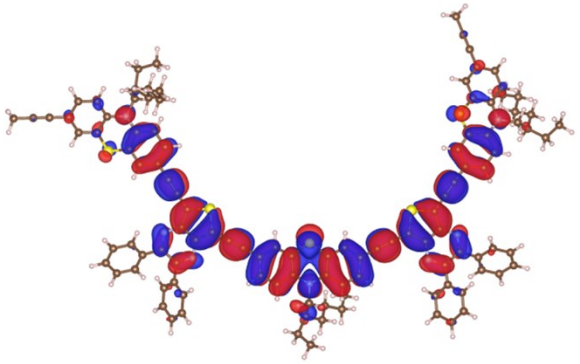


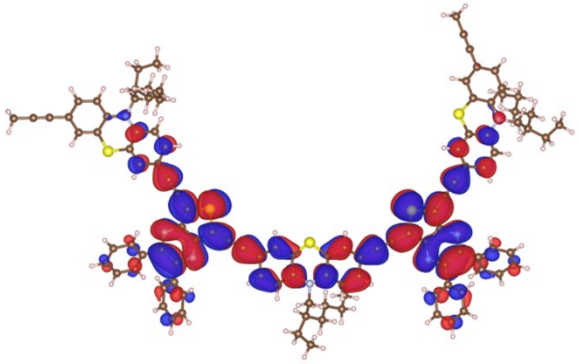

**Figure S20** Natural transition orbitals of the $S_1$ excited state in the model compound **M3** ($E$ = 3.10 eV, $\lambda$ = 400 nm, $f$ = 2.747). Occupied particle and virtual hole states with % contributions to the transition > 10 % are shown. The isosurfaces are drawn to a contour value of 2.5 $\times$ $10^{-2}$ $e$ bohr$^{-3}$.



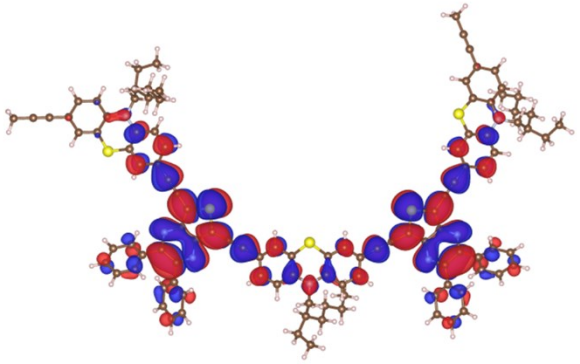
Occ. (33.0 %)



Occ. (61.7 %)

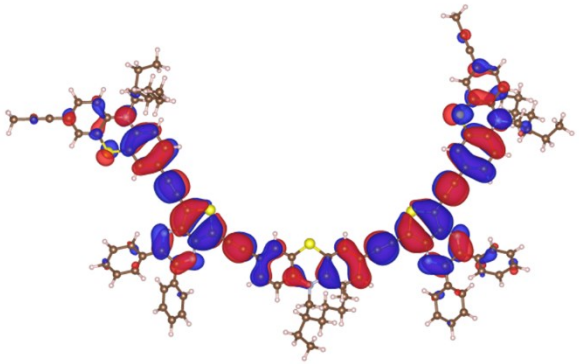


Virt. (61.7 %)

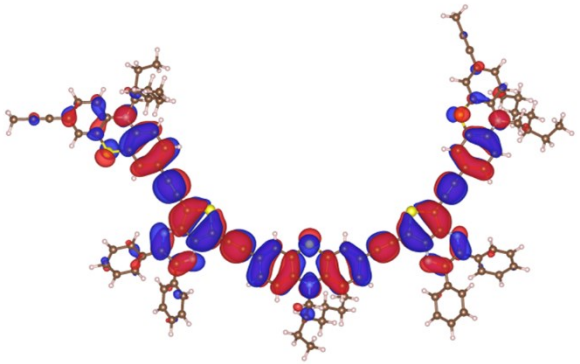


Virt. (33.0 %)

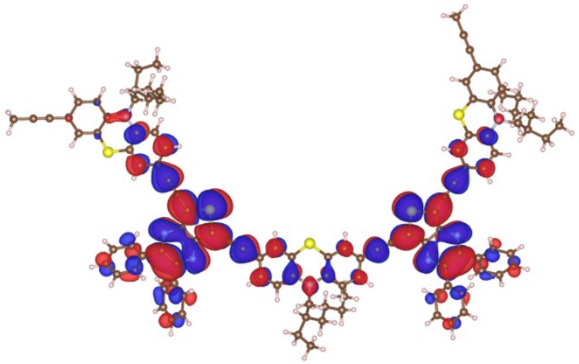
**Figure S21** Natural transition orbitals of the $S_1$ excited state in the model compound **M4** ($E$ = 2.42 eV, $\lambda$ = 513 nm, $f$ = 1.660). Occupied particle and virtual hole states with % contributions to the transition > 10 % are shown. The isosurfaces are drawn to a contour value of 2.5 $\times$ $10^{-2}$ $e$ bohr$^{-3}$.



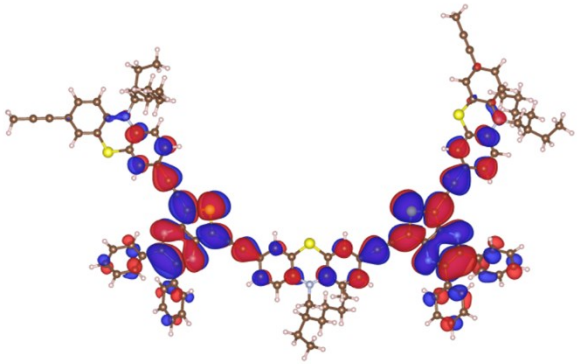
Occ. (42.6 %)



Occ. (53.8 %)



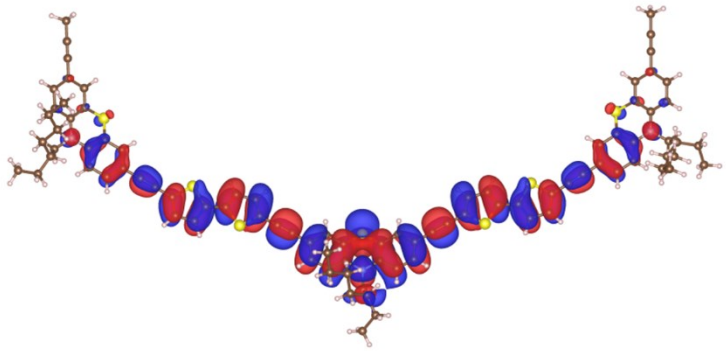
Virt. (53.8 %)



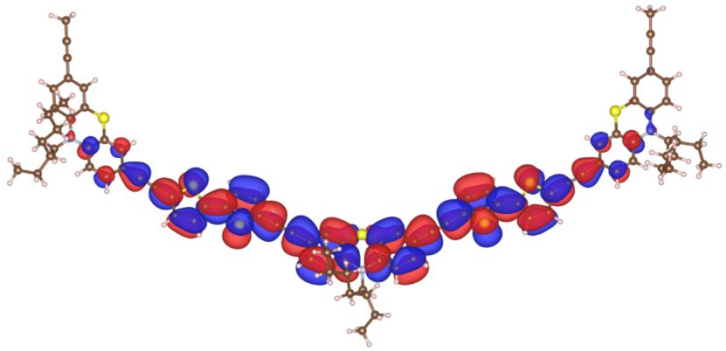
Virt. (42.6 %)

**Figure S22** Natural transition orbitals of the $S_2$ excited state in the model compound **M4** ($E$ = 2.56 eV, $\lambda$ = 484 nm, $f$ = 1.022). Occupied particle and virtual hole states with % contributions to the transition > 10 % are shown. The isosurfaces are drawn to a contour value of 2.5 $\times$ $10^{-2}$ $e$ bohr$^{-3}$.

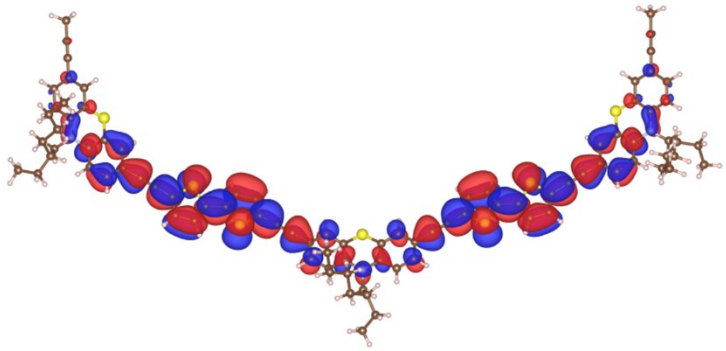
Occ. (25.9 %)



Occ. (56.9 %)



Virt. (56.9 %)



Virt. (25.9 %)

**Figure S23** Natural transition orbitals of the $S_1$ excited state in the model compound **M5** ($E$ = 2.98 eV, $\lambda$ = 416 nm, $f$ = 4.161). Occupied particle and virtual hole states with % contributions to the transition > 10 % are shown. The isosurfaces are drawn to a contour value of 2.5 $\times$ $10^{-2}$ $e$ bohr$^{-3}$.

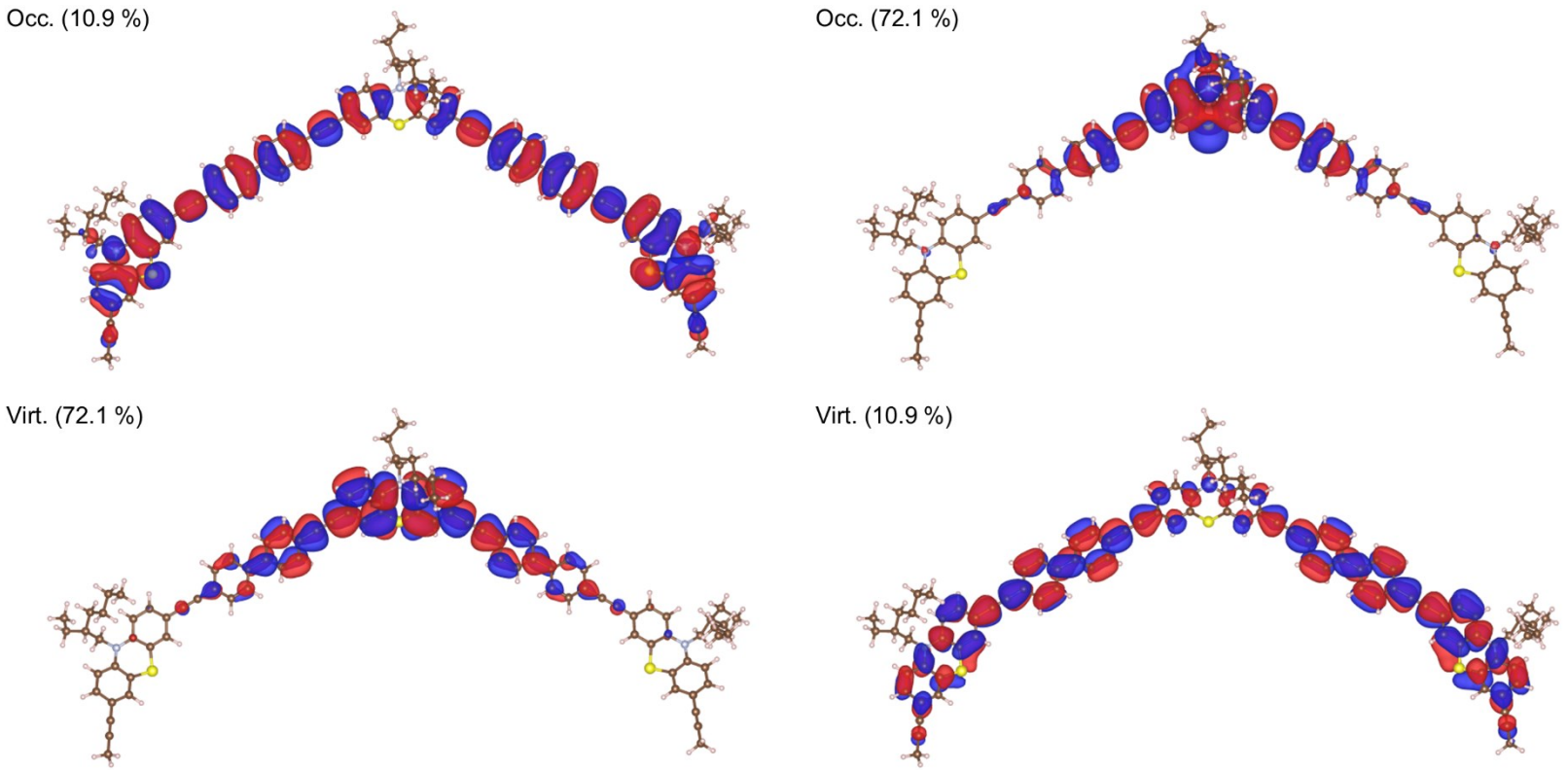



**Figure S24** Natural transition orbitals of the $S_1$ excited state in the model compound **M6** ($E$ = 3.29 eV, $\lambda$ = 377 nm, $f$ = 2.599). Occupied particle and virtual hole states with % contributions to the transition > 10 % are shown. The isosurfaces are drawn to a contour value of 2.5 $\times$ $10^{-2}$ $e$ bohr$^{-3}$.

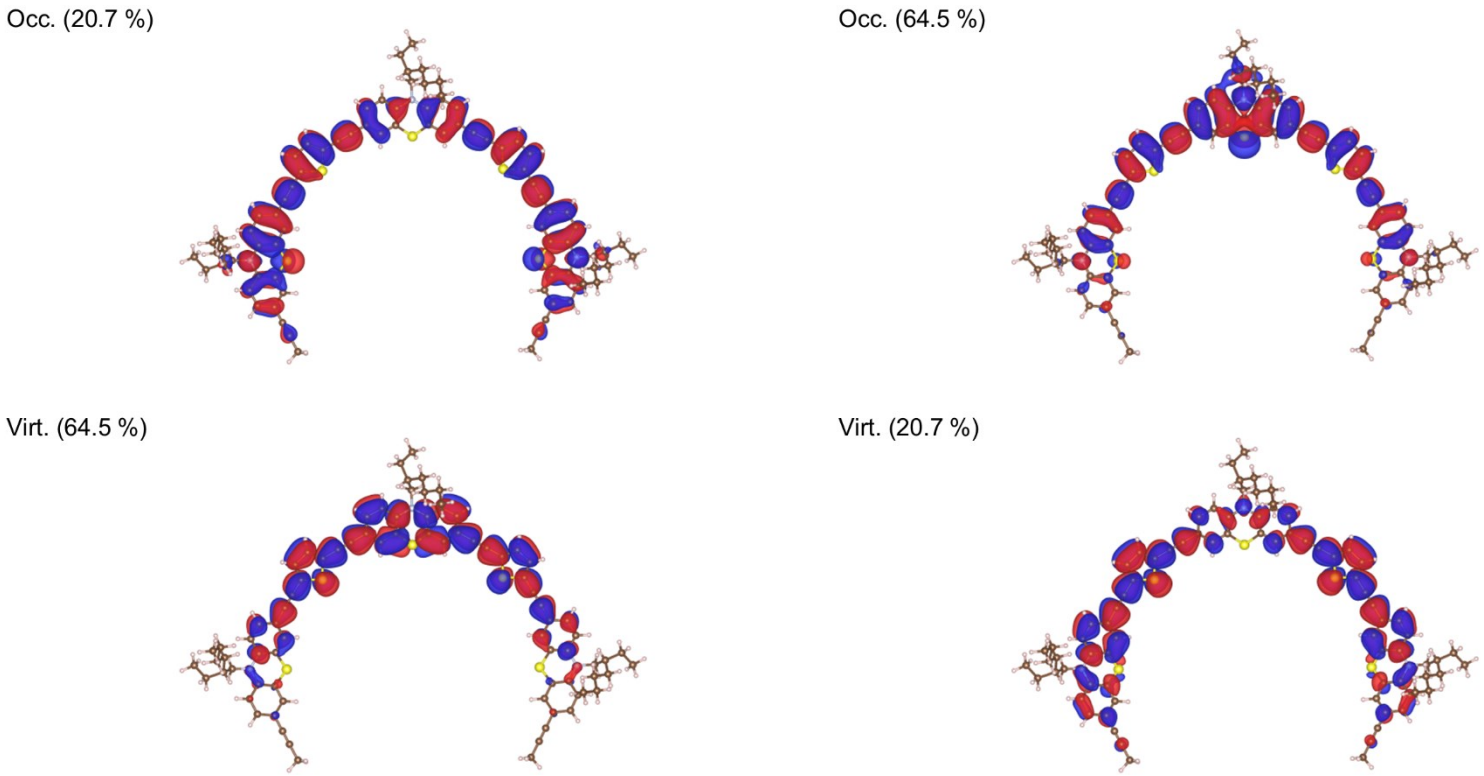



**Figure S25** Natural transition orbitals of the $S_1$ excited state in the model compound **M7** ($E$ = 3.06 eV, $\lambda$ = 405 nm, $f$ = 1.772). Occupied particle and virtual hole states with % contributions to the transition > 10 % are shown. The isosurfaces are drawn to a contour value of 2.5 $\times$ $10^{-2}$ $e$ bohr$^{-3}$.

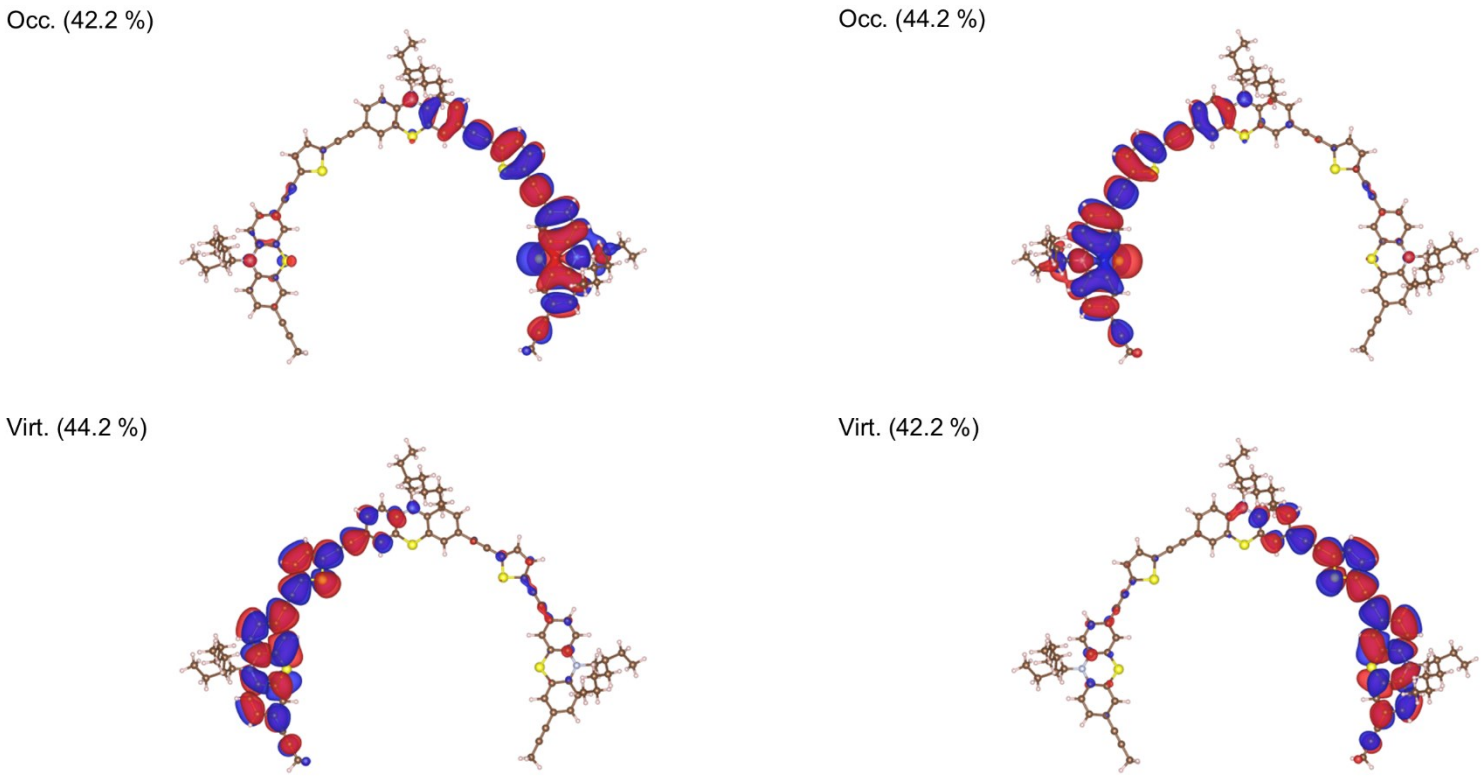



**Figure S26** Natural transition orbitals of the $S_2$ excited state in the model compound **M7** ($E$ = 3.29 eV, $\lambda$ = 376 nm, $f$ = 1.941). Occupied particle and virtual hole states with % contributions to the transition > 10 % are shown. The isosurfaces are drawn to a contour value of 2.5 $\times$ $10^{-2}$ $e$ bohr$^{-3}$.

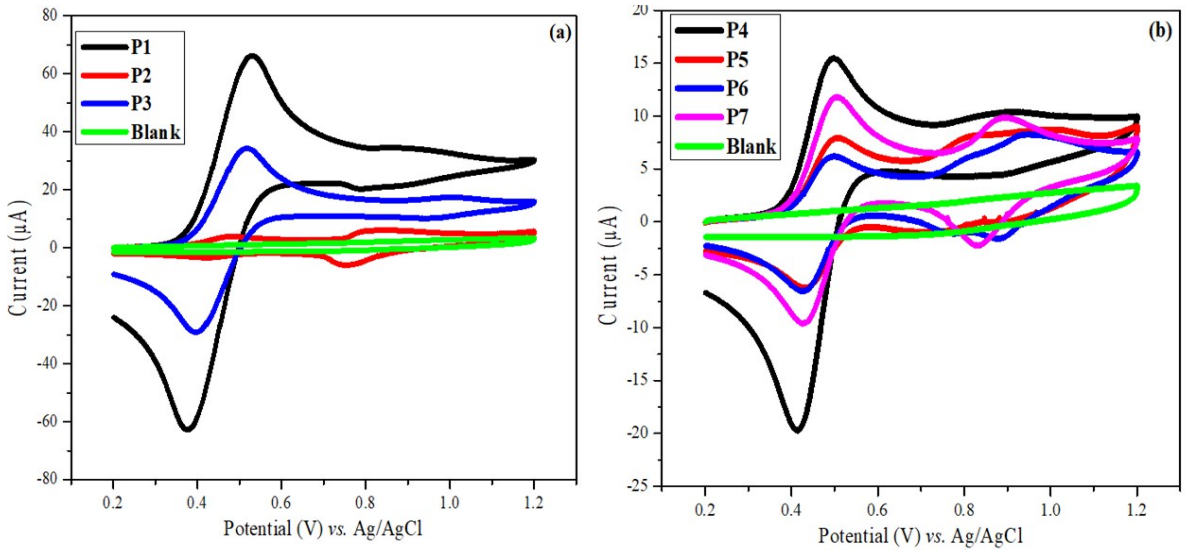



**Figure S27** Cyclic voltammograms of polymer-modified interfaces with **P1**-**P7** in 0.1M $Bu_4NPF_6/CH_3CN$ solution with 1.0 mM ferrocene as an internal reference, at a scan rate of 100 mV/s, at positive potentials.

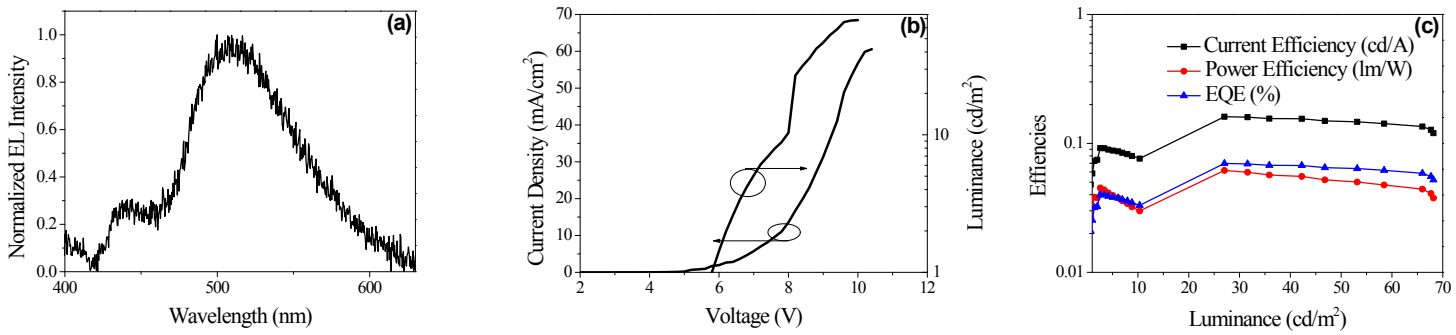



**Figure S28** Device performance of a polymer light-emitting dioide (PLED) based on an emitter layer of poly(9-vinylcarbazole) (PVK) doped with 5 wt. % **P7**: (a) electroluminescence spectra, (b) current density-voltage-luminance (*J*-*V*-*L*) curve, and (c) and current efficiency, power efficiency and external quantum efficiency (EQE) as a function of luminance.

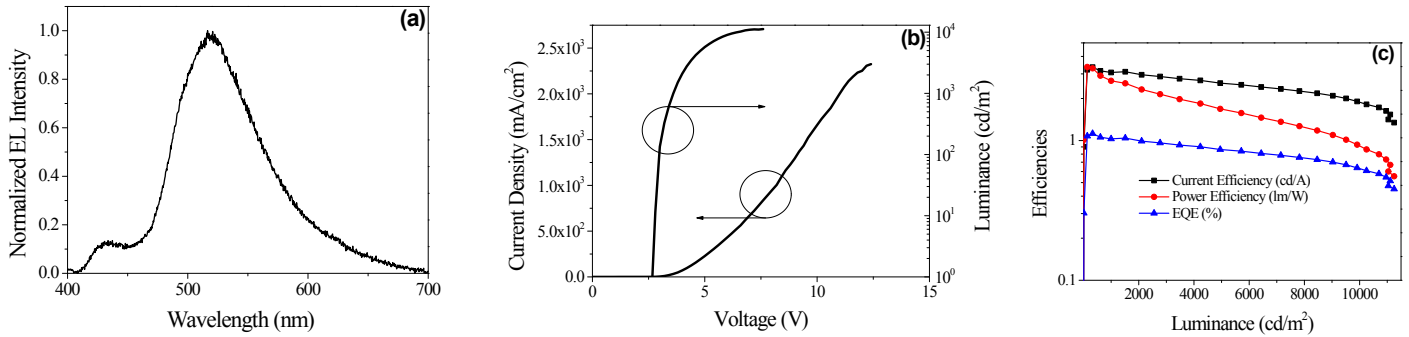



**Figure S29** Device performance of a polymer light-emitting dioide (PLED) based on an emitter layer of poly(9-vinylcarbazole) (PVK) doped with 10 wt. % **P7**: (a) electroluminescence spectra, (b) current density-voltage-luminance (*J*-*V*-*L*) curve, and (c) current efficiency-luminance (CE-*L*), power efficiency-luminance (PE-*L*) and external quantum efficiency-luminance (EQE-*L*) curves.

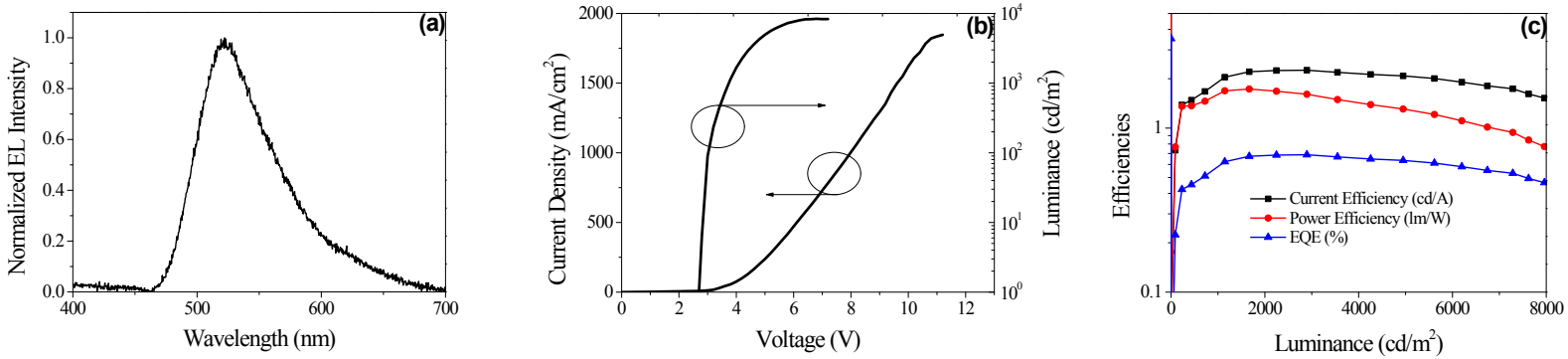



**Figure S30** Device performance of a polymer light-emitting dioide (PLED) based on an emitter layer of poly(9-vinylcarbazole) (PVK) doped with 20 wt. % **P7**: (a) electroluminescence spectra, (b) current density-voltage-luminance (*J*-*V*-*L*) curve, and (c) current efficiency-luminance (CE-*L*), power efficiency-luminance (PE-*L*) and external quantum efficiency-luminance (EQE-*L*) curves.

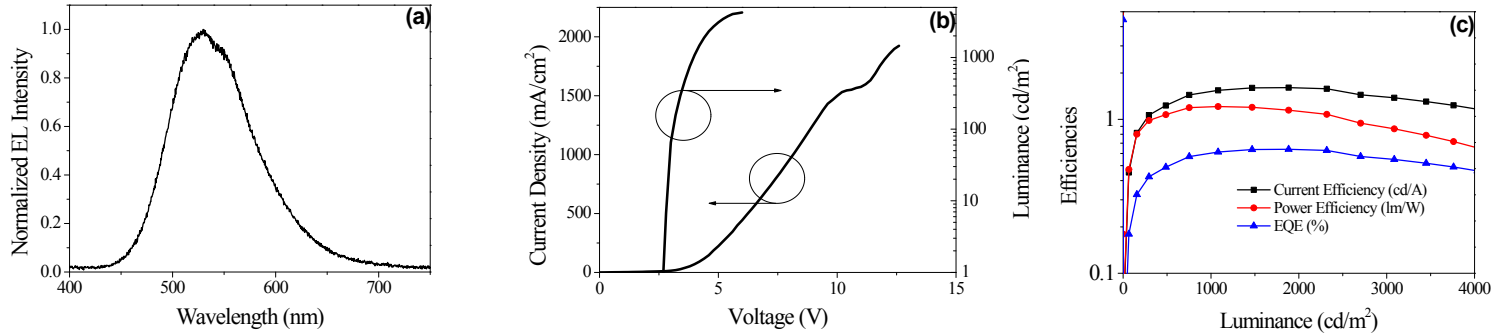



**Figure S31** Device performance of a polymer light-emitting dioide (PLED) based on an emitter layer of pure **P7**: (a) electroluminescence spectra, (b) current density-voltage-luminance (*J*-*V*-*L*) curve, and (c) current efficiency-luminance (CE-*L*), power efficiency-luminance (PE-*L*) and external quantum efficiency-luminance (EQE-*L*) curves.

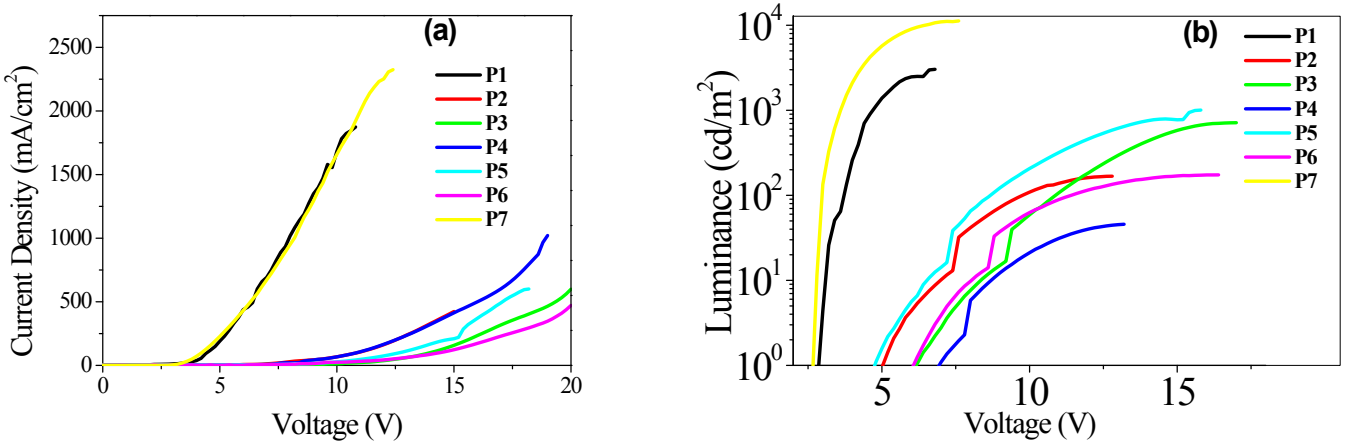



**Figure S32** (a) Current density-voltage-luminance (*J*-*V*-*L*) cirves of polymer light-emitting diode (PLED) devices based on emitter layers of poly(9-vinylcarbazole) (PVK) doped with 10 wt. % **P1**-**P7**. (b) Plot shows the luminance as a function of voltage for each of the materials.

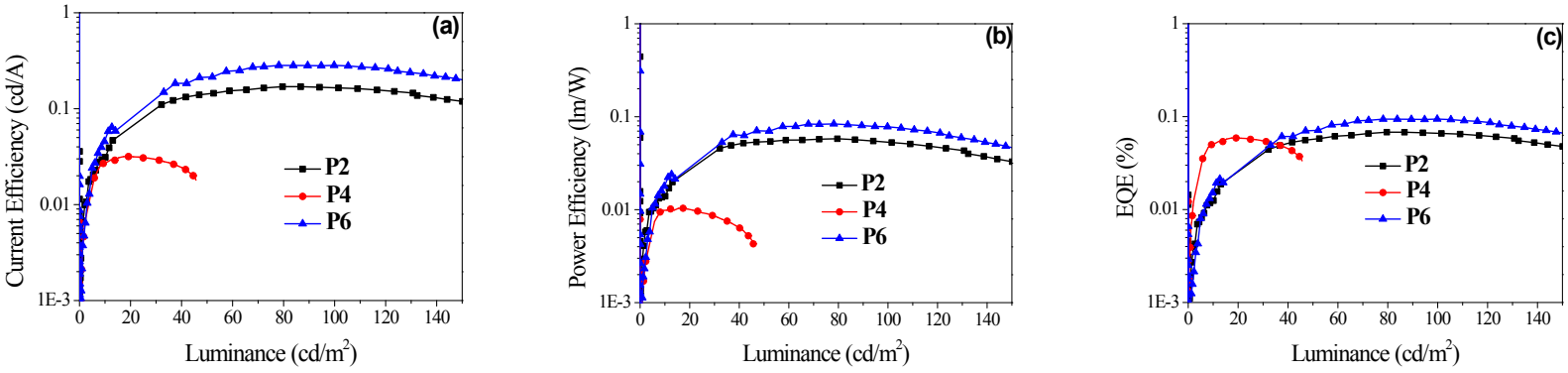



**Figure S33** Current efficiency-luminance (CE-*L*) (a), power efficiency-luminance (PE-*L*) (b), and external quantum efficiency-luminance (EQE-*L*) (c) curves for polymer light-emitting diode (PLED) devices based on the organic co-poly-ynes **P2**, **P4**, and **P6**.

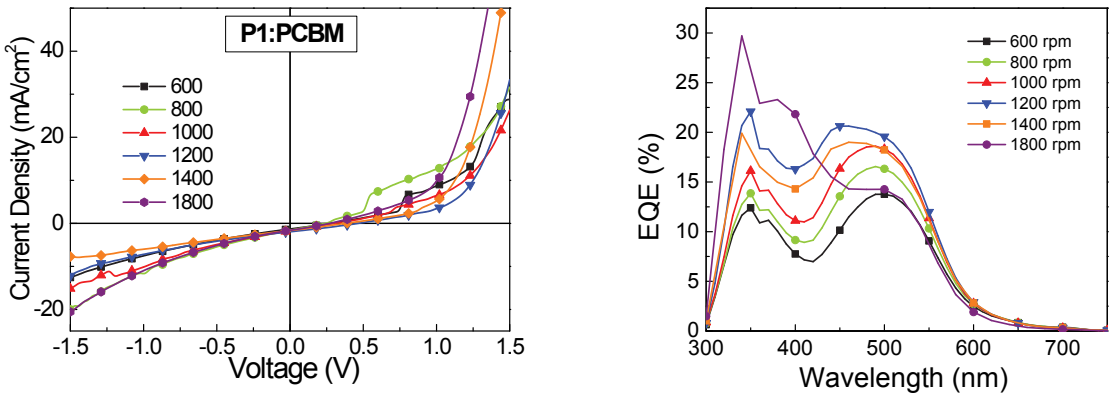



**Figure S34** Current density-voltage (*J-V*) and external quantum efficiency (EQE) curves for polymer solar cells made with a 1:1 blend of **P1** and phenyl-C61-butyric acid methyl ester (PCBM) spin coated at different speeds, resulting in the film thicknesses shown in **Table S11**

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**Table S1** Breakdown of the $S_1$ excited state in the precursor PTZ moiety **4** ($E$ = 3.56 eV, $\lambda$ = 348 nm, $f$ = 0.135) into individual transitions between occupied and virtual states. The % contributions are obtained from the sum of the squared coefficients.

| Occupied | Virtual | Coefficient *c* | % |
|---|---|---|---|
| HOMO | LUMO | 0.673 | 97.47 |
| HOMO | LUMO + 1 | -0.108 | 2.53 |

**Table S2** Breakdown of the $S_1$ excited state in the model compound **M1** ($E$ = 2.68 eV, $\lambda$ = 462 nm, $f$ = 2.712) into individual transitions between occupied and virtual states. The % contributions are obtained from the sum of the squared coefficients.

| Occupied | Virtual | Coefficient *c* | % |
|---|---|---|---|
| HOMO - 4 | LUMO | -0.143 | 4.48 |
| HOMO - 3 | LUMO + 1 | 0.241 | 12.64 |
| HOMO - 2 | LUMO | 0.120 | 3.15 |
| HOMO - 2 | LUMO + 4 | -0.120 | 3.15 |
| HOMO - 1 | LUMO + 1 | -0.283 | 17.51 |
| HOMO | LUMO | 0.521 | 59.07 |

**Table S3** Breakdown of the $S_1$ excited state in the model compound **M2** ($E$ = 3.03 eV, $\lambda$ = 410 nm, $f$ = 3.681) into individual transitions between occupied and virtual states. The % contributions are obtained from the sum of the squared coefficients.

| Occupied | Virtual | Coefficient *c* | % |
|---|---|---|---|
| HOMO - 3 | LUMO + 1 | 0.175 | 6.93 |
| HOMO - 2 | LUMO | 0.164 | 6.11 |
| HOMO - 2 | LUMO + 2 | -0.218 | 10.82 |
| HOMO - 1 | LUMO + 1 | -0.277 | 17.51 |
| HOMO | LUMO | 0.508 | 58.62 |

**Table S4** Breakdown of the $S_1$ excited state in the model compound **M3** ($E$ = 3.10 eV, $\lambda$ = 400 nm, $f$ = 2.747) into individual transitions between occupied and virtual states. The % contributions are obtained from the sum of the squared coefficients.

| Occupied | Virtual | Coefficient *c* | % |
|---|---|---|---|
| HOMO - 3 | LUMO + 1 | -0.150 | 5.02 |
| HOMO - 2 | LUMO | -0.286 | 18.19 |
| HOMO - 2 | LUMO + 2 | 0.250 | 13.85 |
| HOMO - 1 | LUMO | 0.117 | 3.07 |
| HOMO - 1 | LUMO + 1 | 0.231 | 11.87 |
| HOMO - 1 | LUMO + 3 | 0.107 | 2.54 |
| HOMO | LUMO | 0.452 | 45.46 |

**Table S5** Breakdown of the $S_1$ excited state in the model compound **M4** ($E$ = 2.42 eV, $\lambda$ = 513 nm, $f$ = 1.660) into individual transitions between occupied and virtual states. The % contributions are obtained from the sum of the squared coefficients.

| Occupied | Virtual | Coefficient *c* | % |
|---|---|---|---|
| HOMO - 4 | LUMO | -0.122 | 3.24 |
| HOMO - 3 | LUMO + 1 | 0.209 | 9.53 |
| HOMO - 1 | LUMO | -0.104 | 2.37 |
| HOMO - 1 | LUMO + 1 | -0.331 | 23.76 |
| HOMO | LUMO | 0.519 | 58.63 |
| HOMO | LUMO + 1 | -0.107 | 2.48 |
| HOMO - 4 | LUMO | -0.122 | 3.24 |

**Table S6** Breakdown of the $S_2$ excited state in the model compound **M4** ($E$ = 2.56 eV, $\lambda$ = 484 nm, $f$ = 1.022) into individual transitions between occupied and virtual states. The % contributions are obtained from the sum of the squared coefficients.

| Occupied | Virtual | Coefficient *c* | % |
|---|---|---|---|
| HOMO - 4 | LUMO + 1 | -0.153 | 5.02 |
| HOMO - 3 | LUMO | 0.219 | 10.28 |
| HOMO - 1 | LUMO | -0.396 | 33.61 |
| HOMO | LUMO + 1 | 0.488 | 51.09 |

**Table S7** Breakdown of the $S_1$ excited state in the model compound **M5** ($E$ = 2.98 eV, $\lambda$ = 416 nm, $f$ = 4.161) into individual transitions between occupied and virtual states. The % contributions are obtained from the sum of the squared coefficients.

| Occupied | Virtual | Coefficient *c* | % |
|---|---|---|---|
| HOMO - 3 | LUMO + 1 | 0.213 | 10.57 |
| HOMO - 2 | LUMO | 0.142 | 4.66 |
| HOMO - 2 | LUMO + 2 | 0.212 | 10.44 |
| HOMO - 1 | LUMO + 1 | 0.286 | 18.98 |
| HOMO | LUMO | 0.488 | 55.35 |

**Table S8** Breakdown of the $S_1$ excited state in the model compound **M6** ($E$ = 3.29 eV, $\lambda$ = 377 nm, $f$ = 2.599) into individual transitions between occupied and virtual states. The % contributions are obtained from the sum of the squared coefficients.

| Occupied | Virtual | Coefficient *c* | % |
|---|---|---|---|
| HOMO - 3 | LUMO + 1 | 0.132 | 4.03 |
| HOMO - 2 | LUMO | 0.249 | 14.41 |
| HOMO - 2 | LUMO + 2 | 0.308 | 22.02 |
| HOMO - 1 | LUMO + 1 | -0.185 | 7.98 |
| HOMO | LUMO | 0.444 | 45.72 |
| HOMO | LUMO + 2 | 0.102 | 2.43 |
| HOMO | LUMO + 4 | 0.121 | 3.42 |

**Table S9** Breakdown of the $S_1$ excited state in the model compound **M7** ($E$ = 3.06 eV, $\lambda$ = 405 nm, $f$ = 1.772) into individual transitions between occupied and virtual states. The % contributions are obtained from the sum of the squared coefficients.

| Occupied | Virtual | Coefficient *c* | % |
|---|---|---|---|
| HOMO - 3 | LUMO + 1 | -0.158 | 5.63 |
| HOMO - 2 | LUMO | 0.161 | 5.80 |
| HOMO - 2 | LUMO + 2 | -0.214 | 10.32 |
| HOMO - 1 | LUMO + 1 | 0.275 | 16.94 |
| HOMO | LUMO | 0.523 | 61.32 |

**Table S10** Breakdown of the $S_2$ excited state in the model compound **M7** ($E$ = 3.29 eV, $\lambda$ = 376 nm, $f$ = 1.941) into individual transitions between occupied and virtual states. The % contributions are obtained from the sum of the squared coefficients.

| Occupied | Virtual | Coefficient *c* | % |
|---|---|---|---|
| HOMO - 3 | LUMO | -0.126 | 3.52 |
| HOMO - 2 | LUMO + 1 | -0.120 | 3.23 |
| HOMO - 2 | LUMO + 3 | -0.187 | 7.80 |
| HOMO - 1 | LUMO | 0.381 | 32.28 |
| HOMO - 1 | LUMO + 2 | 0.241 | 12.94 |
| HOMO | LUMO + 1 | 0.412 | 37.81 |
| HOMO | LUMO + 3 | 0.104 | 2.42 |

**Table S11** Device characteristics of polymer solar cells made with 1:1 blends of **P1** and phenyl-C61-butyric acid methyl ester (PCBM) as the donor material prepared with the different spin-coating speeds and film thicknesses shown: short-circuit current density ($J_{sc}$), open-circuit voltage ($V_{oc}$), fill factor (FF), power-conversion efficiency (PCE), and integrated current from external quantum efficiency (EQE).

| Spin speed/rpm | Film thickness (nm) | $J_{sc}$ (mA/cm$^2$) | $V_{oc}$ (mV) | FF (%) | PCE (%) | Integrated current (EQE) (mA/cm$^2$) |
|---|---|---|---|---|---|---|
| 600 | 115 | 1.30 | 0.28 | 25.65 | 0.09 | 1.34 |
| 800 | 108 | 1.60 | 0.24 | 25.95 | 0.10 | 1.58 |
| 1000 | 92 | 1.72 | 0.30 | 26.33 | 0.13 | 1.80 |
| 1200 | 84 | 1.94 | 0.46 | 27.18 | 0.24 | 2.09 |
| 1400 | 60 | 1.65 | 0.37 | 26.49 | 0.16 | 1.92 |
| 1800 | 54 | 1.61 | 0.27 | 27.22 | 0.12 | 1.73 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | -0.15676 | 1.29236 | -0.57420 | H | -2.22768 | 0.87438 | -1.00925 |
| C | 0.70300 | 2.32930 | -0.16640 | H | -3.05670 | 3.09041 | -0.51752 |
| S | 2.45894 | 2.14386 | -0.19612 | H | 0.90668 | 4.34913 | 0.49532 |
| C | 2.58225 | 0.39635 | 0.02753 | H | 4.52566 | 0.61498 | 0.88394 |
| C | 1.56881 | -0.47412 | -0.41613 | H | 3.28635 | -3.39049 | 0.02517 |
| N | 0.31657 | -0.00474 | -0.86036 | H | 1.16566 | -2.56686 | -0.78299 |
| C | -1.51465 | 1.61861 | -0.69309 | H | -1.23799 | -0.38833 | -2.18439 |
| C | -1.99778 | 2.88581 | -0.40572 | H | 0.09056 | -1.50508 | -2.25746 |
| C | -1.14424 | 3.89182 | 0.04294 | H | -0.63066 | -2.36952 | 0.06078 |
| C | 0.21369 | 3.58369 | 0.16245 | H | -2.15337 | -0.58119 | 0.70093 |
| C | 3.77986 | -0.08791 | 0.52807 | H | -3.25026 | -0.97982 | -0.61022 |
| C | 4.06153 | -1.45739 | 0.54783 | H | -3.70141 | -3.19835 | 0.39124 |
| C | 3.09309 | -2.32376 | 0.04573 | H | -2.47363 | -2.92747 | 1.61682 |
| C | 1.87642 | -1.84303 | -0.41500 | H | -3.78929 | -0.99579 | 2.50764 |
| C | -0.55091 | -0.95879 | -1.55842 | H | -5.00386 | -1.24008 | 1.26597 |
| C | -1.32412 | -1.99161 | -0.69806 | H | -5.73316 | -2.27707 | 3.42124 |
| C | -2.51269 | -1.40981 | 0.08108 | H | -5.50500 | -3.53082 | 2.19511 |
| C | -3.21871 | -2.41662 | 0.99092 | H | -4.28119 | -3.28594 | 3.44649 |
| C | -4.26938 | -1.76554 | 1.89027 | H | -0.79507 | -3.59473 | -2.04137 |
| C | -4.98796 | -2.76867 | 2.78846 | H | -2.09126 | -3.99687 | -0.94203 |
| C | -1.70857 | -3.19493 | -1.58132 | H | -2.93159 | -3.80514 | -3.26662 |
| C | -2.72985 | -2.90298 | -2.68160 | H | -3.68411 | -2.56148 | -2.26839 |
| C | 5.30809 | -1.94381 | 1.05217 | H | -2.37629 | -2.13632 | -3.37872 |
| C | 6.35715 | -2.35394 | 1.47762 | H | -2.40722 | 7.26836 | 0.87636 |
| C | -2.04400 | 6.29530 | 0.63611 | H | 7.28617 | -2.71623 | 1.85467 |
| C | -1.63268 | 5.19663 | 0.36505 | | | | |

**Listing 1** Cartesian coordinates of the optimized model of the precursor PTZ moiety **4**.

| | | | |
|---|---|---|---|
| C | -1.24367 | -3.86106 | -1.38047 |
| S | 0.09578 | -2.92891 | -2.05512 |
| C | -1.10981 | -5.22552 | -1.05994 |
| C | 1.46116 | -3.82462 | -1.38295 |
| C | 1.36502 | -5.19650 | -1.08012 |
| N | 0.13594 | -5.88444 | -1.08753 |
| C | -2.28846 | -5.90488 | -0.71886 |
| C | -3.52038 | -5.27298 | -0.67774 |
| C | -3.63464 | -3.90979 | -0.95303 |
| C | -2.46812 | -3.21844 | -1.29697 |
| C | 2.66945 | -3.15288 | -1.30423 |
| C | 3.85803 | -3.82180 | -0.98998 |
| C | 3.78429 | -5.19447 | -0.75281 |
| C | 2.56831 | -5.85827 | -0.78854 |
| C | 0.18375 | -7.34980 | -1.03862 |
| C | 0.45066 | -8.01572 | 0.33544 |
| C | -0.72333 | -7.93422 | 1.32131 |
| C | -0.41726 | -8.50145 | 2.70869 |
| C | -1.53378 | -8.23107 | 3.71682 |
| C | -1.24346 | -8.81397 | 5.09717 |
| C | 0.95468 | -9.45414 | 0.10532 |
| C | -0.06633 | -10.42064 | -0.49678 |
| C | 5.10147 | -3.13049 | -0.93590 |
| C | 6.16786 | -2.56233 | -0.89090 |
| C | 7.42050 | -1.89822 | -0.84530 |
| C | 7.55186 | -0.54525 | -1.05831 |
| C | 8.80494 | 0.11942 | -1.02103 |
| C | 9.98799 | -0.53666 | -0.76937 |
| C | 9.90169 | -1.95297 | -0.53755 |
| C | 8.62944 | -2.62764 | -0.57476 |
| N | 10.92069 | -2.76438 | -0.27753 |
| S | 10.29416 | -4.25510 | -0.09829 |
| N | 8.71807 | -3.93241 | -0.34190 |
| C | 11.24058 | 0.12794 | -0.73894 |
| C | 12.30940 | 0.69310 | -0.71727 |
| C | 16.11877 | 2.62643 | -0.62205 |
| C | 14.93468 | 3.34251 | -0.88477 |
| S | 14.96594 | 5.03752 | -1.37947 |
| C | 16.47198 | 5.55103 | -0.61263 |
| C | 17.52707 | 4.64821 | -0.38778 |
| N | 17.37672 | 3.25538 | -0.56088 |
| C | 15.98228 | 1.24298 | -0.43380 |
| C | 14.75174 | 0.60881 | -0.47781 |
| C | 13.57956 | 1.33545 | -0.69079 |
| C | 13.69942 | 2.71562 | -0.88643 |
| C | 16.62017 | 6.90776 | -0.37230 |
| C | 17.84274 | 7.44940 | 0.03768 |
| C | 18.91205 | 6.57034 | 0.19909 |
| C | 18.75355 | 5.20658 | 0.00030 |
| C | 18.59719 | 2.44340 | -0.58767 |
| C | 19.27505 | 2.11231 | 0.76661 |
| C | 18.50898 | 1.10611 | 1.63733 |
| C | 19.12849 | 0.87608 | 3.01713 |
| C | 18.24595 | 0.02185 | 3.92681 |
| C | 18.86659 | -0.22174 | 5.29973 |
| C | 20.73813 | 1.70185 | 0.50724 |
| C | 20.92907 | 0.38705 | -0.25059 |
| C | -7.24675 | -2.08168 | -0.80320 |
| C | -8.43187 | -2.84102 | -0.51058 |
| C | -9.72273 | -2.20279 | -0.47279 |
| C | -9.85168 | -0.79341 | -0.72591 |
| C | -8.69011 | -0.10761 | -0.99758 |
| C | -7.41868 | -0.73648 | -1.03558 |
| N | -8.48078 | -4.14393 | -0.25661 |
| S | -10.04474 | -4.50803 | 0.00580 |
| N | -10.71565 | -3.03902 | -0.19128 |
| C | -11.12271 | -0.16468 | -0.69639 |
| C | -12.20715 | 0.36995 | -0.67707 |
| C | -17.52037 | 4.18306 | -0.35885 |
| C | -16.50319 | 5.11085 | -0.64401 |
| S | -14.99636 | 4.61888 | -1.42332 |
| C | -14.90367 | 2.94327 | -0.87084 |
| C | -16.06529 | 2.19834 | -0.58854 |
| N | -17.33798 | 2.79287 | -0.51913 |
| C | -18.73639 | 4.70922 | 0.09507 |
| C | -18.93373 | 6.07082 | 0.26769 |
| C | -17.90665 | 6.98090 | 0.02022 |
| C | -16.68642 | 6.46862 | -0.43089 |
| C | -13.65187 | 2.35164 | -0.86821 |
| C | -13.49473 | 0.97702 | -0.65503 |
| C | -14.64610 | 0.21874 | -0.44059 |
| C | -15.89502 | 0.81790 | -0.40041 |
| C | -18.50607 | 1.90740 | -0.57994 |
| C | -18.92897 | 1.11787 | 0.69022 |
| C | -19.69683 | 1.90266 | 1.76947 |
| C | -18.80992 | 2.67291 | 2.75005 |
| C | -19.60935 | 3.51227 | 3.74450 |
| C | -18.72456 | 4.24372 | 4.75017 |
| C | -19.72319 | -0.12716 | 0.24524 |
| C | -21.05517 | 0.16617 | -0.44705 |
| C | 17.98693 | 8.85395 | 0.26532 |
| C | -5.97625 | -2.71080 | -0.85056 |
| C | -4.89511 | -3.25021 | -0.89737 |
| C | -18.08881 | 8.38599 | 0.21496 |
| C | -18.24240 | 9.57062 | 0.37920 |
| C | -18.42769 | 11.00409 | 0.57814 |
| C | 18.10817 | 10.03815 | 0.45748 |
| C | 18.25441 | 11.47110 | 0.68998 |
| H | -2.25997 | -6.95329 | -0.46955 |
| H | -4.40550 | -5.84110 | -0.41444 |
| H | -2.52476 | -2.16065 | -1.53133 |
| H | 2.69725 | -2.09066 | -1.52322 |
| H | 4.68952 | -5.74691 | -0.52725 |
| H | 2.57785 | -6.91847 | -0.58775 |
| H | -0.74106 | -7.72696 | -1.47584 |
| H | 0.97539 | -7.65698 | -1.72946 |
| H | 1.27239 | -7.46868 | 0.80986 |
| H | -1.01156 | -6.88356 | 1.43628 |
| H | -1.60289 | -8.45152 | 0.91507 |
| H | -0.24946 | -9.58403 | 2.64806 |
| H | 0.52051 | -8.06691 | 3.08235 |
| H | -1.69098 | -7.14826 | 3.79996 |
| H | -2.47511 | -8.64620 | 3.33369 |
| H | -2.05603 | -8.60365 | 5.79921 |
| H | -1.11778 | -9.90127 | 5.04872 |
| H | -0.32307 | -8.39378 | 5.51731 |
| H | 1.83506 | -9.41313 | -0.54978 |
| H | 1.31416 | -9.86082 | 1.05598 |
| H | 0.37874 | -11.41027 | -0.63600 |
| H | -0.93929 | -10.54350 | 0.15180 |
| H | -0.42428 | -10.08534 | -1.47567 |
| H | 6.66160 | 0.03820 | -1.26535 |
| H | 8.83033 | 1.18847 | -1.20063 |
| H | 16.84929 | 0.63270 | -0.23890 |
| H | 14.69612 | -0.46390 | -0.33019 |
| H | 12.80891 | 3.30746 | -1.07025 |
| H | 15.77416 | 7.56709 | -0.53531 |
| H | 19.88134 | 6.95520 | 0.49604 |
| H | 19.61966 | 4.58051 | 0.15071 |
| H | 18.37564 | 1.52928 | -1.13944 |
| H | 19.31775 | 2.98773 | -1.20666 |
| H | 19.30944 | 3.03843 | 1.35018 |
| H | 17.48581 | 1.47151 | 1.77754 |
| H | 18.42238 | 0.13954 | 1.12306 |
| H | 20.10849 | 0.39245 | 2.91877 |
| H | 19.31331 | 1.84607 | 3.49968 |
| H | 17.27017 | 0.50967 | 4.04501 |
| H | 18.04718 | -0.94066 | 3.43768 |
| H | 18.21424 | -0.83249 | 5.93126 |
| H | 19.82755 | -0.74075 | 5.21286 |
| H | 19.04804 | 0.72316 | 5.82360 |
| H | 21.23109 | 2.50865 | -0.05134 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| H | 21.26503 | 1.64194 | 1.46492 | H | -18.11405 | 3.32418 | 2.21138 |
| H | 21.99321 | 0.18482 | -0.40435 | H | -20.21438 | 4.24318 | 3.19167 |
| H | 20.51169 | -0.46259 | 0.29875 | H | -20.32115 | 2.86773 | 4.27703 |
| H | 20.45693 | 0.40853 | -1.23810 | H | -19.31960 | 4.84207 | 5.44703 |
| H | -8.74783 | 0.95732 | -1.19348 | H | -18.13021 | 3.53743 | 5.34010 |
| H | -6.54740 | -0.13104 | -1.25950 | H | -18.02795 | 4.91810 | 4.24081 |
| H | -19.55663 | 4.04982 | 0.33141 | H | -19.09839 | -0.73275 | -0.42484 |
| H | -19.89593 | 6.43005 | 0.61563 | H | -19.90912 | -0.74813 | 1.12925 |
| H | -15.86946 | 7.15008 | -0.64347 | H | -21.56867 | -0.76488 | -0.70452 |
| H | -12.77869 | 2.96378 | -1.06790 | H | -21.72502 | 0.74335 | 0.19800 |
| H | -14.56026 | -0.85190 | -0.29246 | H | -20.91875 | 0.72937 | -1.37573 |
| H | -16.74673 | 0.17991 | -0.22130 | H | -17.57426 | 11.56813 | 0.18886 |
| H | -19.34462 | 2.49577 | -0.95491 | H | -19.32648 | 11.36149 | 0.06511 |
| H | -18.28804 | 1.17696 | -1.36627 | H | -18.53141 | 11.24643 | 1.64094 |
| H | -18.01818 | 0.75190 | 1.17520 | H | 17.37745 | 12.01879 | 0.33078 |
| H | -20.43438 | 2.57459 | 1.31240 | H | 18.37084 | 11.68976 | 1.75661 |
| H | -20.29157 | 1.18518 | 2.35028 | H | 19.13235 | 11.86829 | 0.17017 |
| H | -18.18784 | 1.95277 | 3.29883 | | | | |

**Listing 2** Cartesian coordinates of the optimized model compound **M1**.

| | | | |
|---|---|---|---|
| C | -1.09054 | -6.18922 | -0.84817 |
| C | -1.23702 | -4.83778 | -1.21215 |
| S | 0.09193 | -3.92436 | -1.93202 |
| C | 1.46599 | -4.78759 | -1.23363 |
| C | 1.37982 | -6.15085 | -0.89303 |
| N | 0.15507 | -6.84575 | -0.88126 |
| C | -2.25496 | -6.86000 | -0.45005 |
| C | -3.49054 | -6.23467 | -0.40844 |
| C | -3.61947 | -4.88475 | -0.73827 |
| C | -2.46403 | -4.19939 | -1.13005 |
| C | 2.66948 | -4.10523 | -1.17320 |
| C | 3.86234 | -4.75824 | -0.84036 |
| C | 3.79750 | -6.12458 | -0.56686 |
| C | 2.58576 | -6.79735 | -0.58445 |
| C | 0.20719 | -8.31236 | -0.87169 |
| C | 0.51199 | -9.05170 | 0.46053 |
| C | -0.65333 | -9.18706 | 1.45779 |
| C | -0.84944 | -7.97915 | 2.37657 |
| C | -2.07141 | -8.11076 | 3.28307 |
| C | -2.22985 | -6.93319 | 4.24098 |
| C | 1.11232 | -10.43220 | 0.12545 |
| C | 0.16686 | -11.39457 | -0.59527 |
| C | 5.09918 | -4.05335 | -0.80353 |
| C | 6.14909 | -3.45238 | -0.77681 |
| C | 12.65040 | 0.10645 | -0.64472 |
| C | 13.70835 | 0.69378 | -0.63353 |
| C | 17.46261 | 2.73621 | -0.57861 |
| C | 16.25533 | 3.41511 | -0.83361 |
| S | 16.23122 | 5.10827 | -1.33432 |
| C | 17.72889 | 5.66944 | -0.58447 |
| C | 18.81274 | 4.79971 | -0.36624 |
| N | 18.70232 | 3.40234 | -0.53182 |
| C | 17.36864 | 1.35061 | -0.38357 |
| C | 16.15708 | 0.67970 | -0.41494 |
| C | 14.96176 | 1.36944 | -0.62025 |
| C | 15.03900 | 2.75199 | -0.82188 |
| C | 17.83872 | 7.03107 | -0.35137 |
| C | 19.04851 | 7.61094 | 0.04402 |
| C | 20.14532 | 6.76509 | 0.19817 |
| C | 20.02574 | 5.39630 | 0.00687 |
| C | 19.94532 | 2.62602 | -0.56912 |
| C | 20.64712 | 2.31800 | 0.77819 |
| C | 19.90980 | 1.30913 | 1.67034 |
| C | 20.54850 | 1.11091 | 3.04632 |
| C | 19.69312 | 0.25274 | 3.97798 |
| C | 20.33280 | 0.04249 | 5.34767 |
| C | 22.11286 | 1.92839 | 0.50199 |
| C | 22.31501 | 0.60918 | -0.24528 |
| C | -12.54320 | -0.27620 | -0.48824 |
| C | -13.62956 | 0.25623 | -0.46316 |
| C | -18.86929 | 4.18427 | -0.44507 |
| C | -17.89890 | 4.98272 | -1.07550 |
| S | -16.49716 | 4.27214 | -1.88203 |
| C | -16.33535 | 2.78015 | -0.95013 |
| C | -17.45218 | 2.16038 | -0.35634 |
| N | -18.70598 | 2.79276 | -0.27514 |
| C | -20.01849 | 4.84215 | 0.01166 |
| C | -20.19718 | 6.20876 | -0.13965 |
| C | -19.21373 | 6.99855 | -0.73421 |
| C | -18.05868 | 6.35539 | -1.18909 |
| C | -15.09190 | 2.17089 | -0.95490 |
| C | -14.90769 | 0.88355 | -0.43611 |
| C | -16.02378 | 0.23240 | 0.08933 |
| C | -17.25859 | 0.86019 | 0.13460 |
| C | -19.87023 | 1.95675 | 0.03782 |
| C | -20.11763 | 1.51434 | 1.50646 |
| C | -20.69381 | 2.57409 | 2.46243 |
| C | -19.65302 | 3.51623 | 3.07119 |
| C | -20.27147 | 4.60110 | 3.95033 |
| C | -19.22816 | 5.51106 | 4.59268 |
| C | -20.99738 | 0.24776 | 1.48938 |
| C | -22.41295 | 0.44427 | 0.94405 |
| C | 19.15219 | 9.02022 | 0.26436 |
| C | -5.95859 | -3.67710 | -0.64652 |
| C | -4.88076 | -4.22553 | -0.68756 |
| C | -19.37453 | 8.41227 | -0.87868 |
| C | -19.50891 | 9.60426 | -1.00112 |
| C | -19.67009 | 11.04671 | -1.14977 |
| C | 19.23787 | 10.20853 | 0.45011 |
| C | 19.34005 | 11.64656 | 0.67459 |
| C | -11.28950 | -0.92073 | -0.51133 |
| S | -11.15123 | -2.59217 | 0.02026 |
| C | -9.45216 | -2.58701 | -0.31305 |
| C | -9.04363 | -1.35621 | -0.80322 |
| C | -10.08581 | -0.40304 | -0.91819 |
| C | -8.41073 | -3.54063 | -0.20094 |
| C | -7.20746 | -3.02372 | -0.61064 |
| S | -7.34510 | -1.35169 | -1.13895 |
| C | 7.38510 | -2.77487 | -0.74475 |
| S | 8.86716 | -3.66407 | -0.41615 |
| C | 9.80215 | -2.21394 | -0.55988 |
| C | 8.99306 | -1.12460 | -0.84401 |
| C | 7.61536 | -1.43800 | -0.95028 |
| C | 11.17994 | -1.90126 | -0.45626 |
| C | 11.41069 | -0.56473 | -0.66453 |
| S | 9.92878 | 0.32506 | -0.99011 |
| H | -2.20743 | -7.89626 | -0.15471 |
| H | -4.36422 | -6.79880 | -0.10158 |
| H | -2.53220 | -3.15129 | -1.40164 |
| H | 2.69049 | -3.04940 | -1.42149 |
| H | 4.70476 | -6.66712 | -0.32570 |
| H | 2.59967 | -7.85167 | -0.35478 |
| H | -0.72712 | -8.67668 | -1.30097 |
| H | 0.98552 | -8.58884 | -1.59064 |
| H | 1.29211 | -8.48925 | 0.98381 |
| H | -1.58822 | -9.42698 | 0.93490 |
| H | -0.45494 | -10.06023 | 2.09312 |
| H | 0.05105 | -7.86131 | 2.99451 |
| H | -0.93571 | -7.05815 | 1.79074 |
| H | -2.97214 | -8.19943 | 2.66117 |
| H | -2.00240 | -9.04601 | 3.85427 |
| H | -3.11293 | -7.04961 | 4.87671 |
| H | -1.35709 | -6.83778 | 4.89612 |
| H | -2.33567 | -5.99177 | 3.69140 |
| H | 2.01519 | -10.29492 | -0.48454 |
| H | 1.44698 | -10.89514 | 1.06107 |
| H | 0.65580 | -12.35816 | -0.76624 |
| H | -0.73745 | -11.58483 | -0.00877 |
| H | -0.14380 | -11.01085 | -1.57242 |
| H | 18.25501 | 0.76709 | -0.19378 |
| H | 16.13848 | -0.39373 | -0.26280 |
| H | 14.12983 | 3.31656 | -0.99978 |
| H | 16.97180 | 7.66411 | -0.50866 |
| H | 21.10564 | 7.18011 | 0.48342 |
| H | 20.91159 | 4.79690 | 0.15091 |
| H | 19.74427 | 1.70458 | -1.11661 |
| H | 20.64382 | 3.18902 | -1.19673 |
| H | 20.67533 | 3.25012 | 1.35243 |
| H | 18.88113 | 1.65658 | 1.81629 |
| H | 19.83695 | 0.33389 | 1.17063 |
| H | 21.53673 | 0.64523 | 2.94387 |
| H | 20.71927 | 2.09112 | 3.51307 |
| H | 18.70894 | 0.72259 | 4.09943 |
| H | 19.50896 | -0.72091 | 3.50535 |
| H | 19.69966 | -0.57175 | 5.99519 |
| H | 21.30323 | -0.45815 | 5.25834 |
| H | 20.50024 | 0.99866 | 5.85544 |
| H | 22.58492 | 2.73737 | -0.07118 |
| H | 22.65388 | 1.88659 | 1.45277 |
| H | 23.38021 | 0.42232 | -0.41064 |
| H | 21.91834 | -0.24143 | 0.31777 |
| H | 21.83022 | 0.61323 | -1.22685 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| H | -20.79879 | 4.28640 | 0.50737 | H | -18.62692 | 6.01736 | 3.83002 |
| H | -21.10816 | 6.67079 | 0.22443 | H | -20.49402 | -0.53227 | 0.90263 |
| H | -17.27738 | 6.93897 | -1.66448 | H | -21.06035 | -0.13763 | 2.51365 |
| H | -14.25119 | 2.69168 | -1.40088 | H | -22.97865 | -0.49058 | 0.99742 |
| H | -15.92334 | -0.77427 | 0.47951 | H | -22.96456 | 1.19523 | 1.51820 |
| H | -18.08098 | 0.30731 | 0.56169 | H | -22.40879 | 0.76165 | -0.10359 |
| H | -20.75255 | 2.46282 | -0.35600 | H | -19.44487 | 11.36571 | -2.17260 |
| H | -19.76123 | 1.05000 | -0.56671 | H | -20.69588 | 11.35347 | -0.92229 |
| H | -19.15418 | 1.21870 | 1.93421 | H | -19.00106 | 11.59154 | -0.47554 |
| H | -21.49037 | 3.14963 | 1.97419 | H | 20.29823 | 11.90561 | 1.13600 |
| H | -21.19164 | 2.04815 | 3.28801 | H | 19.26172 | 12.20092 | -0.26646 |
| H | -18.94946 | 2.92073 | 3.66894 | H | 18.54352 | 12.00030 | 1.33724 |
| H | -19.05592 | 3.99031 | 2.28564 | H | -9.97476 | 0.61104 | -1.27887 |
| H | -20.95892 | 5.20589 | 3.34410 | H | -8.52214 | -4.55540 | 0.15775 |
| H | -20.88505 | 4.13238 | 4.73113 | H | 6.82395 | -0.73244 | -1.16634 |
| H | -19.69610 | 6.28074 | 5.21421 | H | 11.97156 | -2.60718 | -0.24228 |
| H | -18.54339 | 4.93944 | 5.22865 | | | | |

**Listing 3** Cartesian coordinates of the optimized model compound **M2**.

| | | | |
|---|---|---|---|
| C | -1.10264 | -5.69057 | -0.80947 |
| C | -1.24843 | -4.33941 | -1.17646 |
| S | 0.08354 | -3.42394 | -1.88726 |
| C | 1.45343 | -4.28303 | -1.17665 |
| C | 1.36770 | -5.64588 | -0.83255 |
| N | 0.14479 | -6.34317 | -0.82791 |
| C | -2.26897 | -6.36555 | -0.42315 |
| C | -3.50656 | -5.74387 | -0.39410 |
| C | -3.63363 | -4.39454 | -0.72527 |
| C | -2.47763 | -3.70451 | -1.10616 |
| C | 2.65536 | -3.59899 | -1.10993 |
| C | 3.84556 | -4.25120 | -0.76735 |
| C | 3.78263 | -5.61625 | -0.48886 |
| C | 2.57206 | -6.29052 | -0.51245 |
| C | 0.20101 | -7.81029 | -0.80748 |
| C | 0.49502 | -8.53815 | 0.53331 |
| C | -0.68102 | -8.67291 | 1.51813 |
| C | -0.89250 | -7.46088 | 2.42801 |
| C | -2.12272 | -7.59351 | 3.32319 |
| C | -2.29653 | -6.41112 | 4.27246 |
| C | 1.10693 | -9.91742 | 0.21461 |
| C | 0.17566 | -10.88973 | -0.51122 |
| C | 5.08146 | -3.54475 | -0.72790 |
| C | 6.13243 | -2.95017 | -0.69902 |
| C | 7.36833 | -2.25668 | -0.67186 |
| C | 7.44259 | -0.88464 | -0.93194 |
| C | 8.64876 | -0.21124 | -0.91251 |
| C | 9.84927 | -0.87178 | -0.63245 |
| C | 9.77433 | -2.24352 | -0.37026 |
| C | 8.56847 | -2.91664 | -0.38928 |
| F | 8.55663 | -4.22489 | -0.13373 |
| C | 11.08813 | -0.18379 | -0.61974 |
| C | 12.14660 | 0.39840 | -0.61378 |
| C | 15.89342 | 2.44922 | -0.58975 |
| C | 14.68410 | 3.12313 | -0.85240 |
| S | 14.65646 | 4.80836 | -1.37858 |
| C | 16.15352 | 5.38300 | -0.63807 |
| C | 17.23850 | 4.51842 | -0.40729 |
| N | 17.13040 | 3.11771 | -0.55312 |
| C | 15.80356 | 1.06543 | -0.37668 |
| C | 14.59373 | 0.39169 | -0.39696 |
| C | 13.39788 | 1.07769 | -0.60976 |
| C | 13.46968 | 2.45755 | -0.83008 |
| C | 16.26136 | 6.74810 | -0.42498 |
| C | 17.47030 | 7.33510 | -0.03771 |
| C | 18.56809 | 6.49304 | 0.12971 |
| C | 18.45034 | 5.12145 | -0.04177 |
| C | 18.37572 | 2.34389 | -0.58337 |
| C | 19.08128 | 2.05362 | 0.76582 |
| C | 18.34969 | 1.05230 | 1.67117 |
| C | 18.99337 | 0.87087 | 3.04716 |
| C | 18.14289 | 0.02140 | 3.99120 |
| C | 18.78762 | -0.17207 | 5.36098 |
| C | 20.54762 | 1.66571 | 0.49018 |
| C | 20.75209 | 0.33972 | -0.24438 |
| C | -7.22558 | -2.52719 | -0.63625 |
| C | -8.39936 | -3.21167 | -0.30562 |
| C | -9.62499 | -2.57492 | -0.28854 |
| C | -9.74675 | -1.21719 | -0.60090 |
| C | -8.57253 | -0.53221 | -0.92978 |
| C | -7.34681 | -1.16911 | -0.94718 |
| C | -11.00401 | -0.56344 | -0.58812 |
| C | -12.07425 | -0.00320 | -0.58174 |
| C | -17.18424 | 4.07747 | -0.39131 |
| C | -16.13104 | 4.93276 | -0.75849 |
| S | -14.67093 | 4.31770 | -1.53886 |
| C | -14.64813 | 2.67765 | -0.88322 |
| C | -15.83880 | 2.00944 | -0.53393 |
| N | -17.07656 | 2.67126 | -0.46971 |
| C | -18.35843 | 4.69113 | 0.06218 |
| C | -18.48389 | 6.06893 | 0.15444 |
| C | -17.42132 | 6.90880 | -0.17730 |
| C | -16.24112 | 6.30866 | -0.62629 |
| C | -13.42705 | 2.02591 | -0.86732 |
| C | -13.33435 | 0.65966 | -0.57621 |
| C | -14.51602 | -0.02812 | -0.30114 |
| C | -15.73298 | 0.63423 | -0.27334 |
| C | -18.29175 | 1.84832 | -0.45216 |
| C | -18.72935 | 1.15413 | 0.86716 |
| C | -19.35362 | 2.04905 | 1.95285 |
| C | -18.34269 | 2.79406 | 2.82659 |
| C | -19.00295 | 3.72948 | 3.83750 |
| C | -17.99501 | 4.43104 | 4.74356 |
| C | -19.66761 | -0.01639 | 0.50826 |
| C | -21.00253 | 0.38479 | -0.12158 |
| C | 17.57238 | 8.74760 | 0.16155 |
| C | -5.96841 | -3.18145 | -0.66051 |
| C | -4.89660 | -3.73768 | -0.68718 |
| C | -17.52879 | 8.33065 | -0.06753 |
| C | -17.61906 | 9.52949 | 0.02452 |
| C | -17.72728 | 10.98020 | 0.13575 |
| C | 17.65724 | 9.93862 | 0.32939 |
| C | 17.75879 | 11.37992 | 0.53192 |
| F | -8.62968 | 0.76315 | -1.23587 |
| F | -6.26080 | -0.46798 | -1.26969 |
| F | -10.71147 | -3.27725 | 0.03250 |
| F | -8.34220 | -4.50802 | -0.00050 |
| F | 10.88757 | -2.92391 | -0.09707 |
| F | 6.32987 | -0.20555 | -1.20718 |
| F | 8.66075 | 1.09598 | -1.16945 |
| H | -2.22121 | -7.40135 | -0.12664 |
| H | -4.38260 | -6.30897 | -0.09597 |
| H | -2.54795 | -2.65684 | -1.37883 |
| H | 2.67850 | -2.54380 | -1.36080 |
| H | 4.68981 | -6.15536 | -0.23999 |
| H | 2.58531 | -7.34380 | -0.27855 |
| H | -0.72767 | -8.18039 | -1.24356 |
| H | 0.98670 | -8.08896 | -1.51730 |
| H | 1.26597 | -7.96737 | 1.06126 |
| H | -1.60897 | -8.91989 | 0.98630 |
| H | -0.48604 | -9.54162 | 2.16048 |
| H | 0.00122 | -7.33488 | 3.05412 |
| H | -0.97767 | -6.54348 | 1.83628 |
| H | -3.01693 | -7.69069 | 2.69327 |
| H | -2.05437 | -8.52492 | 3.90062 |
| H | -3.18548 | -6.52830 | 4.89971 |
| H | -1.43097 | -6.30752 | 4.93585 |
| H | -2.40148 | -5.47343 | 3.71634 |
| H | 2.01645 | -9.77920 | -0.38526 |
| H | 1.43276 | -10.37221 | 1.15728 |
| H | 0.67200 | -11.85167 | -0.66946 |
| H | -0.73487 | -11.08115 | 0.06516 |
| H | -0.12475 | -10.51449 | -1.49486 |
| H | 16.69178 | 0.48699 | -0.18067 |
| H | 14.57590 | -0.67963 | -0.23073 |
| H | 12.55806 | 3.01601 | -1.01468 |
| H | 15.39366 | 7.37762 | -0.59172 |
| H | 19.52763 | 6.91347 | 0.40954 |
| H | 19.33673 | 4.52524 | 0.11177 |
| H | 18.17599 | 1.41565 | -1.11970 |
| H | 19.07094 | 2.90165 | -1.21911 |
| H | 19.10774 | 2.99220 | 1.32951 |
| H | 17.32050 | 1.39831 | 1.81703 |
| H | 18.27811 | 0.07151 | 1.18228 |
| H | 19.98218 | 0.40607 | 2.94663 |
| H | 19.16362 | 1.85661 | 3.50233 |
| H | 17.15811 | 0.49052 | 4.11071 |
| H | 17.95919 | -0.95787 | 3.53019 |
| H | 18.15796 | -0.78043 | 6.01735 |
| H | 19.75882 | -0.67163 | 5.27401 |
| H | 18.95463 | 0.79007 | 5.85751 |
| H | 21.01605 | 2.47038 | -0.09196 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| H | 21.09068 | 1.63500 | 1.44016 | H | -19.59378 | 4.48141 | 3.29792 |
| H | 21.81752 | 0.15412 | -0.40950 | H | -19.71697 | 3.16116 | 4.44835 |
| H | 20.35857 | -0.50635 | 0.32763 | H | -18.49232 | 5.09456 | 5.45775 |
| H | 20.26589 | 0.33276 | -1.22524 | H | -17.40689 | 3.70527 | 5.31590 |
| H | -19.20168 | 4.08920 | 0.36191 | H | -17.29493 | 5.03577 | 4.15740 |
| H | -19.41645 | 6.49716 | 0.50491 | H | -19.14368 | -0.70168 | -0.17128 |
| H | -15.39787 | 6.93337 | -0.90129 | H | -19.86304 | -0.58842 | 1.42261 |
| H | -12.52847 | 2.57977 | -1.11778 | H | -21.61626 | -0.49971 | -0.31607 |
| H | -14.48202 | -1.09196 | -0.09433 | H | -21.57667 | 1.04398 | 0.53691 |
| H | -16.61144 | 0.05068 | -0.04546 | H | -20.86751 | 0.90199 | -1.07676 |
| H | -19.10535 | 2.46128 | -0.84196 | H | -16.91087 | 11.47694 | -0.39788 |
| H | -18.13456 | 1.06349 | -1.19984 | H | -18.67085 | 11.33940 | -0.28765 |
| H | -17.83912 | 0.70941 | 1.32373 | H | -17.68688 | 11.30152 | 1.18177 |
| H | -20.07157 | 2.75316 | 1.51397 | H | 18.46791 | 11.61676 | 1.33157 |
| H | -19.95484 | 1.40770 | 2.61107 | H | 18.10025 | 11.88508 | -0.37768 |
| H | -17.73039 | 2.05490 | 3.36089 | H | 16.78948 | 11.80756 | 0.80719 |
| H | -17.64857 | 3.37060 | 2.20705 | | | | |

**Listing 4** Cartesian coordinates of the optimized model compound **M3**.

| | | | |
|---|---|---|---|
| C | 1.27752 | -5.62429 | 1.32735 |
| C | 1.39948 | -4.22722 | 1.44546 |
| S | 0.03458 | -3.21967 | 1.93599 |
| C | -1.30088 | -4.21076 | 1.33965 |
| C | -1.19242 | -5.61183 | 1.25293 |
| N | 0.03518 | -6.28098 | 1.42189 |
| C | 2.46304 | -6.34028 | 1.11060 |
| C | 3.69482 | -5.71604 | 1.00489 |
| C | 3.79971 | -4.32591 | 1.08306 |
| C | 2.62426 | -3.59673 | 1.29679 |
| C | -2.50228 | -3.56561 | 1.09936 |
| C | -3.67407 | -4.28309 | 0.82944 |
| C | -3.59078 | -5.67611 | 0.80972 |
| C | -2.37931 | -6.31892 | 1.00818 |
| C | -0.00758 | -7.72739 | 1.66754 |
| C | -0.24441 | -8.69461 | 0.47474 |
| C | 0.95936 | -8.96608 | -0.44622 |
| C | 1.17014 | -7.91875 | -1.54171 |
| C | 2.42463 | -8.16947 | -2.37607 |
| C | 2.60336 | -7.15199 | -3.49940 |
| C | -0.82844 | -10.01141 | 1.02445 |
| C | 0.10795 | -10.81180 | 1.93101 |
| C | -4.90916 | -3.61683 | 0.59848 |
| C | -5.97118 | -3.07217 | 0.39468 |
| C | -9.80471 | 0.43107 | -0.27439 |
| C | -10.45247 | 1.45105 | -0.35375 |
| C | -12.81884 | 4.99848 | -0.61077 |
| C | -13.34052 | 3.73367 | -0.94642 |
| S | -14.93924 | 3.55480 | -1.67494 |
| C | -15.73738 | 4.98363 | -1.01092 |
| C | -15.01234 | 6.14295 | -0.68022 |
| N | -13.60136 | 6.16820 | -0.65899 |
| C | -11.46852 | 5.03507 | -0.23356 |
| C | -10.68882 | 3.89218 | -0.16445 |
| C | -11.23066 | 2.63764 | -0.44711 |
| C | -12.57515 | 2.58495 | -0.83384 |
| C | -17.12203 | 4.96013 | -0.96108 |
| C | -17.86297 | 6.10410 | -0.64728 |
| C | -17.15446 | 7.27449 | -0.38213 |
| C | -15.76731 | 7.28878 | -0.38963 |
| C | -12.95404 | 7.48094 | -0.57577 |
| C | -12.91299 | 8.17538 | 0.80998 |
| C | -11.92545 | 7.55149 | 1.80667 |
| C | -11.96155 | 8.17989 | 3.20109 |
| C | -11.11192 | 7.41524 | 4.21582 |
| C | -11.12967 | 8.04855 | 5.60435 |
| C | -12.69837 | 9.68819 | 0.60850 |
| C | -11.33867 | 10.08898 | 0.03450 |
| C | 10.10371 | 0.26904 | 0.62902 |
| C | 10.78180 | 1.27218 | 0.62023 |
| C | 13.51301 | 7.21087 | 0.28613 |
| C | 12.17348 | 7.51458 | 0.58675 |
| S | 11.11500 | 6.34149 | 1.37620 |
| C | 11.85734 | 4.83963 | 0.81519 |
| C | 13.23284 | 4.76625 | 0.52093 |
| N | 14.04410 | 5.91269 | 0.44074 |
| C | 14.30392 | 8.26941 | -0.17827 |
| C | 13.80048 | 9.55055 | -0.34469 |
| C | 12.46110 | 9.83426 | -0.08018 |
| C | 11.65917 | 8.78558 | 0.38034 |
| C | 11.06070 | 3.70726 | 0.81801 |
| C | 11.60154 | 2.43408 | 0.60013 |
| C | 12.97638 | 2.34362 | 0.37780 |
| C | 13.76548 | 3.48177 | 0.33138 |
| C | 15.49829 | 5.72193 | 0.48200 |
| C | 16.24014 | 5.24405 | -0.79720 |
| C | 16.47675 | 6.29610 | -1.89570 |
| C | 15.29434 | 6.50242 | -2.84476 |
| C | 15.53346 | 7.61548 | -3.86266 |
| C | 14.37782 | 7.77909 | -4.84605 |
| C | 17.56586 | 4.58160 | -0.37130 |
| C | 18.58425 | 5.51898 | 0.27958 |
| C | -19.29243 | 6.07054 | -0.61623 |
| C | 6.14347 | -3.14984 | 0.84823 |
| C | 5.05845 | -3.67641 | 0.95544 |
| C | 11.92250 | 11.14577 | -0.26787 |
| C | 11.46780 | 12.25125 | -0.42624 |
| C | 10.91632 | 13.58835 | -0.61793 |
| C | -20.49759 | 6.04162 | -0.58959 |
| C | -21.95583 | 6.00575 | -0.55730 |
| C | 7.39949 | -2.53823 | 0.72618 |
| C | 8.63762 | -3.14227 | 0.51867 |
| C | 9.71700 | -2.21221 | 0.46433 |
| C | 9.31432 | -0.88990 | 0.63951 |
| S | 7.60140 | -0.82709 | 0.85895 |
| C | -9.04704 | -0.74520 | -0.18039 |
| C | -9.46784 | -2.06251 | -0.34956 |
| C | -8.42408 | -3.01611 | -0.16438 |
| C | -7.19916 | -2.43707 | 0.15941 |
| S | -7.36524 | -0.71767 | 0.21657 |
| N | -10.74157 | -2.45732 | -0.61262 |
| C | -10.95950 | -3.73978 | -0.73059 |
| C | -9.86089 | -4.71179 | -0.65691 |
| N | -8.64610 | -4.34467 | -0.34772 |
| N | 8.85737 | -4.48021 | 0.42123 |
| C | 10.08946 | -4.87281 | 0.23675 |
| C | 11.18358 | -3.90794 | 0.06948 |
| N | 10.98812 | -2.62475 | 0.21576 |
| C | 12.56533 | -4.30520 | -0.31454 |
| C | 10.30065 | -6.34579 | 0.25284 |
| C | -12.38472 | -4.13421 | -0.89550 |
| C | -10.03246 | -6.15717 | -0.96648 |
| C | 13.64729 | -3.65572 | 0.28496 |
| C | 14.94898 | -3.96196 | -0.08886 |
| C | 15.18585 | -4.90707 | -1.08196 |
| C | 14.11358 | -5.54279 | -1.69893 |
| C | 12.81135 | -5.24873 | -1.31519 |
| C | 11.35601 | -6.93253 | 0.95559 |
| C | 11.48117 | -8.31485 | 1.01096 |
| C | 10.56145 | -9.12798 | 0.35721 |
| C | 9.50445 | -8.55154 | -0.33999 |
| C | 9.36926 | -7.17028 | -0.38311 |
| C | -10.77992 | -6.59370 | -2.06322 |
| C | -10.85866 | -7.94710 | -2.36594 |
| C | -10.20178 | -8.88163 | -1.57239 |
| C | -9.45083 | -8.45446 | -0.48192 |
| C | -9.35850 | -7.10076 | -0.18725 |
| C | -12.94015 | -5.20685 | -0.19321 |
| C | -14.29257 | -5.50020 | -0.31283 |
| C | -15.10479 | -4.73348 | -1.14163 |
| C | -14.56073 | -3.65992 | -1.83952 |
| C | -13.21211 | -3.35652 | -1.70956 |
| H | 2.43510 | -7.41382 | 1.01153 |
| H | 4.58643 | -6.31191 | 0.84501 |
| H | 2.67332 | -2.51572 | 1.37389 |
| H | -2.53937 | -2.48265 | 1.15173 |
| H | -4.48362 | -6.26218 | 0.62308 |
| H | -2.37775 | -7.39745 | 0.97149 |
| H | 0.90748 | -7.99720 | 2.19654 |
| H | -0.81720 | -7.88425 | 2.38814 |
| H | -1.01625 | -8.25390 | -0.16446 |
| H | 1.87806 | -9.09636 | 0.13977 |
| H | 0.79829 | -9.93507 | -0.93703 |
| H | 0.29021 | -7.91873 | -2.19930 |
| H | 1.22360 | -6.91437 | -1.10927 |
| H | 3.30372 | -8.14511 | -1.71842 |
| H | 2.38642 | -9.18303 | -2.79691 |
| H | 3.50939 | -7.35095 | -4.08004 |
| H | 1.75316 | -7.17295 | -4.18994 |
| H | 2.67984 | -6.13547 | -3.09914 |
| H | -1.75507 | -9.79296 | 1.57188 |
| H | -1.12091 | -10.63665 | 0.17288 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| H | -0.37192 | -11.73961 | 2.25617 | H | 14.38174 | 6.72249 | -2.28156 |
| H | 1.03296 | -11.08471 | 1.41351 | H | 15.69500 | 8.56130 | -3.32878 |
| H | 0.38179 | -10.25479 | 2.83276 | H | 16.46188 | 7.41320 | -4.41313 |
| H | -11.00105 | 5.97150 | 0.02499 | H | 14.57216 | 8.58309 | -5.56264 |
| H | -9.64850 | 3.97423 | 0.13015 | H | 14.21080 | 6.85795 | -5.41501 |
| H | -13.02133 | 1.62604 | -1.07516 | H | 13.44673 | 8.01732 | -4.32096 |
| H | -17.64195 | 4.03836 | -1.19983 | H | 17.34951 | 3.75507 | 0.31872 |
| H | -17.69415 | 8.18705 | -0.15447 | H | 18.01881 | 4.12404 | -1.25847 |
| H | -15.28138 | 8.22626 | -0.16629 | H | 19.50238 | 4.97742 | 0.52599 |
| H | -11.94896 | 7.38434 | -0.98779 | H | 18.85828 | 6.34223 | -0.38769 |
| H | -13.48950 | 8.13447 | -1.27194 | H | 18.20561 | 5.95510 | 1.20960 |
| H | -13.90301 | 8.05724 | 1.26317 | H | 9.96278 | 13.69904 | -0.09200 |
| H | -12.15473 | 6.48501 | 1.90591 | H | 11.59875 | 14.35534 | -0.23764 |
| H | -10.89946 | 7.61041 | 1.41882 | H | 10.73870 | 13.79570 | -1.67840 |
| H | -11.61331 | 9.21957 | 3.15983 | H | -22.38451 | 6.51765 | -1.42524 |
| H | -13.00081 | 8.21925 | 3.55649 | H | -22.32355 | 4.97480 | -0.56264 |
| H | -11.46929 | 6.37965 | 4.27868 | H | -22.34326 | 6.49390 | 0.34287 |
| H | -10.07782 | 7.35833 | 3.85160 | H | 13.45082 | -2.90403 | 1.04152 |
| H | -10.51660 | 7.48090 | 6.31098 | H | 15.78092 | -3.45799 | 0.39341 |
| H | -10.74346 | 9.07344 | 5.57639 | H | 16.20318 | -5.14436 | -1.37769 |
| H | -12.14816 | 8.09040 | 6.00573 | H | 14.29004 | -6.27108 | -2.48426 |
| H | -13.48898 | 10.06637 | -0.05323 | H | 11.98215 | -5.74887 | -1.80332 |
| H | -12.84662 | 10.19833 | 1.56561 | H | 12.07773 | -6.30756 | 1.46986 |
| H | -11.27941 | 11.17444 | -0.08875 | H | 12.30070 | -8.75735 | 1.56850 |
| H | -10.51664 | 9.78987 | 0.69232 | H | 10.66573 | -10.20798 | 0.39483 |
| H | -11.15797 | 9.64048 | -0.94777 | H | 8.77980 | -9.18004 | -0.84849 |
| H | 15.33953 | 8.10140 | -0.42840 | H | 8.53598 | -6.71180 | -0.90416 |
| H | 14.45495 | 10.33832 | -0.70114 | H | -11.29510 | -5.87301 | -2.68864 |
| H | 10.61472 | 8.97390 | 0.60538 | H | -11.43540 | -8.27163 | -3.22637 |
| H | 10.00061 | 3.80863 | 1.02513 | H | -10.27153 | -9.93961 | -1.80594 |
| H | 13.43026 | 1.37084 | 0.22525 | H | -8.93143 | -9.17787 | 0.13906 |
| H | 14.81995 | 3.34770 | 0.14491 | H | -8.75726 | -6.75539 | 0.64657 |
| H | 15.93916 | 6.64964 | 0.84939 | H | -12.31609 | -5.80939 | 0.45749 |
| H | 15.68230 | 4.98090 | 1.26720 | H | -14.71288 | -6.33043 | 0.24608 |
| H | 15.63404 | 4.45878 | -1.26042 | H | -16.16018 | -4.96872 | -1.23914 |
| H | 16.78860 | 7.25352 | -1.45936 | H | -15.18989 | -3.05283 | -2.48304 |
| H | 17.33455 | 5.96854 | -2.49821 | H | -12.78354 | -2.50753 | -2.23056 |
| H | 15.10362 | 5.55925 | -3.37463 | | | | |

**Listing 5** Cartesian coordinates of the optimized model compound **M4**.

| | | | |
|---|---|---|---|
| C | -1.10744 | -5.90884 | -0.71960 |
| C | -1.23395 | -4.70224 | -1.43241 |
| S | 0.11401 | -4.03250 | -2.35635 |
| C | 1.46753 | -4.67612 | -1.42083 |
| C | 1.36263 | -5.89672 | -0.72747 |
| N | 0.13140 | -6.55943 | -0.55908 |
| C | -2.28388 | -6.44031 | -0.17462 |
| C | -3.51145 | -5.81310 | -0.31365 |
| C | -3.61991 | -4.59572 | -0.98751 |
| C | -2.45287 | -4.05150 | -1.53559 |
| C | 2.67459 | -4.00427 | -1.51733 |
| C | 3.85409 | -4.54471 | -0.99111 |
| C | 3.77192 | -5.78684 | -0.36145 |
| C | 2.55570 | -6.43814 | -0.22673 |
| C | 0.16867 | -7.97180 | -0.16240 |
| C | 0.44152 | -8.33729 | 1.32352 |
| C | -0.74779 | -8.21524 | 2.29422 |
| C | -0.95467 | -6.81416 | 2.87365 |
| C | -2.19613 | -6.71044 | 3.75732 |
| C | -2.36735 | -5.32818 | 4.38115 |
| C | 1.04930 | -9.75368 | 1.37247 |
| C | 0.12023 | -10.87539 | 0.90580 |
| C | 5.09433 | -3.85503 | -1.11162 |
| C | 6.14550 | -3.26519 | -1.21775 |
| C | 14.78935 | -0.39807 | -0.59724 |
| C | 15.81020 | 0.25075 | -0.56288 |
| C | 19.41400 | 2.54631 | -0.43568 |
| C | 18.19643 | 3.10291 | -0.87269 |
| S | 18.11543 | 4.72080 | -1.57574 |
| C | 19.49770 | 5.47125 | -0.77193 |
| C | 20.60835 | 4.71274 | -0.35960 |
| N | 20.60076 | 3.30149 | -0.36640 |
| C | 19.38699 | 1.18945 | -0.08250 |
| C | 18.22663 | 0.43410 | -0.13524 |
| C | 17.01569 | 1.00796 | -0.52363 |
| C | 17.02723 | 2.36010 | -0.88383 |
| C | 19.49968 | 6.85476 | -0.69352 |
| C | 20.62841 | 7.56226 | -0.26730 |
| C | 21.75662 | 6.82136 | 0.07958 |
| C | 21.74150 | 5.43466 | 0.04261 |
| C | 21.88796 | 2.62066 | -0.19800 |
| C | 22.47450 | 2.53157 | 1.23455 |
| C | 21.75548 | 1.53774 | 2.15828 |
| C | 22.28036 | 1.52653 | 3.59528 |
| C | 21.42536 | 0.67207 | 4.53076 |
| C | 21.95594 | 0.64316 | 5.96154 |
| C | 23.99288 | 2.28306 | 1.14125 |
| C | 24.40301 | 0.92783 | 0.56314 |
| C | -14.62742 | -0.65809 | -0.56944 |
| C | -15.66733 | -0.04084 | -0.52662 |
| C | -20.62955 | 4.22411 | -0.28017 |
| C | -19.60227 | 4.99184 | -0.85661 |
| S | -18.25254 | 4.23728 | -1.71054 |
| C | -18.19517 | 2.68381 | -0.87126 |
| C | -19.35457 | 2.10679 | -0.31771 |
| N | -20.56369 | 2.81682 | -0.20256 |
| C | -21.73262 | 4.92965 | 0.21726 |
| C | -21.81315 | 6.31262 | 0.15740 |
| C | -20.77263 | 7.06855 | -0.38137 |
| C | -19.66361 | 6.37683 | -0.87789 |
| C | -16.99539 | 1.99336 | -0.90984 |
| C | -16.90111 | 0.66820 | -0.46773 |
| C | -18.06167 | 0.06434 | 0.01629 |
| C | -19.25188 | 0.77009 | 0.09651 |
| C | -21.78075 | 2.04344 | 0.06569 |
| C | -22.04856 | 1.53633 | 1.51025 |
| C | -22.61958 | 2.56223 | 2.50656 |
| C | -21.56530 | 3.42575 | 3.20241 |
| C | -22.17082 | 4.48889 | 4.11650 |
| C | -21.11509 | 5.31595 | 4.84493 |
| C | -22.94678 | 0.28563 | 1.43122 |
| C | -24.35313 | 0.52908 | 0.88117 |
| C | 20.62264 | 8.99115 | -0.20737 |
| C | -5.93421 | -3.36167 | -1.23281 |
| C | -4.87211 | -3.92999 | -1.11847 |
| C | -20.83205 | 8.49666 | -0.42995 |
| C | -20.88131 | 9.70073 | -0.47108 |
| C | -20.93964 | 11.15773 | -0.52104 |
| C | 20.61605 | 10.19587 | -0.15686 |
| C | 20.60676 | 11.65361 | -0.09624 |
| C | -13.41044 | -1.36831 | -0.62126 |
| S | -11.93415 | -0.58688 | -1.11806 |
| C | -11.02285 | -2.05395 | -0.92422 |
| C | -11.83177 | -3.07294 | -0.48733 |
| C | -13.18161 | -2.68689 | -0.31421 |
| C | -9.60129 | -2.09160 | -1.20866 |
| C | -8.85042 | -1.20177 | -1.93525 |
| C | -7.48208 | -1.55265 | -2.01689 |
| C | -7.18207 | -2.71622 | -1.35293 |
| S | -8.60723 | -3.38185 | -0.60253 |
| C | 7.37939 | -2.59235 | -1.33127 |
| S | 8.82704 | -3.25237 | -0.61975 |
| C | 9.78742 | -1.92378 | -1.19673 |
| C | 9.00973 | -1.02704 | -1.88569 |
| C | 7.64779 | -1.40270 | -1.96169 |
| C | 11.21168 | -1.86471 | -0.93005 |
| C | 12.04864 | -2.87719 | -0.53254 |
| C | 13.39282 | -2.46698 | -0.36962 |
| C | 13.58896 | -1.13623 | -0.64494 |
| S | 12.08875 | -0.37391 | -1.09814 |
| H | -2.25189 | -7.36346 | 0.38208 |
| H | -4.39506 | -6.26702 | 0.12104 |
| H | -2.50509 | -3.11209 | -2.07559 |
| H | 2.70968 | -3.05401 | -2.03944 |
| H | 4.66903 | -6.24518 | 0.03953 |
| H | 2.55562 | -7.39144 | 0.27914 |
| H | -0.76146 | -8.43178 | -0.49934 |
| H | 0.95736 | -8.43088 | -0.76766 |
| H | 1.20919 | -7.65354 | 1.70003 |
| H | -1.67238 | -8.57613 | 1.82522 |
| H | -0.57258 | -8.90050 | 3.13406 |
| H | -0.06665 | -6.54509 | 3.46168 |
| H | -1.02215 | -6.07098 | 2.07232 |
| H | -3.08438 | -6.95354 | 3.15911 |
| H | -2.14451 | -7.47026 | 4.54830 |
| H | -3.26516 | -5.27827 | 5.00481 |
| H | -1.50875 | -5.07047 | 5.01082 |
| H | -2.45432 | -4.55707 | 3.60830 |
| H | 1.96584 | -9.77405 | 0.76770 |
| H | 1.36245 | -9.95565 | 2.40338 |
| H | 0.61393 | -11.84731 | 0.99762 |
| H | -0.79505 | -10.91409 | 1.50465 |
| H | -0.17172 | -10.75748 | -0.14270 |
| H | 20.28595 | 0.69679 | 0.25143 |
| H | 18.25967 | -0.61309 | 0.14411 |
| H | 16.10571 | 2.83372 | -1.20549 |
| H | 18.61338 | 7.40097 | -0.99872 |
| H | 22.65813 | 7.33481 | 0.39501 |
| H | 22.64602 | 4.92234 | 0.33271 |
| H | 21.79982 | 1.62725 | -0.63941 |
| H | 22.60517 | 3.15512 | -0.82936 |
| H | 22.34647 | 3.51369 | 1.70193 |
| H | 20.69021 | 1.79149 | 2.18502 |
| H | 21.81915 | 0.51974 | 1.75053 |
| H | 23.31230 | 1.15472 | 3.62102 |
| H | 22.31650 | 2.55607 | 3.97819 |
| H | 20.39591 | 1.05197 | 4.52720 |
| H | 21.37295 | -0.35187 | 4.13815 |
| H | 21.32541 | 0.02712 | 6.60991 |
| H | 22.97171 | 0.23427 | 5.99823 |
| H | 21.99004 | 1.65081 | 6.39000 |
| H | 24.43873 | 3.07944 | 0.53065 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| H | 24.43305 | 2.39450 | 2.13737 | H | -20.46504 | 5.83583 | 4.13311 |
| H | 25.49295 | 0.84298 | 0.52107 | H | -22.45042 | -0.47673 | 0.81581 |
| H | 24.03439 | 0.09788 | 1.17414 | H | -23.02628 | -0.14228 | 2.43736 |
| H | 24.02675 | 0.78373 | -0.45482 | H | -24.93503 | -0.39732 | 0.88818 |
| H | -22.55330 | 4.39900 | 0.67382 | H | -24.89815 | 1.26390 | 1.48195 |
| H | -22.69137 | 6.81283 | 0.55039 | H | -24.33272 | 0.89157 | -0.15170 |
| H | -18.84038 | 6.93377 | -1.31270 | H | -20.48617 | 11.53877 | -1.44169 |
| H | -16.11872 | 2.48193 | -1.32180 | H | -21.97489 | 11.51176 | -0.48697 |
| H | -18.03119 | -0.96782 | 0.34710 | H | -20.40563 | 11.60513 | 0.32384 |
| H | -20.11173 | 0.24981 | 0.48963 | H | 21.50908 | 12.03270 | 0.39388 |
| H | -22.62880 | 2.62765 | -0.29389 | H | 20.56217 | 12.09145 | -1.09891 |
| H | -21.73118 | 1.16840 | -0.59099 | H | 19.74188 | 12.02000 | 0.46632 |
| H | -21.09216 | 1.20858 | 1.93063 | H | -11.46920 | -4.07924 | -0.31192 |
| H | -23.37595 | 3.19495 | 2.02461 | H | -13.96862 | -3.35263 | 0.01683 |
| H | -23.16635 | 2.01241 | 3.28408 | H | -9.27381 | -0.32640 | -2.41407 |
| H | -20.91063 | 2.76939 | 3.79186 | H | -6.73640 | -0.97825 | -2.55188 |
| H | -20.91905 | 3.91383 | 2.46559 | H | 9.40946 | -0.12871 | -2.34177 |
| H | -22.80827 | 5.15492 | 3.51992 | H | 6.88402 | -0.82708 | -2.46915 |
| H | -22.83334 | 4.00698 | 4.84764 | H | 11.71024 | -3.89534 | -0.37854 |
| H | -21.57305 | 6.07055 | 5.49184 | H | 14.19866 | -3.12439 | -0.06858 |
| H | -20.47919 | 4.68075 | 5.47123 | | | | |

**Listing 6** Cartesian coordinates of the optimized model compound **M5**.

| | | | |
|---|---|---|---|
| C | 1.04305 | 7.07018 | -0.27641 |
| C | 1.14962 | 5.80224 | -0.87717 |
| S | -0.21584 | 5.06482 | -1.72027 |
| C | -1.55097 | 5.80043 | -0.82713 |
| C | -1.42764 | 7.07683 | -0.24655 |
| N | -0.18926 | 7.74218 | -0.15520 |
| C | 2.23248 | 7.63878 | 0.19840 |
| C | 3.45217 | 6.98790 | 0.10246 |
| C | 3.54073 | 5.71077 | -0.45265 |
| C | 2.36114 | 5.13190 | -0.93360 |
| C | -2.76373 | 5.13209 | -0.84563 |
| C | -3.93221 | 5.72431 | -0.35227 |
| C | -3.83205 | 7.01658 | 0.16268 |
| C | -2.60998 | 7.66906 | 0.22121 |
| C | -0.21078 | 9.18072 | 0.13209 |
| C | -0.45684 | 9.66091 | 1.58966 |
| C | 0.74064 | 9.58601 | 2.55492 |
| C | 0.93702 | 8.22325 | 3.22247 |
| C | 2.18580 | 8.16265 | 4.09975 |
| C | 2.35238 | 6.81892 | 4.80383 |
| C | -1.03560 | 11.08941 | 1.53997 |
| C | -0.09022 | 12.15421 | 0.98165 |
| C | -5.17724 | 5.03061 | -0.39233 |
| C | -14.87481 | -0.54184 | -0.69895 |
| C | -15.91553 | -1.15662 | -0.72868 |
| C | -19.56775 | -3.37731 | -0.80710 |
| C | -18.31727 | -4.01440 | -0.70124 |
| S | -18.16784 | -5.77250 | -0.77967 |
| C | -19.74950 | -6.23715 | -0.14355 |
| C | -20.87765 | -5.41484 | -0.31587 |
| N | -20.77788 | -4.09656 | -0.80788 |
| C | -19.55005 | -1.98013 | -0.91690 |
| C | -18.37020 | -1.25299 | -0.90988 |
| C | -17.13774 | -1.89006 | -0.76197 |
| C | -17.14049 | -3.28490 | -0.64965 |
| C | -19.85933 | -7.50481 | 0.40525 |
| C | -21.10201 | -8.04864 | 0.74686 |
| C | -22.23175 | -7.26540 | 0.51667 |
| C | -22.11924 | -5.97967 | 0.00793 |
| C | -22.00744 | -3.45824 | -1.28890 |
| C | -23.01754 | -2.88333 | -0.25655 |
| C | -22.67895 | -1.50769 | 0.34716 |
| C | -21.75143 | -1.55879 | 1.56316 |
| C | -21.35956 | -0.17429 | 2.07507 |
| C | -20.47793 | -0.22895 | 3.31968 |
| C | -24.41950 | -2.87347 | -0.89837 |
| C | -24.57975 | -1.93416 | -2.09477 |
| C | 14.52486 | -0.47113 | -0.94876 |
| C | 15.57772 | -1.06469 | -0.98201 |
| C | 20.72575 | -5.06309 | -0.35251 |
| C | 19.65086 | -5.89769 | 0.00138 |
| S | 18.00611 | -5.57021 | -0.55299 |
| C | 18.09083 | -3.81404 | -0.72692 |
| C | 19.30002 | -3.16569 | -1.04353 |
| N | 20.53789 | -3.83561 | -1.02232 |
| C | 22.00580 | -5.51280 | -0.00425 |
| C | 22.21257 | -6.71085 | 0.66238 |
| C | 21.13799 | -7.51358 | 1.04359 |
| C | 19.85429 | -7.07485 | 0.70526 |
| C | 16.89281 | -3.12075 | -0.68165 |
| C | 16.81972 | -1.76396 | -1.01825 |
| C | 18.00153 | -1.13111 | -1.40281 |
| C | 19.20838 | -1.81355 | -1.40573 |
| C | 21.67101 | -3.19689 | -1.70069 |
| C | 22.42349 | -2.03061 | -1.00164 |
| C | 23.37774 | -2.40731 | 0.14554 |
| C | 22.69702 | -2.60608 | 1.50140 |
| C | 23.66171 | -3.06615 | 2.59231 |
| C | 22.98985 | -3.21597 | 3.95446 |
| C | 23.15507 | -1.20964 | -2.08309 |
| C | 24.27640 | -1.94734 | -2.81658 |
| C | -21.20304 | -9.36517 | 1.29655 |
| C | 5.83753 | 4.42656 | -0.58623 |
| C | 4.78374 | 5.01650 | -0.52844 |
| C | 21.33447 | -8.74095 | 1.75100 |
| C | 21.49991 | -9.77558 | 2.34774 |
| C | 21.69917 | -11.02760 | 3.06990 |
| C | -21.28659 | -10.47498 | 1.76054 |
| C | -21.38663 | -11.81791 | 2.32208 |
| C | 10.82527 | 1.61464 | -0.81330 |
| C | 9.53668 | 2.34278 | -0.75987 |
| C | 8.34928 | 1.74006 | -1.19008 |
| C | 7.14170 | 2.41631 | -1.13721 |
| C | 7.08047 | 3.72806 | -0.64844 |
| C | 8.26668 | 4.33711 | -0.21818 |
| C | 9.46998 | 3.65365 | -0.27465 |
| C | 12.01213 | 2.27413 | -1.15182 |
| C | 13.21996 | 1.59793 | -1.19859 |
| C | 13.28212 | 0.22905 | -0.90595 |
| C | 12.09633 | -0.43661 | -0.56796 |
| C | 10.89269 | 0.24721 | -0.52380 |
| C | -9.91605 | 2.32619 | -0.54932 |
| C | -11.19873 | 1.58678 | -0.58863 |
| C | -11.23425 | 0.19833 | -0.41727 |
| C | -12.43061 | -0.49829 | -0.45297 |
| C | -13.64150 | 0.17516 | -0.66218 |
| C | -13.61197 | 1.56540 | -0.83393 |
| C | -12.41081 | 2.25428 | -0.79737 |
| C | -9.83158 | 3.59382 | 0.03739 |
| C | -8.63292 | 4.28674 | 0.07883 |
| C | -7.46931 | 3.73066 | -0.46875 |
| C | -7.54833 | 2.46198 | -1.05838 |
| C | -8.75106 | 1.77645 | -1.09618 |
| C | -6.23025 | 4.43746 | -0.42673 |
| H | 2.21761 | 8.61037 | 0.66637 |
| H | 4.34599 | 7.47124 | 0.48106 |
| H | 2.39717 | 4.14554 | -1.38376 |
| H | -2.81250 | 4.13936 | -1.28034 |
| H | -4.72021 | 7.51519 | 0.53459 |
| H | -2.59690 | 8.66350 | 0.64045 |
| H | 0.71631 | 9.60652 | -0.25442 |
| H | -1.00632 | 9.59883 | -0.49354 |
| H | -1.23355 | 9.02326 | 2.02399 |
| H | 1.66488 | 9.90409 | 2.05559 |
| H | 0.58151 | 10.32653 | 3.35002 |
| H | 0.05180 | 8.00316 | 3.83462 |
| H | 0.98918 | 7.42905 | 2.47070 |
| H | 3.06997 | 8.36176 | 3.47967 |
| H | 2.14781 | 8.96895 | 4.84421 |
| H | 3.25413 | 6.80022 | 5.42360 |
| H | 1.49656 | 6.60496 | 5.45338 |
| H | 2.42920 | 6.00264 | 4.07775 |
| H | -1.95897 | 11.08417 | 0.94538 |
| H | -1.33189 | 11.37334 | 2.55643 |
| H | -0.56263 | 13.14059 | 1.00831 |
| H | 0.83369 | 12.21664 | 1.56504 |
| H | 0.18483 | 11.95417 | -0.05897 |
| H | -20.47606 | -1.43353 | -1.00137 |
| H | -18.40832 | -0.17332 | -1.00370 |
| H | -16.19805 | -3.81206 | -0.54573 |
| H | -18.96225 | -8.09891 | 0.54413 |
| H | -23.21396 | -7.66123 | 0.74999 |
| H | -23.03102 | -5.42069 | -0.13760 |
| H | -21.71973 | -2.68709 | -2.00507 |
| H | -22.53030 | -4.22098 | -1.87546 |
| H | -23.06390 | -3.57927 | 0.58735 |
| H | -22.26991 | -0.83583 | -0.41849 |
| H | -23.61805 | -1.03478 | 0.66362 |
| H | -22.25788 | -2.11308 | 2.36506 |
| H | -20.84333 | -2.12518 | 1.33194 |
| H | -20.83243 | 0.36723 | 1.27832 |
| H | -22.26705 | 0.40591 | 2.28878 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| H | -20.20876 | 0.77414 | 3.66466 | H | 23.56986 | -0.31293 | -1.60822 |
| H | -20.98924 | -0.73911 | 4.14335 | H | 24.75854 | -1.28748 | -3.54394 |
| H | -19.54927 | -0.77346 | 3.11852 | H | 25.05054 | -2.29434 | -2.12504 |
| H | -24.68070 | -3.89413 | -1.20855 | H | 23.90431 | -2.81824 | -3.36553 |
| H | -25.14726 | -2.59592 | -0.12698 | H | 20.83894 | -11.69330 | 2.94731 |
| H | -25.60525 | -1.96584 | -2.47458 | H | 22.58567 | -11.55655 | 2.70541 |
| H | -24.36221 | -0.89638 | -1.82335 | H | 21.83369 | -10.85005 | 4.14207 |
| H | -23.91829 | -2.20806 | -2.92295 | H | -22.39530 | -12.01204 | 2.70029 |
| H | 22.87201 | -4.91725 | -0.24568 | H | -21.15971 | -12.58014 | 1.56936 |
| H | 23.22383 | -7.01860 | 0.90445 | H | -20.68669 | -11.95145 | 3.15332 |
| H | 18.99626 | -7.68030 | 0.97767 | H | 8.37736 | 0.73324 | -1.59441 |
| H | 15.98668 | -3.65115 | -0.40863 | H | 6.23205 | 1.93631 | -1.48170 |
| H | 17.97995 | -0.08631 | -1.69220 | H | 8.23188 | 5.34933 | 0.17016 |
| H | 20.08849 | -1.26493 | -1.70419 | H | 10.37242 | 4.13520 | 0.08829 |
| H | 22.37328 | -3.98527 | -1.97518 | H | 11.98320 | 3.32900 | -1.40567 |
| H | 21.27751 | -2.81354 | -2.64827 | H | 14.12918 | 2.12323 | -1.47057 |
| H | 21.67428 | -1.36570 | -0.56014 | H | 12.13185 | -1.49453 | -0.33116 |
| H | 23.97366 | -3.29082 | -0.11598 | H | 9.99069 | -0.28257 | -0.23448 |
| H | 24.11008 | -1.59620 | 0.25507 | H | -10.31123 | -0.34029 | -0.22811 |
| H | 22.23322 | -1.65678 | 1.80226 | H | -12.44057 | -1.57339 | -0.30960 |
| H | 21.87946 | -3.32924 | 1.41932 | H | -14.54124 | 2.09790 | -1.00562 |
| H | 24.10521 | -4.02629 | 2.29711 | H | -12.40865 | 3.32761 | -0.95849 |
| H | 24.49508 | -2.35491 | 2.66682 | H | -10.71463 | 4.03210 | 0.49138 |
| H | 23.70100 | -3.54641 | 4.71787 | H | -8.58383 | 5.26436 | 0.54619 |
| H | 22.55895 | -2.26583 | 4.28872 | H | -6.65677 | 2.02403 | -1.49410 |
| H | 22.17896 | -3.95087 | 3.91274 | H | -8.79442 | 0.80602 | -1.58021 |
| H | 22.42257 | -0.85170 | -2.81881 | | | | |

**Listing 7** Cartesian coordinates of the optimized model compound **M6**.

| | | | |
|---|---|---|---|
| C | 1.14177 | 7.91136 | -0.70118 |
| C | 1.27754 | 6.54089 | -0.99007 |
| S | -0.05867 | 5.60162 | -1.66129 |
| C | -1.42378 | 6.50702 | -1.00015 |
| C | -1.32883 | 7.88641 | -0.73539 |
| N | -0.09979 | 8.57353 | -0.76894 |
| C | 2.31173 | 8.59415 | -0.34187 |
| C | 3.54225 | 7.96175 | -0.26392 |
| C | 3.65986 | 6.59415 | -0.51563 |
| C | 2.49891 | 5.89787 | -0.87048 |
| C | -2.62923 | 5.83436 | -0.89111 |
| C | -3.81648 | 6.50984 | -0.58375 |
| C | -3.74397 | 7.88925 | -0.38943 |
| C | -2.52969 | 8.55490 | -0.45523 |
| C | -0.14221 | 10.03837 | -0.84089 |
| C | -0.43893 | 10.85364 | 0.44831 |
| C | 0.72811 | 11.03384 | 1.43664 |
| C | 0.91305 | 9.87577 | 2.41961 |
| C | 2.13271 | 10.04680 | 3.32280 |
| C | 2.28045 | 8.91899 | 4.34039 |
| C | -1.02828 | 12.21797 | 0.03646 |
| C | -0.07812 | 13.12797 | -0.74367 |
| C | -5.05278 | 5.80880 | -0.49076 |
| C | -6.10536 | 5.21765 | -0.40927 |
| C | -9.81464 | 1.54032 | -0.40345 |
| C | -10.41465 | 0.49255 | -0.48303 |
| C | -12.52479 | -3.21615 | -0.74197 |
| C | -11.15168 | -3.12276 | -1.04093 |
| S | -10.25654 | -4.48306 | -1.72386 |
| C | -11.19861 | -5.82602 | -1.06933 |
| C | -12.56892 | -5.69068 | -0.78155 |
| N | -13.22133 | -4.43911 | -0.79468 |
| C | -13.16951 | -2.01923 | -0.39793 |
| C | -12.49661 | -0.81009 | -0.32738 |
| C | -11.12564 | -0.73795 | -0.57552 |
| C | -10.46925 | -1.92259 | -0.92773 |
| C | -10.56177 | -7.05389 | -0.98513 |
| C | -11.26451 | -8.22367 | -0.67859 |
| C | -12.63561 | -8.10901 | -0.45726 |
| C | -13.26646 | -6.87413 | -0.49886 |
| C | -14.68675 | -4.44468 | -0.76321 |
| C | -15.37710 | -4.70220 | 0.60133 |
| C | -15.29767 | -3.52710 | 1.58615 |
| C | -15.89835 | -3.81947 | 2.96235 |
| C | -15.62999 | -2.70483 | 3.97306 |
| C | -16.24360 | -2.98258 | 5.34267 |
| C | -16.81765 | -5.18989 | 0.35085 |
| C | -17.76220 | -4.15852 | -0.26814 |
| C | 9.75912 | 1.75293 | -0.35214 |
| C | 10.37685 | 0.71541 | -0.43021 |
| C | 12.63033 | -5.42741 | -0.55561 |
| C | 11.25556 | -5.60580 | -0.78935 |
| S | 10.25789 | -4.31213 | -1.46077 |
| C | 11.15132 | -2.90694 | -0.87081 |
| C | 12.54253 | -2.95961 | -0.65790 |
| N | 13.25868 | -4.17038 | -0.68428 |
| C | 13.35461 | -6.56783 | -0.18628 |
| C | 12.75558 | -7.81075 | -0.04821 |
| C | 11.38449 | -7.97124 | -0.24546 |
| C | 10.64872 | -6.83949 | -0.60967 |
| C | 10.45199 | -1.71645 | -0.76710 |
| C | 11.10717 | -0.50411 | -0.51891 |
| C | 12.49468 | -0.53578 | -0.37909 |
| C | 13.18933 | -1.73399 | -0.43860 |
| C | 14.71786 | -4.09584 | -0.81371 |
| C | 15.57603 | -3.74153 | 0.43270 |
| C | 15.80725 | -4.86739 | 1.45721 |
| C | 14.68081 | -5.03740 | 2.47870 |
| C | 14.90395 | -6.21557 | 3.42466 |
| C | 13.80384 | -6.35050 | 4.47381 |
| C | 16.91541 | -3.15078 | -0.05177 |
| C | 17.81023 | -4.11672 | -0.83013 |
| C | -10.59768 | -9.48713 | -0.61220 |
| C | 5.97902 | 5.35661 | -0.34512 |
| C | 4.91295 | 5.92370 | -0.42228 |
| C | 10.74892 | -9.24243 | -0.08554 |
| C | 10.21177 | -10.31351 | 0.04916 |
| C | 9.56040 | -11.60880 | 0.21248 |
| C | -10.03364 | -10.55140 | -0.55625 |
| C | -9.34965 | -11.83839 | -0.48871 |
| C | 7.21057 | 4.67401 | -0.26234 |
| C | 8.45241 | 5.18987 | 0.02437 |
| C | 9.47521 | 4.21497 | 0.02208 |
| C | 9.01874 | 2.95040 | -0.26638 |
| S | 7.30057 | 2.95880 | -0.53982 |
| C | -9.09607 | 2.75087 | -0.31621 |
| C | -9.57329 | 4.00357 | -0.01011 |
| C | -8.56977 | 4.99826 | -0.01182 |
| C | -7.32189 | 4.50954 | -0.31918 |
| S | -7.38207 | 2.79546 | -0.61160 |
| H | 2.27271 | 9.64592 | -0.10587 |
| H | 4.42040 | 8.53496 | 0.01187 |
| H | 2.55847 | 4.83566 | -1.08268 |
| H | -2.65655 | 4.76625 | -1.07887 |
| H | -4.64700 | 8.44853 | -0.17166 |
| H | -2.53749 | 9.62070 | -0.28604 |
| H | 0.79372 | 10.37200 | -1.29093 |
| H | -0.92032 | 10.28005 | -1.57263 |
| H | -1.22337 | 10.32831 | 1.00259 |
| H | 1.66519 | 11.23585 | 0.90188 |
| H | 0.53770 | 11.94221 | 2.02334 |
| H | 0.00974 | 9.79696 | 3.03968 |
| H | 0.99511 | 8.92438 | 1.88394 |
| H | 3.03620 | 10.09797 | 2.70074 |
| H | 2.06737 | 11.01051 | 3.84507 |
| H | 3.16161 | 9.06303 | 4.97310 |
| H | 1.40449 | 8.86210 | 4.99576 |
| H | 2.38315 | 7.95010 | 3.84026 |
| H | -1.93527 | 12.05336 | -0.56054 |
| H | -1.35420 | 12.73766 | 0.94493 |
| H | -0.56072 | 14.08290 | -0.97180 |
| H | 0.82920 | 13.34713 | -0.17205 |
| H | 0.22700 | 12.68304 | -1.69630 |
| H | -14.22300 | -2.01497 | -0.16894 |
| H | -13.04215 | 0.08811 | -0.06020 |
| H | -9.40630 | -1.89905 | -1.14346 |
| H | -9.49813 | -7.11079 | -1.19119 |
| H | -13.21855 | -8.99652 | -0.23733 |
| H | -14.32892 | -6.85494 | -0.30989 |
| H | -15.03323 | -3.50647 | -1.19795 |
| H | -15.00797 | -5.22314 | -1.46278 |
| H | -14.84616 | -5.52900 | 1.08496 |
| H | -14.24518 | -3.25592 | 1.72256 |
| H | -15.79165 | -2.64031 | 1.16629 |
| H | -16.98215 | -3.96957 | 2.88044 |
| H | -15.48702 | -4.76318 | 3.34715 |
| H | -14.54666 | -2.56429 | 4.07668 |
| H | -16.02311 | -1.75813 | 3.57991 |
| H | -16.03444 | -2.17158 | 6.04692 |
| H | -17.33155 | -3.09202 | 5.27371 |
| H | -15.84543 | -3.90815 | 5.77273 |
| H | -16.77702 | -6.07184 | -0.30217 |
| H | -17.24350 | -5.54260 | 1.29569 |
| H | -18.75504 | -4.59145 | -0.42230 |
| H | -17.88429 | -3.28281 | 0.37694 |
| H | -17.40675 | -3.80658 | -1.24208 |
| H | 14.41280 | -6.49575 | 0.01004 |
| H | 13.36034 | -8.66577 | 0.23317 |
| H | 9.58123 | -6.93116 | -0.78008 |
| H | 9.37697 | -1.72157 | -0.91272 |
| H | 13.03796 | 0.38708 | -0.20898 |
| H | 14.26049 | -1.69434 | -0.31316 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| H | 15.05642 | -5.03748 | -1.24790 | H | 18.74792 | -3.62918 | -1.11288 |
| H | 14.91337 | -3.33513 | -1.57716 | H | 18.06566 | -4.99835 | -0.23385 |
| H | 15.06123 | -2.94299 | 0.97664 | H | 17.33418 | -4.46429 | -1.75263 |
| H | 16.01240 | -5.81988 | 0.95189 | H | 8.70636 | -11.70805 | -0.46507 |
| H | 16.72776 | -4.63803 | 2.01041 | H | 10.25378 | -12.42844 | -0.00143 |
| H | 14.59787 | -4.11165 | 3.06428 | H | 9.19205 | -11.74126 | 1.23519 |
| H | 13.71788 | -5.16235 | 1.97302 | H | -10.06734 | -12.66418 | -0.45470 |
| H | 14.96348 | -7.14147 | 2.83735 | H | -8.70689 | -11.99005 | -1.36194 |
| H | 15.87745 | -6.10591 | 3.92078 | H | -8.71994 | -11.90603 | 0.40458 |
| H | 13.98523 | -7.20157 | 5.13745 | H | 8.61235 | 6.24105 | 0.22864 |
| H | 13.73874 | -5.45056 | 5.09509 | H | 10.51792 | 4.42445 | 0.22480 |
| H | 12.82708 | -6.49765 | 4.00087 | H | -10.61722 | 4.19071 | 0.20763 |
| H | 16.71490 | -2.26927 | -0.67532 | H | -8.74739 | 6.04414 | 0.20466 |
| H | 17.46357 | -2.78375 | 0.82365 | | | | |

**Listing 8** Cartesian coordinates of the optimized model compound **M7**.