Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Supporting Information

Application of stimuli-responsive FRET behavior toward cyanide detection in photo-switchable [2]pseudorotaxane polymer containing BODIPY donor and merocyanine acceptor

Chinmayananda Gouda,[a] Debashis Barik,[a] Chandrima Maitra,[a] Kai-Chieh Liang,[a] Feng-Cheng Ho,[a] Venkatesan Srinivasadesikan,[b] Sarala Chandran,[b] Shu-Pao Wu,[b] Ming-Chang Lin[b] and Hong-Cheu Lin[a,c,]*

[a] Department of Materials Science and Engineering, National Chiao Tung University, Hsinchu, Taiwan.

[b] Department of Applied Chemistry, National Chiao Tung University, Hsinchu 300, Taiwan.

[c] Center for Emergent Functional Matter Science, National Chiao Tung University, Hsinchu 30010, Taiwan.

Corresponding Author

*E-mail: linhc@mail.nctu.edu.tw (H. C. Lin)

Prof. H. C. Lin

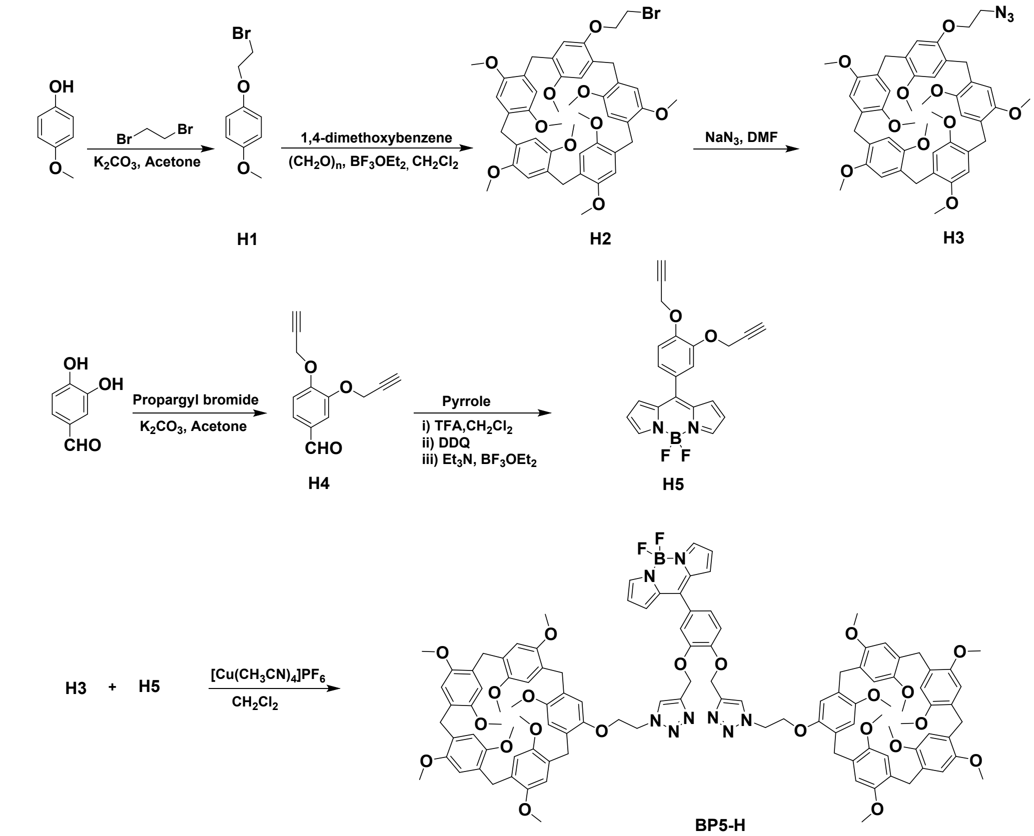
Department of Materials Science and Engineering

National Chiao Tung University

1001 Ta Hsueh Rd.

Hsinchu, Taiwan 300

1. Synthetic procedures



Scheme S1 Synthetic routes of host **BP5-H**.

Compounds **H1**-**H5** were synthesized according to the previous literature[S1] with modifications.

Synthesis of compound H1: A solution of 4-methoxy phenol (10.1 g, 81.3 mmol) and finely powdered K_2CO_3 (35 g, 0.25 mol) were dissolved in acetone (200 mL). Then, 1,2-dibromoethane (35 mL, 0.41 mmol) was added, and the reaction mixture was refluxed for 48 h before K_2CO_3 was removed by filtration. After that, it was dried over anhydrous $MgSO_4$, and the volatiles were evaporated under reduced pressure to yield an orange solid. Then, the crude was purified by column chromatography (silica gel, Hexane/EtOAc = 70/30 v/v) to give compound **H1** as a white solid**.** Yield: 8.42 g (45%). ^{1}H-NMR (300 MHz, $CDCl_3$, δ, ppm): 6.89-6.82 (m, 4H), 4.24 (t, *J* = 6.3 Hz), 3.77(s, 3H), 3.61 (t, *J* = 6.3 Hz, 2H).

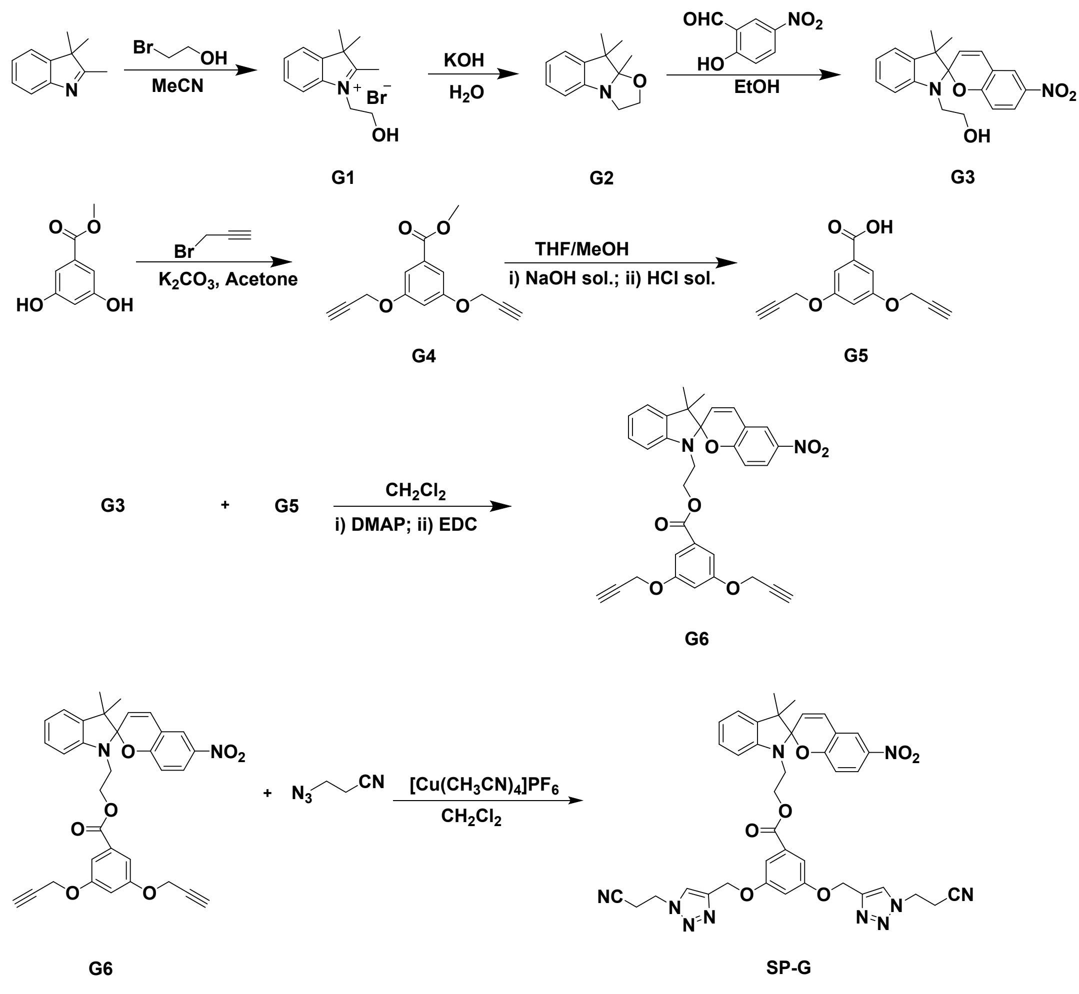
Synthesis of compound H2: Paraformaldehyde (1.09 g, 36.2 mmol) was added to a solution of compound **H1** (5.00 g, 36.2 mmol) and 1,4-dimethoxybenzene (1.67 g, 7.18 mmol) in dry DCM (100 mL) to react for 1 h under nitrogen atmosphere. Then, boron trifluoride etherate $BF_3.OEt_2$ (4.6 mL, 36 mmol) was then added to the previous solution, and the mixture was stirred for further reaction at room temperature for 3 h. Consequently, MeOH (50 mL) was poured into the reaction mixture, and the solution was concentrated and dissolved in DCM (100 mL). The solution was then washed with aqueous $NaHCO_3$ (2 x 50mL) and H_2O (50 mL) sequentially. The organic layer was dried by Na_2SO_4 and concentrated under reduced pressure, and the crude was purified by column chromatography (silica gel, Hexane/DCM = 60/40 v/v) to acquire compound **H2** as a white solid. Yield: 8.42 g (10 %). ^{1}H-NMR (300 MHz, $CDCl_3$, δ, ppm): 6.80−6.76 (m, 9H), 6.69 (s, 1H), 4.04 (t, *J* = 6.4 Hz, 2H), 3.80-3.76 (m, 10H), 3.68−3.64 (m, 27H), 3.44 (t, *J* = 6.14 Hz, 2H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 152.0, 151.5, 151.4, 149.8, 129.6, 129.1, 129.0, 128.9, 128.8, 128.7, 116.4, 114.7, 69.5, 56.7, 56.5, 56.4, 53.7, 30.7, 30.6, 30.3, 30.2. HRMS (ESI$^+$) $[M+H]^+$: calcd. for $C_{46}H_{51}BrO_{10}$ 843.2738, found 843.2747. mp. 131-133.0 °C.

Synthesis of compound H3: Sodium azide (65 mg, 1.00 mmol) was added to a solution of **H2** (0.57 g, 0.71 mmol) in dry N,N-dimethylformamide (50 mL). Then, the reaction mixture was stirred to react at 80°C for 12 h. The reaction mixture was dissolved in DCM (100 mL). Consequently, the solution was washed with H_2O (2 x 50 mL) and brine (2 x 50 mL) and dried (Na_2SO_4) sequentially. The organic layer was removed under vacuum to obtain **H3** as a pale white solid**.** Yield: 0.53 g (93 %). ^{1}H-NMR (300 MHz, $CDCl_3$, δ, ppm): 6.80-6.74 (m, 9H), 6.68

(s, 1H), 3.88 (t, *J* = 4.96 Hz, 2H), 3.81-3.76 (m, 10H), 3.68-3.64 (m, 27H), 3.43 (t, *J* = 4.92 Hz, 2H).

Synthesis of compound H4: 3,4-Dihydroxybenzaldehyde (2.12 g, 15.0 mmol) and K_2CO_3 (12.2 g, 45 mmol) were dissolved in DMF (25 mL) and stirred for 30 min, then propargyl bromide (4.2 g, 33 mmol) was added. Then, the reaction mixture was stirred to react at 60°C for 24 h. Consequently, the insoluble salts were removed by filtration, and the obtained filtrate was dried under reduced pressure to yield a crude product. The crude product was dissolved in EtOAc and washed with water (30 mL x 3). The combined organic extracts were dried over anhydrous Na_2SO_4 and concentrated under reduced pressure. The crude was purified by column chromatography (silica gel, Hexane/EtOAc = 60/40, v/v) to afford compound **H4** as a white solid**.** Yield: 2.6 g (81 %). ^{1}H-NMR (300 MHz, $CDCl_3$, δ, ppm): 9.88 (s, 1H), 7.58-7.51 (m, 2H), 7.17 (d, *J* = 8.1 Hz, 1H), 4.86 (d, *J* = 2.4 Hz, 2H), 4.83 (d, *J* = 2.4 Hz, 2H), 2.58-2.54 (m, 2H).

Synthesis of compound H5: Pyrrole (0.62 g, 6.6 mmol) and compound **H4** (0.64 g, 3 mmol) were dissolved in dry DCM (200 mL) under nitrogen atmosphere. Three drops of trifluoroacetic acid (TFA) were added, and the mixture was stirred to react at room temperature for 24 h in the dark. Then, 2,3-dichloro-5,6-dicyanoquinone (DDQ, 0.68 g, 3 mmol) was added to the previous reaction mixture, and it was stirred for another 2 h. The reaction mixture was then treated with triethylamine (5 mL) for 15 min. Boron trifluoride etherate (6 mL) was added dropwise to the mixture which was cooled in an ice-water bath and stirred for additional 3 h at room temperature. The dark-brown solution was washed with H_2O (2 × 20mL) and brine (30 mL), dried over anhydrous Na_2SO_4 and concentrated under reduced pressure. The crude was purified by column chromatography (silica gel, DCM/Hexane = 50/50, v/v) to give compound **H5** as an orange solid**.** Yield: 0.44 g (34 %). ^{1}H-NMR (300 MHz, $CDCl_3$, δ, ppm): 7.93 (br. s, 2H), 7.34 (d, *J* = 1.9 Hz, 1H), 7.27-7.19 (m, 2H), 7.05 (d, *J* = 4.2 Hz, 2H), 6.55 (dd, J_1 = 4.14 Hz, J_2 = 1.56 Hz, 2H), 4.87 (d, *J* = 2.34 Hz, 2H), 4.82 (d, *J* = 2.4 Hz, 2H), 2.60 (t, *J* = 2.43 Hz, 1H), 2.57 (t, *J* = 2.28 Hz, 1H).



Scheme S2 Synthetic routes of guest **SP-G**.

Compounds **G1**-**G6** were synthesized according to the previous literatures[S2,S3] with modifications.

Synthesis of compound G1: A solution of 2,3,3-trimethyl-3H-indole (6.00 mL, 6.00g, 37.7mmol) and 2-bromoethanol (3.33 mL, 5.88g, 47.1mmol) were dissolved in 45 mL of MeCN, and the reaction mixture was heated to 85 °C for 2 days. After the resulting suspension was cooled to room temperature, the solid product was collected by vacuum filtration and washed several times with Hexane to yield **G1** as a pink solid**.** Yield: 9.34 g (87%). ^{1}H-NMR (300 MHz, $CDCl_3$, δ, ppm): 7.83-7.77 (m, 1H,), 7.74-7.67 (m, 1H,), 7.66-7.57 (m, 2H), 4.58 (t, *J* = 5.1 Hz, 2H), 4.02 (t, *J* = 5.1 Hz, 2H), 2.82 (s, 3H), 1.59 (s, 6H).

Synthesis of compound G3: G1 (6.00g, 21.1mmol) was added in the aqueous solution (40 mL) of KOH (1.91g, 34.0mmol) and stirred for 15 min to react at room temperature. Then, the reaction mixture was extracted with EtOAc repeatedly until the organic phase no longer developed a yellow color. The combined organic layers were dried over MgSO4 and filtered, and concentrated under reduced pressure to afford **G2** as a yellow oil, which was dissolved in EtOH (80mL). To this ethanolic solution, 2-hydroxy-5-nitrobenzaldehyde (3.73g, 22.3 mmol) was added, and the reaction mixture was heated to 60 °C under nitrogen atmosphere for 6 h. After the suspension was cooled to room temperature, the precipitate was filtered with ethanol and dried to afford **G3** as a purple solid. ^{1}H-NMR (300 MHz, $CDCl_3$, δ, ppm): 8.04-7.99 (m, 2H), 7.22-7.17 (m, 1H), 7.12-7.09 (m, 1H), 6.93-6.88 (m, 2H), 6.77 (d, *J* = 8.4 Hz, 1H), 6.67 (d, *J* = 7.8 Hz, 1H), 5.88 (d, *J* = 10.5 Hz, 1H), 3.86-3.70 (m, 2H), 3.51-3.29 (m, 2H), 1.29 (s, 3H), 1.19 (s, 3H).

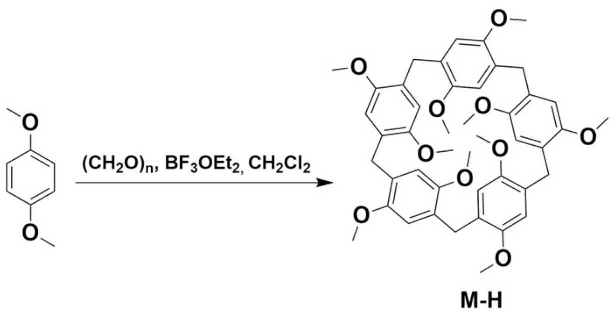
Synthesis of compound G4: Methyl 3, 5-dihydroxybenzoate (20.0 g, 119.6 mmol) and K_2CO_3 (110.2 g, 801.3 mmol) were dissolved in acetone (300 mL) and stirred for 20 min, then propargyl bromide (29.8 g, 299 mmol) was added dropwise to the reaction mixture. The reaction mixture was stirred to react at 80 °C for 24 h under nitrogen atmosphere. Then, the insoluble salts were removed by filtration, and the obtained filtrate was dried under reduced pressure to yield a crude product. The crude product was further dissolved in EtOAc and washed with water (100 mL x 3). The purification process was continued by column chromatography (silica gel, Hexane/EtOAc = 2:1, v/v) to give compound **G4** as a pale white solid**.** Yield: 63%. ^{1}H-NMR (300 MHz, $CDCl_3$, δ, ppm): (300 MHz, $CDCl_3$, δ, ppm): 7.29 (d, *J* = 2.4 Hz, 2H), 6.81 (t, *J* = 2.4 Hz, 1H), 4.71 (d, *J* = 2.4 Hz, 4H), 3.91 (s, 3H), 2.55 (t, *J* = 2.4 Hz, 2H).

Synthesis of compound G5: 4N NaOH (2 mL, 1.5 equiv) was added in a solution of compound **G4** (20.6 g, 104.8 mmol) dissolved in THF/MeOH (250 mL, 1:3 v/v). The obtained reaction mixture was stirred for 5 h at room temperature. Then, the reaction mixture was neutralized by the addition of 1N HCl and the solvents were removed by evaporation. The residue was re-dissolved in EtOAc (400 mL) and the organic phase was washed with brine (3 x 100 mL), and dried over Na_2SO_4 and evaporated under reduced pressure. The residual solid was obtained as a white solid and used without further purification in the next step. Yield: 90%. ^{1}H-NMR (500 MHz, DMSO-d_6, δ, ppm): 7.20 (d, *J* = 2.5 Hz, 2H), 6.89 (t, *J* = 2.5 Hz, 1H), 4.88 (d, *J* = 2.5 Hz, 4H), 3.61 (t, *J* = 2.0 Hz, 2H).

Synthesis of compound G6: Compound **G3** (500 mg, 0.20 mmol) and compound **G5** (756 mg, 0.40 mmol) were dissolved in dry DCM (30 mL). Then, EDCl (300mg, 0.60 mmol) and 4-dimethylaminopyridine (45mg, 0.05mmol) were added and the mixture was stirred to react at room temperature for 24 h. Consequently, the mixture was quenched with water (5mL) and extracted by DCM (3 × 10 mL). The combined organic extracts were dried over anhydrous Na_2SO_4 and concentrated under reduced pressure. The crude was purified by column chromatography (silica gel, Hexane/ EtOAc = 3:1, v/v) to give compound **G6** as an orange solid. Yield: 0.36 g 60%. ^{1}H-NMR (300 MHz, CD_3CN, δ, ppm): 8.0-7.97 (m, 2H), 7.22-7.20 (m, 3H), 7.10 (d, *J* = 7.2 Hz, 1H), 6.94-6.88 (m, 2H), 6.80 (t, *J* = 2.1 Hz, 1H), 6.75-6.71 (m, 2H), 5.88 (d, *J* = 10.2 Hz, 1H), 4.68 (d, *J* = 2.1 Hz, 4H), 4.46 (t, *J* = 6 Hz, 2H), 3.70-3.49 (m, 2H), 2.54 (t, *J* = 2.3 Hz, 2H) 1.28 (s, 3H), 1.16 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 166.5, 160.0, 159.2, 147.4, 141.8, 136.5, 132.5, 129.1, 128.6, 126.7, 123.5, 122.6, 122.4, 120.7, 119.1, 116.2, 109.6, 108.2, 107.4, 107.1, 64.1, 56.8, 53.5, 43.1, 26.6, 20.5. HRMS (ESI$^+$) $[M+H]^+$: calcd. for $C_{33}H_{29}N_2O_7$ 565.1969, found 565.1976. mp. 167-169.0 °C.

Synthetic procedures of model host-guest system

Host **M-H** was synthesized according to the previous literature[67] with modifications.



Scheme S3 Synthetic route of model host **M-H**.

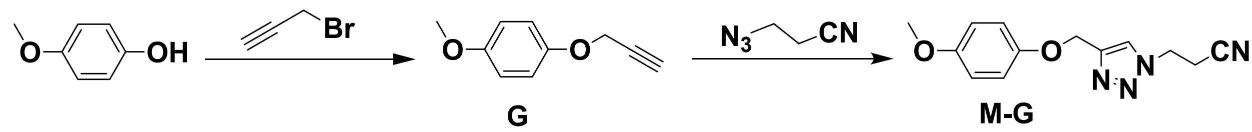
Synthesis of model host

Paraformaldehyde (1.86 g, 60 mmol) was added to a solution of 1,4-dimethoxybenzene (2.76 g, 20 mmol) in dry DCM (70 mL) to react for 1 h under nitrogen atmosphere. Then, boron trifluoride etherate $BF_3.OEt_2$ (2.5 mL, 20 mmol) was added to the previous solution, and the mixture was stirred for further reaction at room temperature for 3 h. Consequently, MeOH (50 mL) was poured into the reaction mixture, and the resulting precipitate was collected from chloroform/acetone (1:1 v/v) to acquire compound **M-H** as a white solid.

Yield: 1.6 g (70 %). ^{1}H-NMR (500 MHz, $CDCl_3$, δ, ppm): δ 6.78 (s, 10H), 3.78 (s, 10H), 3.65 (s, 30H). ^{13}C NMR ($CDCl_3$, 125 MHz) δ 151.5, 128.9, 114.7, 56.5, 30.3. HRMS (ESI$^+$) $[M+H]^+$: calcd. for $C_{33}H_{29}N2O_7$ 751.3477, found 751.3487.

Synthesis of model guest

Compounds **G and M-G** were synthesized according to the previous literature[68] with modifications.



Scheme S4 Synthetic routes of guest **M-G**.

Synthesis of model guest

Compound 3-azidopropanenitrile (31.6 mg, 0.33 mmol, 1.1 equiv.) and **G** (50 mg, 0.3 mmol, 1 equiv.) were dissolved in dry DCM (50 mL). Then, $[Cu(MeCN)_4]PF_6$ (122.9 mg, 0.33 mmol, 1.1 equiv.) was added to the mixture and stir to react at room temperature for 1 day, monitoring by thin-layer chromatography (DCM:MeOH= 99:1 v/v). Consequently, the mixture was quenched with water (25 mL) and extracted by DCM (3 × 30 mL). The combined organic extracts were dried over anhydrous Na_2SO_4 and concentrated under reduced pressure. The resultant crude was purified by silica gel column chromatography (DCM:MeOH= 99:1 v/v) to give **M-G** as a white solid. Yield: 46 mg, (50%). ^{1}H NMR (500 MHz, $CDCl_3$, 298 K): δ 7.74 (s, 1H), 6.91 (d, *J* = 9.0 Hz, 2H), 6.83 (d, *J* = 9.0 Hz, 2H), 5.16 (s, 2H), 4.64 (t, *J* = 6.5, 2H), 3.76 (s, 3H), 3.03 (t, *J* = 6.5 Hz, 2H). ^{13}C NMR ($CDCl_3$, 125 MHz) δ 155.0, 152.9, 145.8, 123.9, 116.9, 116.5, 115.4, 63.2, 56.4, 46.3, 20.1. HRMS (ESI^+) $[M+H]^+$: calcd. for $C_{13}H_{15}N_4O_2$ 259.1190, found 259.1190.

2. Characterizations of intermediate compounds and host-guest [2]pseudorotaxane

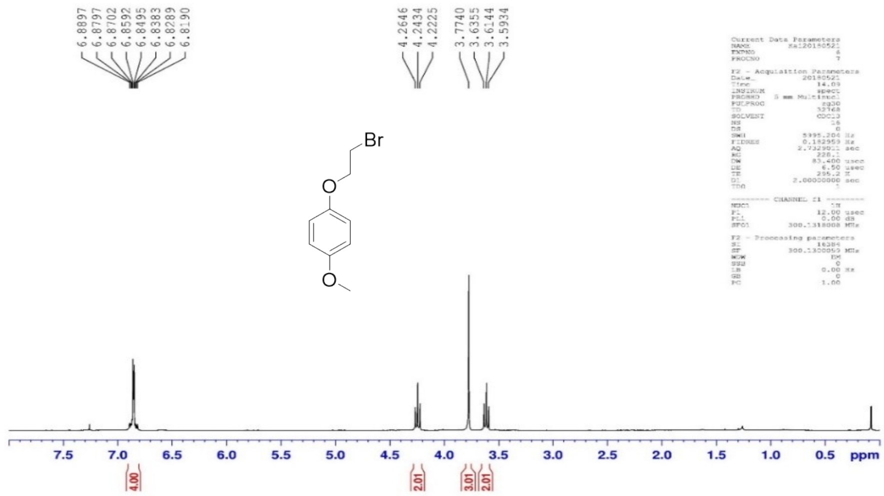


Fig. S1 ^{1}H NMR spectrum of compound **H1** ($CDCl_3$, 300 MHz, 298K).

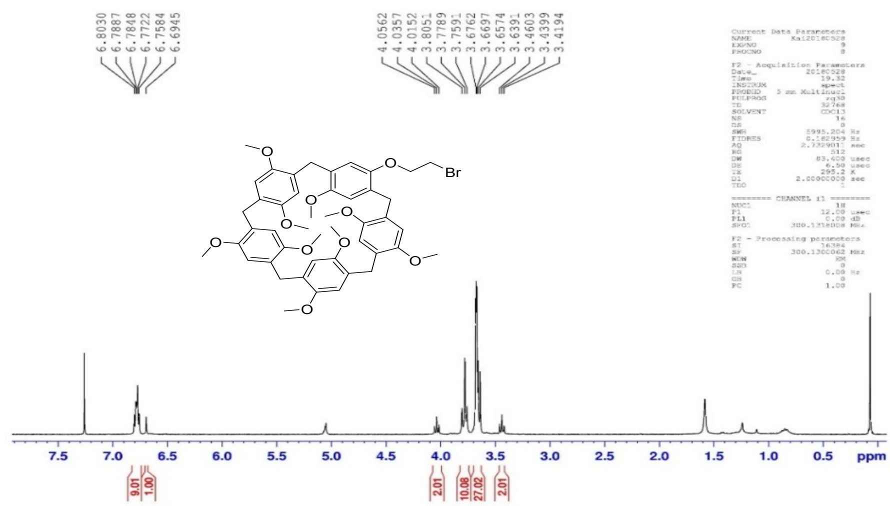


Fig. S2 ^{1}H NMR spectrum of compound **H2** ($CDCl_3$, 300 MHz, 298K).

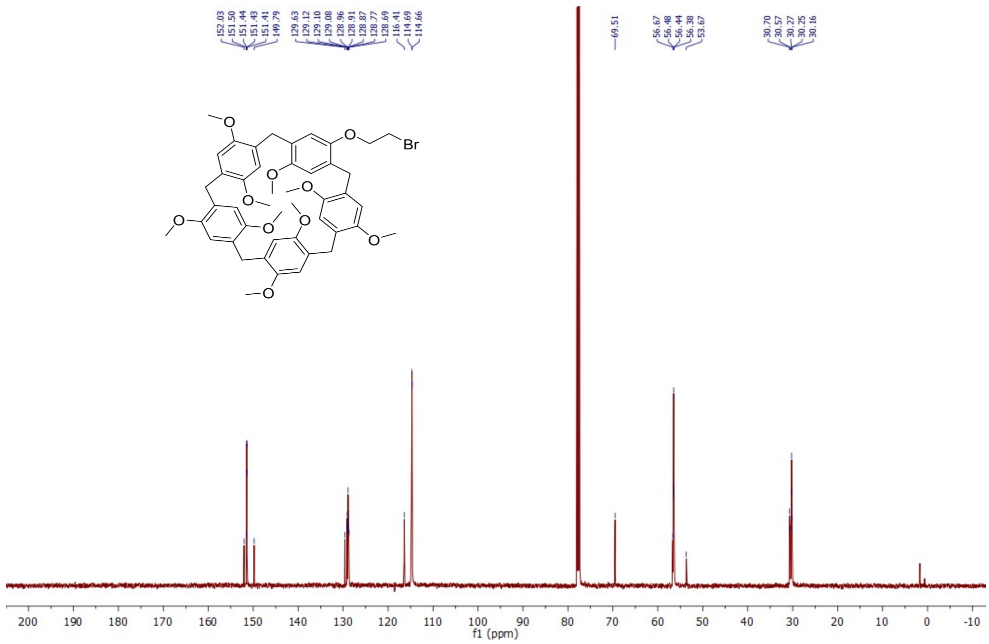
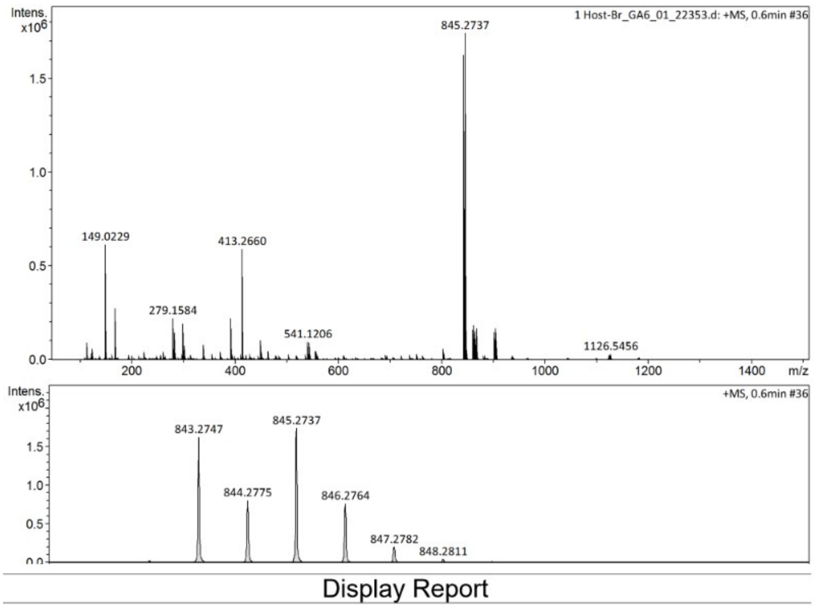


Fig. S3 ^{13}C NMR spectrum of compound **H2** ($CDCl_3$, 125 MHz, 298K).



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Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e⁻ Conf	N-Rule	Adduct
843.2747	1	C46H52BrO10	843.2738	1.0	19.7	1	100.00	20.5	even	ok	M+H

Fig. S4 HRMS-ESI spectra of compound **H2**.

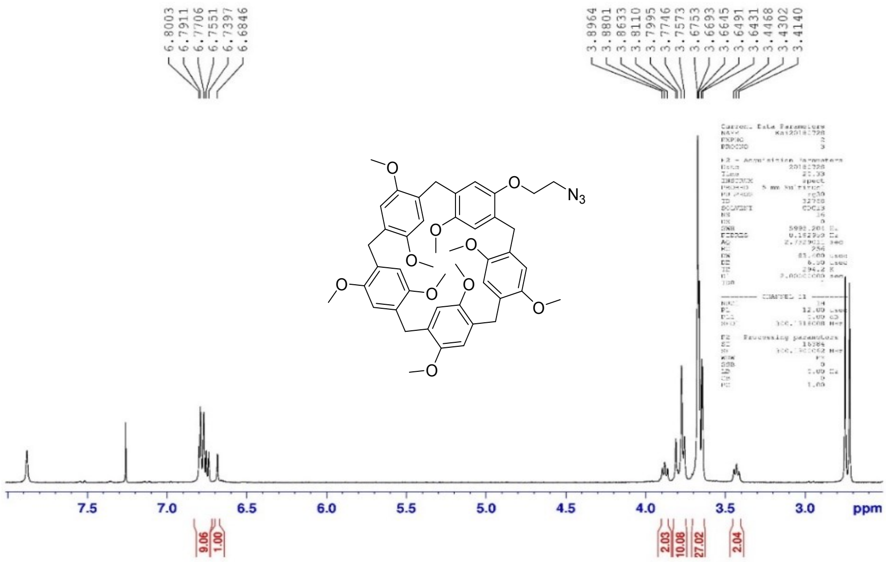


Fig. S5 ¹H NMR spectrum of compound **H3** ($CDCl_3$, 300 MHz, 298K).

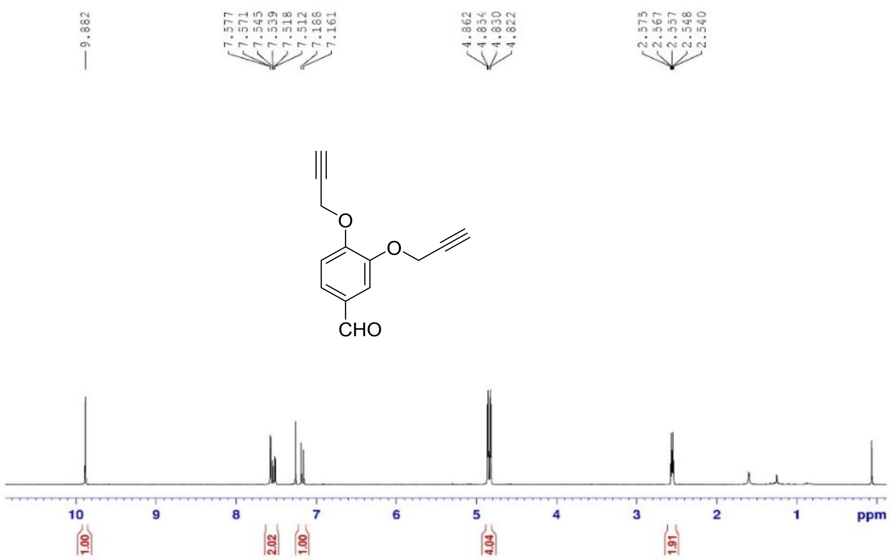


Fig. S6 ¹H NMR spectrum of compound **H4** ($CDCl_3$, 300 MHz, 298K).

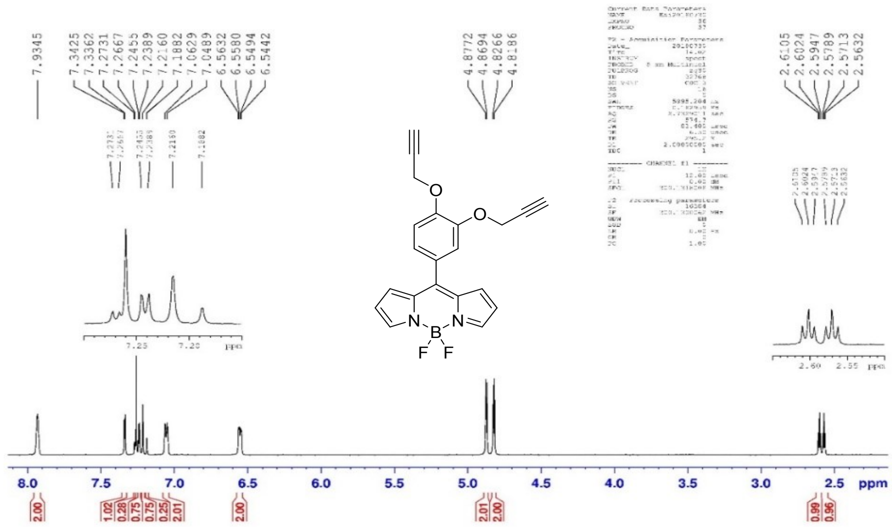


Fig. S7 ^{1}H NMR spectrum of compound **H5** ($CDCl_3$, 300 MHz, 298K).

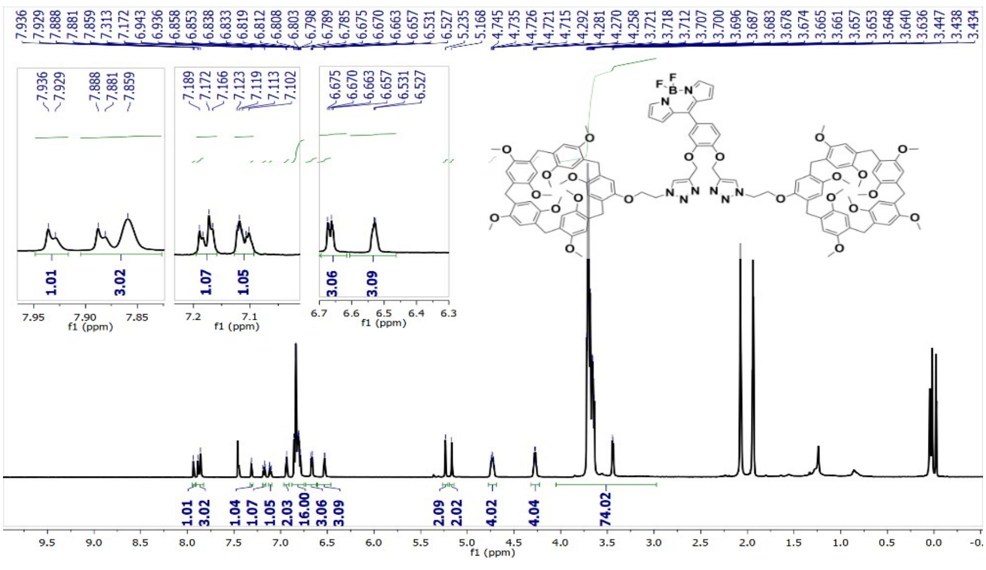


Fig. S8 ^{1}H NMR spectrum of host **BP5-H** ($CDCl_3$, 500 MHz, 298K).

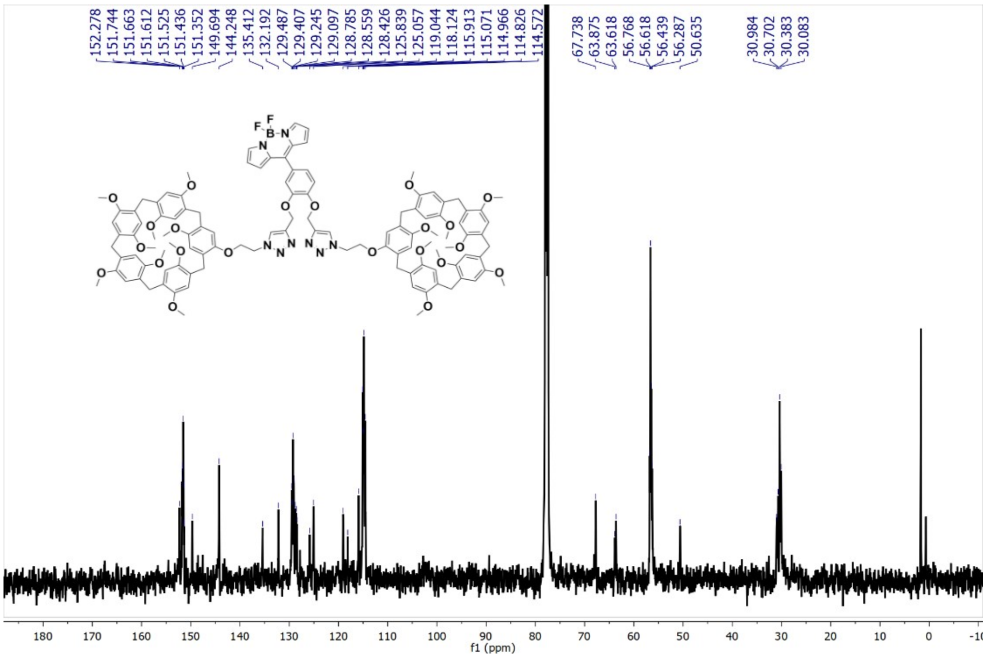
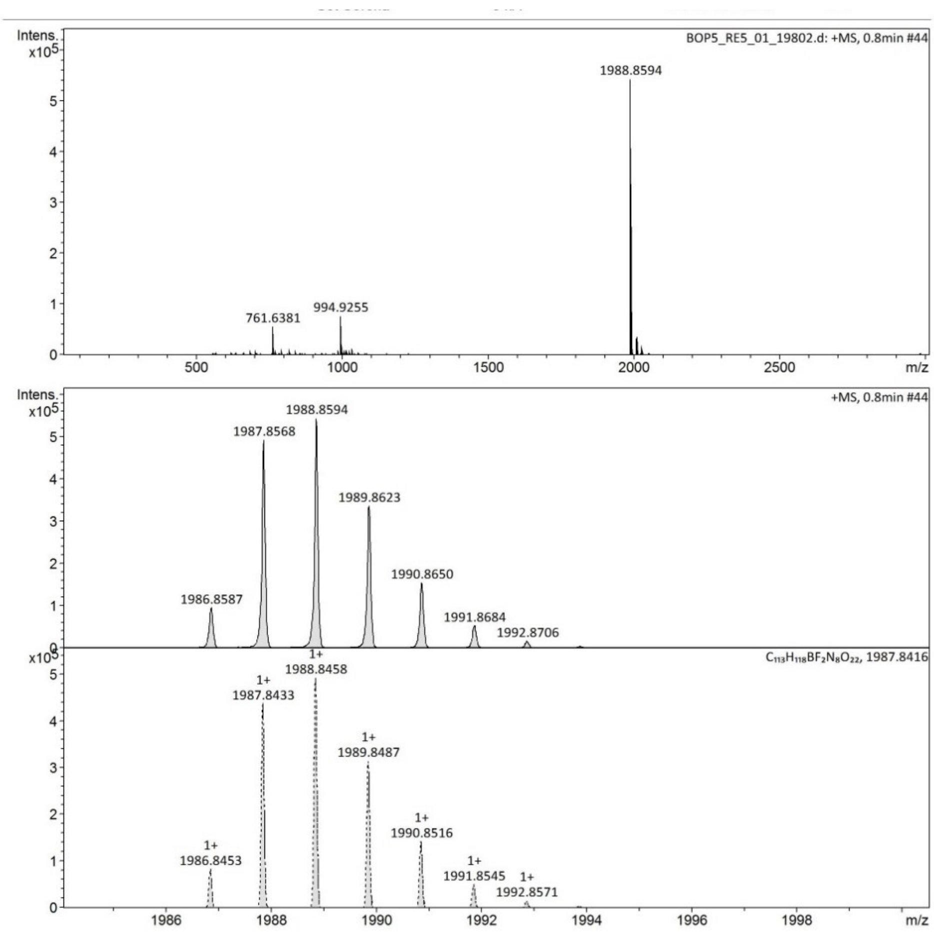


Fig. S9 ^{13}C NMR spectrum of host **BP5-H** ($CDCl_3$, 125 MHz, 298K).



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Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e⁻ Conf	N-Rule	Adduct
1987.8568	1	C113H118BF2N8O22	1988.8458	-7.6	10.3	1	100.00	58.5	even	ok	M+H

Fig. S10 HRMS-ESI spectra of host **BP5-H**.

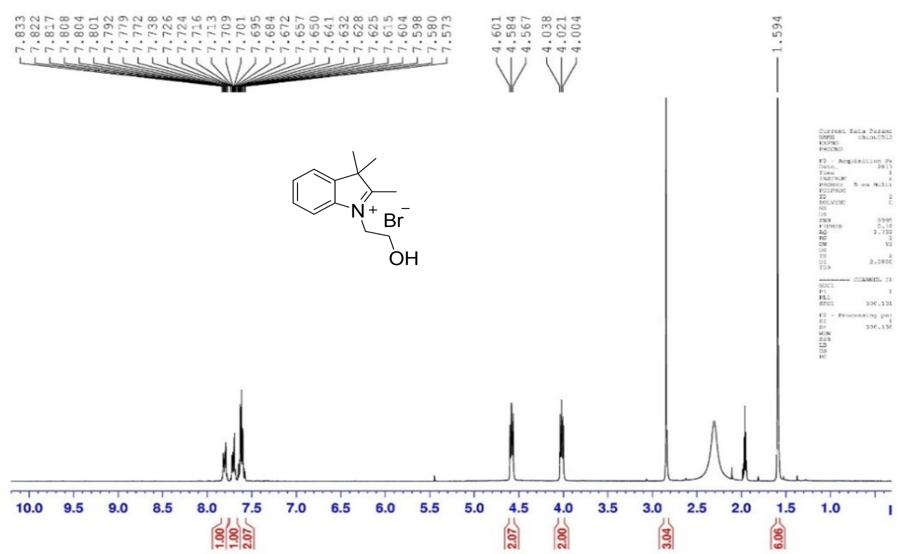

Fig. S11 ^{1}H N MR spectrum of compound **G1** ($CDCl_3$, 300 MHz, 298K).

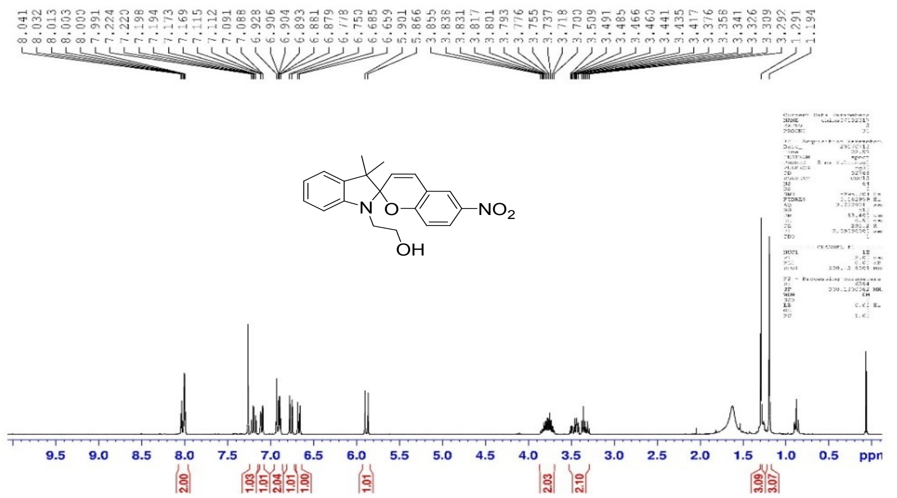

Fig. S12 ^{1}H NMR spectrum of compound **G3** ($CDCl_3$, 300 MHz, 298K).

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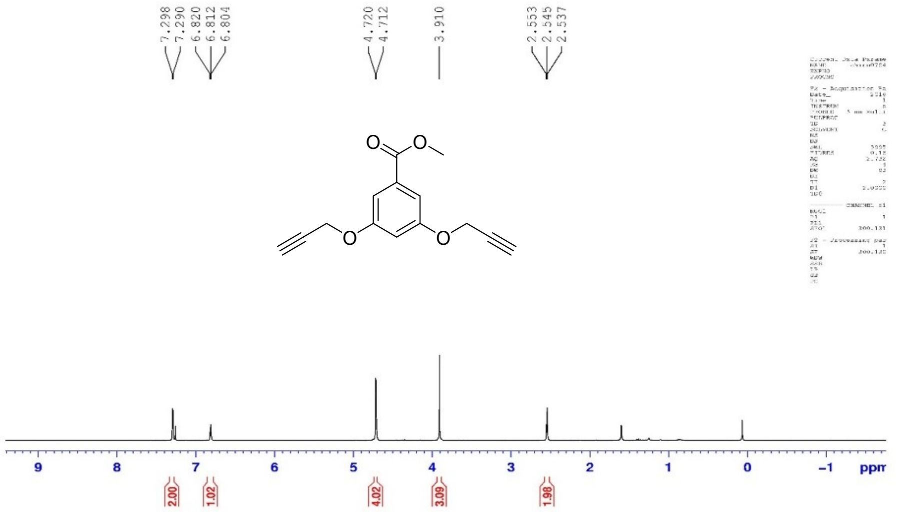


Fig. S13 ^{1}H NMR spectrum of compound **G4** ($CDCl_3$, 300 MHz, 298K).

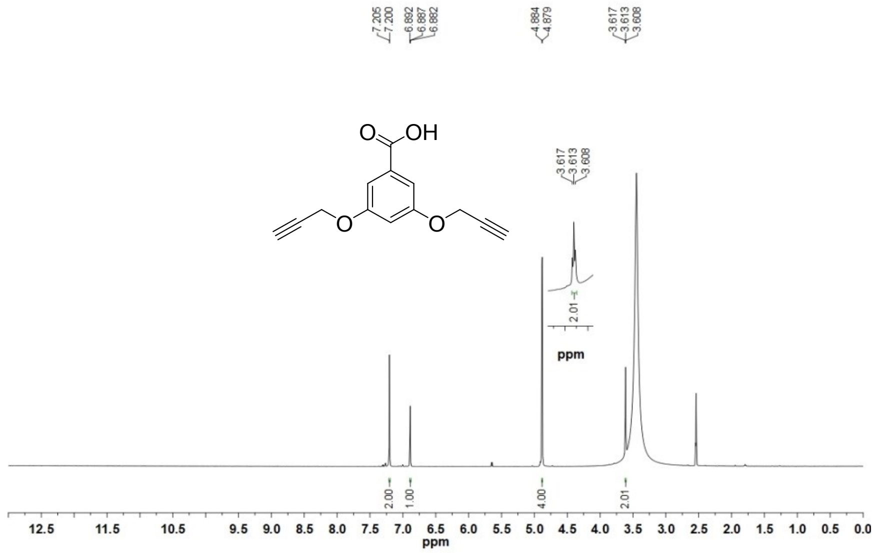


Fig. S14 ^{1}H NMR spectrum of compound **G5** (DMSO-d_6, 500 MHz, 298K).

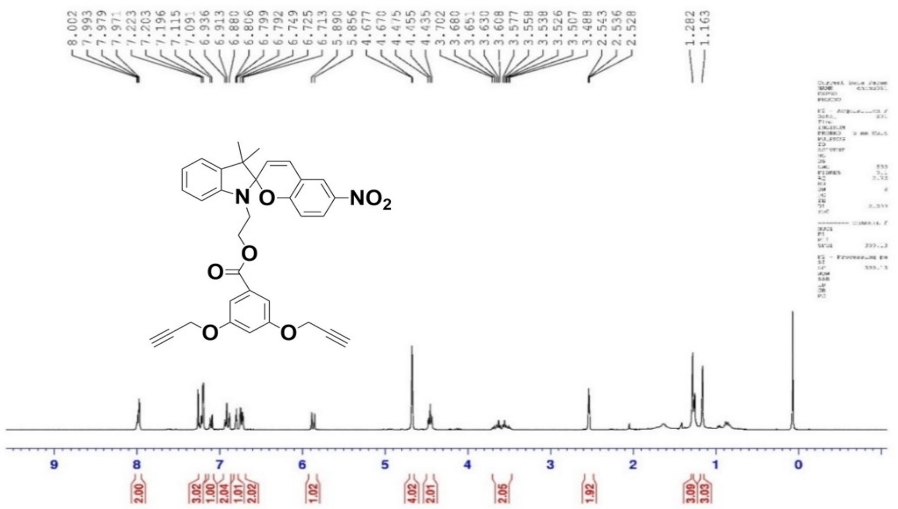


Fig. S15 ^{1}H NMR spectrum of guest **G6** (300 MHz, $CDCl_3$).

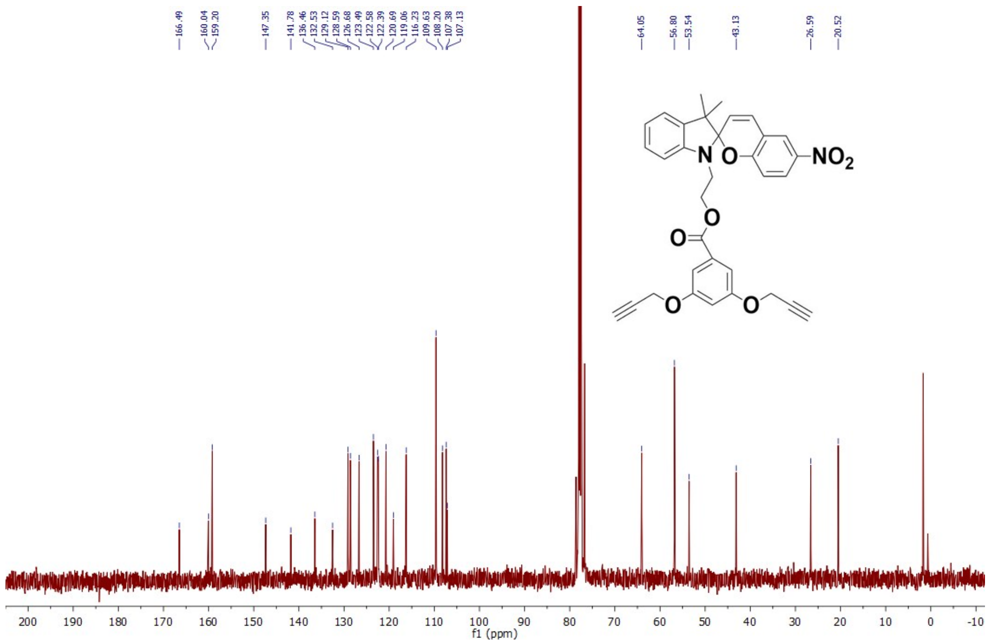
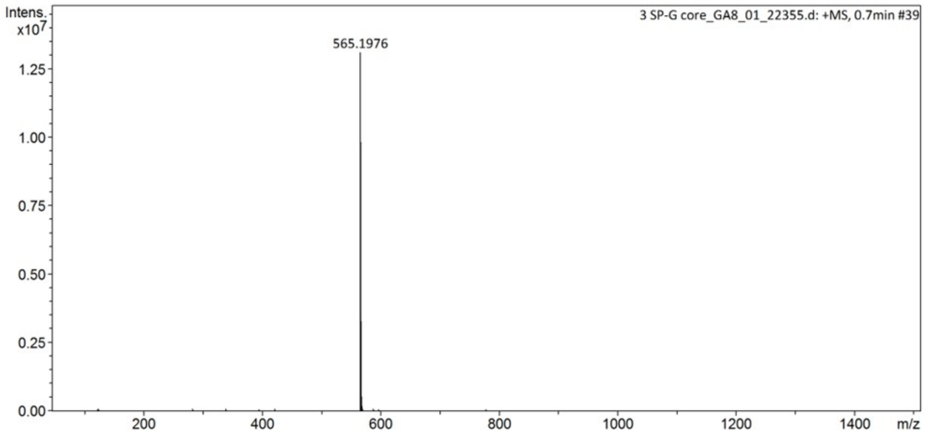


Fig. S16 ^{1}H NMR spectrum of compound **G6** ($CDCl_3$, 125 MHz, 298K).



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Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e⁻ Conf	N-Rule	Adduct
565.1976	1	C33H29N2O7	565.1969	1.1	21.3	1	100.00	20.5	even	ok	M+H

Fig. S17 HRMS-ESI spectrum of **G6**.

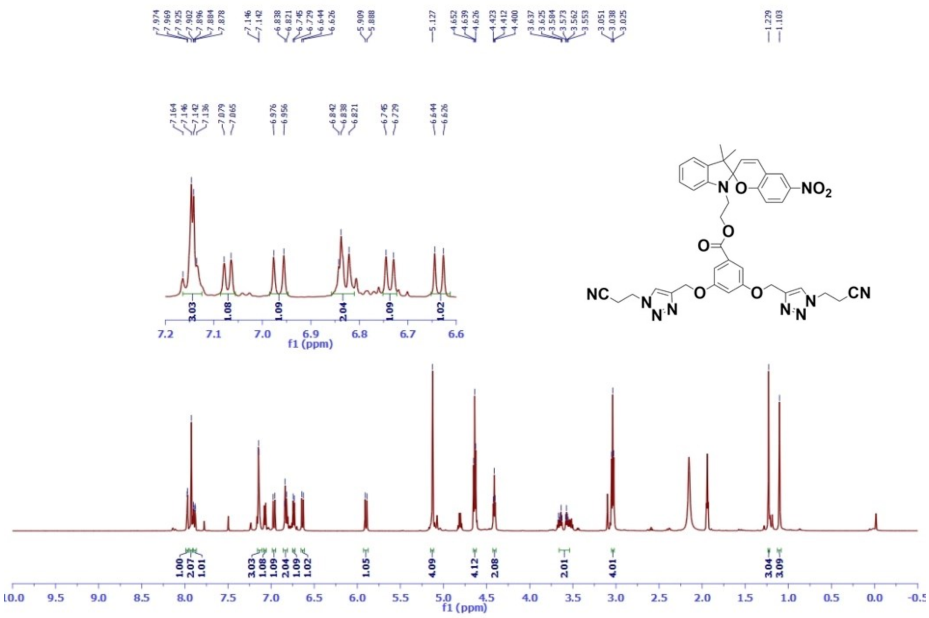


Fig. S18 ^{1}H NMR spectrum of guest **SP-G** (500 MHz, 1:1 $CDCl_3$-CD_3CN).

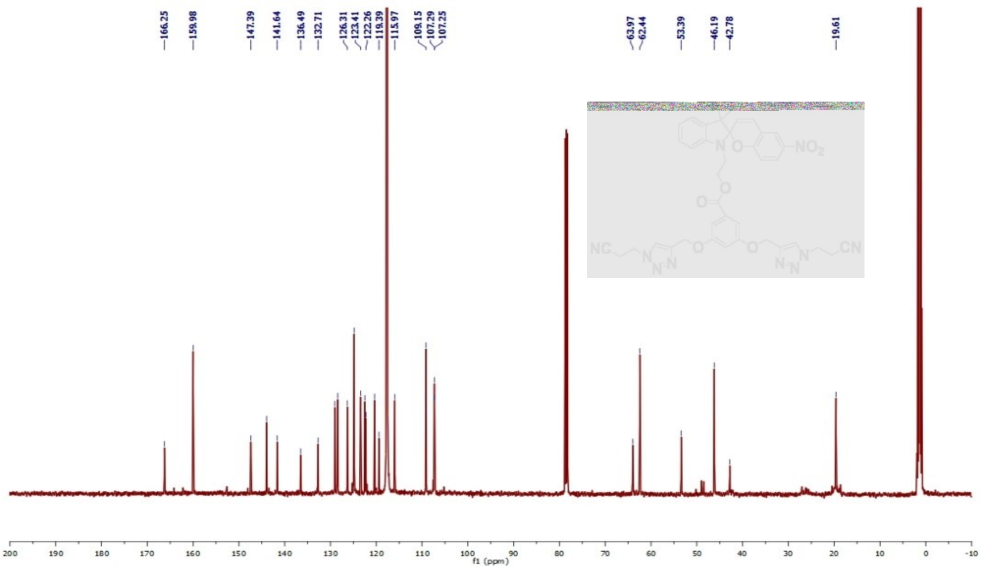


Fig. S19 ^{13}C NMR spectrum of guest **SP-G** (125 MHz, 1:1 $CDCl_3$-CD_3CN).

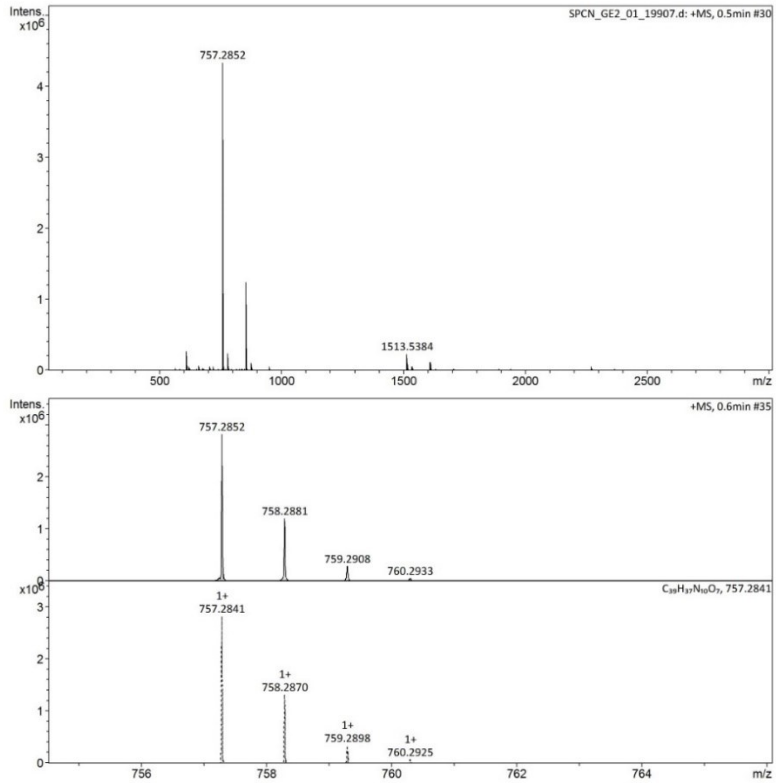


Fig. S20 HRMS-ESI spectra of guest **SP-G**.

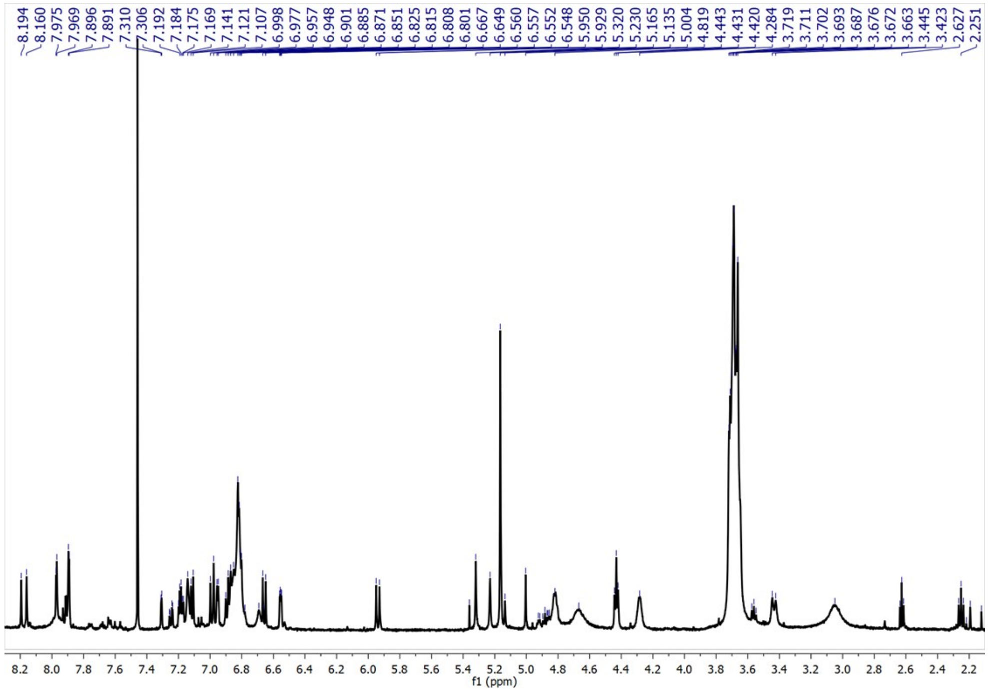


Fig. S21 ^{1}H NMR spectrum of **BP5-H⊃MC-G** (1:1 mixture, 5.0 mM each) after UV exposure (2 min.) of **BP5-H⊃SP-G** (500 MHz, 1:1 $CDCl_3$-CD_3CN).

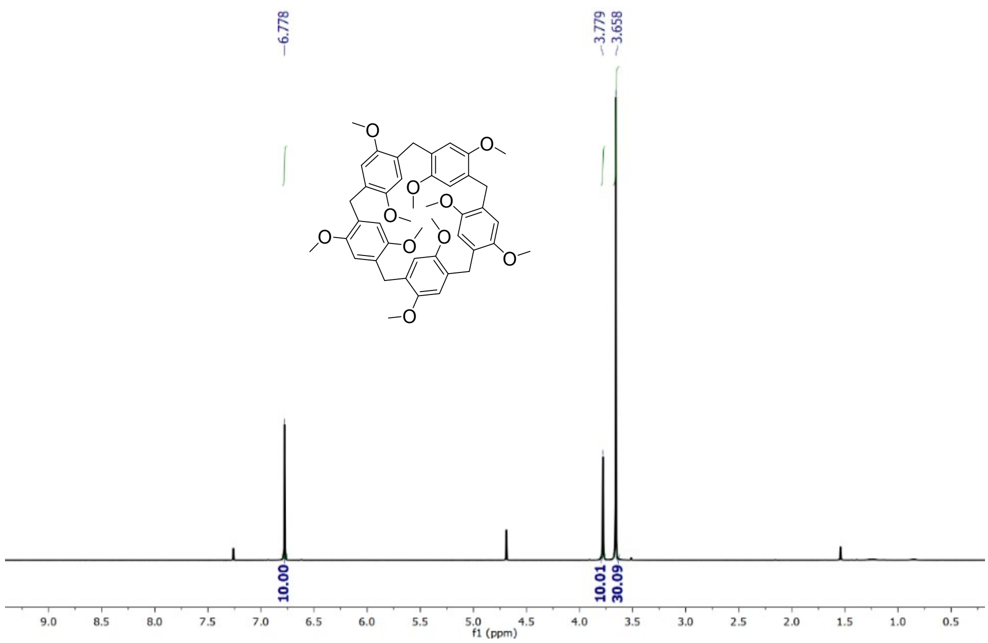


Fig. S22 ^{1}H NMR spectrum of compound **M-H** ($CDCl_3$, 500 MHz, 298K).

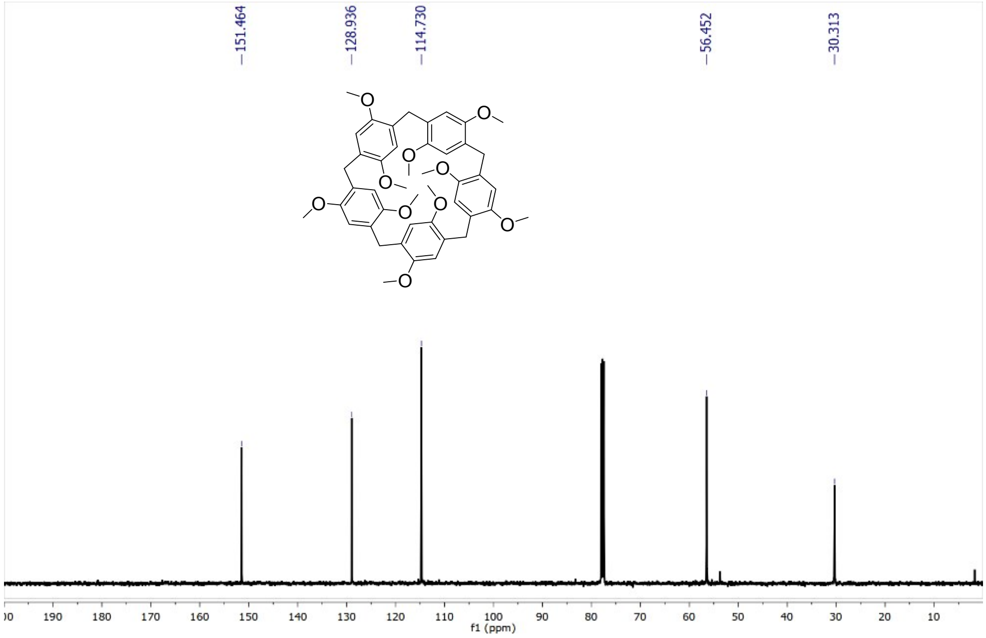
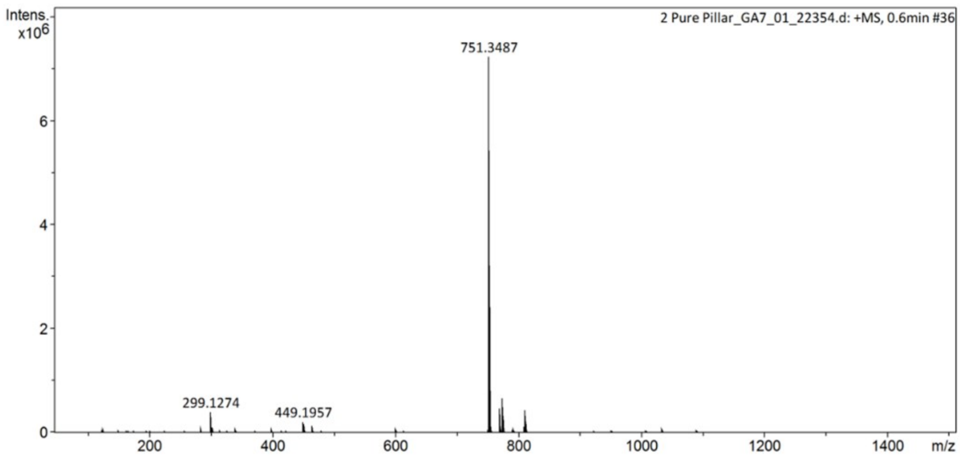


Fig. S23 ^{13}C NMR spectrum of compoud **M-H** ($CDCl_3$, 125 MHz, 298K).



Display Report

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e⁻ Conf	N-Rule	Adduct
751.3487	1	C45H51O10	751.3477	1.3	27.0	1	100.00	20.5	even	ok	M+H

Fig. S24 HRMS-ESI spectrum of compound **M-H.**

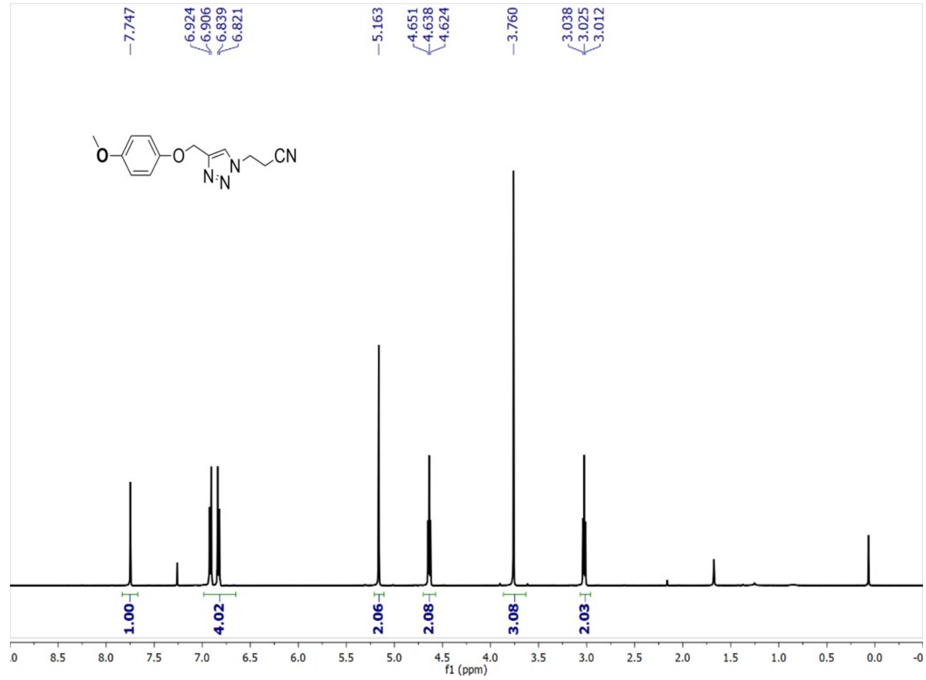


Fig. S25 ^{1}H NMR spectrum of compound **M-G** ($CDCl_3$, 500 MHz, 298K).

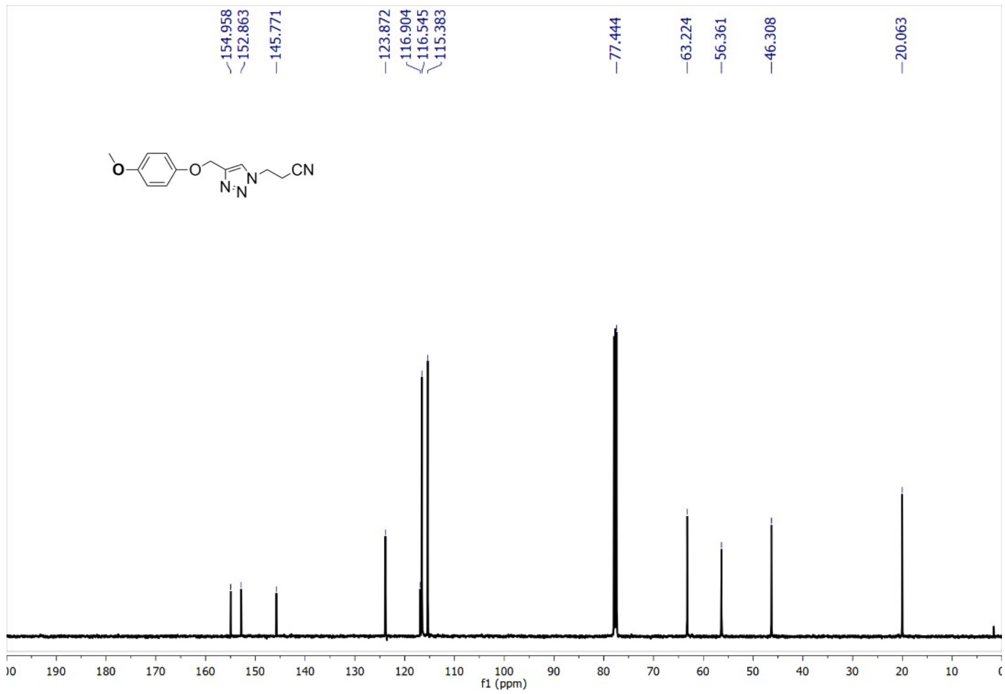
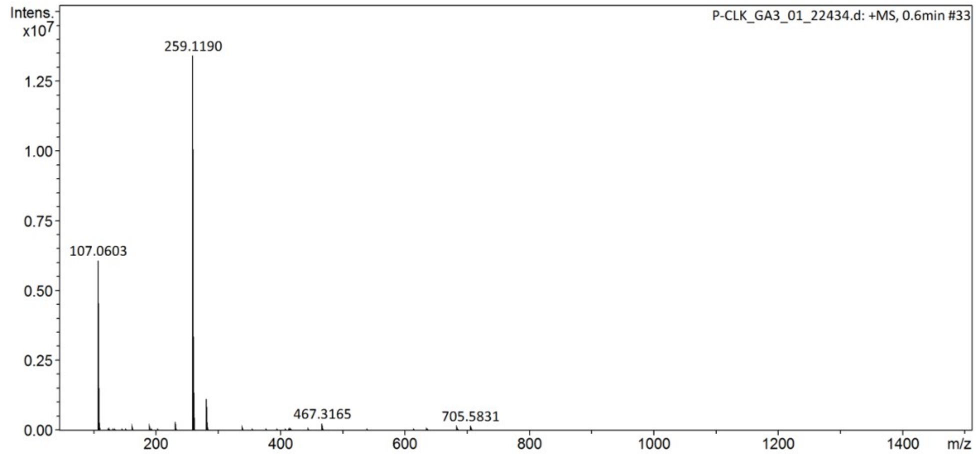


Fig. S26 ^{13}C NMR spectrum of compound **M-G** ($CDCl_3$, 125 MHz, 298K).



Display Report

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e⁻ Conf	N-Rule	Adduct
259.1190	1	C13H15N4O2	259.1190	0.0	13.4	1	100.00	8.5	even	ok	M+H

Fig. S27 HRMS-ESI spectrum of compound **M-G.**

3. Host-guest complexation of model compounds

Confirmation of host-guest interaction in pseudo-rotaxane

The host-guest interactions of host **M-H** and guest **M-G** were studied by ^{1}H NMR spectroscopy in $CDCl_3$. As shown in **Fig. S28**, the complexation between **M-H** and **M-G** is a fast exchange process on the NMR time scale based on the proton signals of **M-H**, **M-G** and 1:1 equiv. host-guest mixture of **M-H** and **M-G** (i.e., **M-H⊃M-G**).

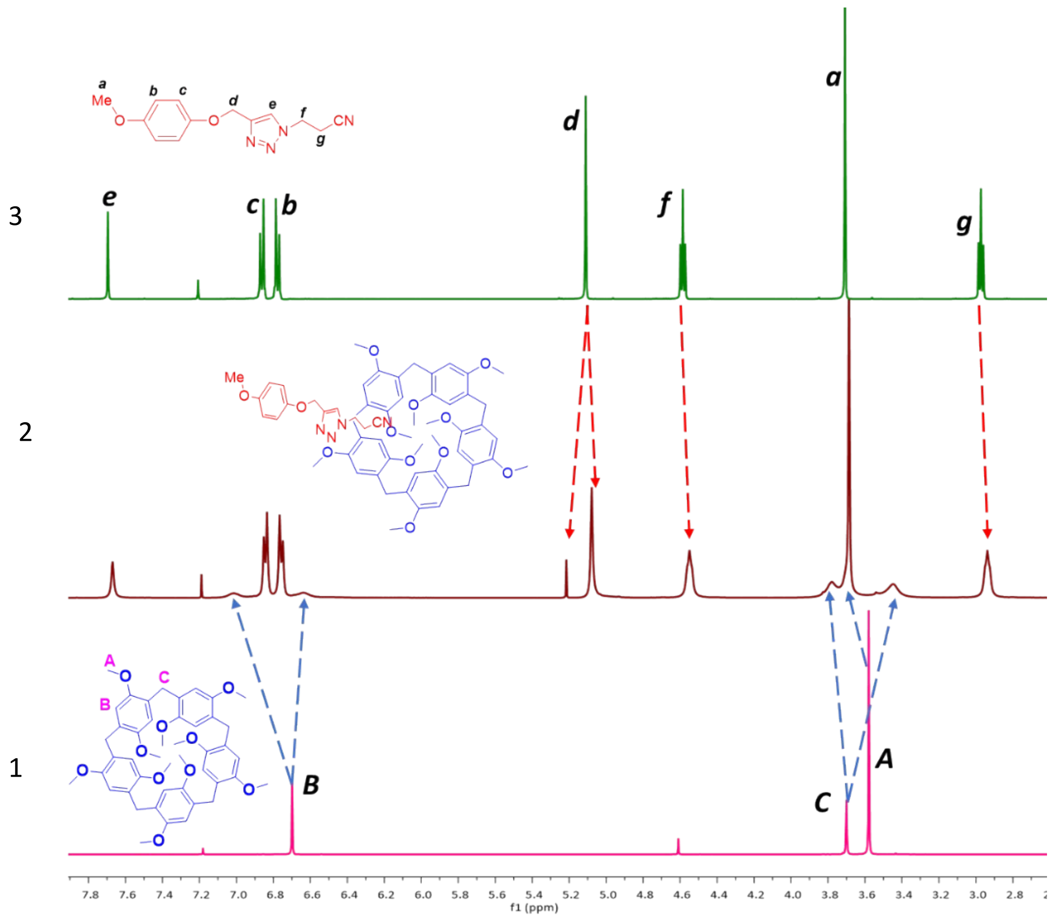


Fig. S28 ^{1}H NMR spectra (500 MHz, $CDCl_3$, 298 K) of (1) **M-H** (5.0 mM), (2) 1:1 mixture of **M-H** and **M-G** (5.0 mM each) and (3) **M-G** (5.0 mM).

Upon the addition of 1.0 equiv. of **M-G** to **M-H** solution, the resonance values for H_A, H_C and H_B of **M-G** showed small upfield shifts due to the shielding effect of electron-rich cavity provided by pillar[5]arene macrocycle. Besides, the H_f, H_g, and $H_{A,}$ H_B and H_c protons of **M-H** appeared in the small downfield region because of the de-shielding effects on the protons exposed outside the electron-rich pillar[5]arene. There are also peak broadenings of H_f, H_g protons of **M-G** along with the $H_{A,}$ H_B and H_c protons of **BP5-H** clearly indicating the occurrence of host-guest pseudorotaxane due to the interaction between electron-deficient nitrile unit of **M-G** and electron-rich cavity of **M-H**.

4. Photo-physical studies

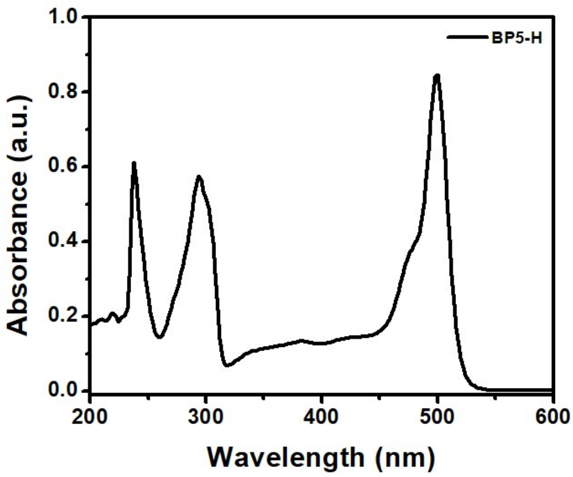


Fig. S29 Absorption spectrum of **BP5-H** in THF/water solution (60% H_2O, v/v).

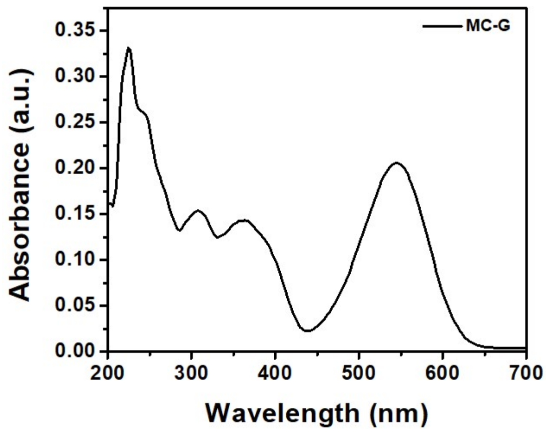


Fig. S30 Absorption spectrum of **MC-G** in THF/water solution (60% H_2O, v/v).

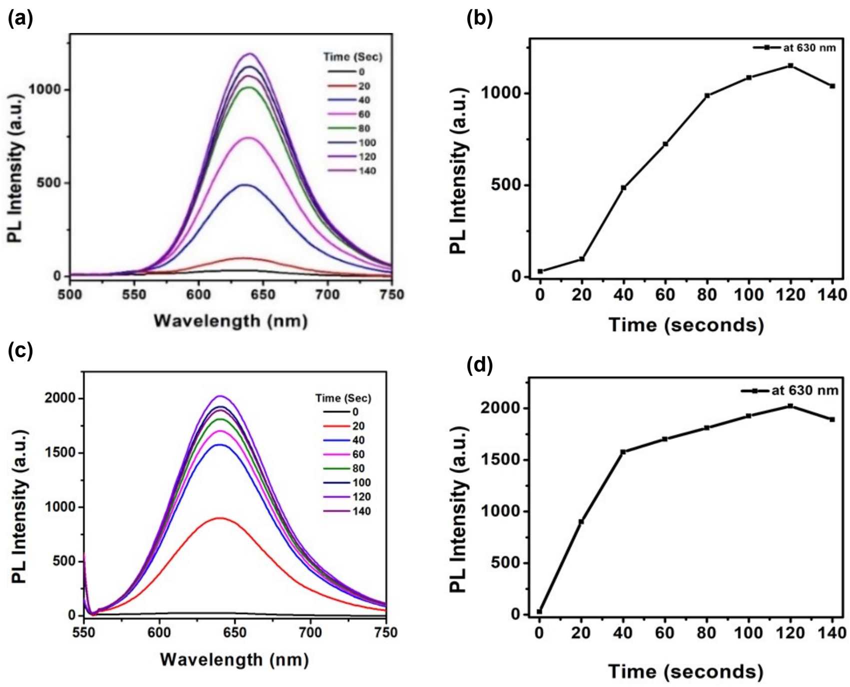


Fig. S31 (a) Time-dependent fluorescence spectra and (b) relative maximum PL intensity of **MC-G** (63 μM) in THF/water solutions (60% H_2O, v/v) with an excitation wavelength at λ_{ex} = 490 nm. (c) Time-dependent fluorescence spectra and (d) relative maximum PL intensity of **MC-G** (63 μM) in THF/water solutions (60% H_2O, v/v) with an excitation wavelength at λ_{ex} = 540 nm.

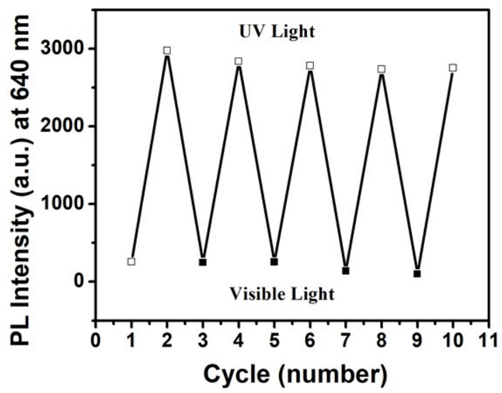


Fig. S32 Photo-switching of **SP-G** (63 μM) at 540 nm upon irradiation of UV (365 nm) and visible light for 10 min alternatively in THF/water solution (60% H_2O, v/v) with an excitation wavelength at λ_{ex} = 540 nm.

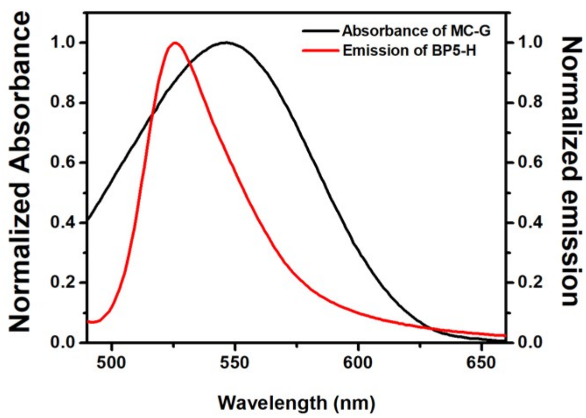


Fig. S33 Emission and absorption spectra of **BP5-H** and **MC-G** in THF/water solutions (60% H_2O, v/v) with an excitation wavelength at λ_{ex} = 490 nm.

The FRET efficiency E can be defined as the fraction of the donor de-excited via energy transfer to the acceptor. In our system, the efficiency E was calculated according to the following eqn. (1):

$$E = 1 - I_{DA}/I_D \quad (1)$$

where I_{DA} and I_D are the fluorescence intensities of the donor in the presence and absence of the acceptor, respectively. The I_{DA}, I_D values were measured as 446, 2759 counts in the **BP5-H⊃SP-G** system. According to eqn. (1), the FRET efficiency was calculated to be 84 % for **BP5-H⊃SP-G**.

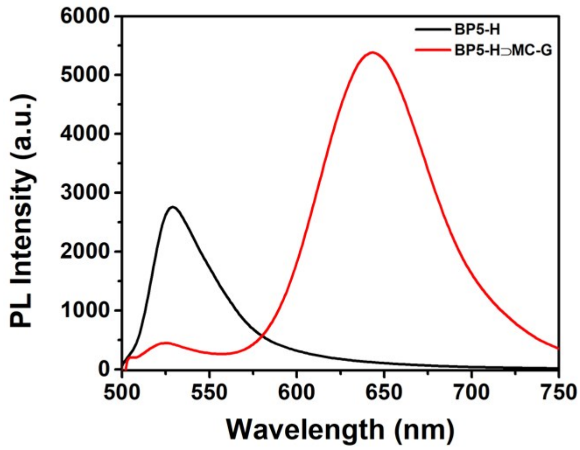


Fig. S34 PL spectra of host **BP5** and host-guest **BP5-H⊃MC-G** in THF/water solutions (60% H_2O, v/v) with an excitation wavelength at λ_{ex} = 490 nm.

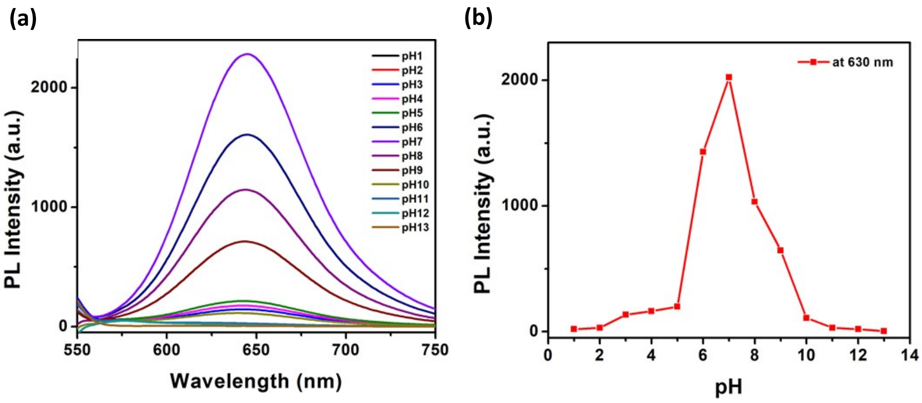


Fig. S35 (a) Fluorescence spectra and (b) relative maximum PL intensity of **MC-G** (63 μM) under UV exposure with different pH values in THF/water solutions (60% H_2O, v/v) with an excitation wavelength at λ_{ex} = 540 nm.

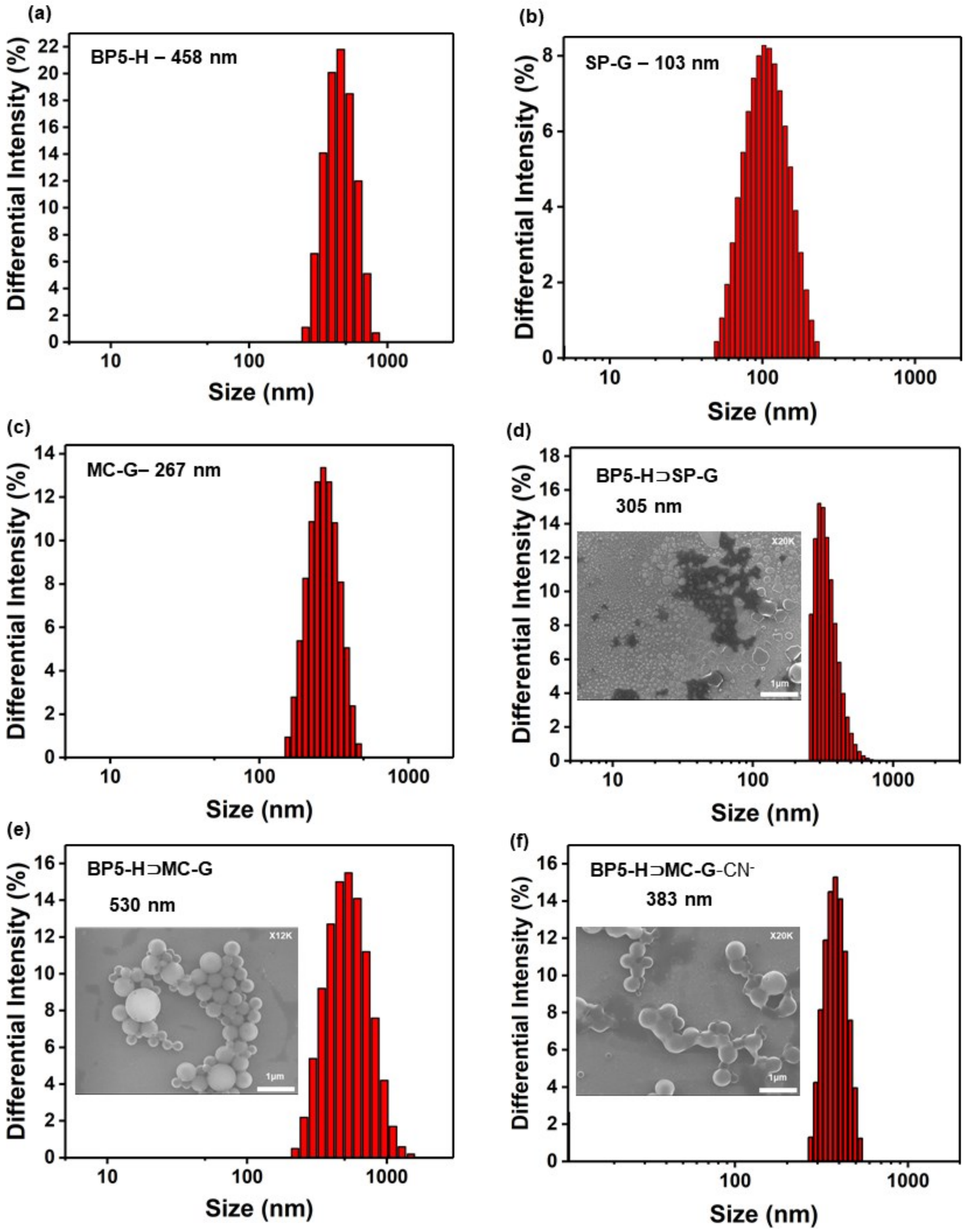


Fig. S36 DLS results of (a) **BP5-H** (b) **SP-G** (c) **MC-G** (d) **BP5-H⊃SP-G** (e) **BP5-H⊃MC-G** (f) **BP5-H⊃MC-G**-CN^- in THF/water solutions (60% H_2O, v/v) at 25 °C. Insets: Scanning electron microscope (SEM) images of host-guest systems **BP5**-**H⊃SP**-**G, BP5**-**H⊃MC**-**G** and **BP5-H⊃MC-G**-CN^- from their THF/Water (60% H_2O, v/v) solutions (63 μM) before and after detections.

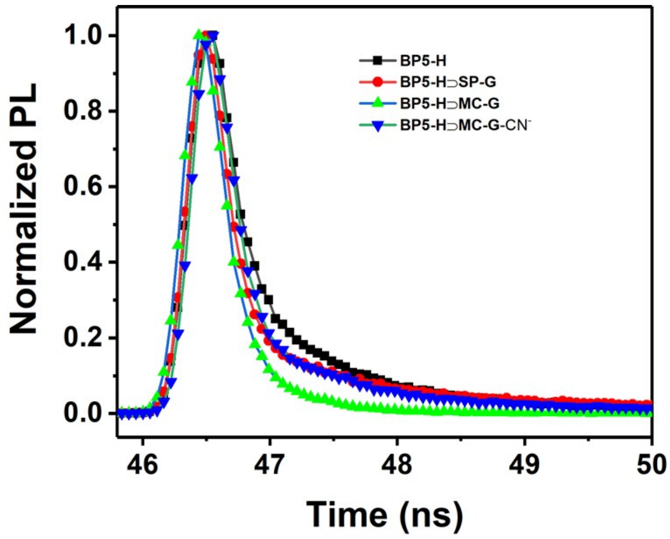


Fig. S37 Time-resolved photoluminescence spectra of **BP5-H**, **BP5-H⊃SP-G**, **BP5-H⊃MC-G** and **BP5-H⊃MC-G**-CN^- in THF/water solutions (60% H_2O, v/v) at 25 °C. (63 μM of each component used in these mixtures with an excitation wavelength of λ_{ex} = 375 nm).

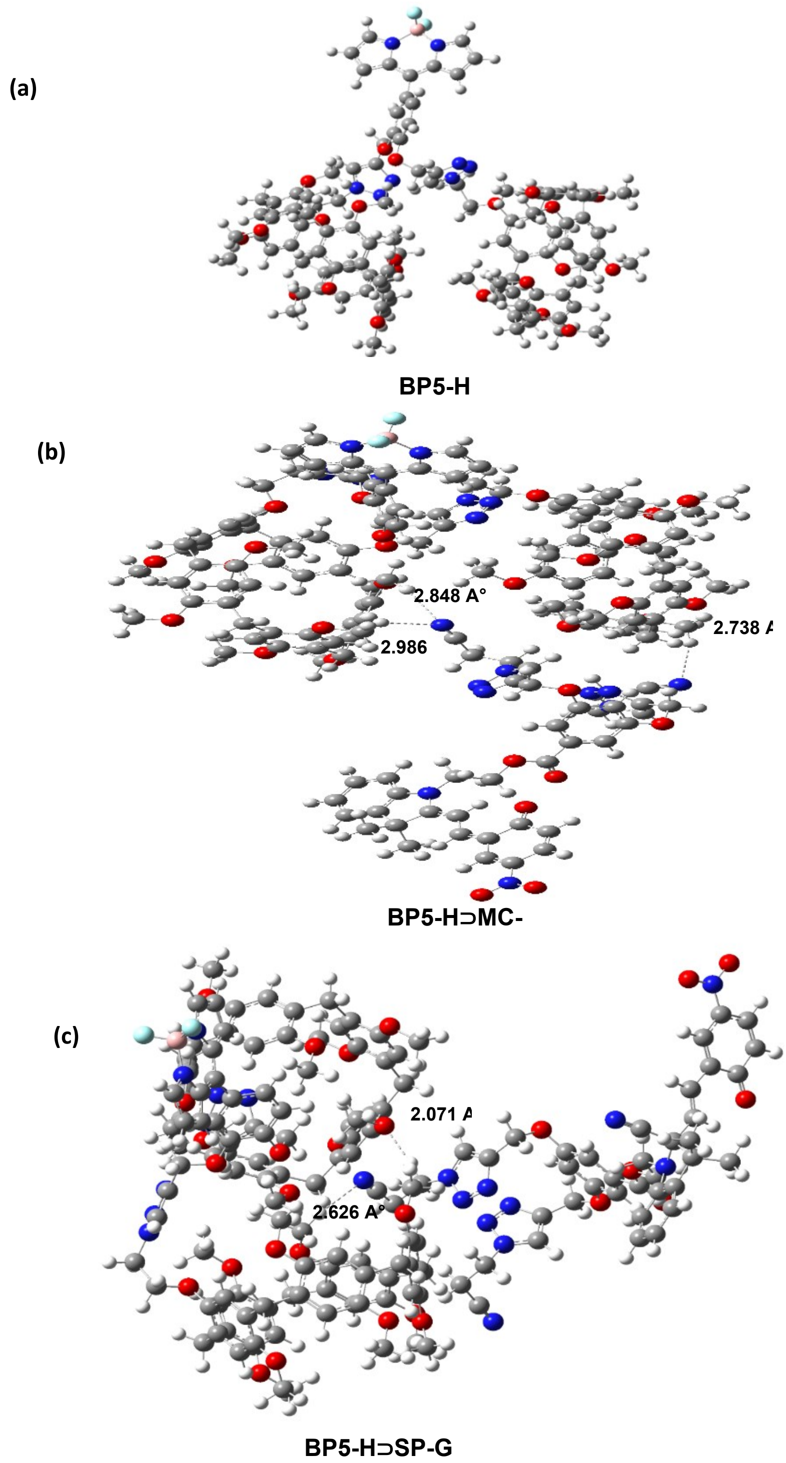


Fig. S38 Molecular structures of (a) **BP5-H** (b) **BP5-H⊃MC-G** (c) **BP5-H⊃SP-G** optimized at B3LYP/6-31g(d,p)//HF level in the gas phase.

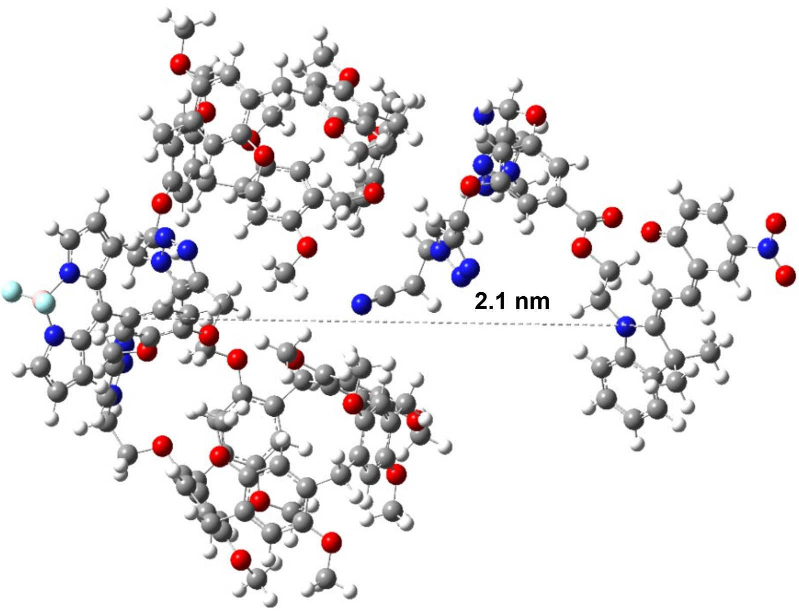


Fig. S39 Optimized structure of **BP5-H⊃MC-G** at B3LYP/6-31g(d,p)//HF level in gas phase.

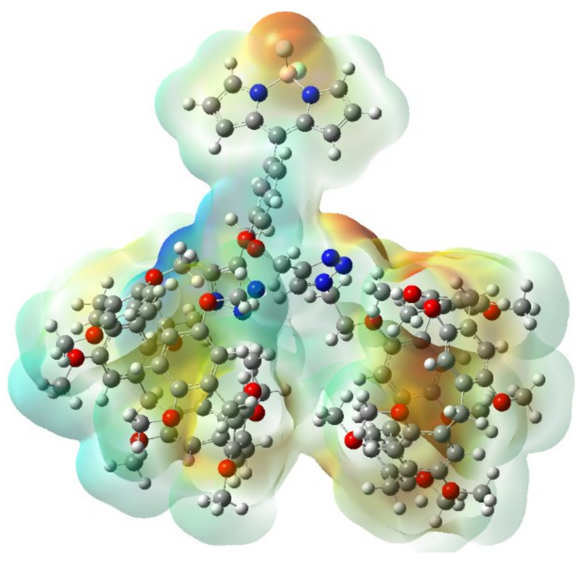


Fig. S40 Electrostatic potential of **BP5-H** obtained at B3LYP/6-31g(d,p)//HF level in the gas phase. Scale: The scale was maintained for this structure -5.627e^{-2} to 5.627e^{-2}.

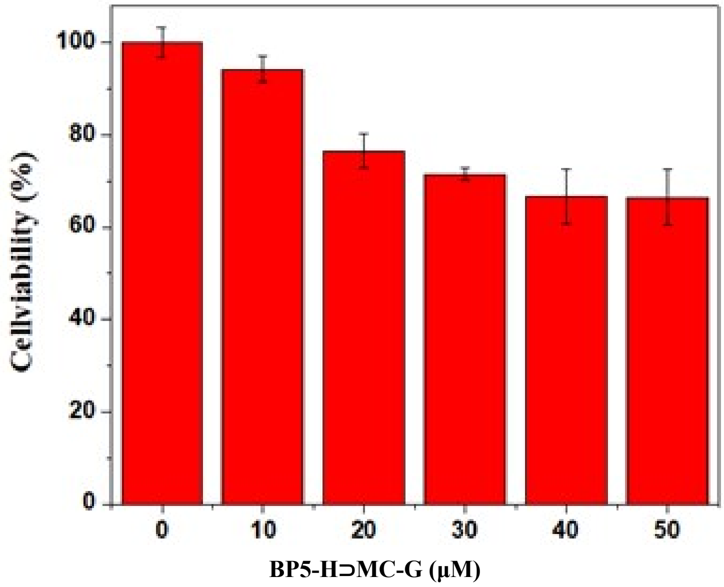


Fig. S41 MTT assay of HeLa cells in the presence of **BP5-H⊃MC-G** (10-50 μM) at 37°C for 24h.

XYZ Coordinates of **BP5-H**, optimized at B3LYP/6-31g(d,p)//HF level of theory in gas phase

O	-3.15952	2.696614	1.513203
O	-4.10976	3.505651	-0.84209
O	-5.59751	-1.54537	-3.77905
C	-0.73407	-4.13132	1.379062
C	-0.50795	-5.29645	2.100075
C	-0.12977	-6.45635	1.416156
C	-0.01853	-6.42662	0.024452
C	-0.26544	-5.27014	-0.69457
C	-0.61824	-4.10125	-0.00346
C	-0.18929	-5.25372	-2.22652
C	-1.57154	-5.04724	-2.8625
C	-2.58051	-5.9747	-2.6459
C	-3.85905	-5.7881	-3.15916
C	-4.1405	-4.63207	-3.89912
C	-3.12682	-3.71924	-4.13963
C	-1.84021	-3.91385	-3.64029
C	-5.56306	-4.36509	-4.40963
C	-6.45428	-3.76924	-3.30961
C	-7.26995	-4.59885	-2.54208
C	-8.03944	-4.09216	-1.50479
C	-7.99407	-2.71701	-1.20012
C	-7.19812	-1.89793	-1.97436
C	-6.44001	-2.40623	-3.03163
C	-8.79598	-2.15586	-0.01818
C	-8.05732	-2.33444	1.31523
C	-8.30285	-3.44251	2.108958
C	-7.61528	-3.64271	3.303199
C	-6.6632	-2.7043	3.716487
C	-6.42657	-1.58686	2.928188
C	-7.10839	-1.38952	1.731251
C	-5.86056	-2.92624	5.004995
C	-4.4912	-3.55316	4.709356
C	-3.31571	-2.81081	4.853769

C	-2.09177	-3.3961	4.52801
C	-2.01717	-4.69561	4.0573
C	-3.19718	-5.44455	3.929471
C	-4.41532	-4.86545	4.260132
C	-0.67819	-5.30351	3.627955
O	-3.48534	-1.49065	5.304317
O	-3.0183	-6.74956	3.447511
C	-2.27153	-0.79973	5.616517
O	-6.9374	-0.29726	0.867731
C	-5.95461	0.6561	1.2886
O	-7.77637	-4.75189	4.151844
O	-8.89564	-4.84761	-0.69208
O	-0.75235	-3.05649	-3.85752
O	-4.93797	-6.67284	-2.99596
C	-1.05111	-1.88202	-4.61947
O	0.12036	-7.57731	2.22268
O	-0.81801	-2.97318	-0.8122
C	-4.60381	8.176527	0.862483
C	-4.20346	6.732593	1.045248
C	-3.68245	6.295465	2.253676
C	-3.32324	4.963937	2.413067
C	-3.45686	4.066387	1.36579
C	-3.98821	4.505677	0.131831
C	-4.36297	5.833336	-0.01218
C	-3.66706	9.190362	1.070597
C	-5.92434	8.494634	0.48263
C	-7.05301	7.673727	0.268401
C	-8.11298	8.487948	-0.04913
C	-7.6343	9.807777	-0.02244
N	-6.33096	9.829586	0.295551
N	-4.00828	10.5531	0.909352
C	-2.90748	11.26927	1.14869
C	-1.81979	10.42301	1.467152
C	-2.28726	9.140561	1.414224

B	-5.43867	11.15477	0.46207
F	-5.30954	11.78008	-0.72737
F	-5.93832	11.92491	1.451233
O	4.46069	-3.36444	-0.26602
C	8.699554	2.272968	2.571486
C	7.605171	2.743707	3.285738
C	7.015213	1.916772	4.247498
C	7.511821	0.626964	4.439704
C	8.585131	0.149376	3.707972
C	9.200506	0.993178	2.771531
C	9.082087	-1.29092	3.896531
C	8.537878	-2.22563	2.807343
C	9.306955	-2.53408	1.695831
C	8.808027	-3.33257	0.670988
C	7.502638	-3.83315	0.757607
C	6.744437	-3.54915	1.882762
C	7.244949	-2.75403	2.909885
C	6.910768	-4.65748	-0.39412
C	6.418634	-3.76144	-1.53949
C	7.187495	-3.58217	-2.67605
C	6.779003	-2.73224	-3.70465
C	5.572183	-2.03668	-3.58116
C	4.787615	-2.23819	-2.4528
C	5.189417	-3.09288	-1.43458
C	5.118679	-1.04766	-4.66578
C	4.887933	2.974757	-3.05604
C	6.109885	2.430519	-3.43361
C	6.195806	1.150412	-3.96422
C	5.028192	0.386144	-4.12889
C	3.811263	0.935436	-3.76714
C	3.725618	2.221281	-3.23114
C	4.835088	4.373386	-2.42648
C	5.405581	4.367308	-1.0029
C	6.712827	4.796605	-0.75526

C	7.218657	4.740921	0.542269
C	6.456766	4.258065	1.593242
C	5.140653	3.837943	1.3449
C	4.632709	3.901866	0.052057
C	7.048723	4.14844	3.004531
O	7.430355	5.233025	-1.8837
O	4.444759	3.374486	2.468971
C	8.663564	5.897592	-1.59032
O	2.533311	2.829508	-2.79777
O	7.479794	-2.52496	-4.90303
O	6.551499	-2.41323	4.082861
O	9.511719	-3.69783	-0.48847
O	5.96143	2.488898	4.976107
O	10.30448	0.43866	2.102709
C	0.405824	-8.78425	1.509137
C	5.243302	1.576663	5.812381
C	5.249925	-2.9962	4.201356
C	3.203597	-2.68691	-0.16983
H	-1.02039	-3.24381	1.919986
H	0.260903	-7.31688	-0.51691
H	0.236431	-6.19503	-2.57029
H	0.463086	-4.44853	-2.55606
H	-2.35231	-6.84596	-2.05223
H	-3.36088	-2.83789	-4.7151
H	-6.00428	-5.29633	-4.75808
H	-5.51273	-3.67623	-5.24941
H	-7.27739	-5.65252	-2.76963
H	-7.15252	-0.83979	-1.75185
H	-9.75544	-2.66545	0.036334
H	-8.97828	-1.09713	-0.18676
H	-9.03514	-4.15785	1.769403
H	-5.69122	-0.87273	3.265309
H	-6.42506	-3.58273	5.663555
H	-5.71073	-1.9761	5.510551

H	-1.17628	-2.83481	4.631225
H	-5.3364	-5.4191	4.163313
H	-0.6085	-6.33098	3.975699
H	0.133157	-4.73843	4.085858
H	-2.56536	0.167594	6.028731
H	-1.66957	-1.32637	6.362669
H	-1.65255	-0.6222	4.732042
H	-5.9187	1.426932	0.516586
H	-4.95762	0.216823	1.379303
H	-6.21461	1.129371	2.239751
H	-0.11905	-1.31819	-4.68859
H	-1.38479	-2.11841	-5.63417
H	-1.80504	-1.24859	-4.14298
H	-3.5711	6.986291	3.078734
H	-2.92616	4.620291	3.359464
H	-4.76305	6.195112	-0.94626
H	-7.06556	6.597582	0.354289
H	-9.1238	8.191708	-0.27163
H	-8.17753	10.72625	-0.21465
H	-2.91818	12.35246	1.083661
H	-0.82035	10.75098	1.697556
H	-1.72362	8.235642	1.589922
H	9.151699	2.92616	1.842623
H	7.056421	-0.03221	5.161688
H	8.763366	-1.65037	4.872306
H	10.16929	-1.30392	3.864119
H	10.30248	-2.12381	1.638218
H	5.744468	-3.94928	1.935119
H	6.079268	-5.24794	-0.01549
H	7.667935	-5.33773	-0.77763
H	8.125167	-4.11067	-2.74367
H	3.854298	-1.70317	-2.37825
H	4.142087	-1.34634	-5.04378
H	5.828993	-1.08716	-5.48734

H	6.994845	3.031969	-3.29465
H	2.918345	0.344798	-3.90384
H	3.801571	4.709141	-2.40164
H	5.411116	5.066347	-3.03548
H	8.223606	5.074947	0.747463
H	3.621933	3.587231	-0.15863
H	6.280333	4.369974	3.739978
H	7.847611	4.880662	3.111556
H	9.044348	6.275996	-2.54109
H	9.412009	5.221306	-1.16656
H	8.532931	6.742407	-0.90804
H	0.533016	-9.56341	2.263171
H	-0.40912	-9.07857	0.841425
H	1.328337	-8.7163	0.92486
H	4.410569	2.140674	6.237092
H	4.839813	0.726563	5.254914
H	5.854793	1.194444	6.635373
H	4.851004	-2.66577	5.162451
H	4.569868	-2.66371	3.411718
H	5.279027	-4.08968	4.197396
H	2.752508	-3.00816	0.770946
H	3.317639	-1.59913	-0.14556
H	2.522117	-2.94855	-0.98439
C	-1.73445	2.467408	1.628873
C	-4.37632	4.000518	-2.16968
H	-3.62711	4.744515	-2.466
H	-5.36414	4.471879	-2.22467
H	-1.32271	2.968521	2.511698
H	-1.63418	1.386839	1.775081
C	-4.34008	2.825729	-3.13256
C	-5.36554	2.19166	-3.75177
H	-6.43321	2.351891	-3.72836
C	-0.94611	2.918633	0.409072
C	-1.02587	2.499487	-0.8781

N	-0.00139	3.950698	0.489257
N	0.495075	4.166542	-0.71018
N	-0.13323	3.27929	-1.57274
N	-3.13707	2.219098	-3.52176
N	-3.40757	1.238428	-4.35578
N	-4.78372	1.204853	-4.514
C	-5.42255	0.226529	-5.42325
H	-4.61021	-0.32941	-5.8928
C	-6.37832	-0.74168	-4.67999
H	-7.14485	-0.16392	-4.1517
H	-6.88713	-1.35607	-5.4331
H	-5.97507	0.768121	-6.19571
C	0.173543	3.240156	-3.01971
H	0.438845	4.253277	-3.32568
H	-0.73678	2.926076	-3.53601
C	1.337684	2.270312	-3.3531
H	1.399219	2.172185	-4.44293
H	1.114446	1.281743	-2.93548
H	-1.6399	1.759037	-1.36981
O	7.378098	0.513911	-4.36613
C	8.563108	1.304284	-4.22723
C	8.794376	-3.08885	-4.93601
H	8.526575	2.221066	-4.823
H	8.76539	1.573563	-3.18641
H	9.386963	0.687696	-4.59148
H	9.424669	-2.73006	-4.11734
H	8.780592	-4.18266	-4.91057
H	9.240099	-2.77354	-5.88148
C	10.94471	1.31522	1.170625
C	10.85658	-3.21305	-0.55191
H	11.33396	2.220181	1.646272
H	11.78526	0.758668	0.751422
H	10.28266	1.609687	0.350992
H	11.4725	-3.57792	0.275214

H	11.27635	-3.59064	-1.48639
H	10.9066	-2.12042	-0.56692
C	3.090542	2.981626	2.219304
H	2.47727	3.798621	1.827933
H	3.02543	2.136133	1.528222
H	2.681542	2.671872	3.182703
C	-1.33502	-1.82731	-0.12845
H	-1.50903	-1.06747	-0.89238
H	-2.28279	-2.03332	0.377248
H	-0.62878	-1.42494	0.604118
C	-4.62485	-7.87699	-2.28865
C	-4.21416	-7.53312	3.381141
H	-5.53984	-8.47244	-2.27367
H	-3.84203	-8.46028	-2.78202
H	-4.31923	-7.68723	-1.25549
H	-4.94486	-7.12036	2.679305
H	-3.91436	-8.52126	3.026902
H	-4.69498	-7.6459	4.357199
C	-8.97802	-6.2369	-1.02805
C	-8.88318	-5.59962	3.827497
H	-9.69336	-6.67924	-0.33199
H	-9.34129	-6.39894	-2.04692
H	-8.01923	-6.75075	-0.91357
H	-9.83269	-5.05731	3.802761
H	-8.75011	-6.11122	2.869675
H	-8.93527	-6.35354	4.615531

XYZ coordinates of BP5-H⊃MC-G, optimized at B3LYP/6-31g(d,p)//HF level of theory in gas phase

O	-2.94652	-2.9476	2.798061
O	-5.40458	-3.97229	2.935944
O	-6.96145	-5.46314	-2.62628
C	-0.55897	-1.49053	-3.90292
C	0.486349	-1.42891	-4.82652

C	0.197336	-1.04729	-6.13089
C	-1.12212	-0.76012	-6.50245
C	-2.1597	-0.84309	-5.59998
C	-1.86318	-1.20565	-4.26828
C	-3.61399	-0.58273	-6.01069
C	-4.46286	-1.8596	-5.92782
C	-4.14441	-2.95637	-6.71591
C	-4.85016	-4.15018	-6.61628
C	-5.8979	-4.25329	-5.69184
C	-6.23609	-3.14992	-4.92601
C	-5.53925	-1.94809	-5.0362
C	-6.63739	-5.5842	-5.50025
C	-5.88039	-6.50928	-4.53584
C	-4.96375	-7.43638	-5.03027
C	-4.22466	-8.24274	-4.17761
C	-4.38	-8.12263	-2.78136
C	-5.29958	-7.21469	-2.29938
C	-6.05892	-6.41761	-3.16003
C	-3.52944	-8.97315	-1.82809
C	-2.12047	-8.39715	-1.63183
C	-1.05485	-8.88343	-2.37081
C	0.224243	-8.35084	-2.23142
C	0.442893	-7.31057	-1.32152
C	-0.62183	-6.83257	-0.57044
C	-1.90183	-7.35928	-0.71449
C	1.832548	-6.67457	-1.18472
C	1.934334	-5.38631	-2.01182
C	1.951209	-4.13366	-1.38804
C	1.981506	-2.98181	-2.17211
C	1.98723	-3.04959	-3.55654
C	1.997791	-4.30588	-4.17811
C	1.972367	-5.45556	-3.39692
C	1.923724	-1.76718	-4.39123
O	1.899704	-4.1547	0.013767

O	2.008022	-4.28764	-5.58405
C	2.141921	-2.89135	0.6443
O	-3.03738	-6.94391	-0.00333
C	-2.81606	-5.85598	0.902431
O	1.351929	-8.757	-2.96641
O	-3.2994	-9.21294	-4.58467
O	-5.83652	-0.77736	-4.32345
O	-4.6004	-5.30821	-7.37149
C	-6.84001	-0.92668	-3.31345
O	1.2415	-0.87393	-7.07001
O	-2.96917	-1.23747	-3.41352
C	-4.86485	-4.8442	7.824297
C	-4.34465	-4.32923	6.504528
C	-3.07563	-3.77754	6.413347
C	-2.60908	-3.30865	5.192588
C	-3.40917	-3.36445	4.062299
C	-4.70171	-3.92993	4.148372
C	-5.15288	-4.41224	5.367649
C	-4.91658	-3.99751	8.931697
C	-5.29872	-6.18391	7.932095
C	-5.28755	-7.24022	6.997236
C	-5.78133	-8.36146	7.621362
C	-6.08785	-7.99123	8.939168
N	-5.80315	-6.69492	9.14247
N	-5.40206	-4.44765	10.18186
C	-5.34631	-3.41461	11.02477
C	-4.8354	-2.26573	10.37573
C	-4.57555	-2.62373	9.083795
B	-5.99141	-5.9107	10.52974
F	-7.30438	-5.80324	10.82833
F	-5.24283	-6.4874	11.49317
O	-3.86481	4.067597	-3.26108
C	-1.53479	8.102113	3.07171
C	-0.93474	7.147302	3.881361

C	0.252634	6.541035	3.455441
C	0.774777	6.867357	2.202854
C	0.152695	7.789647	1.378438
C	-1.00415	8.438864	1.833431
C	0.704699	8.08928	-0.022
C	-0.2686	7.687583	-1.14152
C	-0.87221	8.663371	-1.93049
C	-1.78528	8.330345	-2.92396
C	-2.10006	6.980638	-3.1578
C	-1.47787	6.014366	-2.39193
C	-0.57586	6.3493	-1.38346
C	-3.14531	6.583793	-4.20867
C	-4.51097	6.331992	-3.556
C	-5.42051	7.366297	-3.4137
C	-6.64165	7.177518	-2.76705
C	-6.94914	5.919835	-2.23479
C	-6.04762	4.877505	-2.40287
C	-4.83659	5.062082	-3.05882
C	-8.25139	5.689774	-1.4519
C	-7.39888	5.030732	2.753229
C	-7.57362	6.31632	2.259265
C	-7.86114	6.544032	0.918664
C	-7.98477	5.455464	0.041662
C	-7.83053	4.172241	0.540054
C	-7.53566	3.944323	1.883565
C	-7.03921	4.821796	4.231446
C	-5.62082	5.315701	4.542619
C	-5.41017	6.594421	5.066078
C	-4.10827	7.036444	5.298508
C	-3.01566	6.235245	5.016133
C	-3.22852	4.945797	4.502424
C	-4.52653	4.503152	4.27519
C	-1.58598	6.752078	5.215643
O	-6.57111	7.358794	5.284991

O	-2.06147	4.215035	4.247698
C	-6.37346	8.533158	6.079483
O	-7.33567	2.678829	2.462219
O	-7.63314	8.15848	-2.61674
O	0.09942	5.33986	-0.65606
O	-2.46236	9.248454	-3.74075
O	0.824571	5.634695	4.358844
O	-1.53058	9.400786	0.956935
C	1.318486	-1.99575	-7.96855
C	2.004251	4.973442	3.890155
C	-0.8128	4.579787	0.159634
C	-4.27164	2.745226	-2.89127
H	-0.33062	-1.77839	-2.89015
H	-1.32222	-0.47014	-7.52614
H	-3.63004	-0.19441	-7.02783
H	-4.05566	0.165462	-5.35676
H	-3.31743	-2.8667	-7.40274
H	-7.04779	-3.24825	-4.22281
H	-6.74435	-6.08164	-6.46159
H	-7.63056	-5.38322	-5.10623
H	-4.83658	-7.50088	-6.09881
H	-5.42978	-7.1091	-1.23026
H	-3.44669	-9.98172	-2.22743
H	-4.0316	-9.02681	-0.8648
H	-1.24362	-9.68164	-3.0711
H	-0.43222	-6.03236	0.128305
H	2.582068	-7.38566	-1.5246
H	2.026216	-6.43921	-0.14158
H	1.992293	-2.00818	-1.70712
H	1.967421	-6.43354	-3.85267
H	2.541628	-1.86731	-5.27954
H	2.322739	-0.9414	-3.80181
H	2.178244	-3.0863	1.717797
H	3.09396	-2.44815	0.33888

H	1.342143	-2.16999	0.451766
H	-3.78292	-5.62225	1.352211
H	-2.44858	-4.95932	0.39644
H	-2.11547	-6.11624	1.700953
H	-6.90997	0.037065	-2.80579
H	-7.82164	-1.1643	-3.73407
H	-6.58375	-1.69084	-2.57422
H	-2.44109	-3.72639	7.288134
H	-1.61542	-2.88561	5.119161
H	-6.13935	-4.83815	5.461475
H	-4.93726	-7.16702	5.978642
H	-5.90814	-9.34375	7.19956
H	-6.49332	-8.60478	9.735675
H	-5.67205	-3.51361	12.05521
H	-4.69305	-1.30162	10.83372
H	-4.1872	-1.99016	8.299325
H	-2.44075	8.570515	3.421815
H	1.672933	6.387899	1.846629
H	1.643909	7.554023	-0.14887
H	0.913764	9.153894	-0.11154
H	-0.62706	9.695758	-1.73856
H	-1.71896	4.975944	-2.57245
H	-2.81915	5.678809	-4.71641
H	-3.23519	7.379882	-4.94298
H	-5.15469	8.33335	-3.81128
H	-6.30394	3.910854	-1.99997
H	-8.76847	4.822624	-1.85966
H	-8.89029	6.559864	-1.57449
H	-7.47156	7.13864	2.950278
H	-7.94212	3.341736	-0.13915
H	-7.11427	3.763193	4.465583
H	-7.74718	5.365232	4.853665
H	-3.93276	8.0216	5.7019
H	-4.70969	3.514227	3.883235

H	-0.97598	5.981763	5.680423
H	-1.60884	7.614599	5.880287
H	-7.3658	8.943504	6.277151
H	-5.78565	9.295293	5.559134
H	-5.89063	8.315833	7.036442
H	2.149415	-1.80635	-8.65117
H	1.507317	-2.92749	-7.42806
H	0.40378	-2.10875	-8.55797
H	2.313836	4.29692	4.689009
H	1.821232	4.382935	2.987825
H	2.823337	5.671042	3.691693
H	-0.21766	3.851641	0.714048
H	-1.34591	5.211175	0.875127
H	-1.54898	4.037752	-0.4398
H	-3.45492	2.078073	-3.17325
H	-4.43839	2.647057	-1.8146
H	-5.17518	2.423437	-3.41654
C	-2.82825	-1.50541	2.724098
C	-6.81107	-4.25507	3.076857
H	-7.28345	-3.54847	3.76992
H	-6.97454	-5.26845	3.460499
H	-2.10322	-1.13113	3.454894
H	-2.43666	-1.30237	1.722005
C	-7.459	-4.14312	1.7069
C	-7.88955	-5.12818	0.881551
H	-7.89132	-6.20306	0.983049
C	-4.14901	-0.78247	2.939918
C	-5.27273	-0.78559	2.181156
N	-4.38456	-0.01508	4.089442
N	-5.61492	0.448634	4.047219
N	-6.18388	-0.02311	2.872235
N	-7.70111	-2.90567	1.092912
N	-8.26245	-3.1164	-0.07783
N	-8.3883	-4.48838	-0.22993

C	-9.0347	-5.06035	-1.43318
H	-9.23229	-4.22045	-2.10033
C	-8.14697	-6.11569	-2.14038
H	-7.91041	-6.92265	-1.43856
H	-8.73212	-6.55239	-2.95928
H	-9.98705	-5.51583	-1.1471
C	-7.58118	0.287762	2.501255
H	-8.14231	0.419896	3.42751
H	-7.97326	-0.57276	1.953767
C	-7.69583	1.568718	1.634017
H	-8.72823	1.644994	1.273731
H	-7.03785	1.476497	0.762278
H	-5.52214	-1.26909	1.247871
O	-8.04478	7.804108	0.331703
C	-7.97398	8.906689	1.241234
C	-7.24901	9.471885	-3.03468
H	-8.72956	8.847928	2.030147
H	-6.98968	8.999502	1.709484
H	-8.16091	9.804501	0.649092
H	-6.36462	9.837972	-2.50531
H	-7.05902	9.52939	-4.11069
H	-8.09015	10.12666	-2.7989
C	-2.75174	10.00622	1.392047
C	-2.04902	10.61054	-3.58829
H	-2.63129	10.56756	2.323356
H	-3.04658	10.704	0.605931
H	-3.55592	9.276801	1.525941
H	-2.61687	11.18768	-4.32069
H	-2.26962	11.00411	-2.59176
C	-2.27613	2.871028	3.801205
H	-2.8528	2.275034	4.514341
H	-2.77872	2.833068	2.830318
H	-1.28625	2.42372	3.694377
C	-2.69208	-1.68064	-2.0791

H	-3.64977	-1.68646	-1.55586
H	-2.2791	-2.69305	-2.05599
H	-2.00987	-1.00855	-1.55029
C	-3.56372	-5.17518	-8.34926
C	2.239054	-5.5644	-6.19084
H	-3.5104	-6.1312	-8.87384
H	-3.77763	-4.39138	-9.08161
H	-2.58757	-4.9738	-7.89826
H	1.409408	-6.25865	-6.02842
H	2.332296	-5.38626	-7.26385
H	3.16051	-6.03481	-5.83669
C	-3.13952	-9.33883	-6.00175
C	1.175611	-9.96262	-3.71744
H	-2.40024	-10.1267	-6.15853
H	-4.06743	-9.63103	-6.50184
H	-2.7694	-8.4186	-6.46277
H	0.849495	-10.8003	-3.09442
H	0.462604	-9.84211	-4.53846
H	2.15117	-10.2064	-4.14286
N	3.818015	2.42866	-9.49858
C	3.386524	2.151904	-8.46417
C	2.830784	1.783332	-7.13107
C	3.938032	1.605156	-6.0607
H	2.142086	2.564628	-6.80906
H	2.273549	0.844587	-7.21639
N	4.605674	2.884198	-5.72954
H	3.494553	1.204436	-5.14505
H	4.707453	0.915117	-6.40899
C	5.946541	3.193381	-5.76181
N	3.895784	3.926946	-5.15313
C	6.045839	4.429238	-5.21476
H	6.687302	2.51345	-6.15661
N	4.765843	4.864444	-4.84609
C	7.284693	5.285702	-4.97341

O	8.449963	4.512422	-4.64344
H	7.054556	6.039529	-4.21318
H	7.557405	5.819975	-5.89081
C	8.396376	3.821433	-3.42382
C	9.414212	2.880085	-3.24897
C	7.460556	4.014188	-2.412
C	9.492283	2.14137	-2.08042
H	10.14458	2.73346	-4.03359
C	7.545778	3.263772	-1.23804
H	6.661045	4.732834	-2.50502
C	10.61864	1.125367	-1.93617
C	8.560124	2.329614	-1.06549
O	6.638047	3.556362	-0.19717
O	10.50872	0.399943	-0.75569
O	11.50308	0.94953	-2.75621
H	8.632197	1.7566	-0.15161
C	5.721874	2.467263	0.056483
C	11.58082	-0.54686	-0.58241
C	4.559549	2.435219	-0.92873
H	5.338584	2.635638	1.068303
H	6.226772	1.496548	0.041189
C	11.27398	-1.35233	0.707221
H	11.65042	-1.21358	-1.44753
H	12.54326	-0.03474	-0.47812
N	4.472151	1.479769	-1.95036
C	3.490445	3.265759	-1.02139
N	12.30811	-2.38612	0.937062
H	11.28371	-0.66504	1.553026
H	10.27285	-1.78653	0.63577
N	3.384824	1.707242	-2.65505
N	2.753837	2.805265	-2.0862
H	3.183448	4.123996	-0.44138
C	12.1165	-3.70639	0.402984
C	12.79988	-2.56185	2.347465

C	1.552062	3.415794	-2.69865
C	11.34229	-4.11059	-0.6674
C	12.89644	-4.62586	1.115153
C	13.6688	-3.88822	2.21828
C	13.55515	-1.32378	2.831587
C	0.511189	2.335069	-3.08593
H	1.130472	4.12022	-1.97496
H	1.850795	3.95639	-3.60165
C	11.35789	-5.45959	-1.02113
H	10.7312	-3.41129	-1.21841
C	12.91028	-5.95045	0.752134
C	15.09367	-3.54786	1.704037
C	13.77787	-4.67198	3.547141
C	13.49682	-0.82325	4.055401
H	14.19498	-0.8622	2.097185
C	0.025906	1.559193	-1.90799
H	-0.34045	2.822696	-3.56199
H	0.949179	1.639685	-3.80213
C	12.12774	-6.37034	-0.32664
H	10.75147	-5.79309	-1.85408
H	13.51267	-6.66809	1.294707
H	15.04145	-2.95268	0.798399
H	15.64628	-2.98938	2.452523
H	15.63263	-4.46522	1.485969
H	14.43721	-5.52504	3.42181
H	14.19145	-4.03339	4.322103
H	12.8094	-5.03335	3.876412
C	14.23678	0.342152	4.562046
H	12.84723	-1.30028	4.785146
N	-0.3533	0.954058	-1.00092
H	12.12513	-7.41266	-0.61485
C	15.16883	1.101214	3.683655
C	14.0578	0.719232	5.869801
C	15.84149	2.24615	4.354253

O	15.3877	0.826949	2.489301
C	14.72322	1.805267	6.432887
H	13.37691	0.161112	6.504881
C	15.62662	2.566585	5.638077
H	16.52717	2.823984	3.751469
N	14.49991	2.162192	7.830666
H	16.12989	3.406452	6.10421
O	15.12716	3.172749	8.331461
O	13.6812	1.461198	8.540285
H	-0.98278	10.7486	-3.78929
C	11.59917	-2.84802	3.235085
N	10.65877	-3.06026	3.871078

XYZ coordinates of BP5-SPCN, optimized at B3LYP/6-31g(d,p)//HF level of theory in gas phase

O	-2.946515	-2.947601	2.798061
O	-5.404577	-3.972294	2.935944
O	-6.961450	-5.463144	-2.626279
C	-0.558973	-1.490532	-3.902916
C	0.486349	-1.428905	-4.826524
C	0.197336	-1.047292	-6.130893
C	-1.122123	-0.760119	-6.502446
C	-2.159695	-0.843092	-5.599977
C	-1.863183	-1.205654	-4.268279
C	-3.613988	-0.582732	-6.010691
C	-4.462859	-1.859601	-5.927819
C	-4.144409	-2.956369	-6.715905
C	-4.850164	-4.150181	-6.616278
C	-5.897903	-4.253288	-5.691837
C	-6.236087	-3.149916	-4.926008
C	-5.539252	-1.948086	-5.036198

C	-6.637392	-5.584196	-5.500253
C	-5.880394	-6.509275	-4.535843
C	-4.963752	-7.436377	-5.030272
C	-4.224655	-8.242742	-4.177607
C	-4.380000	-8.122634	-2.781358
C	-5.299576	-7.214694	-2.299384
C	-6.058922	-6.417607	-3.160034
C	-3.529439	-8.973150	-1.828093
C	-2.120473	-8.397146	-1.631831
C	-1.054853	-8.883431	-2.370811
C	0.224243	-8.350844	-2.231422
C	0.442893	-7.310565	-1.321521
C	-0.621825	-6.832566	-0.570443
C	-1.901831	-7.359275	-0.714489
C	1.832548	-6.674570	-1.184720
C	1.934334	-5.386308	-2.011824
C	1.951209	-4.133664	-1.388040
C	1.981506	-2.981813	-2.172111
C	1.987230	-3.049588	-3.556540
C	1.997791	-4.305884	-4.178112
C	1.972367	-5.455556	-3.396923
C	1.923724	-1.767184	-4.391232
O	1.899704	-4.154695	0.013767
O	2.008022	-4.287639	-5.584047
C	2.141921	-2.891350	0.644300
O	-3.037375	-6.943913	-0.003326
C	-2.816060	-5.855982	0.902431
O	1.351929	-8.757001	-2.966408
O	-3.299397	-9.212944	-4.584667
O	-5.836516	-0.777358	-4.323454
O	-4.600395	-5.308212	-7.371493
C	-6.840014	-0.926683	-3.313454

O	1.241500	-0.873932	-7.070007
O	-2.969166	-1.237473	-3.413515
C	-4.864853	-4.844204	7.824297
C	-4.344649	-4.329228	6.504528
C	-3.075633	-3.777537	6.413347
C	-2.609083	-3.308650	5.192588
C	-3.409167	-3.364454	4.062299
C	-4.701707	-3.929933	4.148372
C	-5.152876	-4.412243	5.367649
C	-4.916583	-3.997512	8.931697
C	-5.298722	-6.183905	7.932095
C	-5.287550	-7.240220	6.997236
C	-5.781330	-8.361459	7.621362
C	-6.087845	-7.991230	8.939168
N	-5.803153	-6.694922	9.142470
N	-5.402060	-4.447645	10.181859
C	-5.346312	-3.414606	11.024770
C	-4.835398	-2.265727	10.375732
C	-4.575554	-2.623729	9.083795
B	-5.991414	-5.910701	10.529735
F	-7.304376	-5.803242	10.828330
F	-5.242832	-6.487399	11.493168
O	-3.864811	4.067597	-3.261077
C	-1.534792	8.102113	3.071710
C	-0.934743	7.147302	3.881361
C	0.252634	6.541035	3.455441
C	0.774777	6.867357	2.202854
C	0.152695	7.789647	1.378438
C	-1.004145	8.438864	1.833431
C	0.704699	8.089280	-0.021995
C	-0.268599	7.687583	-1.141518
C	-0.872206	8.663371	-1.930485

C	-1.785284	8.330345	-2.923961
C	-2.100060	6.980638	-3.157802
C	-1.477874	6.014366	-2.391933
C	-0.575858	6.349300	-1.383459
C	-3.145311	6.583793	-4.208672
C	-4.510968	6.331992	-3.556004
C	-5.420511	7.366297	-3.413695
C	-6.641652	7.177518	-2.767046
C	-6.949138	5.919835	-2.234794
C	-6.047624	4.877505	-2.402873
C	-4.836591	5.062082	-3.058820
C	-8.251393	5.689774	-1.451901
C	-7.398884	5.030732	2.753229
C	-7.573616	6.316320	2.259265
C	-7.861141	6.544032	0.918664
C	-7.984773	5.455464	0.041662
C	-7.830530	4.172241	0.540054
C	-7.535664	3.944323	1.883565
C	-7.039206	4.821796	4.231446
C	-5.620815	5.315701	4.542619
C	-5.410165	6.594421	5.066078
C	-4.108274	7.036444	5.298508
C	-3.015657	6.235245	5.016133
C	-3.228515	4.945797	4.502424
C	-4.526526	4.503152	4.275190
C	-1.585982	6.752078	5.215643
O	-6.571108	7.358794	5.284991
O	-2.061472	4.215035	4.247698
C	-6.373463	8.533158	6.079483
O	-7.335674	2.678829	2.462219
O	-7.633141	8.158480	-2.616744
O	0.099420	5.339860	-0.656064

O	-2.462355	9.248454	-3.740745
O	0.824571	5.634695	4.358844
O	-1.530576	9.400786	0.956935
C	1.318486	-1.995746	-7.968547
C	2.004251	4.973442	3.890155
C	-0.812801	4.579787	0.159634
C	-4.271643	2.745226	-2.891270
H	-0.330618	-1.778389	-2.890146
H	-1.322224	-0.470143	-7.526137
H	-3.630039	-0.194408	-7.027825
H	-4.055658	0.165462	-5.356762
H	-3.317430	-2.866700	-7.402742
H	-7.047785	-3.248251	-4.222814
H	-6.744348	-6.081638	-6.461592
H	-7.630559	-5.383220	-5.106234
H	-4.836582	-7.500877	-6.098812
H	-5.429781	-7.109101	-1.230260
H	-3.446688	-9.981722	-2.227427
H	-4.031598	-9.026811	-0.864801
H	-1.243615	-9.681643	-3.071099
H	-0.432216	-6.032355	0.128305
H	2.582068	-7.385657	-1.524601
H	2.026216	-6.439212	-0.141583
H	1.992293	-2.008175	-1.707118
H	1.967421	-6.433542	-3.852670
H	2.541628	-1.867314	-5.279540
H	2.322739	-0.941396	-3.801814
H	2.178244	-3.086295	1.717797
H	3.093960	-2.448152	0.338880
H	1.342143	-2.169987	0.451766
H	-3.782924	-5.622247	1.352211
H	-2.448582	-4.959317	0.396440

H	-2.115471	-6.116242	1.700953
H	-6.909969	0.037065	-2.805785
H	-7.821644	-1.164303	-3.734068
H	-6.583745	-1.690840	-2.574218
H	-2.441094	-3.726390	7.288134
H	-1.615415	-2.885607	5.119161
H	-6.139352	-4.838151	5.461475
H	-4.937259	-7.167024	5.978642
H	-5.908138	-9.343751	7.199560
H	-6.493316	-8.604783	9.735675
H	-5.672045	-3.513614	12.055205
H	-4.693048	-1.301621	10.833719
H	-4.187199	-1.990157	8.299325
H	-2.440745	8.570515	3.421815
H	1.672933	6.387899	1.846629
H	1.643909	7.554023	-0.148872
H	0.913764	9.153894	-0.111544
H	-0.627056	9.695758	-1.738563
H	-1.718960	4.975944	-2.572454
H	-2.819153	5.678809	-4.716409
H	-3.235187	7.379882	-4.942984
H	-5.154690	8.333350	-3.811280
H	-6.303938	3.910854	-1.999967
H	-8.768469	4.822624	-1.859663
H	-8.890285	6.559864	-1.574490
H	-7.471557	7.138640	2.950278
H	-7.942117	3.341736	-0.139147
H	-7.114267	3.763193	4.465583
H	-7.747178	5.365232	4.853665
H	-3.932758	8.021600	5.701900
H	-4.709685	3.514227	3.883235
H	-0.975983	5.981763	5.680423

H	-1.608841	7.614599	5.880287
H	-7.365799	8.943504	6.277151
H	-5.785645	9.295293	5.559134
H	-5.890631	8.315833	7.036442
H	2.149415	-1.806345	-8.651173
H	1.507317	-2.927491	-7.428055
H	0.403780	-2.108749	-8.557968
H	2.313836	4.296920	4.689009
H	1.821232	4.382935	2.987825
H	2.823337	5.671042	3.691693
H	-0.217662	3.851641	0.714048
H	-1.345907	5.211175	0.875127
H	-1.548981	4.037752	-0.439795
H	-3.454922	2.078073	-3.173248
H	-4.438390	2.647057	-1.814602
H	-5.175178	2.423437	-3.416536
C	-2.828251	-1.505413	2.724098
C	-6.811065	-4.255073	3.076857
H	-7.283450	-3.548469	3.769920
H	-6.974542	-5.268447	3.460499
H	-2.103217	-1.131127	3.454894
H	-2.436662	-1.302368	1.722005
C	-7.458996	-4.143117	1.706900
C	-7.889553	-5.128181	0.881551
H	-7.891317	-6.203061	0.983049
C	-4.149012	-0.782470	2.939918
C	-5.272727	-0.785588	2.181156
N	-4.384555	-0.015076	4.089442
N	-5.614920	0.448634	4.047219
N	-6.183879	-0.023110	2.872235
N	-7.701114	-2.905672	1.092912
N	-8.262448	-3.116398	-0.077834

N	-8.388301	-4.488378	-0.229932
C	-9.034699	-5.060345	-1.433178
H	-9.232291	-4.220454	-2.100329
C	-8.146971	-6.115689	-2.140380
H	-7.910409	-6.922653	-1.438559
H	-8.732124	-6.552393	-2.959278
H	-9.987045	-5.515826	-1.147099
C	-7.581183	0.287762	2.501255
H	-8.142308	0.419896	3.427510
H	-7.973262	-0.572763	1.953767
C	-7.695829	1.568718	1.634017
H	-8.728232	1.644994	1.273731
H	-7.037852	1.476497	0.762278
H	-5.522139	-1.269094	1.247871
O	-8.044781	7.804108	0.331703
C	-7.973978	8.906689	1.241234
C	-7.249005	9.471885	-3.034676
H	-8.729562	8.847928	2.030147
H	-6.989682	8.999502	1.709484
H	-8.160912	9.804501	0.649092
H	-6.364617	9.837972	-2.505307
H	-7.059024	9.529390	-4.110686
H	-8.090151	10.126659	-2.798904
C	-2.751741	10.006223	1.392047
C	-2.049016	10.610541	-3.588287
H	-2.631290	10.567558	2.323356
H	-3.046582	10.704002	0.605931
H	-3.555915	9.276801	1.525941
H	-2.616868	11.187678	-4.320686
H	-2.269619	11.004110	-2.591761
C	-2.276134	2.871028	3.801205
H	-2.852796	2.275034	4.514341

H	-2.778717	2.833068	2.830318
H	-1.286245	2.423720	3.694377
C	-2.692077	-1.680643	-2.079098
H	-3.649766	-1.686459	-1.555863
H	-2.279096	-2.693047	-2.055986
H	-2.009868	-1.008553	-1.550286
C	-3.563718	-5.175179	-8.349255
C	2.239054	-5.564398	-6.190842
H	-3.510401	-6.131201	-8.873838
H	-3.777631	-4.391381	-9.081611
H	-2.587573	-4.973795	-7.898261
H	1.409408	-6.258646	-6.028415
H	2.332296	-5.386256	-7.263851
H	3.160510	-6.034806	-5.836687
C	-3.139516	-9.338830	-6.001748
C	1.175611	-9.962616	-3.717437
H	-2.400235	-10.126674	-6.158526
H	-4.067430	-9.631025	-6.501839
H	-2.769398	-8.418601	-6.462766
H	0.849495	-10.800326	-3.094419
H	0.462604	-9.842105	-4.538462
H	2.151170	-10.206437	-4.142864
N	3.818015	2.428660	-9.498582
C	3.386524	2.151904	-8.464167
C	2.830784	1.783332	-7.131072
C	3.938032	1.605156	-6.060702
H	2.142086	2.564628	-6.809055
H	2.273549	0.844587	-7.216393
N	4.605674	2.884198	-5.729538
H	3.494553	1.204436	-5.145049
H	4.707453	0.915117	-6.408992
C	5.946541	3.193381	-5.761805

N	3.895784	3.926946	-5.153127
C	6.045839	4.429238	-5.214763
H	6.687302	2.513450	-6.156605
N	4.765843	4.864444	-4.846086
C	7.284693	5.285702	-4.973408
O	8.449963	4.512422	-4.643441
H	7.054556	6.039529	-4.213176
H	7.557405	5.819975	-5.890813
C	8.396376	3.821433	-3.423822
C	9.414212	2.880085	-3.248970
C	7.460556	4.014188	-2.411998
C	9.492283	2.141370	-2.080418
H	10.144582	2.733460	-4.033591
C	7.545778	3.263772	-1.238043
H	6.661045	4.732834	-2.505022
C	10.618639	1.125367	-1.936169
C	8.560124	2.329614	-1.065493
O	6.638047	3.556362	-0.197167
O	10.508718	0.399943	-0.755694
O	11.503082	0.949530	-2.756206
H	8.632197	1.756600	-0.151608
C	5.721874	2.467263	0.056483
C	11.580821	-0.546862	-0.582412
C	4.559549	2.435219	-0.928729
H	5.338584	2.635638	1.068303
H	6.226772	1.496548	0.041189
C	11.273975	-1.352325	0.707221
H	11.650418	-1.213584	-1.447530
H	12.543263	-0.034742	-0.478117
N	4.472151	1.479769	-1.950362
C	3.490445	3.265759	-1.021392
N	12.308107	-2.386118	0.937062

H	11.283714	-0.665043	1.553026
H	10.272850	-1.786531	0.635770
N	3.384824	1.707242	-2.655047
N	2.753837	2.805265	-2.086195
H	3.183448	4.123996	-0.441379
C	12.116501	-3.706389	0.402984
C	12.799877	-2.561846	2.347465
C	1.552062	3.415794	-2.698651
C	11.342287	-4.110587	-0.667403
C	12.896441	-4.625860	1.115153
C	13.668796	-3.888218	2.218280
C	13.555146	-1.323775	2.831587
C	0.511189	2.335069	-3.085933
H	1.130472	4.120220	-1.974960
H	1.850795	3.956390	-3.601651
C	11.357892	-5.459593	-1.021130
H	10.731204	-3.411293	-1.218405
C	12.910277	-5.950453	0.752134
C	15.093673	-3.547855	1.704037
C	13.777873	-4.671981	3.547141
C	13.496819	-0.823250	4.055401
H	14.194980	-0.862198	2.097185
C	0.025906	1.559193	-1.907989
H	-0.340447	2.822696	-3.561993
H	0.949179	1.639685	-3.802126
C	12.127744	-6.370337	-0.326642
H	10.751469	-5.793091	-1.854078
H	13.512670	-6.668089	1.294707
H	15.041454	-2.952676	0.798399
H	15.646284	-2.989377	2.452523
H	15.632631	-4.465219	1.485969
H	14.437208	-5.525040	3.421810

H	14.191448	-4.033387	4.322103
H	12.809402	-5.033354	3.876412
C	14.236778	0.342152	4.562046
H	12.847234	-1.300282	4.785146
N	-0.353303	0.954058	-1.000918
H	12.125131	-7.412662	-0.614847
C	15.168829	1.101214	3.683655
C	14.057797	0.719232	5.869801
C	15.841493	2.246150	4.354253
O	15.387696	0.826949	2.489301
C	14.723217	1.805267	6.432887
H	13.376905	0.161112	6.504881
C	15.626623	2.566585	5.638077
H	16.527167	2.823984	3.751469
N	14.499912	2.162192	7.830666
H	16.129888	3.406452	6.104210
O	15.127162	3.172749	8.331461
O	13.681201	1.461198	8.540285
H	-0.982781	10.748595	-3.789288
C	11.599165	-2.848015	3.235085
N	10.658768	-3.060263	3.871078

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