Table of contents

General and methods:

Air-sensitive syntheses have been performed under argon using Schlenk techniques. Anhydrous solvents were dried using standard methods, when necessary. Chemicals and solvents have been used as received unless otherwise stated. Thin layer chromatography (TLC) has been performed on silica gel 60 F_{254} while column chromatography has been carried out on silica gel 60 (0.063-0.2 mm).

UV/vis spectroscopy: UV/vis spectra have been recorded on a Varian Cary 5000 spectrometer. Cyclization and cycloreversion of the investigated photochromes have been induced by light irradiation with a lamp (Oriel Hg(Xe) 200 W) equipped with narrow-band interference filters of appropriate wavelengths (Semrock: 320 ± 20 nm, 340 ± 13 nm; Andover Corporation 600 ± 40 nm).

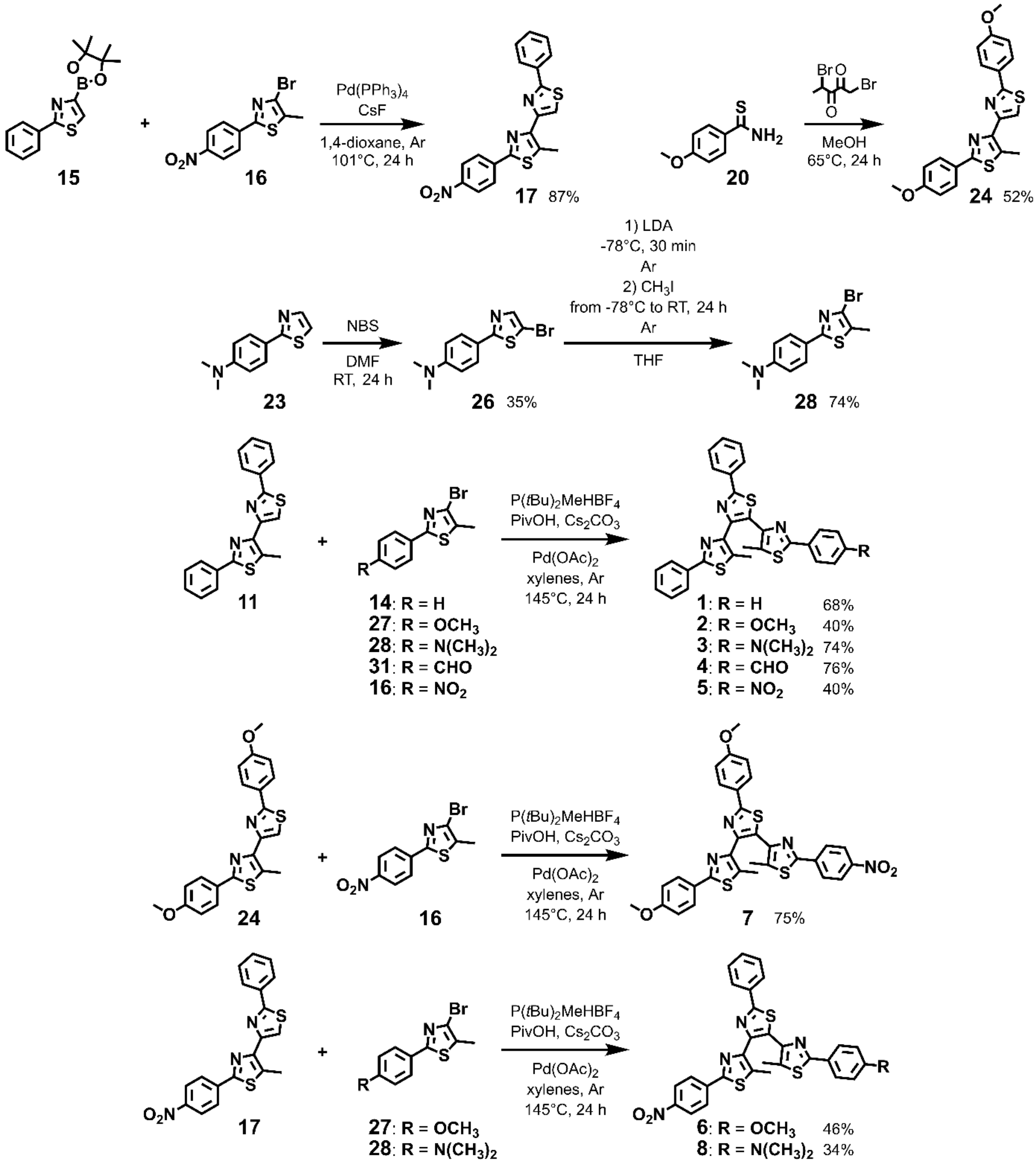
Photochromism quantum yield determination: The photochromic reactions have been induced by continuous irradiation through a Hg/Xe lamp (Hamamatsu, LC6 Lightingcure, 200 W) equipped with narrow-band interference filters of appropriate wavelengths (Semrock) and attenuation filters (Melles Griot, DO 1 or 2). The irradiation power has been measured by a photodiode from Ophir (PD300-UV). The photochromic quantum yields have been determined by probing the sample with a Xenon lamp during the photochromic reaction. Absorption changes have been monitored by a CCD camera mounted with a spectrometer (Princeton Instruments). Kinetic profiles have been analysed by an Igor-implemented in-house procedure.

Computational details: The molecular calculations of the studied photochromes have been carried out with Gaussian 09 program package[1] in the frame of density functional theory (DFT). Since weak interactions like van der Waals and dispersive ones may be important especially for the parallel conformations on the open forms, ωB97XD functional,[2] which includes dispersive corrections, in conjunction with 6-311G(d,p) basis set has been used to fully optimize the ground state geometries. Tight SCF convergence criteria (10^{-8} a.u.) and integration grid of 10^{-8} have been used for all calculations. Frequency calculations have been performed on the optimized geometries to verify the nature of the computed geometries and the lack of imaginary values in the wavenumber calculations confirmed the successful optimization as a minimum geometry.
For the excited state calculations, we have employed time-dependent density functional theory (TD-DFT). We have selected the CAM-B3LYP functional,[3] which includes long-range corrections to improve some deficiencies of B3LYP and showed good performance for the lowest maximum absorption of the photoswitches for both colorless and colored forms of the set of investigated compounds. TD-DFT calculations have been performed along with the 6-311G(d,p) basis set. The conductor-like polarizable continuum model (C-PCM) has been employed for the simulation of UV–vis spectra. Solvent effect (acetonitrile) has been undertaken using the Polarizable Continuum Model (PCM) based on the integral equation formalism variant (IEFPCM). Ground-state optimized structures have been used to compute absorption wavelength maxima (λ_{max}), excitation energy (E_g) and oscillator strength (f) for 10 states.

The potential energy surface (PES) for ring-closure has been determined by changing the bond length distance between the reactive carbon atoms starting from the distance in the open forms (in antiparallel conformation) to 2.1 Å using a step of 0.1 Å. A smaller distance between the reactive carbons leads to a region close to a conical intersection where standard TD-DFT cannot be used due to the multideterminental character of the wavefunction. For each step, the distance between the reactive carbon atoms, i.e. a large part of the reaction coordinate, has been kept frozen while all other geometry parameters have been relaxed. The structure corresponding to the maximum on this curve served as starting point for further optimization of the transition state for ring-closure which has been confirmed as transition state with one imaginary frequency corresponding to the carbon-carbon bond formation. Due to the high computational cost of the excited state optimization, the first excited state potential energy surface (PES) has been obtained by vertical excitation energies using a TD-DFT approach and each of the ground state optimized structures. This very simple approach allows to obtain an approximate picture of the excited state energy landscape, even if geometry optimization at this excited state is required to get a more accurate description.

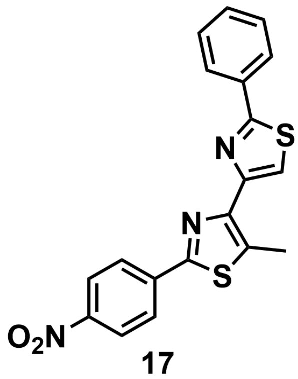
Synthetic procedures:

The eight switches **1** – **8** have been prepared according to the synthetic routes shown in Scheme S1. All new compounds have been fully characterized by standard techniques: ^{1}H-NMR, ^{13}C-NMR and HRMS.



Scheme S1: Synthetic routes for the preparation of terthiazoles **1** – **8**.

*5-methyl-2-(4-nitrophenyl)-2'-phenyl-4,4'-bithiazole, **17***

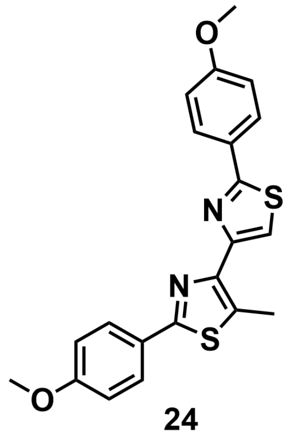


17

2-(4-nitrophenyl)-4-bromo-5-methylthiazole, **16**[4] (299 mg, 1 mmol), 2-phenyl-4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)thiazole, **15**[5] (373 mg, 1.3 mmol), CsF (380 mg, 2.50 mmol) and $Pd(PPh_3)_4$ (46 mg, 0.04 mmol) were partially solubilized in dry 1,4-dioxane (20 mL) and the obtained yellow mixture was stirred at reflux under argon for 24 h. The reaction was then quenched with water (20 mL) and extracted with chloroform. The combined extracts were washed with water (20 mL), dried over anhydrous Na_2SO_4 and filtered. Evaporation of the solvents under reduced pressure left a dark yellow solid, which afforded the pure title compound, **17** (327 mg, 0.87 mmol, 87%) as a dark yellow crystalline solid after a simple recrystallization (dichloromethane and methanol).

^{1}H-NMR ($CDCl_3$, 300 MHz): δ (ppm) 8.31 (d, *J* = 8.9 Hz, 2H), 8.14 (d, *J* = 8.9 Hz, 2H), 8.04 (m, 2H), 7.95 (s, 1H), 7.48 (m, 3H), 3.03 (s, 3H).
^{13}C-NMR ($CDCl_3$, 91 MHz): δ (ppm) 167.90, 160.76, 152.15, 148.29, 146.98, 139.29, 133.79, 133.75, 130.28, 129.12, 126.93, 126.61, 124.43, 117.14, 13.49.
HRMS (ESI): calcd. for $C_{19}H_{14}N_3O_2S_2^+$ $[M+H]^+$ 380.0522, found $[M+H]^+$ 380.0510; calcd. for $C_{19}H_{13}N_3NaO_2S_2^+$ $[M+Na]^+$ 402.0341, found $[M+Na]^+$ 402.0327.

2,2'-bis(4-methoxyphenyl)-5-methyl-4,4'-bithiazole, ***24***

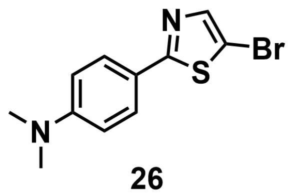


24

4-methoxybenzothioamide, **20**[6] (2.90 g, 17 mmol) was partially dissolved in CH_3OH (60 mL) and crude 1,4-dibromopentane-2,3-dione[7] (2.20 g, 8.5 mmol) was added. The mixture was stirred at room temperature for 20 min and then refluxed 24 h. After cooling down to room temperature, the title compound, **24** (1.73 g, 4.4 mmol, 52%) precipitated as beige crystalline solid that was used without further purification.

^{1}H-NMR ($CDCl_3$, 300 MHz): δ (ppm) 7.96 (m, 5H), 6.97 (m, 4H), 3.88 (s, 3H), 3.87 (s, 3H), 2.95 (s, 3H).
^{13}C-NMR ($CDCl_3$,101 MHz): δ (ppm) 167.41, 163.89, 161.20, 161.07, 152.42, 145.49, 130.17, 128.09, 127.95, 127.01, 126.78, 115.70, 114.37, 114.31, 55.55, 13.20.
HRMS (ESI): calcd. for $C_{21}H_{19}N_2O_2S_2^+$ [M+H]$^+$ 395.0882, found [M+H]$^+$ 395.0877; calcd. for $C_{21}H_{18}N_2NaO_2S_2^+$ [M+Na]$^+$ 417.0702, found [M+Na]$^+$ 417.0692.

4-(5-bromothiazol-2-yl)-N,N-dimethylaniline, ***26***

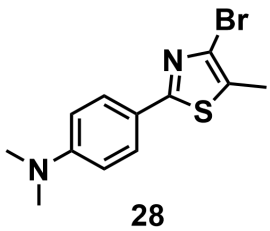


26

N-bromosuccinimide (410 mg, 2.3 mmol) was added to a solution of N,N-dimethyl-4-(thiazol-2-yl)aniline, **23**[8] (430 mg, 2.1 mmol) in DMF (10 mL) and the obtained solution was stirred at room temperature for 24 hours. Sodium thiosulfate pentahydrate (124 mg, 0.5 mmol) in distilled water (25 mL) was added to the solution to induce a solid precipitation that was filtered and washed with water (20 mL). The crude product was dissolved in diethyl ether to remove insoluble impurities by filtration. After removal of the solvent, the residue was purified by silica gel column chromatography (eluent: dichloromethane / petroleum ether 1:1) and 4-(5-bromothiazol-2-yl)-N,N-dimethylaniline, **26** (208 mg, 0.74 mmol, 35%) was isolated as light yellow crystalline solid.

[1]H-NMR ($CDCl_3$, 300 MHz): δ (ppm) 7.72 (d, *J* = 8.8 Hz, 2H), 7.61 (s, 1H), 6.70 (d, *J* = 8.9 Hz, 2H), 3.03 (s, 6H).
[13]C-NMR ($CDCl_3$, 63 MHz): δ (ppm) 170.58, 151.77, 144.28, 127.48, 121.31, 111.82, 105.69, 40.18.
HRMS (ESI): calcd. for $C_{11}H_{12}BrN_2S^+$ $[M+H]^+$ 282.9899, found $[M+H]^+$ 282.9896.

*4-(4-bromo-5-methylthiazol-2-yl)-N,N-dimethylaniline, **28***

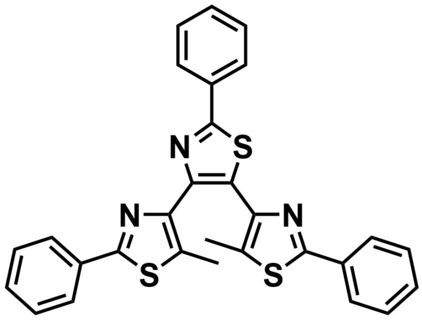


28

4-(5-bromothiazol-2-yl)-N,N-dimethylaniline, **26** (205 mg, 0.72 mmol) was dissolved in distilled dry THF (10 mL) under argon and the obtained solution was cooled at -78°C with a dry ice/acetone bath. Lithium diisopropylamine (2M solution, 550 µL, 1.1 mmol) was added dropwise and the system was stirred at -78°C for 30 min. Iodomethane (160 mg, 70 µL, 1.1 mmol) was finally added and the resulting solution was stirred for 24 h letting the temperature rise to room temperature under argon. The system was quenched with NH_4Cl 1M solution (15 mL) and the organic layer has been extracted with diethyl ether. The combined extracts have been washed with water (30 mL), dried over anhydrous Na_2SO_4 and filtered. The solvent was evaporated under vacuum and the crude product was purified by silica gel column chromatography (eluent: dichloromethane / petroleum ether 1:1) to afford the pure title compound, **28** (159 mg, 0.53 mmol, 74%) as a pale yellow crystalline solid.

[1]H-NMR ($CDCl_3$, 360 MHz): δ (ppm) 7.74 (d, *J* = 9.0 Hz, 2H), 6.70 (d, *J* = 8.6 Hz, 2H), 3.02 (s, 6H), 2.39 (s, 3H).
[13]C-NMR ($CDCl_3$ + drops of CD_3OD, 63 MHz): δ (ppm) 166.79, 151.75, 127.23, 125.98, 124.15, 120.90, 111.76, 40.14, 12.88.
HRMS (ESI): calcd. for $C_{12}H_{14}BrN_2S^+$ $[M+H]^+$ 297.0055, found $[M+H]^+$ 297.0054.

*Terthiazole **1***[9]

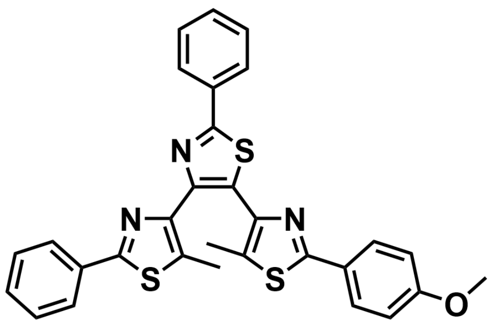


1

Title compound **1**[9] was prepared by following a different procedure:
5-methyl-2,2'-diphenyl-4,4'-bithiazole, **11**[7] (334 mg, 1 mmol), 2-phenyl-4-bromo-5-methylthiazole, **14**[10] (240 mg, 1 mmol), $P(tBu)_2MeHBF_4$ (32.3 mg, 0.13 mmol), Cs_2CO_3 (424 mg, 1.30 mmol), pivalic acid (31 mg, 0.30 mmol) and $Pd(OAc)_2$ (23 mg, 0.10 mmol) were partially solubilized in dry xylenes (5 mL) and the obtained mixture was stirred at reflux for 24 h. The reaction was diluted with chloroform and filtered through a Celite pad. The obtained solution was washed with water (20 mL), dried over anhydrous Na_2SO_4 and filtered. The filtrate was concentrated under vacuum and silica gel column chromatography (eluent: dichloromethane) of the residue afforded pure terthiazole **1** (344 mg, 0.68 mmol, 68%) as a whitish-light blue crystalline solid. Characterization data consistent with the literature.[9]

^{1}H-NMR ($CDCl_3$, 300 MHz): δ (ppm) 8.07 (m, 2H), 7.94 (m, 2H), 7.80 (m, 2H), 7.45 (m, 6H), 7.35 (m, 3H), 2.53 (s, 3H), 2.12 (s, 3H).
HRMS (ESI): calcd. for $C_{29}H_{22}N_3S_3^+$ $[M+H]^+$ 508.0970, found $[M+H]^+$ 508.0974.

*Terthiazole **2***[7]



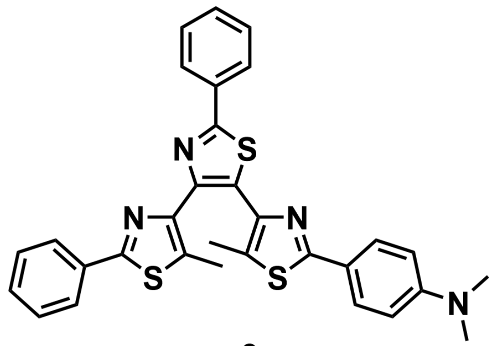
2

Title compound **2**[7] was prepared by following a different procedure:
5-methyl-2,2'-diphenyl-4,4'-bithiazole, **11**[7] (167 mg, 0.50 mmol), 2-(4-methoxyphenyl)-4-bromo-5-methylthiazole, **27**[7] (142 mg, 0.50 mmol), $P(tBu)_2MeHBF_4$ (16 mg, 0.06 mmol), Cs_2CO_3 (212 mg, 0.65 mmol), pivalic acid (15 mg, 0.15 mmol) and $Pd(OAc)_2$ (11 mg, 0.05 mmol) were partially solubilized in dry xylenes (5 mL) and the obtained mixture has been stirred at reflux for 24 h. The reaction has been diluted with chloroform (20 mL) and filtered through a Celite

pad. The obtained solution has been washed with water (15 mL), dried over anhydrous Na_2SO_4 and filtered. The filtrate was concentrated under vacuum and silica gel column chromatography (eluent: initially dichloromethane, then dichloromethane / ethyl acetate 95:5) of the residue afforded pure terthiazole **2** (108 mg, 0.20 mmol, 40%) as an off-white solid. Characterization data consistent with the literature.[7]

^{1}H-NMR ($CDCl_3$, 300 MHz): δ (ppm) 8.04 (m, 2H), 7.88 (d, *J* = 8.9 Hz, 2H), 7.81 (m, 2H), 7.46 (m, 3H), 7.35 (m, 3H), 6.95 (d, *J* = 8.9 Hz, 2H), 3.86 (s, 3H), 2.51 (s, 3H), 2.08 (s, 3H).
^{13}C-NMR ($CDCl_3$, 100 MHz): δ (ppm) 167.19, 164.27, 164.02, 161.19, 147.72, 146.59, 143.44, 133.86, 133.77, 133.09, 131.45, 130.28, 129.79, 129.72, 129.04, 128.86, 128.00, 126.77, 126.64, 126.47, 114.36, 55.58, 12.81, 12.41.
HRMS (ESI): calcd. for $C_{30}H_{24}N_3OS_3^+$ $[M+H]^+$ 538.1076, found $[M+H]^+$ 538.1087.

*Terthiazole **3***

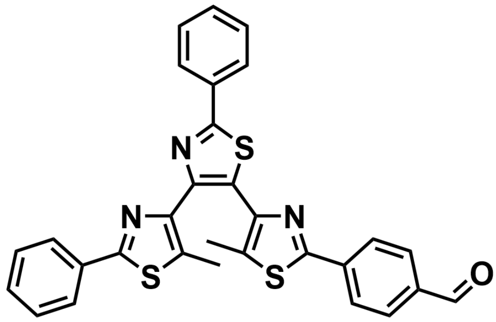


3

The same procedure used for **1** and **2** was followed by replacing **14** and **27**, respectively, with 4-(4-bromo-5-methylthiazol-2-yl)-N,N-dimethylaniline, **28** (149 mg, 0.50 mmol) to afford pure terthiazole **3** (205 mg, 0.37 mmol, 74%) as a greenish solid after purification by silica gel column chromatography (eluent: dichloromethane / acetonitrile 99:1) and precipitation in cyclohexane.

^{1}H-NMR ($CDCl_3$, 300 MHz): δ (ppm) 8.07 (m, 2H), 7.84 (m, 2H), 7.81 (d, *J* = 9.0 Hz, 2H), 7.46 (m, 3H), 7.36 (m, 3H), 6.71 (d, *J* = 9.0 Hz, 2H), 3.03 (s, 6H), 2.45 (s, 3H), 2.04 (s, 3H).
^{13}C-NMR ($CDCl_3$, 75 MHz): δ (ppm) 167.06, 165.28, 164.01, 151.62, 147.50, 146.72, 142.95, 133.90, 133.83, 132.97, 130.28, 130.16, 130.09, 129.65, 128.98, 128.82, 127.69, 126.75, 126.49, 121.94, 111.95, 40.37, 12.70, 12.31.
HRMS (ESI): calcd. for $C_{31}H_{27}N_4S_3^+$ $[M+H]^+$ 551.1392, found $[M+H]^+$ 551.1373; calcd. for $C_{31}H_{26}N_4NaS_3^+$ $[M+Na]^+$ 573.1212, found $[M+Na]^+$ 573.1185.

*Terthiazole **4***

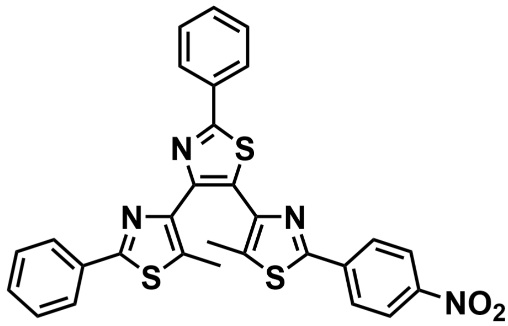


4

The same procedure was followed on 2-(4-formylphenyl)-4-bromo-5-methylthiazole, **31**[11] (141 mg, 0.50 mmol) to afford pure terthiazole **4** (203 mg, 0.38 mmol, 76%) as a light green crystalline solid after purification by silica gel column chromatography (eluent: dichloromethane / acetonitrile 99:1).

^{1}H-NMR ($CDCl_3$, 300 MHz): δ (ppm) 10.05 (s, 1H), 8.11 (d, *J* = 8.3 Hz, 2H), 8.07 (m, 2H), 7.94 (d, *J* = 8.4 Hz, 2H), 7.75 (m, 2H), 7.48 (m, 3H), 7.33 (m, 3H), 2.60 (s, 3H), 2.17 (s, 3H).
^{13}C-NMR ($CDCl_3$,75 MHz): δ (ppm) 191.55, 167.23, 163.75, 162.19, 148.17, 146.21, 144.92, 138.67, 136.93, 134.38, 133.70, 133.59, 133.30, 130.37, 129.71, 129.05, 128.81, 128.61, 126.80, 126.67, 126.27, 12.93, 12.56.
HRMS (ESI): calcd. for $C_{30}H_{22}N_3OS_3^+$ $[M+H]^+$ 536.0919, found $[M+H]^+$ 536.0892.

*Terthiazole **5***



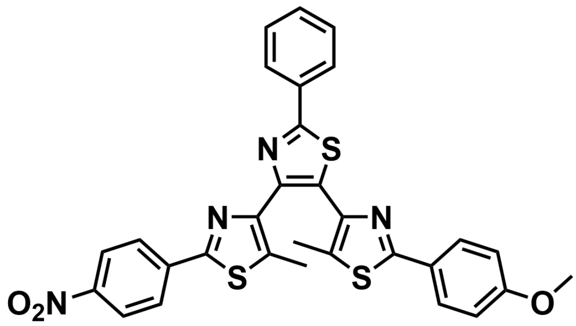
5

The same procedure was followed on 2-(4-nitrophenyl)-4-bromo-5-methylthiazole, **16**[4] (299 mg, 1 mmol) to afford pure terthiazole **5** (200 mg, 0.40 mmol, 40%) as a yellow-brownish solid after purification by silica gel column chromatography (eluent: initially dichloromethane, then dichloromethane / acetonitrile 99:1) and precipitation in diethyl ether.

^{1}H-NMR ($CDCl_3$, 300 MHz): δ (ppm) 8.29 (d, *J* = 8.9 Hz, 2H), 8.09 (d, *J* = 8.9 Hz, 2H), 8.06 (m, 2H), 7.73 (m, 2H), 7.49 (dd, *J* = 5.1, 1.9 Hz, 3H), 7.33 (dd, *J* = 5.3, 2.0 Hz, 3H), 2.65 (s, 3H), 2.20 (s, 3H).

^{13}C-NMR ($CDCl_3$, 75 MHz): δ (ppm) 167.19, 163.65, 160.83, 148.18, 146.01, 145.23, 138.96, 135.11, 133.53, 133.44, 133.36, 130.39, 129.73, 129.02, 128.78, 128.19, 126.81, 126.59, 126.16, 124.29, 12.95, 12.56.
HRMS (ESI): calcd. for $C_{29}H_{21}N_4O_2S_3^+$ [M+H]$^+$ 553.0821, found [M+H]$^+$ 553.0798.

*Terthiazole **6***

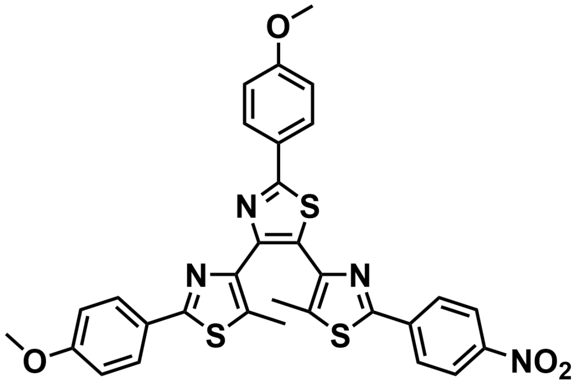


6

5-methyl-2-(4-nitrophenyl)-2'-phenyl-4,4'-bithiazole, **17** (304 mg, 0.80 mmol), 2-(4-methoxyphenyl)-4-bromo-5-methylthiazole, **27**[7] (227 mg, 0.80 mmol), $P(tBu)_2MeHBF_4$ (25 mg, 0.10 mmol), Cs_2CO_3 (326 mg, 1 mmol), pivalic acid (25 mg, 0.24 mmol) and $Pd(OAc)_2$ (18 mg, 0.08 mmol) were partially solubilized in dry xylenes (5 mL) and the obtained mixture was stirred at reflux for 24 h. The reaction was diluted with chloroform (25 mL) and filtered through a Celite pad. The obtained solution was washed with water (20 mL), dried over anhydrous Na_2SO_4 and filtered. The solvent was evaporated under vacuum and silica gel column chromatography (eluent: initially dichloromethane / acetonitrile 99:1, then 97:3) of the residue afforded pure terthiazole **6** (216 mg, 0.37 mmol, 46%) as a light orange crystalline solid.

^{1}H-NMR ($CDCl_3$, 300 MHz): δ (ppm) 8.18 (d, J = 9.0 Hz, 2H), 8.06 (m, 2H) 7.91 (d, J = 9.0 Hz, 2H), 7.86 (d, J = 8.8 Hz, 2H) 7.48 (m, 3H), 6.95 (d, J = 8.9 Hz, 2H), 3.86 (s, 3H), 2.63 (s, 3H), 2.12 (s, 3H).
^{13}C-NMR ($CDCl_3$, 101 MHz): δ (ppm) 167.31, 164.40, 161.39, 160.49, 148.17, 147.62, 147.51, 143.19, 139.29, 135.80, 133.60, 131.49, 130.43, 129.11, 128.01, 126.81, 126.70, 126.28, 124.28, 114.45, 55.56, 13.17, 12.41.
HRMS (ESI): calcd. for $C_{30}H_{23}N_4O_3S_3^+$ [M+H]$^+$ 583.0926, found [M+H]$^+$ 583.0902; calcd. for $C_{30}H_{22}N_4NaO_3S_3^+$ [M+Na]$^+$ 605.0746, found [M+Na]$^+$ 605.0721.

*Terthiazole **7***

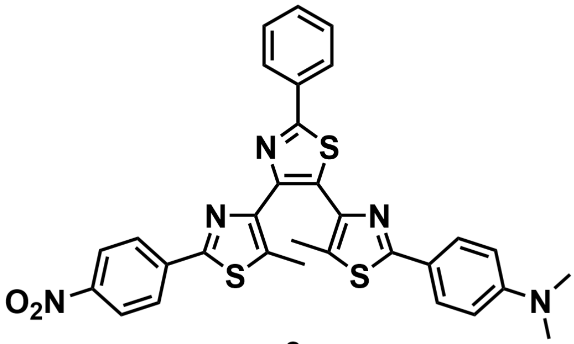


7

2,2'-bis(4-methoxyphenyl)-5-methyl-4,4'-bithiazole, **24** (395 mg, 1 mmol), 2-(4-nitrophenyl)-4-bromo-5-methylthiazole, **16**[4] (299 mg, 1 mmol), $P(tBu)_2MeHBF_4$ (31 mg, 0.12 mmol), Cs_2CO_3 (652 mg, 2 mmol), pivalic acid (40 mg, 0.40 mmol) and $Pd(OAc)_2$ (23 mg, 0.10 mmol) were partially solubilized in dry xylenes (5 mL) and the obtained mixture was stirred at reflux for 24 hours. The reaction was diluted with chloroform (40 mL) and water (30 mL). The organic layer was extracted with chloroform. The obtained solution was washed with water, dried over anhydrous Na_2SO_4 and filtered. The filtrate was concentrated under vacuum and silica gel column chromatography (eluent dichloromethane) of the residue followed by recrystallization from methanol afforded pure terthiazole **7** (460 mg, 0.75 mmol, 75%) as a yellow crystalline solid.

^{1}H-NMR ($CDCl_3$, 360 MHz): δ (ppm) 8.27 (d, *J* = 8.9 Hz, 2H), 8.06 (d, *J* = 8.9 Hz, 2H), 8.01 (d, *J* = 8.9 Hz, 2H), 7.74 (d, *J* = 8.9 Hz, 2H), 6.99 (d, *J* = 8.9 Hz, 2H), 6.86 (d, *J* = 8.9 Hz, 2H), 3.89 (s, 3H), 3.82 (s, 3H), 2.55 (s, 3H), 2.22 (s, 3H).
^{13}C-NMR ($CDCl_3$, 91 MHz): δ (ppm) 167.18, 163.73, 161.44, 160.92, 160.77, 148.17, 147.92, 145.82, 145.40, 139.00, 134.86, 132.20, 128.15, 127.69, 127.28, 126.82, 126.54, 126.39, 124.31, 114.34, 114.12, 55.47, 55.40, 12.80, 12.56.
HRMS (ESI): calcd. for $C_{31}H_{25}N_4O_4S_3^+$ $[M+H]^+$ 613.1032, found $[M+H]^+$ 613.1007; calcd. for $C_{31}H_{24}N_4NaO_4S_3^+$ $[M+Na]^+$ 635.0852, found $[M+Na]^+$ 635.0822.

*Terthiazole **8***

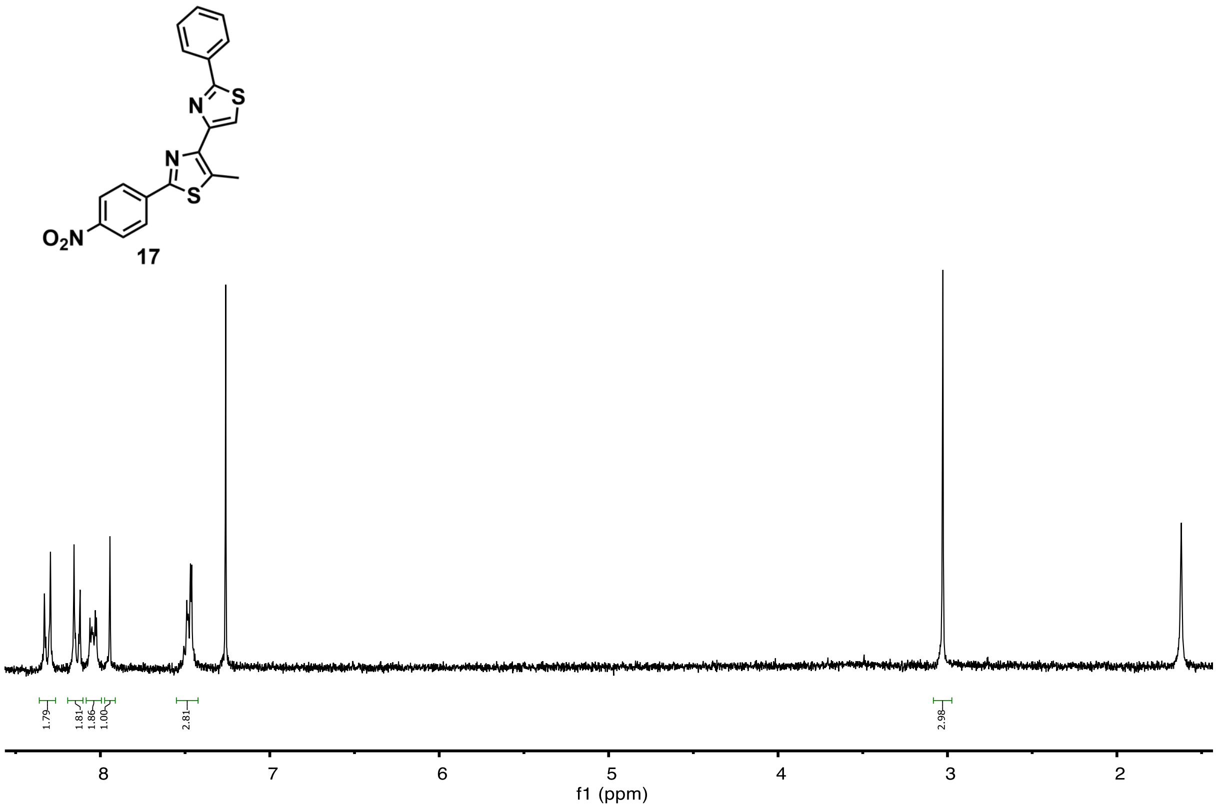


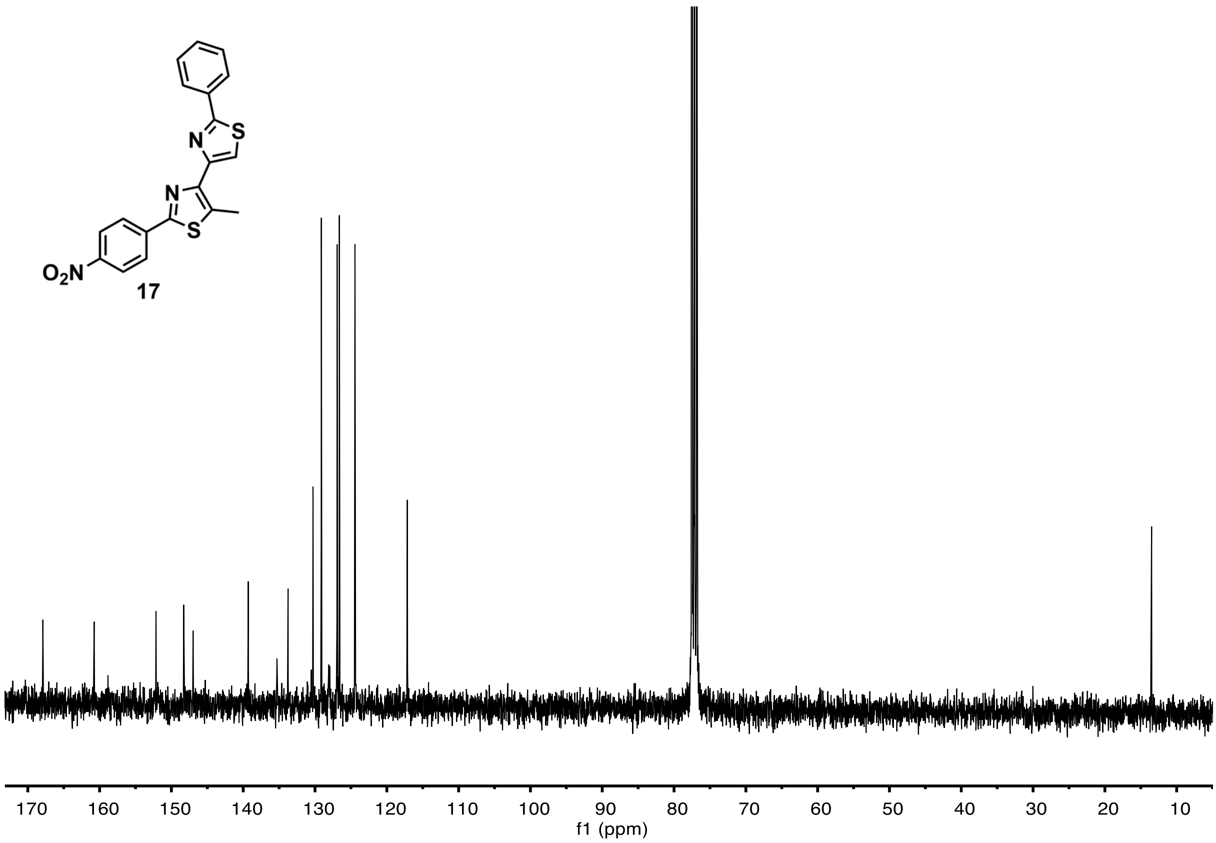
8

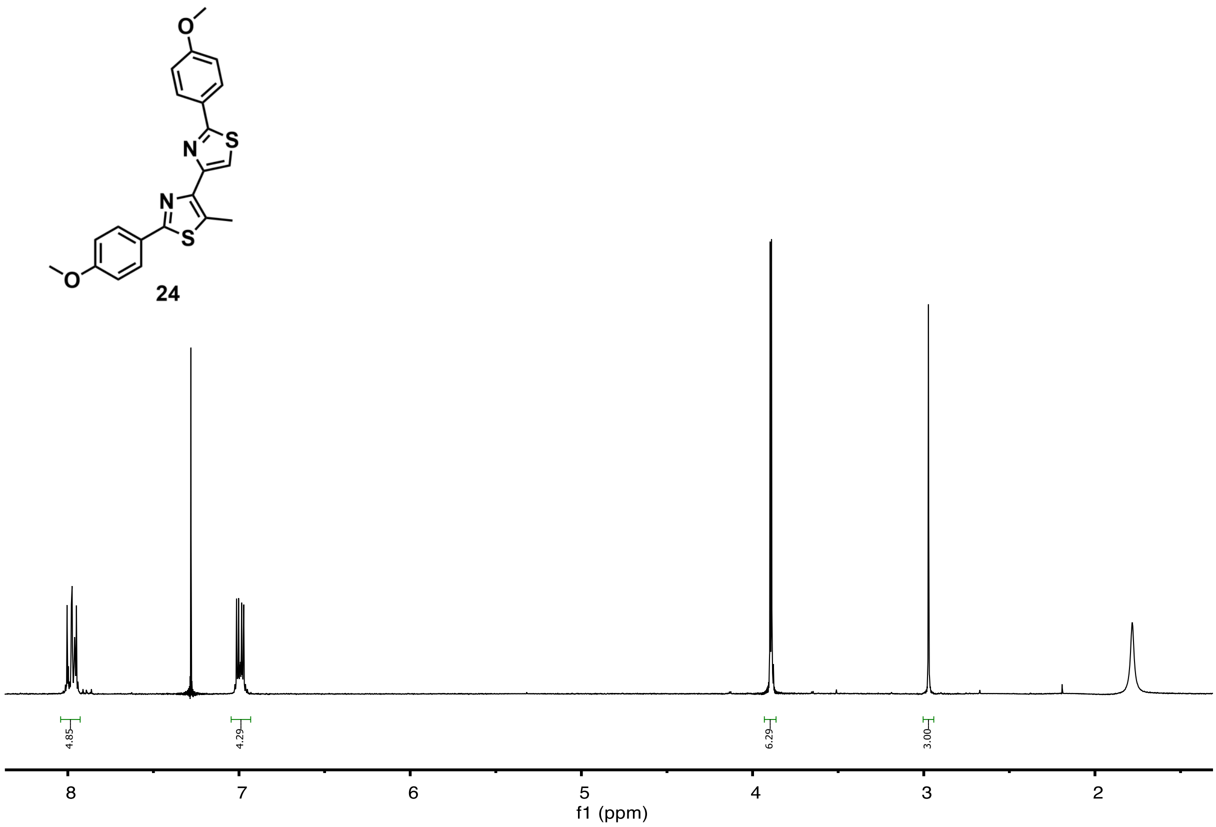
5-methyl-2-(4-nitrophenyl)-2'-phenyl-4,4'-bithiazole, **17** (190 mg, 0.50 mmol), 4-(4-bromo-5-methylthiazol-2-yl)-N,N-dimethylaniline, **28** (149 mg, 0.50 mmol), $P(tBu)_2MeHBF_4$ (16 mg, 0.07 mmol), Cs_2CO_3 (212 mg, 0.65 mmol), pivalic acid (15 mg, 0.15 mmol) and $Pd(OAc)_2$ (11 mg, 0.05 mmol) were partially solubilized in dry xylenes (5 mL) and the obtained mixture has been stirred at reflux for 24 h. The reaction has been diluted with chloroform (20 mL) and filtered through a Celite pad. The obtained solution has been washed with water (20 mL), dried over anhydrous Na_2SO_4 and filtered. The filtrate was concentrated under vacuum and silica gel column chromatography (eluent: initially dichloromethane / acetonitrile 99:1, then 98:2 and finally 96:4) of the residue afforded pure terthiazole **8** (100 mg, 0.17 mmol, 34%) as a light orange crystalline solid.

^{1}H-NMR ($CDCl_3$, 300 MHz): δ (ppm) 8.17 (d, *J* = 8.9 Hz, 2H), 8.06 (m, 2H), 7.92 (d, *J* = 8.9 Hz, 2H), 7.80 (d, *J* = 8.9 Hz, 2H), 7.47 (m, 3H), 6.72 (d, *J* = 8.9 Hz, 2H), 3.03 (s, 6H), 2.63 (s, 3H), 2.10 (s, 3H).
^{13}C-NMR ($CDCl_3$, 75 MHz): δ (ppm) 167.08, 165.26, 160.45, 151.55, 148.03, 147.68, 147.20, 142.78, 139.25, 135.60, 133.59, 130.30, 130.09, 129.03, 127.61, 126.79, 126.63, 124.21, 121.71, 111.95, 40.34, 13.05, 12.32.
HRMS (ESI): calcd. for $C_{31}H_{26}N_5O_2S_3^+$ $[M+H]^+$ 596.1243, found $[M+H]^+$ 596.1227.

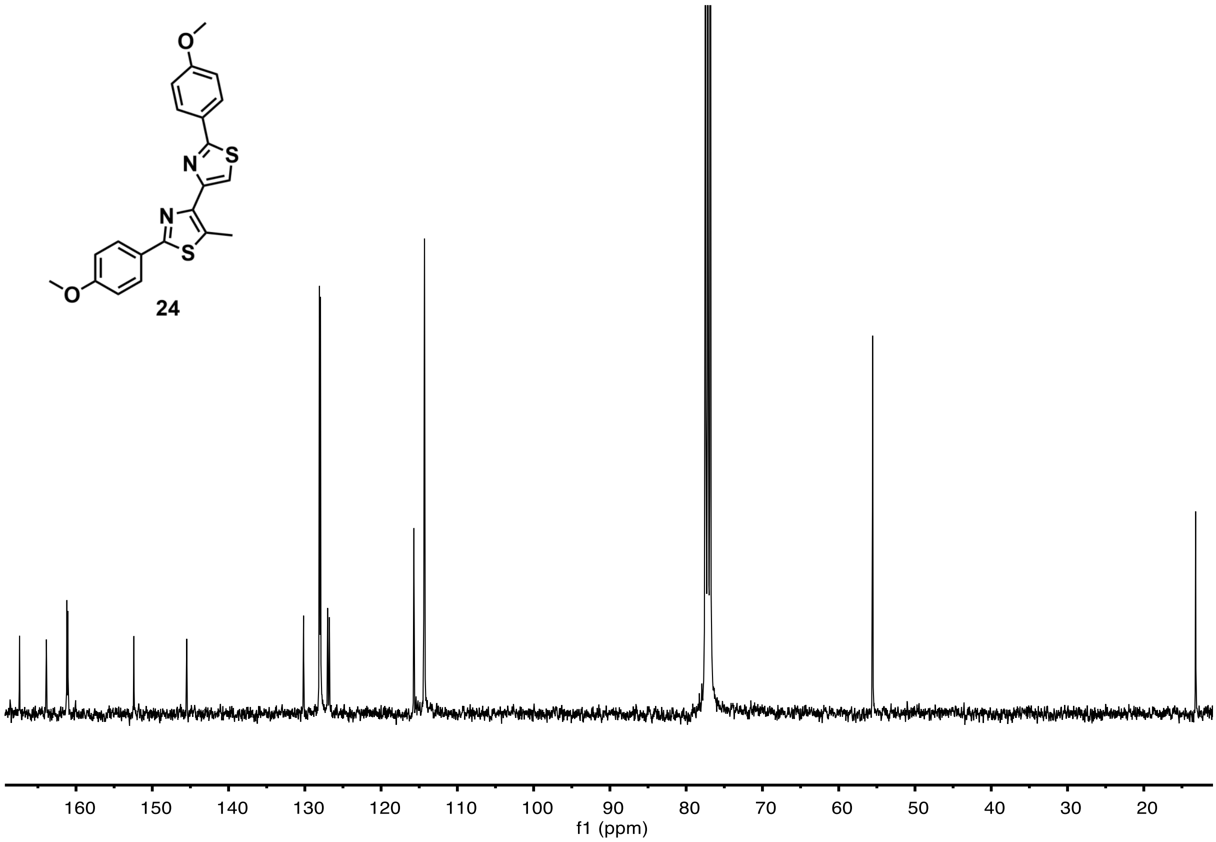
^{1}H- and ^{13}C-NMR spectra:



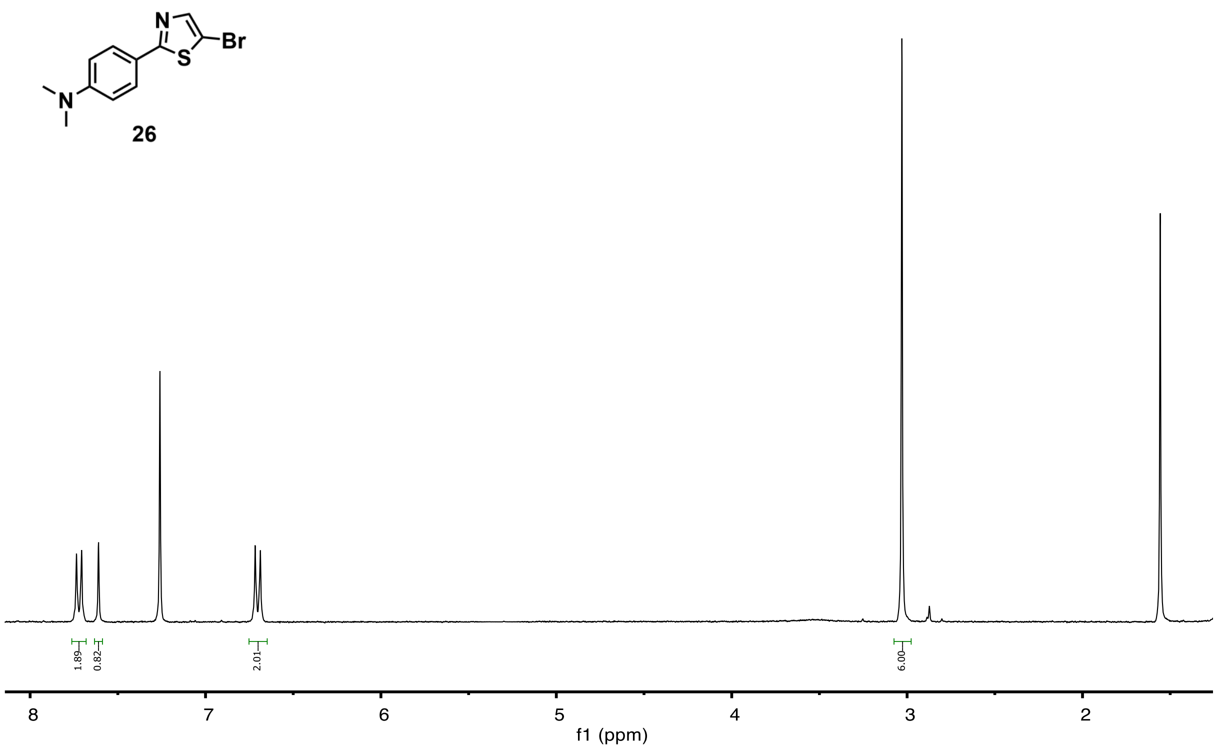


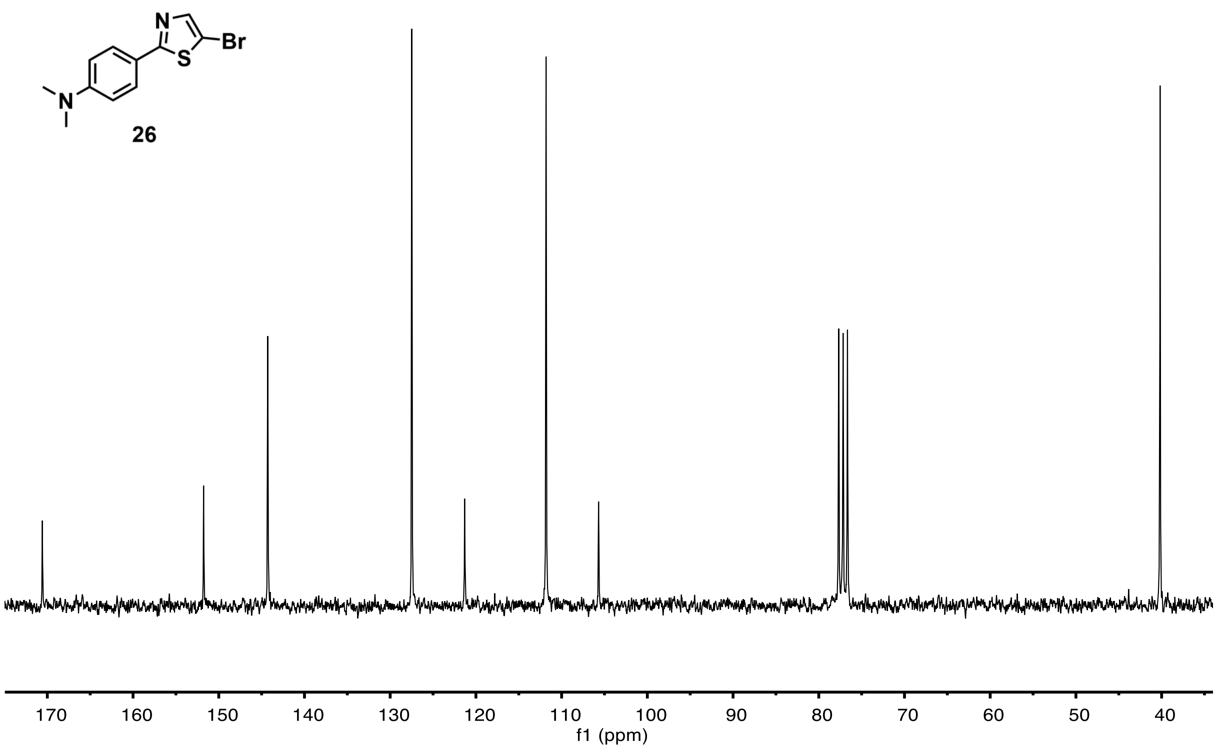


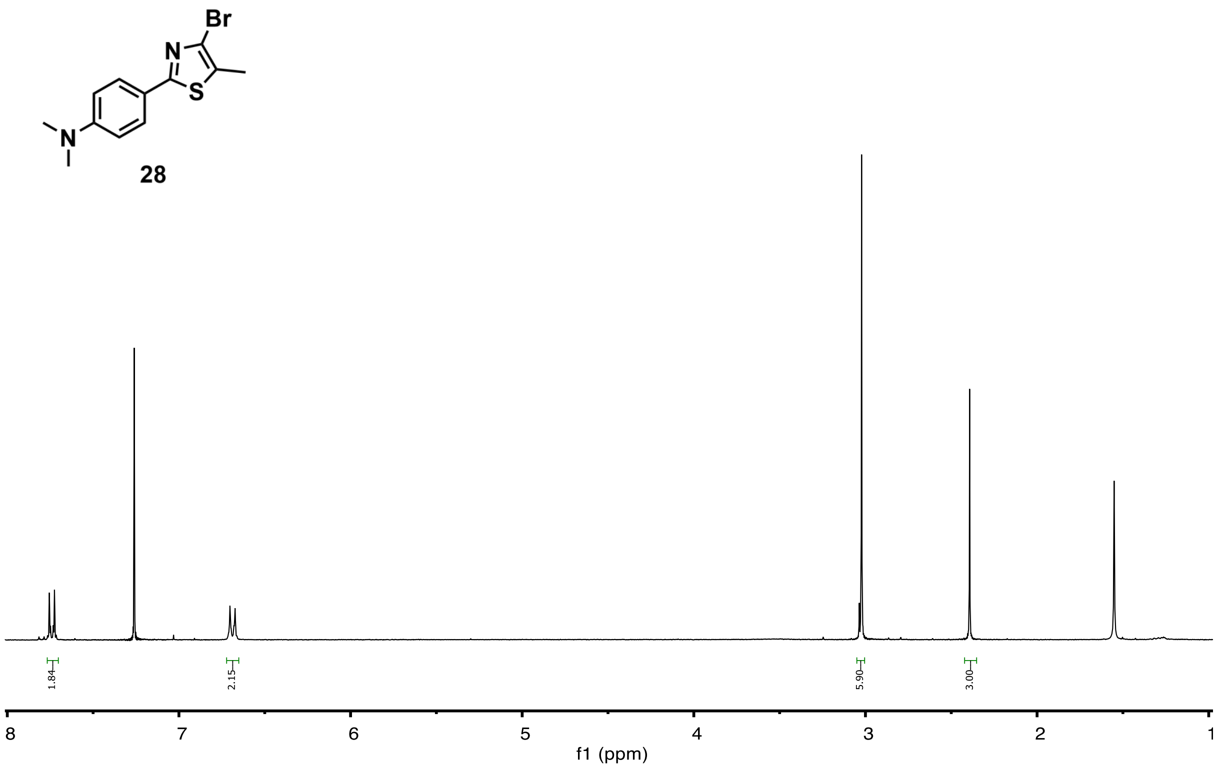
24
4.85
4.29
6.29
3.00
8 7 6 5 4 3 2
f1 (ppm)



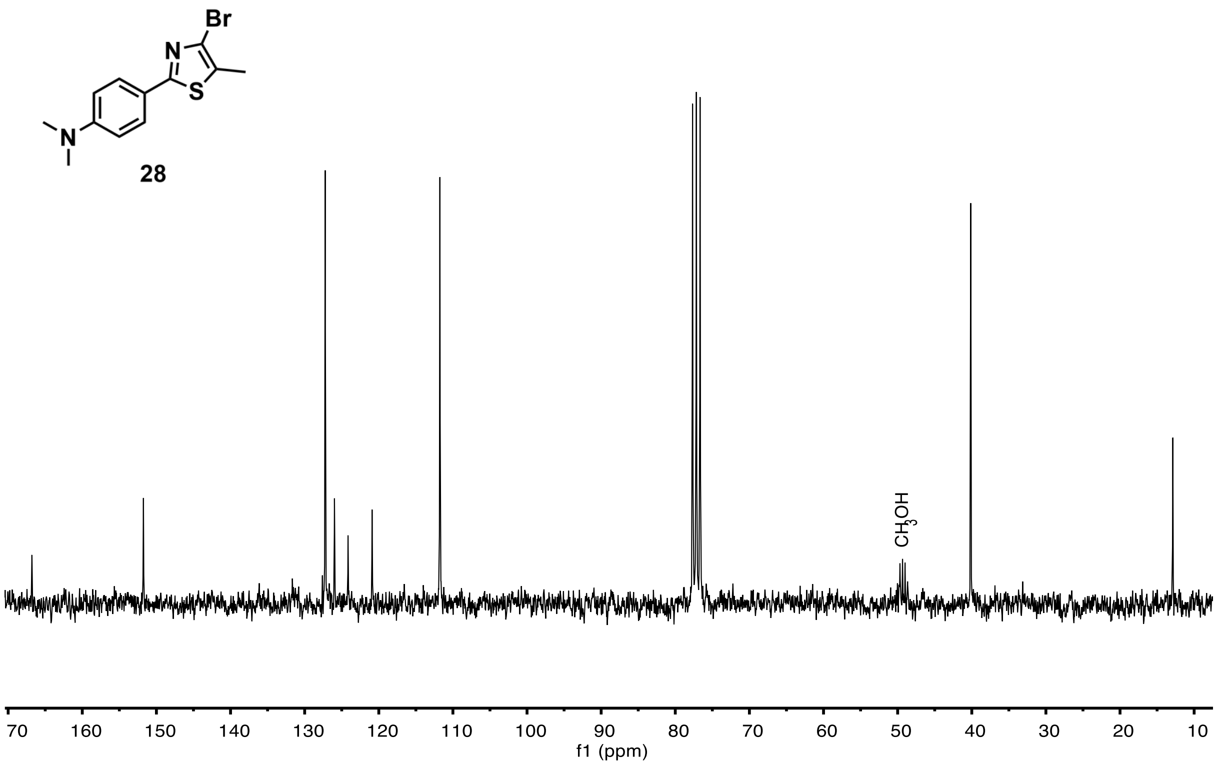
24
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20
f1 (ppm)


N
S
Br
26
1.89
0.82
2.01
6.00
8 7 6 5 4 3 2
f1 (ppm)

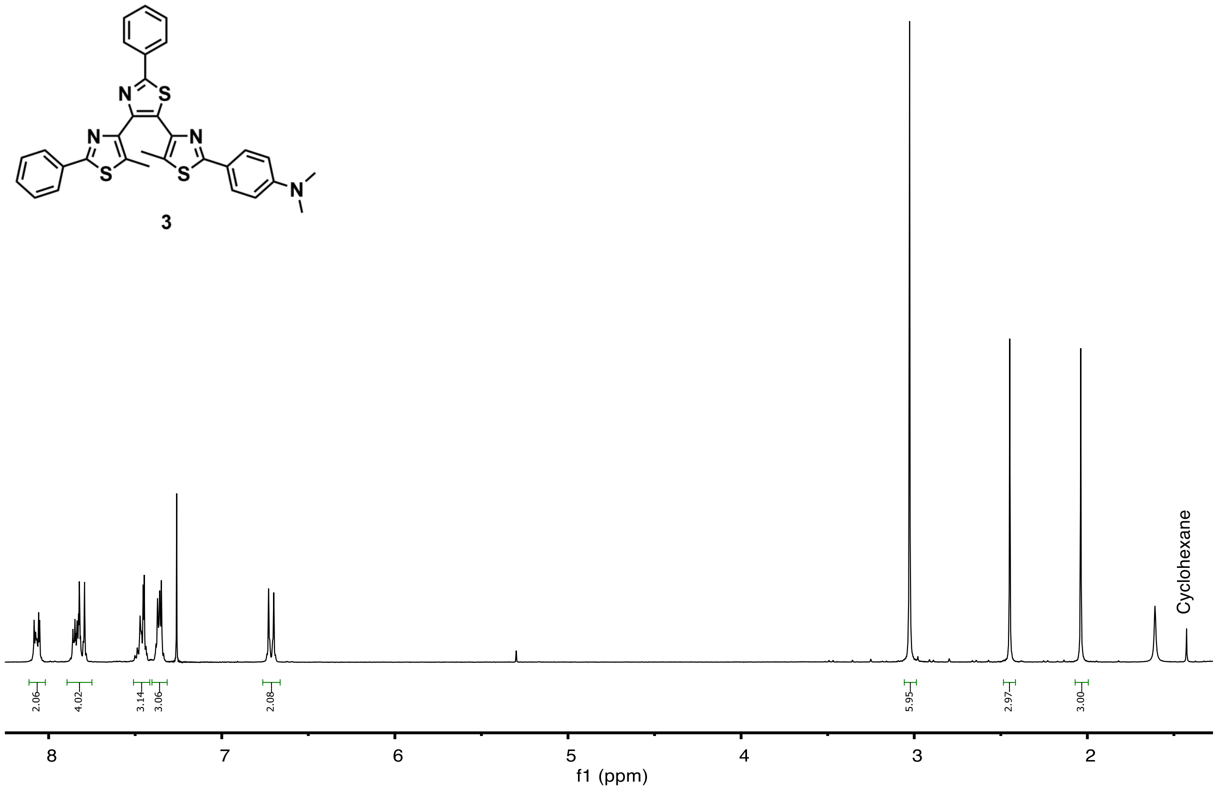

N
S
Br
26
170 160 150 140 130 120 110 100 90 80 70 60 50 40
f1 (ppm)



Br
N
S
28
1.84
2.15
5.90
3.00
8
7
6
5
4
3
2
1
f1 (ppm)



Br
N
S
28
CH3OH
70
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


N
S
3
Cyclohexane
2.06
4.02
3.14
3.06
2.08
5.95
2.97
3.00
8
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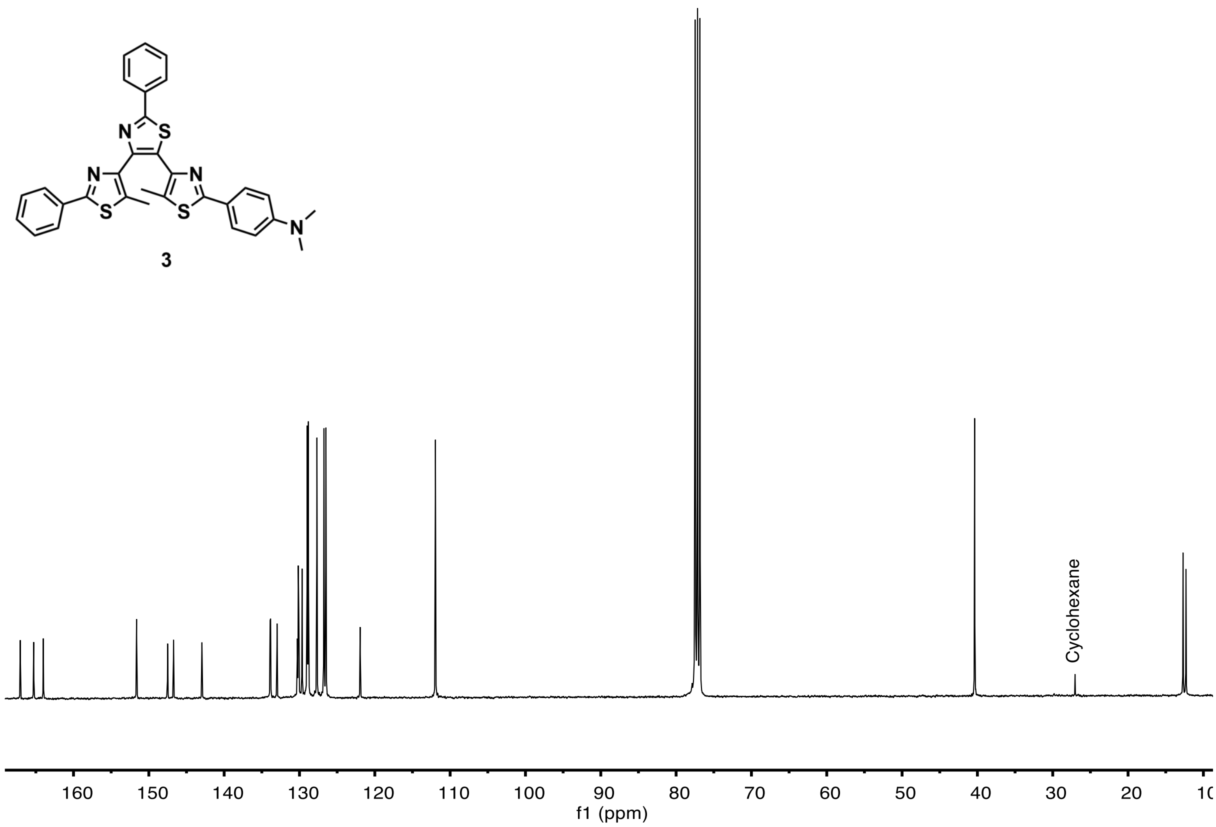
4
3
2
f1 (ppm)


N
S
3
Cyclohexane
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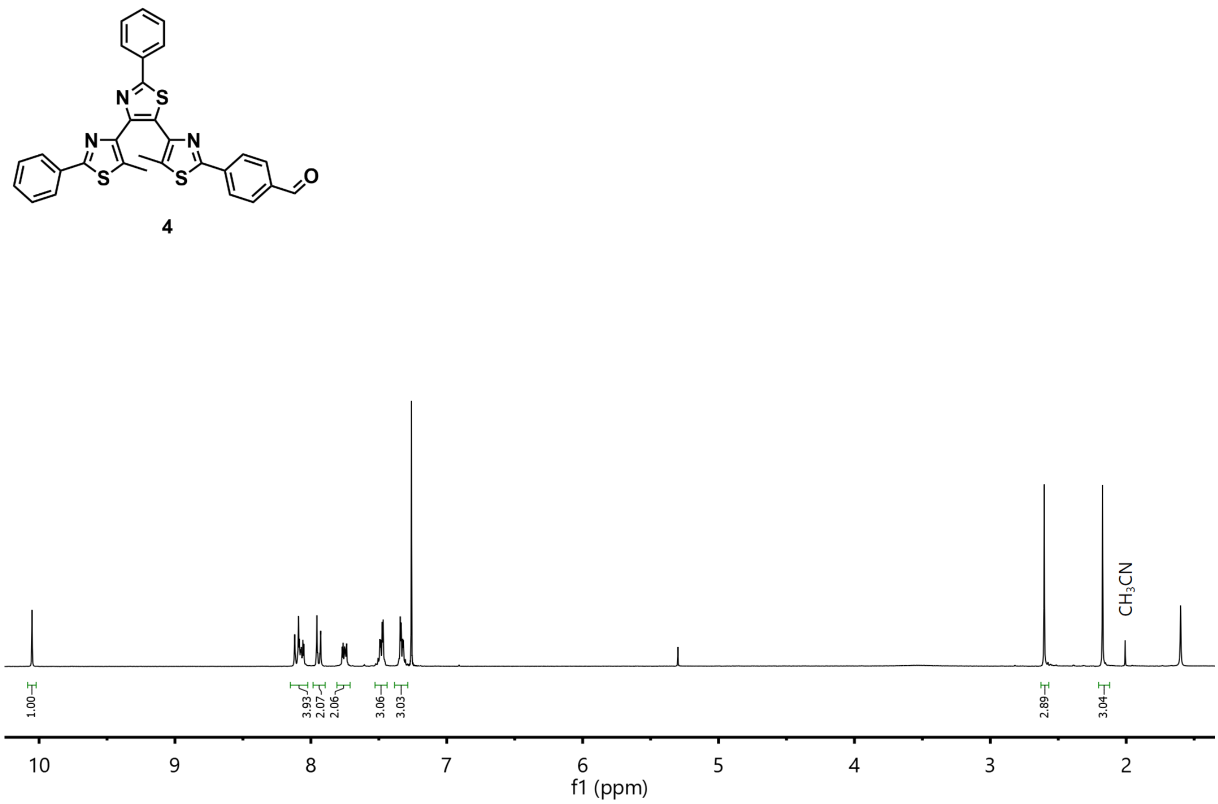
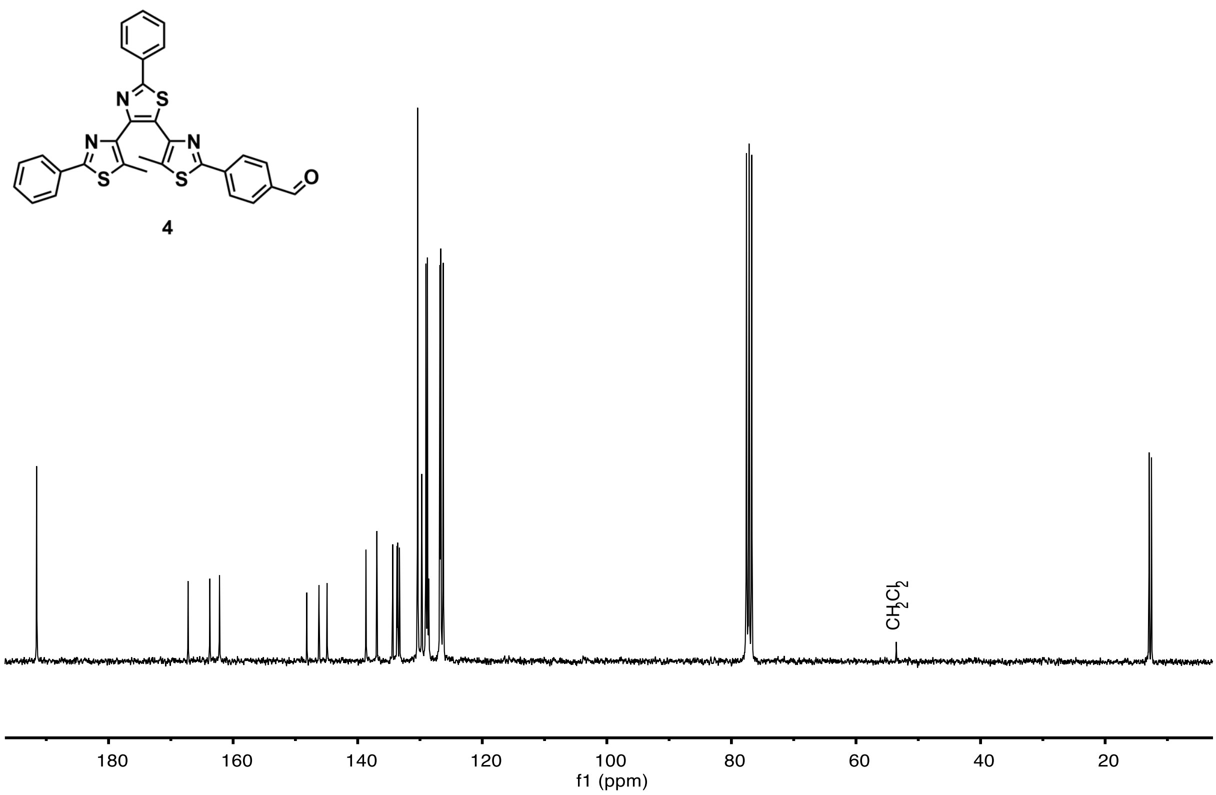
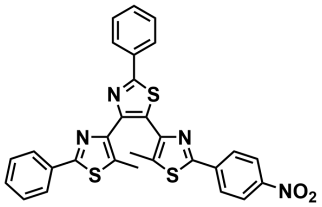
150
140
130
120
110
100
90
80
70
60
50
40
30
20
f1 (ppm)



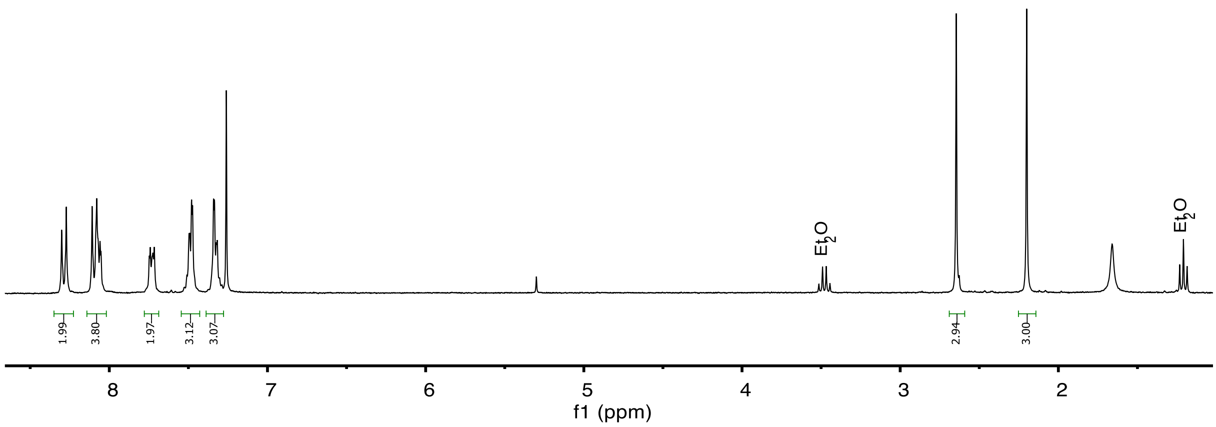
4
CH3CN
1.00
3.93
2.07
2.06
3.06
3.03
2.89
3.04
10
9
8
7
6
5
4
3
2
f1 (ppm)



4
CH2Cl2
180
160
140
120
100
80
60
40
20
f1 (ppm)


N
S
N
S
N
S
NO2

5


Et2O
Et2O
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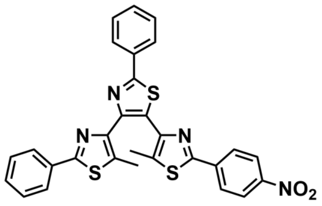
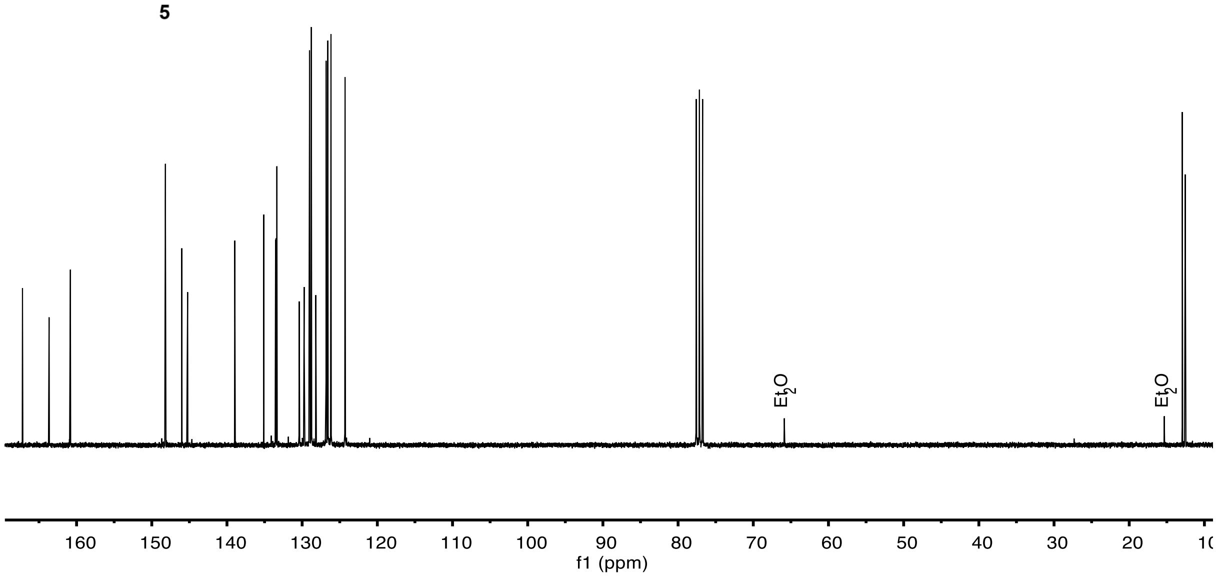
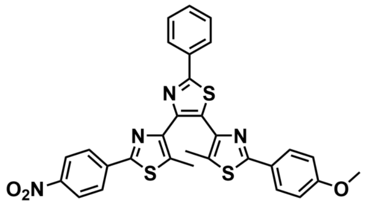
3.80
1.97
3.12
3.07
2.94
3.00
8
7
6
5
4
3
2
f1 (ppm)

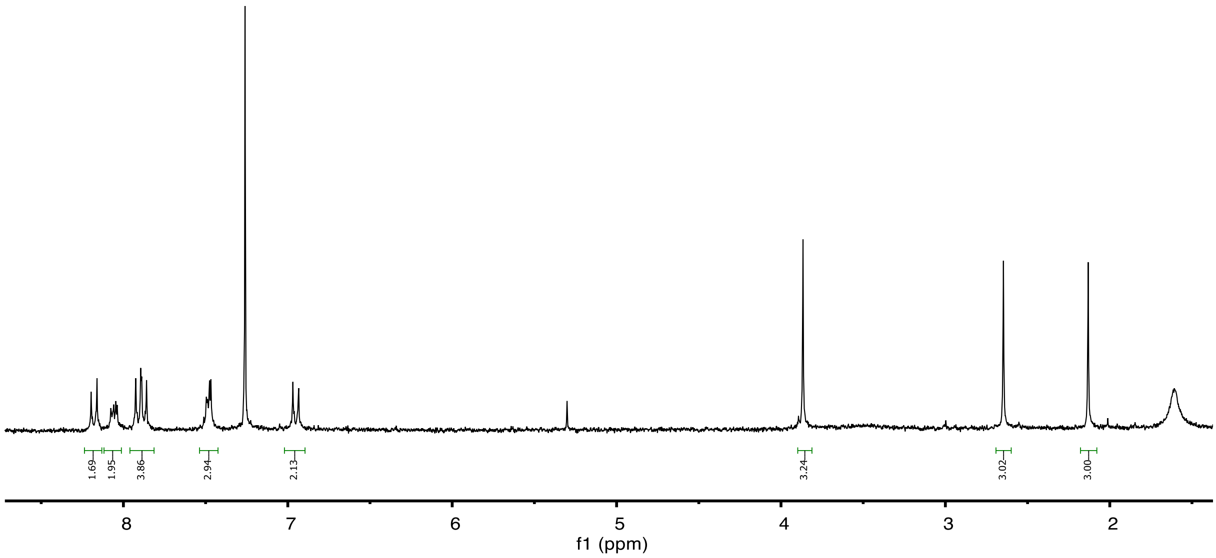

N
S
N
S
N
S
NO2

5


Et2O
Et2O
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
f1 (ppm)


N
S
N
S
N
S
O2N
O

6


1.69
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2.13
3.24
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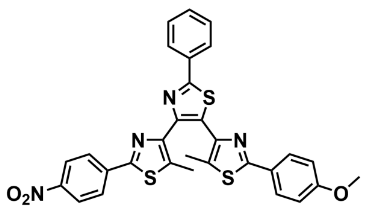
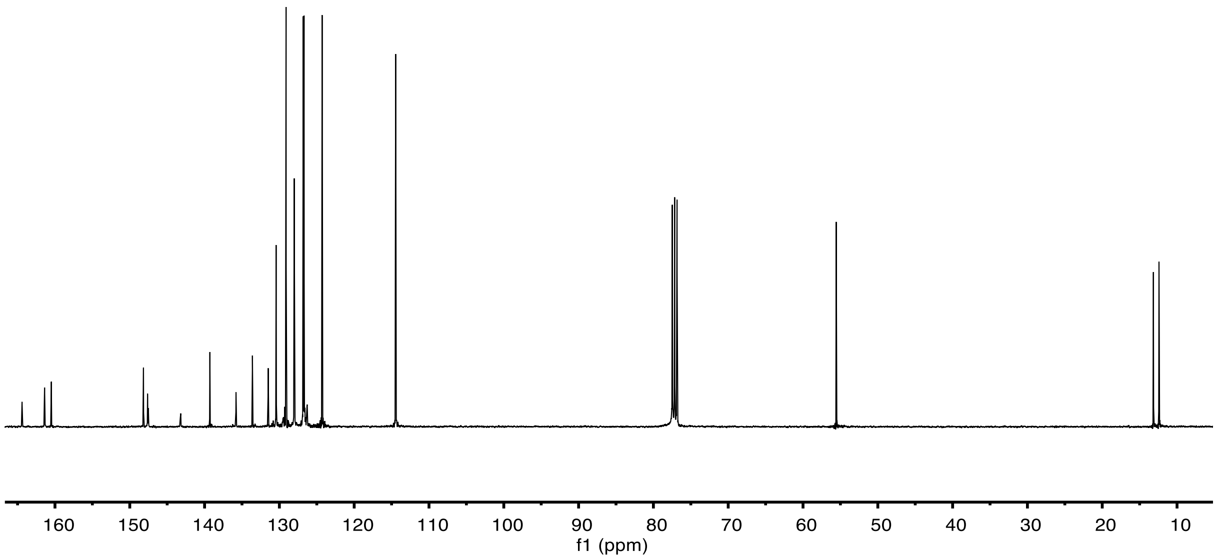
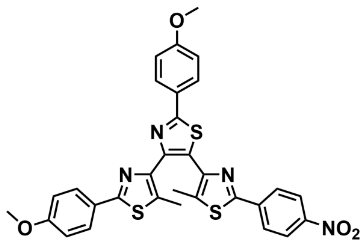
3.00
8
7
6
5
4
3
2
f1 (ppm)

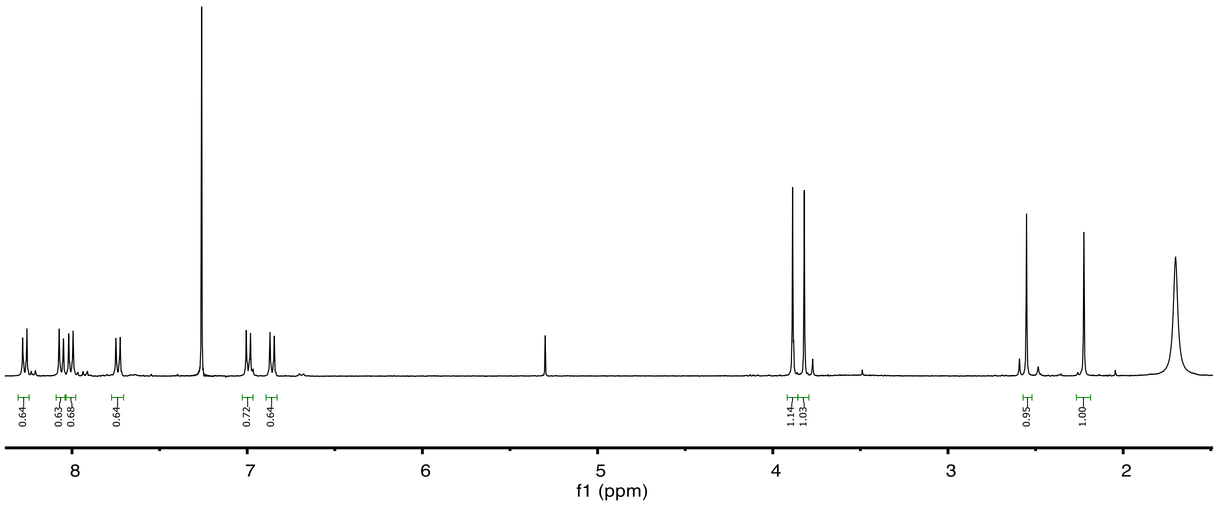

N
S
N
S
N
S
O2N
O

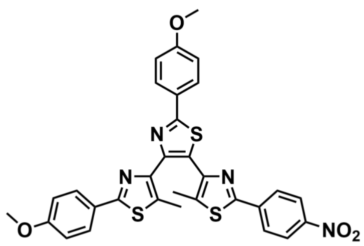
6


160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

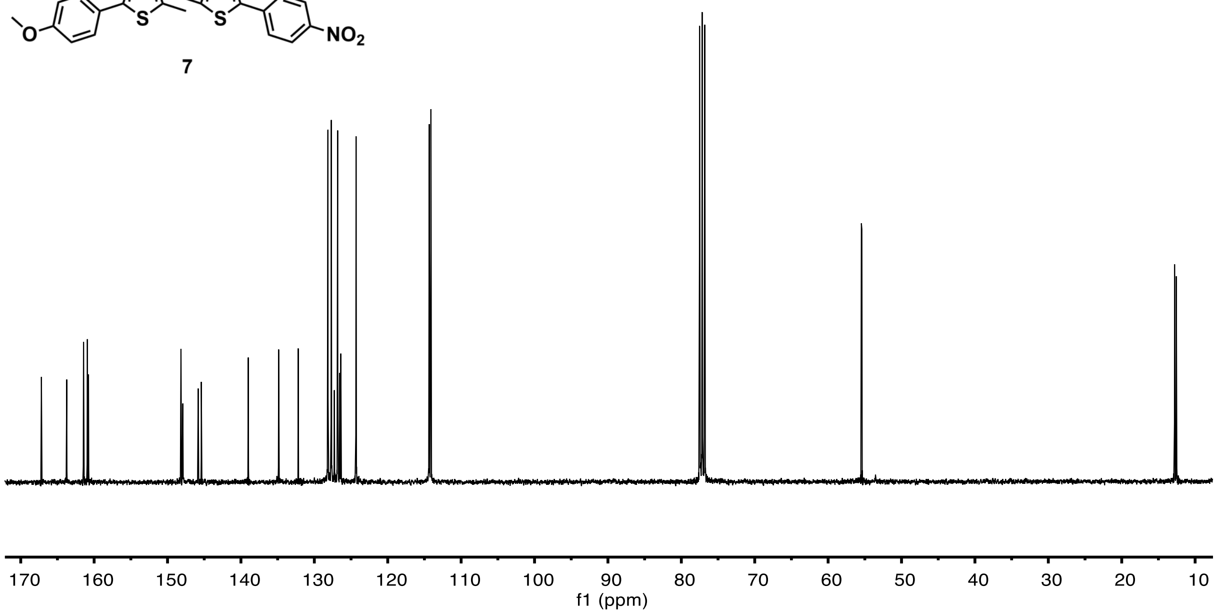


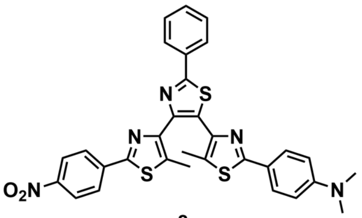
7



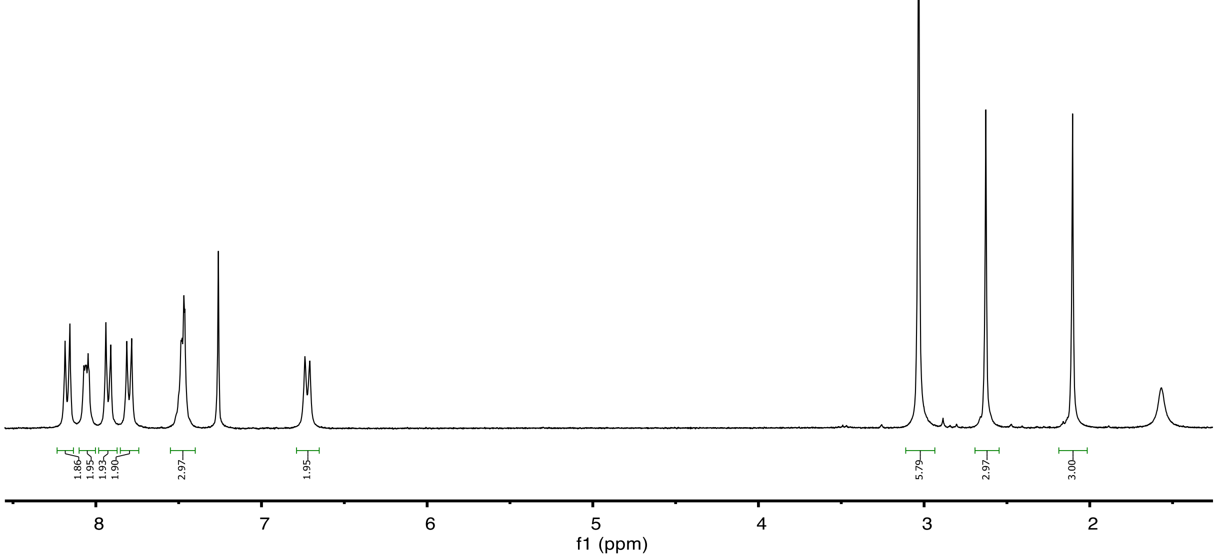


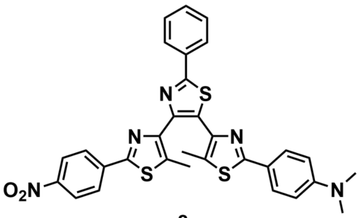
7



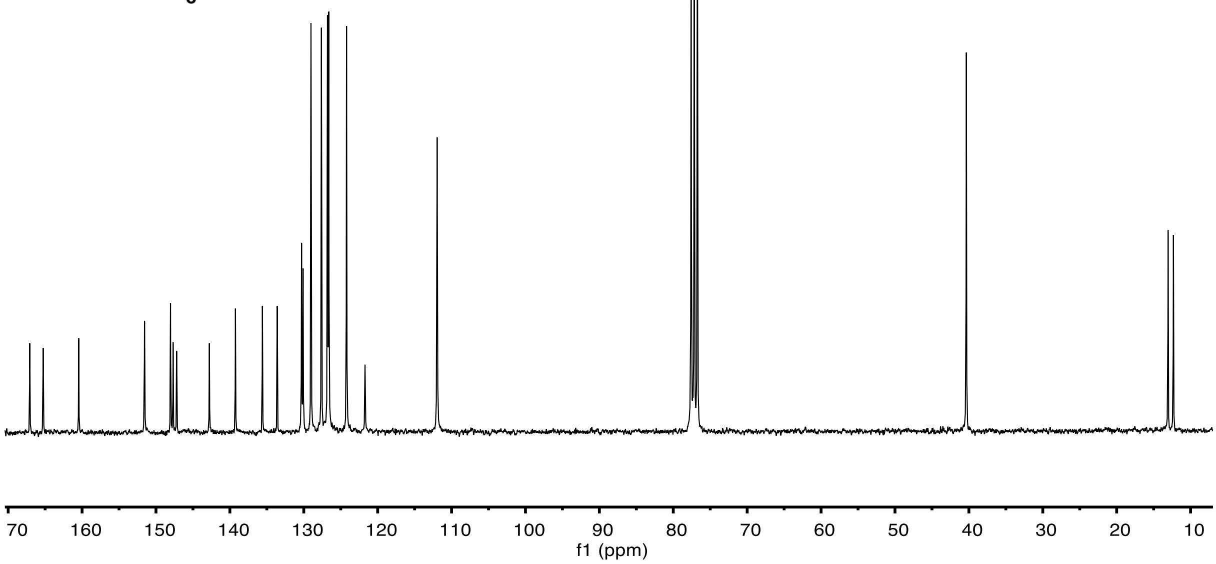

O2N
N
S
N
S
N
S
N

8


1.86
1.95
1.93
1.90
2.97
1.95
5.79
2.97
3.00
8
7
6
5
4
3
2
f1 (ppm)


O2N
N
S
N
S
N
S
N

8


70
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

Additional spectroscopic data:

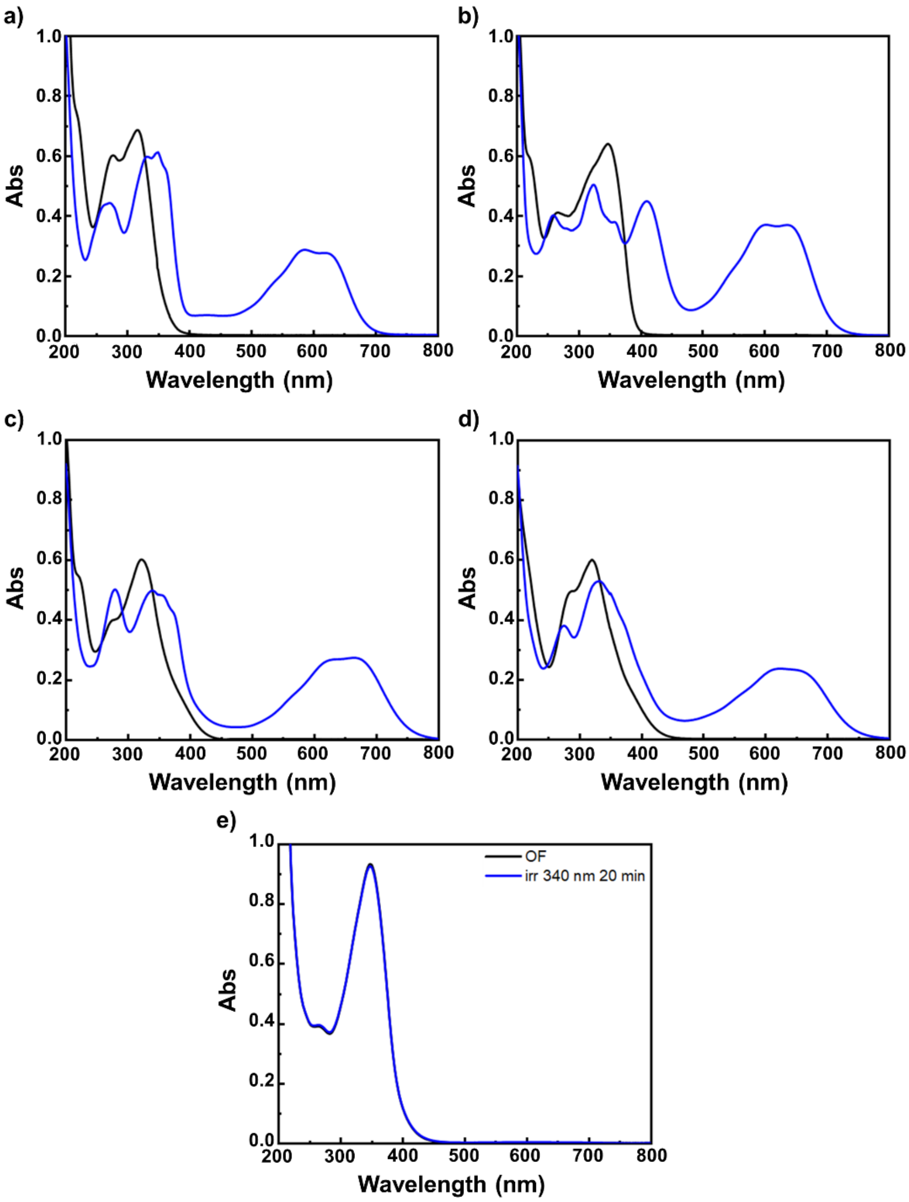


Figure S1: Absorption spectra in CH_3CN at room temperature of (a) **2** (1.85×10^{-5} M), (b) **3** (1.76×10^{-5} M), (c) **6** (1.60×10^{-5} M), (d) **7** (1.70×10^{-5} M) and (e) **8** (2.15×10^{-5} M), showing the evolution under UV light irradiation (at 320 nm for **2**, **3**, **6** and **7**, at 340 nm for **8**) from the black lines for (open forms) to the blue lines (respective photo-stationary states). Optical path of the cuvette: 1 cm.

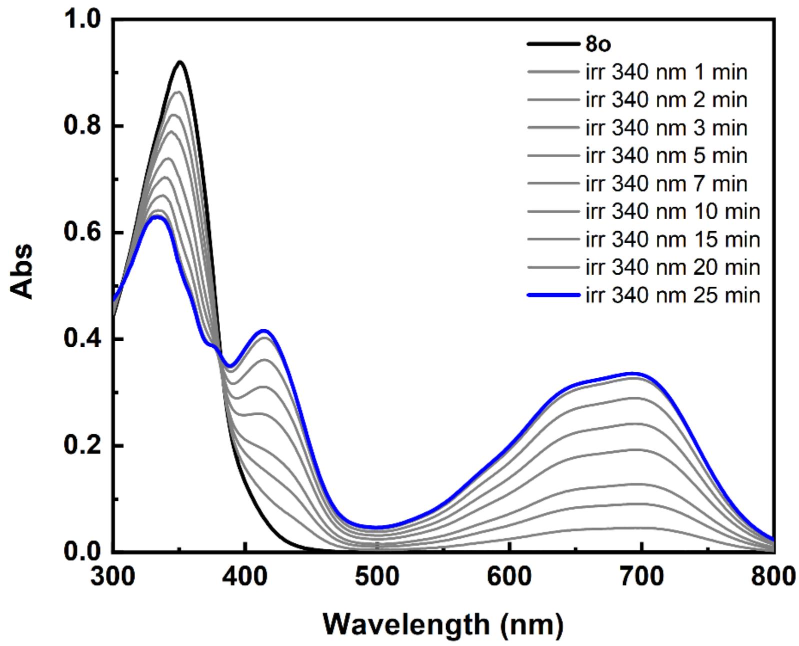


Figure S2: Photochromic behavior of **8** (2.04×10^{-5} M) in toluene at room temperature. The spectrum of the OF is shown with a black solid line while the PSS is indicated in blue. The solution has been irradiated at 340 nm. Optical path of the cuvette: 1 cm.

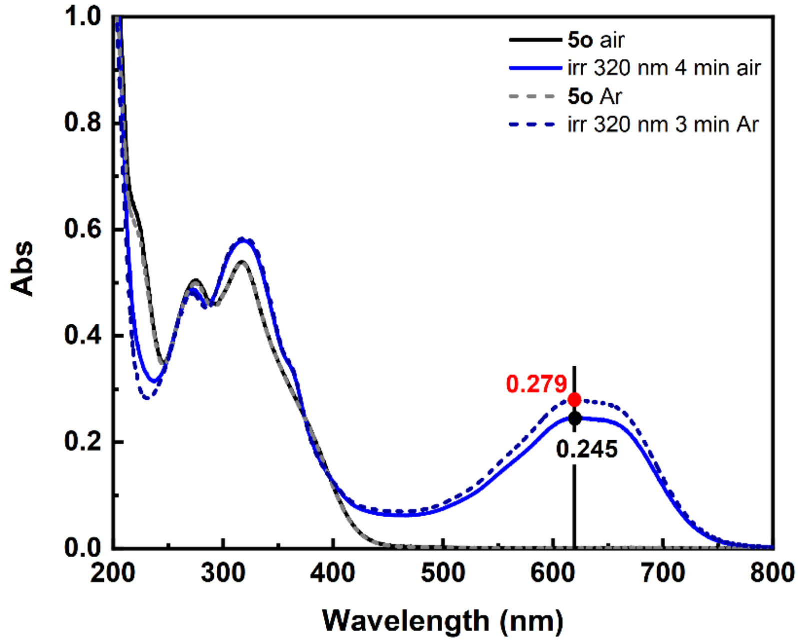


Figure S3: Absorption spectra of **5** (2.00×10^{-5} M) in acetonitrile at room temperature. **5o** in aerated solution in black solid line; **5o** in degassed solution in grey dashed line; PPS in aerated solution by irradiating at 320 nm in blue solid line; PSS in degassed solution by irradiating at 320 nm in dashed blue line. Optical path of the cuvette: 1 cm.

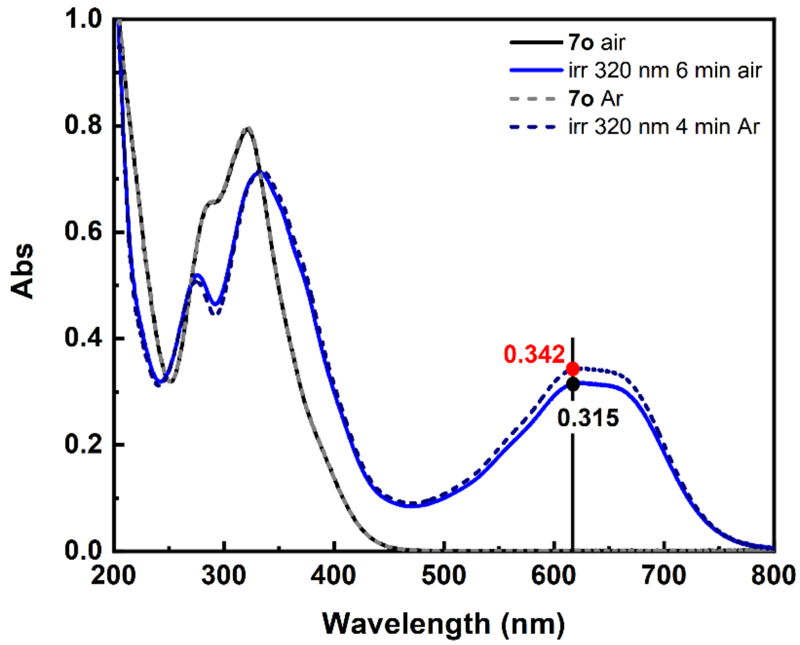


Figure S4: Absorption spectra of **7** (2.24×10^{-5} M) in acetonitrile at room temperature. **7o** in aerated solution in black solid line; **7o** in degassed solution in grey dashed line; PPS in aerated solution by irradiating at 320 nm in blue solid line; PSS in degassed solution by irradiating at 320 nm in dashed blue line. Optical path of the cuvette: 1 cm.

Additional calculation data:

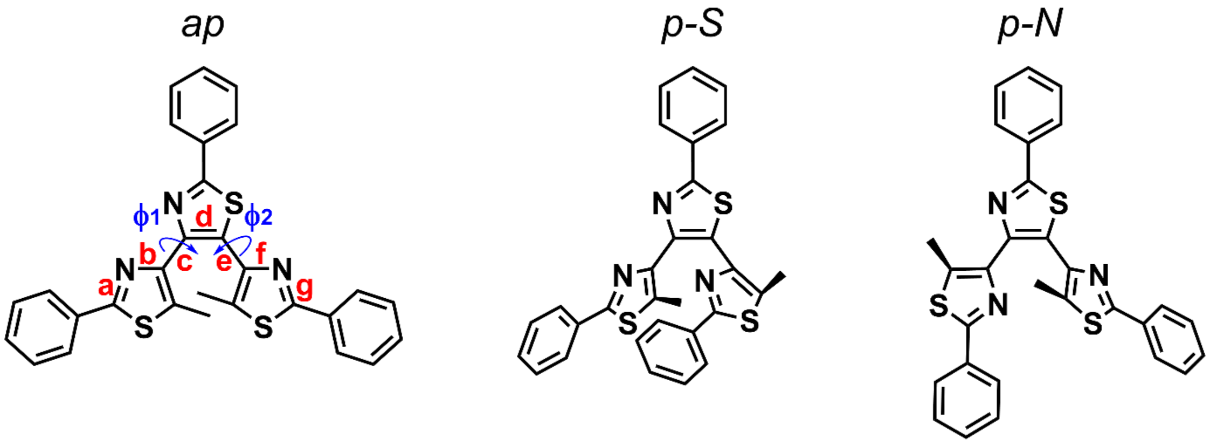
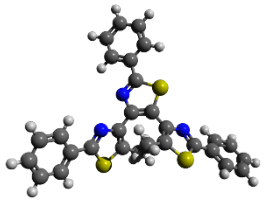
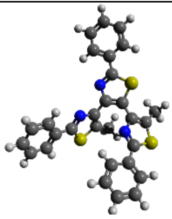
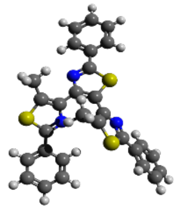
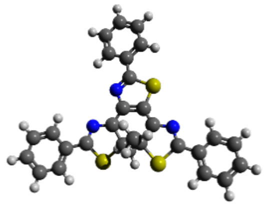
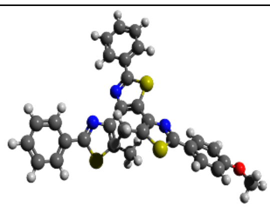
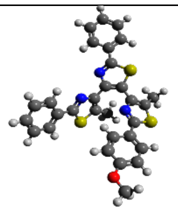
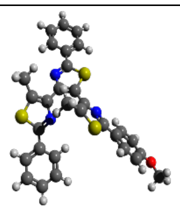
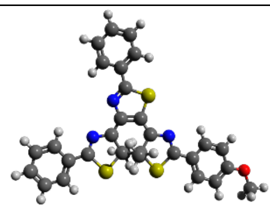
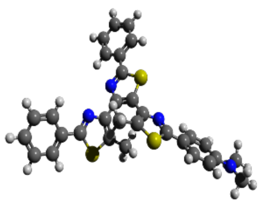
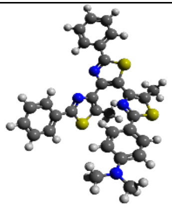
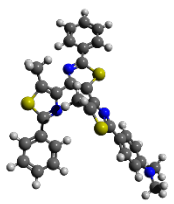
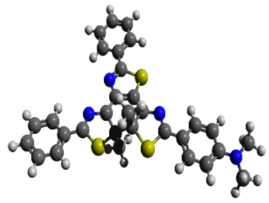
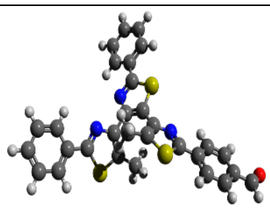
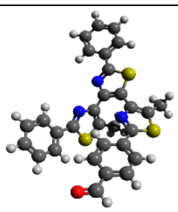
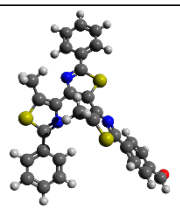
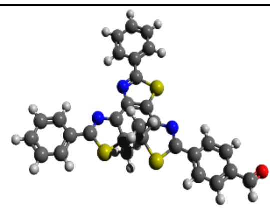
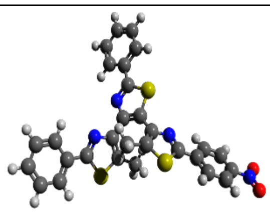
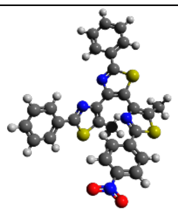
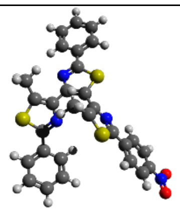
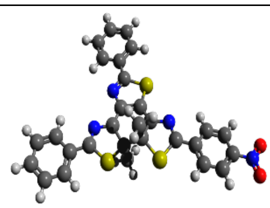


Figure S5: Antiparallel (*ap*) and parallel (*p-S* and *p-N*) conformers of the open form.

	ap	*p-S*	*p-N*	CF
1				
2				
3				
4				
5				

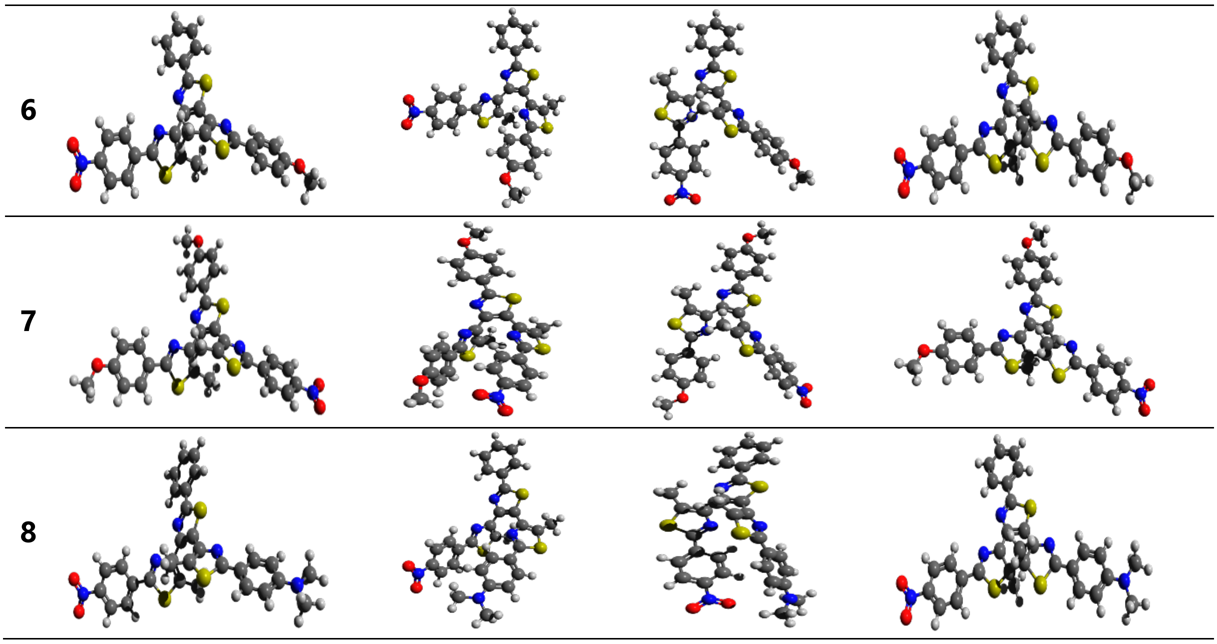


Figure S6: Optimized geometries (ωB97XD/6-311G(d,p); calculations in acetonitrile) of the open (*ap*, *p-S* and *p-N*) and closed forms of **1-8**.

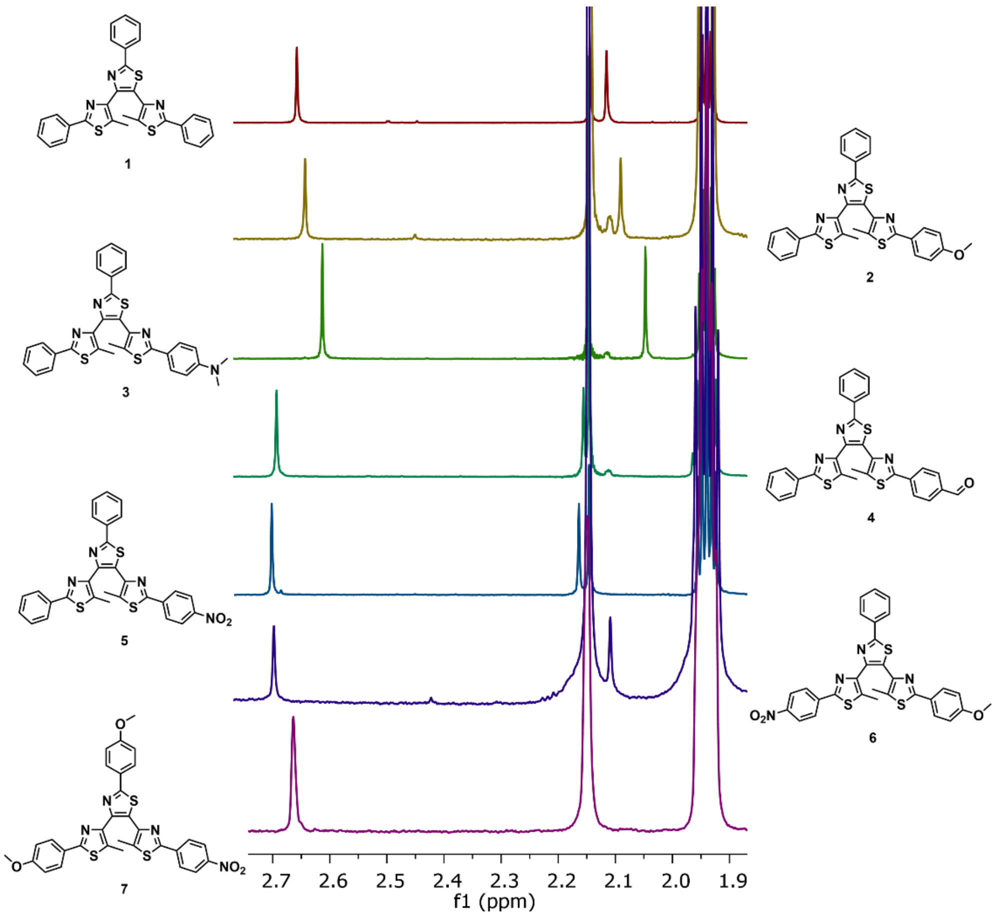


Figure S7: Zoom of the ^{1}H-NMR spectra of **1** – **7** in CD_3CN showing only two singlets associated to the methyl groups on the reactive carbons. In the case of **7**, one singlet is covered by the peak of residual H_2O in CD_3CN.

Table S1: Geometric parameters of the open and closed forms calculated at the ωB97XD/6-311G(d,p) level in acetonitrile of **1-8**.

	a	b	c	d	e	f	g	ϕ1	ϕ2	d_{C-C} (Å)
1										
ap	1.301	1.378	1.465	1.372	1.475	1.377	1.301	132.9	130.6	3.477
p-S	1.295	1.375	1.466	1.370	1.474	1.374	1.297	-40.8	124.9	
p-N	1.298	1.374	1.465	1.371	1.473	1.375	1.294	127.0	-36.0	
CF	1.290	1.377	1.356	1.463	1.346	1.379	1.290	176.1	176.5	
2										
ap	1.298	1.377	1.464	1.369	1.474	1.375	1.297	132.1	129.2	3.469
p-S	1.295	1.376	1.466	1.370	1.474	1.373	1.298	-39.8	123.4	
p-N	1.298	1.376	1.464	1.371	1.471	1.374	1.295	130.9	-36.5	
CF	1.288	1.377	1.343	1.461	1.353	1.375	1.286	176.3	176.4	
3										
ap	1.299	1.377	1.464	1.369	1.473	1.375	1.297	131.2	129.5	3.467
p-S	1.298	1.373	1.474	1.370	1.466	1.377	1.296	122.6	-39.3	
p-N	1.300	1.379	1.467	1.374	1.475	1.376	1.301	-38.5	124.1	
CF	1.291	1.374	1.344	1.460	1.353	1.376	1.285	176.2	176.4	
4										
ap	1.298	1.374	1.464	1.369	1.473	1.375	1.297	131.8	128.8	3.466
p-S	1.294	1.372	1.467	1.370	1.475	1.374	1.298	-40.0	111.8	
p-N	1.299	1.372	1.465	1.371	1.472	1.374	1.295	128.0	-34.9	
CF	1.285	1.377	1.343	1.461	1.354	1.374	1.287	176.1	176.1	
5										
ap	1.298	1.373	1.464	1.369	1.473	1.375	1.297	131.5	129.0	3.473
p-S	1.295	1.372	1.466	1.370	1.474	1.373	1.298	-38.7	122.4	
p-N	1.299	1.371	1.465	1.371	1.472	1.374	1.294	123.6	-34.9	
CF	1.285	1.377	1.344	1.461	1.354	1.374	1.287	176.0	176.3	
6										
ap	1.298	1.377	1.464	1.369	1.473	1.371	1.298	131.7	130.2	3.468
p-S	1.295	1.376	1.466	1.370	1.473	1.370	1.298	-39.6	126.5	
p-N	1.298	1.376	1.465	1.371	1.471	1.371	1.296	129.3	-34.3	
CF	1.289	1.375	1.344	1.460	1.354	1.375	1.285	176.7	175.7	
7										
ap	1.298	1.373	1.464	1.368	1.473	1.376	1.297	131.5	128.7	3.468
p-S	1.293	1.370	1.469	1.368	1.480	1.376	1.297	-46.7	102.9	
p-N	1.299	1.371	1.465	1.370	1.472	1.376	1.295	127.6	-34.6	
CF	1.289	1.373	1.354	1.461	1.344	1.377	1.284	176.1	176.1	
8										
ap	1.299	1.377	1.464	1.369	1.473	1.371	1.298	132.8	130.2	3.471

p-S	1.295	1.375	1.468	1.369	1.478	1.370	1.298	-43.4	105.2
p-N	1.299	1.376	1.471	1.369	1.474	1.369	1.293	103.9	-39.3
CF	1.293	1.372	1.345	1.459	1.354	1.375	1.284	177.0	175.4

Charge density analysis on the HT moiety. An important parameter that could control the photochromism relies to the charge density on the hexatriene (HT) part of the molecule, the unit responsible of the electrocyclization reaction. A general accepted idea is that a large electron density on the HT unit should favour the ring-closing reaction. To compare the effect of the substituents on the charge density on the HT moiety, we determined the Mulliken charges in ground and first excited states.

Table S2. Mulliken charges on the HT moieties of compounds **1** – **8** in the open forms. Data in bracket correspond to the average values on the reactive carbon atoms.

	HT's Mulliken charge		
	S_0	**S_1**	**$\Delta(S_1$-$S_0)$**
1	-0.465965 (-0.292571)	-0.485274 (-0.2890935)	-0.019309
2	-0.488963 (-0.290701)	-0.52393 (-0.2887825)	-0.034967
3	-0.513030 (-0.2918355)	-0.708059 (-0.3004295)	-0.195029
4	-0.442851 (-0.2893125)	-0.311262 (-0.2705065)	0.131589
5	-0.427694 (-0.2885065)	-0.211872 (-0.2705065)	0.215822
6	-0.436385 (-0.2907715)	-0.218063 (-0.272632)	0.218322
7	-0.441427 (-0.2905895)	-0.224398 (-0.2722915)	0.217029
8	-0.457879 (-0.292759)	-0.306258 (-0.2792105)	0.151621

The Mulliken densities are found ranging between -0.427694 (terarylene **5**) and -0.51303 (terarylene **3**) in the ground state. As expected, the Mulliken charge becomes more negative for the derivatives holding a single donor substituent (i.e. **2** and **3**) when compared to non-substituted terarylene **1**. Interestingly, the negative charge significantly increases in the S_1 state for the first three compounds, from -0.019e for **1** to -0.195e for **3**. For all the other derivatives, the charge density on the HT is less negative than in the reference **1** in the ground state and the excited state process induces a depletion of the electron density in the core unit. The calculated $\Delta(S_1$-$S_0)$ is found positive for **4** – **8**.

The variation of the electronic density on the HT core unit can be linked to some extent to the impact of the electron-donating and withdrawing characters of the substituents. However, the resulting value of the charge density is only poorly correlated to the photocyclization quantum yield, thus suggesting that the Mulliken charge on the HT unit cannot be used to rationalize the variation of the efficiency of the ring-closing reaction.

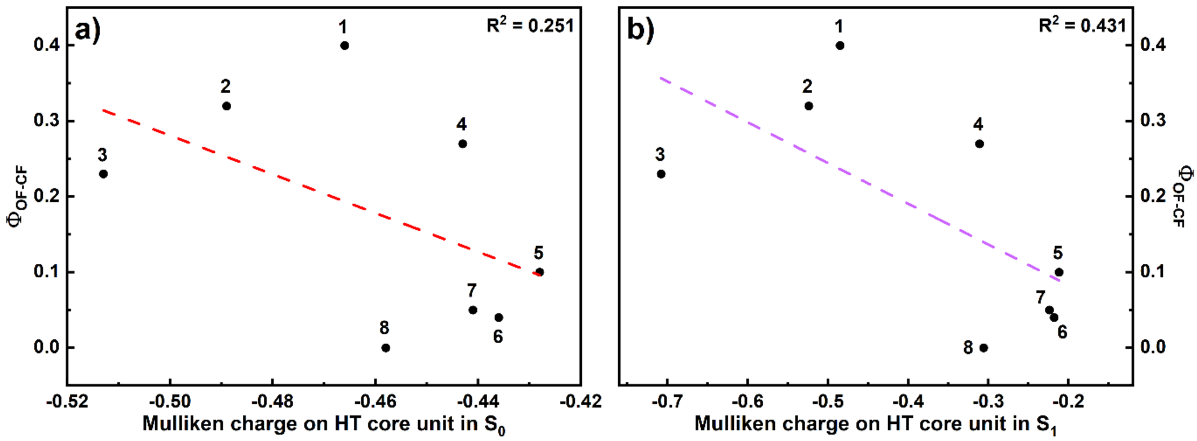


Figure S8: Correlation between Φ_{OF-CF} and the Mulliken charge on the HT moiety in a) the ground state (S_0) and b) the first excited state (S_1).

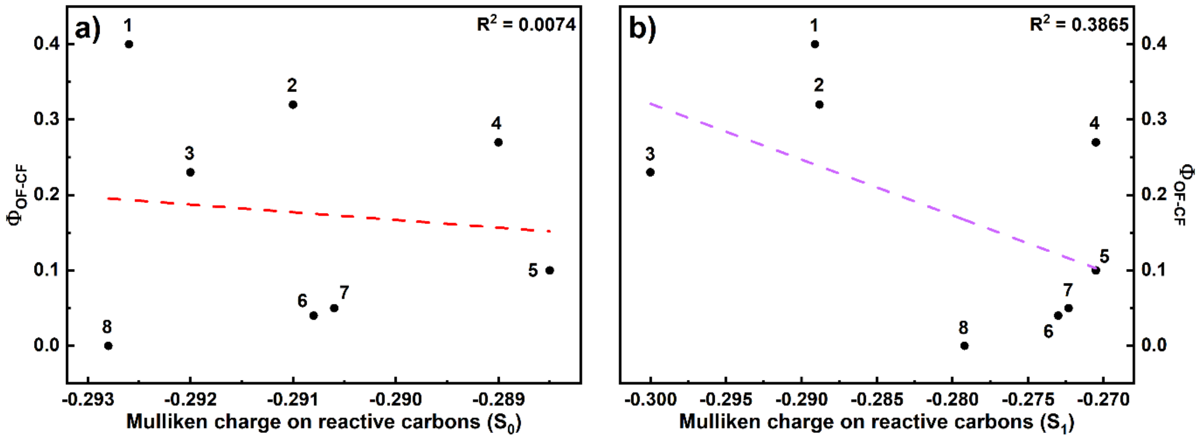


Figure S9: Correlation between Φ_{OF-CF} and the Mulliken charge on the reactive carbons in a) the ground state (S_0) and b) the first excited state (S_1).

Table S3: Excitation energies of the OFs (antiparallel form) calculated at the CAM-B3LYP/6-311G(d,p)//ωB97XD/6-311G(d,p) level in acetonitrile. λ: calculated wavelength, in nm; f: oscillator strength; H = HOMO and L = LUMO; Exp: experimental wavelength; AD: absolute deviation, in eV.

	λ (nm)	*f*	Assignment	Exp	AD
1	311	0.643	H->L (75%)	314	0.04
	299	1.353	H->L+1 (55%)	274	0.38
	295	0.003	H->L+2 (65%)		
2	313	0.515	H->L (75%)	317	0.05
	305	1.323	H->L+2 (63%)	279	0.38
	294	0.378	H-1->L+1 (38%)		
3	330	1.063	H->L+2 (77%)	348	0.19
	314	0.803	H-1->L (43%)		
	295	0.508	H-1->L+1 (58%)		
4	324	1.000	H->L (50%)	317	0.08
	307	0.0036	H-1->L (69%)		
	291	0.7379	H->L+1 (79%)		
5	335	0.814	H->L (54%)	317	0.21
	307	0.779	H->L+1 (79%)	274	0.49
	291	0.556	H->L+2 (64%)		
6	336	0.854	H->L (37%)	322	0.16
	309	0.402	H->L+1 (73%)	276	0.48
	303	1.092	H-1->L+1 (14%)		
7	340	0.7814	H->L (49%)	320	0.23
	315	0.9720	H-1->L+1 (20%)	286	0.40
	298	0.7050	H-1->L+2 (32%)		
8	340	1.1393	H-1->L (32%)	348	0.08
	331	0.4505	H->L+1 (11%)		
	315	0.8129	H-1->L+1 (48%)		
					0.24*

*MAD = Mean Absolute Deviation

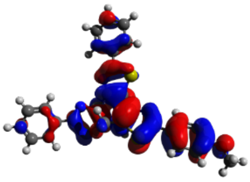
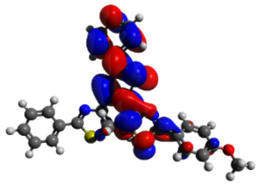
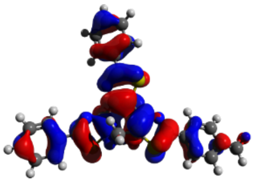
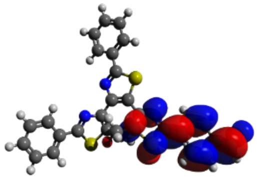
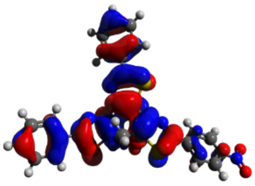
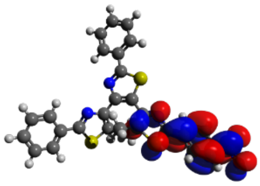
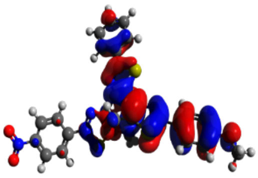
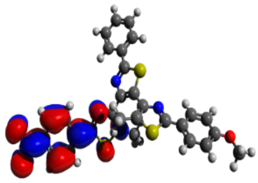
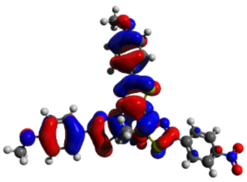
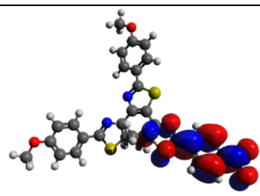
	HOMO	LUMO
2		
4		
5		
6		
7		

Figure S10: CAM-B3LYP/6-311G(d,p)//ωB97XD/6-311G(d,p) HOMOs and LUMOs of terthiazoles **2**, **4** – **7** in the antiparallel form (*ap*).

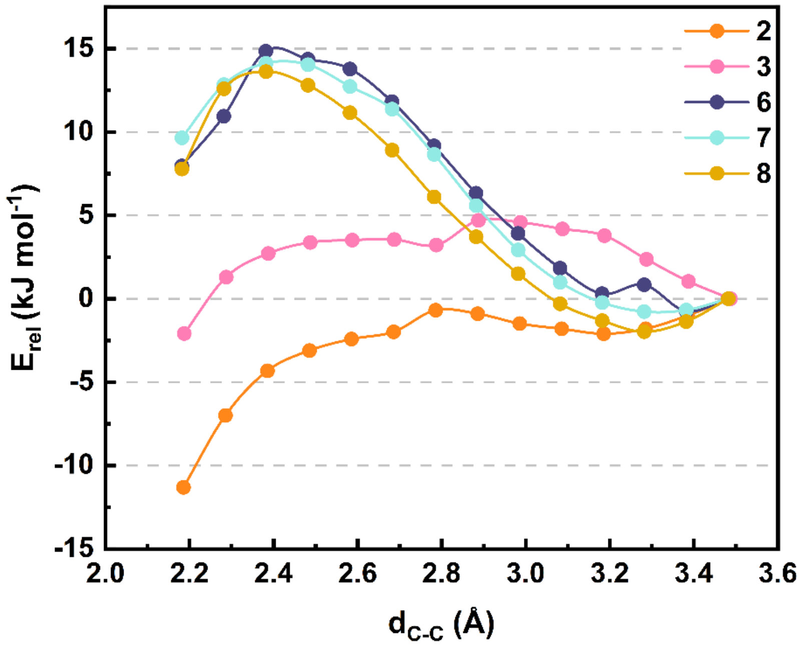


Figure S11: S_1 PES for the ring-closing reaction of terthiazoles **2**, **3** and **6** – **8** in the antiparallel form (*ap*).

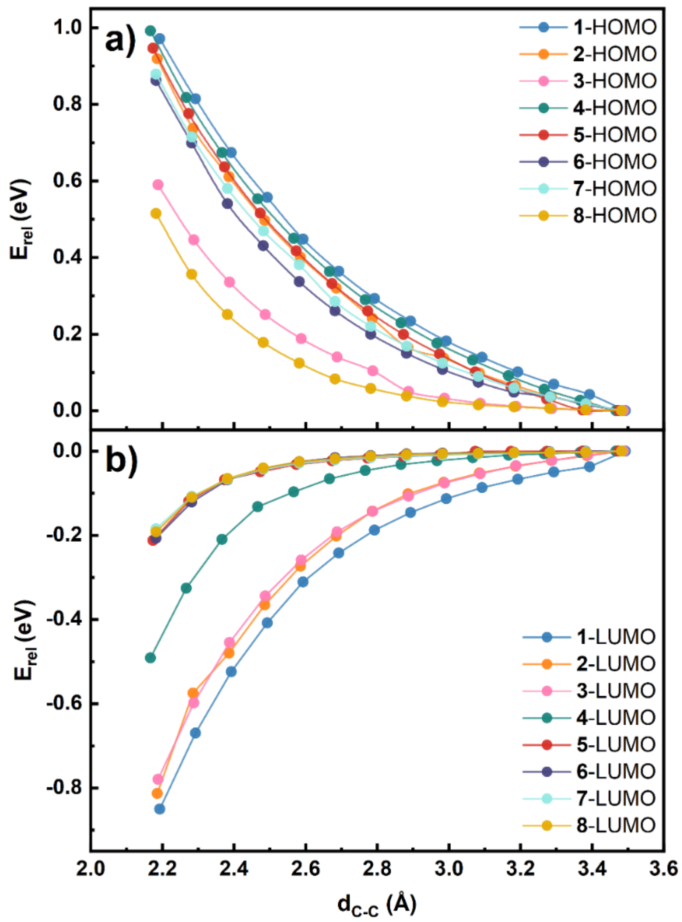


Figure S12: Evolution of the relative energies of a) HOMO and b) LUMO of the antiparallel (*ap*) open form of terarylenes **1** – **8** along the ground state ring-closure reaction. CAM-B3LYP/6-311G(d,p)//ωB97XD/6-311G(d,p) calculations.

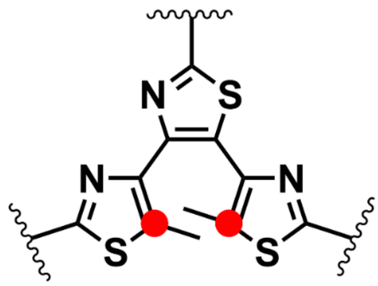
Molecular orbital composition. The analysis of the molecular orbital composition provides an interesting way to investigate and understand the photo-reactivity in S_0 and S_1 states as function of the substituents. As the ring-closure proceeds through an electrocyclic reaction involving the bridge and the two (hetero)aryl rings directly connected to it, we focus our attention on the composition of HOMO and LUMO on this electrocyclic core unit.

It is worth noting that while the HOMO is mainly localized on the electrocyclic unit for most of the studied derivatives (**1**, **2** and **4** – **7**), this is not always the case for the LUMO, as a significant percentage (higher than 50%) is observed only for **1**, **2** and **3**.

For most of the compounds, the contribution on the electrocyclic unit is larger for HOMO than for the LUMO. However, the difference between the percentages decreases as the reaction progresses along the reaction coordinate.

Table S4. Percentage of the molecular orbitals (HOMO and LUMO) localized on the HT moiety for compounds **1** – **8** in the antiparallel open form. CAM-B3LYP/6-311G(d,p)//ωB97XD/6-311G(d,p) calculations. The values in bracket correspond to the percentage on the reactive carbon atoms. The red dots indicate the reactive carbon atoms involved in the ring-closing reaction.

	Percentage of molecular orbitals	
	HOMO	**LUMO**
1	73,7 (18.5)	66,2 (11.1)
2	62,2 (17.4)	65,9 (8.8)
3	25,8 (8.5)	65,0 (7.2)
4	73,7 (17.9)	28,8 (6.4)
5	74,1 (17.6)	15,6 (3.5)
6	59,0 (16.4)	15,1 (3.5)
7	58,1 (16.6)	15,4 (3.4)
8	24,8 (8.2)	15,6 (3.6)



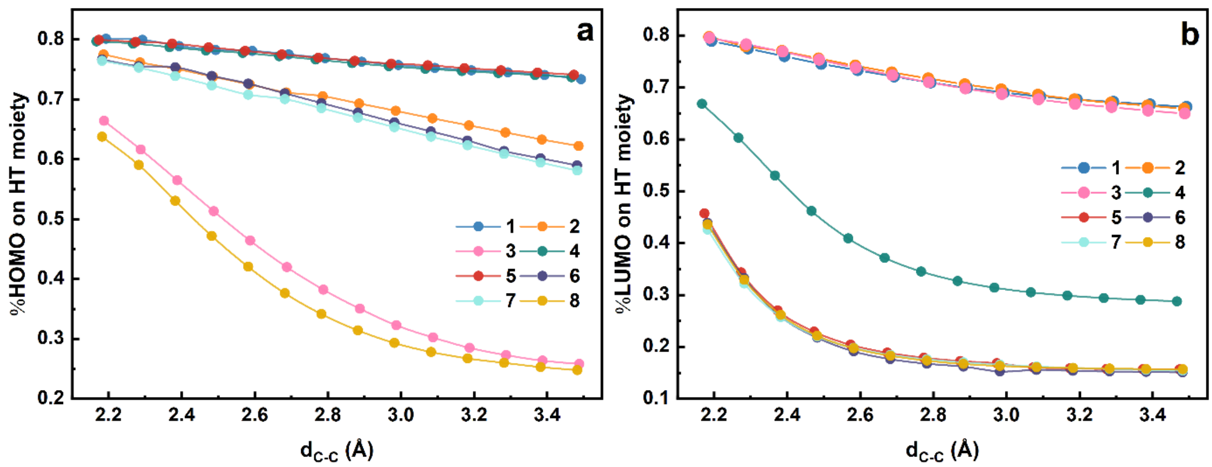


Figure S13: Evolution of the percentage of a) HOMO and b) LUMO, localized on the HT moiety in the antiparallel form for compounds **1** – **8**.

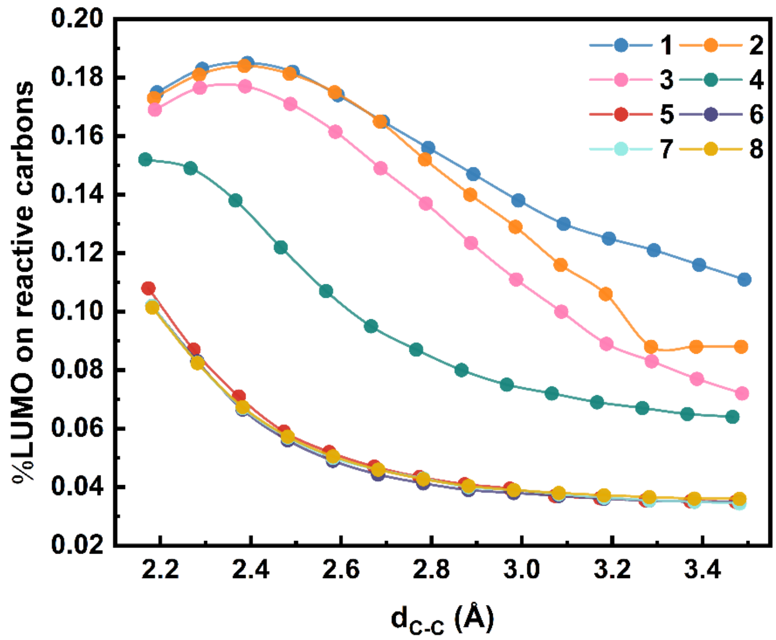


Figure S14: Evolution of the LUMO percentage on the reactive carbon atoms of **1** – **8** along the reaction coordinate.

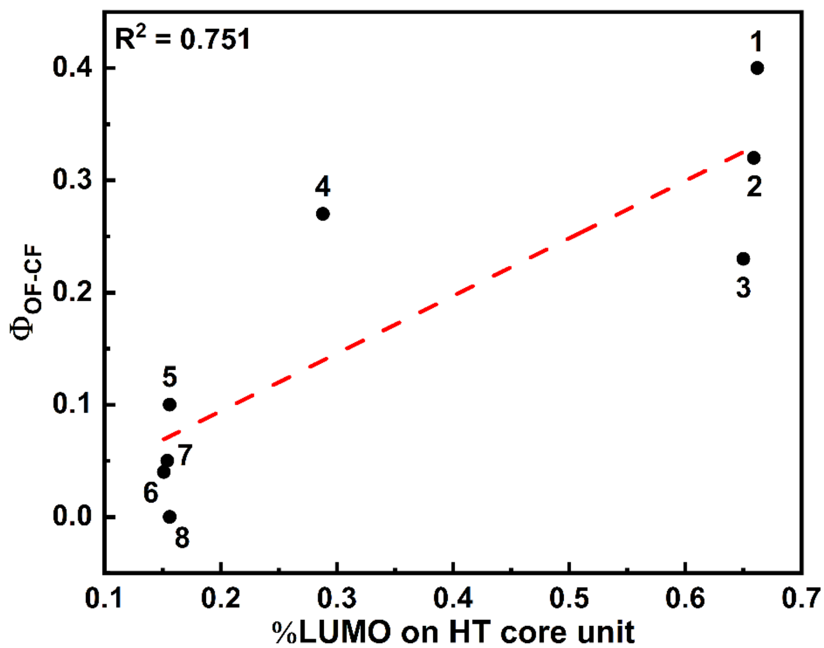


Figure S15: Correlation between the Φ_{OF-CF} quantum yield and the percentage of LUMO localized on the HT moiety.

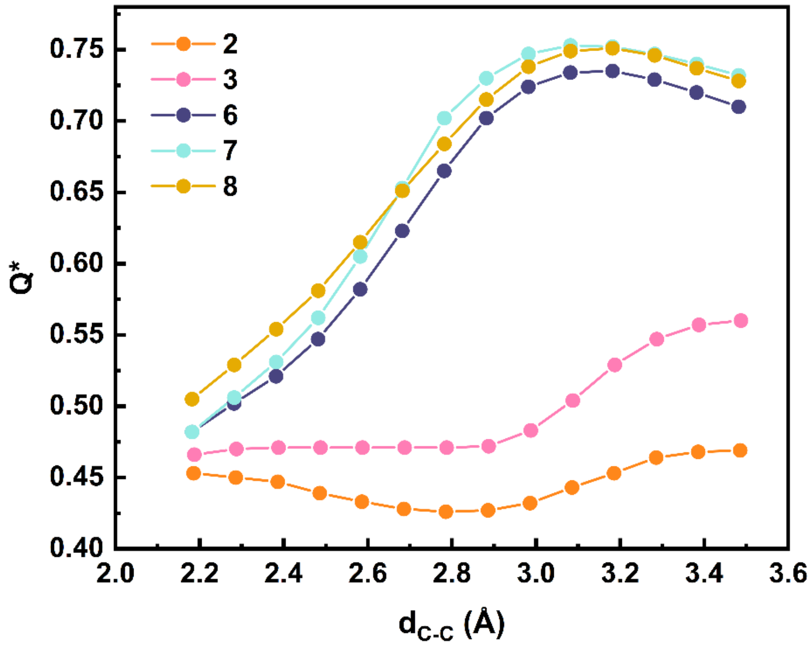


Figure S16: Evolution of the amount charge (Q*) transferred in the first excited state along the ring-closing reaction coordinate, starting from the antiparallel (*ap*) open forms of terthiazoles **2**, **3** and **6** – **8**.

Natural transition orbitals. The first electronic transition of the antiparallel form can also be analysed by using the natural transition orbitals (NTOs). From the NTOs, the Φ_S index has been calculated for the first singlet excited state by using the Nancy_EX program packages. The Φ_S index is defined as the spatial overlap between attachment and detachment densities. Typically, a value of Φ_S close to 1 underlines a local excitation character, whereas values approaching 0 imply that the CT character is dominant.[12] The calculated Φ_S indexes for the antiparallel forms of terarylenes **1** – **8** are found between 0.5 (compound **8**) and 0.68 (compound **1**). The report of Φ_S indexes versus the photocyclization quantum yields shows a nice, linear correlation, suggesting that the CT character is an important parameter that controls the efficiency of the excited state ring-closing reaction.

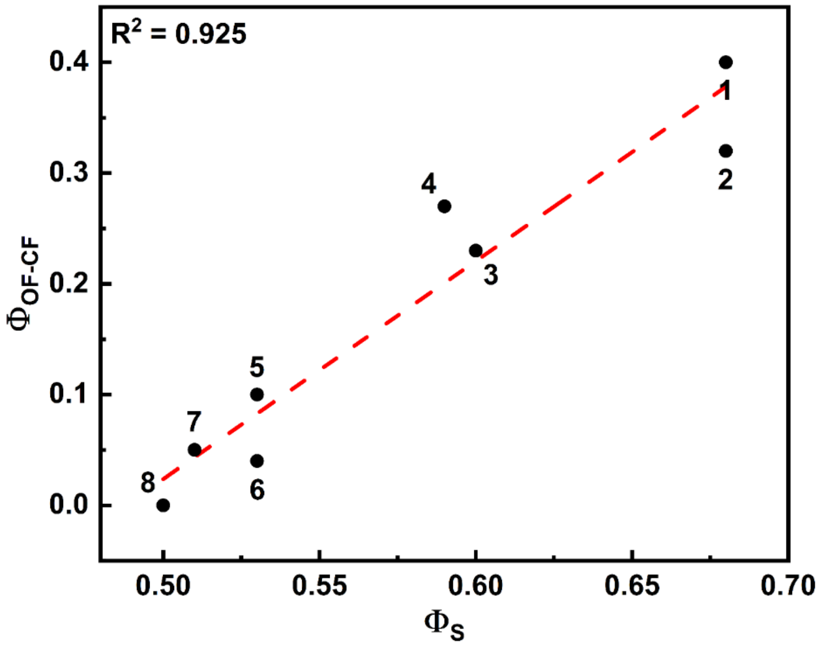


Figure S17: Correlation between Φ_S index and Φ_{OF-CF} of terthiazoles **1** – **8** in the antiparallel form (*ap*).

Additional calculation data on the CFs. The charge transfer analysis was also performed for the closed state. The amount of transferred charge (Q*) in the S_1 state can be correlated to the quantum yield for ring-opening reaction (Φ_{CF-OF}).

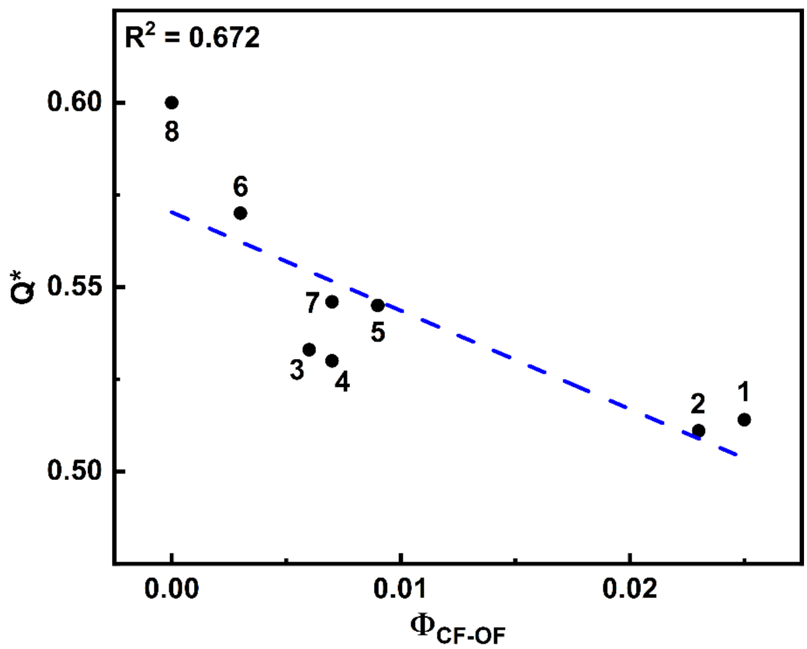


Figure S18: Correlation between the amount of transferred charge between S_0 and S_1 (Q*) and the ring-closing quantum yield (Φ_{CF-OF}).

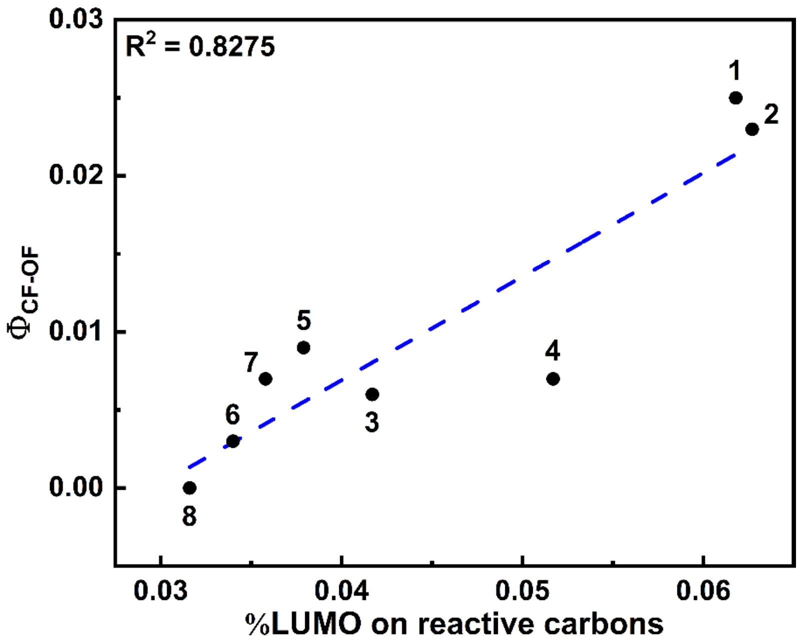


Figure S19: Correlation between the ring-closing quantum yield (Φ_{CF-OF}) and the percentage of LUMO localized on the reactive carbon atoms of the eight closed form isomers.

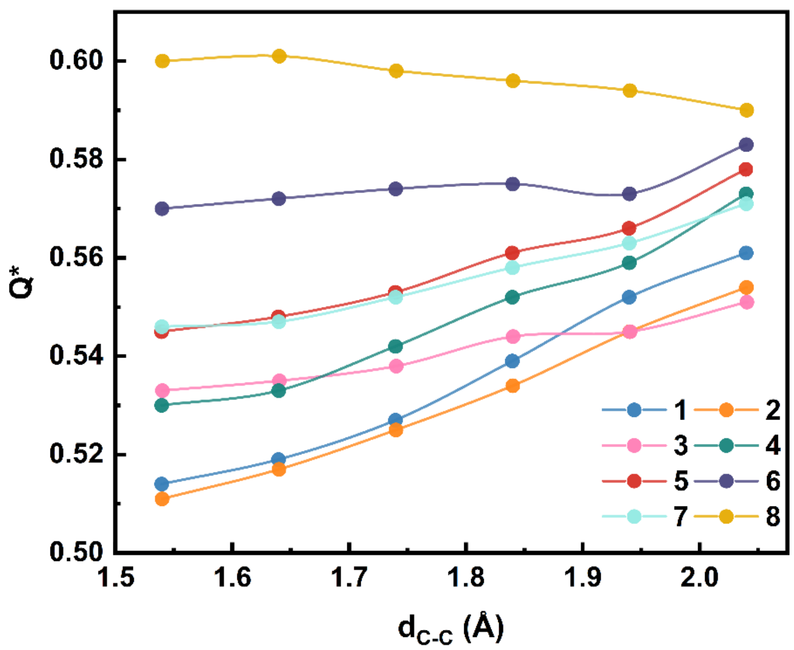


Figure S20: Evolution of the amount charge (Q*) transferred in the first excited state along the ring-opening reaction coordinate, starting from the closed forms of **1** – **8**.

Extension of the model to other photochromes:

The proposed correlation has been applied to four terarylenes investigated by Jaung and co-workers[13] (Figure S21), to four dissymmetric diarylethenes studied by Pu's group[14] (Figure S23) and to three diarylethenes developed by Irie et al.[15] (Figure S25). The model appeared to remain valid.

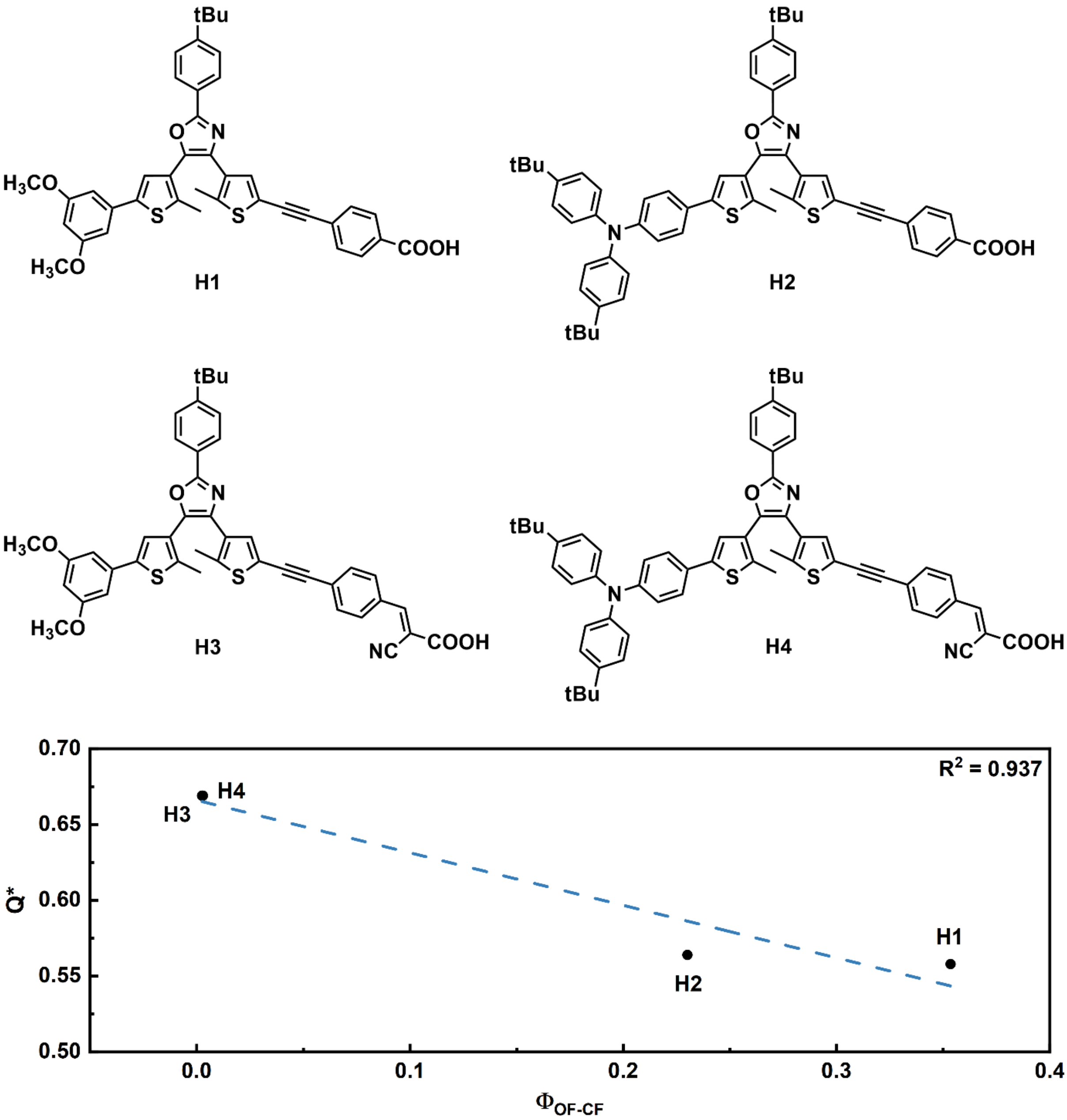


Figure S21: top) Structures of the four photochromes investigated by Jaung and co-workers; bottom) Application of the correlation between the amount of transferred charge between S_0 and S_1 (Q^*) and the ring-closure quantum yield ($\Phi_{OF\text{-}CF}$).

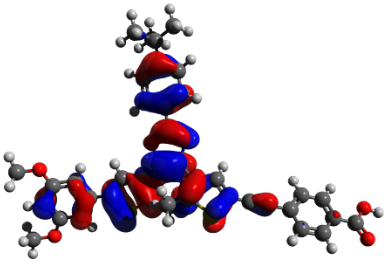
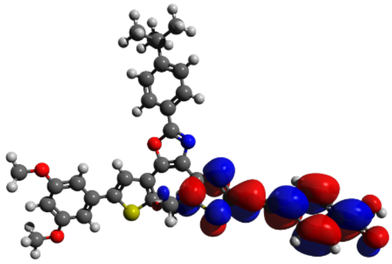
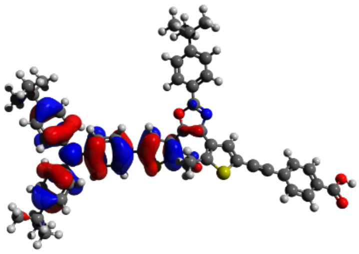
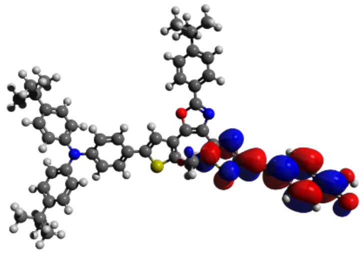
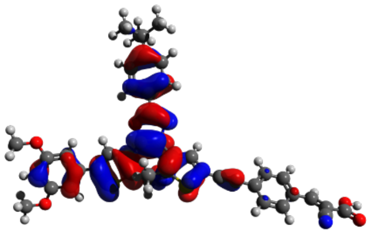
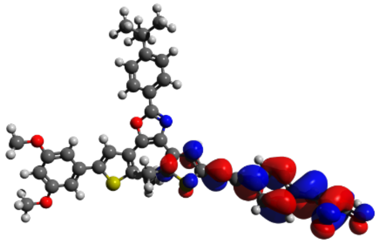
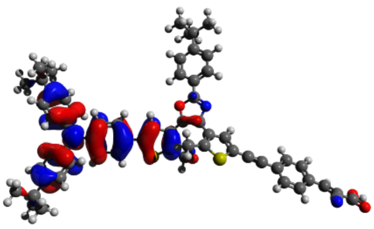
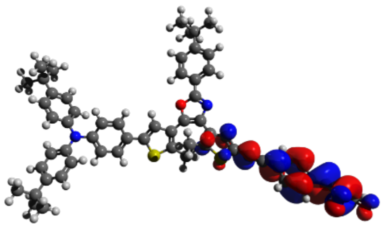
	HOMO	LUMO
H1		
H2		
H3		
H4		

Figure S22: CAM-B3LYP/6-311G(d,p)//ωB97XD/6-311G(d,p) HOMOs and LUMOs of derivatives **H1** – **H4** investigated by Jaung and co-workers.

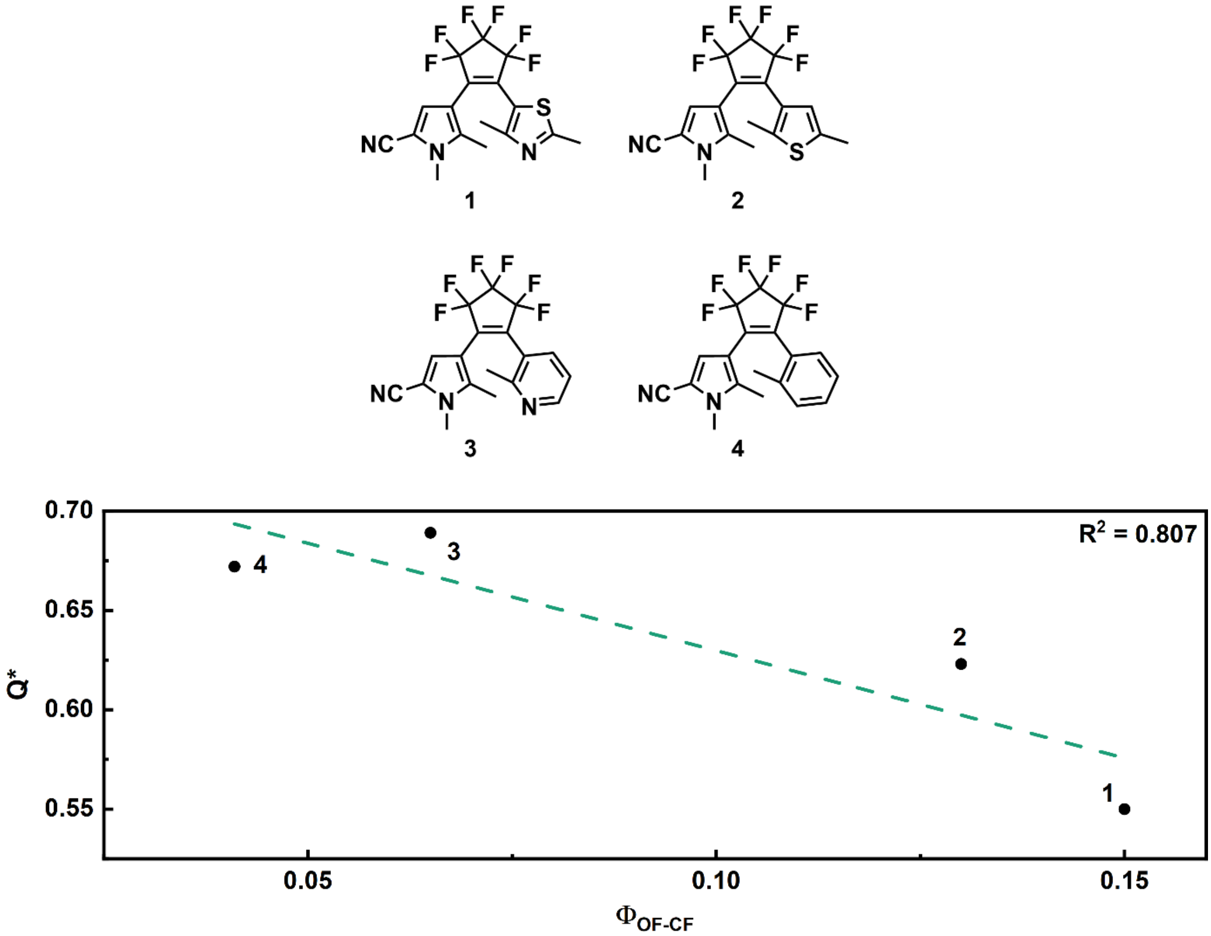


Figure S23: top) Structures of the four photochromes investigated by Pu and co-workers; bottom) Application of the correlation between the amount of transferred charge between S_0 and S_1 (Q^*) and the ring-closure quantum yield ($\Phi_{OF\text{-}CF}$).

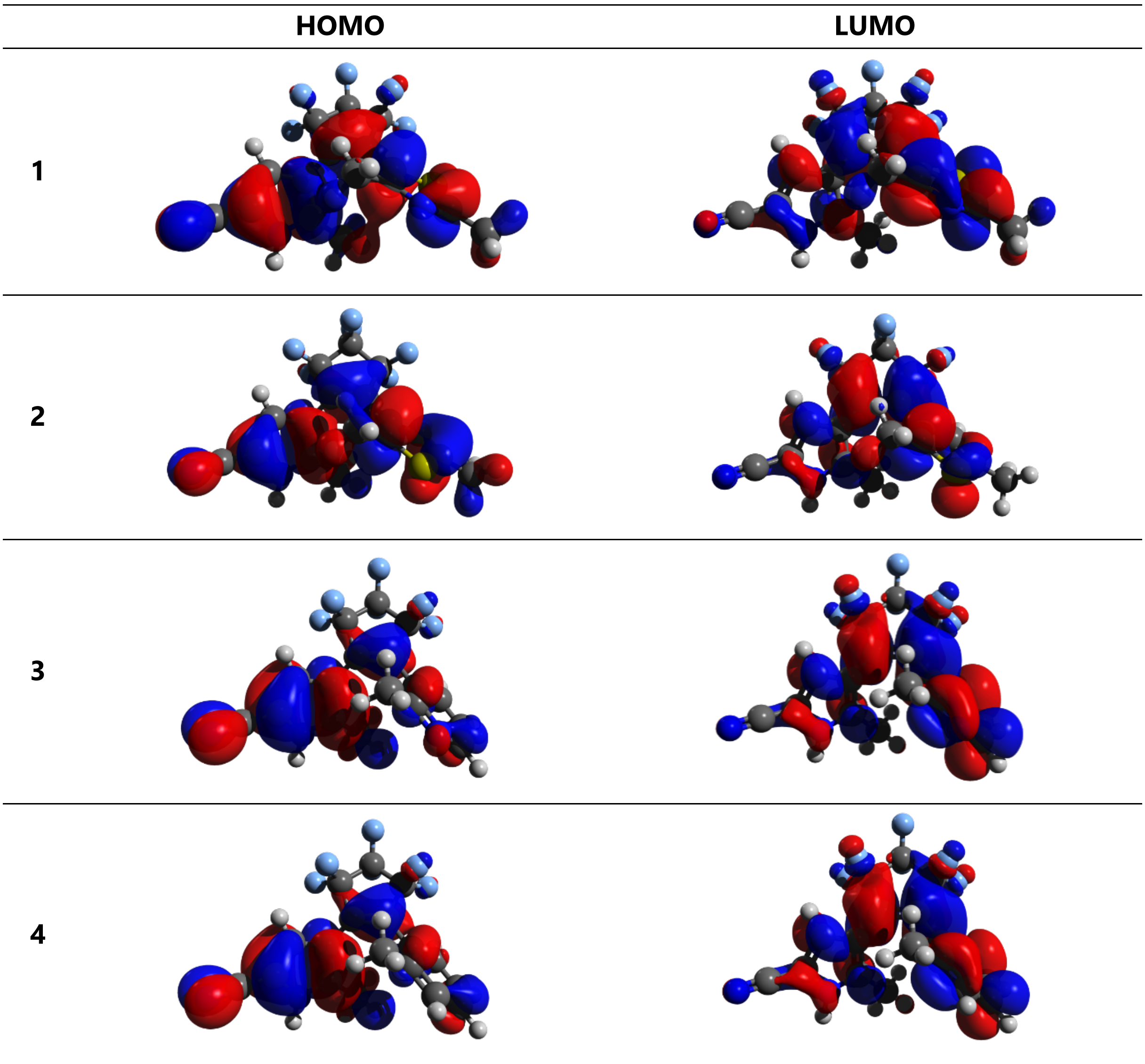
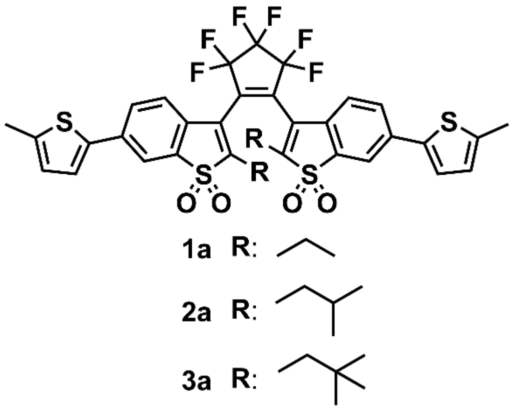


Figure S24: CAM-B3LYP/6-311G(d,p)//ωB97XD/6-311G(d,p) HOMOs and LUMOs of derivatives **1** – **4** investigated by Pu and co-workers.



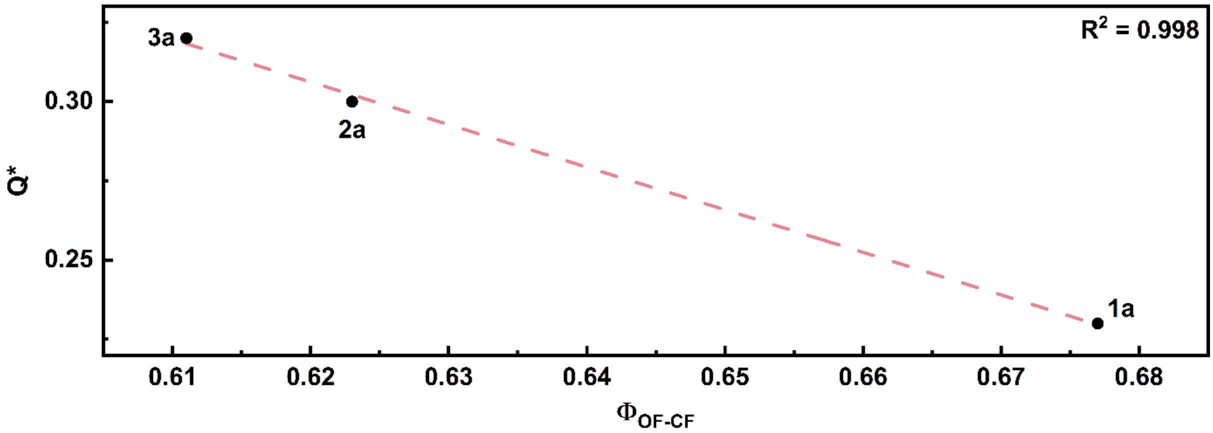


Figure S25: top) Structures of the four photochromes investigated by Irie and co-workers; bottom) Application of the correlation between the amount of transferred charge between S_0 and S_1 (Q^*) and the ring-closure quantum yield ($\Phi_{OF\text{-}CF}$).

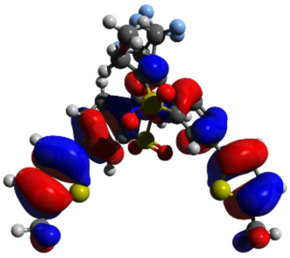
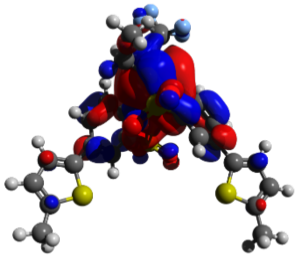
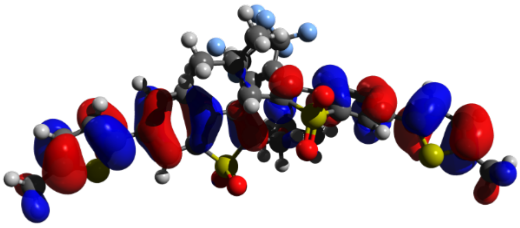
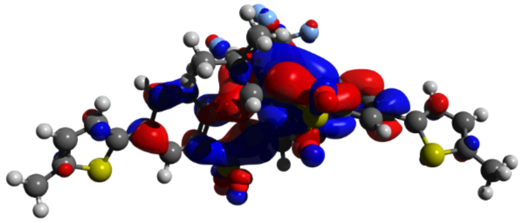
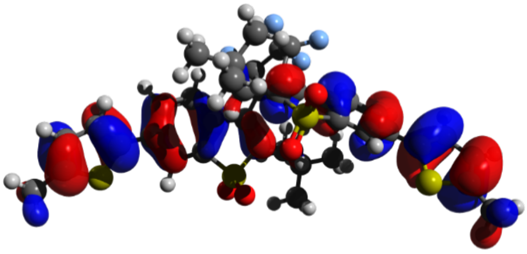
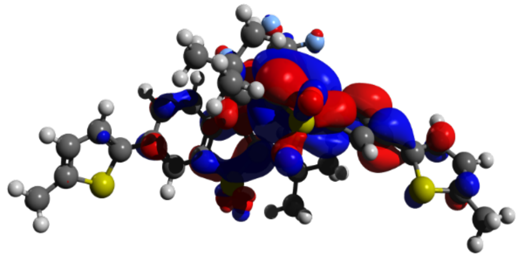
	HOMO	LUMO
1a		
2a		
3a		

Figure S26: CAM-B3LYP/6-311G(d,p)//ωB97XD/6-311G(d,p) HOMOs and LUMOs of derivatives **1a** – **3a** investigated by Irie and co-workers.

Cartesian coordinates of the optimized geometries for *ap*, *p-N*, *p-S* and CF forms of the investigated terarylenes in the ground state:

1-*ap*

1	6	0.835213	6.730222	-0.453804
2	6	0.353218	5.427592	-0.526398
3	6	1.093370	4.369642	0.012160
4	6	2.325693	4.637298	0.621385
5	6	2.804784	5.939356	0.689760
6	6	2.061574	6.989824	0.153420
7	1	0.252574	7.542466	-0.876693
8	1	-0.600540	5.242128	-1.013487
9	1	2.896351	3.815114	1.039317
10	1	3.760686	6.134988	1.165587
11	1	2.437641	8.006717	0.208903
12	6	0.616990	2.977168	-0.047492
13	16	-0.998693	2.557679	-0.557019
14	6	0.657057	0.770344	0.166951
15	6	-0.626033	0.882886	-0.306358
16	7	1.346504	1.952901	0.293100
17	6	1.329847	-0.483041	0.556210
18	6	0.816309	-1.439171	1.390536
19	7	2.586846	-0.731648	0.051164
20	16	1.965950	-2.727880	1.531941
21	6	3.055750	-1.871544	0.466792
22	6	4.376004	-2.399439	0.081956
23	6	4.848662	-3.628530	0.553929
24	6	5.181241	-1.643995	-0.779856
25	6	6.102729	-4.093046	0.171371
26	1	4.241895	-4.233522	1.222578
27	6	6.433091	-2.111053	-1.159765
28	1	4.811544	-0.692160	-1.145606
29	6	6.898827	-3.336415	-0.685145
30	1	6.458508	-5.047554	0.546421
31	1	7.048460	-1.515470	-1.826995
32	1	7.877542	-3.700611	-0.982020
33	6	-1.615738	-0.155642	-0.603901
34	6	-1.381535	-1.300356	-1.320089
35	7	-2.900422	0.012984	-0.133892
36	16	-2.841310	-2.230175	-1.368321
37	6	-3.664091	-0.991363	-0.452106
38	6	-5.080665	-1.093721	-0.064010
39	6	-5.919556	-2.086343	-0.581374
40	6	-5.599822	-0.168204	0.850026
41	6	-7.252388	-2.153851	-0.189307
42	1	-5.541437	-2.808583	-1.300243
43	6	-6.932170	-0.237228	1.236988
44	1	-4.946331	0.598755	1.251569
45	6	-7.762707	-1.230503	0.720176
46	1	-7.893746	-2.927992	-0.598587
47	1	-7.322456	0.484746	1.947637
48	1	-8.803366	-1.284998	1.024422
49	6	-0.128925	-1.772192	-1.985978
50	1	0.557569	-0.933936	-2.128277

51	1	0.385152	-2.523982	-1.376320
52	1	-0.340836	-2.216193	-2.962552
53	6	-0.494983	-1.480479	2.108989
54	1	-0.924492	-0.477096	2.163221
55	1	-1.212023	-2.123175	1.585485
56	1	-0.378803	-1.862590	3.127039

1-*p*-*N*

1	6	6.885313	-2.327599	-0.482574
2	6	5.541451	-2.106585	-0.213859
3	6	4.976248	-0.847710	-0.428292
4	6	5.780734	0.187651	-0.913608
5	6	7.123505	-0.036230	-1.177759
6	6	7.680432	-1.293540	-0.963949
7	1	7.312691	-3.308490	-0.311414
8	1	4.937552	-2.921657	0.170811
9	1	5.338987	1.162167	-1.080139
10	1	7.738439	0.773288	-1.553640
11	1	8.730295	-1.466232	-1.170161
12	6	3.556719	-0.577382	-0.144966
13	16	2.423809	-1.834366	0.263462
14	6	1.689957	0.587902	0.100596
15	6	1.173640	-0.646633	0.397757
16	7	3.028959	0.610147	-0.191893
17	6	0.889719	1.823118	0.056003
18	6	1.275904	3.055106	0.504766
19	7	-0.396599	1.735819	-0.421079
20	16	-0.053647	4.152997	0.327018
21	6	-1.024158	2.864981	-0.339704
22	6	-2.435363	3.031685	-0.723116
23	6	-3.008314	4.289299	-0.916913
24	6	-3.222667	1.887386	-0.886921
25	6	-4.348630	4.401593	-1.263648
26	1	-2.409595	5.187333	-0.806541
27	6	-4.559582	2.004011	-1.236058
28	1	-2.772098	0.914429	-0.730869
29	6	-5.127404	3.260916	-1.423815
30	1	-4.784217	5.382637	-1.412444
31	1	-5.161491	1.110696	-1.357098
32	1	-6.173513	3.351547	-1.692471
33	6	-0.184930	-1.006898	0.811063
34	6	-0.858266	-0.421762	1.846175
35	7	-0.865285	-1.982420	0.122470
36	16	-2.444622	-1.100068	1.928670
37	6	-2.067224	-2.146096	0.584210
38	6	-3.037021	-3.106318	0.030727
39	6	-4.283558	-3.314094	0.624861
40	6	-2.702319	-3.827614	-1.119158
41	6	-5.178733	-4.224925	0.080484
42	1	-4.563399	-2.769706	1.520587
43	6	-3.598679	-4.738028	-1.659213
44	1	-1.736382	-3.663767	-1.580423
45	6	-4.839473	-4.940130	-1.062392
46	1	-6.142192	-4.376760	0.552650
47	1	-3.328688	-5.290502	-2.551823

48	1	-5.538755	-5.651801	-1.485709
49	6	-0.412456	0.654994	2.778333
50	1	0.677627	0.698391	2.801330
51	1	-0.780702	1.631639	2.449202
52	1	-0.774022	0.480070	3.792930
53	6	2.570406	3.495381	1.107016
54	1	3.215241	2.632420	1.266053
55	1	3.096081	4.189951	0.446562
56	1	2.408485	3.997650	2.063448

1-*p*-*S*

1	6	-7.219906	-0.087353	-1.003518
2	6	-5.923462	-0.540589	-0.800232
3	6	-4.921587	0.345052	-0.398114
4	6	-5.240392	1.691842	-0.200233
5	6	-6.536870	2.140457	-0.403117
6	6	-7.530490	1.253284	-0.805801
7	1	-7.987979	-0.784828	-1.316065
8	1	-5.701321	-1.590940	-0.956118
9	1	-4.460864	2.375679	0.111452
10	1	-6.771847	3.186918	-0.247174
11	1	-8.542916	1.606033	-0.964732
12	6	-3.534513	-0.098013	-0.177565
13	16	-3.010151	-1.731444	-0.485604
14	6	-1.399945	0.018941	0.393104
15	6	-1.416268	-1.303398	0.033731
16	7	-2.592179	0.680326	0.263854
17	6	-0.211740	0.745592	0.875093
18	6	0.586116	0.353978	1.911238
19	7	0.166659	1.893903	0.223478
20	16	1.897543	1.472526	2.055910
21	6	1.256978	2.392816	0.719166
22	6	1.904992	3.609301	0.199414
23	6	3.068693	4.130476	0.768623
24	6	1.337040	4.256511	-0.902065
25	6	3.653044	5.276960	0.246057
26	1	3.526509	3.646225	1.624765
27	6	1.923050	5.400928	-1.421011
28	1	0.435733	3.848139	-1.341674
29	6	3.083000	5.915502	-0.849480
30	1	4.555574	5.671841	0.697621
31	1	1.473825	5.892680	-2.276101
32	1	3.540619	6.809637	-1.256634
33	6	-0.272748	-2.219732	-0.013806
34	6	-0.238670	-3.501316	0.462475
35	7	0.912891	-1.734248	-0.512519
36	16	1.365156	-4.121649	0.276741
37	6	1.868404	-2.603635	-0.421016
38	6	3.257425	-2.318525	-0.815865
39	6	4.195468	-3.332745	-1.013309
40	6	3.643070	-0.985062	-0.986668
41	6	5.500413	-3.018903	-1.370804
42	1	3.910960	-4.373196	-0.896484
43	6	4.945954	-0.676647	-1.347389
44	1	2.911865	-0.201791	-0.825982

45	6	5.878907	-1.691626	-1.539256
46	1	6.221543	-3.813535	-1.522039
47	1	5.235220	0.360165	-1.474832
48	1	6.898157	-1.449319	-1.816982
49	6	-1.325616	-4.310010	1.094449
50	1	-2.042240	-3.653075	1.590818
51	1	-1.865784	-4.900783	0.349695
52	1	-0.924943	-4.997462	1.840625
53	6	0.472467	-0.838569	2.802474
54	1	-0.543176	-1.235362	2.765533
55	1	1.154250	-1.631445	2.479695
56	1	0.707563	-0.589468	3.838707

1-CF

1	6	-0.985529	3.073693	-0.004762
2	6	-0.834145	0.864791	-0.026987
3	6	0.592527	1.177735	0.023912
4	16	0.800175	2.914262	-0.065595
5	6	1.524237	0.221013	0.167453
6	6	1.062988	-1.214402	0.441867
7	16	2.559475	-2.186734	-0.022148
8	6	3.535574	-0.696988	0.068082
9	6	-1.234539	-0.421815	-0.152068
10	6	-0.180947	-1.504442	-0.417897
11	16	-1.086936	-3.041743	0.044136
12	6	-2.621560	-2.142503	-0.051549
13	7	-1.656103	1.981642	0.016888
14	7	-2.537046	-0.862014	-0.136886
15	7	2.888699	0.410982	0.154312
16	6	-3.905718	-2.854009	-0.000637
17	6	-3.977771	-4.244045	-0.120130
18	6	-5.083561	-2.117778	0.172591
19	6	-5.207040	-4.887173	-0.067905
20	1	-3.076085	-4.827935	-0.267144
21	6	-6.307559	-2.764039	0.225517
22	1	-5.019264	-1.041310	0.268871
23	1	-5.254171	-5.965045	-0.166932
24	1	-7.215215	-2.188329	0.363100
25	6	5.002248	-0.765627	0.015289
26	6	5.674660	-1.989913	0.006183
27	6	5.740532	0.422516	-0.035279
28	6	7.061129	-2.026876	-0.055806
29	1	5.121256	-2.921171	0.054405
30	6	7.124051	0.380885	-0.095149
31	1	5.215254	1.369222	-0.029336
32	1	7.572797	-2.981776	-0.062262
33	1	7.687655	1.305560	-0.135115
34	6	0.823432	-1.364388	1.954854
35	1	-0.034296	-0.761602	2.263485
36	1	0.634042	-2.403308	2.224194
37	1	1.705053	-1.017529	2.495863
38	6	0.100751	-1.533607	-1.932063
39	1	0.599440	-0.612169	-2.241954
40	1	0.732320	-2.379952	-2.201646
41	1	-0.843717	-1.616564	-2.471824

42	6	-1.608457	4.405638	-0.004859
43	6	-0.849509	5.569093	0.137043
44	6	-2.996649	4.504380	-0.148405
45	6	-1.467737	6.812228	0.133544
46	1	0.226521	5.512670	0.259975
47	6	-3.609485	5.746971	-0.151639
48	1	-3.577875	3.597586	-0.259066
49	6	-2.847034	6.903839	-0.011445
50	1	-0.871151	7.709504	0.246172
51	1	-4.684652	5.816432	-0.267374
52	1	-3.328608	7.874727	-0.015429
53	6	-6.372709	-4.150057	0.104941
54	6	7.787795	-0.843250	-0.106582
55	1	8.870117	-0.873508	-0.155786
56	1	-7.331549	-4.653556	0.146623

2-*ap*

1	6	1.507596	2.976377	-0.040505
2	6	1.302146	0.782906	0.165551
3	6	0.060113	1.032185	-0.354386
4	16	-0.115602	2.733023	-0.623881
5	6	-1.020033	0.102903	-0.690910
6	6	-0.873500	-1.053074	-1.404280
7	16	-2.411682	-1.840533	-1.500329
8	6	-3.140279	-0.532417	-0.602755
9	6	1.806169	-0.539064	0.577534
10	6	1.148245	-1.416717	1.391871
11	16	2.107931	-2.847472	1.554636
12	6	3.324122	-2.147548	0.518039
13	7	2.107396	1.882195	0.321746
14	7	3.027587	-0.955211	0.102578
15	7	-2.295102	0.390440	-0.258397
16	6	4.569073	-2.851923	0.168203
17	6	4.740215	-4.213957	0.423500
18	6	5.603320	-2.137669	-0.443863
19	6	5.926197	-4.848987	0.079975
20	1	3.944947	-4.789702	0.885040
21	6	6.785504	-2.775963	-0.787758
22	1	5.465791	-1.081598	-0.640314
23	1	6.046752	-5.906780	0.282016
24	1	7.582231	-2.212387	-1.259383
25	6	-4.566243	-0.509350	-0.252181
26	6	-5.481244	-1.403586	-0.801505
27	6	-5.032239	0.441851	0.665944
28	6	-6.825923	-1.368728	-0.452647
29	1	-5.158132	-2.145267	-1.524355
30	6	-6.363985	0.487832	1.019399
31	1	-4.330020	1.143285	1.099265
32	1	-7.505118	-2.079554	-0.903184
33	1	-6.726834	1.219006	1.731701
34	6	0.346915	-1.640741	-2.032412
35	1	1.112097	-0.872133	-2.149245
36	1	0.765983	-2.436250	-1.409318
37	1	0.124136	-2.060940	-3.014707
38	6	-0.173256	-1.281467	2.075308

39	1	-0.467244	-0.231742	2.114116
40	1	-0.953413	-1.827617	1.537026
41	1	-0.131849	-1.667267	3.095490
42	6	2.133720	4.307697	0.026124
43	6	1.391487	5.478998	-0.138990
44	6	3.508060	4.398231	0.265430
45	6	2.012808	6.718486	-0.069142
46	1	0.321890	5.431266	-0.314135
47	6	4.124750	5.638292	0.335912
48	1	4.078918	3.486921	0.392929
49	6	3.380234	6.802139	0.168198
50	1	1.426524	7.620780	-0.196965
51	1	5.191238	5.698017	0.519558
52	1	3.863978	7.770349	0.223982
53	6	6.951950	-4.132812	-0.526599
54	6	-7.275189	-0.419691	0.465486
55	1	7.877261	-4.629476	-0.794492
56	8	-8.553689	-0.297703	0.878462
57	6	-9.522377	-1.188787	0.347669
58	1	-9.279836	-2.228583	0.587385
59	1	-10.464345	-0.920711	0.820806
60	1	-9.615094	-1.072747	-0.736496

2-*p*-*N*

1	6	3.501443	-1.606965	-0.139049
2	6	2.218603	0.180358	0.116688
3	6	1.288712	-0.762838	0.471073
4	16	2.000820	-2.335305	0.355165
5	6	-0.097788	-0.600762	0.912799
6	6	-0.516296	0.252742	1.893327
7	16	-2.235842	0.129318	2.036449
8	6	-2.254308	-1.091419	0.787571
9	6	1.953175	1.625196	0.030498
10	6	2.812000	2.616924	0.414459
11	16	2.031130	4.145508	0.188576
12	6	0.609550	3.328899	-0.406413
13	7	3.457089	-0.309715	-0.211543
14	7	0.726713	2.039157	-0.431481
15	7	-1.076332	-1.359923	0.313297
16	6	-0.622155	4.038572	-0.787212
17	6	-0.622039	5.394400	-1.118822
18	6	-1.825654	3.327100	-0.809317
19	6	-1.807856	6.030321	-1.462893
20	1	0.306015	5.956400	-1.120981
21	6	-3.006773	3.965374	-1.156992
22	1	-1.818908	2.276211	-0.545175
23	1	-1.796799	7.083151	-1.719557
24	1	-3.935881	3.407143	-1.168184
25	6	-3.489111	-1.739302	0.325756
26	6	-4.736075	-1.436633	0.866104
27	6	-3.420496	-2.697537	-0.695241
28	6	-5.892453	-2.060952	0.413967
29	1	-4.827737	-0.699578	1.656997
30	6	-4.559828	-3.325138	-1.151758
31	1	-2.457209	-2.939363	-1.126806
32	1	-6.841488	-1.797872	0.860810

33	1	-4.510742	-4.066258	-1.940430
34	6	0.277366	1.187607	2.744078
35	1	1.316765	0.857963	2.788199
36	1	0.263604	2.200639	2.330554
37	1	-0.115221	1.230596	3.761357
38	6	4.193924	2.521140	0.975846
39	1	4.349271	1.537528	1.418199
40	1	4.946108	2.657295	0.194217
41	1	4.361493	3.279902	1.742456
42	6	4.703994	-2.399055	-0.446513
43	6	4.647485	-3.785369	-0.604979
44	6	5.931071	-1.745242	-0.590236
45	6	5.797517	-4.505448	-0.898277
46	1	3.703116	-4.310482	-0.509383
47	6	7.077712	-2.468104	-0.884499
48	1	5.972113	-0.670003	-0.467244
49	6	7.015297	-3.849825	-1.039087
50	1	5.739051	-5.580332	-1.022376
51	1	8.024756	-1.952239	-0.992530
52	1	7.912798	-4.412221	-1.269069
53	6	-3.002067	5.318657	-1.483201
54	6	-5.808955	-3.012980	-0.601678
55	1	-3.926649	5.816548	-1.751539
56	8	-6.863336	-3.679159	-1.116894
57	6	-8.158184	-3.382746	-0.617320
58	1	-8.413478	-2.331565	-0.782601
59	1	-8.844332	-4.013905	-1.177495
60	1	-8.236845	-3.617102	0.448687

2-*p*-*S*

1	6	-3.978098	-0.318066	-0.292799
2	6	-1.899400	-0.023268	0.399710
3	6	-1.787310	-1.345373	0.057272
4	16	-3.305548	-1.904136	-0.553788
5	6	-0.566463	-2.156713	0.084872
6	6	-0.442861	-3.431668	0.560968
7	16	1.223539	-3.896103	0.480574
8	6	1.625233	-2.331423	-0.185027
9	6	-0.800540	0.790761	0.948856
10	6	-0.058445	0.466710	2.047775
11	16	1.175012	1.659965	2.256755
12	6	0.584078	2.512999	0.854173
13	7	-3.130354	0.540247	0.191053
14	7	-0.440654	1.944567	0.296722
15	7	0.598407	-1.557167	-0.337233
16	6	1.200040	3.754498	0.355245
17	6	2.369786	4.274948	0.912894
18	6	0.600406	4.423539	-0.715962
19	6	2.927414	5.443605	0.410845
20	1	2.855593	3.770053	1.741225
21	6	1.161025	5.589152	-1.215792
22	1	-0.305098	4.016103	-1.147810
23	1	3.835117	5.837215	0.853048
24	1	0.687341	6.098061	-2.047342
25	6	2.999293	-1.920065	-0.498316
26	6	4.049217	-2.828357	-0.590967

27	6	3.269090	-0.559844	-0.705619
28	6	5.343182	-2.409000	-0.877714
29	1	3.870787	-3.888758	-0.446550
30	6	4.547696	-0.131721	-0.992928
31	1	2.458442	0.155370	-0.631358
32	1	6.132257	-3.145602	-0.942739
33	1	4.761486	0.918824	-1.149171
34	6	-1.482902	-4.349741	1.117420
35	1	-2.322312	-3.774052	1.511100
36	1	-1.865972	-5.028359	0.350412
37	1	-1.079964	-4.956258	1.930036
38	6	-0.164777	-0.717323	2.951214
39	1	-1.153120	-1.169695	2.856564
40	1	0.577373	-1.476317	2.685082
41	1	-0.008950	-0.441627	3.995626
42	6	-5.378220	0.005723	-0.611668
43	6	-6.345322	-0.988992	-0.769132
44	6	-5.746505	1.346811	-0.753936
45	6	-7.657656	-0.648619	-1.069318
46	1	-6.083065	-2.034170	-0.643811
47	6	-7.058774	1.682367	-1.052126
48	1	-4.992884	2.114821	-0.631430
49	6	-8.017871	0.686765	-1.211949
50	1	-8.401095	-1.428409	-1.185332
51	1	-7.332761	2.724908	-1.165049
52	1	-9.043175	0.950212	-1.444332
53	6	2.325916	6.103871	-0.654554
54	6	5.598686	-1.053091	-1.081337
55	1	2.763495	7.014527	-1.046854
56	8	6.813016	-0.536630	-1.364327
57	6	7.919719	-1.421536	-1.441981
58	1	7.783147	-2.159857	-2.238083
59	1	8.782951	-0.800573	-1.670770
60	1	8.082617	-1.934209	-0.489007

2-CF

1	6	-1.825577	3.003106	0.008874
2	6	-1.465951	0.818867	-0.009162
3	6	-0.075687	1.265244	0.047717
4	16	-0.033790	3.015015	-0.041733
5	6	0.942606	0.401495	0.192441
6	6	0.617469	-1.072136	0.464484
7	16	2.200251	-1.897786	0.006152
8	6	3.033657	-0.322693	0.101868
9	6	-1.742673	-0.499234	-0.138607
10	6	-0.590445	-1.476588	-0.401081
11	16	-1.348421	-3.093869	0.054505
12	6	-2.961922	-2.343733	-0.052734
13	7	-2.390542	1.852479	0.030682
14	7	-2.997958	-1.061063	-0.134341
15	7	2.282133	0.719592	0.184668
16	6	-4.172883	-3.174964	-0.017339
17	6	-4.107131	-4.566457	-0.121556
18	6	-5.419944	-2.555712	0.125707
19	6	-5.268616	-5.326361	-0.084568
20	1	-3.150490	-5.061758	-0.244654

21	6	-6.576096	-3.318209	0.163257
22	1	-5.464262	-1.477091	0.209741
23	1	-5.206905	-6.404535	-0.171490
24	1	-7.537598	-2.831690	0.277402
25	6	4.493178	-0.256725	0.048732
26	6	5.286100	-1.402362	0.100904
27	6	5.125833	0.991565	-0.068010
28	6	6.670563	-1.325367	0.037395
29	1	4.828901	-2.380169	0.204022
30	6	6.497591	1.080933	-0.133651
31	1	4.520102	1.888035	-0.110576
32	1	7.250838	-2.236515	0.084692
33	1	6.991699	2.040067	-0.228864
34	6	0.386166	-1.244711	1.976267
35	1	-0.527276	-0.727905	2.280793
36	1	0.296777	-2.297036	2.245462
37	1	1.227728	-0.814571	2.521259
38	6	-0.299752	-1.476328	-1.913720
39	1	0.115511	-0.512803	-2.218727
40	1	0.407609	-2.260926	-2.181679
41	1	-1.230105	-1.642971	-2.458661
42	6	-2.574601	4.268877	-0.002845
43	6	-1.937181	5.500822	0.156285
44	6	-3.962246	4.231275	-0.176985
45	6	-2.675032	6.677061	0.140583
46	1	-0.863715	5.551883	0.301924
47	6	-4.694581	5.407396	-0.192333
48	1	-4.449439	3.272636	-0.302916
49	6	-4.053297	6.632985	-0.033876
50	1	-2.172113	7.628234	0.267301
51	1	-5.768572	5.369357	-0.331525
52	1	-4.627167	7.552352	-0.047176
53	6	-6.503625	-4.705136	0.057990
54	6	7.285412	-0.078314	-0.083608
55	1	-7.409811	-5.299095	0.086891
56	8	8.614587	0.113188	-0.159317
57	6	9.468482	-1.021496	-0.107489
58	1	9.266898	-1.705808	-0.936732
59	1	10.480689	-0.633902	-0.195250
60	1	9.361035	-1.550721	0.843794

3-*ap*

1	6	-1.761248	2.993167	0.078018
2	6	-1.558910	0.798216	-0.117534
3	6	-0.331546	1.042784	0.438059
4	16	-0.152795	2.744458	0.700779
5	6	0.733563	0.106946	0.803171
6	6	0.559863	-1.043486	1.517210
7	16	2.088137	-1.850435	1.640682
8	6	2.849683	-0.552743	0.748321
9	6	-2.050747	-0.522974	-0.546388
10	6	-1.365473	-1.394419	-1.344639
11	16	-2.314189	-2.827014	-1.544185
12	6	-3.570997	-2.130608	-0.553246
13	7	-2.354336	1.900644	-0.299872

14	7	-3.287644	-0.942578	-0.116637
15	7	2.019143	0.379870	0.390273
16	6	-4.819647	-2.847332	-0.242261
17	6	-5.131826	-4.067347	-0.845715
18	6	-5.716108	-2.292928	0.676121
19	6	-6.315889	-4.722467	-0.536231
20	1	-4.454662	-4.512897	-1.566714
21	6	-6.899185	-2.949652	0.981798
22	1	-5.472895	-1.346408	1.142742
23	1	-6.545145	-5.668190	-1.013007
24	1	-7.586835	-2.511510	1.695948
25	6	4.275005	-0.558581	0.414752
26	6	5.173403	-1.477178	0.963012
27	6	4.779251	0.380942	-0.490786
28	6	6.512814	-1.471907	0.623235
29	1	4.831140	-2.215332	1.681659
30	6	6.113552	0.401501	-0.842201
31	1	4.100490	1.104614	-0.926488
32	1	7.165301	-2.201684	1.082424
33	1	6.449553	1.146948	-1.549853
34	6	-0.679437	-1.615459	2.122655
35	1	-1.438406	-0.838030	2.221213
36	1	-1.095404	-2.408310	1.493791
37	1	-0.481788	-2.034625	3.110881
38	6	-0.022782	-1.252992	-1.984134
39	1	0.260663	-0.200525	-2.027281
40	1	0.743949	-1.781270	-1.409893
41	1	-0.023642	-1.653839	-2.999222
42	6	-2.371342	4.329566	-0.030854
43	6	-1.750731	5.466106	0.491791
44	6	-3.606635	4.461364	-0.671983
45	6	-2.350700	6.712051	0.369865
46	1	-0.796078	5.386465	1.000764
47	6	-4.204010	5.707314	-0.789810
48	1	-4.084971	3.577612	-1.075383
49	6	-3.578334	6.836798	-0.270618
50	1	-1.858967	7.586268	0.779950
51	1	-5.161197	5.798386	-1.289929
52	1	-4.046062	7.809852	-0.365356
53	6	-7.203230	-4.166178	0.378000
54	6	7.025446	-0.533261	-0.299894
55	7	8.344689	-0.529451	-0.654784
56	6	9.264002	-1.474953	-0.052851
57	1	10.253032	-1.332554	-0.483156
58	1	9.342237	-1.337115	1.032327
59	1	8.961185	-2.509736	-0.246259
60	6	8.850426	0.479708	-1.564864
61	1	8.352950	0.428133	-2.539486
62	1	8.719230	1.492241	-1.165034
63	1	9.913960	0.315029	-1.724125
64	1	-8.128423	-4.677077	0.618218

3-*p*-*N*

1	6	3.574910	-1.840458	-0.124139
2	6	2.453812	0.054066	0.117205
3	6	1.460413	-0.796939	0.526851

4	16	2.031622	-2.427008	0.427482
5	6	0.111288	-0.491398	1.007407
6	6	-0.179265	0.411344	1.988829
7	16	-1.898753	0.492125	2.172329
8	6	-2.091305	-0.726933	0.932433
9	6	2.301865	1.513421	0.000818
10	6	3.237041	2.444489	0.356230
11	16	2.570749	4.023276	0.108695
12	6	1.084333	3.305085	-0.455202
13	7	3.635991	-0.546294	-0.233100
14	7	1.104718	2.010155	-0.456954
15	7	-0.962535	-1.136119	0.435718
16	6	-0.091626	4.098407	-0.847869
17	6	0.000408	5.460356	-1.139125
18	6	-1.335311	3.464234	-0.925497
19	6	-1.133175	6.177897	-1.498131
20	1	0.959695	5.965333	-1.096156
21	6	-2.464166	4.183697	-1.288317
22	1	-1.401813	2.407902	-0.693809
23	1	-1.049079	7.234811	-1.722330
24	1	-3.424121	3.683475	-1.344133
25	6	-3.404570	-1.221279	0.513188
26	6	-4.598989	-0.715210	1.031407
27	6	-3.493253	-2.238351	-0.443017
28	6	-5.828389	-1.195565	0.622090
29	1	-4.582225	0.074668	1.775872
30	6	-4.711912	-2.731613	-0.863133
31	1	-2.580523	-2.647433	-0.859589
32	1	-6.720646	-0.768708	1.058769
33	1	-4.722829	-3.521163	-1.602002
34	6	0.737836	1.260214	2.805347
35	1	1.734656	0.816367	2.825835
36	1	0.826742	2.264934	2.380612
37	1	0.382319	1.357005	3.832657
38	6	4.612533	2.255859	0.908695
39	1	4.721718	1.243410	1.296317
40	1	5.370538	2.399826	0.134013
41	1	4.814572	2.964929	1.713940
42	6	4.692860	-2.738735	-0.459843
43	6	4.613639	-4.117776	-0.254370
44	6	5.863856	-2.195965	-0.997059
45	6	5.682920	-4.939366	-0.584436
46	1	3.717369	-4.560548	0.166981
47	6	6.930912	-3.019720	-1.323463
48	1	5.923034	-1.126620	-1.157000
49	6	6.844231	-4.393577	-1.119465
50	1	5.607058	-6.007886	-0.421156
51	1	7.832947	-2.588111	-1.741469
52	1	7.678008	-5.036233	-1.377406
53	6	-2.367366	5.542521	-1.574578
54	6	-5.923851	-2.220969	-0.344447
55	7	-7.135031	-2.698032	-0.761738
56	6	-8.356811	-2.203633	-0.158374
57	1	-9.208619	-2.695847	-0.623097
58	1	-8.394064	-2.404039	0.919495
59	1	-8.471390	-1.125045	-0.310067

60	6	-7.197389	-3.808186	-1.692219
61	1	-6.709092	-3.564675	-2.641691
62	1	-6.725860	-4.711215	-1.285629
63	1	-8.239983	-4.036294	-1.903550
64	1	-3.251166	6.103398	-1.855862

3-*p*-*S*

1	6	-4.190593	-0.271004	-0.326989
2	6	-2.116268	-0.021436	0.400353
3	6	-2.020401	-1.340256	0.041081
4	16	-3.539866	-1.866045	-0.596520
5	6	-0.814128	-2.173055	0.075777
6	6	-0.722349	-3.458168	0.528881
7	16	0.939629	-3.947914	0.475910
8	6	1.382583	-2.374209	-0.149615
9	6	-1.009988	0.771644	0.965524
10	6	-0.281696	0.431309	2.068469
11	16	0.971298	1.602142	2.289611
12	6	0.407000	2.468372	0.884754
13	7	-3.335223	0.563746	0.183679
14	7	-0.624320	1.920294	0.319052
15	7	0.368656	-1.583103	-0.310407
16	6	1.048873	3.698445	0.390242
17	6	2.234341	4.188808	0.941932
18	6	0.457521	4.386388	-0.673574
19	6	2.814911	5.347120	0.441505
20	1	2.714487	3.667941	1.763692
21	6	1.041062	5.541164	-1.171863
22	1	-0.459727	4.001433	-1.101223
23	1	3.734436	5.717710	0.879202
24	1	0.573316	6.064785	-1.997624
25	6	2.767626	-1.981849	-0.414587
26	6	3.817831	-2.899660	-0.470694
27	6	3.071621	-0.629643	-0.606575
28	6	5.118995	-2.495843	-0.705275
29	1	3.625567	-3.959285	-0.333327
30	6	4.364592	-0.208215	-0.841263
31	1	2.270814	0.099488	-0.559934
32	1	5.895503	-3.247457	-0.738631
33	1	4.547198	0.849407	-0.974009
34	6	-1.787759	-4.371304	1.044373
35	1	-2.626492	-3.791625	1.433700
36	1	-2.165873	-5.028355	0.256255
37	1	-1.411137	-5.001158	1.851989
38	6	-0.412206	-0.756878	2.963011
39	1	-1.406347	-1.194130	2.858081
40	1	0.320547	-1.524562	2.695608
41	1	-0.259382	-0.491353	4.010522
42	6	-5.584334	0.081849	-0.645925
43	6	-6.497448	-0.866144	-1.112150
44	6	-6.002556	1.405097	-0.475442
45	6	-7.804334	-0.498451	-1.402817
46	1	-6.196716	-1.899583	-1.248871
47	6	-7.309038	1.768260	-0.765897
48	1	-5.291341	2.137698	-0.115052
49	6	-8.214295	0.818879	-1.230310

50	1	-8.503794	-1.243757	-1.762580
51	1	-7.621920	2.796982	-0.629457
52	1	-9.235501	1.103727	-1.455346
53	6	2.221225	6.026432	-0.616288
54	6	5.432863	-1.132598	-0.901215
55	7	6.715762	-0.723443	-1.137975
56	6	7.800363	-1.684614	-1.109102
57	1	8.736968	-1.172445	-1.319467
58	1	7.891514	-2.172534	-0.130792
59	1	7.666953	-2.462459	-1.868532
60	6	7.017347	0.690248	-1.249692
61	1	6.477183	1.151298	-2.083273
62	1	6.765751	1.237458	-0.332793
63	1	8.082215	0.814189	-1.435357
64	1	2.676512	6.929059	-1.007004

3-CF

1	6	-1.998196	3.031466	0.001620
2	6	-1.708906	0.836198	-0.021534
3	6	-0.306324	1.239003	0.039452
4	16	-0.208718	2.987392	-0.050020
5	6	0.686823	0.346584	0.191350
6	6	0.314407	-1.113920	0.472374
7	16	1.871584	-1.992790	0.030417
8	6	2.757990	-0.441883	0.113697
9	6	-2.026049	-0.473434	-0.148056
10	6	-0.902358	-1.487374	-0.395312
11	16	-1.710924	-3.076652	0.071429
12	6	-3.302551	-2.279642	-0.052956
13	7	-2.600479	1.899280	0.017541
14	7	-3.297938	-0.997851	-0.147284
15	7	2.032757	0.624069	0.186462
16	6	-4.537801	-3.074748	-0.027962
17	6	-4.508441	-4.465581	0.099261
18	6	-5.771907	-2.421836	-0.127163
19	6	-5.691549	-5.191427	0.129413
20	1	-3.562212	-4.990034	0.173590
21	6	-6.949999	-3.150351	-0.100572
22	1	-5.787868	-1.343651	-0.225822
23	1	-5.657013	-6.269561	0.230950
24	1	-7.901383	-2.637860	-0.181143
25	6	4.210032	-0.425692	0.065600
26	6	4.974916	-1.598453	0.052543
27	6	4.894377	0.798323	0.019290
28	6	6.351935	-1.562822	-0.011660
29	1	4.489409	-2.567367	0.103259
30	6	6.267810	0.853439	-0.045299
31	1	4.323172	1.718681	0.032222
32	1	6.893829	-2.498109	-0.011659
33	1	6.747273	1.821824	-0.078406
34	6	0.069088	-1.264539	1.984372
35	1	-0.830882	-0.718451	2.277993
36	1	-0.052765	-2.311034	2.263335
37	1	0.919823	-0.853769	2.530086
38	6	-0.604270	-1.510110	-1.906213
39	1	-0.160796	-0.561325	-2.217850

40	1	0.082220	-2.316530	-2.163657
41	1	-1.536393	-1.655541	-2.454276
42	6	-2.705779	4.321145	0.003003
43	6	-2.025367	5.529303	0.166974
44	6	-4.095351	4.332443	-0.158812
45	6	-2.722274	6.730146	0.167867
46	1	-0.949567	5.540812	0.303980
47	6	-4.786970	5.533089	-0.157873
48	1	-4.615721	3.391705	-0.286898
49	6	-4.102726	6.734679	0.005196
50	1	-2.186519	7.662696	0.298568
51	1	-5.862870	5.533699	-0.287413
52	1	-4.645019	7.673092	0.005220
53	6	-6.913245	-4.536726	0.028556
54	6	7.045449	-0.331154	-0.072375
55	7	8.403169	-0.284521	-0.154552
56	6	9.178131	-1.511460	-0.122909
57	1	10.232802	-1.270846	-0.236781
58	1	9.049789	-2.049551	0.823523
59	1	8.896872	-2.181217	-0.941656
60	6	9.092414	0.992962	-0.144457
61	1	8.777479	1.623378	-0.982019
62	1	8.917627	1.542598	0.787632
63	1	10.161872	0.820458	-0.241480
64	1	-7.836628	-5.103894	0.049822

4-*ap*

1	6	1.273248	2.995864	-0.052533
2	6	1.181570	0.795916	0.168328
3	6	-0.065945	0.975904	-0.365880
4	16	-0.332618	2.663877	-0.641733
5	6	-1.087007	-0.015339	-0.710000
6	6	-0.867006	-1.164463	-1.421237
7	16	-2.351843	-2.038626	-1.532791
8	6	-3.160501	-0.782522	-0.638117
9	6	1.755544	-0.496105	0.582315
10	6	1.144788	-1.412535	1.390713
11	16	2.183450	-2.786571	1.553977
12	6	3.362863	-2.015368	0.525688
13	7	1.924904	1.937168	0.325498
14	7	3.000982	-0.840462	0.112549
15	7	-2.377967	0.192556	-0.289144
16	6	4.648426	-2.645425	0.181589
17	6	4.884229	-4.003261	0.405435
18	6	5.654756	-1.863563	-0.393052
19	6	6.106631	-4.568237	0.067129
20	1	4.111220	-4.630930	0.836056
21	6	6.873583	-2.432123	-0.731902
22	1	5.468200	-0.810770	-0.565468
23	1	6.276850	-5.623631	0.244307
24	1	7.648165	-1.816126	-1.173921
25	6	-4.595397	-0.829514	-0.313100
26	6	-5.375715	-1.948872	-0.608513
27	6	-5.185506	0.277588	0.311451
28	6	-6.724700	-1.961237	-0.289373
29	1	-4.936973	-2.818548	-1.084264

30	6	-6.529434	0.261917	0.628504
31	1	-4.573973	1.141094	0.539481
32	1	-7.326288	-2.833942	-0.521194
33	1	-6.994406	1.114411	1.109480
34	6	0.391111	-1.680317	-2.037533
35	1	1.107727	-0.867068	-2.158523
36	1	0.854839	-2.441680	-1.403616
37	1	0.199692	-2.123698	-3.016020
38	6	-0.186138	-1.356274	2.067176
39	1	-0.540406	-0.325544	2.110908
40	1	-0.930257	-1.943269	1.520790
41	1	-0.128938	-1.745826	3.085123
42	6	1.825030	4.359368	0.024844
43	6	1.154134	5.457685	-0.517006
44	6	3.059741	4.554312	0.650668
45	6	1.706061	6.728654	-0.430417
46	1	0.198972	5.328327	-1.014888
47	6	3.608778	5.824935	0.733238
48	1	3.576160	3.699416	1.068850
49	6	2.934263	6.916076	0.193573
50	1	1.177094	7.573245	-0.855887
51	1	4.566307	5.964965	1.221197
52	1	3.365240	7.908300	0.259629
53	6	7.104396	-3.785180	-0.502170
54	6	-7.308563	-0.858384	0.329100
55	1	8.057941	-4.227736	-0.765843
56	6	-8.748557	-0.884828	0.664389
57	8	-9.341365	0.023433	1.197610
58	1	-9.273585	-1.820189	0.389516

4-*p*-*N*

1	6	3.551249	-1.414655	-0.130408
2	6	2.150358	0.287920	0.075526
3	6	1.293662	-0.702721	0.480222
4	16	2.107992	-2.226981	0.404010
5	6	-0.089239	-0.602861	0.953106
6	6	-0.513783	0.230701	1.951744
7	16	-2.220336	0.054717	2.133056
8	6	-2.229527	-1.151415	0.876141
9	6	1.777396	1.706487	-0.043625
10	6	2.567358	2.776386	0.273396
11	16	1.650527	4.228848	0.046712
12	6	0.275522	3.280670	-0.455706
13	7	3.414485	-0.127561	-0.254630
14	7	0.500971	2.005540	-0.455877
15	7	-1.056012	-1.382636	0.370347
16	6	-1.031299	3.868296	-0.792279
17	6	-1.188461	5.230672	-1.050967
18	6	-2.149019	3.028978	-0.839827
19	6	-2.443683	5.747027	-1.345820
20	1	-0.331083	5.895241	-1.030833
21	6	-3.399895	3.548078	-1.137504
22	1	-2.019579	1.972858	-0.635720
23	1	-2.555049	6.806498	-1.544355
24	1	-4.260124	2.889210	-1.167951
25	6	-3.454261	-1.836852	0.433414

26	6	-4.692104	-1.584370	1.027875
27	6	-3.368599	-2.767895	-0.610872
28	6	-5.824716	-2.253106	0.590383
29	1	-4.780060	-0.866560	1.835608
30	6	-4.498468	-3.432876	-1.043891
31	1	-2.406338	-2.955060	-1.069638
32	1	-6.783391	-2.054574	1.058002
33	1	-4.440573	-4.156321	-1.848636
34	6	0.271237	1.191045	2.781004
35	1	1.326641	0.914699	2.768999
36	1	0.184976	2.207061	2.384222
37	1	-0.074087	1.199648	3.816039
38	6	3.975846	2.816040	0.770916
39	1	4.267705	1.832763	1.137587
40	1	4.667582	3.093020	-0.029161
41	1	4.087571	3.542065	1.578717
42	6	4.800332	-2.133550	-0.432535
43	6	4.960705	-3.486301	-0.125231
44	6	5.855279	-1.440425	-1.033467
45	6	6.152375	-4.135641	-0.416957
46	1	4.158197	-4.039814	0.350703
47	6	7.045482	-2.091847	-1.320370
48	1	5.727090	-0.391536	-1.270263
49	6	7.198006	-3.440918	-1.014682
50	1	6.265142	-5.185631	-0.174104
51	1	7.857380	-1.546044	-1.786840
52	1	8.129053	-3.948015	-1.239633
53	6	-3.552068	4.908603	-1.389182
54	6	-5.735150	-3.181252	-0.444506
55	1	-4.530773	5.314483	-1.617322
56	6	-6.950032	-3.892512	-0.895611
57	8	-6.970943	-4.713119	-1.782919
58	1	-7.876793	-3.622030	-0.353119

4-*p*-*S*

1	6	-4.045539	0.164960	-0.282077
2	6	-1.948501	0.157797	0.409816
3	6	-1.983693	-1.127922	-0.062042
4	16	-3.553658	-1.454641	-0.704776
5	6	-0.840600	-2.045749	-0.107604
6	6	-0.815952	-3.359807	0.275069
7	16	0.810650	-3.939060	0.175496
8	6	1.334324	-2.366024	-0.363886
9	6	-0.740361	0.742142	1.022927
10	6	-0.142089	0.240869	2.141554
11	16	1.360038	1.061814	2.382958
12	6	1.061760	2.013772	0.952720
13	7	-3.106525	0.872247	0.275185
14	7	-0.068895	1.749609	0.373278
15	7	0.369267	-1.510690	-0.473379
16	6	2.038437	2.986799	0.437381
17	6	3.400124	2.867692	0.723958
18	6	1.602863	4.018413	-0.398180
19	6	4.310903	3.768515	0.187146
20	1	3.757571	2.056875	1.349855
21	6	2.515514	4.916661	-0.931471

22	1	0.546446	4.104504	-0.621541
23	1	5.366318	3.658562	0.407275
24	1	2.168184	5.715026	-1.577050
25	6	2.739513	-2.004392	-0.610953
26	6	3.754904	-2.958595	-0.673204
27	6	3.054168	-0.646047	-0.763627
28	6	5.068688	-2.561367	-0.876226
29	1	3.528064	-4.013303	-0.564603
30	6	4.361787	-0.254605	-0.966982
31	1	2.257529	0.085597	-0.712411
32	1	5.856380	-3.306064	-0.922364
33	1	4.611479	0.794478	-1.078183
34	6	-1.935719	-4.228434	0.749158
35	1	-2.701973	-3.619343	1.232381
36	1	-2.400490	-4.762309	-0.083971
37	1	-1.586888	-4.968093	1.470818
38	6	-0.578099	-0.890258	3.014057
39	1	-1.641562	-1.083929	2.865571
40	1	-0.032609	-1.805012	2.761629
41	1	-0.410218	-0.675031	4.070805
42	6	-5.403868	0.670334	-0.541600
43	6	-6.434531	-0.170600	-0.967097
44	6	-5.666758	2.030223	-0.352402
45	6	-7.703658	0.340294	-1.203322
46	1	-6.256069	-1.230803	-1.111626
47	6	-6.936329	2.536215	-0.587581
48	1	-4.865785	2.679709	-0.022155
49	6	-7.958569	1.693798	-1.014263
50	1	-8.494752	-0.323130	-1.532347
51	1	-7.128309	3.592372	-0.438605
52	1	-8.949924	2.091550	-1.197567
53	6	3.871427	4.794470	-0.641642
54	6	5.379165	-1.211053	-1.021224
55	1	4.582969	5.495848	-1.061682
56	6	6.784510	-0.800032	-1.224576
57	8	7.148251	0.345938	-1.351051
58	1	7.515296	-1.631393	-1.253221

4-*CF*

1	6	-1.525400	3.060947	-0.000034
2	6	-1.337256	0.855559	-0.030798
3	6	0.083166	1.191611	0.031230
4	16	0.263689	2.929928	-0.050351
5	6	1.028890	0.248704	0.178752
6	6	0.591185	-1.193690	0.453392
7	16	2.108642	-2.140895	-0.001506
8	6	3.053890	-0.634322	0.093130
9	6	-1.714530	-0.438061	-0.160040
10	6	-0.642734	-1.505992	-0.413071
11	16	-1.528786	-3.054647	0.049405
12	6	-3.075965	-2.179412	-0.062919
13	7	-2.178075	1.958187	0.010674
14	7	-3.009330	-0.897931	-0.155663
15	7	2.389105	0.462752	0.171414
16	6	-4.350381	-2.908380	-0.025172
17	6	-4.394167	-4.303569	0.031914

18	6	-5.548153	-2.184027	-0.039513
19	6	-5.614449	-4.963740	0.076783
20	1	-3.476139	-4.880898	0.036235
21	6	-6.763435	-2.847069	0.002890
22	1	-5.506734	-1.103060	-0.083435
23	1	-5.638602	-6.045955	0.122021
24	1	-7.686722	-2.279937	-0.008904
25	6	4.523907	-0.666682	0.048660
26	6	5.227165	-1.870301	0.116952
27	6	5.225780	0.541545	-0.070444
28	6	6.613462	-1.868195	0.064600
29	1	4.700327	-2.811491	0.221203
30	6	6.604849	0.539675	-0.122228
31	1	4.671786	1.469647	-0.123939
32	1	7.157514	-2.805041	0.120227
33	1	7.156210	1.467535	-0.216709
34	6	0.346650	-1.346901	1.965028
35	1	-0.522617	-0.758475	2.269045
36	1	0.173085	-2.388771	2.233632
37	1	1.219319	-0.985084	2.510687
38	6	-0.351036	-1.537061	-1.925439
39	1	0.138069	-0.610491	-2.235325
40	1	0.292707	-2.376300	-2.188119
41	1	-1.290860	-1.633769	-2.470914
42	6	-2.167663	4.383380	0.008289
43	6	-1.426685	5.555538	0.171750
44	6	-3.555935	4.464005	-0.145431
45	6	-2.062635	6.789541	0.179898
46	1	-0.351024	5.513255	0.303277
47	6	-4.186443	5.697686	-0.137265
48	1	-4.123113	3.550464	-0.272346
49	6	-3.441925	6.863269	0.024970
50	1	-1.480208	7.693715	0.310002
51	1	-5.261579	5.753281	-0.260561
52	1	-3.937286	7.827189	0.030735
53	6	-6.799916	-4.238088	0.062148
54	6	7.306408	-0.667018	-0.055440
55	1	-7.752176	-4.754450	0.096831
56	6	8.786472	-0.679935	-0.111585
57	8	9.470438	0.309693	-0.220068
58	1	9.247246	-1.684243	-0.044879

5-*ap*

1	6	1.653277	2.981153	-0.069298
2	6	1.467452	0.786690	0.145360
3	6	0.233993	1.020119	-0.400877
4	16	0.041138	2.717947	-0.675890
5	6	-0.825394	0.074115	-0.756416
6	6	-0.649835	-1.079845	-1.473204
7	16	-2.168868	-1.889584	-1.599465
8	6	-2.928909	-0.603932	-0.707505
9	6	1.979364	-0.528825	0.567488
10	6	1.317289	-1.414394	1.369876
11	16	2.292330	-2.832371	1.552036
12	6	3.518675	-2.117199	0.537792

13	7	2.256445	1.895433	0.312530
14	7	3.214555	-0.929141	0.115641
15	7	-2.108556	0.333604	-0.343198
16	6	4.780246	-2.804354	0.214646
17	6	4.959657	-4.166738	0.462180
18	6	5.822462	-2.072922	-0.362658
19	6	6.161733	-4.785326	0.145561
20	1	4.158535	-4.755591	0.896247
21	6	7.020701	-2.694949	-0.679905
22	1	5.679004	-1.016497	-0.552876
23	1	6.288705	-5.843519	0.341393
24	1	7.823513	-2.118084	-1.124328
25	6	-4.362029	-0.598033	-0.373242
26	6	-5.245789	-1.534113	-0.915725
27	6	-4.843996	0.371451	0.512290
28	6	-6.588496	-1.511240	-0.579836
29	1	-4.895622	-2.287218	-1.611689
30	6	-6.183585	0.405782	0.853322
31	1	-4.155852	1.094184	0.930128
32	1	-7.281491	-2.230454	-0.992752
33	1	-6.567800	1.147826	1.538972
34	6	0.591138	-1.644628	-2.080899
35	1	1.344248	-0.862285	-2.182552
36	1	1.011558	-2.432883	-1.449842
37	1	0.392516	-2.067942	-3.066729
38	6	-0.016999	-1.294449	2.031289
39	1	-0.324138	-0.248341	2.065588
40	1	-0.781624	-1.851222	1.481692
41	1	0.012284	-1.679312	3.052196
42	6	2.257347	4.321599	0.018994
43	6	1.630536	5.447491	-0.519152
44	6	3.494621	4.467263	0.653147
45	6	2.227011	6.697015	-0.419426
46	1	0.674511	5.356671	-1.023670
47	6	4.088403	5.716786	0.748771
48	1	3.977629	3.591509	1.068186
49	6	3.456898	6.835685	0.213888
50	1	1.731137	7.563064	-0.841615
51	1	5.047250	5.818895	1.243480
52	1	3.922054	7.811519	0.290869
53	6	7.195366	-4.052187	-0.426347
54	6	-7.036131	-0.539946	0.301752
55	7	-8.459673	-0.511304	0.663704
56	8	-8.833093	0.347605	1.439360
57	8	-9.191002	-1.347946	0.169556
58	1	8.133315	-4.536028	-0.672827

5-*p*-*N*

1	6	3.768718	-1.495425	-0.141380
2	6	2.406885	0.238153	0.055493
3	6	1.545119	-0.723075	0.515622
4	16	2.328099	-2.263767	0.463734
5	6	0.180346	-0.557684	1.023072
6	6	-0.165914	0.296507	2.035142
7	16	-1.877142	0.253739	2.236449
8	6	-1.995661	-0.926862	0.963255

9	6	2.045719	1.657253	-0.090642
10	6	2.849750	2.730094	0.176263
11	16	1.930972	4.181887	-0.052150
12	6	0.536118	3.228604	-0.487956
13	7	3.651843	-0.210061	-0.300214
14	7	0.757985	1.953482	-0.468184
15	7	-0.850509	-1.249672	0.442270
16	6	-0.780537	3.810288	-0.795995
17	6	-0.951694	5.173186	-1.041831
18	6	-1.893674	2.963853	-0.828345
19	6	-2.215798	5.683337	-1.308452
20	1	-0.098692	5.843656	-1.032385
21	6	-3.153502	3.476777	-1.097153
22	1	-1.753489	1.906769	-0.636621
23	1	-2.337854	6.743399	-1.497200
24	1	-4.009623	2.812045	-1.115773
25	6	-3.276318	-1.494478	0.513921
26	6	-4.498224	-1.026818	1.004549
27	6	-3.264306	-2.519025	-0.438327
28	6	-5.690471	-1.571039	0.559118
29	1	-4.531545	-0.229543	1.737561
30	6	-4.448730	-3.069720	-0.891671
31	1	-2.316415	-2.876074	-0.818481
32	1	-6.640785	-1.216025	0.931976
33	1	-4.452222	-3.861570	-1.627304
34	6	0.704441	1.197762	2.845287
35	1	1.730090	0.825396	2.837085
36	1	0.710817	2.207790	2.423869
37	1	0.364731	1.261455	3.879973
38	6	4.273934	2.773123	0.626001
39	1	4.581569	1.788781	0.976510
40	1	4.936725	3.058090	-0.195529
41	1	4.410186	3.494947	1.433884
42	6	4.995423	-2.245574	-0.459209
43	6	5.129112	-3.600166	-0.147839
44	6	6.056381	-1.579950	-1.080305
45	6	6.300774	-4.278363	-0.454667
46	1	4.320831	-4.133230	0.341572
47	6	7.226316	-2.260230	-1.382740
48	1	5.948786	-0.529456	-1.320127
49	6	7.352564	-3.610872	-1.072186
50	1	6.393017	-5.329577	-0.208525
51	1	8.043245	-1.735477	-1.864368
52	1	8.268061	-4.140276	-1.309326
53	6	-3.319431	4.838077	-1.335855
54	6	-5.646198	-2.586090	-0.383736
55	7	-6.907682	-3.167459	-0.860648
56	8	-6.848590	-4.059568	-1.685064
57	8	-7.946607	-2.727165	-0.406536
58	1	-4.305048	5.239131	-1.541672

5-*p*-*S*

1	6	-4.123929	-0.239658	-0.313420
2	6	-2.045476	-0.009277	0.407090
3	6	-1.965367	-1.329332	0.049154
4	16	-3.491859	-1.842375	-0.581013

5	6	-0.765664	-2.170641	0.079499
6	6	-0.680431	-3.463421	0.524330
7	16	0.970060	-3.967574	0.463345
8	6	1.421340	-2.400272	-0.145525
9	6	-0.928498	0.772394	0.967333
10	6	-0.202929	0.427765	2.070753
11	16	1.062600	1.586256	2.286640
12	6	0.506749	2.452820	0.878290
13	7	-3.258586	0.587624	0.193016
14	7	-0.530740	1.913530	0.315292
15	7	0.420215	-1.593060	-0.298807
16	6	1.161499	3.673632	0.377946
17	6	2.347890	4.158904	0.932053
18	6	0.580682	4.357863	-0.694016
19	6	2.939960	5.308725	0.425586
20	1	2.819645	3.641158	1.760624
21	6	1.175601	5.504204	-1.198099
22	1	-0.337481	3.976856	-1.123191
23	1	3.860138	5.675535	0.865020
24	1	0.716007	6.025142	-2.030075
25	6	2.810309	-2.000849	-0.418106
26	6	3.842094	-2.935515	-0.521175
27	6	3.091538	-0.638632	-0.569575
28	6	5.140206	-2.522211	-0.769670
29	1	3.640368	-3.994870	-0.414877
30	6	4.383502	-0.214646	-0.819766
31	1	2.286443	0.079991	-0.483845
32	1	5.948301	-3.234981	-0.853581
33	1	4.614237	0.834863	-0.936383
34	6	-1.758919	-4.366452	1.029676
35	1	-2.537270	-3.782375	1.524390
36	1	-2.220748	-4.924389	0.210709
37	1	-1.368679	-5.087312	1.748955
38	6	-0.348340	-0.754214	2.971375
39	1	-1.345523	-1.183852	2.863681
40	1	0.380336	-1.529510	2.714709
41	1	-0.199732	-0.483670	4.018141
42	6	-5.513933	0.127588	-0.631751
43	6	-6.436554	-0.810442	-1.099235
44	6	-5.917643	1.455112	-0.460024
45	6	-7.739209	-0.428449	-1.390242
46	1	-6.146903	-1.846891	-1.237110
47	6	-7.219934	1.832479	-0.750960
48	1	-5.198773	2.179685	-0.098664
49	6	-8.134826	0.893127	-1.216757
50	1	-8.446382	-1.165839	-1.751126
51	1	-7.521718	2.864384	-0.613859
52	1	-9.152692	1.189289	-1.442320
53	6	2.356756	5.984428	-0.640296
54	6	5.389119	-1.166479	-0.915972
55	7	6.764584	-0.723295	-1.180776
56	8	6.968536	0.470987	-1.285304
57	8	7.628319	-1.573436	-1.282357
58	1	2.820884	6.880562	-1.035485

5-CF

1	6	-1.888062	3.038147	0.006760
2	6	-1.623298	0.841044	-0.012202
3	6	-0.215290	1.226495	0.048598
4	16	-0.095223	2.969072	-0.037122
5	6	0.762931	0.316622	0.193524
6	6	0.377767	-1.141182	0.464861
7	16	1.927379	-2.032356	0.001783
8	6	2.816268	-0.494100	0.100763
9	6	-1.954513	-0.465333	-0.140843
10	6	-0.845951	-1.493872	-0.400228
11	16	-1.674415	-3.074265	0.057035
12	6	-3.251222	-2.255519	-0.054587
13	7	-2.502277	1.913648	0.023519
14	7	-3.232114	-0.971548	-0.138810
15	7	2.114725	0.578796	0.183768
16	6	-4.496328	-3.033663	-0.021009
17	6	-4.490377	-4.425896	-0.138334
18	6	-5.714938	-2.362263	0.131837
19	6	-5.683090	-5.135222	-0.104625
20	1	-3.556296	-4.960368	-0.269775
21	6	-6.902483	-3.074746	0.166344
22	1	-5.711926	-1.283670	0.226397
23	1	-5.668861	-6.214161	-0.201924
24	1	-7.842317	-2.549384	0.288152
25	6	4.287187	-0.470245	0.054187
26	6	5.036682	-1.647315	0.109394
27	6	4.940615	0.762498	-0.053566
28	6	6.420313	-1.601266	0.056794
29	1	4.548334	-2.609464	0.203808
30	6	6.320517	0.820721	-0.105928
31	1	4.354553	1.670680	-0.097301
32	1	7.011686	-2.504619	0.100147
33	1	6.839400	1.764984	-0.190929
34	6	0.143658	-1.309038	1.976519
35	1	-0.744959	-0.753065	2.285465
36	1	0.008119	-2.357316	2.242024
37	1	1.004492	-0.918407	2.521049
38	6	-0.556613	-1.507613	-1.913508
39	1	-0.099811	-0.563666	-2.220103
40	1	0.114729	-2.323237	-2.181346
41	1	-1.493750	-1.633763	-2.457540
42	6	-2.574881	4.337889	-0.001657
43	6	-1.874673	5.536495	0.148830
44	6	-3.964339	4.369371	-0.162760
45	6	-2.551966	6.748268	0.136376
46	1	-0.798708	5.532901	0.284907
47	6	-4.636129	5.581010	-0.175154
48	1	-4.499712	3.435680	-0.280528
49	6	-3.932165	6.773114	-0.026224
50	1	-2.001174	7.673454	0.256091
51	1	-5.711875	5.598057	-0.304508
52	1	-4.459236	7.720048	-0.037383
53	6	-6.889662	-4.462434	0.047721
54	6	7.037811	-0.366274	-0.050112
55	1	-7.820528	-5.016956	0.074250

56	7	8.507382	-0.310327	-0.105080
57	8	9.119486	-1.358856	-0.046951
58	8	9.030937	0.781971	-0.205861

6-*ap*

1	6	0.164170	3.437849	-0.012650
2	6	0.407595	1.253185	0.231578
3	6	-0.844937	1.233193	-0.320955
4	16	-1.358034	2.857145	-0.628786
5	6	-1.695851	0.093569	-0.668553
6	6	-1.289226	-1.009327	-1.364984
7	16	-2.620421	-2.109143	-1.480732
8	6	-3.631237	-0.982218	-0.609772
9	6	1.165663	0.070458	0.675892
10	6	0.684898	-0.923344	1.484542
11	16	1.920850	-2.109421	1.703534
12	6	2.994517	-1.169611	0.706565
13	7	0.966330	2.496216	0.385113
14	7	2.462451	-0.075814	0.253972
15	7	-3.011335	0.104103	-0.262924
16	6	4.374985	-1.579943	0.403178
17	6	4.927012	-2.749931	0.930932
18	6	5.150220	-0.770577	-0.433895
19	6	6.229329	-3.111136	0.631544
20	1	4.345485	-3.390634	1.583098
21	6	6.452462	-1.120444	-0.739477
22	1	4.718458	0.134444	-0.839899
23	1	6.666945	-4.013068	1.035355
24	1	7.061794	-0.502976	-1.384272
25	6	-5.040544	-1.256076	-0.300325
26	6	-5.686826	-2.408727	-0.739058
27	6	-5.770152	-0.331321	0.459840
28	6	-7.021725	-2.649962	-0.438275
29	1	-5.154784	-3.145010	-1.332397
30	6	-7.095454	-0.557960	0.763862
31	1	-5.279685	0.568639	0.809360
32	1	-7.486780	-3.556950	-0.799707
33	1	-7.662785	0.153112	1.352257
34	6	0.039251	-1.321563	-1.971092
35	1	0.616895	-0.403915	-2.090590
36	1	0.616156	-1.999873	-1.335666
37	1	-0.074185	-1.789180	-2.950652
38	6	-0.658315	-1.071275	2.120866
39	1	-1.160238	-0.103652	2.158366
40	1	-1.290683	-1.753908	1.546028
41	1	-0.574376	-1.458946	3.137354
42	6	0.502690	4.870228	0.037897
43	6	-0.463179	5.861184	-0.147800
44	6	1.827089	5.244129	0.283457
45	6	-0.110172	7.202884	-0.093380
46	1	-1.499112	5.593465	-0.326787
47	6	2.175417	6.585447	0.338317
48	1	2.573273	4.472598	0.426859
49	6	1.208972	7.568749	0.149764
50	1	-0.869045	7.963059	-0.236355
51	1	3.205798	6.863931	0.526464

52	1	1.482309	8.616633	0.193644
53	6	6.972638	-2.288822	-0.200617
54	6	-7.735661	-1.720742	0.318149
55	7	8.355045	-2.666481	-0.521347
56	8	8.996304	-1.925656	-1.241813
57	8	8.787717	-3.701026	-0.050264
58	8	-9.031810	-1.850810	0.668321
59	6	-9.728001	-3.018217	0.259804
60	1	-9.264963	-3.919521	0.672824
61	1	-10.735911	-2.916286	0.655668
62	1	-9.771770	-3.093571	-0.830965

6-*p*-*N*

1	6	-4.316292	0.657555	-0.272705
2	6	-2.527898	-0.587852	0.116348
3	6	-1.980388	0.623900	0.451063
4	16	-3.166850	1.862351	0.231409
5	6	-0.641992	0.947713	0.951190
6	6	-0.032854	0.339899	2.011335
7	16	1.547811	1.016583	2.202831
8	6	1.249181	2.095910	0.862522
9	6	-1.794122	-1.862776	0.124084
10	6	-2.302455	-3.078344	0.498122
11	16	-1.042256	-4.258855	0.410726
12	6	0.068969	-3.028402	-0.117276
13	7	-3.841228	-0.552575	-0.276699
14	7	-0.467910	-1.853840	-0.221944
15	7	0.077439	1.939978	0.326119
16	6	1.497315	-3.272068	-0.368270
17	6	2.012382	-4.558282	-0.542859
18	6	2.357028	-2.169239	-0.423556
19	6	3.365922	-4.747788	-0.765231
20	1	1.358609	-5.422196	-0.515345
21	6	3.709413	-2.346248	-0.647307
22	1	1.949526	-1.176531	-0.281959
23	1	3.777783	-5.737265	-0.903947
24	1	4.386750	-1.504725	-0.687861
25	6	2.244836	3.064129	0.384667
26	6	3.425725	3.321051	1.076020
27	6	2.005936	3.759587	-0.808713
28	6	4.354836	4.240410	0.603938
29	1	3.639114	2.808039	2.007924
30	6	2.918702	4.675529	-1.286870
31	1	1.091033	3.567030	-1.355134
32	1	5.259965	4.411961	1.170407
33	1	2.738950	5.211596	-2.211009
34	6	-0.535396	-0.748798	2.899678
35	1	-1.617984	-0.838372	2.798481
36	1	-0.091862	-1.711712	2.628510
37	1	-0.301344	-0.550546	3.947181
38	6	-3.681544	-3.440899	0.945103
39	1	-4.182879	-2.563105	1.351671
40	1	-4.279447	-3.807113	0.106468
41	1	-3.657321	-4.218300	1.710411
42	6	-5.700518	0.992387	-0.646062
43	6	-6.095167	2.310086	-0.887361

44	6	-6.641646	-0.034498	-0.762743
45	6	-7.409020	2.596688	-1.231675
46	1	-5.376896	3.119904	-0.816607
47	6	-7.953241	0.255945	-1.108204
48	1	-6.332580	-1.055747	-0.576705
49	6	-8.341729	1.571683	-1.342449
50	1	-7.701857	3.623317	-1.417402
51	1	-8.676909	-0.546539	-1.191867
52	1	-9.367892	1.796219	-1.609251
53	6	4.193408	-3.636490	-0.813620
54	6	4.104408	4.925029	-0.585183
55	7	5.630415	-3.830779	-1.046866
56	8	6.341124	-2.844217	-1.077810
57	8	6.036412	-4.967459	-1.196685
58	8	4.934584	5.836628	-1.133538
59	6	6.155629	6.121866	-0.468952
60	1	6.782916	5.228453	-0.392665
61	1	6.661229	6.866004	-1.080266
62	1	5.977275	6.533174	0.529295

6-*p*-*S*

1	6	-4.205208	0.471614	-0.292066
2	6	-2.162469	0.057693	0.444434
3	6	-2.466714	-1.216359	0.041242
4	16	-4.066395	-1.234107	-0.617730
5	6	-1.572742	-2.378317	0.036610
6	6	-1.881715	-3.647906	0.437067
7	16	-0.457017	-4.626052	0.332375
8	6	0.446003	-3.245444	-0.240850
9	6	-0.881386	0.468785	1.044639
10	6	-0.278453	-0.133171	2.114803
11	16	1.233994	0.643741	2.412164
12	6	0.931075	1.730851	1.086826
13	7	-3.143010	0.993164	0.244792
14	7	-0.200552	1.519222	0.486907
15	7	-0.267380	-2.169345	-0.346683
16	6	1.869453	2.789598	0.683351
17	6	3.128202	2.924979	1.274610
18	6	1.484947	3.677951	-0.326638
19	6	3.991140	3.929459	0.870956
20	1	3.449122	2.243367	2.053509
21	6	2.338381	4.684112	-0.739111
22	1	0.510140	3.566717	-0.782229
23	1	4.966573	4.043995	1.322019
24	1	2.051929	5.377949	-1.516860
25	6	1.884853	-3.292041	-0.528389
26	6	2.563606	-4.485052	-0.756997
27	6	2.605904	-2.090623	-0.573812
28	6	3.928212	-4.498987	-1.022026
29	1	2.030663	-5.430021	-0.742815
30	6	3.959346	-2.091358	-0.836230
31	1	2.086197	-1.157069	-0.394050
32	1	4.420302	-5.445740	-1.198216
33	1	4.521546	-1.165744	-0.867756
34	6	-3.176635	-4.202907	0.936890
35	1	-3.786957	-3.406741	1.366539

36	1	-3.746666	-4.669844	0.129074
37	1	-3.011776	-4.955695	1.709288
38	6	-0.736753	-1.292708	2.935846
39	1	-1.812713	-1.428556	2.817456
40	1	-0.244887	-2.215382	2.613172
41	1	-0.520840	-1.142891	3.994827
42	6	-5.415712	1.240381	-0.624198
43	6	-6.648070	0.617813	-0.831859
44	6	-5.324114	2.631062	-0.731677
45	6	-7.769003	1.373157	-1.149869
46	1	-6.742552	-0.458337	-0.732782
47	6	-6.446618	3.381692	-1.048186
48	1	-4.366079	3.109452	-0.569930
49	6	-7.671374	2.755734	-1.259752
50	1	-8.721284	0.880333	-1.306180
51	1	-6.363842	4.458763	-1.135732
52	1	-8.547231	3.343594	-1.508825
53	6	3.581297	4.794695	-0.131594
54	6	4.634640	-3.297031	-1.062944
55	7	4.492483	5.861122	-0.565414
56	8	4.113244	6.613567	-1.442552
57	8	5.579868	5.937669	-0.025699
58	8	5.957403	-3.193936	-1.309802
59	6	6.689584	-4.382309	-1.565902
60	1	6.310197	-4.896165	-2.454380
61	1	7.716130	-4.068518	-1.741341
62	1	6.659748	-5.060513	-0.707557

6-CF

1	6	0.269593	3.615418	0.002177
2	6	0.515617	1.416417	0.035518
3	6	-0.942271	1.470426	-0.024255
4	16	-1.456751	3.142972	0.048811
5	6	-1.689736	0.362802	-0.165923
6	6	-0.981615	-0.971886	-0.425269
7	16	-2.287085	-2.186763	0.041026
8	6	-3.510741	-0.893968	-0.078477
9	6	1.136570	0.220614	0.166805
10	6	0.291259	-1.029760	0.439481
11	16	1.457473	-2.386098	-0.014447
12	6	2.803626	-1.226428	0.077254
13	7	1.126416	2.660100	-0.010058
14	7	2.496373	0.018607	0.153034
15	7	-3.064145	0.311455	-0.168826
16	6	4.199949	-1.688884	0.037496
17	6	4.520696	-3.045832	0.116735
18	6	5.222606	-0.741193	-0.083750
19	6	5.842783	-3.457846	0.076871
20	1	3.742573	-3.792238	0.219761
21	6	6.545094	-1.140557	-0.124793
22	1	4.965804	0.307734	-0.147163
23	1	6.104415	-4.504298	0.141401
24	1	7.345715	-0.420627	-0.218955
25	6	-4.934976	-1.218062	-0.047752
26	6	-5.392360	-2.535228	-0.030608
27	6	-5.880832	-0.179776	-0.030411

28	6	-6.748355	-2.827972	0.004215
29	1	-4.688848	-3.360131	-0.052108
30	6	-7.228051	-0.457040	0.003431
31	1	-5.535678	0.846475	-0.042404
32	1	-7.063984	-3.862105	0.014338
33	1	-7.963484	0.337947	0.017929
34	6	-0.713777	-1.086433	-1.936923
35	1	0.028286	-0.346458	-2.246498
36	1	-0.347525	-2.078510	-2.200113
37	1	-1.640076	-0.900011	-2.482255
38	6	0.016280	-1.103056	1.952863
39	1	-0.642852	-0.286824	2.257908
40	1	-0.450907	-2.049130	2.225664
41	1	0.958754	-1.010035	2.494451
42	6	0.645482	5.037070	0.003226
43	6	-0.311248	6.046461	-0.121058
44	6	1.995274	5.381412	0.132255
45	6	0.074488	7.380148	-0.114226
46	1	-1.361841	5.800874	-0.231104
47	6	2.375894	6.713829	0.138534
48	1	2.731733	4.593786	0.229362
49	6	1.417005	7.715872	0.015973
50	1	-0.675138	8.156133	-0.211679
51	1	3.423008	6.972384	0.242822
52	1	1.716534	8.757491	0.022767
53	6	6.832396	-2.496307	-0.043329
54	6	-7.676835	-1.785860	0.021877
55	7	8.238504	-2.927335	-0.085440
56	8	9.092172	-2.070752	-0.208636
57	8	8.472417	-4.116786	0.005024
58	8	-9.010513	-1.952206	0.055941
59	6	-9.531228	-3.274350	0.079184
60	1	-9.192735	-3.815572	0.967365
61	1	-10.612633	-3.165200	0.112026
62	1	-9.247463	-3.825473	-0.822080

7-*ap*

1	6	0.849524	2.880993	-0.132406
2	6	0.761151	0.688949	0.168192
3	6	-0.478280	0.842668	-0.390705
4	16	-0.748134	2.519680	-0.733017
5	6	1.334937	-0.585880	0.632955
6	6	0.715378	-1.479691	1.458034
7	16	1.758770	-2.844613	1.679150
8	6	2.951259	-2.098962	0.643675
9	7	1.498478	1.838647	0.294462
10	7	2.589957	-0.938025	0.191308
11	6	4.240285	-2.733239	0.338163
12	6	4.487507	-4.077898	0.600353
13	6	5.258398	-1.969930	-0.249594
14	6	5.712723	-4.660731	0.299045
15	1	3.716324	-4.702017	1.039514
16	6	6.477816	-2.536453	-0.554626
17	1	5.076670	-0.922858	-0.458430
18	1	5.863881	-5.709613	0.514730

19	1	7.269151	-1.949129	-1.004769
20	6	-0.625805	-1.410892	2.112872
21	1	-0.983008	-0.380324	2.127947
22	1	-1.360929	-2.012739	1.570410
23	1	-0.583069	-1.775594	3.140785
24	6	1.391558	4.245699	-0.103267
25	6	0.722369	5.327403	-0.688008
26	6	2.619180	4.480126	0.514880
27	6	1.263090	6.596637	-0.651762
28	1	-0.231363	5.182702	-1.184474
29	6	3.174366	5.750979	0.557333
30	1	3.144131	3.649053	0.969375
31	6	2.495878	6.820973	-0.029429
32	1	0.749224	7.435286	-1.105322
33	1	4.128304	5.892695	1.046867
34	6	6.718321	-3.888612	-0.282220
35	8	7.942380	-4.349048	-0.615526
36	6	8.243112	-5.711524	-0.355867
37	1	7.579701	-6.376988	-0.916664
38	1	9.267907	-5.859488	-0.688879
39	1	8.172523	-5.935351	0.712901
40	6	-1.487077	-0.166090	-0.719434
41	6	-1.248290	-1.332650	-1.396904
42	7	-2.785240	0.040222	-0.322319
43	16	-2.722515	-2.223395	-1.504328
44	6	0.023042	-1.853486	-1.980690
45	6	-3.553096	-0.951697	-0.656258
46	1	0.737641	-1.038616	-2.102375
47	1	0.478227	-2.600466	-1.323906
48	1	-0.148476	-2.315476	-2.954271
49	6	-4.991255	-1.001141	-0.347895
50	6	-5.764921	-2.126245	-0.643897
51	6	-5.592061	0.106588	0.259103
52	6	-7.116352	-2.149893	-0.345734
53	1	-5.319953	-2.998308	-1.108097
54	6	-6.941375	0.094718	0.561751
55	1	-4.990081	0.975495	0.489530
56	1	-7.723324	-3.015220	-0.570963
57	6	-7.683894	-1.036070	0.252711
58	1	-7.417697	0.945329	1.028538
59	7	-9.118211	-1.054117	0.569541
60	8	-9.601747	-0.062114	1.080385
61	8	-9.748201	-2.060009	0.304127
62	8	2.943018	8.093379	-0.048285
63	6	4.187969	8.380830	0.570239
64	1	5.003799	7.826758	0.096140
65	1	4.349026	9.447548	0.432208
66	1	4.160219	8.152944	1.640125

7-*p*-*N*

1	6	-1.014577	3.000016	0.000495
2	6	-0.933033	0.785826	-0.030056
3	6	0.502511	1.050481	0.035299
4	16	0.769637	2.777003	-0.041331
5	6	-1.374356	-0.487306	-0.165151
6	6	-0.355407	-1.604229	-0.427044

7	16	-1.314108	-3.111930	0.022207
8	6	-2.820062	-2.162449	-0.081608
9	7	-1.718498	1.928259	0.010311
10	7	-2.688925	-0.883210	-0.164591
11	6	-4.119953	-2.828493	-0.044914
12	6	-4.240170	-4.217488	-0.026892
13	6	-5.291692	-2.053962	-0.019942
14	6	-5.482652	-4.834040	0.017111
15	1	-3.355936	-4.844869	-0.053756
16	6	-6.529333	-2.653529	0.022875
17	1	-5.207820	-0.974586	-0.032152
18	1	-5.535047	-5.913939	0.028374
19	1	-7.437234	-2.063068	0.043743
20	6	-0.063711	-1.635655	-1.939323
21	1	0.469511	-0.730794	-2.240613
22	1	0.539273	-2.502559	-2.209068
23	1	-1.006611	-1.682244	-2.486112
24	6	-1.584055	4.348182	-0.002445
25	6	-0.792247	5.487684	0.123845
26	6	-2.972272	4.507506	-0.135323
27	6	-1.350691	6.758851	0.117216
28	1	0.282694	5.400170	0.238632
29	6	-3.537846	5.762427	-0.144819
30	1	-3.595406	3.627513	-0.234257
31	6	-2.731826	6.902942	-0.020147
32	1	-0.703467	7.618834	0.220318
33	1	-4.607634	5.893299	-0.252591
34	6	-6.638451	-4.051627	0.043020
35	8	-7.890338	-4.540855	0.087334
36	6	-8.068923	-5.950255	0.113728
37	1	-7.600692	-6.390630	0.998806
38	1	-9.143414	-6.112177	0.154663
39	1	-7.664212	-6.415844	-0.789490
40	6	1.400941	0.061231	0.178648
41	6	0.891270	-1.359545	0.442571
42	7	2.770387	0.207091	0.174288
43	16	2.360812	-2.377645	-0.019968
44	6	0.639403	-1.511847	1.952943
45	6	3.378441	-0.920962	0.088292
46	1	-0.200339	-0.883825	2.260556
47	1	0.416403	-2.545714	2.215816
48	1	1.528431	-1.195783	2.500813
49	6	4.845913	-1.024923	0.051068
50	6	5.485680	-2.265979	0.026140
51	6	5.609608	0.147807	0.034376
52	6	6.868135	-2.343105	-0.017214
53	1	4.911539	-3.184360	0.046617
54	6	6.989559	0.083281	-0.006054
55	1	5.108112	1.106082	0.053156
56	1	7.376082	-3.296741	-0.037011
57	6	7.596223	-1.164922	-0.031668
58	1	7.591927	0.980501	-0.018791
59	7	9.065035	-1.240135	-0.074299
60	8	9.687856	-0.196284	-0.080930
61	8	9.578054	-2.341840	-0.100618
62	8	-3.378383	8.082860	-0.044160

63	6	-2.618269	9.276992	0.076277
64	1	-1.899386	9.372498	-0.742797
65	1	-3.337206	10.091213	0.024499
66	1	-2.093456	9.315631	1.035340

7-*p*-*S*

1	6	-3.820839	0.237709	0.012717
2	6	-1.964295	-0.947453	0.257840
3	6	-1.458988	0.263409	0.652520
4	16	-2.706494	1.460488	0.557932
5	6	-1.171378	-2.183381	0.159553
6	6	-1.601424	-3.441331	0.474338
7	16	-0.279303	-4.545828	0.274225
8	6	0.747691	-3.223702	-0.222654
9	7	-3.291832	-0.946349	-0.088099
10	7	0.142121	-2.078952	-0.235924
11	6	2.171531	-3.388536	-0.541345
12	6	2.740906	-4.630508	-0.805342
13	6	2.994862	-2.253963	-0.573974
14	6	4.095408	-4.758100	-1.090469
15	1	2.128243	-5.526044	-0.801087
16	6	4.339379	-2.367269	-0.857199
17	1	2.560523	-1.283231	-0.367065
18	1	4.501278	-5.740044	-1.291503
19	1	4.980776	-1.494237	-0.878438
20	6	-2.939088	-3.911675	0.946823
21	1	-3.529045	-3.064740	1.294654
22	1	-3.493114	-4.393577	0.136509
23	1	-2.839444	-4.632264	1.761197
24	6	-5.227869	0.527501	-0.290807
25	6	-5.713893	1.828449	-0.393134
26	6	-6.120142	-0.535602	-0.487985
27	6	-7.050232	2.081013	-0.676496
28	1	-5.048465	2.674903	-0.259939
29	6	-7.448479	-0.298382	-0.769788
30	1	-5.752985	-1.551745	-0.412228
31	6	-7.928375	1.013693	-0.865277
32	1	-7.387822	3.105726	-0.751273
33	1	-8.143224	-1.116355	-0.918121
34	6	4.904136	-3.621995	-1.116998
35	8	6.228105	-3.630653	-1.380079
36	6	6.850427	-4.875012	-1.658894
37	1	6.419758	-5.341740	-2.550101
38	1	7.899278	-4.651051	-1.839948
39	1	6.767571	-5.560006	-0.809405
40	6	-0.116036	0.604615	1.127394
41	6	0.542755	-0.042339	2.138354
42	7	0.565738	1.634610	0.531845
43	16	2.110379	0.653832	2.315363
44	6	0.091660	-1.191060	2.976784
45	6	1.751197	1.783289	1.040667
46	1	-0.996711	-1.262448	2.949243
47	1	0.499179	-2.131943	2.594570
48	1	0.407405	-1.077585	4.015021
49	6	2.708923	2.796988	0.572093
50	6	3.953741	2.970323	1.182600

51	6	2.359005	3.602827	-0.516689
52	6	4.839004	3.927690	0.718205
53	1	4.244496	2.359691	2.029288
54	6	3.234482	4.563065	-0.988848
55	1	1.395090	3.464748	-0.987833
56	1	5.803994	4.070307	1.183476
57	6	4.464198	4.710244	-0.362882
58	1	2.975916	5.191331	-1.829625
59	7	5.399282	5.726727	-0.861400
60	8	5.055877	6.398853	-1.815141
61	8	6.469294	5.844481	-0.295189
62	8	-9.242454	1.142496	-1.140848
63	6	-9.785936	2.450204	-1.240228
64	1	-9.319878	3.011424	-2.055750
65	1	-10.844368	2.316576	-1.451623
66	1	-9.669497	2.998522	-0.300539

7-CF

1	6	4.114336	-0.075871	-0.110001
2	6	2.017623	0.112239	0.553555
3	6	2.102274	1.307140	-0.107825
4	16	3.679987	1.476127	-0.786677
5	6	0.778985	-0.271264	1.266477
6	6	0.334531	0.396421	2.368029
7	16	-1.273849	-0.130788	2.728246
8	6	-1.221229	-1.209002	1.352940
9	7	3.148584	-0.657065	0.542544
10	7	-0.091332	-1.184229	0.715684
11	6	-2.395155	-1.981361	0.922991
12	6	-3.654517	-1.777258	1.481166
13	6	-2.280064	-2.881660	-0.144019
14	6	-4.778609	-2.435299	0.999026
15	1	-3.785664	-1.071060	2.294064
16	6	-3.388325	-3.542900	-0.632532
17	1	-1.308650	-3.042322	-0.595406
18	1	-5.739949	-2.236409	1.452157
19	1	-3.303956	-4.236058	-1.460947
20	6	1.003428	1.483389	3.144291
21	1	2.049633	1.562373	2.845712
22	1	0.523918	2.448461	2.955770
23	1	0.966265	1.292059	4.218816
24	6	5.449989	-0.658652	-0.287784
25	6	6.543027	0.101903	-0.695441
26	6	5.643264	-2.023495	-0.034157
27	6	7.799328	-0.468290	-0.859664
28	1	6.431858	1.164901	-0.881813
29	6	6.884986	-2.601108	-0.193329
30	1	4.801191	-2.624537	0.286235
31	6	7.976410	-1.829150	-0.610345
32	1	8.623479	0.157519	-1.173779
33	1	7.038091	-3.656798	-0.004508
34	6	-4.651653	-3.322420	-0.069633
35	8	-5.674341	-4.000887	-0.628253
36	6	-6.987144	-3.761824	-0.140510
37	1	-7.266010	-2.713057	-0.275496
38	1	-7.643136	-4.392005	-0.737107

39	1	-7.076263	-4.042030	0.913553
40	6	0.966800	2.224039	-0.275272
41	6	0.883876	3.540793	0.086151
42	7	-0.207110	1.647946	-0.685433
43	16	-0.759425	4.062946	-0.084714
44	6	1.949967	4.448358	0.604817
45	6	-1.207509	2.464866	-0.616208
46	1	2.828209	3.864804	0.884956
47	1	2.252840	5.177800	-0.150387
48	1	1.610140	4.995324	1.486268
49	6	-2.584699	2.009292	-0.868861
50	6	-3.698112	2.838354	-0.717173
51	6	-2.766782	0.663046	-1.203946
52	6	-4.976562	2.326346	-0.869802
53	1	-3.578253	3.885305	-0.464056
54	6	-4.035368	0.142484	-1.363419
55	1	-1.899303	0.024285	-1.301136
56	1	-5.848119	2.952095	-0.739204
57	6	-5.123990	0.982813	-1.182128
58	1	-4.183822	-0.902754	-1.596990
59	7	-6.473558	0.422177	-1.305731
60	8	-6.577486	-0.736938	-1.664930
61	8	-7.419464	1.138095	-1.039210
62	8	9.147638	-2.485584	-0.740411
63	6	10.289569	-1.753136	-1.157868
64	1	11.103473	-2.473126	-1.203177
65	1	10.138200	-1.312728	-2.148064
66	1	10.539503	-0.966649	-0.439308

8-*ap*

1	6	0.456691	3.429981	-0.052329
2	6	0.690255	1.244334	0.201515
3	6	-0.558230	1.226575	-0.360192
4	16	-1.066660	2.851994	-0.669239
5	6	-1.420062	0.095874	-0.709358
6	6	-1.023837	-1.023459	-1.383263
7	16	-2.380060	-2.094483	-1.514444
8	6	-3.384750	-0.932566	-0.676464
9	6	1.441899	0.061790	0.657184
10	6	0.953054	-0.925738	1.468692
11	16	2.185080	-2.112792	1.705142
12	6	3.268042	-1.181939	0.709817
13	7	1.251824	2.486517	0.354858
14	7	2.741520	-0.090134	0.246099
15	7	-2.743598	0.143268	-0.330888
16	6	4.650152	-1.596046	0.419323
17	6	5.194691	-2.767684	0.951182
18	6	5.434700	-0.788089	-0.410462
19	6	6.498779	-3.131701	0.662970
20	1	4.605813	-3.407482	1.597631
21	6	6.738642	-1.140805	-0.704951
22	1	5.008541	0.118200	-0.819508
23	1	6.930882	-4.034903	1.069911
24	1	7.354850	-0.524362	-1.344148
25	6	-4.802476	-1.169656	-0.400107
26	6	-5.462998	-2.335265	-0.795814

27	6	-5.546965	-0.203574	0.285516
28	6	-6.803575	-2.535753	-0.528096
29	1	-4.927123	-3.115416	-1.327726
30	6	-6.886589	-0.385566	0.560956
31	1	-5.055925	0.707718	0.605394
32	1	-7.264003	-3.457828	-0.854849
33	1	-7.414847	0.393884	1.092807
34	6	0.307696	-1.375725	-1.960227
35	1	0.912680	-0.475523	-2.077307
36	1	0.854734	-2.063712	-1.308844
37	1	0.200657	-1.848941	-2.937985
38	6	-0.396060	-1.067324	2.093592
39	1	-0.895015	-0.097861	2.123294
40	1	-1.025486	-1.749021	1.514424
41	1	-0.322747	-1.452254	3.111931
42	6	0.790178	4.863280	0.013362
43	6	-0.082829	5.841665	-0.466807
44	6	2.011136	5.253565	0.571375
45	6	0.255319	7.185542	-0.385729
46	1	-1.033353	5.562408	-0.908881
47	6	2.346327	6.597188	0.649071
48	1	2.687478	4.493228	0.941470
49	6	1.469876	7.567513	0.172784
50	1	-0.432716	7.934457	-0.759777
51	1	3.294565	6.888529	1.085655
52	1	1.731793	8.617196	0.237759
53	6	7.251322	-2.310734	-0.162242
54	6	-7.561584	-1.561065	0.158578
55	7	8.635533	-2.691493	-0.470909
56	8	9.061307	-3.727739	0.002772
57	8	9.285246	-1.951436	-1.184593
58	7	-8.889231	-1.745225	0.421607
59	6	-9.548778	-2.970536	0.015337
60	1	-10.602410	-2.912866	0.280148
61	1	-9.483285	-3.121088	-1.067637
62	1	-9.119951	-3.850372	0.509930
63	6	-9.625072	-0.752607	1.180338
64	1	-9.193731	-0.601332	2.176779
65	1	-9.647556	0.214804	0.666352
66	1	-10.652087	-1.088946	1.305746

8-*p*-*N*

1	6	4.785247	-0.706068	-0.348715
2	6	2.930997	0.437170	0.015658
3	6	2.522185	-0.744884	0.573087
4	16	3.790582	-1.906782	0.432072
5	6	1.242124	-0.957825	1.265447
6	6	0.950913	-0.336283	2.442672
7	16	-0.726370	-0.573660	2.793450
8	6	-0.899856	-1.502007	1.318735
9	6	2.039512	1.608942	-0.063184
10	6	2.343091	2.913047	0.217348
11	16	0.894628	3.859423	0.104048
12	6	-0.005021	2.425693	-0.309137
13	7	4.202603	0.449505	-0.489012
14	7	0.727642	1.361187	-0.366396

15	7	0.208200	-1.629727	0.653709
16	6	-1.460759	2.365146	-0.521973
17	6	-2.287226	3.488978	-0.463070
18	6	-2.025062	1.105471	-0.752877
19	6	-3.658191	3.356392	-0.616627
20	1	-1.869980	4.474291	-0.291160
21	6	-3.389605	0.959194	-0.905029
22	1	-1.376129	0.241307	-0.791387
23	1	-4.312099	4.215737	-0.567627
24	1	-3.829998	-0.016652	-1.061711
25	6	-2.210471	-1.952649	0.842543
26	6	-3.388158	-1.694921	1.548080
27	6	-2.328451	-2.552051	-0.414788
28	6	-4.629607	-1.999000	1.024828
29	1	-3.348782	-1.223181	2.524799
30	6	-3.561471	-2.862377	-0.954833
31	1	-1.429557	-2.751459	-0.986315
32	1	-5.508256	-1.758128	1.606595
33	1	-3.595787	-3.308188	-1.939344
34	6	1.826831	0.526290	3.290543
35	1	2.874936	0.343357	3.049019
36	1	1.619168	1.585355	3.107755
37	1	1.678519	0.331051	4.354248
38	6	3.650090	3.518197	0.611935
39	1	4.405789	2.736670	0.684800
40	1	3.987353	4.248112	-0.128027
41	1	3.573638	4.025996	1.576157
42	6	6.153118	-0.986171	-0.818160
43	6	6.764304	-2.225288	-0.615564
44	6	6.857781	0.020716	-1.484791
45	6	8.054823	-2.454062	-1.073595
46	1	6.238576	-3.021296	-0.098903
47	6	8.147249	-0.210951	-1.938994
48	1	6.380828	0.979944	-1.642061
49	6	8.750042	-1.448571	-1.735955
50	1	8.517674	-3.420280	-0.911423
51	1	8.683357	0.577200	-2.454895
52	1	9.757285	-1.628553	-2.093320
53	6	-4.187920	2.091967	-0.830032
54	6	-4.756971	-2.586703	-0.252635
55	7	-5.640442	1.943018	-0.975689
56	8	-6.335695	2.929176	-0.823217
57	8	-6.076742	0.837673	-1.241028
58	7	-5.984611	-2.868349	-0.788134
59	6	-7.181190	-2.377798	-0.128732
60	1	-8.053425	-2.682767	-0.703784
61	1	-7.283070	-2.803211	0.874123
62	1	-7.184694	-1.283798	-0.047464
63	6	-6.082064	-3.310229	-2.166080
64	1	-5.695244	-2.563038	-2.871506
65	1	-5.536317	-4.245427	-2.320998
66	1	-7.127188	-3.497151	-2.404715

8-*p*-*S*

1	6	4.711205	-0.611320	-0.346084
2	6	2.686155	-0.232560	0.442923

3	6	2.864208	0.978748	-0.170510
4	16	4.416048	1.008809	-0.925802
5	6	1.842541	2.029837	-0.258874
6	6	1.976805	3.352287	0.050495
7	16	0.413760	4.104108	-0.048549
8	6	-0.298938	2.566698	-0.488021
9	6	1.449897	-0.535142	1.194069
10	6	1.094215	0.132305	2.331714
11	16	-0.526612	-0.289787	2.743202
12	6	-0.598051	-1.337721	1.354059
13	7	3.723564	-1.116113	0.334989
14	7	0.501087	-1.370234	0.664250
15	7	0.571341	1.611417	-0.574163
16	6	-1.842270	-1.998222	0.928765
17	6	-3.011105	-1.920187	1.690143
18	6	-1.872508	-2.647228	-0.310242
19	6	-4.198836	-2.446917	1.214498
20	1	-3.010705	-1.429353	2.655962
21	6	-3.051668	-3.184028	-0.793901
22	1	-0.965510	-2.702199	-0.897684
23	1	-5.111550	-2.375979	1.789134
24	1	-3.090911	-3.674740	-1.756293
25	6	-1.735012	2.339406	-0.668423
26	6	-2.697378	3.348375	-0.624578
27	6	-2.180006	1.023239	-0.837051
28	6	-4.047076	3.061967	-0.737186
29	1	-2.401498	4.384681	-0.492290
30	6	-3.519502	0.718978	-0.944610
31	1	-1.444649	0.228811	-0.864842
32	1	-4.753821	3.878984	-0.690105
33	1	-3.802868	-0.319286	-1.053572
34	6	3.195322	4.116101	0.455866
35	1	3.961220	3.428382	0.818834
36	1	3.613005	4.676123	-0.385088
37	1	2.971937	4.825550	1.254630
38	6	1.867852	1.154866	3.097632
39	1	2.925999	1.086432	2.841764
40	1	1.524535	2.163116	2.847069
41	1	1.762497	1.016086	4.174954
42	6	5.968445	-1.326943	-0.619356
43	6	7.083674	-0.675182	-1.150263
44	6	6.047323	-2.693983	-0.337149
45	6	8.254517	-1.377812	-1.399815
46	1	7.047895	0.387735	-1.364523
47	6	7.219805	-3.391877	-0.585709
48	1	5.181225	-3.196380	0.075244
49	6	8.326351	-2.737572	-1.118678
50	1	9.113188	-0.860733	-1.811482
51	1	7.270120	-4.452041	-0.366044
52	1	9.241680	-3.284460	-1.312839
53	6	-4.202640	-3.063061	-0.027382
54	6	-4.501157	1.734124	-0.899202
55	7	-5.467218	-3.586274	-0.555767
56	8	-6.490117	-3.322131	0.049366
57	8	-5.430142	-4.249856	-1.573742
58	7	-5.833677	1.438106	-1.007786

59	6	-6.822027	2.481409	-0.814416
60	1	-7.816061	2.056232	-0.937537
61	1	-6.760817	2.930558	0.185222
62	1	-6.707200	3.278226	-1.555893
63	6	-6.264954	0.053173	-1.005098
64	1	-5.825349	-0.501125	-1.840298
65	1	-6.001980	-0.462267	-0.072491
66	1	-7.346252	0.014579	-1.120829

8-CF

1	6	0.604630	3.632482	0.006200
2	6	0.809031	1.428854	0.042969
3	6	-0.646259	1.510962	-0.017188
4	16	-1.128919	3.194170	0.051051
5	6	-1.418353	0.418885	-0.156767
6	6	-0.735957	-0.931097	-0.408006
7	16	-2.064903	-2.117047	0.062509
8	6	-3.267602	-0.800716	-0.069475
9	6	1.407441	0.221134	0.175788
10	6	0.536775	-1.009901	0.456048
11	16	1.673832	-2.392823	0.007391
12	6	3.044901	-1.260094	0.085437
13	7	1.443704	2.660870	-0.004614
14	7	2.762448	-0.009011	0.155974
15	7	-2.790562	0.396846	-0.164913
16	6	4.431342	-1.749730	0.037178
17	6	4.727525	-3.112624	0.111912
18	6	5.471309	-0.821458	-0.089752
19	6	6.041303	-3.549486	0.061415
20	1	3.936414	-3.844740	0.219038
21	6	6.785460	-1.245617	-0.141181
22	1	5.234040	0.232239	-0.149714
23	1	6.283278	-4.600880	0.121961
24	1	7.598852	-0.540751	-0.239929
25	6	-4.687590	-1.099258	-0.049402
26	6	-5.179140	-2.404889	0.074454
27	6	-5.623201	-0.057684	-0.149668
28	6	-6.531683	-2.668126	0.103686
29	1	-4.492225	-3.241861	0.145483
30	6	-6.976710	-0.301567	-0.127510
31	1	-5.263722	0.959452	-0.248724
32	1	-6.858462	-3.694122	0.199175
33	1	-7.657152	0.534416	-0.211462
34	6	-0.469850	-1.055977	-1.919340
35	1	0.287513	-0.332383	-2.230816
36	1	-0.124201	-2.056269	-2.179228
37	1	-1.392057	-0.852202	-2.465468
38	6	0.260868	-1.070385	1.969569
39	1	-0.379661	-0.238146	2.271173
40	1	-0.227486	-2.004523	2.246681
41	1	1.205481	-0.996013	2.510411
42	6	1.008387	5.046862	0.010378
43	6	0.071591	6.074626	-0.115185
44	6	2.363715	5.365448	0.146445
45	6	0.482374	7.400725	-0.102359
46	1	-0.982968	5.849453	-0.230577

47	6	2.769544	6.690509	0.158634
48	1	3.084652	4.563686	0.244746
49	6	1.830303	7.710859	0.035249
50	1	-0.252366	8.190773	-0.200553
51	1	3.820861	6.928820	0.268732
52	1	2.149540	8.746579	0.047215
53	6	7.048193	-2.606686	-0.064333
54	6	-7.478638	-1.620701	0.005553
55	7	8.445309	-3.063523	-0.117863
56	8	8.658067	-4.257576	-0.034372
57	8	9.314067	-2.222335	-0.242915
58	7	-8.815191	-1.868627	0.036920
59	6	-9.302883	-3.230222	0.161428
60	1	-10.389852	-3.216866	0.196266
61	1	-8.996235	-3.850774	-0.688202
62	1	-8.941842	-3.701207	1.081477
63	6	-9.766143	-0.782028	-0.115439
64	1	-9.659021	-0.038153	0.680991
65	1	-9.649584	-0.275659	-1.079931
66	1	-10.775094	-1.184873	-0.064613

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