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ELECTRONIC SUPPORTING INFORMATION (ESI) FOR

Switching Cation Selectivity via Steric Tuning in Sumanene-Based Receptors

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S1. Experimental section

S1.1. Materials and methods

Materials. Chemical reagents and solvents were of the higher possible purity and were commercially purchased and purified according to the standard methods, if necessary. Sumanene[1] (**1**), 2-ethynylsumanene[2] (**7**) and tris((1-benzyl-1*H*-1,2,3-triazol-4-yl)methyl)amine (TBTA)[3] were synthesized according to the literature protocols. Thin layer chromatography (TLC) and preparative thin layer chromatography (PTLC; 2 mm) were performed on SiO_2using Merck Silica gel 60 F254 plates or on Al_2O_3 Alox-100 UV254 plates. Regarding potentiometric experiments, all inorganic salts, 1-morpholinoethanesulfonic acid (MES), were of analytical grade and were purchased from Fluka. The solutions of inorganic salts (0.01 M) were prepared with deionised water. High-molecular-weight poly(vinyl chloride) (PVC), o-nitrophenyl octyl ether (o-NPOE), potassium tetrakis[3,5-bis(trifluoromethyl)phenyl]borate (KTFPB), were obtained from Fluka (Selectophore). Freshly distilled tetrahydrofuran (THF, Fluka) was used as a solvent for membrane components.

The NMR experiments were carried out using a JEOL 600 MHz or Varian 500 MHz spectrometer (^{1}H NMR and {^{1}H}^{13}C NMR) equipped with a multinuclear z-gradient inverse probe head. The spectra were recorded at 297.15 K and standard 5 mm NMR tubes were used. ^{1}H NMR (δ_H) and {^{1}H}^{13}C NMR (δ_C) chemical shifts were reported in parts per million (ppm) relative to the solvent signal, *i.e.*, $CDCl_3$, δ_H (residual $CHCl_3$) 7.26 ppm, δ_C (residual $CHCl_3$) 77.16 ppm, THF-d_8, δ_H (residual THF) 1.73 ppm, δ_C (residual THF) 25.37 ppm, DMSO-d_6, δ_H (residual DMSO) 2.50 ppm, δ_C (residual DMSO) 39.52 ppm. NMR spectra were analyzed with the MestReNova v12.0 software (Mestrelab Research S.L).

ESI-HRMS (TOF) measurements were performed with a Q-Exactive ThermoScientific spectrometer. **APCI-HRMS (q-TOF)** measurements were recorded using Synapt G2-S HDMS mass spectrometer (*Waters*) equipped with the atmospheric-pressure chemical ionization (APCI) ion source and quadrupole-Time-of-Flight (q-TOF) mass analyzer. Methanol (Honeywell, HPLC-MS Chromasolv, purity ≥ 99.9%) was used as a solvent and mobile phase with the flow rate of 100 µl/min. Sample was dissolved and injected directly into the APCI source. Injection volume was 1 µl. The measurements were recorded in the positive and negative ion modes with the resolving power of TOF analyzer 20 000 FWHM. The lock-spray spectrum of Leucine-enkephalin was generated by the lock-spray source and the correction was performed for recorded mass spectra in the mass range of m/z = 50 – 1200. The exact mass measurements were performed within 3 mDa mass error. Nitrogen was used as the desolvation and cone gas, and their flow values were set to 600 L/h and 100 L/h, respectively. Nebulizer gas pressure was set to 5.0 bar. Source and probe temperatures were set to 120˚C and 550˚C, respectively. Corona current was set to 13.0 µA, sampling

cone voltage and source offset were set to 40 V. The instrument was controlled, and data were processed using the MassLynx V4.1 software package (*Waters*).

UV-vis spectra were recorded with a WVR UV-1600PC spectrometer, with the spectral resolution of 2 cm^{-1}. For the UV-Vis measurements, the wavelengths for the absorption maxima λ_{max} were reported in nm. **Fluorescence spectra** were recorded with a HITACHI F-7100 FL spectrometer (parameters: scan speed: 1200 nm/min, delay: 0.0 s, EX slit: 5.0 nm, EM slit: 5.0 nm). The wavelengths for the emission maxima (λ_{em}) were reported in nm.

S1.2. Synthesis

S1.2.1. Synthesis of 2-([1,1':3',1''-terphenyl]-5'-yl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (18)

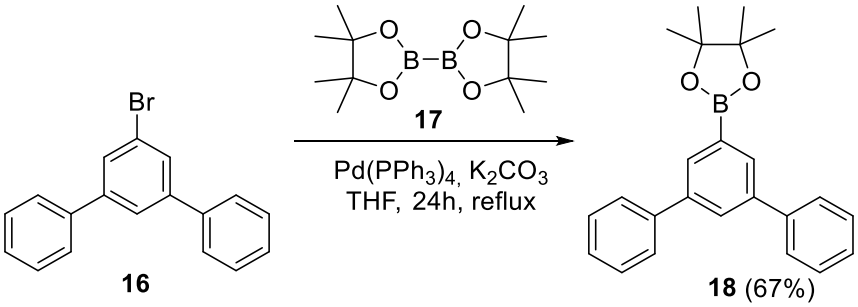
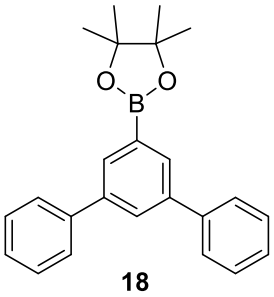


Fig. S1. Synthesis of compound **18**.



5'-Bromo-1,1':3',1''-terphenyl (**16**; 500 mg, 1.617 mmol, 1 eq) was placed in 25ml round bottom flask. Next, bis(pinacolato)diboron (**17**; 862 mg, 3.396 mmol, 2.1 eq) and tetrakis(triphenylphosphine)palladium(0) (500 mg, 0.485 mmol, 0.3 eq) were added. Flask was evacuated with vacuum and flushed with argon. Then 15ml of dry THF was added followed by 2ml of degassed solution of 2M potassium bicarbonate. Reaction mixture was stirred for 24 h under reflux conditions. Distilled water was added (20 ml) and crude product was extracted with CH_2Cl_2 (3x20ml). Organic layers were combined, dried with $MgSO_4$ and volatiles were distilled off using a rotary evaporator. Finally, the product was purified using column chromatography (SiO_2; CH_2Cl_2:hexane 1:1 v/v) to obtain 2-([1,1':3',1''-terphenyl]-5'-yl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (**18**) as a white solid. Yield 67% (385 mg). The NMR spectra were consistent with literature.[4]

S1.2.2. Synthesis of amines 20, 22, 25

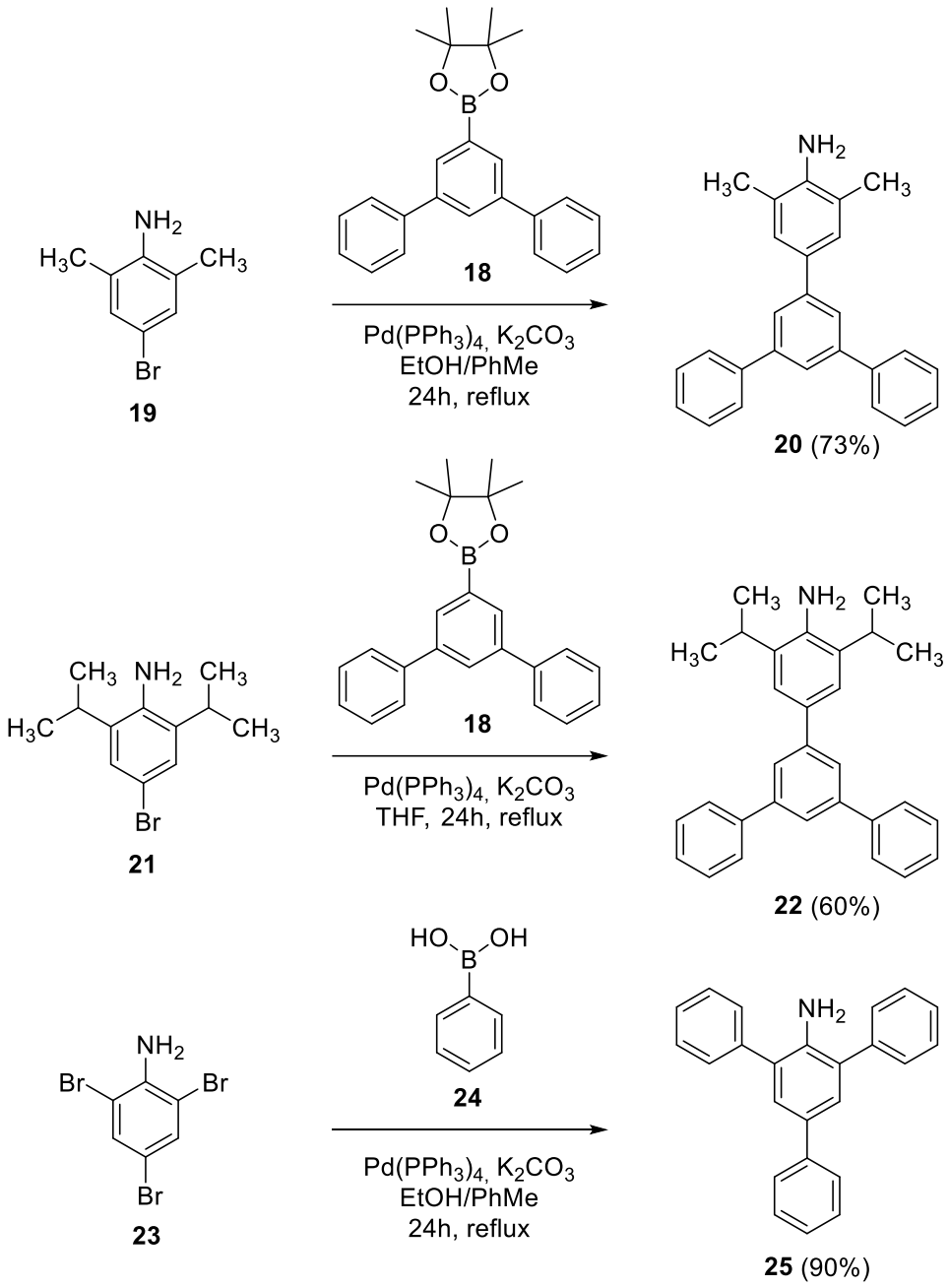
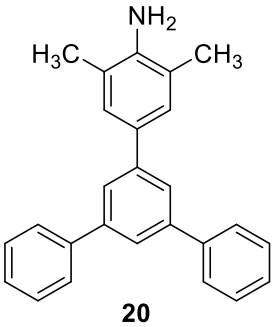


Fig. S2. Synthesis of amines **20**, **22**, **25**.

Synthesis of 3,5-dimethyl-5'-phenyl-[1,1':3',1''-terphenyl]-4-amine (20)

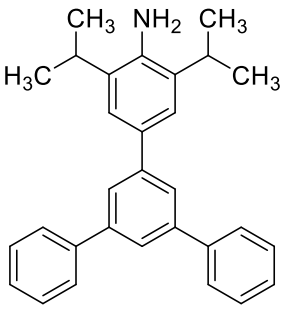


20

2-([1,1':3',1''-Terphenyl]-5'-yl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (**18**; 32.8 mg, 0.653 mmol, 2 eq) was placed in 25ml round bottom flask. Next, 4-bromo-2,6-dimethylaniline (**19**; 65.4 mg, 0.327 mmol, 1 eq) and tetrakis(triphenylphosphine)palladium(0) (19 mg, 0.016 mmol, 0.05 eq) were added. Flask was evacuated with vacuum and flushed with argon. Then 10ml of dry toluene and 5ml of 96% ethanol were added followed by 3ml of degassed solution of 2M potassium bicarbonate. Reaction mixture was stirred for 24 h under reflux conditions. Distilled water was added (20 ml) and crude product was extracted with CH_2Cl_2 (3x20ml). Organic layers were combined, dried with $MgSO_4$ and volatiles were distilled off using a rotary evaporator. Finally, the product was purified using column chromatography (SiO_2; CH_2Cl_2:hexane 3:1 v/v) to obtain 3,5-dimethyl-5'-phenyl-[1,1':3',1''-terphenyl]-4-amine (**20**) as a yellowish solid. Yield 73% (83.8 mg).

^{1}H NMR ($CDCl_3$, 600 MHz, ppm), δ_H δ 7.75 (m, 2H), 7.73–7.71 (m, 4H), 7.51–7.48 (m, 4H), 7.41–7.38 (m, 2H), 7.34 (s, 2H), 7.08–7.08 (m, 1H), 4.45 (bs, 2H), 2.34 (s, 6H). {^{1}H}^{13}C NMR ($CDCl_3$, 151 MHz, ppm), δ_C ^{13}C 142.6, 142.3, 141.6, 131.9, 130.8, 128.9, 127.5, 127.5, 127.4, 124.8, 124.4, 123.2, 18.1. ESI-HRMS (TOF) m/z $[M+H]^+$ calcd. for $C_{26}H_{24}N$ 350.1903 found 350.1905. TLC R_f (SiO_2, CH_2Cl_2:hexane 3:1 v/v) = 0.48.

Synthesis of 3,5-diisopropyl-5'-phenyl-[1,1':3',1''-terphenyl]-4-amine (22)

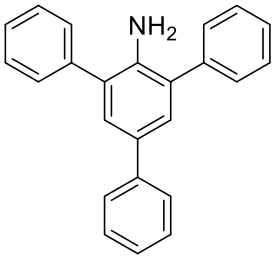


22

2-([1,1':3',1''-Terphenyl]-5'-yl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (**18**; 47 mg, 0.133 mmol, 1.2 eq) was placed in 25ml round bottom flask. Next, 4-bromo-2,6-diisopropylaniline (**19**; 28 mg, 0.111 mmol, 1 eq) and tetrakis(triphenylphosphine)palladium(0) (38 mg, 0.003 mmol, 0.3 eq) were added. Flask was evacuated with vacuum and flushed with argon. Then 8ml of dry THF was added followed by 0.5ml of degassed solution of 2M potassium bicarbonate. Reaction mixture was stirred for 24h under reflux conditions. Distilled water was added (20 ml) and crude product was extracted with CH_2Cl_2 (3x20ml). Organic layers were combined, dried with $MgSO_4$ and volatiles were distilled off using a rotary evaporator. Finally, the product was purified using column chromatography (SiO_2; CH_2Cl_2:hexane 1:1 v/v) to obtain 3,5-diisopropyl-5'-phenyl-[1,1':3',1''-terphenyl]-4-amine (**22**) as a yellowish solid. Yield 60% (25.0 mg).

^{1}H NMR ($CDCl_3$, 500 MHz, ppm), δ_H 7.73–7.69 (m, 7H), 7.51–7.47 (m, 4H), 7.41–7.36 (m, 4H), 3.85 (bs, 2H), 3.01 (p, $^3J_{H-H}$ = 6.8 Hz, 2H), 1.36 (d, $^3J_{H-H}$ = 6.8 Hz, 12H). {^{1}H}^{13}C NMR ($CDCl_3$, 151 MHz, ppm), δ_C 143.7, 142.3, 141.7, 140.3, 133.0, 131.5, 129.0, 127.6, 127.5, 125.0, 124.4, 122.2, 28.3, 22.7. ESI-HRMS (TOF) m/z $[M+H]^+$ calcd. for $C_{30}H_{32}N$ 406.2529 found 406.2530. TLC R_f (SiO_2, CH_2Cl_2:hexane 1:1 v/v) = 0.35.

Synthesis of 5'-phenyl-[1,1':3',1''-terphenyl]-2'-amine (25)



25

2,4,6-tribromoaniline (**23**; 400 mg, 1.213 mmol, 1 eq) was placed in 25ml round bottom flask. Next, phenylboronic acid (**24**; 739 mg, 6.064 mmol, 5 eq) and tetrakis(triphenylphosphine)palladium(0) (100 mg, 0.086 mmol, 0.07 eq) were added. Flask was evacuated with vacuum and flushed with argon. Then 20ml of dry toluene and 5ml of 96% ethanol were added followed by 5 ml of degassed solution of 2M potassium bicarbonate. Reaction mixture was stirred for 24 h under reflux conditions. Distilled water was added (20 ml) and crude product was extracted with CH_2Cl_2 (3x20ml). Organic layers were combined, dried with $MgSO_4$ and volatiles were distilled off using a rotary evaporator. Finally, the product was purified using column chromatography (SiO_2; CH_2Cl_2:hexane 1:1 v/v) to obtain 5'-phenyl-[1,1':3',1''-terphenyl]-2'-amine (**25**) as a yellowish solid. Yield 90% (358mg). The NMR spectra were consistent with literature.[5]

S1.2.3. Synthesis of azides 8-11

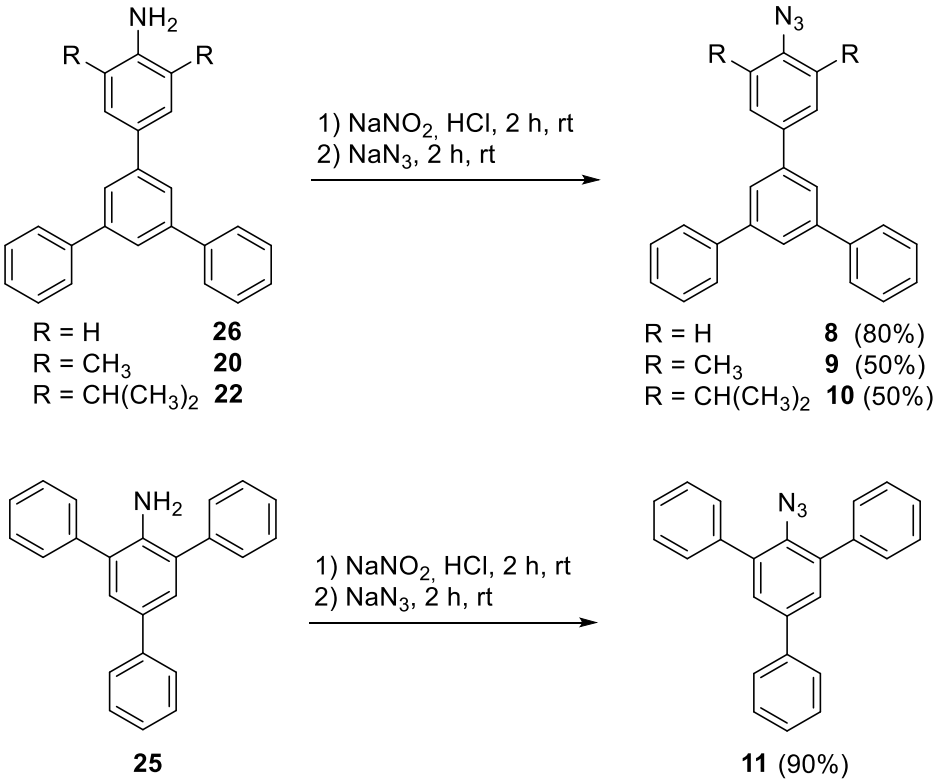
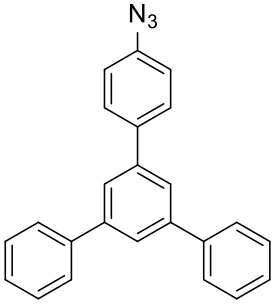


Fig. S3. Synthesis of azides **8**-**11**.

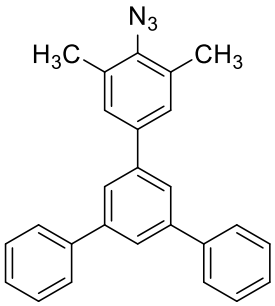
Synthesis of 4-azido-5'-phenyl-1,1':3',1''-terphenyl (8)



8

5'-Phenyl-[1,1':3',1''-terphenyl]-4-amine (**26**; 100 mg, 0.311 mmol, 1 eq) was placed in 50ml round bottom flask. Next 15 ml of water was added followed by 37% hydrochloric acid (0.28 ml, 2.800 mmol, 9 eq) followed by sodium nitrite (200 mg, 2.900 mmol, 9 eq). Reaction mixture was stirred at room temperature for 2 h with exclusion of light. Then sodium azide (80 mg, 1.231 mmol, 4 eq) was added in portions, then mixture was stirred at room temperature for 2 h with exclusion of light. Crude product was extracted with chloroform (3x20ml). Organic layers were combined, dried with $MgSO_4$ and volatiles were distilled off using a rotary evaporator. Finally, the product was purified using column chromatography (SiO_2; cyclohexane:$CHCl_3$ 2:3 v/v) to obtain 4-azido-5'-phenyl-1,1':3',1''-terphenyl (**8**) as a yellow solid. Yield 80% (93mg). The NMR spectra were consistent with literature.[6]

Synthesis of 4-azido-3,5-dimethyl-5'-phenyl-1,1':3',1''-terphenyl (9)



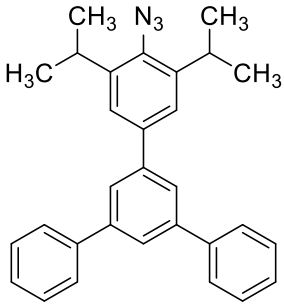
9

3,5-Dimethyl-5'-phenyl-[1,1':3',1''-terphenyl]-4-amine (**20**; 22 mg, 0.062 mmol, 1 eq) was placed in 50ml round bottom flask. Next 5 ml of water was added followed by 37% hydrochloric acid (50 µl, 0.560 mmol, 9 eq) followed by sodium nitrite (37 mg, 0.560 mmol, 9 eq). Reaction mixture was stirred at room temperature for 2 h with exclusion of light. Then sodium azide (16 mg, 0.249 mmol, 4 eq) was added in portions, then mixture was stirred at room temperature for 2 h with exclusion of light. Crude product was extracted with chloroform (3x20ml). Organic layers were combined, dried with $MgSO_4$ and volatiles were distilled off using a rotary evaporator. Finally, the product was purified using column chromatography (SiO_2; CH_2Cl_2:hexane 1:1 v/v) to obtain 4-azido-3,5-dimethyl-5'-phenyl-1,1':3',1''-terphenyl (**9**) as a yellow solid. Yield 50% (11.5 mg).

^{1}H NMR ($CDCl_3$, 600 MHz, ppm), δ_H 7.78–7.77 (m, 1H), 7.73–7.70 (m, 6H), 7.51–7.48 (m, 4H), 7.42–7.39 (m, 2H), 7.36–7.36 (m, 2H), 2.46 (s, 6H). $\{^1H\}^{13}C$ NMR ($CDCl_3$, 151 MHz, ppm), δ_C 142.5, 141.6, 141.3x2, 138.7, 136.6, 132.7, 129.0, 127.9, 127.7, 127.5, 125.4, 125.1, 18.5. HRMS: significant fragmentation observed both in the case of ESI and APCI ionization. TLC R_f (SiO_2, CH_2Cl_2:hexane 1:1 v/v) = 0.71.

Synthesis of 4-azido-3,5-diisopropyl-5'-phenyl-1,1':3',1''-terphenyl (10)

3,5-Diisopropyl-5'-phenyl-[1,1':3',1''-terphenyl]-4-amine (**22**; (12.5 mg, 0.031 mmol, 1 eq) was placed in 50ml round bottom flask. Next 5 ml of water was added followed by 37% hydrochloric acid (23 µl, 0.277 mmol, 9 eq) followed by sodium nitrite (20 mg, 0.277 mmol, 9 eq). Reaction mixture was stirred at room temperature for 2 h with exclusion of light. Then

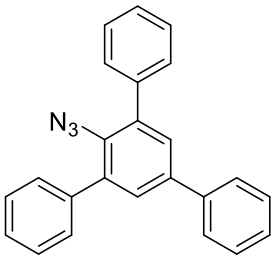


10

sodium azide (8 mg, 0.123 mmol, 4 eq) was added in portions, then mixture was stirred at room temperature for 2 h with exclusion of light. Crude product was extracted with chloroform (3x20ml). Organic layers were combined, dried with $MgSO_4$ and volatiles were distilled off using a rotary evaporator. Finally, the product was purified using column chromatography (SiO_2; CH_2Cl_2:hexane 1:1 v/v) to obtain 4-azido-3,5-diisopropyl-5'-phenyl-1,1':3',1''-terphenyl (**10**) as a yellow solid. Yield 50% (7 mg).

^{1}H NMR ($CDCl_3$, 600 MHz, ppm), δ_H δ 7.78–7.77 (m, 1H), 7.71–7.69 (m, 6H), 7.51–7.49 (m, 4H), 7.42–7.39 (m, 4H), 3.44 (hept, $^3J_{H\text{-}H}$ = 6.9 Hz, 2H), 1.34 (d, $^3J_{H\text{-}H}$ = 6.9 Hz, 12H). {^{1}H}^{13}C NMR ($CDCl_3$, 126 MHz, ppm), δ_C 143.7, 142.6, 141.3, 139.9, 135.1, 129.0, 127.8, 127.6, 125.5, 125.4, 123.3, 29.2, 23.7. HRMS: significant fragmentation observed both in the case of ESI and APCI ionization. TLC R_f (SiO_2, CH_2Cl_2:hexane 1:1 v/v) = 0.71.

Synthesis of 2'-azido-5'-phenyl-1,1':3',1''-terphenyl (11)

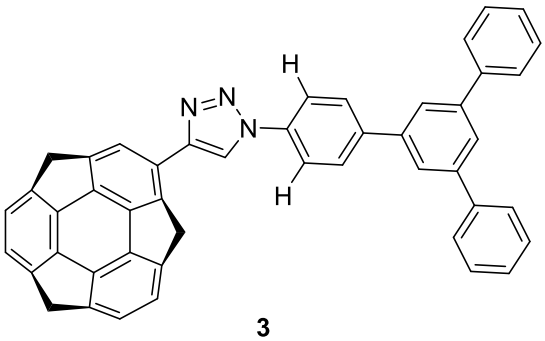


11

5'-Phenyl-[1,1':3',1''-terphenyl]-2'-amine (**25**; 7 mg, 0.022 mmol, 1 eq) was placed in 50ml round bottom flask. Next 5 ml of water was added followed by 37% hydrochloric acid (16µl, 0.196mmol, 9eq) followed by sodium nitrite (14mg, 0.196mmol, 9eq). Reaction mixture was stirred at room temperature for 2h with exclusion of light. Then sodium azide (6 mg, 0.087 mmol, 4 eq) was added in portions, then mixture was stirred at room temperature for 2 h with exclusion of light. Crude product was extracted with chloroform (3x20ml). Organic layers were combined, dried with $MgSO_4$ and volatiles were distilled off using a rotary evaporator. Finally, the product was purified using column chromatography (SiO_2 CH_2Cl_2:hexane 1:2 v/v) to obtain 2'-azido-5'-phenyl-1,1':3',1''-terphenyl (**11**) as a yellow solid. Yield 90% (6.8 mg). The NMR spectra were consistent with literature.[7]

S1.2.4. Synthesis of sumanene receptors 3-6

Synthesis of 4-(4,7-dihydro-1H-tricyclopenta[def,jkl,pqr]triphenylen-2-yl)-1-(5'-phenyl-[1,1':3',1''-terphenyl]-4-yl)-1H-1,2,3-triazole (3)



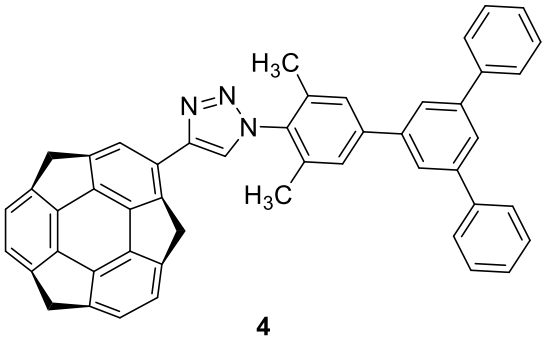
3

2-Ethynylsumanene (**7**; 4.5 mg, 0.016 mmol, 1 eq) was placed in 25 ml round bottom flask. Next, 4-azido-5'-phenyl-1,1':3',1''-terphenyl (**8**; 6.7 mg, 0.019 mmol, 1.2 eq) and copper(I) thiophene-2-carboxylate (CuTC; 0.62 mg, 0.003 mmol, 0.3 eq) were added. Flask was evacuated with vacuum and flushed with argon. Then 2 ml of DMF were added followed by *N*,*N*-diisopropylethylamine

(DIPEA; 3.3 µl, 0.019 mmol, 1.2 eq). Reaction mixture was stirred for 24 h at 55°C. Distilled water was added (30 ml), and the mixture was filtered on a 0.45 µm nylon filter under reduced pressure and washed with distilled water. Collected solids were dissolved in 30 ml of $CHCl_3$ and resulting solution was dried with $MgSO_4$. After filtration, volatiles were distilled off using rotary evaporator. Finally, the product was purified using preparative thin layer chromatography (PTLC, SiO_2; 5% cyclohexane in CH_2Cl_2). Yield 40% (4 mg; yellowish solid).

^{1}H NMR ($CDCl_3$, 500 MHz, ppm), δ_H 8.25 (s, 1H), 7.96–7.82 (m, 8H), 7.73–7.61 (m, 4H), 7.53–7.49 (m, 4H), 7.44–7.41 (m, 2H), 7.17–7.13 (m, 4H), 5.02 (d, $^2J_{H\text{-}H}$ = 19.7 Hz, 1H), 4.81–4.71 (m, 2H), 3.75 (d, $^2J_{H\text{-}H}$= 19.7 Hz, 1H), 3.56–3.43 (m, 2H). {^{1}H}^{13}C NMR ($CDCl_3$, 151 MHz, ppm), δ_C 149.9, 149.3, 149.2, 149.1, 148.9, 148.8, 148.7x3, 148.5, 145.4, 142.9, 141.8, 141.1, 140.9, 136.5, 129.1, 128.8, 127.9, 127.5, 126.0x2, 125.2, 123.9, 123.7, 123.6, 123.5, 121.4, 121.0, 118.5, 43.2, 42.0, 41.9. APCI-HRMS (q-TOF) m/z [M]$^+$ calcd. for $C_{47}H_{30}N_3$ 636.2442 found 636.2440. TLC R_f (SiO_2, 5% cyclohexane in CH_2Cl_2) = 0.78.

Synthesis of 4-(4,7-dihydro-1H-tricyclopenta[def,jkl,pqr]triphenylen-2-yl)-1-(3,5-dimethyl-5'-phenyl-[1,1':3',1''-terphenyl]-4-yl)-1H-1,2,3-triazole (4)

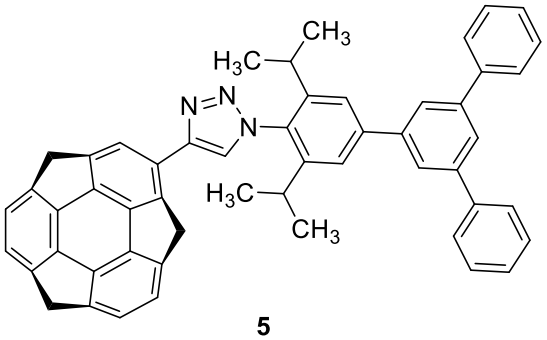


4

2-Ethynylsumanene (**7**; 4 mg, 0.014 mmol, 1 eq) was placed in 25 ml round bottom flask. Next, 4-azido-3,5-dimethyl-5'-phenyl-1,1':3',1''-terphenyl (**9**; 6.2 mg, 0.017 mmol, 1.2 eq) and copper(I) thiophene-2-carboxylate (CuTC; 0.8 mg, 0.004 mmol, 0.3 eq) were added. Flask was evacuated with vacuum and flushed with argon. Then 1 ml of DMF were added followed by *N*,*N*-diisopropylethylamine (DIPEA; 3 µl, 0.017 mmol, 1.2 eq). Reaction mixture was stirred for 24 h at 55°C. Distilled water was added (30 ml), and the mixture was filtered on a 0.45 µm nylon filter under reduced pressure and washed with distilled water. Collected solids were dissolved in 30 ml of $CHCl_3$ and resulting solution was dried with $MgSO_4$. After filtration, volatiles were distilled off using rotary evaporator. Finally, the product was purified using preparative thin layer chromatography (PTLC, SiO_2; 5% cyclohexane in CH_2Cl_2). Yield 50% (4.6 mg; yellowish solid).

^{1}H NMR ($CDCl_3$, 600 MHz, ppm), δ_H 7.96–7.94 (m, 2H), 7.84–7.84 (m, 1H), 7.80–7.80 (m, 2H), 7.73–7.92 (m, 4H), 7.54–7.50 (m, 7H), 7.44–7.41 (m, 2H), 7.16–7.13 (m, 4H), 4.99 (d, $^2J_{H\text{-}H}$ = 19.5 Hz, 1H), 4.82–4.72 (m, 2H), 3.71 (d, $^2J_{H\text{-}H}$ = 19.5 Hz, 1H), 3.55 (d, $^2J_{H\text{-}H}$ = 19.4 Hz, 1H), 3.45 (d, $^2J_{H\text{-}H}$ = 19.4 Hz, 1H), 2.16 (s, 6H). {^{1}H}^{13}C NMR ($CDCl_3$, 126 MHz, ppm), δ_C 150.1, 149.3, 149.2x2, 148.9x2, 148.8, 148.7, 148.6, 148.5, 147.7, 145.3, 143.2, 142.8, 141.3, 141.1, 136.2, 135.5, 129.1, 127.9, 127.6, 127.5, 126.0, 125.3, 123.9, 123.6x2, 123.5, 122.6, 121.3, 43.2, 41.9x2, 17.8. ESI-HRMS (TOF) m/z [M+H]$^+$ calcd. for $C_{49}H_{34}N_3$ 664.2747 found 664.2744. TLC R_f (SiO_2, 5% cyclohexane in CH_2Cl_2) = 0.23.

Synthesis of 4-(4,7-dihydro-1H-tricyclopenta[def,jkl,pqr]triphenylen-2-yl)-1-(3,5-diisopropyl-5'-phenyl-[1,1':3',1''-terphenyl]-4-yl)-1H-1,2,3-triazole (5)

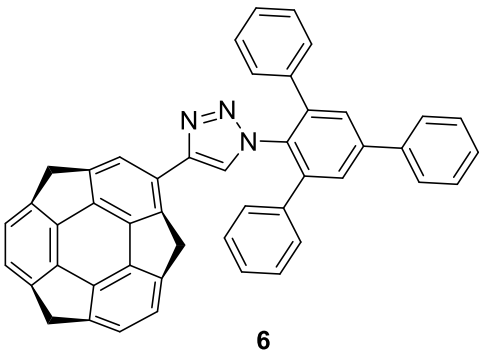


5

2-Ethynylsumanene (**7**; 1.5 mg, 0.005 mmol, 1 eq) was placed in 25 ml round bottom flask. Next, 4-azido-3,5-diisopropyl-5'-phenyl-1,1':3',1''-terphenyl (**10**; 2.5 mg, 0.006 mmol, 1.2 eq) and copper(I) thiophene-2-carboxylate (CuTC; 0.30 mg, 0.001 mmol, 0.3 eq) were added. Flask was evacuated with vacuum and flushed with argon. Then 1 ml of DMF were added followed by *N*,*N*-diisopropylethylamine (DIPEA; 1 µl, 0.006 mmol, 1.2 eq). Reaction mixture was stirred for 24 h at 55°C. Distilled water was added (30 ml), and the mixture was filtered on a 0.45 µm nylon filter under reduced pressure and washed with distilled water. Collected solids were dissolved in 30 ml of $CHCl_3$ and resulting solution was dried with $MgSO_4$. After filtration, volatiles were distilled off using rotary evaporator. Finally, the product was purified using preparative thin layer chromatography (PTLC, SiO_2; 20% cyclohexane in CH_2Cl_2). Yield 40% (1.3 mg; yellowish solid).

^{1}H NMR ($CDCl_3$, 600 MHz, ppm), δ_H 7.94-7.93 (m, 2H), 7.84-7.84 (m, 1H), 7.78-7.78 (m, 2H), 7.73-7.71 (m, 4H), 7.58 (s, 2H), 7.54-7.51 (m, 4H), 7.45-7.42 (m, 2H), 7.16-7.13 (m, 4H), 4.99 (d, $^2J_{H\text{-}H}$ = 19.6 Hz, 1H), 4.82-4.72 (m, 4H), 3.72 (d, $^2J_{H\text{-}H}$ = 19.6 Hz, 1H), 3.54 (d, $^2J_{H\text{-}H}$ = 19.4 Hz, 1H), 3.44 (d, $^2J_{H\text{-}H}$ = 19.4 Hz, 1H), 2.47-2.34 (m, 2H), 1.24-1.20 (m, 12H). {^{1}H}^{13}C NMR ($CDCl_3$, 151 MHz, ppm), δ_C 150.2, 149.3, 149.2x2, 149.0, 148.9, 148.8x2, 148.6, 147.6, 145.3, 144.1, 142.8, 142.3, 141.2, 138.3, 132.9, 129.1, 127.9, 127.6, 126.1, 125.5, 123.8, 123.6x2, 123.5, 123.3x2, 121.3, 41.9, 29.9x2, 24.4x2, 24.3. . ESI-HRMS (TOF) m/z $[M+H]^+$ calcd. for $C_{53}H_{42}N_3$ 720.3373 found 720.3370. TLC R_f (SiO_2, 20% cyclohexane in CH_2Cl_2) = 0.55.

Synthesis of 4-(4,7-dihydro-1H-tricyclopenta[def,jkl,pqr]triphenylen-2-yl)-1-(5'-phenyl-[1,1':3',1''-terphenyl]-4'-yl)-1H-1,2,3-triazole (6)



6

2-Ethynylsumanene (**7**; 3.0 mg, 0.010 mmol, 1 eq) was placed in 25 ml round bottom flask. Next, 2'-azido-5'-phenyl-1,1':3',1''-terphenyl (**11**; 5.5 mg, 0.016 mmol, 1.5 eq), copper(I) thiophene-2-carboxylate (CuTC; 3.0 mg, 0.016 mmol, 1.5 eq) and tris((1-benzyl-1*H*-1,2,3-triazol-4-yl)methyl)amine (TBTA; 8.0 mg, 0.016 mmol, 1.5 eq) were added. Flask was evacuated with vacuum and flushed with argon. Then 2 ml of DMF were added followed by *N*,*N*-diisopropylethylamine (DIPEA; 9 µl, 0.052 mmol, 5 eq). Reaction mixture was stirred for 24 h at 55°C. Distilled water was added (30 ml), and the mixture was filtered on a 0.45 µm nylon filter under reduced pressure and

washed with distilled water. Collected solids were dissolved in 30 ml of $CHCl_3$ and resulting solution was dried with $MgSO_4$. After filtration, volatiles were distilled off using rotary evaporator. Finally, the product was purified using preparative thin layer chromatography (PTLC, Al_2O_3; 50% cyclohexane in CH_2Cl_2). Yield 60% (4 mg; yellowish solid).

^{1}H NMR (THF-d_8, 600 MHz, ppm), δ_H 7.89 (s, 1H), 7.87–7.82 (m, 5H), 7.68 (s, 1H), 7.50–7.48 (m, 2H), 7.42–7.39 (m, 1H), 7.29–7.27 (m, 4H), 7.23–7.15 (m, 6H), 7.11–7.05 (m, 4H), 4.67 (d, $^2J_{H\text{-}H}$= 18.3 Hz, 2H), 4.57 (d, $^2J_{H\text{-}H}$ = 20.0 Hz, 1H), 3.42–3.37 (m, 2H), 2.95 ($^2J_{H\text{-}H}$, J = 20.0 Hz, 1H). {^{1}H}^{13}C NMR ($CDCl_3$, 151 MHz, ppm), δ_C 150.7, 150.1x2, 150.0, 149.9, 149.7x2, 149.6, 149.5, 149.3, 149.1, 147.2, 146.0, 144.0, 141.9, 140.6, 139.3, 133.6, 129.8, 129.5, 129.0, 128.5, 128.2, 127.9, 126.2, 124.3, 124.2, 124.0, 121.7, 43.13, 42.1x2. ESI-HRMS (TOF) m/z $[M+H]^+$ calcd. for $C_{47}H_{30}N_3$ 636.2434 found 636.2428. TLC R_f (Al_2O_3, 50% cyclohexane in CH_2Cl_2) = 0.17.

Table S1. Selected optimization experiments for the synthesis of sumanene receptor **6**.

Compound 7 (equiv)	Compound 11 (equiv)	Copper source (equiv)	Additives (equiv)	Isolated yield (%)[a]
1	1.2	CuTC (0.5)	DIPEA (2.5)	0
1	2	CuI (1)	DIPEA (5) TBTA (1)	Traces
1	1.5	CuTC (1.5)	DIPEA (5) TBTA (1.5)	60

[a] DMF, 55°C, 24 hours

S1.2.5. Synthesis of compounds 12-15

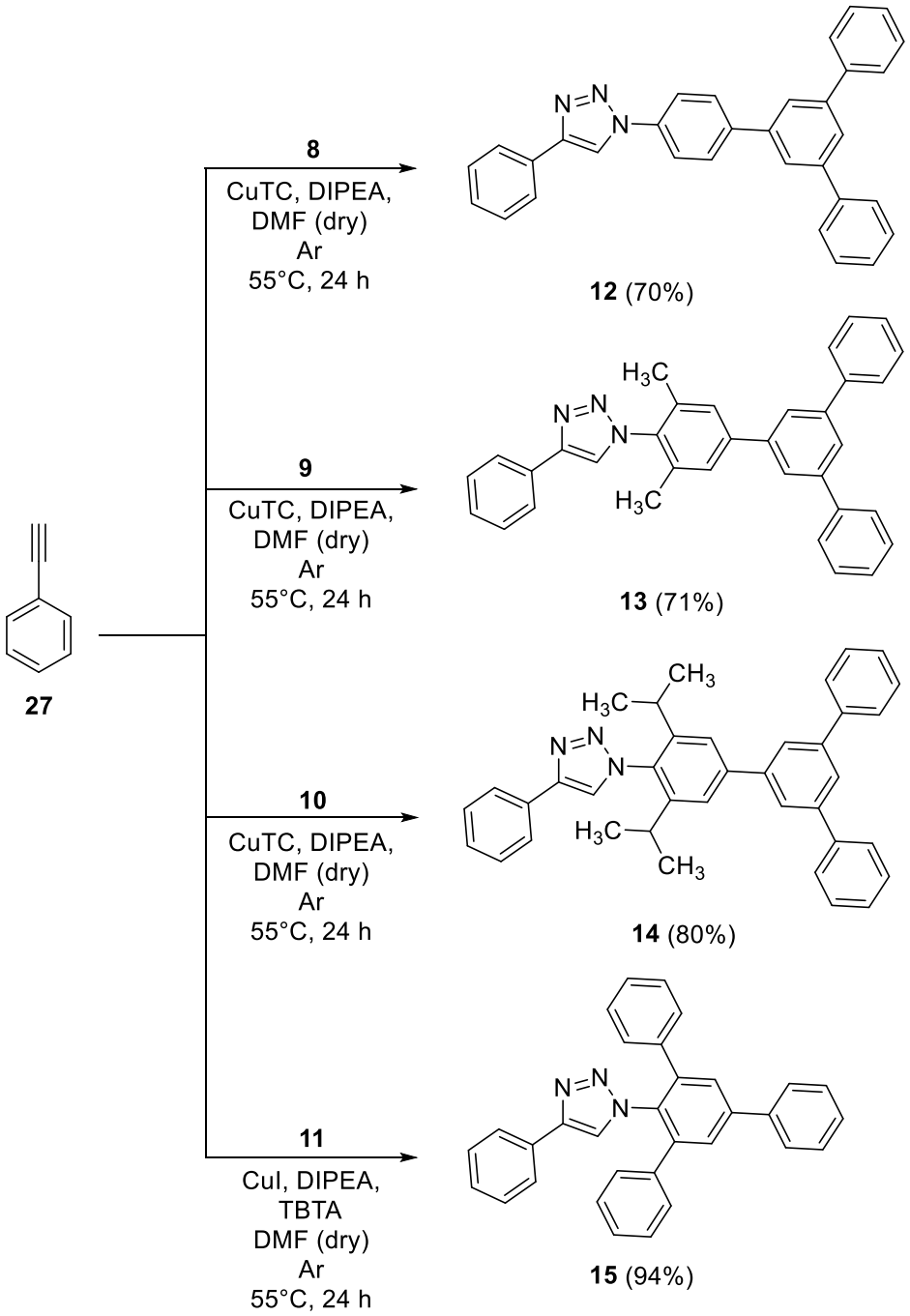
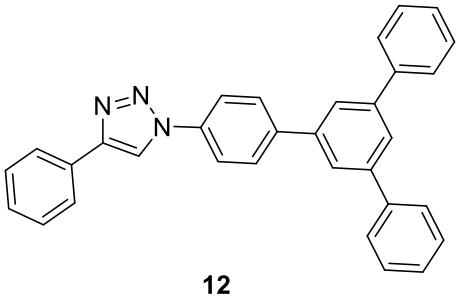


Fig. S4. Synthesis of compounds **12-15**.

Synthesis of 4-phenyl-1-(5'-phenyl-[1,1':3',1''-terphenyl]-4-yl)-1H-1,2,3-triazole (12)

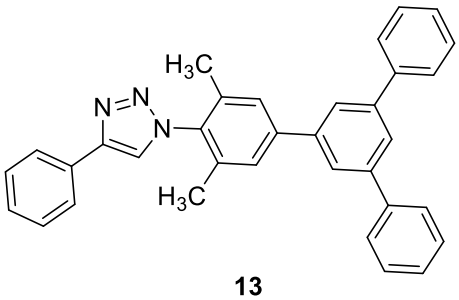


12

4-Azido-5'-phenyl-1,1':3',1''-terphenyl (**8**; 48.135 mg, 0.014 mmol, 1.2 eq) was placed in 25 ml round bottom flask. Next copper(I) thiophene-2-carboxylate (CuTC; 6.6 mg, 0.035 mmol, 0.3 eq) was added. Flask was evacuated with vacuum and flushed with argon. Then 1 ml of DMF was added followed by phenylacetylene (**27**; 12.5 µl, 0.115 mmol, 1 eq) and *N*,*N*-diisopropylethylamine (DIPEA; 24 µl, 0.014 mmol, 1.2 eq). Reaction mixture was stirred for 24 h at 55°C. Distilled water was added (30 ml), and mixture was extracted with chloroform (3x20ml). Organic layers were combined, dried with $MgSO_4$ and volatiles were distilled off using a rotary evaporator. Then to remove residual DMF, 10 ml of toluene was added and mixture was distilled off using a rotary evaporator. Finally, the product was purified using preparative thin layer chromatography (PTLC, SiO_2; 10% hexane in CH_2Cl_2). Yield 70% (36 mg; white solid).

^{1}H NMR ($CDCl_3$, 600 MHz, ppm), δ_H 8.25 (s, 1H), 7.96–7.91 (m, 4H), 7.88–7.82 (m, 5H), 7.73–7.71 (m, 4H), 7.52–7.47 (m, 6H), 7.44 – 7.38 (m, 3H). {^{1}H}^{13}C NMR ($CDCl_3$, 151 MHz, ppm), δ_C 148.7, 142.8, 141.8, 141.0, 140.9, 136.5, 130.4, 129.1x2, 128.8, 128.6, 127.9, 127.5, 126.1, 126.0, 125.2, 121.0, 117.6. ESI-HRMS (TOF) m/z $[M+H]^+$ calcd. for $C_{32}H_{24}N_3$ 450.1965 found 450.1960. TLC R_f (SiO_2, 10% hexane in CH_2Cl_2) = 0.65.

Synthesis of 1-(3,5-dimethyl-5'-phenyl-[1,1':3',1''-terphenyl]-4-yl)-4-phenyl-1H-1,2,3-triazole (13)

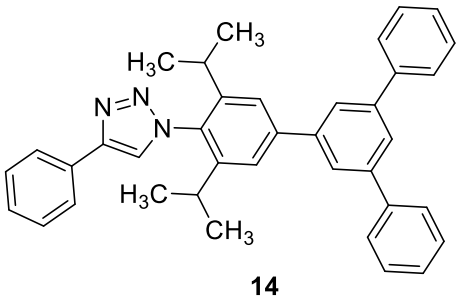


13

4-Azido-3,5-dimethyl-5'-phenyl-1,1':3',1''-terphenyl (**9**; 8.9 mg, 0.024 mmol, 1.2 eq) was placed in 25 ml round bottom flask. Next copper(I) thiophene-2-carboxylate (CuTC; 1.1 mg, 0.006 mmol, 0.3 eq) was added. Flask was evacuated with vacuum and flushed with argon. Then 1 ml of DMF was added followed by phenylacetylene (**27**; 2.2 µl, 0.020 mmol, 1 eq) and *N*,*N*-diisopropylethylamine (DIPEA; 4 µl, 0.024 mmol, 1.2 eq). Reaction mixture was stirred for 24 h at 55°C. Distilled water was added (30 ml), and mixture was extracted with chloroform (3x20ml). Organic layers were combined, dried with $MgSO_4$ and volatiles were distilled off using a rotary evaporator. Then to remove residual DMF, 10 ml of toluene was added and mixture was distilled off using a rotary evaporator. Finally, the product was purified using preparative thin layer chromatography (PTLC, SiO_2; CH_2Cl_2). Yield 71% (9.5 mg; yellowish solid).

^{1}H NMR ($CDCl_3$, 600 MHz, ppm), δ_H 7.97–7.95 (m, 2H), 7.92 (s, 1H), 7.84–7.83 (m, 1H), 7.80–7.79 (m, 2H), 7.73–7.71 (m, 4H), 7.53–7.47 (m, 8H), 7.43–7.37 (m, 3H), 2.17 (s, 6H). {^{1}H}^{13}C NMR ($CDCl_3$, 151 MHz, ppm), δ_C 148.0, 143.2, 142.8, 141.3, 141.1, 136.2, 135.5, 130.6, 129.1x2, 128.5, 127.9, 127.6, 127.5, 126.0, 125.3, 121.5, 17.9. ESI-HRMS (TOF) m/z $[M+H]^+$ calcd. for $C_{34}H_{28}N_3$ 478.2278 found 478.2272. TLC R_f (SiO_2, CH_2Cl_2) = 0.24.

Synthesis of 1-(3,5-diisopropyl-5'-phenyl-[1,1':3',1''-terphenyl]-4-yl)-4-phenyl-1H-1,2,3-triazole (14)

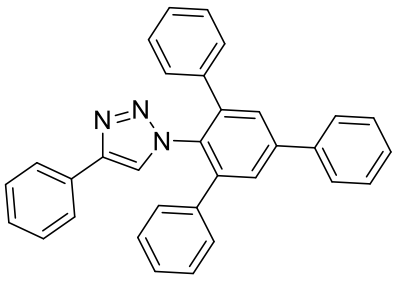


14

4-Azido-3,5-diisopropyl-5'-phenyl-1,1':3',1''-terphenyl (**10**; 6.6 mg, 0.015 mmol, 1.3 eq) was placed in 25 ml round bottom flask. Next copper(I) thiophene-2-carboxylate (CuTC; 0.9 mg, 0.004 mmol, 0.4 eq) was added. Flask was evacuated with vacuum and flushed with argon. Then 1 ml of DMF was added followed by phenylacetylene (**27**; 1.3 µl, 0.012 mmol, 1 eq) and *N*,*N*-diisopropylethylamine (DIPEA; 4 µl, 0.023 mmol, 1.2 eq). Reaction mixture was stirred for 24 h at 55°C. Distilled water was added (30 ml), and mixture was extracted with chloroform (3x20ml). Organic layers were combined, dried with $MgSO_4$ and volatiles were distilled off using a rotary evaporator. Then to remove residual DMF, 10 ml of toluene was added and mixture was distilled off using a rotary evaporator. Finally, the product was purified using preparative thin layer chromatography (PTLC, SiO_2; 10% hexane in CH_2Cl_2). Yield 80% (5 mg; yellowish solid).

^{1}H NMR ($CDCl_3$, 600 MHz, ppm), δ_H δ 7.98–7.96 (m, 2H), 7.91 (s, 1H), 7.83–7.82 (m, 1H), 7.77–7.76 (m, 2H), 7.72–7.70 (m, 4H), 7.56 (s, 2H), 7.52–7.47 (m, 6H), 7.43–7.37 (m, 3H), 2.42 (hept, $^3J_{H-H}$ = 6.9 Hz, 2H), 1.23 (2x, 2x $^3J_{H-H}$ = 6.9 Hz, 12H). {^{1}H}^{13}C NMR ($CDCl_3$, 151 MHz, ppm), 147.7, 146.8, 144.1, 142.8, 142.3, 141.2, 132.9, 130.5, 129.1x2, 128.6, 127.9, 127.6, 126.1, 126.0, 125.5, 123.2, 122.7, 28.8, 24.5, 24.3. ESI-HRMS (TOF) m/z $[M+H]^+$ calcd. for $C_{38}H_{36}N_3$ 534.2904 found 534.2904. TLC R_f (SiO_2, 10% hexane in CH_2Cl_2) = 0.23.

Synthesis of 4-phenyl-1-(5'-phenyl-[1,1':3',1''-terphenyl]-4'-yl)-1H-1,2,3-triazole (15)



15

2'-Azido-5'-phenyl-1,1':3',1''-terphenyl (**11**; 6.55 mg, 0.019 mmol, 2 eq) was placed in 25 ml round bottom flask. Next copper(I) iodide (CuI; 1.7 mg, 0.009 mmol, 1 eq) and tris((1-benzyl-1*H*-1,2,3-triazol-4-yl)methyl)amine (TBTA; 5 mg, 0.009 mmol, 1 eq) were added. Flask was evacuated with vacuum and flushed with argon. Then 1 ml of DMF was added followed by phenylacetylene (**27**; 1 µl, 0.009 mmol, 1 eq) and *N*,*N*-diisopropylethylamine (DIPEA; 8 µl, 0.047 mmol, 5 eq). Reaction mixture was stirred for 24 h at 55°C. Distilled water was added (30 ml), and mixture

was extracted with chloroform (3x20ml). Organic layers were combined, dried with $MgSO_4$ and volatiles were distilled off using a rotary evaporator. Then to remove residual DMF, 10 ml of toluene was added and mixture was distilled off using a rotary evaporator. Finally, the product was purified using preparative thin layer chromatography (PTLC, Al_2O_3; CH_2Cl_2). Yield 94% (4 mg; yellowish solid).

^{1}H NMR (DMSO-d_6, 600 MHz, ppm), δ_H 8.53 (s, 1H), 7.92–7.90 (m, 2H), 7.85 (s, 2H), 7.65–7.63 (m, 2H), 7.55–7.47 (m, 2H), 7.48–7.45 (m, 1H), 7.39–7.36 (m, 2H), 7.30–7.26 (m, 11H). {^{1}H}^{13}C NMR ($CDCl_3$, 151 MHz, ppm), δ_C 145.8, 142.4, 140.3, 138.6, 137.4, 131.8, 130.2, 129.1, 128.9, 128.3, 127.8, 127.4, 125.1. ESI-HRMS (TOF) m/z $[M+H]^+$ calcd. for $C_{32}H_{24}N_3$ 450.1965 found 450.1964. TLC R_f (SiO_2, Al_2O_3; CH_2Cl_2) = 0.34.

Table S2. Selected optimization experiments for the synthesis of compound **15**.

Compound 27 (equiv)	Compound 11 (equiv)	Copper source (equiv)	Additives (equiv)	Isolated yield (%)[a]
1	1.2	CuTC (0.3)	DIPEA (2.5)	0[b]
1	1.2	$CuSO_4 \cdot 5H_2O$ (0.3)	Sodium ascorbate (1.2)	0[b]
1	1.2	CuTC (0.3)	DIPEA (2.5) 1,10-phenantroline (0.3eq)	0[b]
1	1.2	copper mesh	Sodium ascorbate (1.2)	0[c]
1	1.5	CuTC (0.3)	DIPEA (1.2)	0[d]
1	2	CuI (1)	DIPEA (5) TBTA (1)	94

[a] DMF, 55°C, 24 hours; [b] no product observed also for longer reaction times (up to 4 days); [c] mechanochemistry (Retsch MM 400); [d] sonochemistry

S1.3. Potentiometric experiments: Sensors preparation, EMF measurements and determination of potentiometric selectivity coefficients

The method of the membranes and sensors preparation was the same as for standard ion-selective electrodes. The membranes contained: 1% wt receptor, 65-66% wt plasticizer NPOE, 32-33% wt PVC and 10% mol (vs receptor) KTFPB. The membrane components (200 mg in total) were dissolved in 1.5 ml of THF. The solution was poured into a glass ring placed on a glass. After solvent evaporation, membrane discs of appropriate size were cut off and mounted in electrode bodies (type IS 561, Philips) for electromotive force (EMF) measurements. NaCl solution (0.01 M) was used as an internal filling; the electrodes were conditioned for a week in NaCl solution (0.001 M). For each membrane composition at least three sensor specimens were prepared.

All measurements were carried out with cells of the following type: Ag, AgCl; KCl 1 M / CH_3COOLi 1 M / sample solution // membrane // internal filling solution; AgCl, Ag.

Potentiometric multiplexer (EMF 16 Interface, Lawson Labs Inc., Malvern, USA) was used for the EMF measurements. The values of the potentiometric selectivity coefficients (log $K_{Na, Me}$) of the ion-selective electrodes were determined by the separate solution method (SSM)

using 0.01 M solutions of nitrate salts containing 0.01M MES pH 5.0.[8] The activities of ions in aqueous solutions were calculated according to the Debye-Hueckel approximation. Determination of potentiometric selectivity was repeated four times during the period of one month.

Potentiometric selectivity coefficients compare quantitatively the influence of an arbitrary chosen primary ion (in our case: Na^+) and given interfering ion (Me) on the signal of the ion-selective electrode. Additionally, a highly lipophilic anionic additive (potassium tetrakis[3,5-bis(trifluoro-methyl)-phenyl]borate (KTFPB) was introduced into the membranes to prevent anion interference (permselectivity for cations) and ensure theoretical operation of the sensors[9]. Since the presence of anionic sites ($TFPB^-$) imposes specific selectivity pattern with higher affinity towards lipophilic cations, the selectivity of the membranes doped with the studied receptors should be assessed against the selectivity of the membranes containing only KTFPB (blank membranes) to reliably evaluate the cation binding properties of the studied receptors.

S1.4. Spectrofluorimetric receptor studies: Titration experiments methodology

Stock solutions of receptors were prepared by dissolving weighted amounts of investigated compounds in such amount of THF to obtain concentration of $2 \cdot 10^{-4}$ M. Solutions used for fluorescence experiments were prepared by diluting stock solutions with THF and then with MES buffer (0.01M, pH=5.0) in such amounts to yield final concentration of sumanene derivatives equal to $2 \cdot 10^{-5}$ M and equal proportions (by volume) of THF and water. Metal cations were introduced to the solution in the form of the corresponding hexafluorophosphate salts (PF_6^-) in the case of Li^+ and a nitrate salt was used in the case of Cu^{2+} and Pb^{2+} cations.

Each fluorescence titration experiment was carried out in 10 steps. First, the fluorescence of solution containing only sumanene derivative was measured, then metal salts were added as a solution in a mixture of THF and water (50% water by volume) to achieve following proportions of metal cation to sumanene derivative: 0.1, 0.2, 0.3, 0.5, 0.75, 1, 2 ,5 and 10 eq. To guarantee good mixing, a magnetic stir bar was placed in a cuvette. To prevent magnetic stir bar obstructing light path in spectrometer, a small permanent magnet was placed on the side of the cuvette to hold the magnetic stir bar above light beam.

S2. NMR spectra

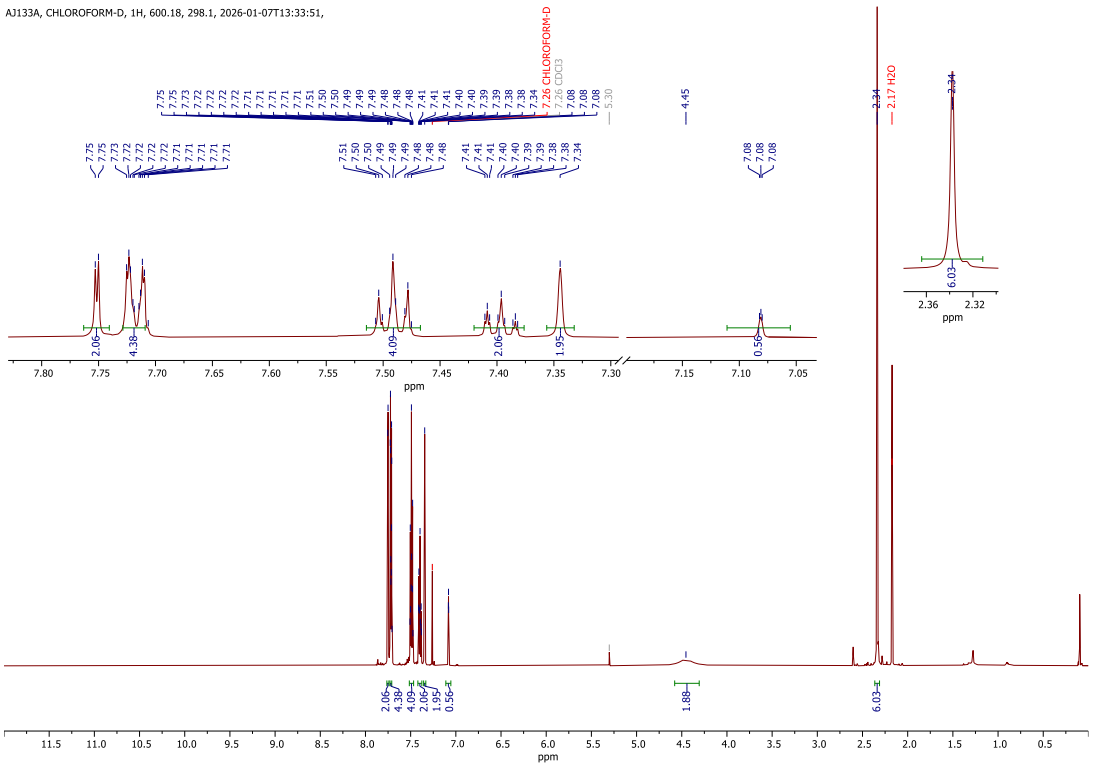


Fig. S5. ^{1}H NMR spectrum (600 MHz, $CDCl_3$) of 3,5-dimethyl-5'-phenyl-[1,1':3',1''-terphenyl]-4-amine (**20**).

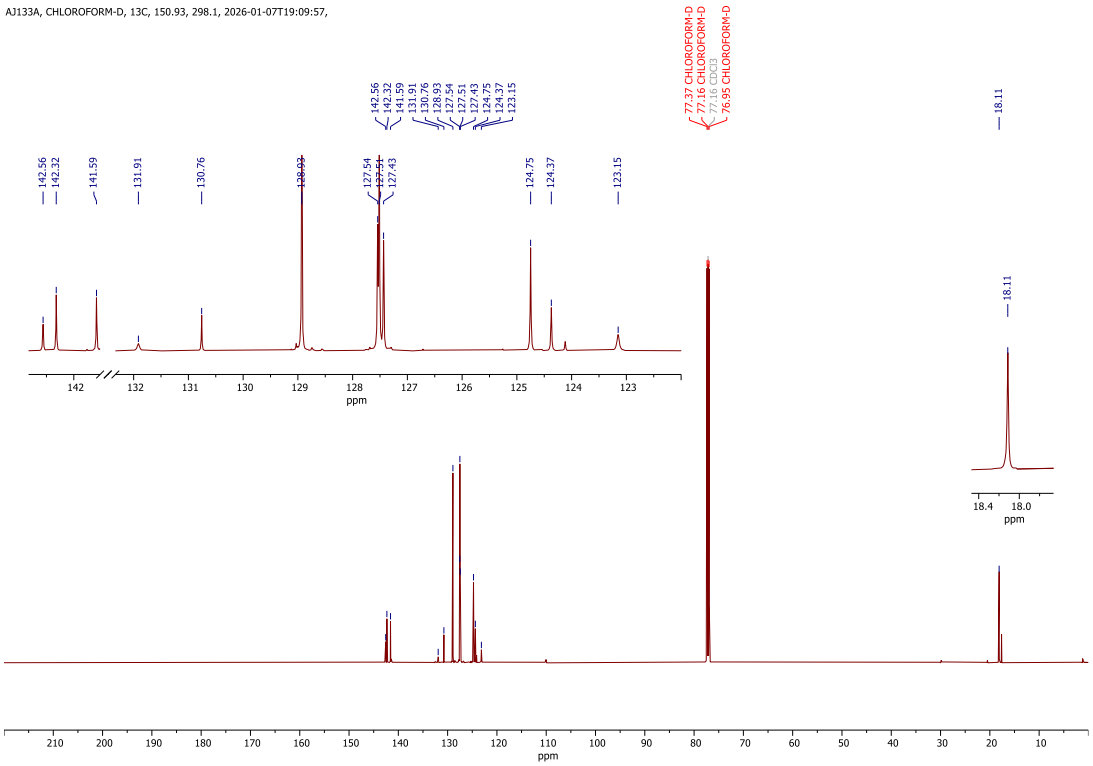


Fig. S6. $\{^{1}H\}^{13}C$ NMR spectrum (151 MHz, $CDCl_3$) of 3,5-dimethyl-5'-phenyl-[1,1':3',1''-terphenyl]-4-amine (**20**).

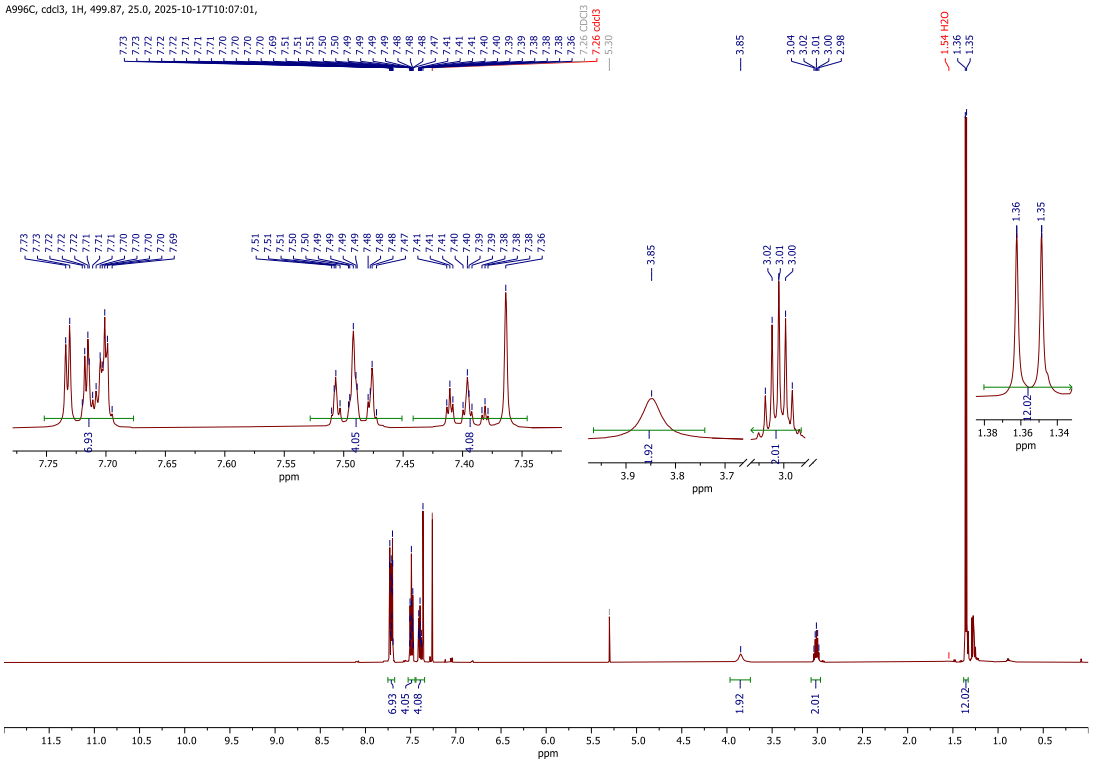


Fig. S7. ^{1}H NMR spectrum (500 MHz, $CDCl_3$) of 3,5-diisopropyl-5'-phenyl-[1,1':3',1''-terphenyl]-4-amine (**20**).

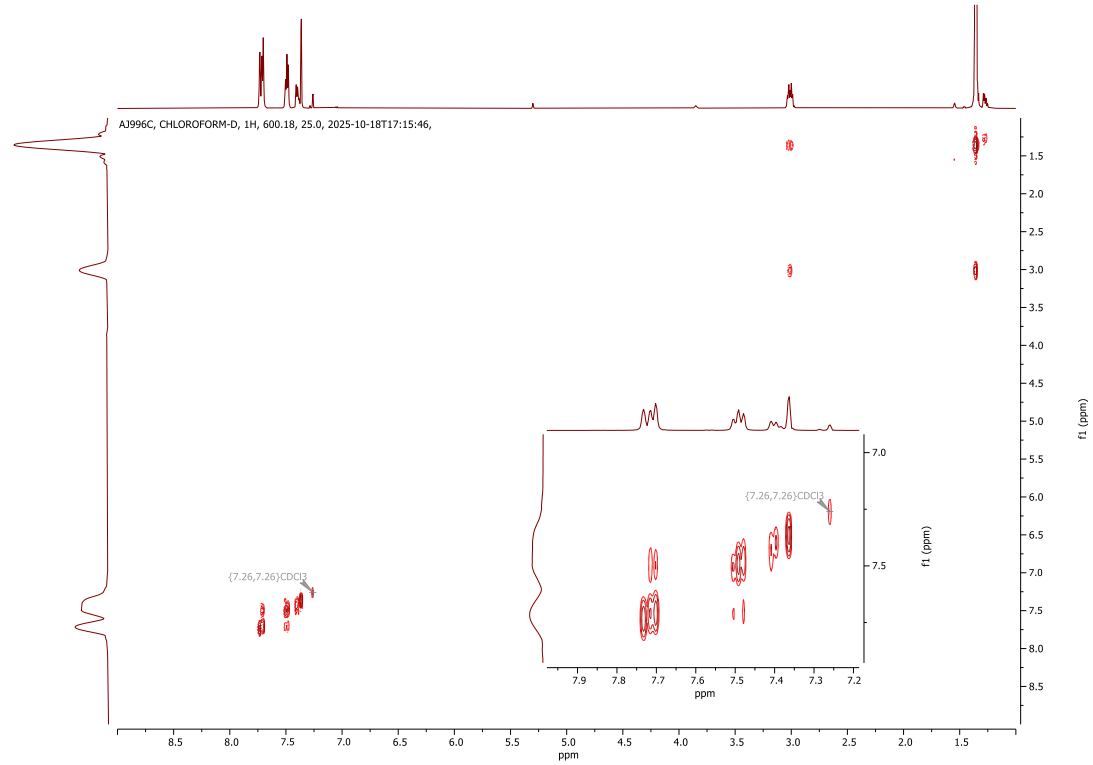


Fig. S8. ^{1}H-^{1}H COSY NMR spectrum (600 MHz, $CDCl_3$) of 3,5-diisopropyl-5'-phenyl-[1,1':3',1''-terphenyl]-4-amine (**20**).

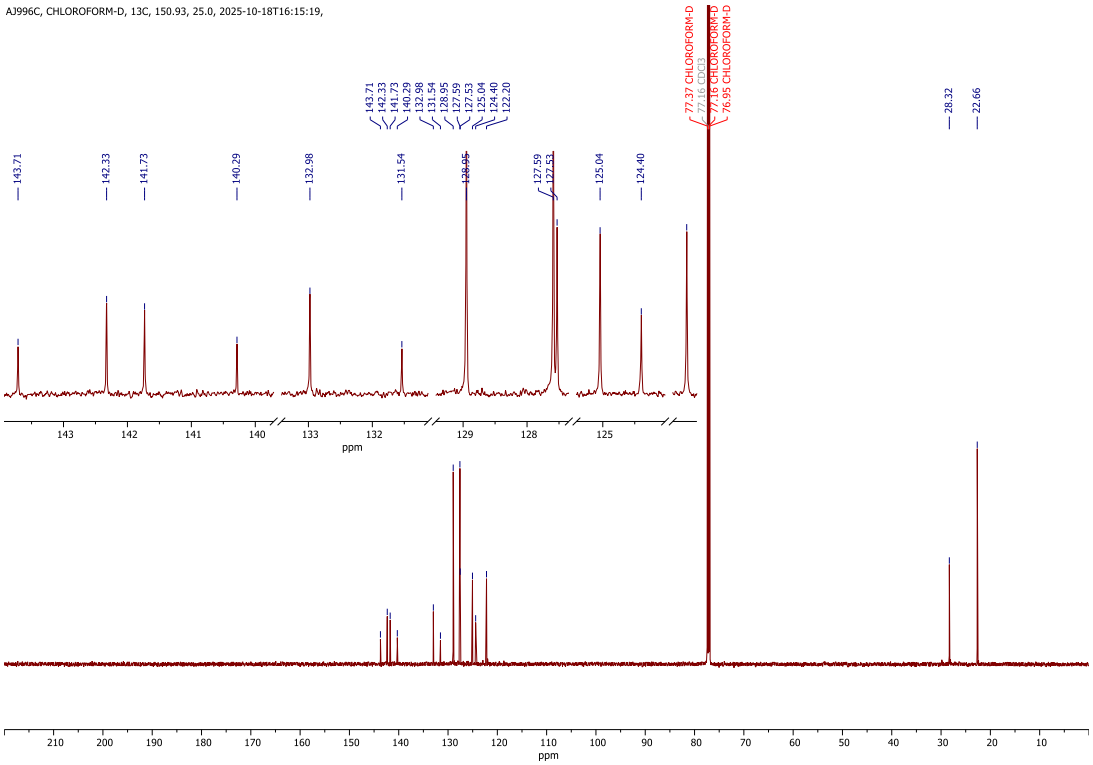


Fig. S9. $\{^1H\}^{13}C$ NMR spectrum (151 MHz, $CDCl_3$) of 3,5-diisopropyl-5'-phenyl-[1,1':3',1''-terphenyl]-4-amine (**20**).

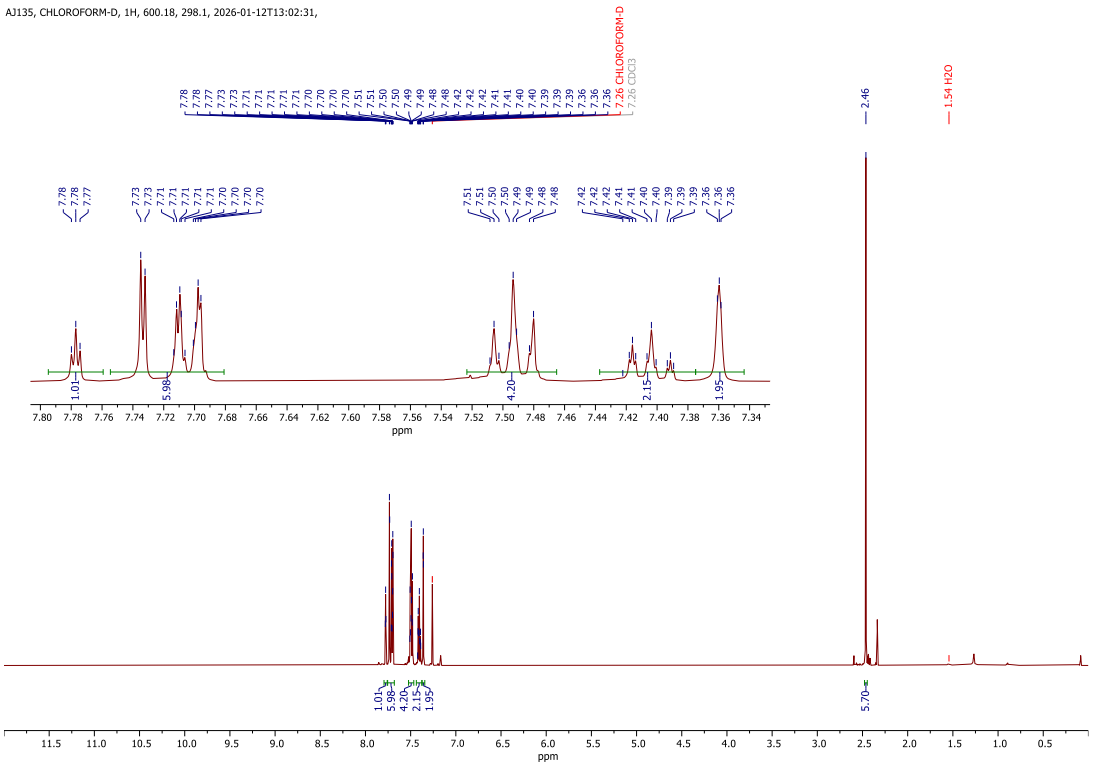


Fig. S10. ^1H NMR spectrum (600 MHz, $CDCl_3$) of 4-azido-3,5-dimethyl-5'-phenyl-1,1':3',1''-terphenyl (**9**).

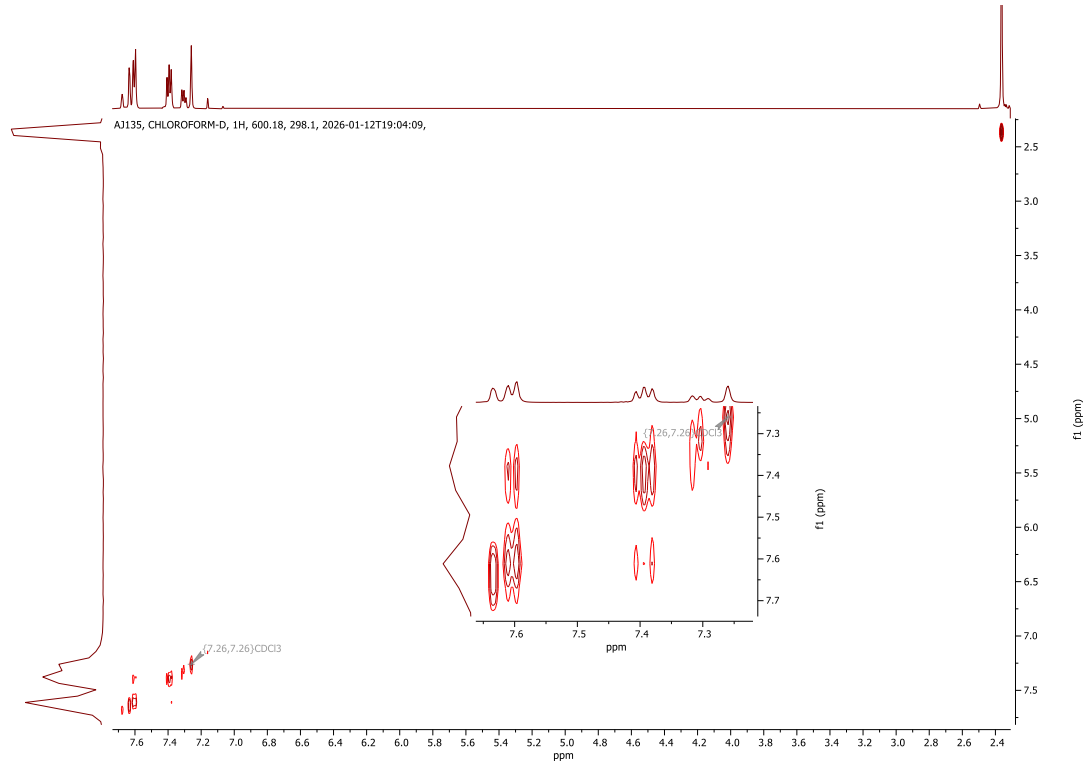


Fig. S11. ^{1}H-^{1}H COSY NMR spectrum (600 MHz, $CDCl_3$) of 4-azido-3,5-dimethyl-5'-phenyl-1,1':3',1''-terphenyl (**9**).

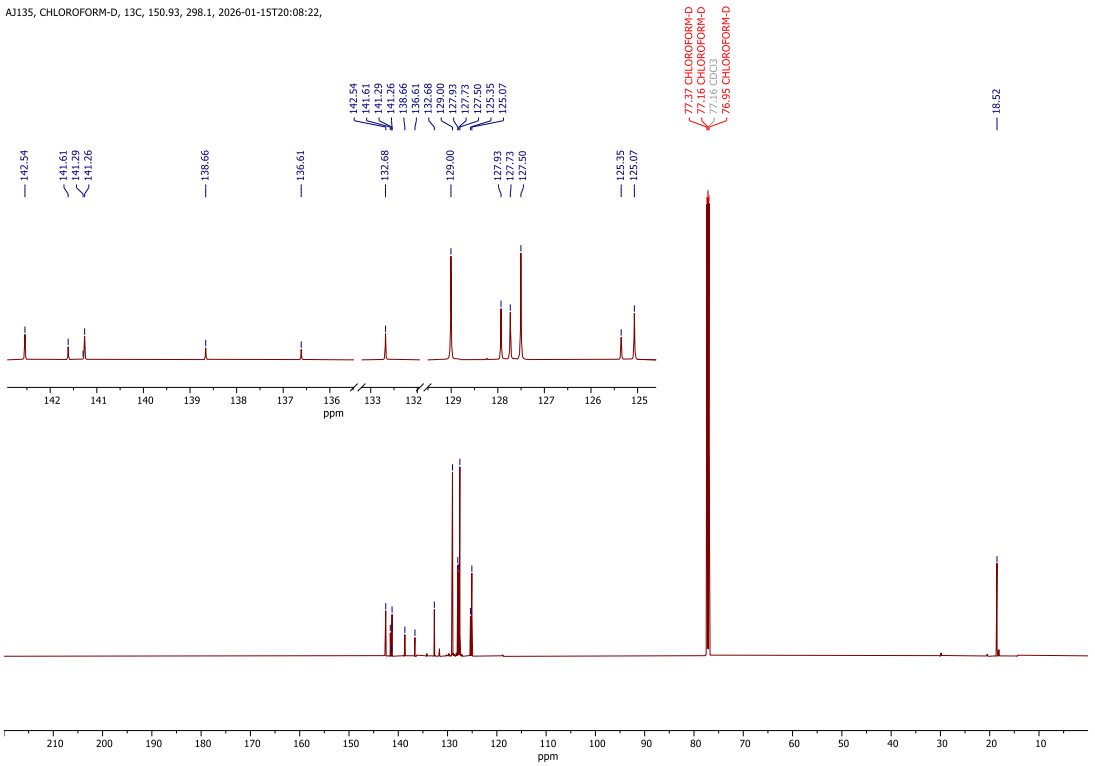


Fig. S12. {^{1}H}^{13}C NMR spectrum (151 MHz, $CDCl_3$) of 4-azido-3,5-dimethyl-5'-phenyl-1,1':3',1''-terphenyl (**9**).

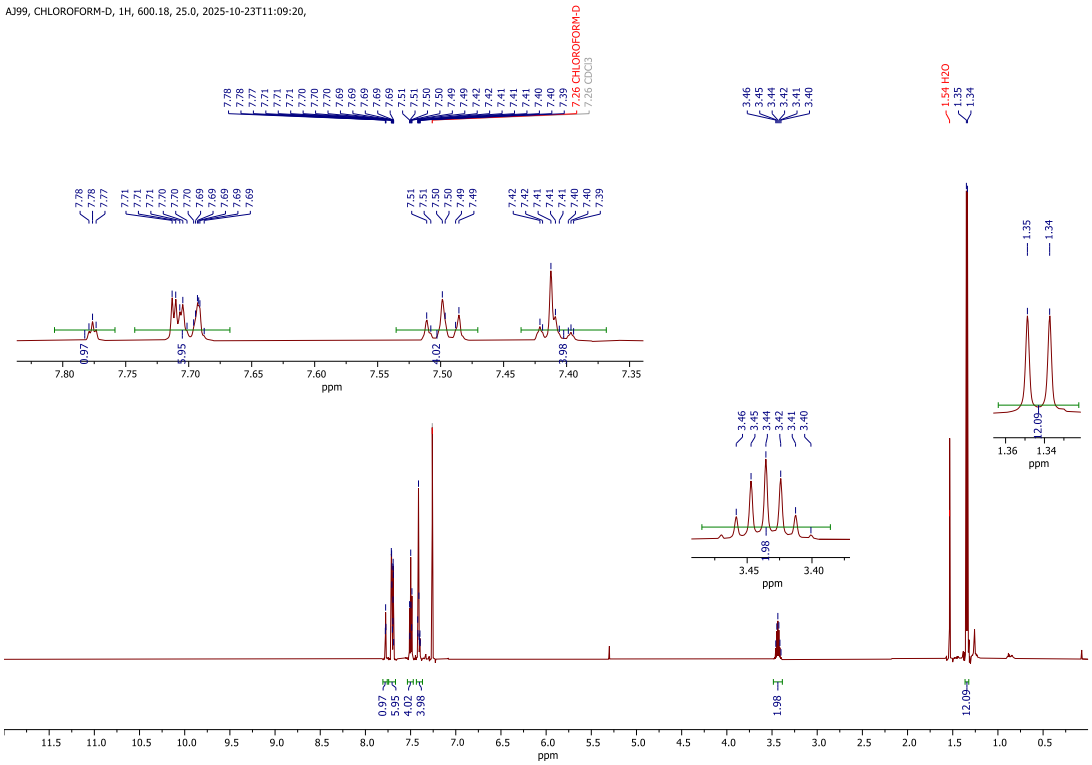


Fig. S13. ^{1}H NMR spectrum (600 MHz, $CDCl_3$) of 4-azido-3,5-diisopropyl-5'-phenyl-1,1':3',1''-terphenyl (**10**).

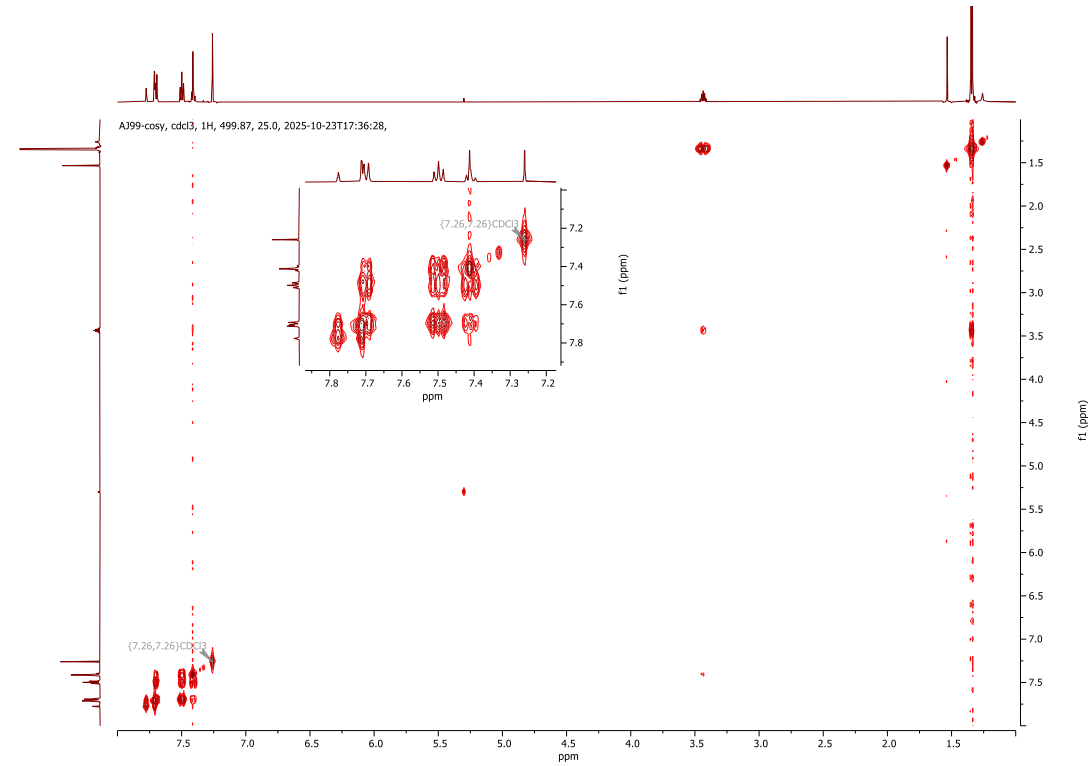


Fig. S14. ^{1}H-^{1}H COSY NMR spectrum (500 MHz, $CDCl_3$) of 4-azido-3,5-diisopropyl-5'-phenyl-1,1':3',1''-terphenyl (**10**).

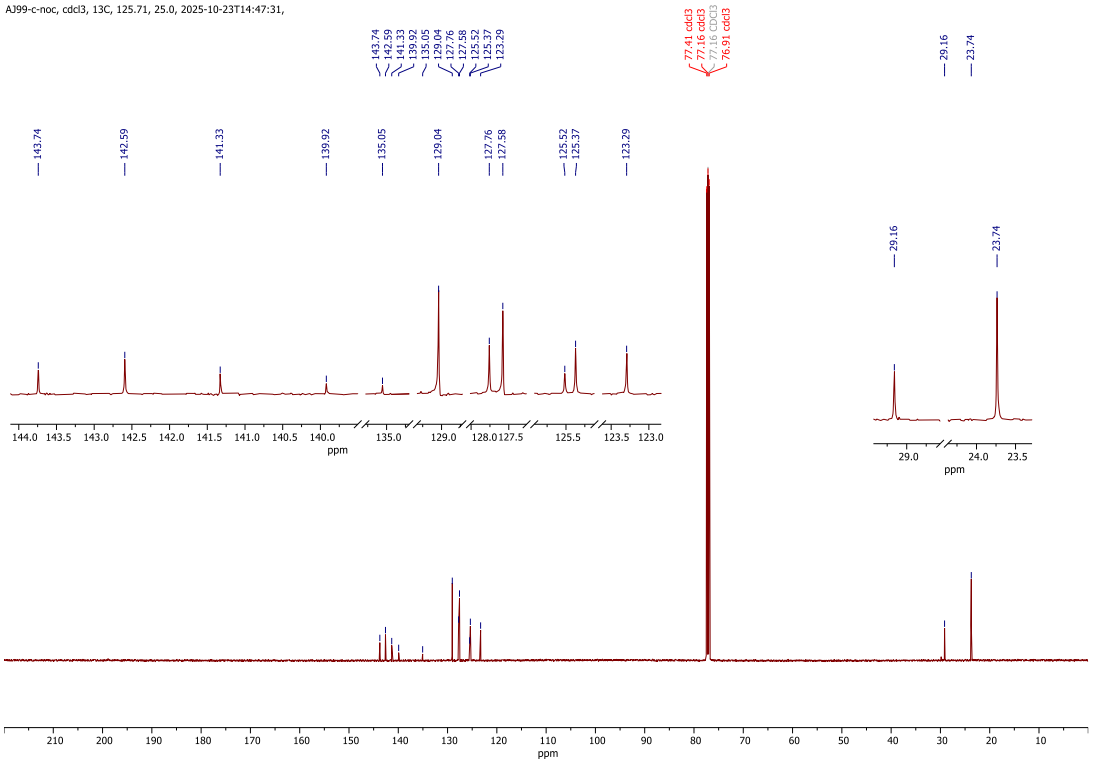


Fig. S15. {^{1}H}^{13}C NMR spectrum (126 MHz, $CDCl_3$) of 4-azido-3,5-diisopropyl-5'-phenyl-1,1':3',1''-terphenyl (**10**).

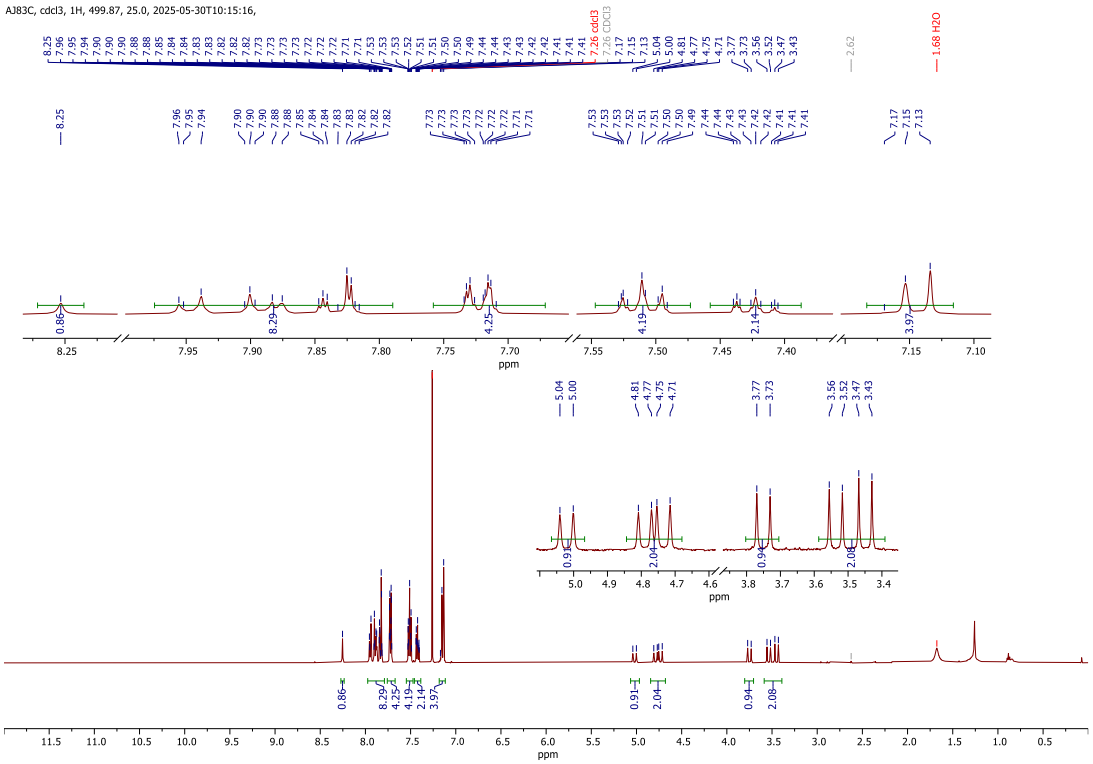


Fig. S16. ^{1}H NMR spectrum (500 MHz, $CDCl_3$) of 4-(4,7-dihydro-1*H*-tricyclopenta[*def*,*jkl*,*pqr*]triphenylen-2-yl)-1-(5'-phenyl-[1,1':3',1''-terphenyl]-4-yl)-1*H*-1,2,3-triazole (**3**).

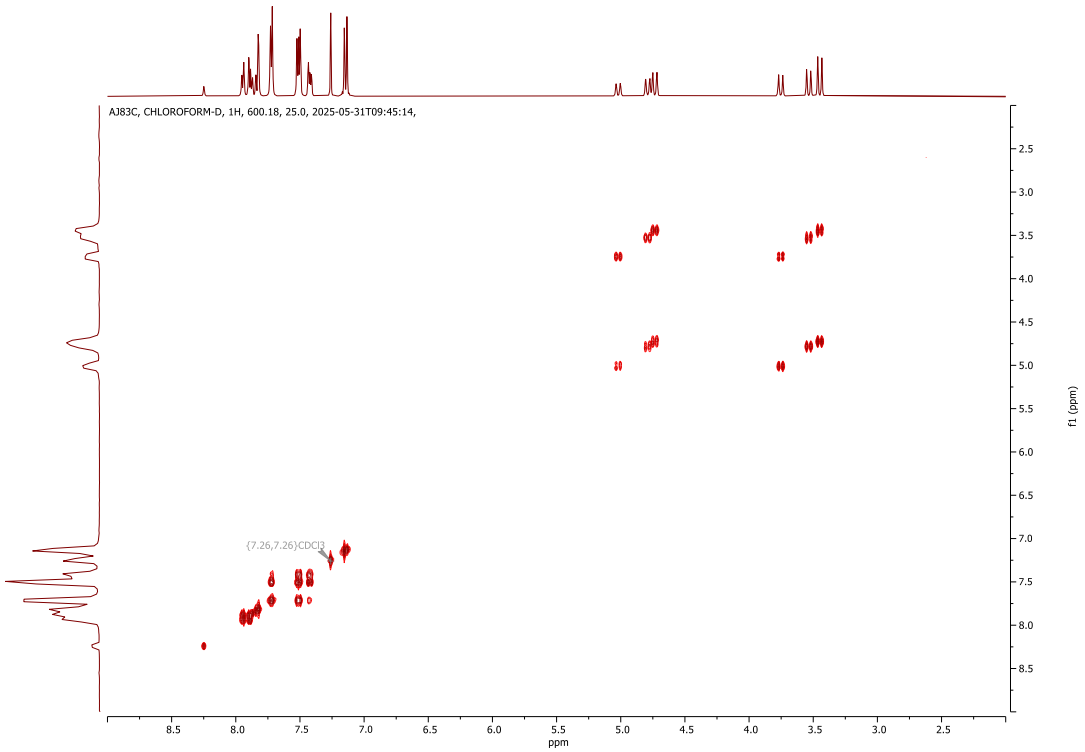


Fig. S17. ^{1}H-^{1}H COSY NMR spectrum (600 MHz, $CDCl_3$) of 4-(4,7-dihydro-1*H*-tricyclopenta[*def*,*jkl*,*pqr*]triphenylen-2-yl)-1-(5'-phenyl-[1,1':3',1''-terphenyl]-4-yl)-1*H*-1,2,3-triazole (**3**).

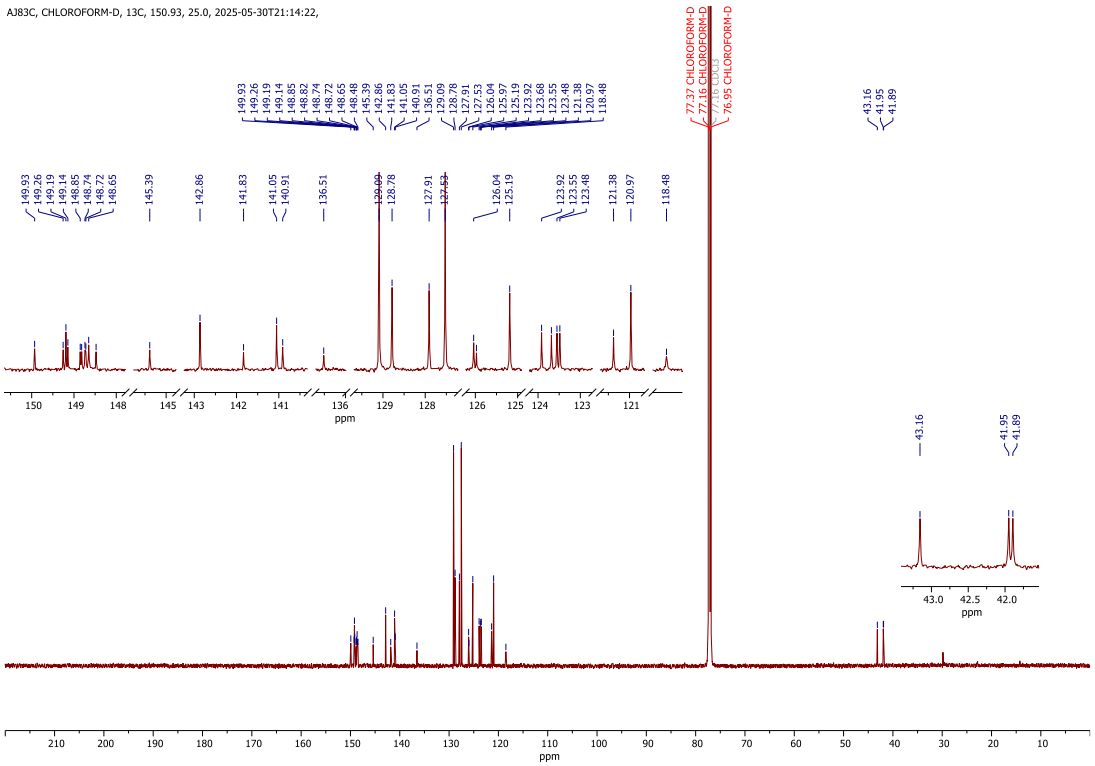


Fig. S18. {^{1}H}^{13}C NMR spectrum (151 MHz, $CDCl_3$) of 4-(4,7-dihydro-1*H*-tricyclopenta[*def*,*jkl*,*pqr*]triphenylen-2-yl)-1-(5'-phenyl-[1,1':3',1''-terphenyl]-4-yl)-1*H*-1,2,3-triazole (**3**).

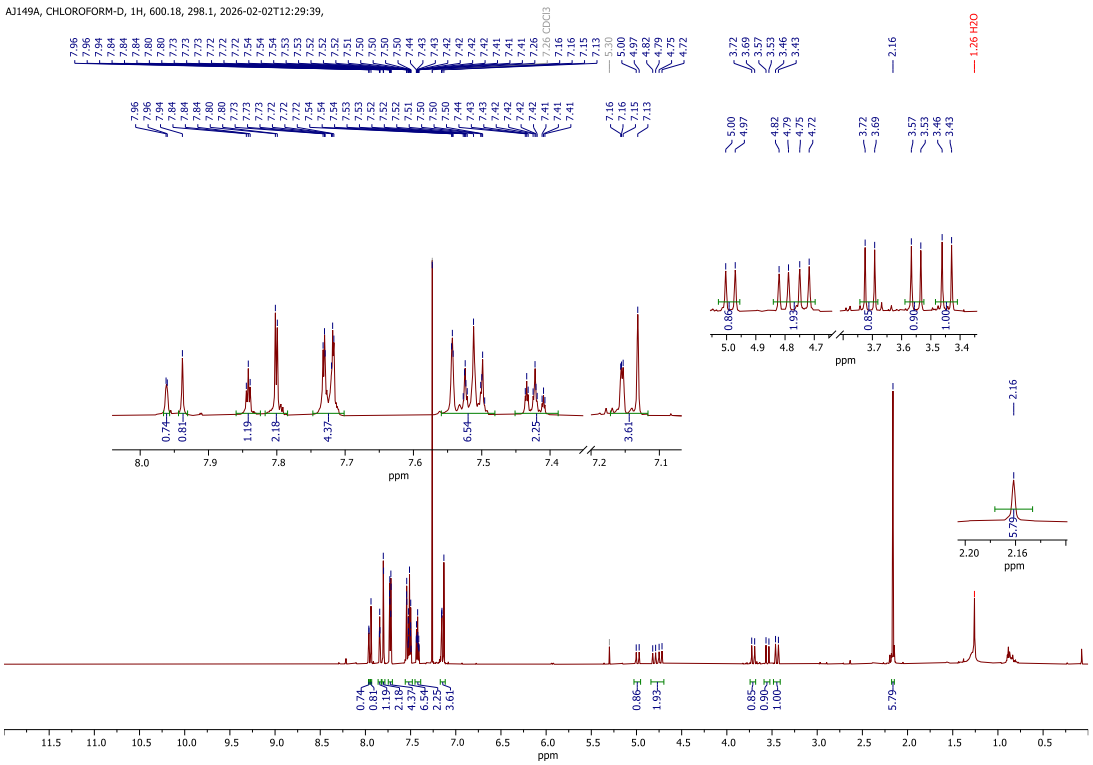


Fig. S19. ^{1}H NMR spectrum (600 MHz, $CDCl_3$) of 4-(4,7-dihydro-1*H*-tricyclopenta[*def*,*jkl*,*pqr*]triphenylen-2-yl)-1-(3,5-dimethyl-5'-phenyl-[1,1':3',1''-terphenyl]-4-yl)-1*H*-1,2,3-triazole (**4**).

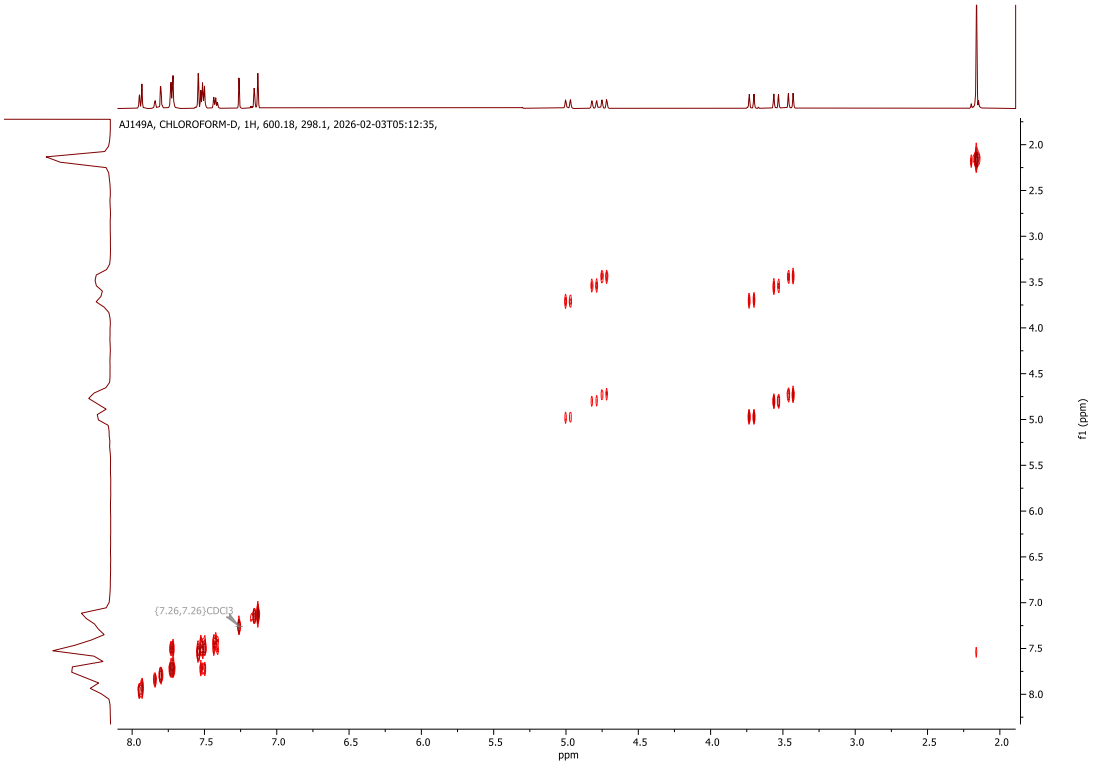


Fig. S20. ^{1}H-^{1}H COSY NMR spectrum (600 MHz, $CDCl_3$) of 4-(4,7-dihydro-1*H*-tricyclopenta[*def*,*jkl*,*pqr*]triphenylen-2-yl)-1-(3,5-dimethyl-5'-phenyl-[1,1':3',1''-terphenyl]-4-yl)-1*H*-1,2,3-triazole (**4**).

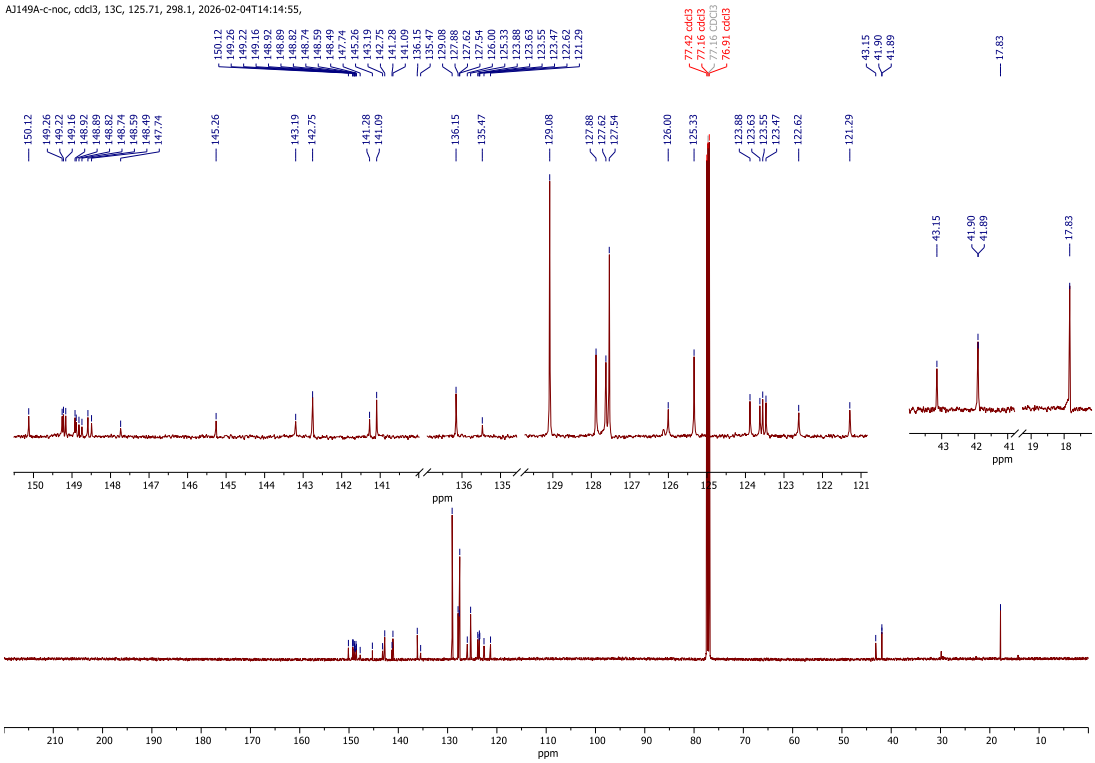


Fig. S21. $\{^1H\}^{13}C$ NMR spectrum (126 MHz, $CDCl_3$) of 4-(4,7-dihydro-1*H*-tricyclopenta[*def*,*jkl*,*pqr*]triphenylen-2-yl)-1-(3,5-dimethyl-5'-phenyl-[1,1':3',1''-terphenyl]-4-yl)-1*H*-1,2,3-triazole (**4**).

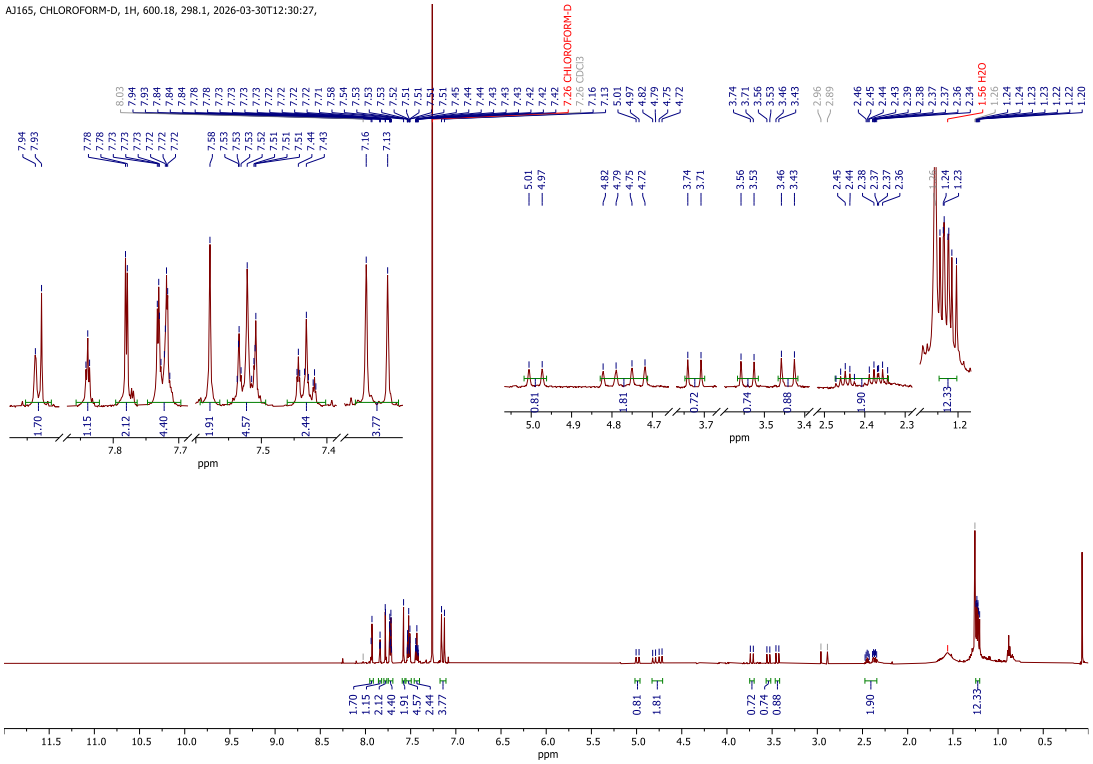


Fig. S22. ^1H NMR spectrum (600 MHz, $CDCl_3$) of 4-(4,7-diisopropyl-1*H*-tricyclopenta[*def*,*jkl*,*pqr*]triphenylen-2-yl)-1-(3,5-dimethyl-5'-phenyl-[1,1':3',1''-terphenyl]-4-yl)-1*H*-1,2,3-triazole (**5**).

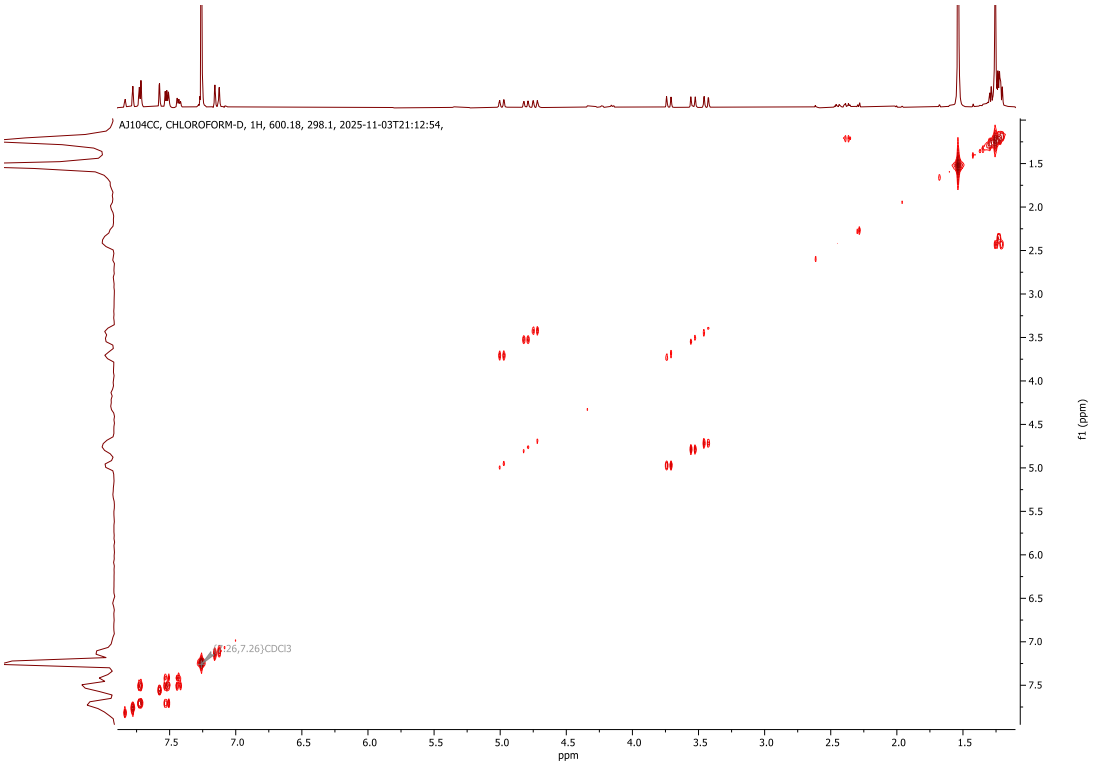


Fig. S23. ^{1}H-^{1}H COSY NMR spectrum (600 MHz, $CDCl_3$) of 4-(4,7-diisopropyl-1*H*-tricyclopenta[*def*,*jkl*,*pqr*]triphenylen-2-yl)-1-(3,5-dimethyl-5'-phenyl-[1,1':3',1''-terphenyl]-4-yl)-1*H*-1,2,3-triazole (**5**).

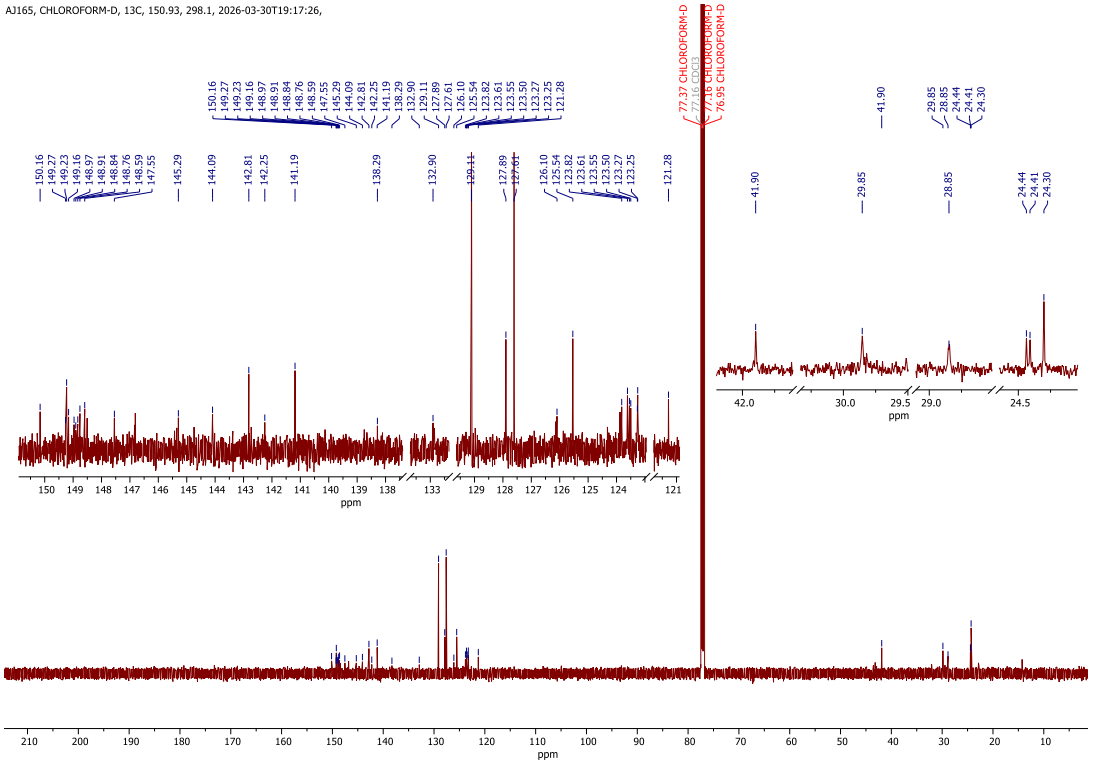


Fig. S24. {^{1}H}^{13}C NMR spectrum (151 MHz, $CDCl_3$) of 4-(4,7-diisopropyl-1*H*-tricyclopenta[*def*,*jkl*,*pqr*]triphenylen-2-yl)-1-(3,5-dimethyl-5'-phenyl-[1,1':3',1''-terphenyl]-4-yl)-1*H*-1,2,3-triazole (**5**).

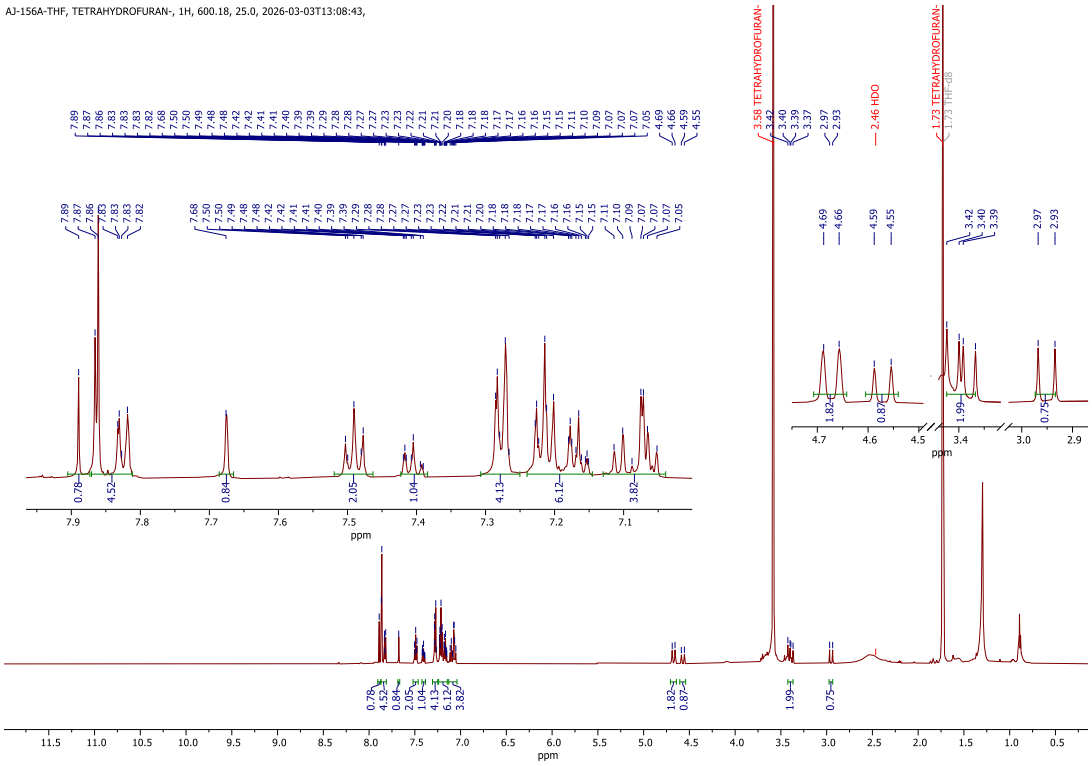


Fig. S25. ^{1}H NMR spectrum (600 MHz, THF-d_8) of 4-(4,7-dihydro-1*H*-tricyclopenta[*def*,*jkl*,*pqr*]triphenylen-2-yl)-1-(5'-phenyl-[1,1':3',1''-terphenyl]-4'-yl)-1*H*-1,2,3-triazole (**6**).

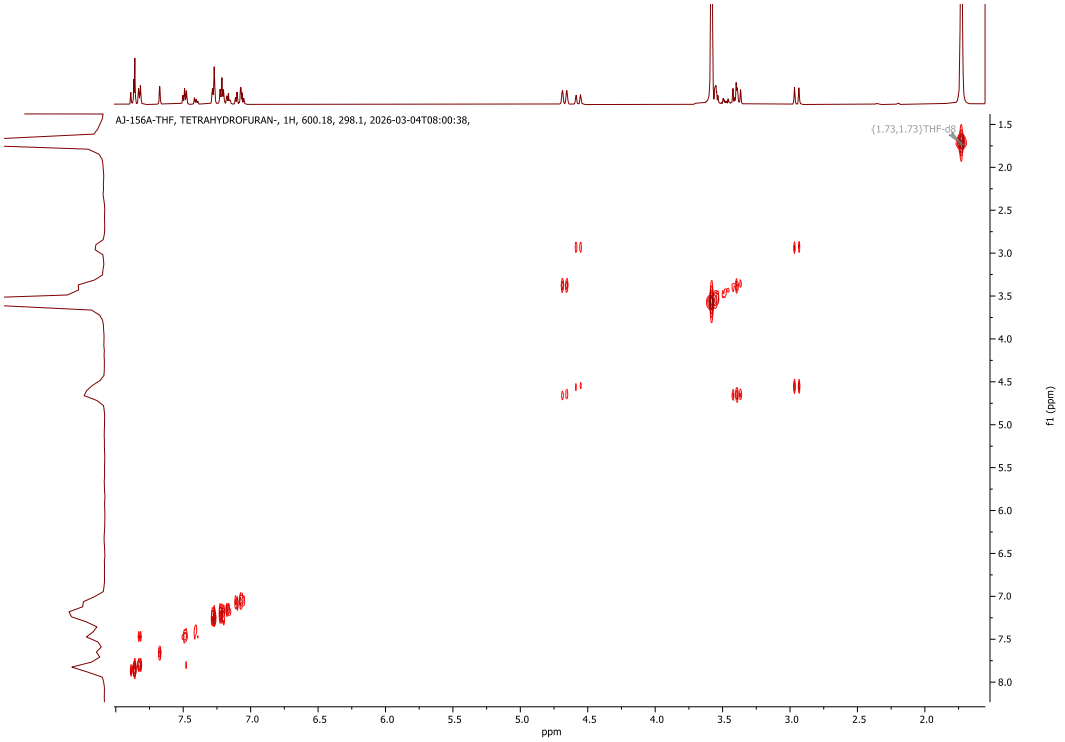


Fig. S26. ^{1}H-^{1}H COSY NMR spectrum (600 MHz, THF-d_8) of 4-(4,7-dihydro-1*H*-tricyclopenta[*def*,*jkl*,*pqr*]triphenylen-2-yl)-1-(5'-phenyl-[1,1':3',1''-terphenyl]-4'-yl)-1*H*-1,2,3-triazole (**6**).

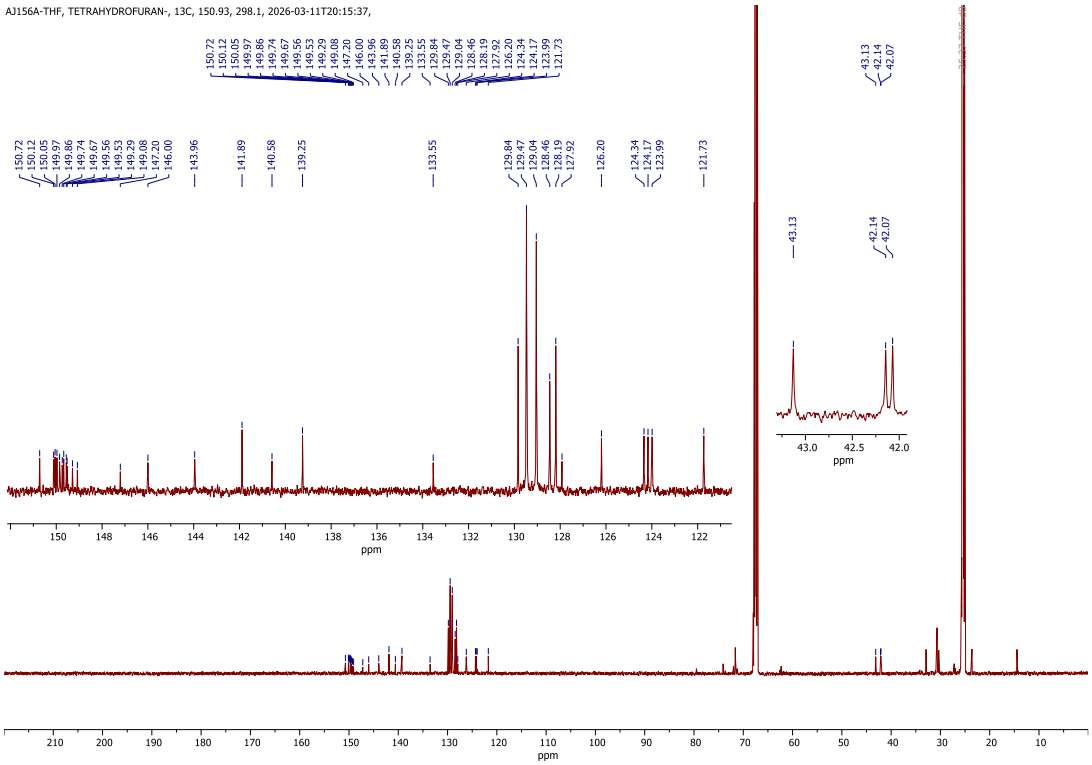


Fig. S27. {^{1}H}^{13}C NMR spectrum (151 MHz, THF-d_8) of 4-(4,7-dihydro-1*H*-tricyclopenta[*def*,*jkl*,*pqr*]triphenylen-2-yl)-1-(5'-phenyl-[1,1':3',1''-terphenyl]-4'-yl)-1*H*-1,2,3-triazole (**6**).

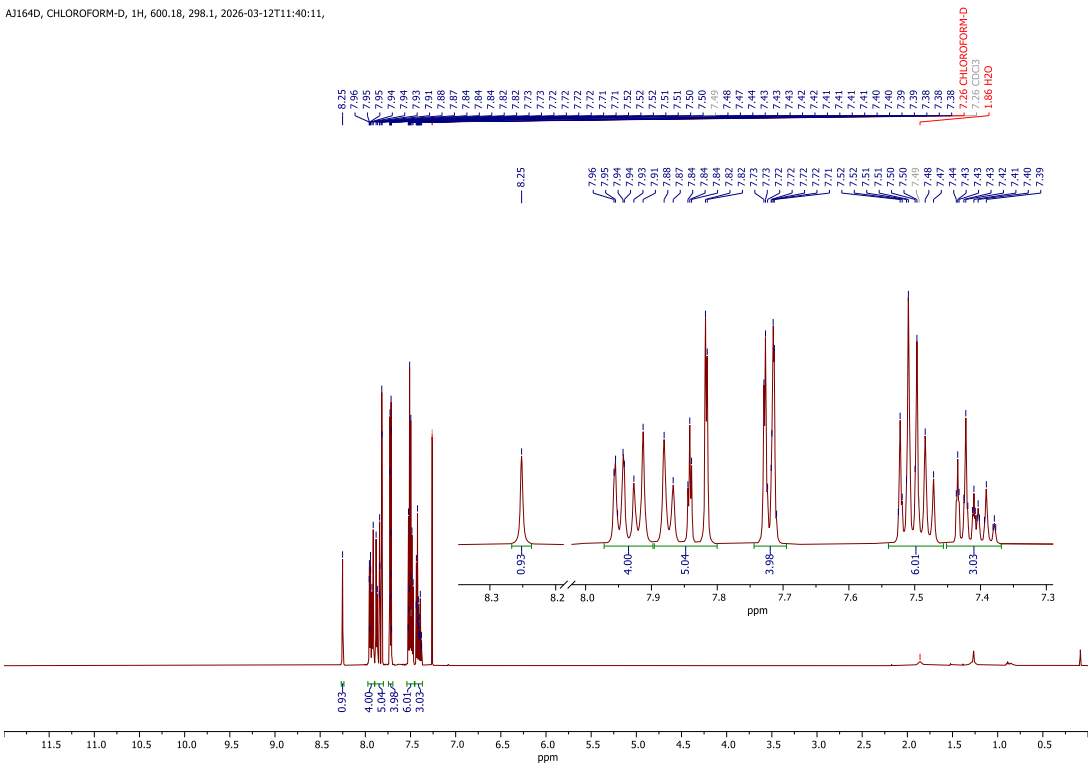


Fig. S28. ^{1}H NMR spectrum (600 MHz, $CDCl_3$) of 4-phenyl-1-(5'-phenyl-[1,1':3',1''-terphenyl]-4-yl)-1*H*-1,2,3-triazole (**12**).

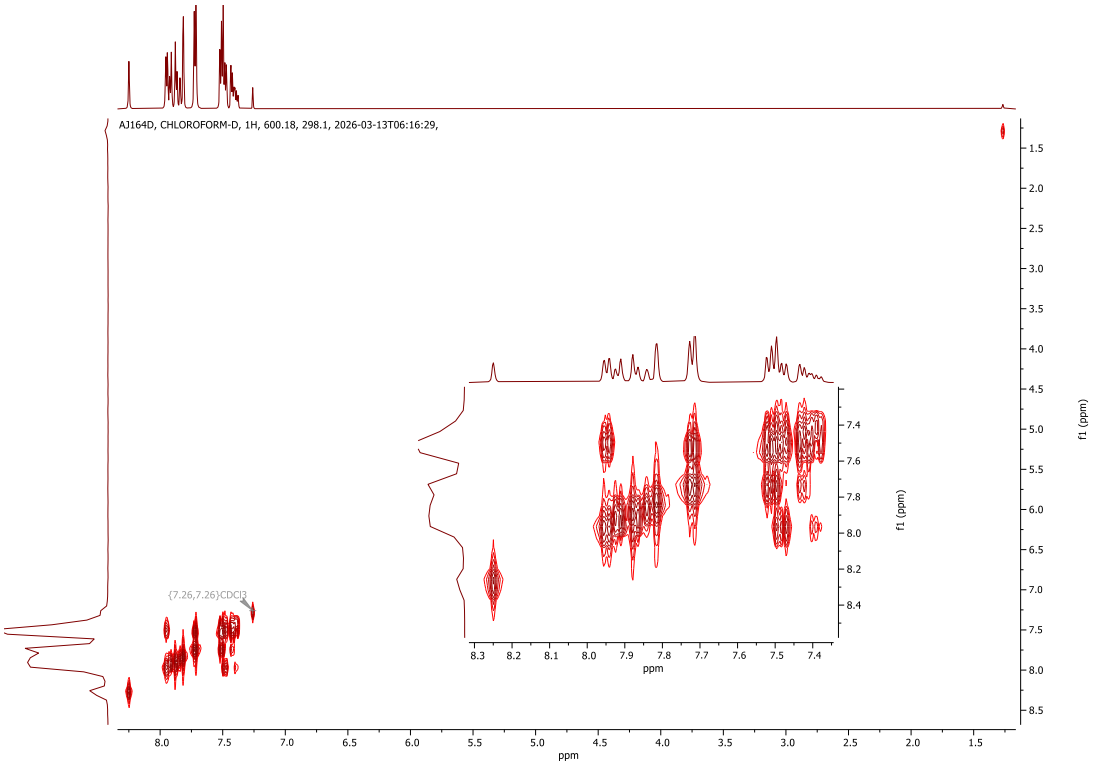


Fig. S29. ^{1}H-^{1}H COSY NMR spectrum (600 MHz, $CDCl_3$) of 4-phenyl-1-(5'-phenyl-[1,1':3',1''-terphenyl]-4-yl)-1*H*-1,2,3-triazole (**12**).

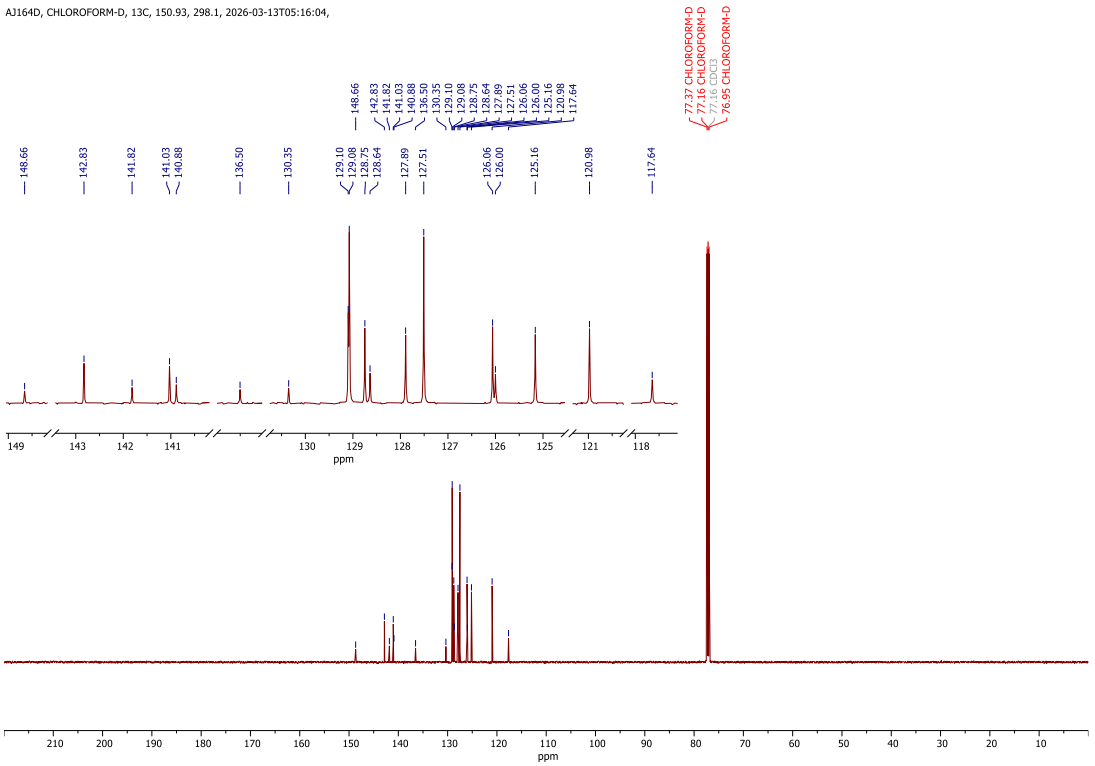


Fig. S30. {^{1}H}^{13}C NMR spectrum (151 MHz, $CDCl_3$) of 4-phenyl-1-(5'-phenyl-[1,1':3',1''-terphenyl]-4-yl)-1*H*-1,2,3-triazole (**12**).

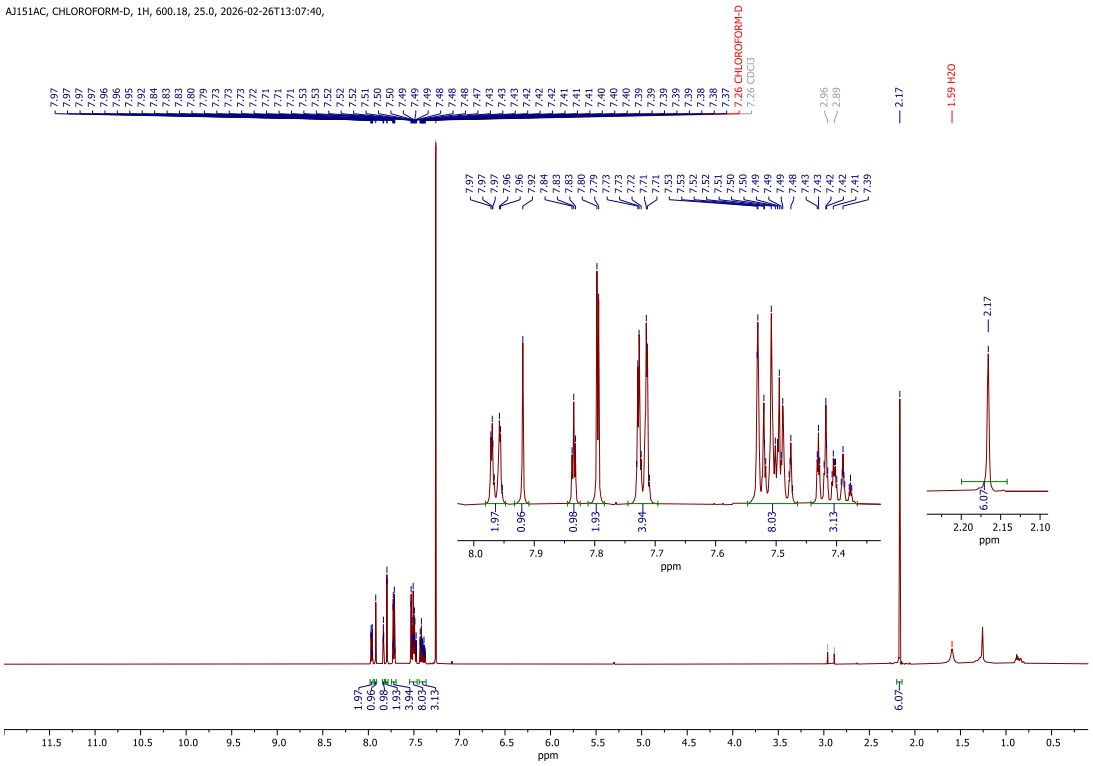


Fig. S31. ^{1}H NMR spectrum (600 MHz, $CDCl_3$) of 1-(3,5-dimethyl-5'-phenyl-[1,1':3',1''-terphenyl]-4-yl)-4-phenyl-1*H*-1,2,3-triazole (**13**).

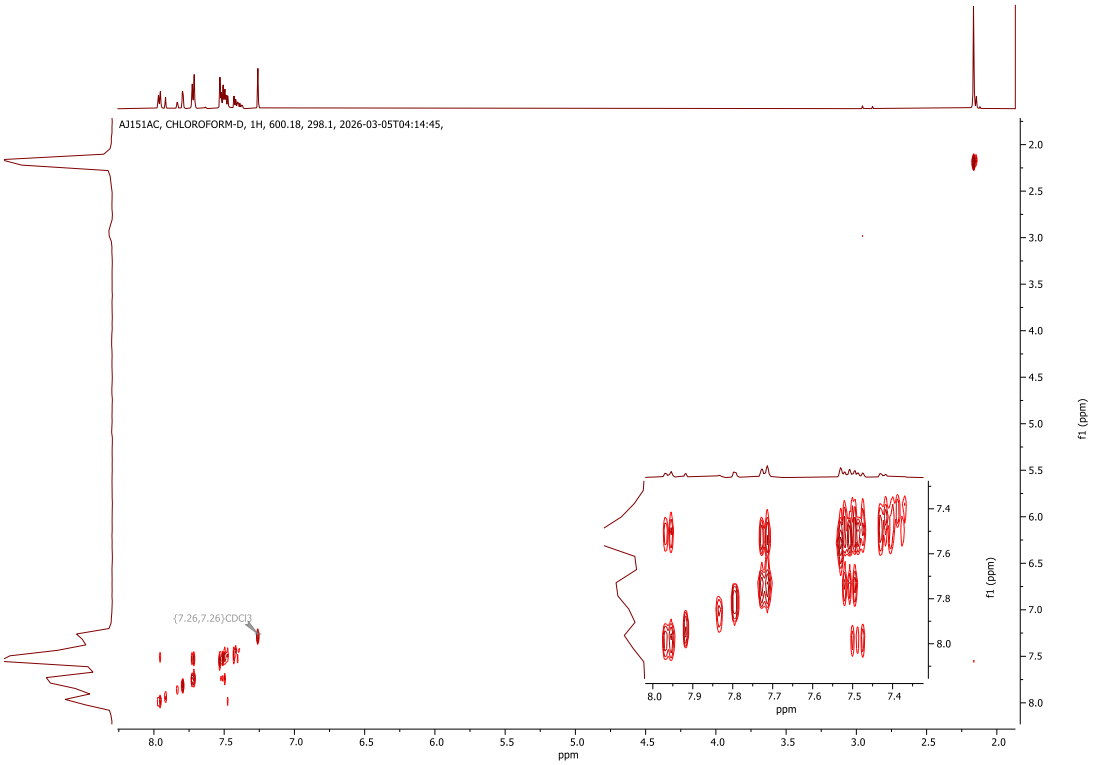


Fig. S32. ^{1}H-^{1}H COSY NMR spectrum (600 MHz, $CDCl_3$) of 1-(3,5-dimethyl-5'-phenyl-[1,1':3',1''-terphenyl]-4-yl)-4-phenyl-1*H*-1,2,3-triazole (**13**).

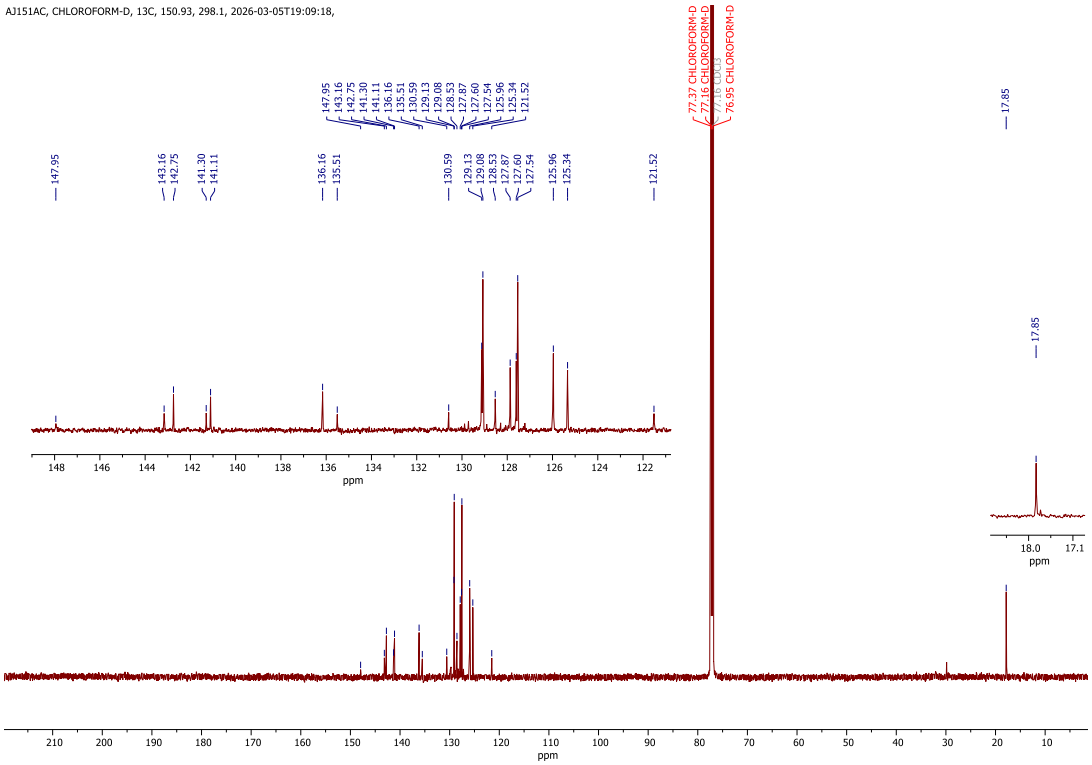


Fig. S33. $\{^1H\}^{13}C$ NMR spectrum (151 MHz, $CDCl_3$) of 1-(3,5-dimethyl-5'-phenyl-[1,1':3',1''-terphenyl]-4-yl)-4-phenyl-1*H*-1,2,3-triazole (**13**).

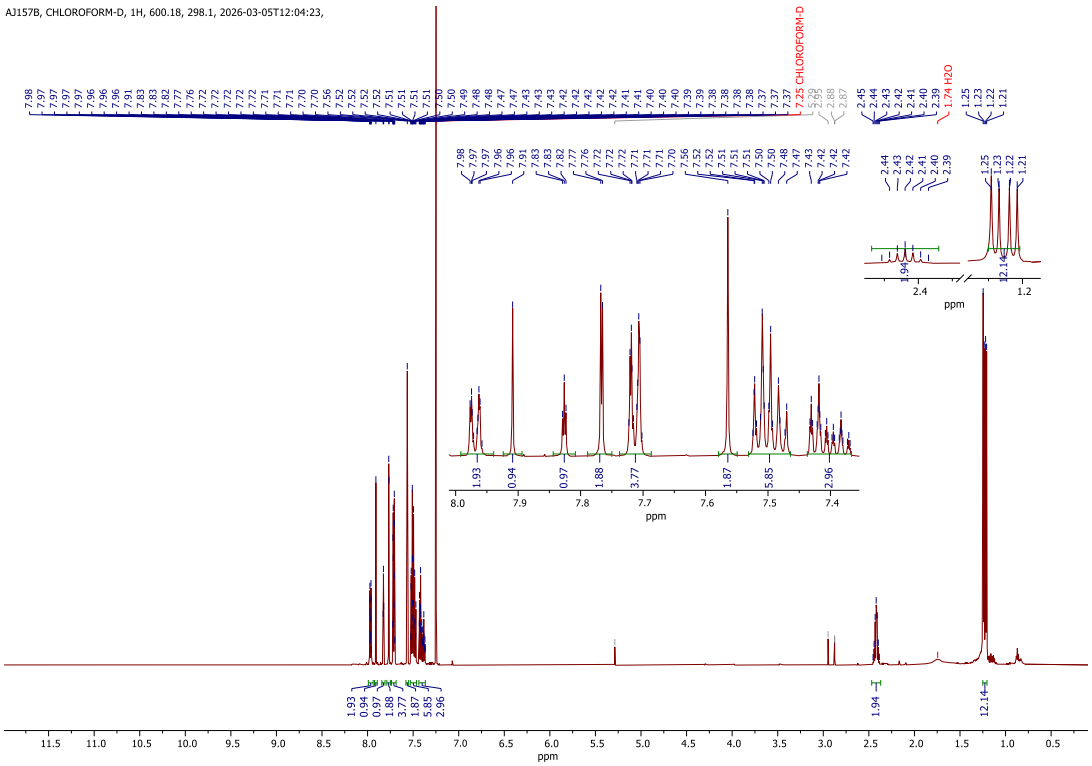


Fig. S34. ^1H NMR spectrum (600 MHz, $CDCl_3$) of 1-(3,5-diisopropyl-5'-phenyl-[1,1':3',1''-terphenyl]-4-yl)-4-phenyl-1*H*-1,2,3-triazole (**14**).

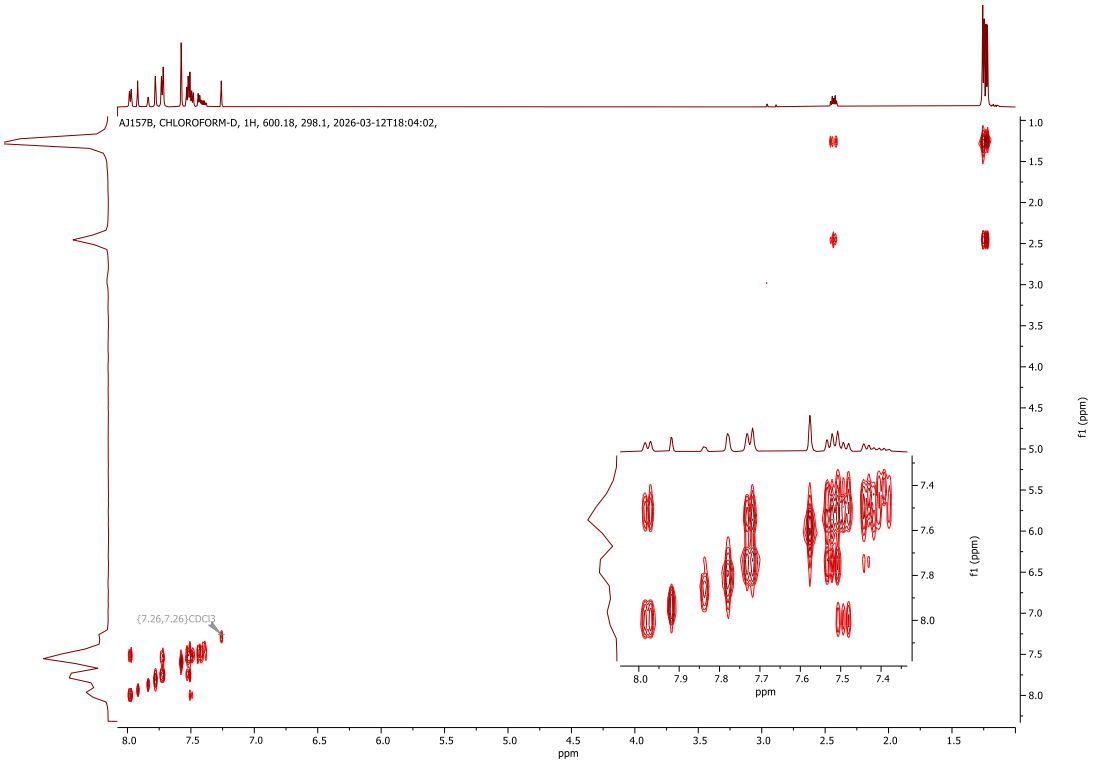


Fig. S35. ^{1}H-^{1}H COSY NMR spectrum (600 MHz, $CDCl_3$) of 1-(3,5-diisopropyl-5'-phenyl-[1,1':3',1''-terphenyl]-4-yl)-4-phenyl-1*H*-1,2,3-triazole (**14**).

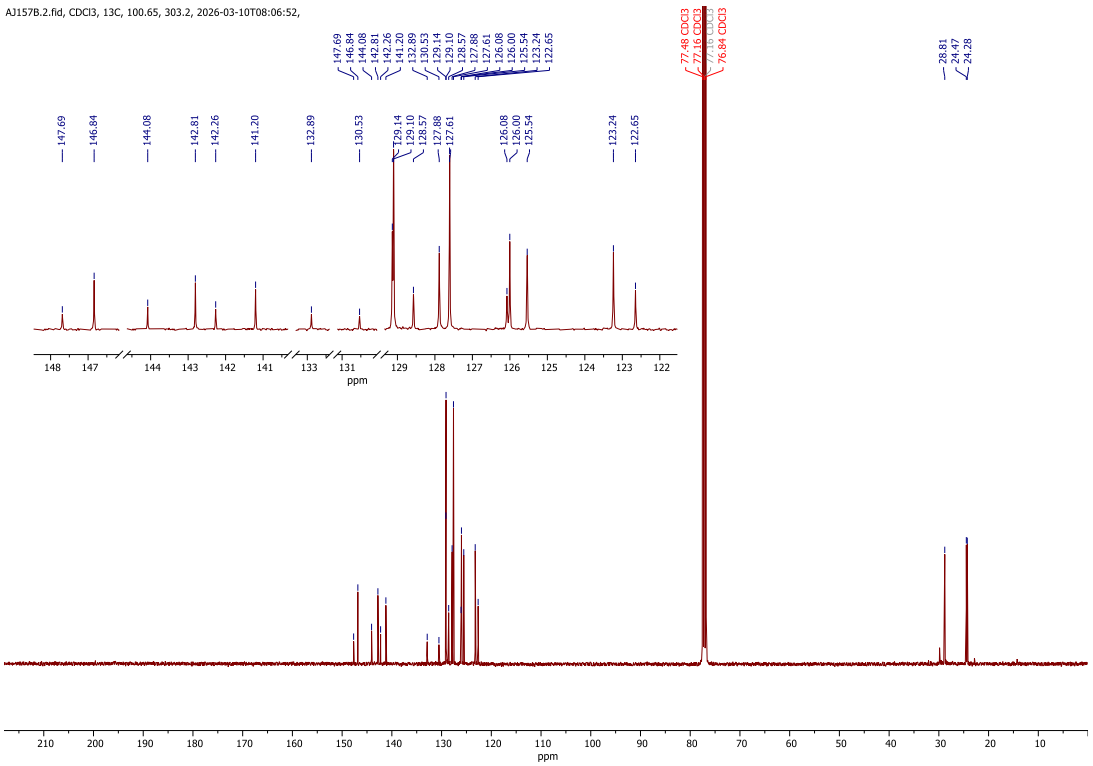


Fig. S36. {^{1}H}^{13}C NMR spectrum (126 MHz, $CDCl_3$) of 1-(3,5-diisopropyl-5'-phenyl-[1,1':3',1''-terphenyl]-4-yl)-4-phenyl-1*H*-1,2,3-triazole (**14**).

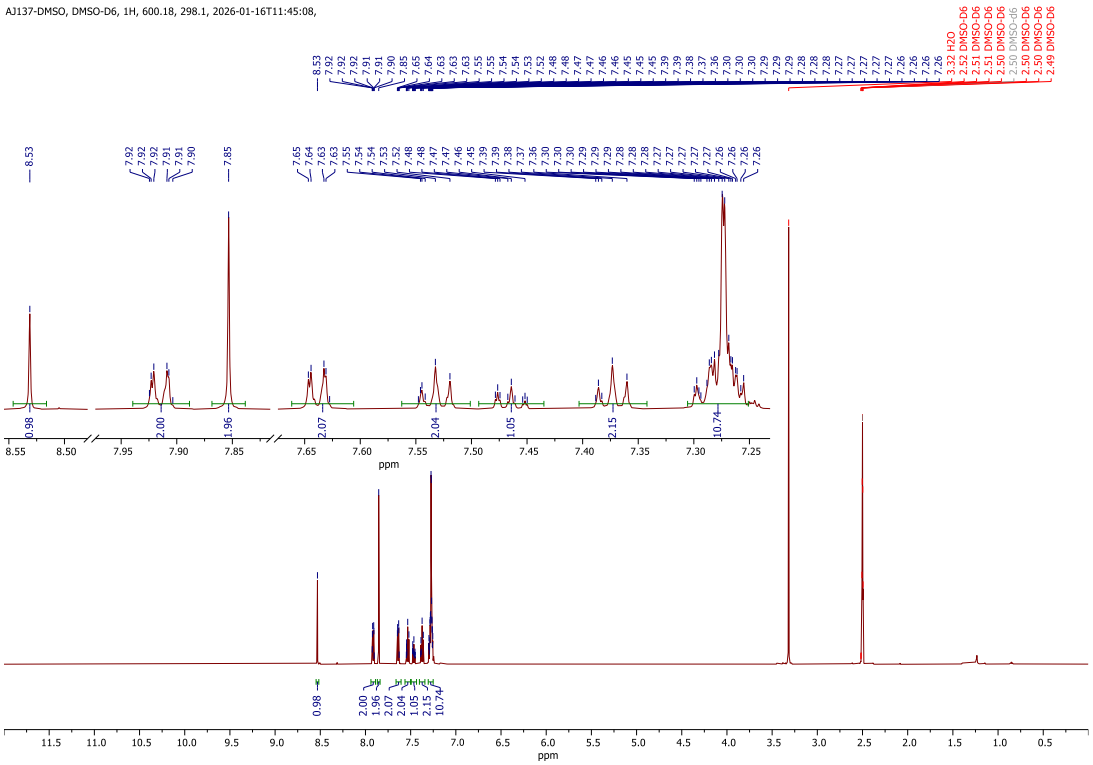


Fig. S37. ^{1}H NMR spectrum (600 MHz, DMSO-d_6) of 4-phenyl-1-(5'-phenyl-[1,1':3',1''-terphenyl]-4'-yl)-1*H*-1,2,3-triazole (**15**).

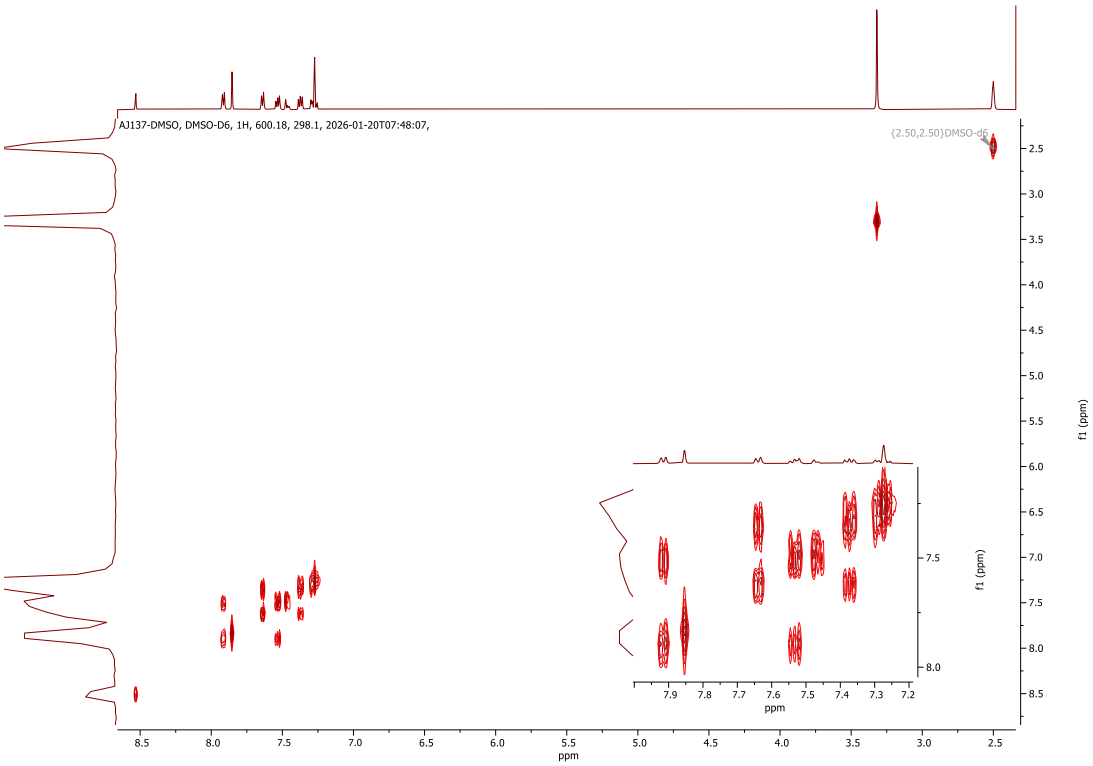


Fig. S38. ^{1}H-^{1}H COSY NMR spectrum (600 MHz, DMSO-d_6) of 4-phenyl-1-(5'-phenyl-[1,1':3',1''-terphenyl]-4'-yl)-1*H*-1,2,3-triazole (**15**).

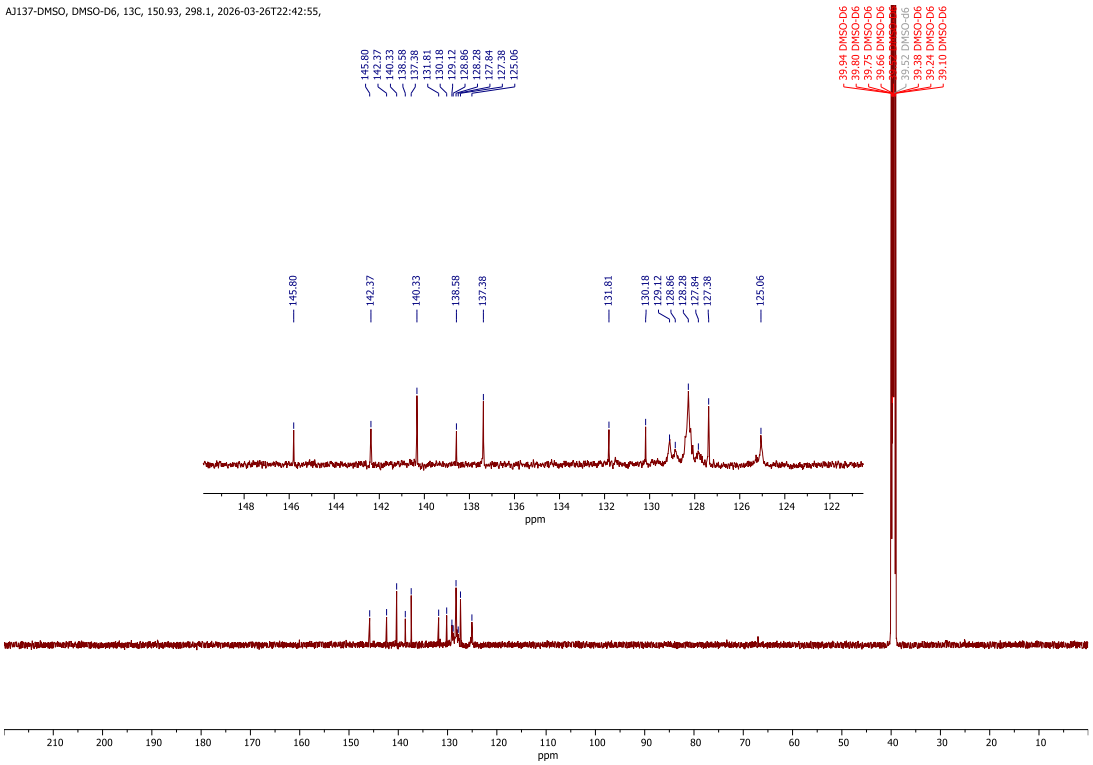


Fig. S39. {^{1}H}^{13}C NMR spectrum (151 MHz, DMSO-d_6) of 4-phenyl-1-(5'-phenyl-[1,1':3',1''-terphenyl]-4'-yl)-1*H*-1,2,3-triazole (**15**).

S3. HRMS spectra

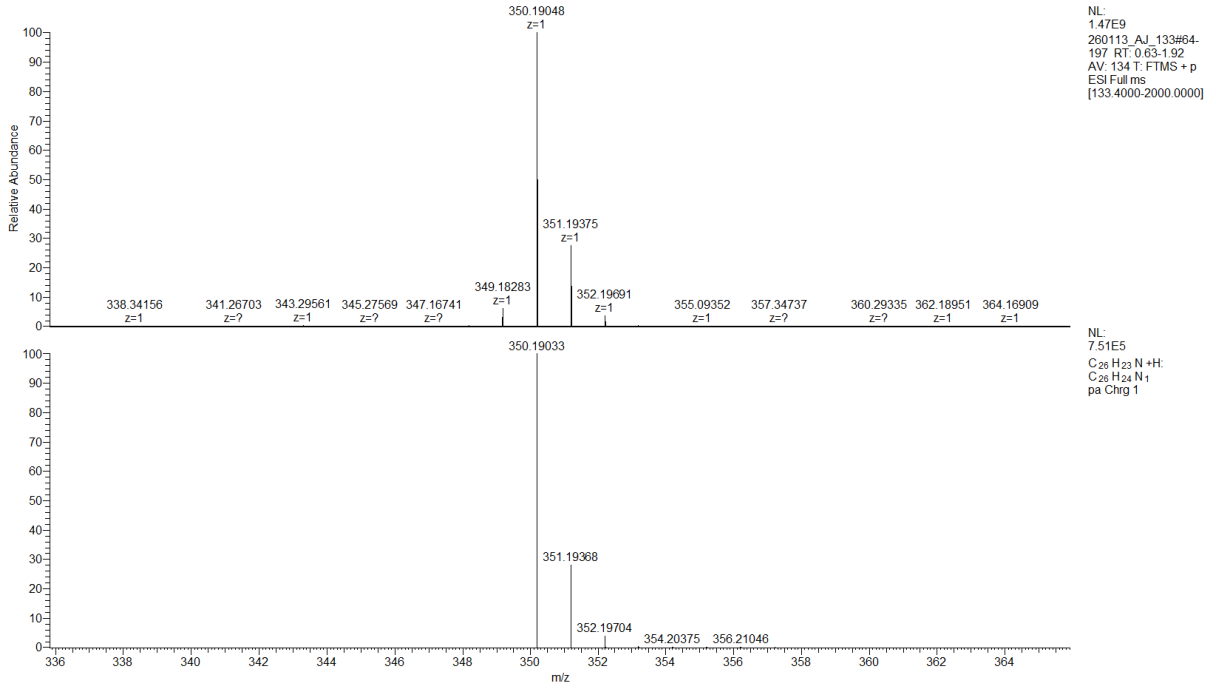


Fig. S40. ESI-HRMS (TOF) spectrum of 3,5-dimethyl-5'-phenyl-[1,1':3',1''-terphenyl]-4-amine (**20**).

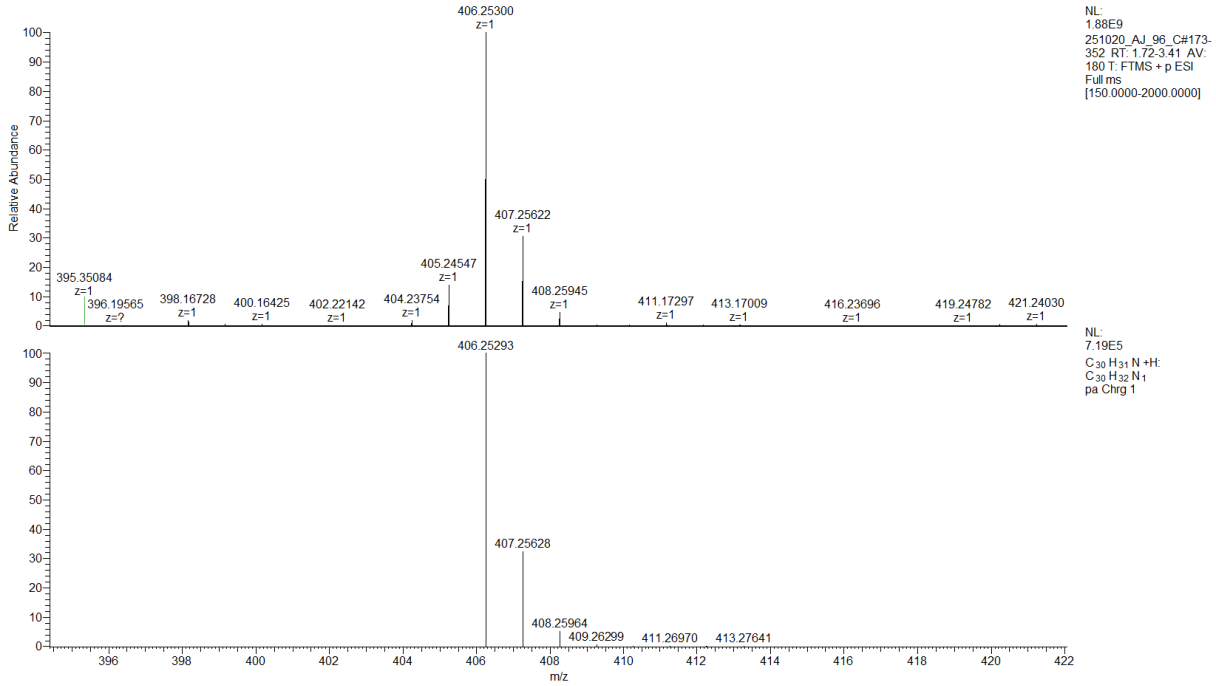


Fig. S41. ESI-HRMS (TOF) spectrum of 3,5-diisopropyl-5'-phenyl-[1,1':3',1''-terphenyl]-4-amine (**22**).

Single Mass Analysis
Tolerance = 3.0 PPM / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3
Monoisotopic Mass, Even Electron Ions
24 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-200 H: 0-200 N: 1-3

Mass	Calc. Mass	mDa	PPM	DBE	Formula	i-FIT	i-FIT Norm	Fit Conf %	C	H	N
636.2442	636.2440	0.2	0.3	34.5	C47 H30 N3	540.6	n/a	n/a	47	30	3

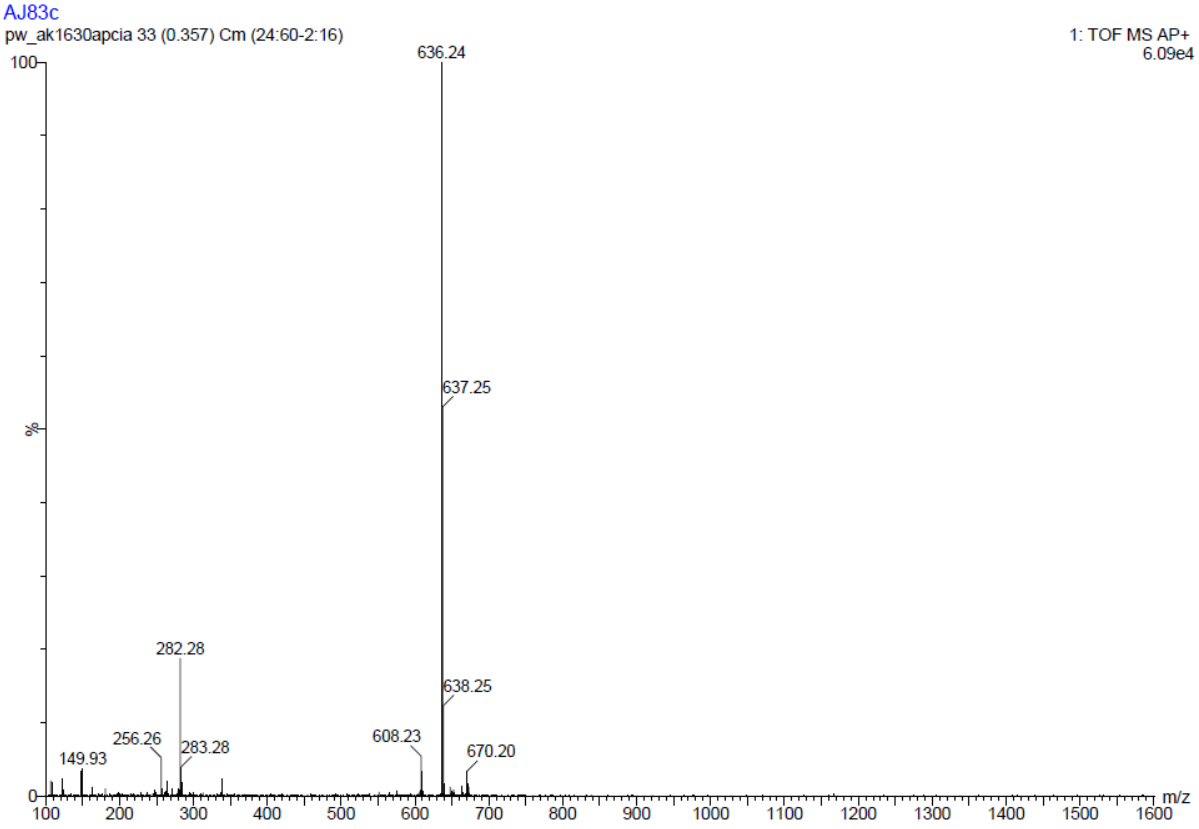


Fig. S42. APCI-HRMS (q-TOF) spectrum of 4-(4,7-dihydro-1*H*-tricyclopenta[*def*,*jkl*,*pqr*]triphenylen-2-yl)-1-(5'-phenyl-[1,1':3',1''-terphenyl]-4-yl)-1*H*-1,2,3-triazole (**3**).

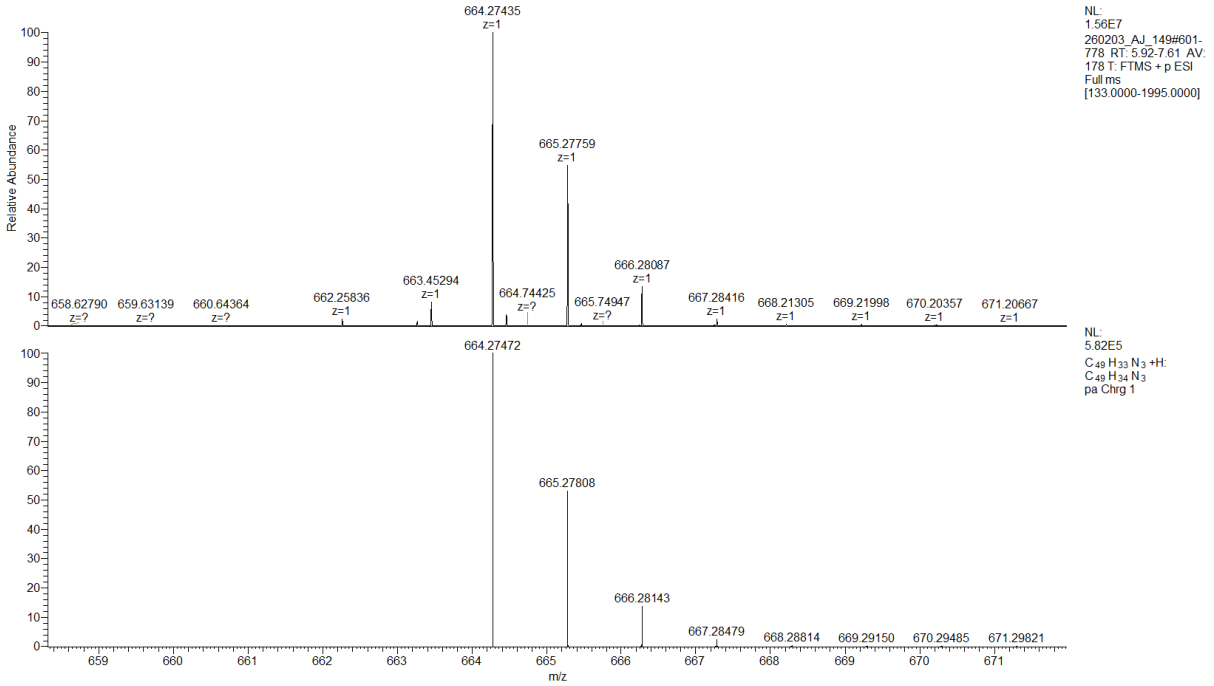


Fig. S43. ESI-HRMS (TOF) spectrum of 4-(4,7-dihydro-1*H*-tricyclopenta[*def*,*jkl*,*pqr*]triphenylen-2-yl)-1-(3,5-dimethyl-5'-phenyl-[1,1':3',1''-terphenyl]-4-yl)-1*H*-1,2,3-triazole (**4**).

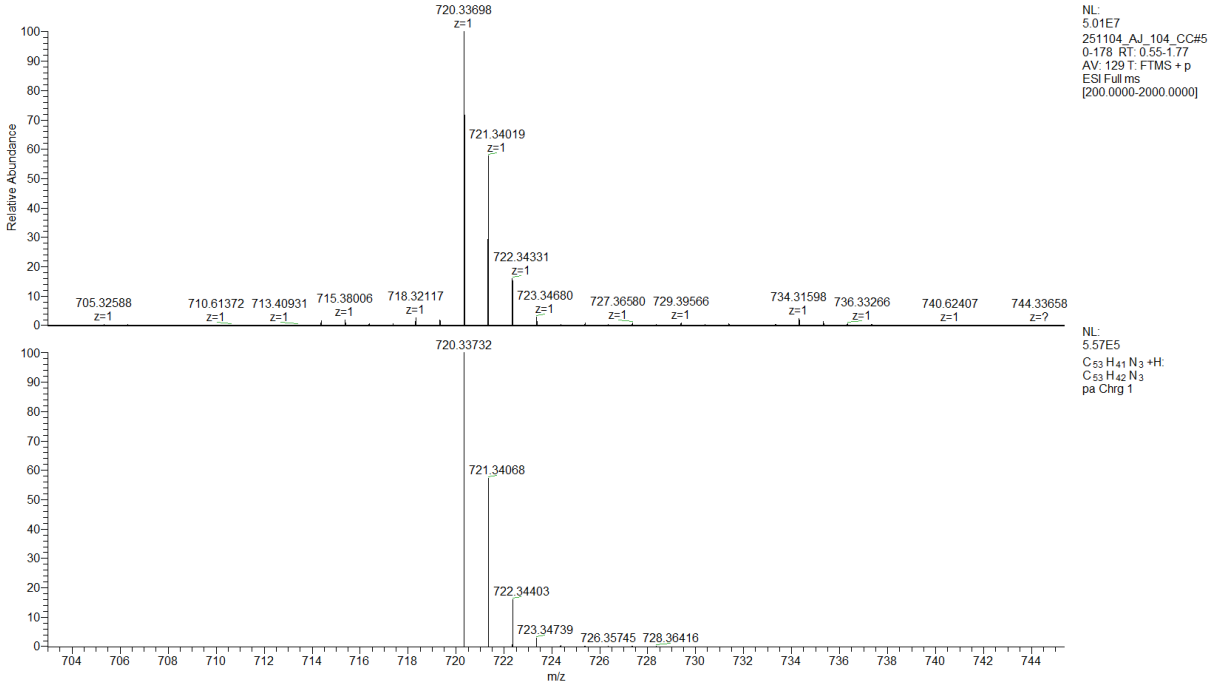


Fig. S44. ESI-HRMS (TOF) spectrum of 4-(4,7-dihydro-1*H*-tricyclopenta[*def*,*jkl*,*pqr*]triphenylen-2-yl)-1-(3,5-diisopropyl-5'-phenyl-[1,1':3',1''-terphenyl]-4-yl)-1*H*-1,2,3-triazole (**5**).

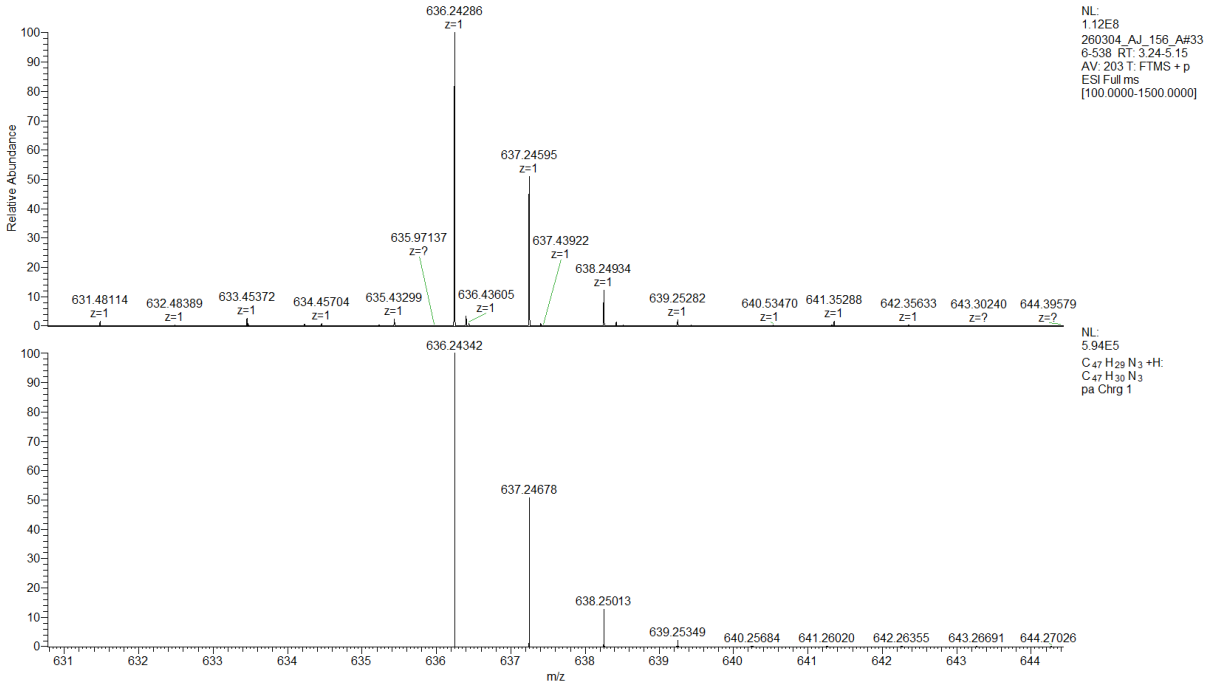


Fig. S45. ESI-HRMS (TOF) spectrum of 4-(4,7-dihydro-1*H*-tricyclopenta[*def*,*jkl*,*pqr*]triphenylen-2-yl)-1-(5'-phenyl-[1,1':3',1''-terphenyl]-4'-yl)-1*H*-1,2,3-triazole (**6**).

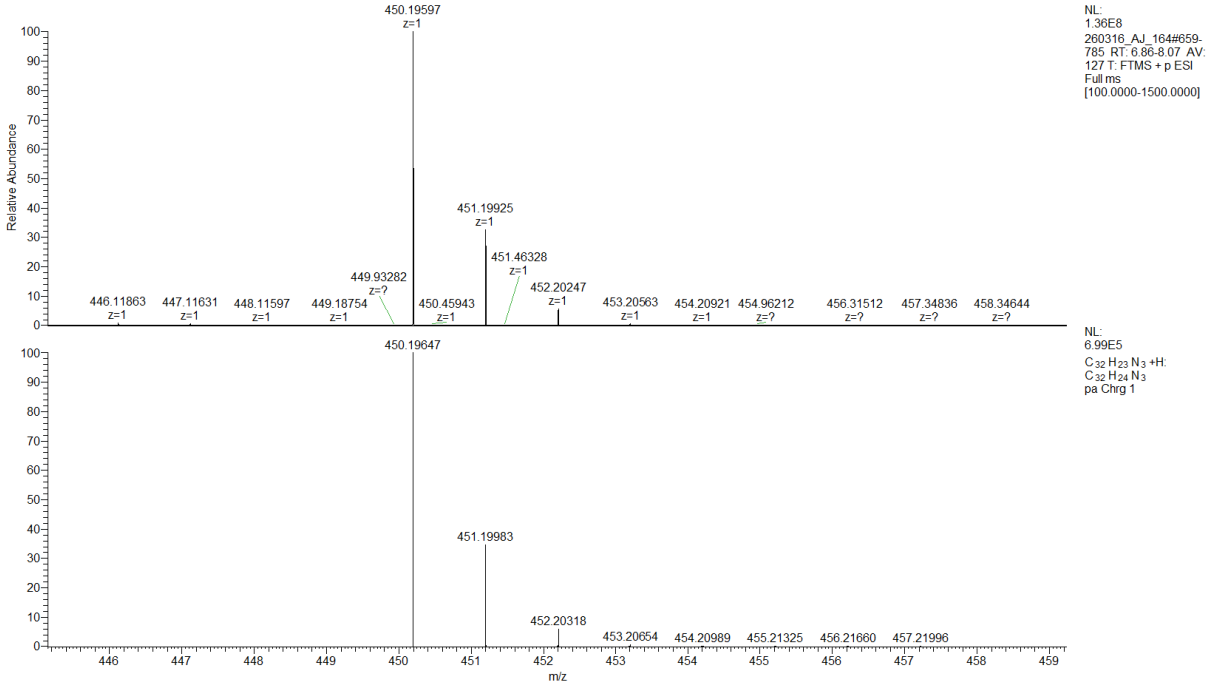


Fig. S46. ESI-HRMS (TOF) spectrum of 4-phenyl-1-(5'-phenyl-[1,1':3',1''-terphenyl]-4-yl)-1*H*-1,2,3-triazole (**12**).

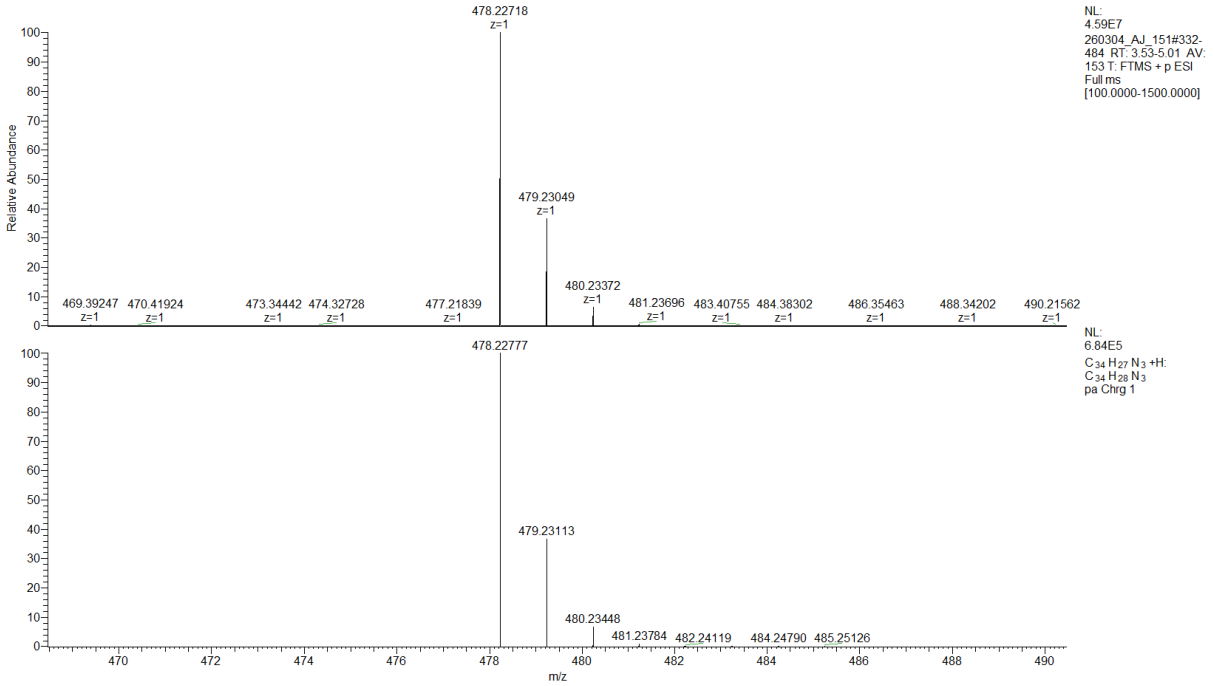


Fig. S47. ESI-HRMS (TOF) spectrum of 1-(3,5-dimethyl-5'-phenyl-[1,1':3',1''-terphenyl]-4-yl)-4-phenyl-1*H*-1,2,3-triazole (**13**).

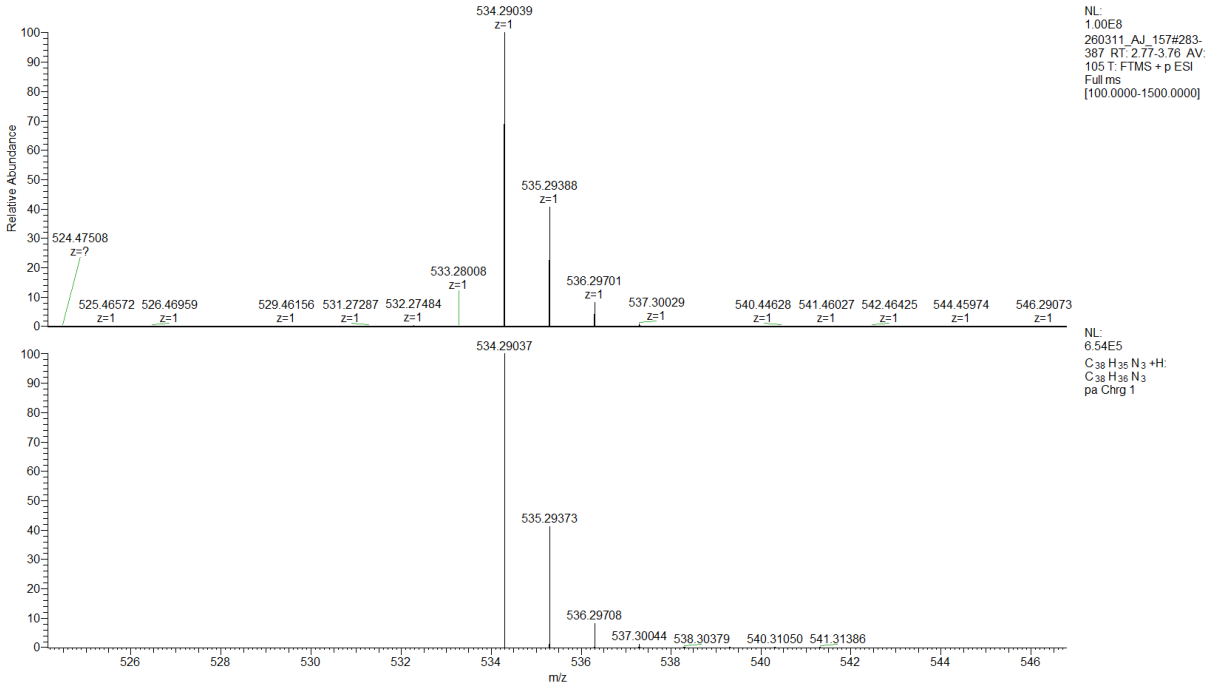


Fig. S48. ESI-HRMS (TOF) spectrum of 1-(3,5-diisopropyl-5'-phenyl-[1,1':3',1''-terphenyl]-4-yl)-4-phenyl-1*H*-1,2,3-triazole (**14**).

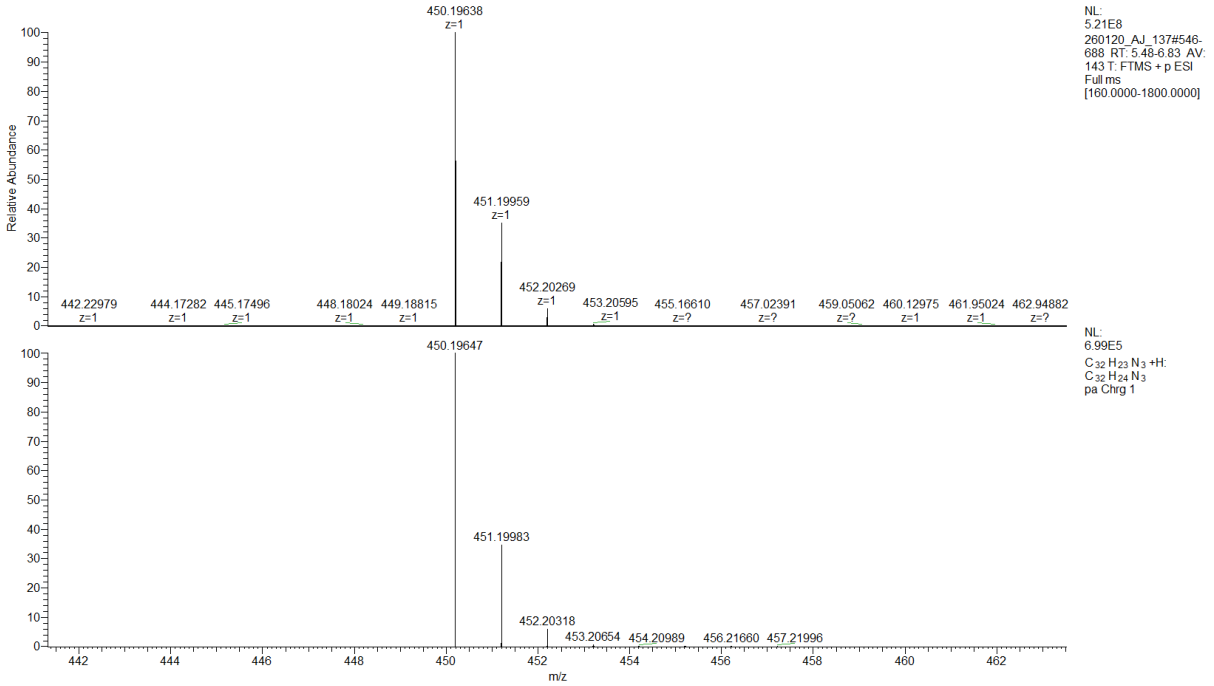


Fig. S49. ESI-HRMS (TOF) spectrum of 4-phenyl-1-(5''-phenyl-[1,1':3',1''-terphenyl]-4'-yl)-1*H*-1,2,3-triazole (**15**).

S4. Photophysical characterization

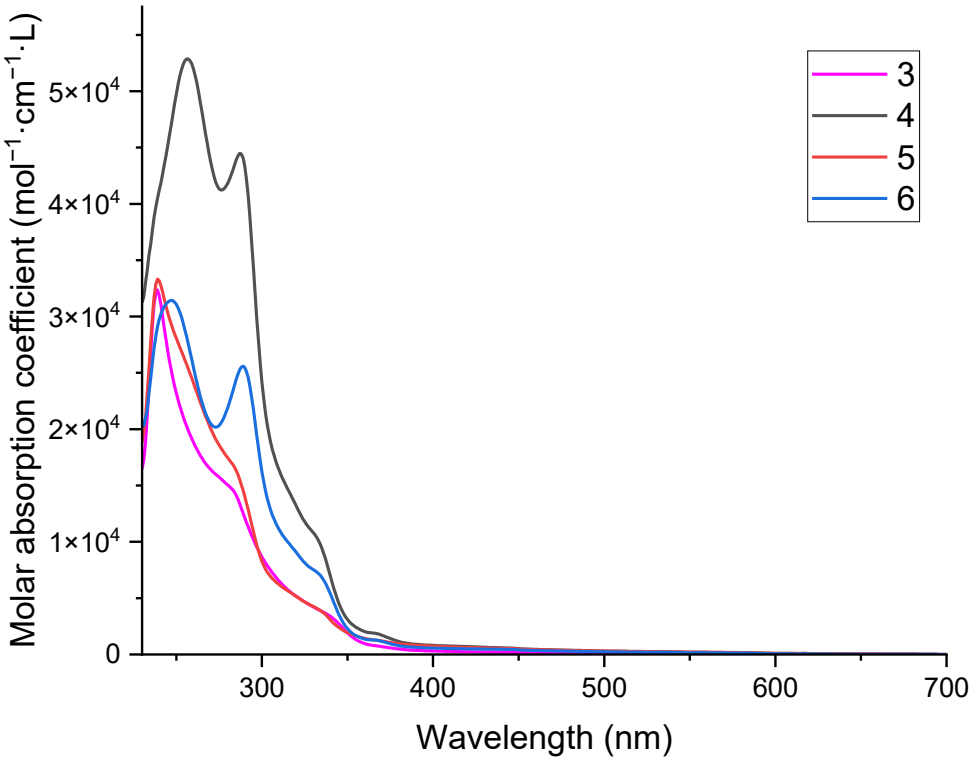


Fig. S50. UV-vis spectra of compounds **3-6** (THF, $C = 2 \cdot 10^{-5}$ M).

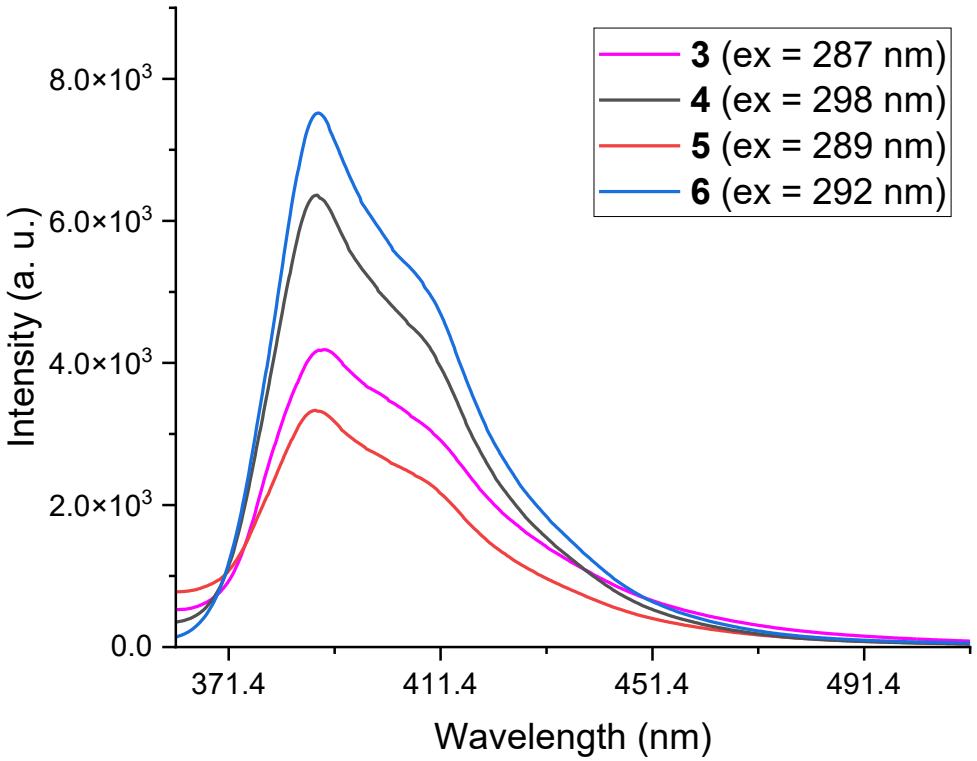


Fig. S51. Fluorescence spectra of compounds **3-6** (THF, $C = 2 \cdot 10^{-5}$ M).

S5. Potentiometric studies

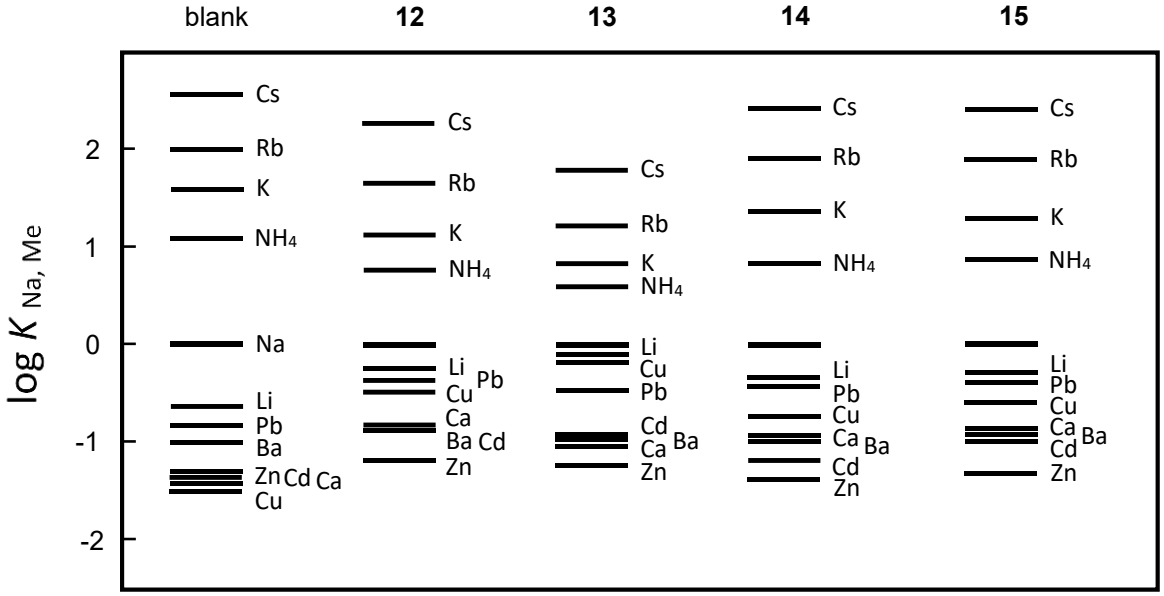


Fig. S52. Graphical presentation of the selectivity (values of log $K_{Na,\ Me}$) of PVC/o-NPOE membranes formulated with receptors **12-15** (10 mol% KTFPB) and without receptor (blank membrane); mean values were calculated for 3 electrode specimens.

Table S3. Values of selectivity coefficients (log $K_{Na,\ Me}$) of potentiometric sensors formulated with receptors **3-6** (10 mol% KTFPB) and without receptor (blank membrane) in PVC/o-NPOE membranes (mean values calculated for 3 electrode specimens).

	blank	**3**	**4**	**5**	**6**
log $K_{Na,\ Li}$	-0.70	-0.25	-0.30	-0.25	-0.70
log $K_{Na,\ NH4}$	1.10	0.75	0.70	0.45	0.10
log $K_{Na,\ K}$	1.60	0.95	1.15	0.60	0.65
log $K_{Na,\ Rb}$	2.00	1.30	1.75	1.05	0.75
log $K_{Na,\ Cs}$	2.55	2.00	2.25	1.60	0.80
log $K_{Na,\ Ca}$	-1.40	-1.20	-0.85	-0.85	-1.20
log $K_{Na,\ Ba}$	-1.00	-1.00	-0.90	-0.15	-0.10
log $K_{Na,\ Cu}$	-1.50	-0.90	-0.75	-0.70	-1.45
log $K_{Na,\ Pb}$	-0.80	-0.55	-0.40	0.40	0.60
log $K_{Na,\ Zn}$	-1.30	-1.20	-1.40	-0.95	-1.30
log $K_{Na,\ Cd}$	-1.35	-1.10	-1.10	-0.90	-1.60

Table S4. Values of selectivity coefficients (log $K_{Na, Me}$) of potentiometric sensors formulated with receptors **12-15** (10 mol% KTFPB) and without receptor (blank membrane) in PVC/o-NPOE membranes (mean values calculated for 3 electrode specimens).

	blank	**12**	**13**	**14**	**15**
log $K_{Na, Li}$	-0.70	-0.25	-0.15	-0.35	-0.30
log $K_{Na, NH4}$	1.10	0.75	0.55	0.80	0.85
log $K_{Na, K}$	1.60	1.10	0.80	1.35	1.25
log $K_{Na, Rb}$	2.00	1.65	1.20	1.90	1.85
log $K_{Na, Cs}$	2.55	2.25	1.75	2.40	2.40
log $K_{Na, Ca}$	-1.40	-0.85	-1.05	-0.95	-0.90
log $K_{Na, Ba}$	-1.00	-0.90	-1.00	-1.00	-0.95
log $K_{Na, Cu}$	-1.50	-0.50	-0.20	-0.80	-0.60
log $K_{Na, Pb}$	-0.80	-0.35	-0.50	-0.45	-0.40
log $K_{Na, Zn}$	-1.30	-1.20	-1.25	-1.40	-1.30
log $K_{Na, Cd}$	-1.35	-0.90	-0.95	-1.20	-1.00

S6. Spectrofluorimetric titrations

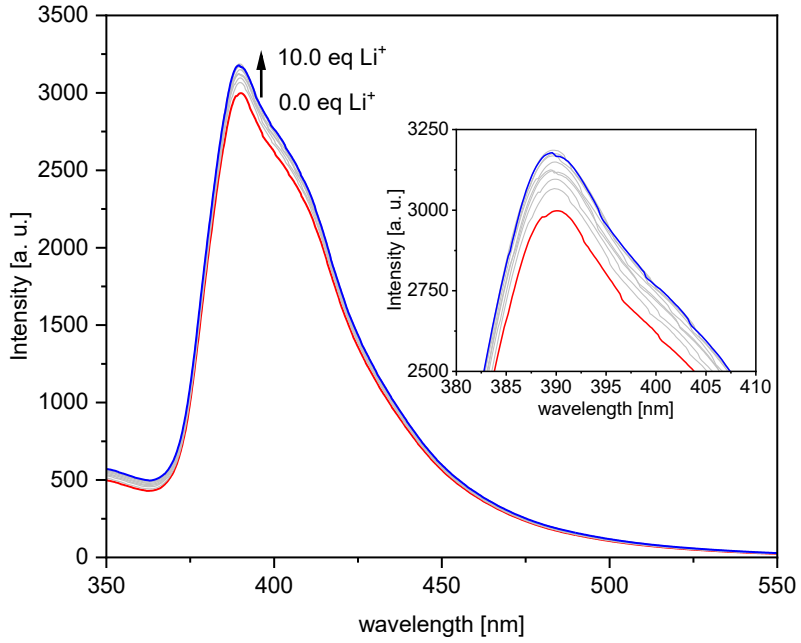


Fig. S53. Emission spectra of receptor **3** in the presence of various amounts (equivalents = eq) of lithium cations (λ_{ex} = 287 nm).

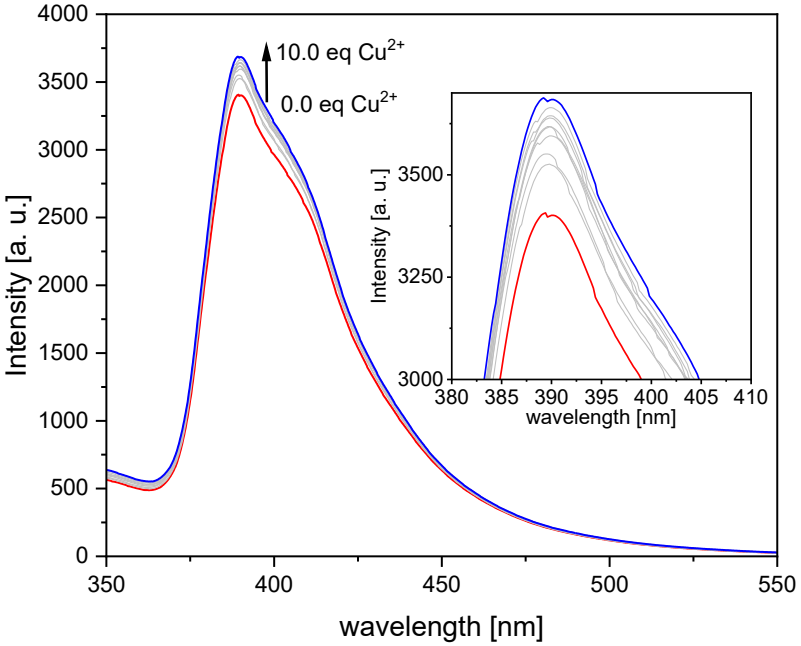


Fig. S54. Emission spectra of receptor **3** in the presence of various amounts (equivalents = eq) of copper(II) cations (λ_{ex} = 287 nm).

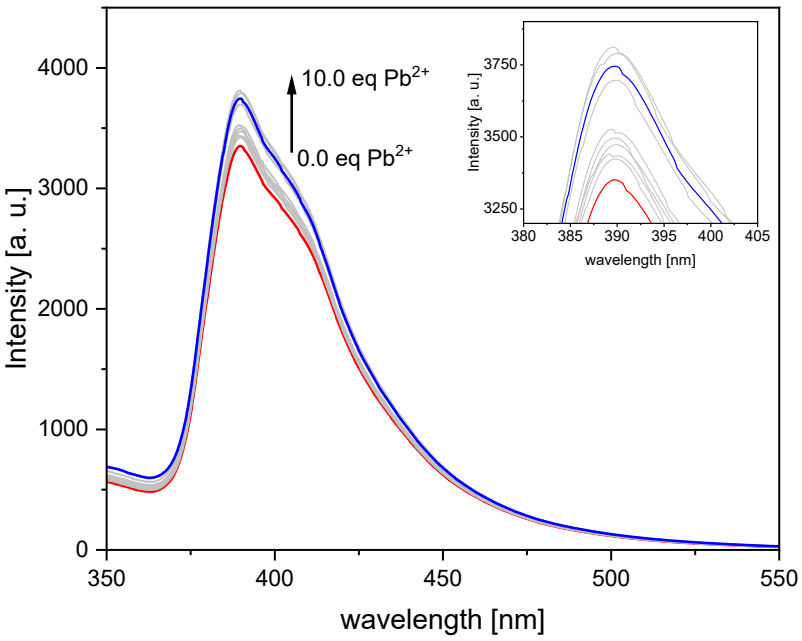


Fig. S55. Emission spectra of receptor **3** in the presence of various amounts (equivalents = eq) of lead(II) cations (λ_{ex} = 287 nm).

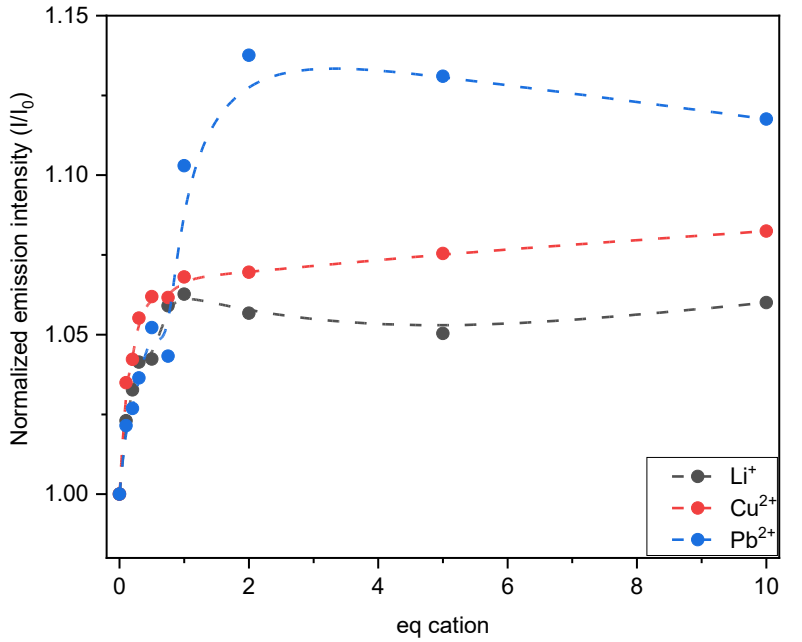


Fig. S56. Fluorescence spectra titration curves for receptor **3** with Li^+, Cu^{2+} and Pb^{2+} cations (THF:water = 1:1 v/v, *C* = 0.02 mM).

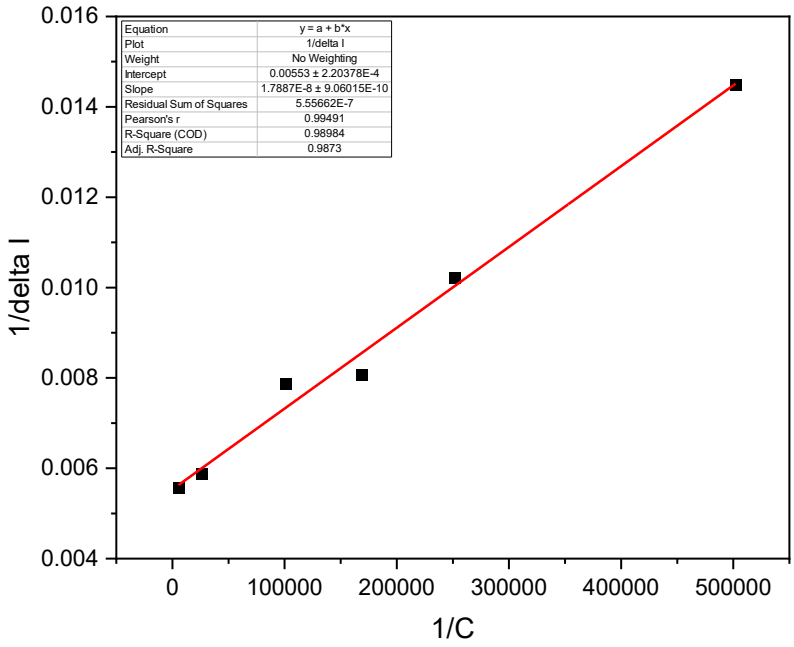


Fig. S57. Benesi-Hildebrand plot regarding the interactions between **3** and **Li^{+}**. The data for the linear plot are also presented.

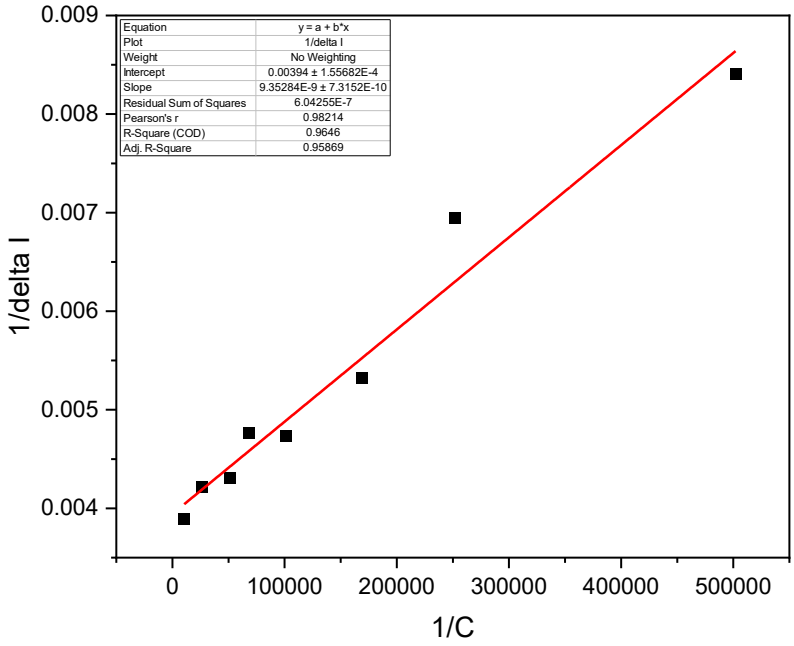


Fig. S58. Benesi-Hildebrand plot regarding the interactions between **3** and **Cu^{2+}**. The data for the linear plot are also presented.

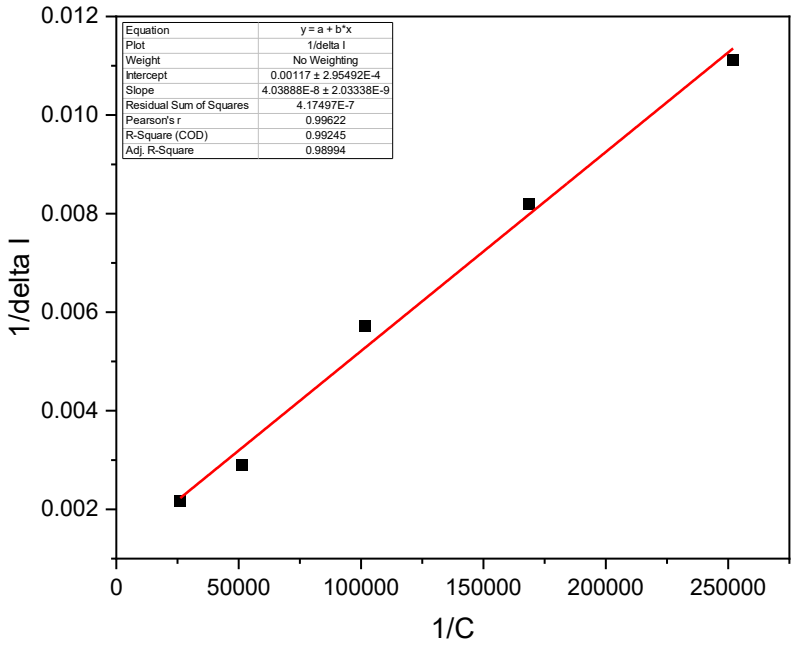


Fig. S59. Benesi-Hildebrand plot regarding the interactions between **3** and Pb^{2+}. The data for the linear plot are also presented.

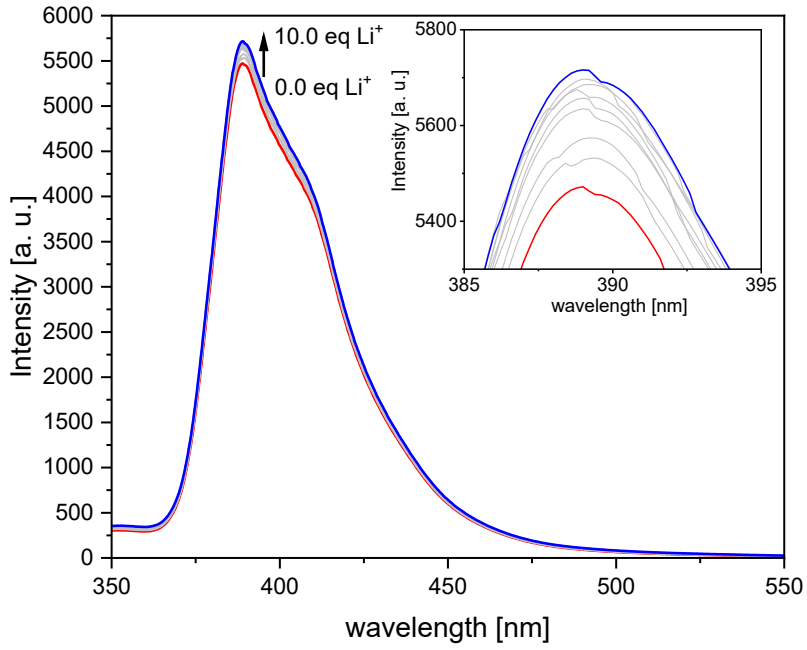


Fig. S60. Emission spectra of receptor **4** in the presence of various amounts (equivalents = eq) of lithium cations (λ_{ex} = 298 nm).

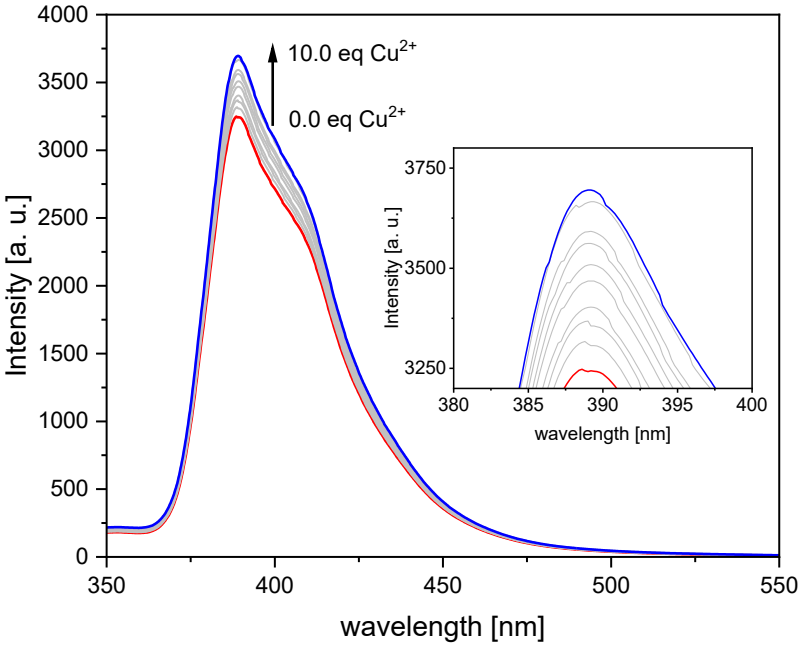


Fig. S61. Emission spectra of receptor **4** in the presence of various amounts (equivalents = eq) of copper(II) cations (λ_{ex} = 298 nm).

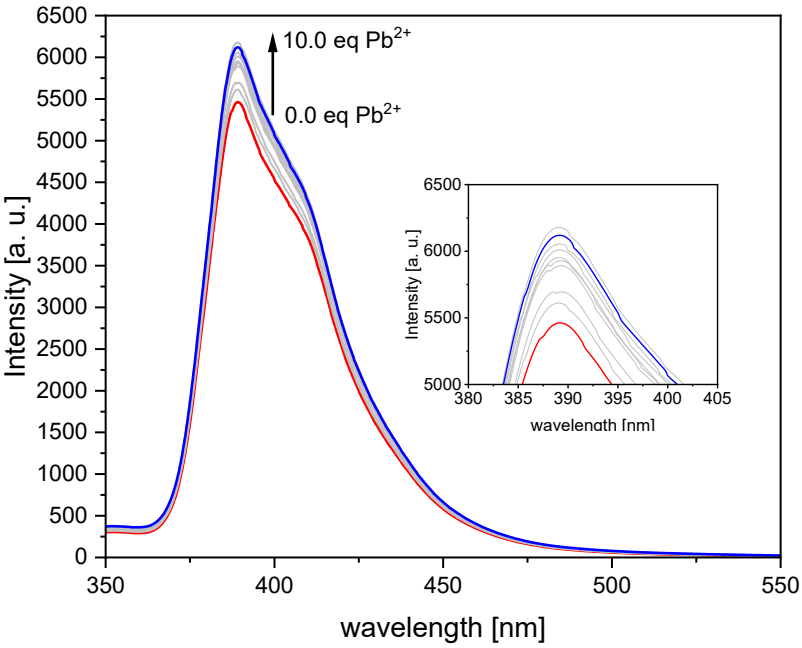


Fig. S62. Emission spectra of receptor **4** in the presence of various amounts (equivalents = eq) of lead(II) cations (λ_{ex} = 298 nm).

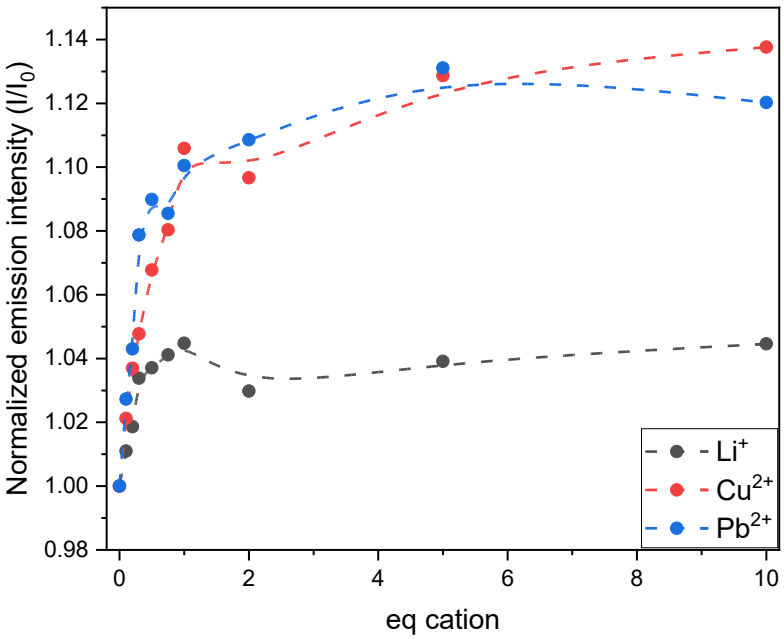


Fig. S63. Fluorescence spectra titration curves for receptor **4** with Li^+, Cu^{2+} and Pb^{2+} cations (THF:water = 1:1 v/v, *C* = 0.02 mM).

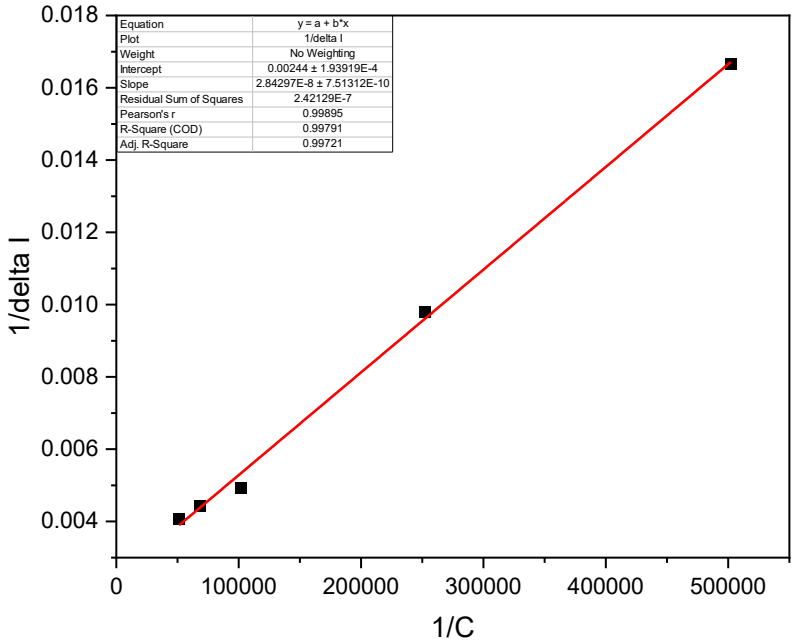


Fig. S64. Benesi-Hildebrand plot regarding the interactions between **4** and **Li^+**. The data for the linear plot are also presented.

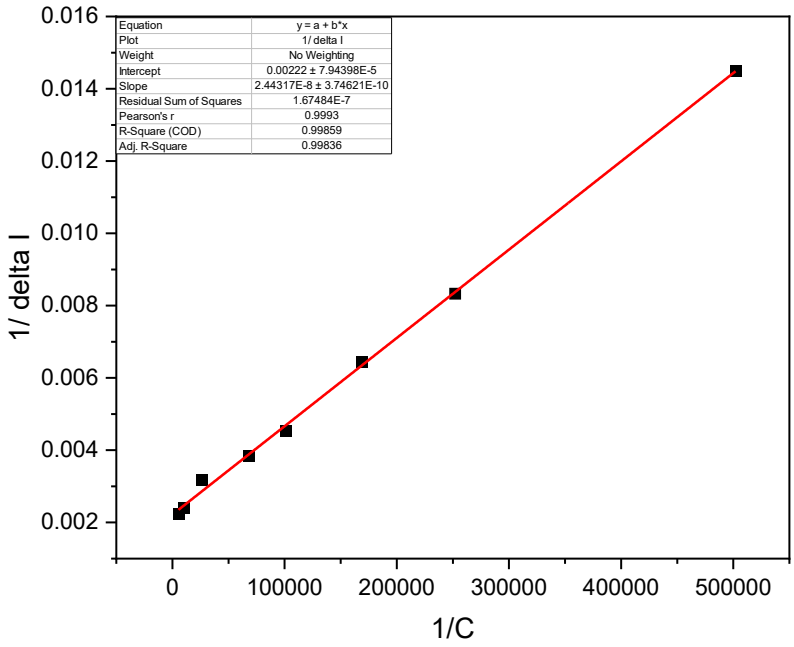


Fig. S65. Benesi-Hildebrand plot regarding the interactions between **4** and **Cu^{2+}**. The data for the linear plot are also presented.

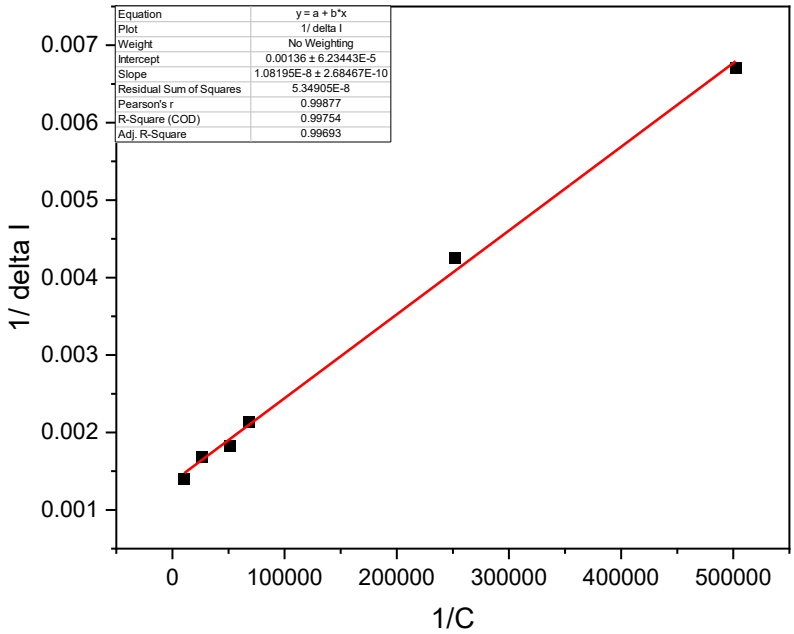


Fig. S66. Benesi-Hildebrand plot regarding the interactions between **4** and **Pb^{2+}.** The data for the linear plot are also presented.

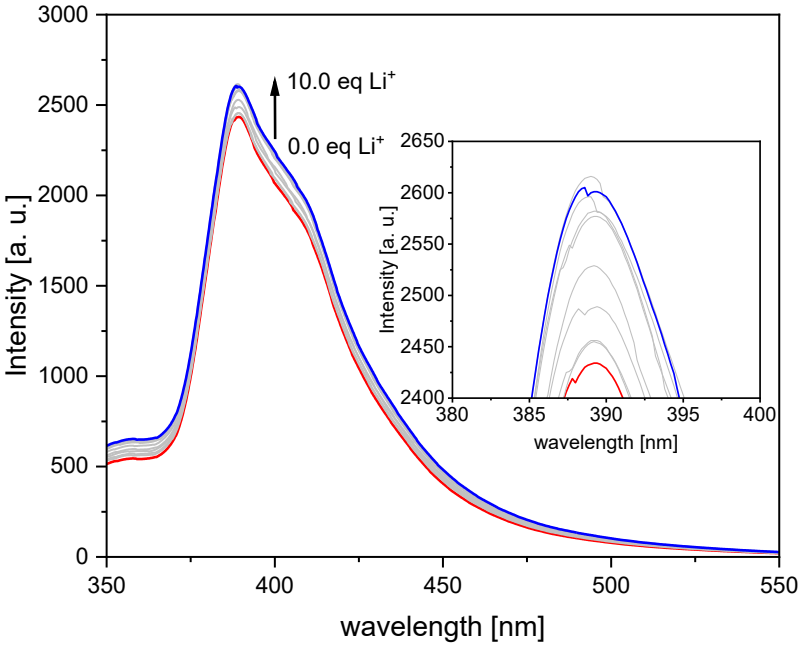


Fig. S67. Emission spectra of receptor **5** in the presence of various amounts (equivalents = eq) of lithium cations (λ_{ex} = 289 nm).

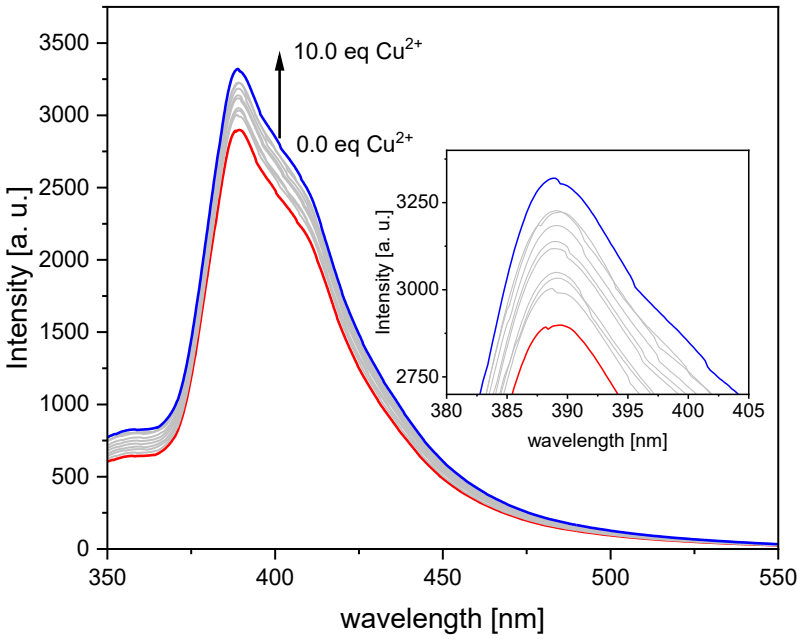


Fig. S68. Emission spectra of receptor **5** in the presence of various amounts (equivalents = eq) of copper(II) cations (λ_{ex} = 289 nm).

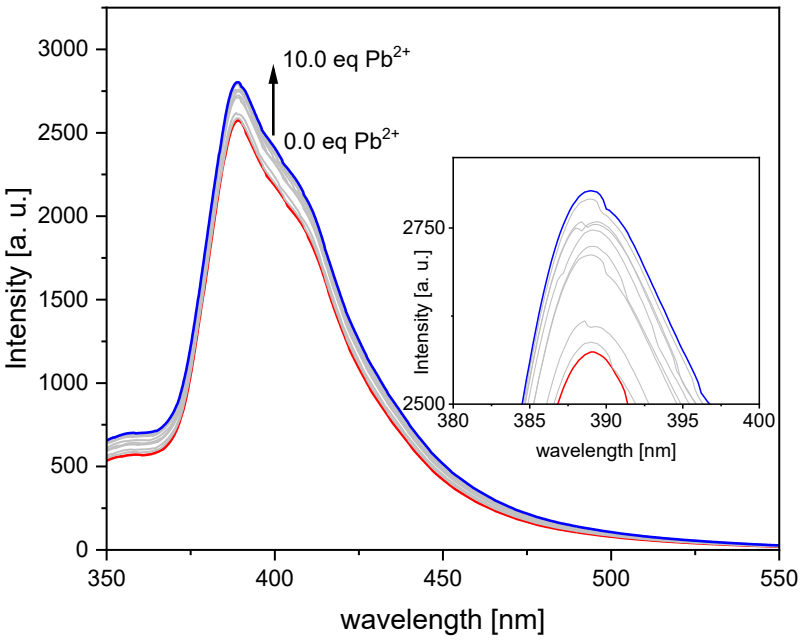


Fig. S69. Emission spectra of receptor **5** in the presence of various amounts (equivalents = eq) of lead(II) cations (λ_{ex} = 289 nm).

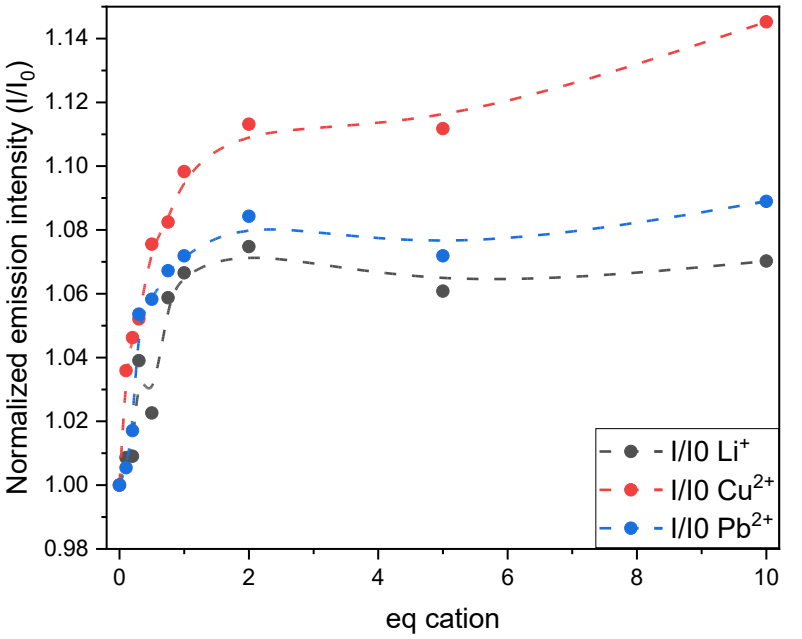


Fig. S70. Fluorescence spectra titration curves for receptor **5** with Li^+, Cu^{2+} and Pb^{2+} cations (THF:water = 1:1 v/v, *C* = 0.02 mM).

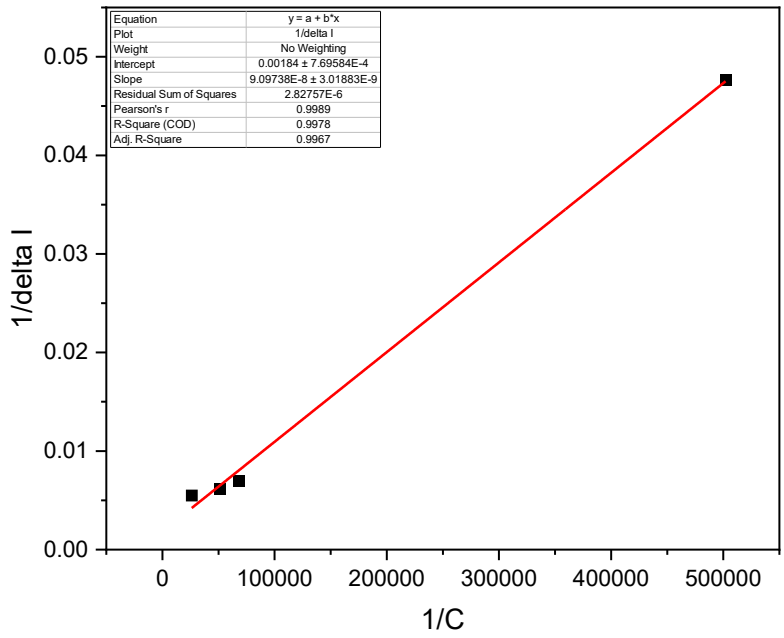


Fig. S71. Benesi-Hildebrand plot regarding the interactions between **5** and **Li^{+}**. The data for the linear plot are also presented.

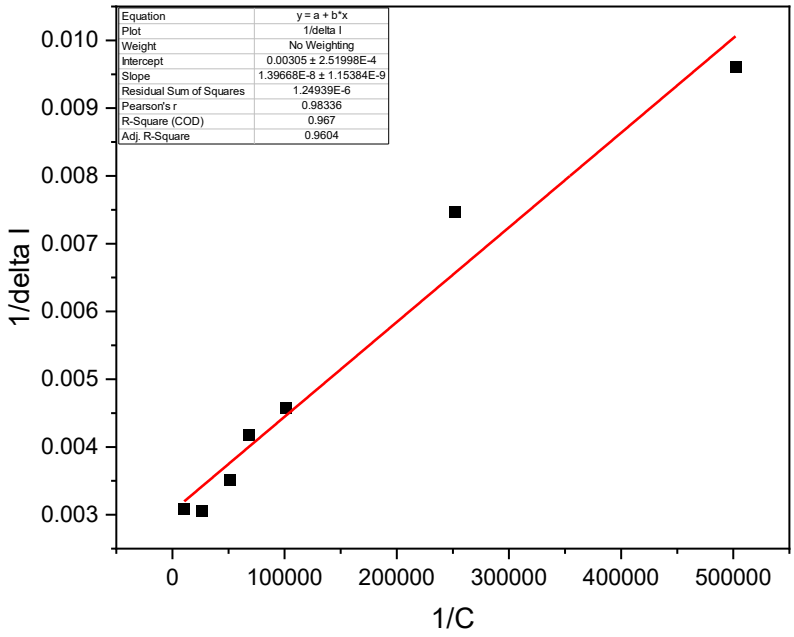


Fig. S72. Benesi-Hildebrand plot regarding the interactions between **5** and **Cu^{2+}**. The data for the linear plot are also presented.

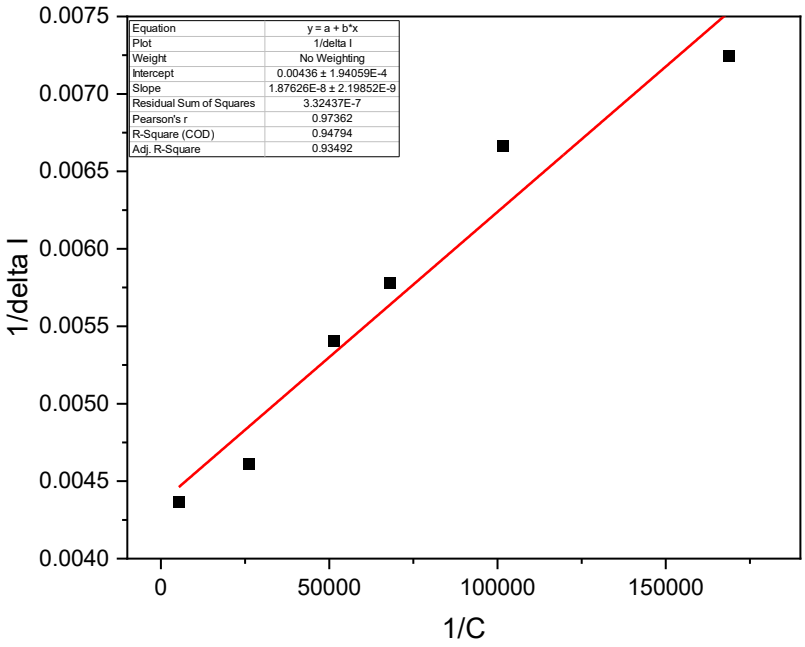


Fig. S73. Benesi-Hildebrand plot regarding the interactions between **5** and **Pb^{2+}**. The data for the linear plot are also presented.

Table S5. Summary of association constants (*K*) from Benesi-Hildebrand plots regarding the interactions between receptors **3**, **4**, **5** and **Li^{+}**, **Cu^{2+}** and **Pb^{2+}** cations.

Cation	Receptor 3	Receptor 4	Receptor 5
Li^{+}	$3.09 \cdot 10^5$	$0.86 \cdot 10^5$	$0.20 \cdot 10^5$
Cu^{2+}	$4.21 \cdot 10^5$	$0.91 \cdot 10^5$	$2.51 \cdot 10^5$
Pb^{2+}	$0.28 \cdot 10^5$	$1.26 \cdot 10^5$	$2.32 \cdot 10^5$

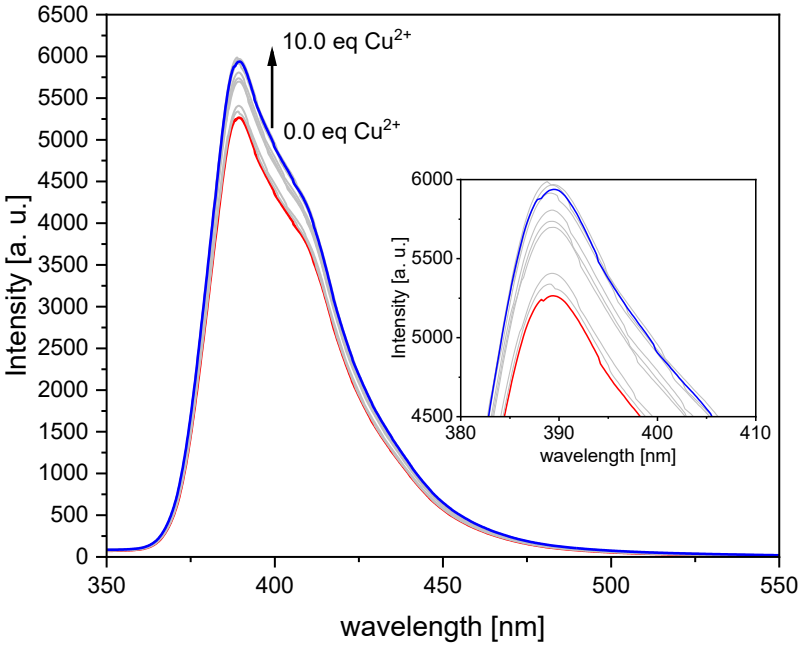


Fig. S74. Emission spectra of receptor **6** in the presence of various amounts (equivalents = eq) of copper(II) cations (λ_{ex} = 292 nm).

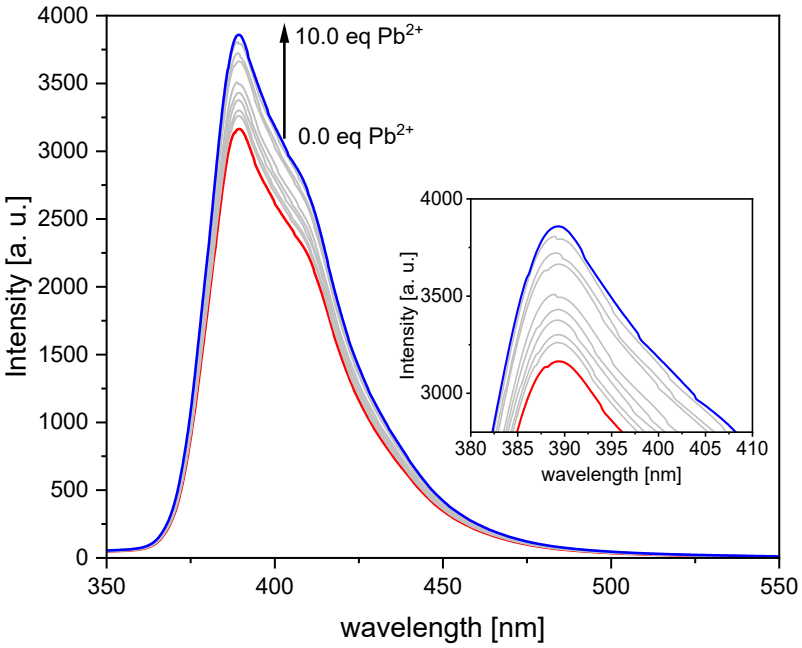


Fig. S75. Emission spectra of receptor **6** in the presence of various amounts (equivalents = eq) of lead(II) cations (λ_{ex} = 292 nm).

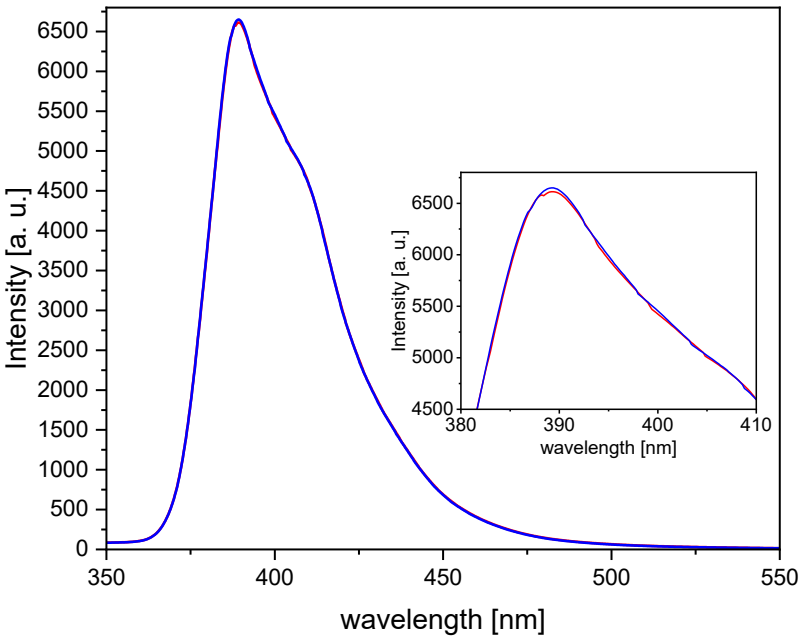


Fig. S76. Emission spectra of receptor **6** in the presence of 0 eq (red spectrum) or 10 eq (blue spectrum) of lithium cations (λ_{ex} = 292 nm).

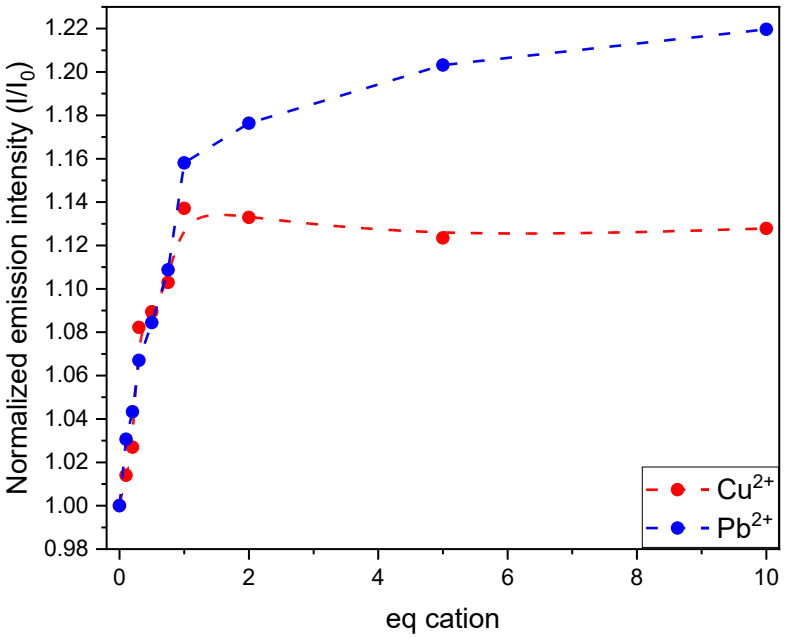


Fig. S77. Fluorescence spectra titration curves for receptor **6** with Cu^{2+} and Pb^{2+} cations (THF:water = 1:1 v/v, *C* = 0.02 mM).

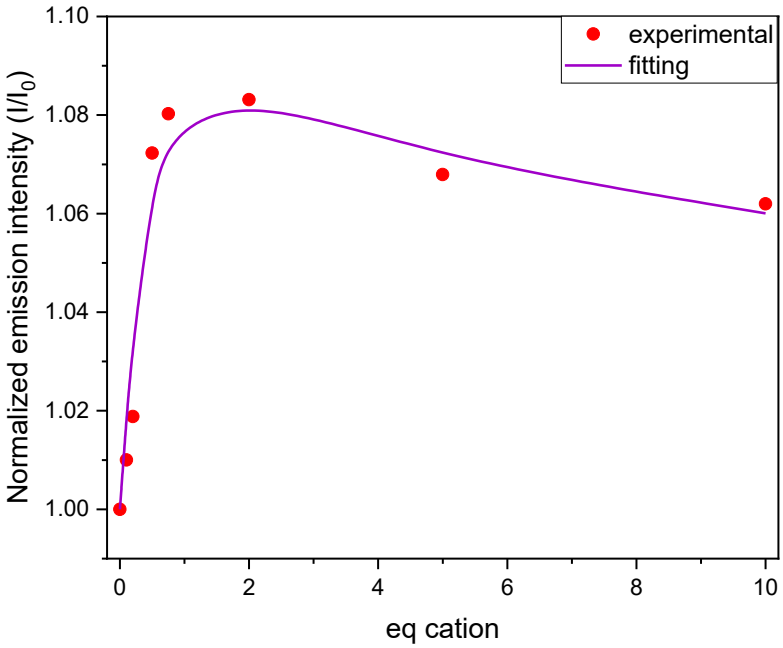


Fig. S78. Titration curve and global fitting (Bindfit) regarding interactions between **6** and copper(II) cations in THF:water = 1:1 v/v, C = 0.02 mM (K = (7.67±2.02)·10^4 M^{-1}, model: 2:1 non-cooperative, covariance = 0.04752755).

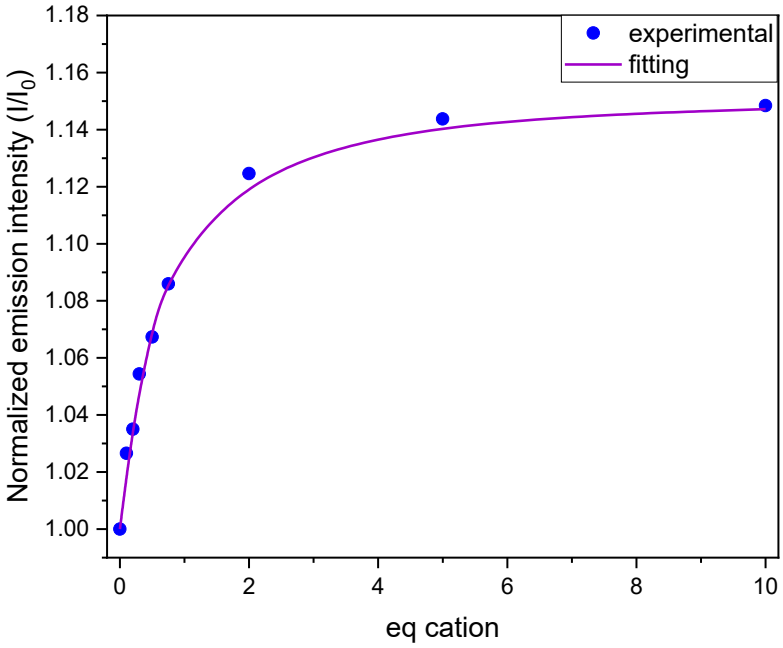


Fig. S79. Titration curve and global fitting (Bindfit) regarding interactions between **6** and lead(II) cations in THF:water = 1:1 v/v, C = 0.02 mM (K = (8.66±1.33)·10^4 M^{-1}, model: 2:1 non-cooperative, covariance = 0.005432837).

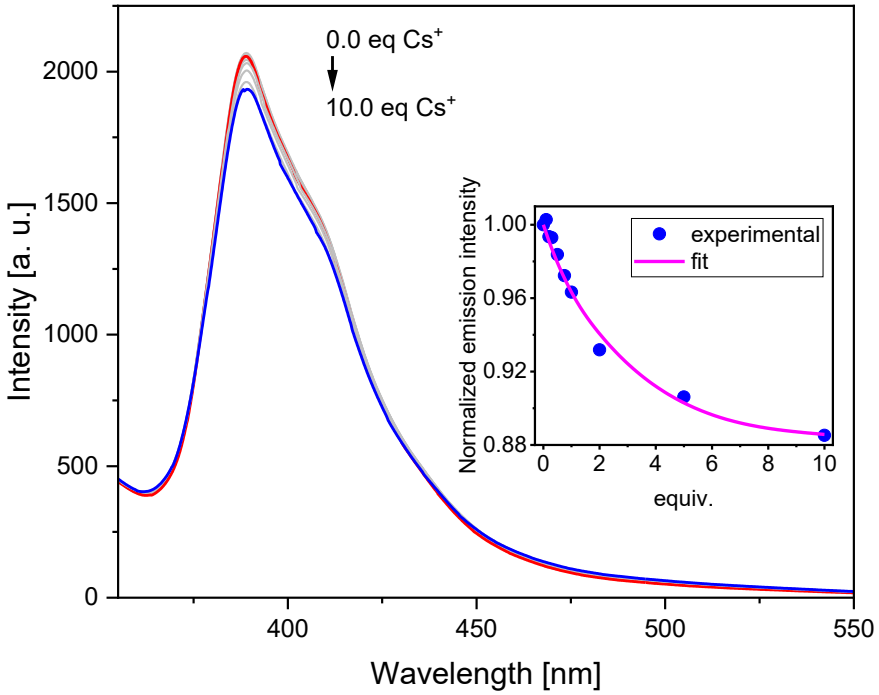


Fig. S80. Emission spectra of receptor **6** in the presence of various amounts (equivalents = eq) of caesium cations (λ_{ex} = 292 nm; THF:water = 1:1 v/v, C = 0.02 mM). Inset: titration curve and global fitting with Bindfit (K = (6.2±0.4)·10^3 M^{-1}, model: 2:1 non-cooperative, covariance = 0.011584289).

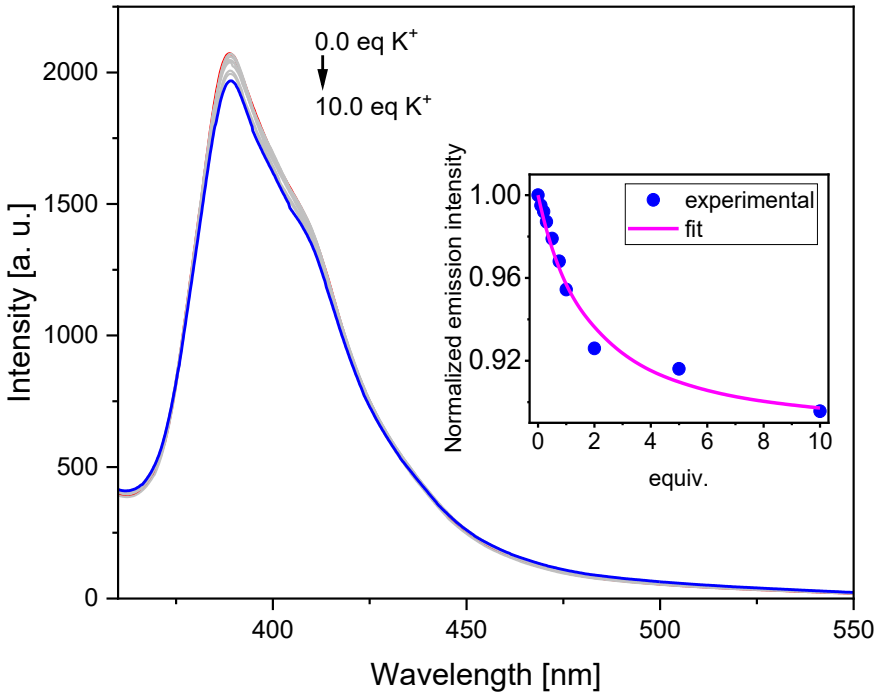


Fig. S81. Emission spectra of receptor **6** in the presence of various amounts (equivalents = eq) of potassium cations (λ_{ex} = 292 nm; THF:water = 1:1 v/v, C = 0.02 mM). Inset: titration curve and global fitting with Bindfit (K = (26.0±4.4)·10^3 M^{-1}, model: 2:1 statistical, covariance = 0.017307740).

S7. DFT computations

Density functional theory (DFT) and time-dependent DFT (TD-DFT) computations were performed with B3LYP functional[10] and 6-311G(d,p) basis set[11] using Gaussian[12], GaussView[13] and Avogadro[14,15] software.

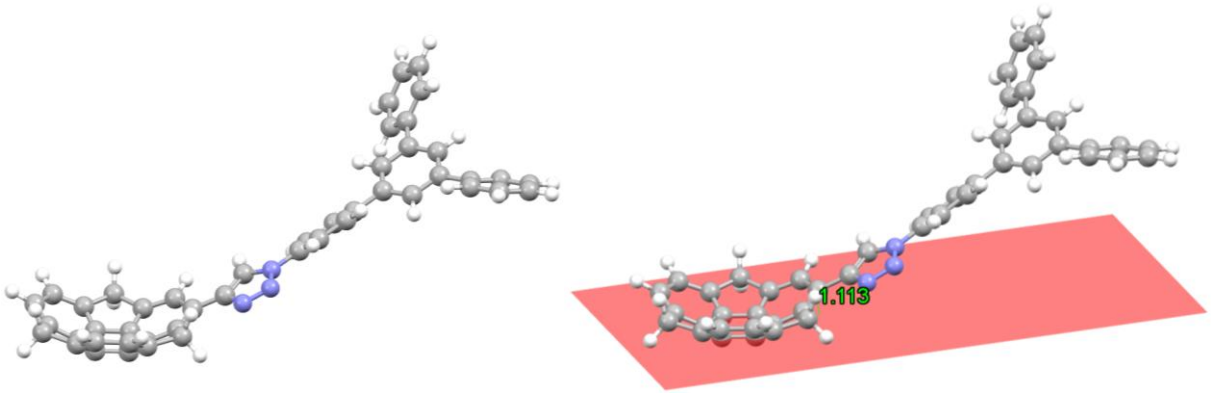


Fig. S82. DFT optimized (B3LYP/6-311g(d,p)) structure of compound **3**. Right image shows the method of estimating the bowl depth.

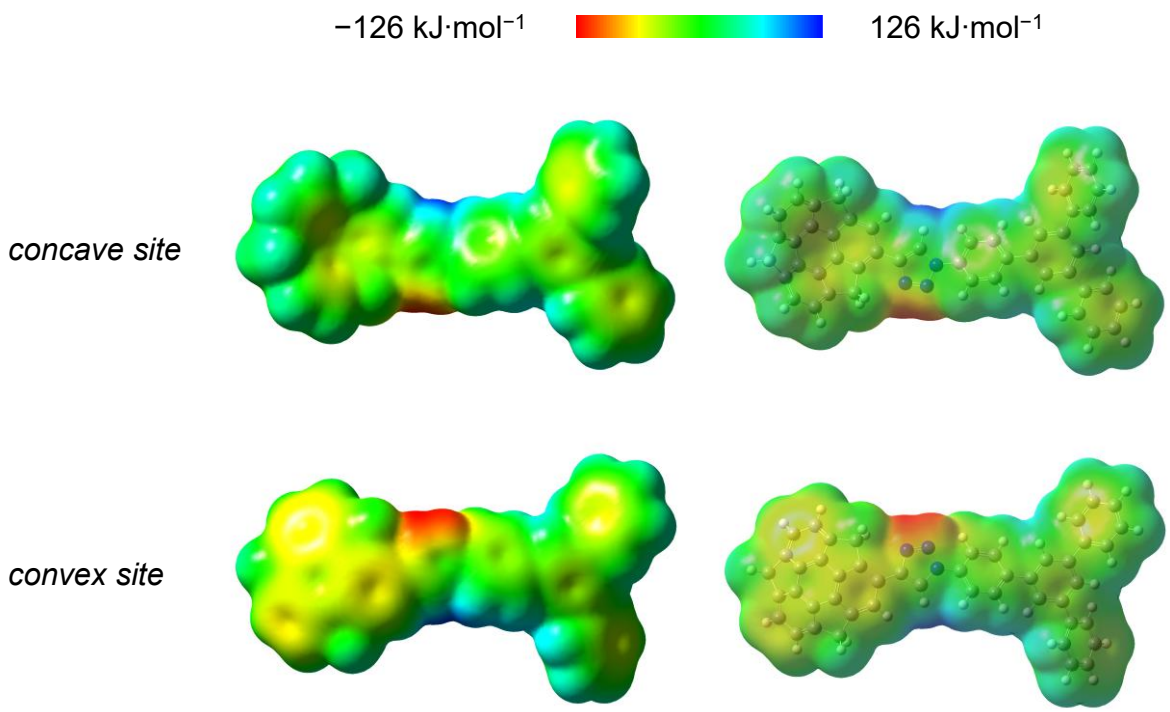


Fig. S83. DFT optimized (B3LYP/6-311g(d,p)) ESP plot of compound **3**.

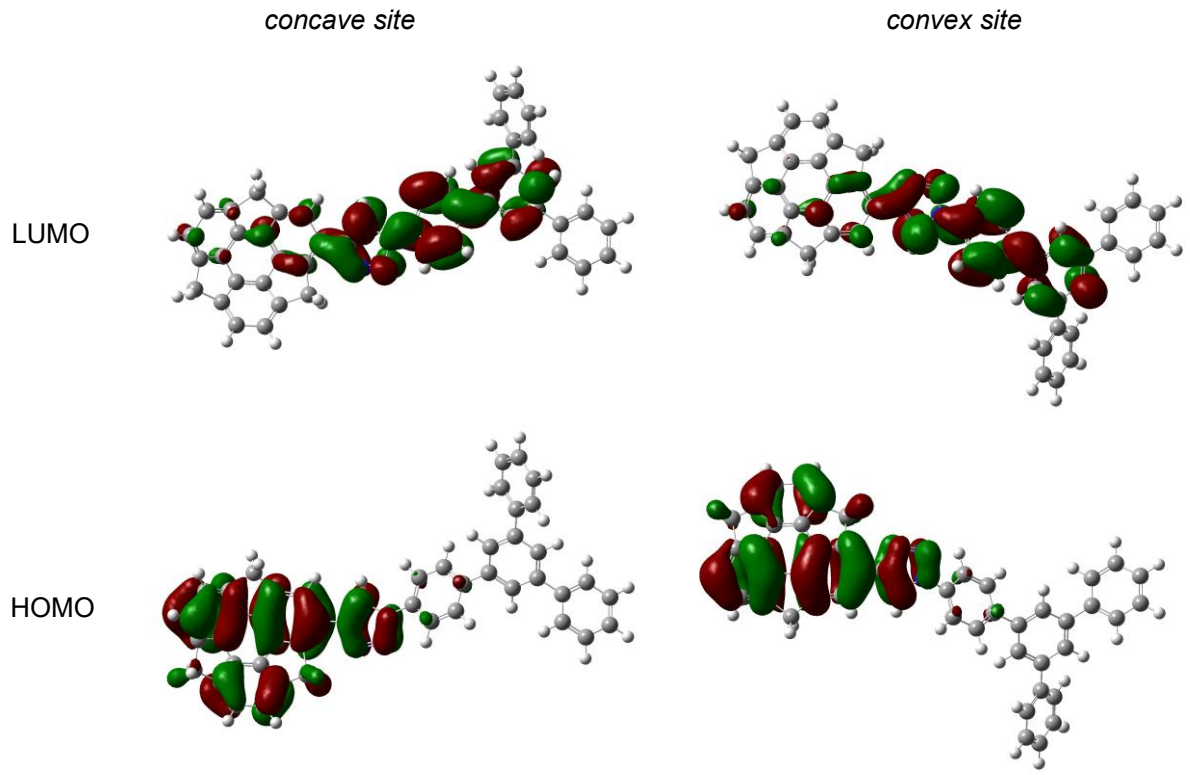


Fig. S84. HOMO and LUMO (B3LYP/6-311g(d,p)) distributions for compound **3**.

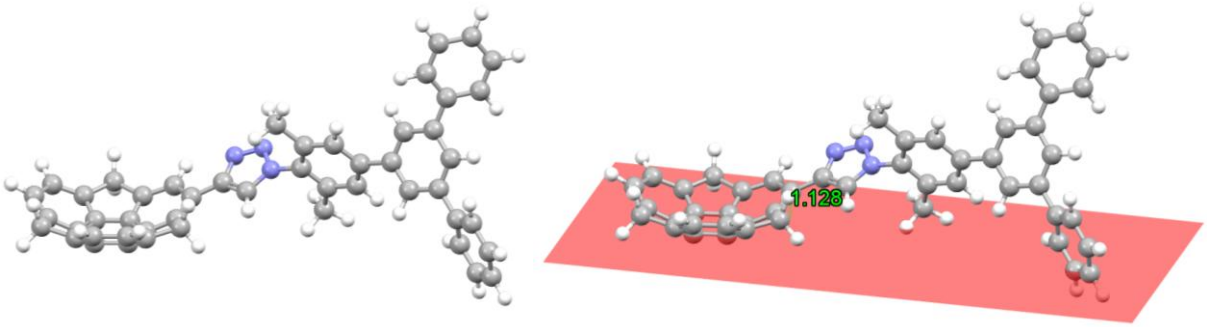


Fig. S85. DFT optimized (B3LYP/6-311g(d,p)) structure of compound **4**. Right image shows the method of estimating the bowl depth.

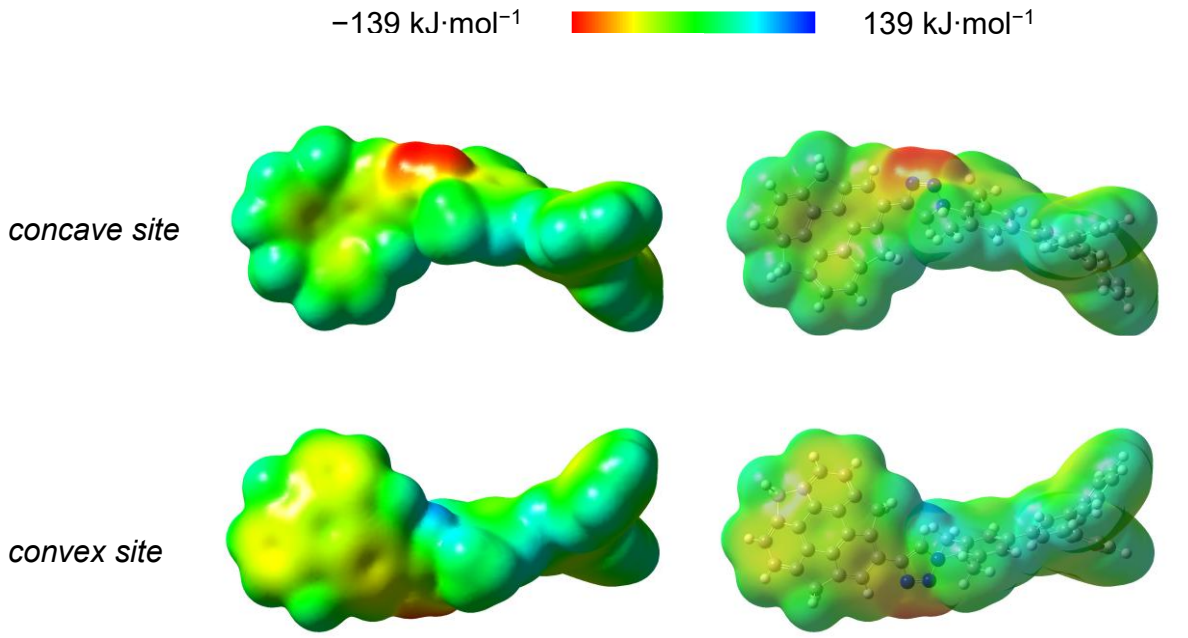


Fig. S86. DFT optimized (B3LYP/6-311g(d,p)) ESP plot of compound **4**.

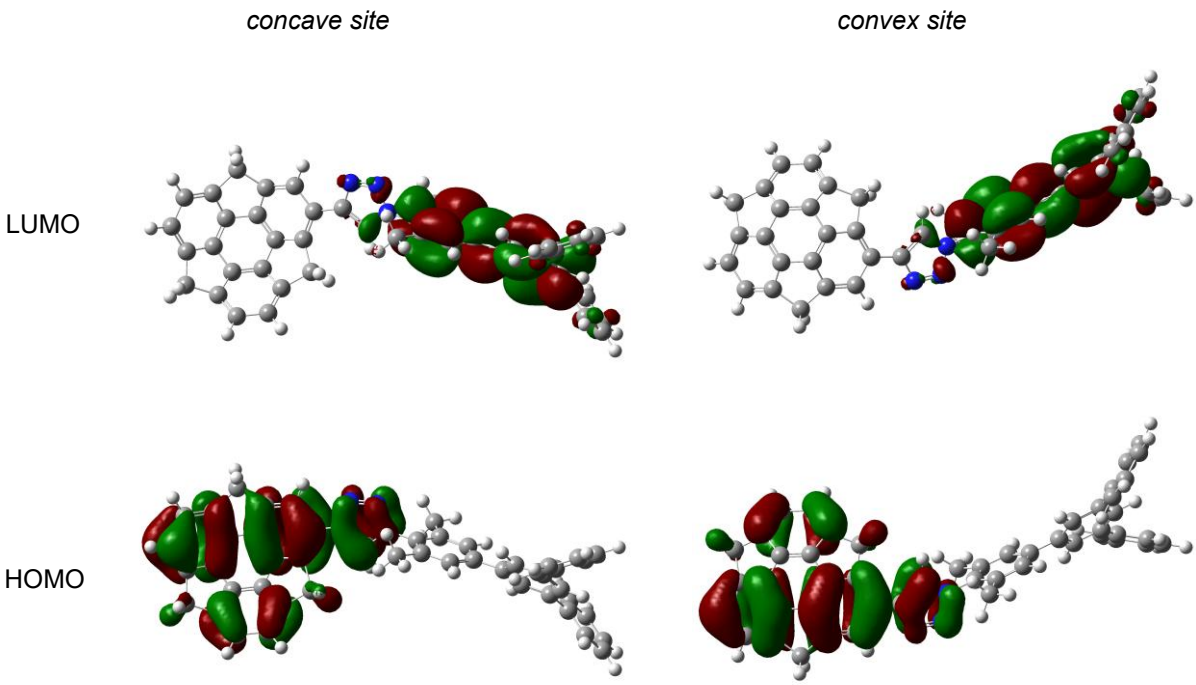


Fig. S87. HOMO and LUMO (B3LYP/6-311g(d,p)) distributions for compound **4**.

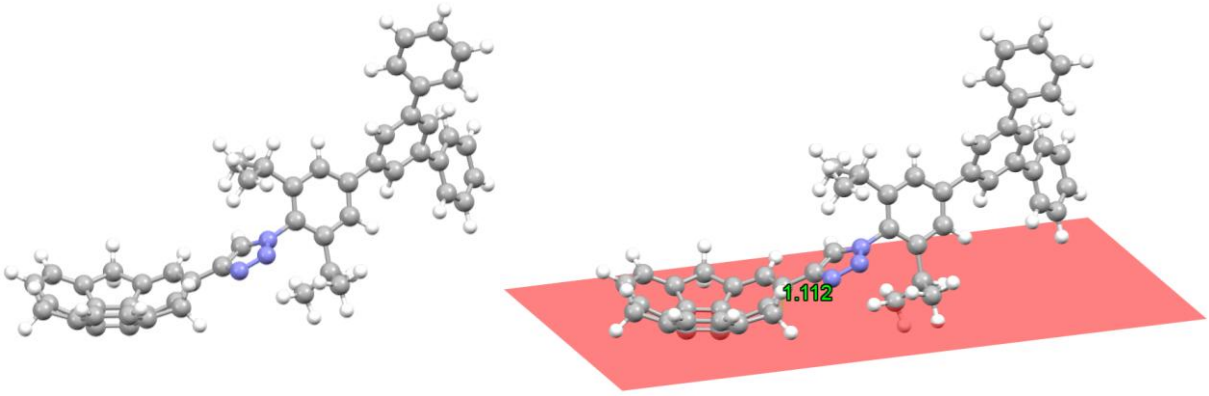


Fig. S88. DFT optimized (B3LYP/6-311g(d,p)) structure of compound **5**. Right image shows the method of estimating the bowl depth.

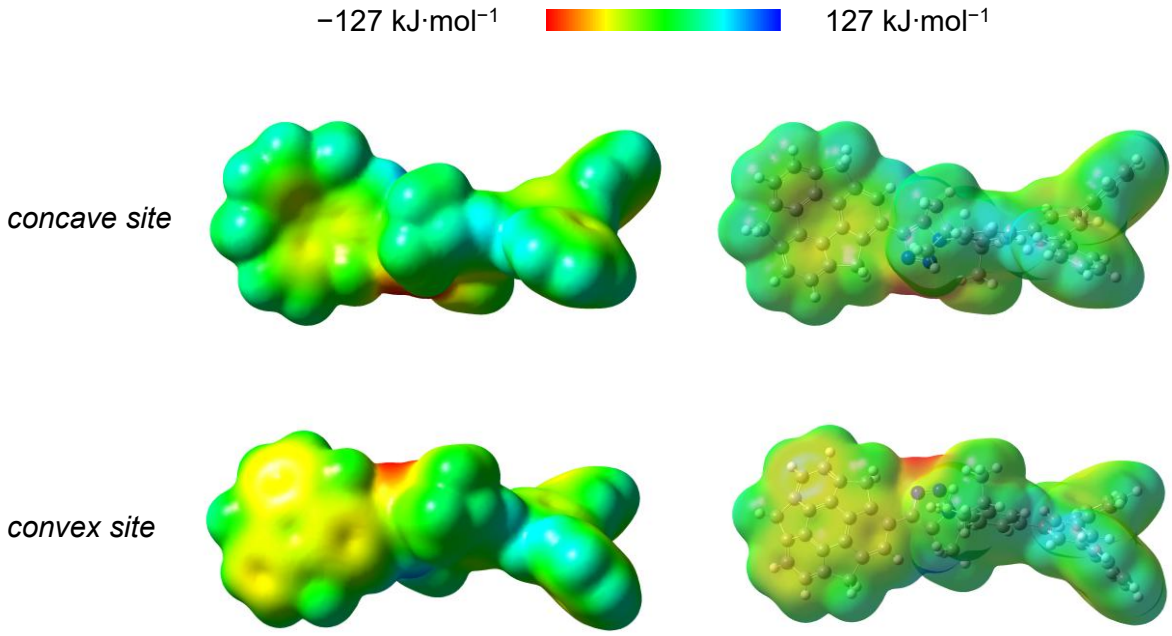


Fig. S89. DFT optimized (B3LYP/6-311g(d,p)) ESP plot of compound **5**.

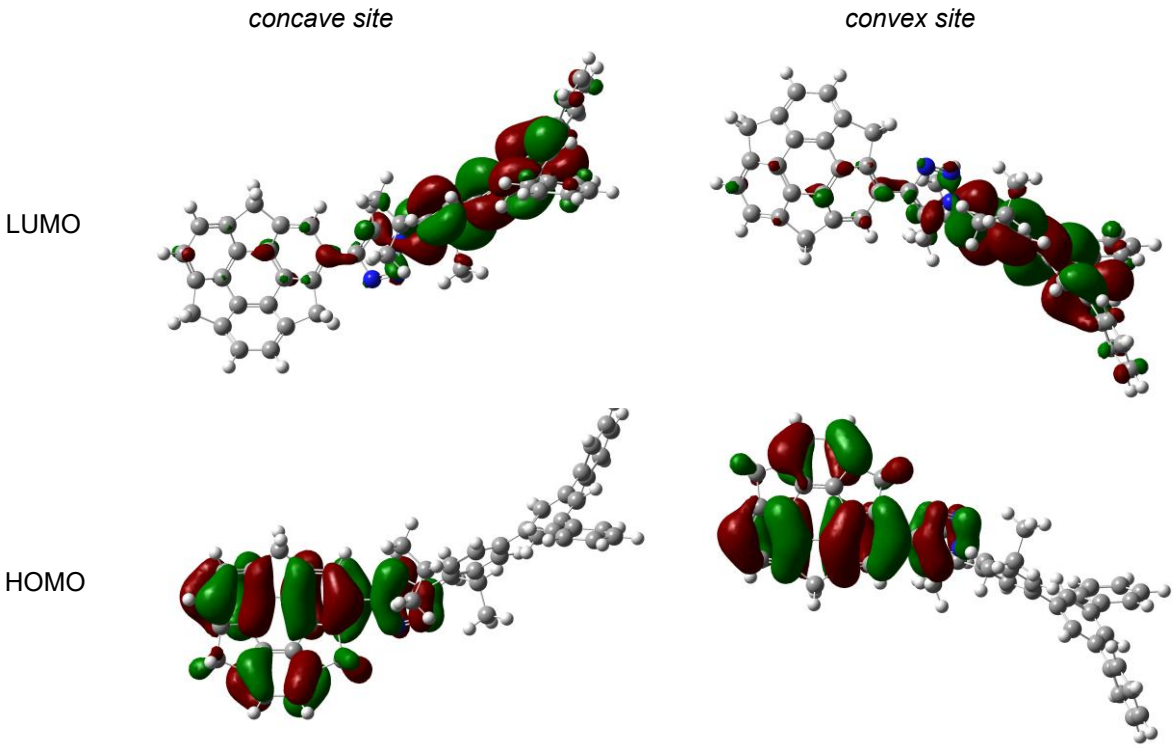


Fig. S90. HOMO and LUMO (B3LYP/6-311g(d,p)) distributions for compound **5**.

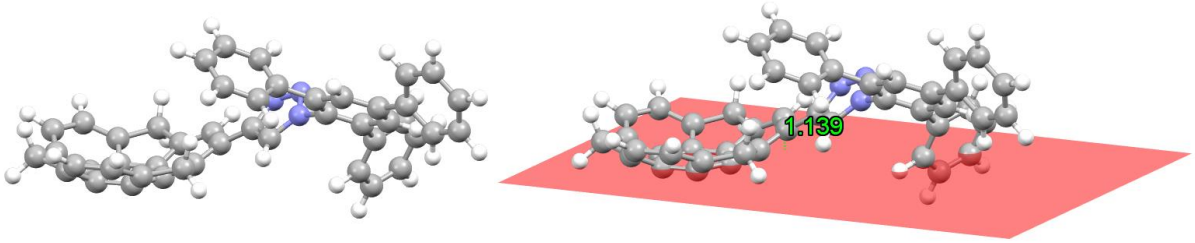


Fig. S91. DFT optimized (B3LYP/6-311g(d,p)) structure of compound **6**. Right image shows the method of estimating the bowl depth.

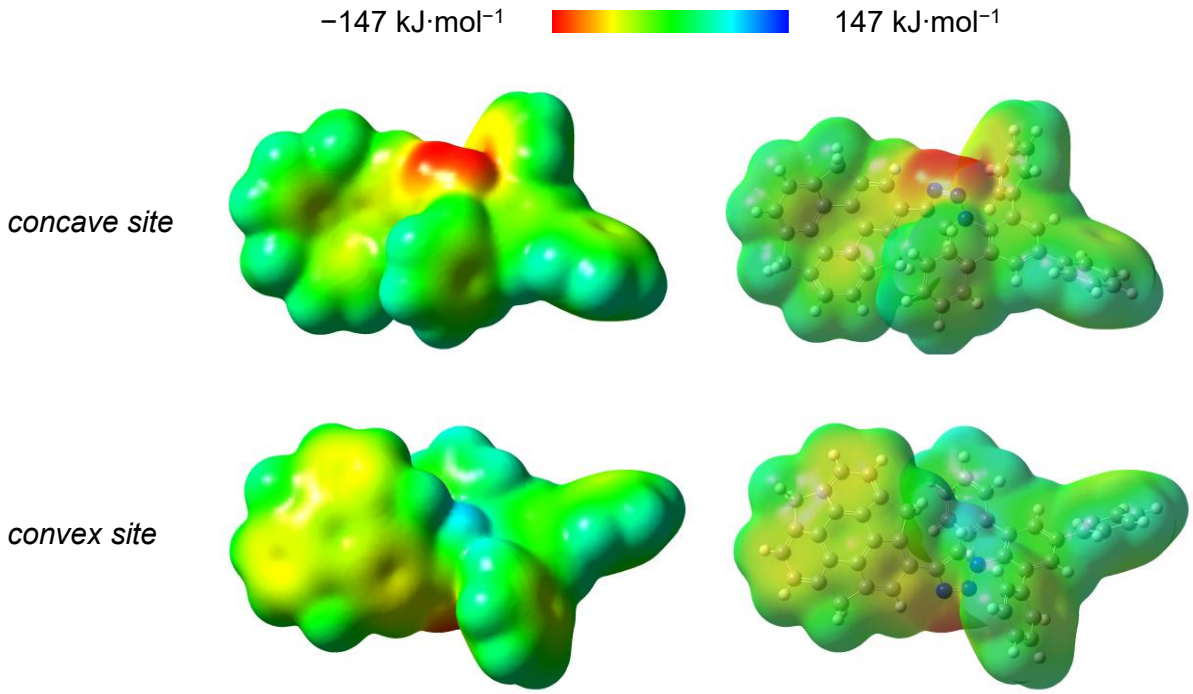


Fig. S92. DFT optimized (B3LYP/6-311g(d,p)) ESP plot of compound **6**.

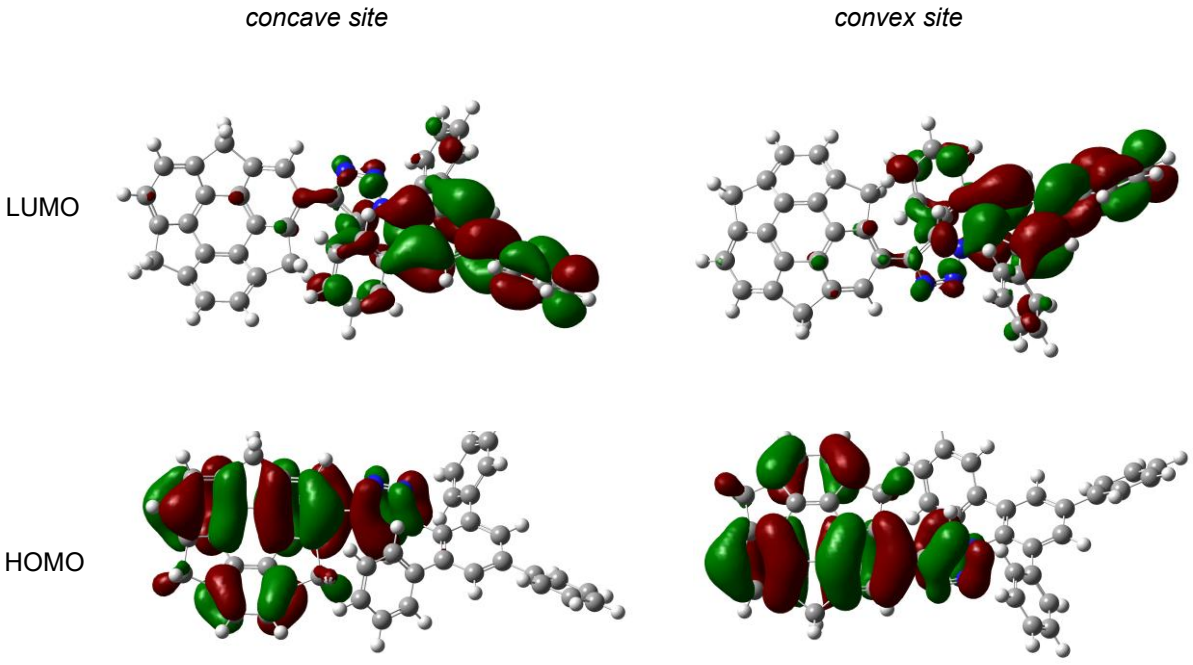


Fig. S93. HOMO and LUMO (B3LYP/6-311g(d,p)) distributions for compound **6**.

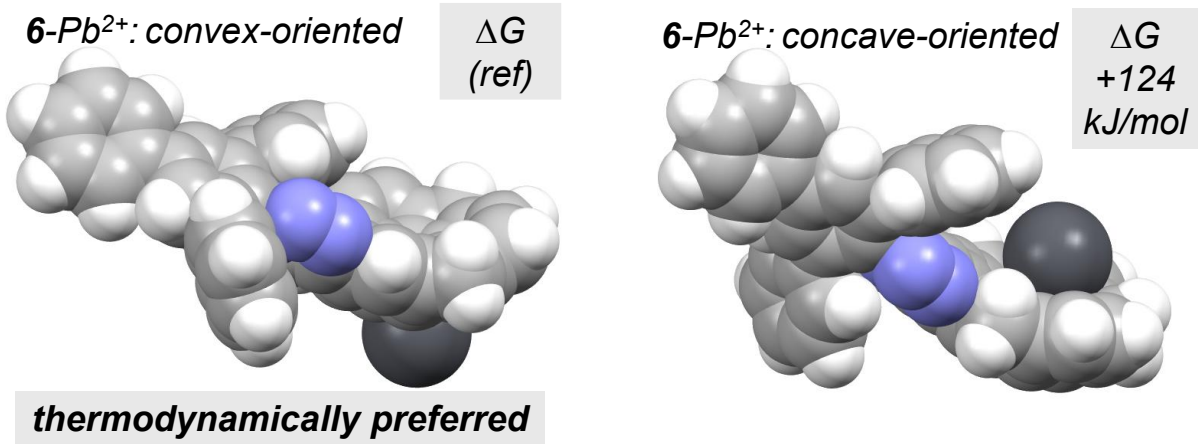


Fig. S94. DFT optimized **6**-Pb^{2+} complexes: *left* – convex-bound cation, *right* - concave-bound cation. Interaction energies (*Δ*G) are also presented and compared, taking the value for the **6**-Pb^{2+} convex complex as the reference one. Basis set and functionals: M06-2X, def2-svp (for C, H, N), def2-ecp (for Pb).

Table S6. Atomic coordinates for the DFT optimized (B3LYP/6-311G(d,p)) compound **3**.

	x	*y*	*z*
C	-9.6309000000	2.4244000000	1.0578000000
C	-8.7809000000	-2.4800000000	1.6994000000
C	-8.6366000000	3.2480000000	0.4444000000
C	-7.6943000000	2.7097000000	-0.4344000000
C	-7.8614000000	1.3646000000	-0.7728000000
C	-6.2595000000	3.1110000000	-0.8741000000
C	-9.2829000000	-1.3171000000	1.1099000000
C	-4.3009000000	1.2386000000	-1.0773000000
C	-10.2304000000	-0.1793000000	1.5785000000
C	-7.5446000000	-3.0528000000	1.2706000000
C	-6.7912000000	-2.4684000000	0.2487000000
C	-9.6938000000	1.0529000000	0.8004000000
C	-8.8241000000	0.5669000000	-0.1781000000
C	-5.5970000000	1.7363000000	-1.1632000000
C	-6.6236000000	0.7903000000	-1.2012000000
C	-8.5794000000	-0.8315000000	0.0058000000
C	-4.0307000000	-0.1648000000	-0.8985000000
C	-5.2880000000	-2.4654000000	-0.1282000000
C	-7.3790000000	-1.3855000000	-0.4067000000
C	-5.1024000000	-1.0730000000	-0.7875000000
C	-6.3796000000	-0.5589000000	-1.0143000000
C	-2.6460000000	-0.6010000000	-0.7015000000
C	-1.4667000000	0.1189000000	-0.7039000000
N	-0.4927000000	-0.8017000000	-0.4722000000

N	-1.0401000000	-2.0360000000	-0.3318000000
N	-2.3203000000	-1.9146000000	-0.4706000000
C	0.9130000000	-0.6181000000	-0.3737000000
C	1.5339000000	0.4507000000	-1.0198000000
C	2.9071000000	0.6251000000	-0.8996000000
C	3.6925000000	-0.2626000000	-0.1515000000
C	3.0449000000	-1.3380000000	0.4752000000
C	1.6724000000	-1.5177000000	0.3755000000
C	5.1601000000	-0.0733000000	-0.0304000000
C	6.0267000000	-1.1720000000	-0.0668000000
C	7.4123000000	-1.0099000000	0.0462000000
C	7.9247000000	0.2834000000	0.1998000000
C	7.0850000000	1.4022000000	0.2402000000
C	5.7040000000	1.2075000000	0.1229000000
C	7.6465000000	2.7661000000	0.4240000000
C	8.3218000000	-2.1839000000	-0.0149000000
C	9.5287000000	-2.1244000000	-0.7266000000
C	10.3798000000	-3.2240000000	-0.7829000000
C	10.0431000000	-4.4068000000	-0.1281000000
C	8.8473000000	-4.4806000000	0.5831000000
C	7.9960000000	-3.3811000000	0.6386000000
C	7.1451000000	3.8547000000	-0.3041000000
C	7.6710000000	5.1319000000	-0.1340000000
C	8.7096000000	5.3484000000	0.7691000000
C	9.2176000000	4.2765000000	1.4999000000
C	8.6921000000	2.9992000000	1.3290000000
H	-10.2508000000	2.8753000000	1.8262000000
H	-9.2513000000	-2.9042000000	2.5809000000
H	-8.5589000000	4.2764000000	0.7825000000
H	-5.7334000000	3.6546000000	-0.0855000000
H	-6.2685000000	3.7560000000	-1.7606000000
H	-3.4611000000	1.9233000000	-1.0176000000
H	-10.1746000000	-0.0282000000	2.6594000000
H	-11.2785000000	-0.3915000000	1.3365000000
H	-7.1465000000	-3.8792000000	1.8506000000
H	-5.0200000000	-3.2764000000	-0.8135000000
H	-4.6407000000	-2.5814000000	0.7422000000
H	-1.2521000000	1.1654000000	-0.8199000000
H	0.9577000000	1.1261000000	-1.6399000000
H	3.3809000000	1.4444000000	-1.4271000000
H	3.6209000000	-2.0291000000	1.0790000000
H	1.1778000000	-2.3414000000	0.8714000000
H	5.6221000000	-2.1627000000	-0.2360000000

H	8.9955000000	0.4217000000	0.2895000000
H	5.0409000000	2.0607000000	0.2035000000
H	9.7888000000	-1.2178000000	-1.2610000000
H	11.3038000000	-3.1592000000	-1.3467000000
H	10.7061000000	-5.2633000000	-0.1720000000
H	8.5795000000	-5.3938000000	1.1028000000
H	7.0798000000	-3.4420000000	1.2149000000
H	6.3540000000	3.6931000000	-1.0275000000
H	7.2744000000	5.9578000000	-0.7141000000
H	9.1193000000	6.3432000000	0.9021000000
H	10.0200000000	4.4358000000	2.2116000000
H	9.0782000000	2.1773000000	1.9210000000

Table S7. Atomic coordinates for the DFT optimized (B3LYP/6-311G(d,p)) compound **4**.

	x	*y*	*z*
C	-8.2396000000	-0.1512000000	-0.7558000000
C	-6.8876000000	-0.3285000000	-1.1885000000
C	-8.0667000000	-1.2873000000	2.6251000000
C	-7.7254000000	-1.3971000000	1.2753000000
C	-8.6539000000	-0.6785000000	0.4558000000
C	-5.9876000000	-1.0221000000	-0.3983000000
C	-8.7769000000	1.0283000000	-1.2776000000
C	-6.4856000000	0.7298000000	-2.0074000000
C	-6.4165000000	-1.5658000000	0.8559000000
C	-9.6366000000	-0.0678000000	1.2376000000
C	-4.6247000000	-0.7246000000	-0.3740000000
C	-5.3520000000	-1.6387000000	1.7554000000
H	-11.0315000000	1.5868000000	1.2286000000
H	-4.9120000000	-1.6874000000	3.8742000000
C	-7.7527000000	1.5748000000	-2.3084000000
C	-5.1175000000	0.9611000000	-2.1035000000
C	-9.8513000000	1.5812000000	-0.5771000000
H	-8.0977000000	1.4411000000	-3.3403000000
H	-7.5668000000	2.6421000000	-2.1673000000
H	-7.2114000000	-1.3910000000	4.6105000000
C	-2.7612000000	0.6344000000	-1.3719000000
C	-4.1705000000	0.2368000000	-1.2970000000
C	-4.0658000000	-1.2969000000	0.9588000000

C	-5.6843000000	-1.6641000000	3.1118000000
H	-3.4382000000	-2.1832000000	0.8021000000
H	-3.4531000000	-0.5581000000	1.4831000000
H	-10.3036000000	2.5140000000	-0.8987000000
H	-9.4747000000	0.2106000000	3.4177000000
C	-9.4576000000	-0.6000000000	2.6851000000
C	-10.2789000000	1.0366000000	0.6728000000
C	-7.0345000000	-1.4898000000	3.5442000000
H	-10.2507000000	-1.3037000000	2.9644000000
H	-4.7182000000	1.7784000000	-2.6920000000
C	-1.6327000000	0.0215000000	-0.8592000000
N	-2.3452000000	1.7588000000	-2.0375000000
N	-0.5985000000	0.8131000000	-1.2421000000
H	-1.4813000000	-0.8811000000	-0.2943000000
C	0.8026000000	0.6438000000	-0.9778000000
N	-1.0570000000	1.8696000000	-1.9617000000
C	1.5513000000	-0.2026000000	-1.8061000000
H	3.1914000000	1.6781000000	1.1714000000
C	2.9082000000	-0.3560000000	-1.5230000000
C	0.9211000000	-0.9042000000	-2.9838000000
C	3.5203000000	0.3130000000	-0.4570000000
H	3.5080000000	-0.9856000000	-2.1702000000
C	2.7371000000	1.1628000000	0.3329000000
C	4.9681000000	0.1313000000	-0.1753000000
C	1.3764000000	1.3458000000	0.0906000000
C	0.5515000000	2.2725000000	0.9483000000
C	9.5677000000	4.4517000000	1.5025000000
H	9.6492000000	1.6433000000	-0.4012000000
C	8.2839000000	4.3207000000	2.0277000000
H	11.0505000000	3.5746000000	0.2130000000
C	10.0562000000	3.4775000000	0.6346000000
H	6.5078000000	3.1212000000	2.1211000000
C	7.4960000000	3.2252000000	1.6876000000
H	7.8970000000	5.0693000000	2.7101000000
H	10.1814000000	5.3053000000	1.7667000000
H	0.1022000000	3.0650000000	0.3452000000
C	9.2683000000	2.3817000000	0.2951000000
C	8.4555000000	-3.1082000000	0.8807000000
H	-0.2682000000	1.7404000000	1.4398000000
H	1.1676000000	2.7330000000	1.7215000000
H	1.6843000000	-1.3817000000	-3.5995000000
H	9.1215000000	-6.2290000000	-0.2874000000
H	8.7137000000	-2.4526000000	1.7045000000

C	9.0245000000	-4.3761000000	0.8062000000
C	5.5578000000	-1.1348000000	-0.2656000000
H	5.3328000000	2.2139000000	0.2098000000
C	6.9190000000	-1.3241000000	0.0000000000
H	4.9389000000	-1.9934000000	-0.4975000000
C	7.6916000000	-0.2136000000	0.3582000000
C	7.5269000000	-2.6781000000	-0.0783000000
C	7.1324000000	1.0658000000	0.4545000000
H	8.7467000000	-0.3472000000	0.5651000000
C	5.7676000000	1.2218000000	0.1862000000
C	7.9743000000	2.2363000000	0.8159000000
C	7.1876000000	-3.5604000000	-1.1143000000
H	9.7338000000	-4.6913000000	1.5634000000
C	7.7570000000	-4.8280000000	-1.1894000000
H	6.4909000000	-3.2398000000	-1.8806000000
C	8.6780000000	-5.2415000000	-0.2292000000
H	7.4870000000	-5.4906000000	-2.0042000000
H	0.2166000000	-1.6777000000	-2.6635000000
H	0.3647000000	-0.2013000000	-3.6081000000

Table S8. Atomic coordinates for the DFT optimized (B3LYP/6-311G(d,p)) compound **5**.

	x	*y*	*z*
C	-9.6527000000	0.1883000000	-2.8523000000
C	-8.9996000000	2.0911000000	1.7458000000
C	-8.6029000000	-0.5571000000	-3.4730000000
C	-7.6379000000	-1.2187000000	-2.7106000000
C	-7.8335000000	-1.2158000000	-1.3274000000
C	-6.1711000000	-1.6655000000	-2.9581000000
C	-9.4333000000	1.2008000000	0.7602000000
C	-4.2688000000	-1.2825000000	-1.0563000000
C	-10.3636000000	1.3145000000	-0.4781000000
C	-7.7640000000	1.8893000000	2.4334000000
C	-6.9428000000	0.7965000000	2.1422000000
C	-9.7491000000	0.2818000000	-1.4619000000
C	-8.8499000000	-0.4930000000	-0.7263000000
C	-5.5420000000	-1.5633000000	-1.5418000000
C	-6.5966000000	-1.4177000000	-0.6381000000
C	-8.6613000000	0.0507000000	0.5844000000
C	-4.0542000000	-0.7421000000	0.2614000000
C	-5.4238000000	0.5155000000	2.2647000000
C	-7.4616000000	-0.1419000000	1.2489000000
C	-5.1599000000	-0.4630000000	1.0892000000

C	-6.4069000000	-0.8820000000	0.6237000000
C	-2.6927000000	-0.3705000000	0.6593000000
C	-1.4817000000	-0.5835000000	0.0267000000
N	-0.5497000000	-0.0454000000	0.8522000000
N	-1.1459000000	0.4750000000	1.9534000000
N	-2.4225000000	0.2772000000	1.8377000000
C	0.8781000000	0.0019000000	0.6699000000
C	1.6872000000	-0.9283000000	1.3542000000
C	3.0635000000	-0.8787000000	1.1209000000
C	3.6493000000	0.0503000000	0.2594000000
C	2.8106000000	0.9697000000	-0.3720000000
C	1.4257000000	0.9784000000	-0.1866000000
C	5.1176000000	0.0662000000	0.0311000000
C	5.8301000000	-1.1310000000	-0.1019000000
C	7.2128000000	-1.1346000000	-0.3198000000
C	7.8807000000	0.0926000000	-0.4005000000
C	7.1972000000	1.3068000000	-0.2695000000
C	5.8143000000	1.2770000000	-0.0553000000
C	7.9276000000	2.5995000000	-0.3378000000
C	7.9531000000	-2.4134000000	-0.4799000000
C	8.9589000000	-2.5481000000	-1.4479000000
C	9.6522000000	-3.7457000000	-1.5963000000
C	9.3553000000	-4.8347000000	-0.7795000000
C	8.3586000000	-4.7157000000	0.1867000000
C	7.6651000000	-3.5183000000	0.3345000000
C	7.3859000000	3.6968000000	-1.0226000000
C	8.0695000000	4.9072000000	-1.0884000000
C	9.3100000000	5.0469000000	-0.4698000000
C	9.8605000000	3.9656000000	0.2148000000
C	9.1769000000	2.7550000000	0.2799000000
C	0.6486000000	2.0571000000	-0.9512000000
C	0.0567000000	1.5391000000	-2.2775000000
C	-0.3949000000	2.8433000000	-0.1381000000
C	1.2118000000	-1.9501000000	2.3919000000
C	1.0173000000	-1.2916000000	3.7737000000
C	-0.0012000000	-2.8148000000	2.0070000000
H	-10.2936000000	0.7828000000	-3.4957000000
H	-9.5261000000	3.0236000000	1.9233000000
H	-8.5071000000	-0.4855000000	-4.5518000000
H	-5.6652000000	-1.0111000000	-3.6723000000
H	-6.1155000000	-2.6847000000	-3.3584000000
H	-3.4110000000	-1.3448000000	-1.7180000000
H	-10.3551000000	2.3238000000	-0.8970000000

H	-11.4053000000	1.0763000000	-0.2328000000
H	-7.4223000000	2.6798000000	3.0940000000
H	-5.1501000000	0.0738000000	3.2289000000
H	-4.8236000000	1.4210000000	2.1684000000
H	-1.2084000000	-1.0837000000	-0.8845000000
H	3.6999000000	-1.5751000000	1.6551000000
H	3.2430000000	1.6990000000	-1.0478000000
H	5.2942000000	-2.0725000000	-0.0843000000
H	8.9512000000	0.1029000000	-0.5675000000
H	5.2818000000	2.2083000000	0.0964000000
H	9.1810000000	-1.7154000000	-2.1055000000
H	10.4201000000	-3.8305000000	-2.3571000000
H	9.8956000000	-5.7674000000	-0.8949000000
H	8.1257000000	-5.5545000000	0.8333000000
H	6.9088000000	-3.4290000000	1.1061000000
H	6.4325000000	3.5920000000	-1.5281000000
H	7.6358000000	5.7402000000	-1.6306000000
H	9.8425000000	5.9898000000	-0.5204000000
H	10.8212000000	4.0665000000	0.7075000000
H	9.6031000000	1.9284000000	0.8369000000
H	1.4181000000	2.7840000000	-1.2311000000
H	-0.7861000000	0.8667000000	-2.1077000000
H	0.8075000000	1.0081000000	-2.8681000000
H	-0.3107000000	2.3794000000	-2.8739000000
H	-1.3144000000	2.2818000000	0.0260000000
H	-0.6615000000	3.7523000000	-0.6853000000
H	-0.0036000000	3.1386000000	0.8374000000
H	2.0533000000	-2.6439000000	2.4917000000
H	0.2034000000	-0.5657000000	3.7515000000
H	1.9266000000	-0.7746000000	4.0913000000
H	0.7832000000	-2.0555000000	4.5213000000
H	-0.9452000000	-2.2760000000	2.0840000000
H	-0.0599000000	-3.6670000000	2.6899000000
H	0.0908000000	-3.2111000000	0.9922000000

Table S9. Atomic coordinates for the DFT optimized (B3LYP/6-311G(d,p)) compound **6**.

	x	*y*	*z*
C	-6.1095000000	1.1787000000	-0.2478000000
C	-4.7210000000	1.4233000000	-0.4910000000
C	-6.4031000000	-2.2631000000	-1.1524000000
C	-5.8989000000	-0.9779000000	-1.3645000000
C	-6.6912000000	-0.0015000000	-0.6795000000

C	-3.9524000000	0.4815000000	-1.1533000000
C	-6.5352000000	1.8397000000	0.9073000000
C	-4.1823000000	2.2496000000	0.4987000000
C	-4.5543000000	-0.7411000000	-1.5964000000
C	-7.7423000000	-0.6101000000	0.0098000000
C	-2.5940000000	0.3014000000	-0.8903000000
C	-3.6141000000	-1.7720000000	-1.6331000000
H	-9.0659000000	-0.3163000000	1.6966000000
H	-3.4451000000	-3.9274000000	-1.5435000000
C	-5.3709000000	2.7639000000	1.3547000000
C	-2.8060000000	2.1825000000	0.6887000000
C	-7.6688000000	1.3196000000	1.5356000000
H	-5.5879000000	3.8209000000	1.1604000000
H	-5.1669000000	2.6689000000	2.4238000000
H	-5.8082000000	-4.3437000000	-1.1386000000
C	-0.5768000000	1.1260000000	0.3555000000
C	-1.9948000000	1.2164000000	-0.0039000000
C	-2.2267000000	-1.1265000000	-1.3816000000
C	-4.1151000000	-3.0735000000	-1.5552000000
H	-1.6177000000	-1.1098000000	-2.2942000000
H	-1.6563000000	-1.6739000000	-0.6263000000
H	-8.0437000000	1.7560000000	2.4561000000
H	-7.8468000000	-2.7702000000	0.4332000000
C	-7.7657000000	-2.1000000000	-0.4262000000
C	-8.2693000000	0.1021000000	1.0896000000
C	-5.5021000000	-3.3177000000	-1.3166000000
H	-8.6118000000	-2.3204000000	-1.0878000000
H	-2.3080000000	2.7634000000	1.4560000000
C	0.4613000000	0.4745000000	-0.2816000000
N	-0.0522000000	1.7428000000	1.4629000000
N	1.5559000000	0.7356000000	0.4759000000
H	0.5141000000	-0.1147000000	-1.1795000000
C	2.9031000000	0.2889000000	0.2893000000
N	1.2182000000	1.5110000000	1.5404000000
C	3.8925000000	1.2235000000	-0.0604000000
H	4.7751000000	-2.5269000000	0.4196000000
C	5.2054000000	0.7695000000	-0.2118000000
C	3.2120000000	-1.0700000000	0.4795000000
C	5.5475000000	-0.5768000000	-0.0510000000
H	5.9736000000	1.4910000000	-0.4618000000
C	4.5348000000	-1.4790000000	0.2879000000
C	9.6026000000	-1.9015000000	-0.5722000000
C	9.0586000000	-0.9512000000	-1.4338000000

H	9.2398000000	-3.1520000000	1.1412000000
H	10.6255000000	-2.2352000000	-0.7035000000
C	7.7459000000	-0.5215000000	-1.2645000000
C	4.0479000000	4.9922000000	0.2687000000
H	9.6549000000	-0.5480000000	-2.2446000000
C	4.2766000000	3.6358000000	0.4820000000
C	3.1434000000	5.4048000000	-0.7067000000
C	3.6007000000	2.6703000000	-0.2736000000
H	4.9671000000	3.3187000000	1.2552000000
H	2.1729000000	2.3640000000	-1.8572000000
C	2.1950000000	-2.0812000000	0.8870000000
C	1.3982000000	-1.8955000000	2.0253000000
H	1.0322000000	-5.1459000000	-0.0437000000
C	0.4835000000	-2.8698000000	2.4134000000
H	1.4999000000	-0.9892000000	2.6099000000
C	0.3458000000	-4.0428000000	1.6729000000
H	-0.1215000000	-2.7114000000	3.2988000000
C	1.1329000000	-4.2378000000	0.5403000000
H	-0.3687000000	-4.7990000000	1.9776000000
C	2.0517000000	-3.2658000000	0.1521000000
H	2.6552000000	-3.4189000000	-0.7358000000
C	6.9490000000	-1.0349000000	-0.2311000000
C	7.5093000000	-1.9912000000	0.6282000000
H	7.3259000000	0.2012000000	-1.9547000000
C	8.8227000000	-2.4191000000	0.4598000000
H	6.9200000000	-2.3821000000	1.4499000000
H	4.5717000000	5.7261000000	0.8707000000
C	2.4690000000	4.4522000000	-1.4672000000
H	2.9632000000	6.4609000000	-0.8717000000
C	2.6948000000	3.0958000000	-1.2523000000
H	1.7654000000	4.7642000000	-2.2307000000

Table S10. Atomic coordinates for the DFT optimized (M06-2X/def2-svp/def2-ecp) **6**-Pb^{2+} complex with convex-bound cation.

	x	*y*	*z*
C	1.0022568400	-4.8693677400	-0.7428428700
C	1.3417948900	-3.6034807100	-0.1416314900
C	-2.5609990100	-5.0040847400	-0.3542281800
C	-1.2860591300	-4.6599232600	0.1173877100
C	-0.2760405500	-5.4100130200	-0.5864194400
C	0.3370849300	-2.8496633900	0.4884787800
C	1.8232608500	-5.1475944700	-1.8493134600

C	2.3625904600	-2.9845312600	-0.9046564400
C	-0.9833373200	-3.4030256800	0.6449388900
C	-0.8634940200	-6.2600020900	-1.5397811800
C	0.2971767800	-1.4612874200	0.4996525200
C	-1.9299258400	-2.3712723400	0.7324109600
H	-0.4035353500	-7.2405830200	-3.4116749100
H	-4.0266561500	-1.9861959400	0.3679787800
C	2.9056365800	-4.0433411800	-1.8940576800
C	2.3871518400	-1.6042951800	-0.8582748900
C	1.2995273600	-6.0783692200	-2.7409445500
H	3.8990566600	-4.4214585800	-1.5989228200
H	3.0144101800	-3.6242786100	-2.9043243400
H	-4.5556088200	-4.1822198000	-0.5320094900
C	1.3947487900	0.6034297000	-0.3267762500
C	1.3782452900	-0.8268082900	-0.1487415800
C	-1.1523943400	-1.0402760000	0.8313103200
C	-3.2303039900	-2.7344007800	0.3812976700
H	-1.2560904200	-0.5682170100	1.8229171700
H	-1.5274366000	-0.3107090000	0.0910272000
H	1.8303640600	-6.3207232300	-3.6649685100
H	-2.9410633000	-6.0749572700	-2.2397604200
C	-2.3912692300	-6.2184810700	-1.2986825500
C	-0.0273357700	-6.6266731500	-2.5895673900
C	-3.5415951200	-4.0323532400	-0.1530315300
H	-2.7683103200	-7.1531809300	-0.8503514300
H	3.0719367900	-1.0174666400	-1.4766377700
C	0.6506918600	1.5940413500	0.3013965900
N	2.1447234700	1.2074888100	-1.2997828800
N	0.9943327700	2.7148493300	-0.3439772800
H	-0.0614478700	1.5996297200	1.1218717400
C	0.4257297200	4.0175156100	-0.1752550100
N	1.8934182000	2.4559160300	-1.3158690700
C	1.2615776900	5.1046720100	0.1149979200
H	-2.5982265300	5.5476930500	-0.2467766700
C	0.6666059600	6.3624852800	0.2402050400
C	2.7293477600	4.9503098900	0.2978486100
C	-0.7165338900	6.5456578800	0.1203592200
H	1.3096454200	7.2210643400	0.4456888900
C	-1.5168632300	5.4271787100	-0.1518125400
C	-1.3214722900	7.8901870100	0.2818961100
C	-0.9648877900	4.1573740300	-0.3227236700
C	-1.8497709300	3.0058990000	-0.6621317800
C	-2.9837971300	9.5420722000	-0.3469828900

C	-2.4200778800	8.2776922000	-0.4980211100
C	-2.4613103600	10.4340927300	0.5894715600
H	-2.9040363500	11.4247056400	0.7082076000
C	-0.8018444600	8.7954740500	1.2177793500
H	-2.8183094000	7.5962679300	-1.2535049300
C	-1.3699663600	10.0573223500	1.3721121700
C	-1.5998666600	2.2074140000	-1.7894160900
H	-2.2702161000	0.5722892200	-3.0197990400
C	3.6112178200	5.7497830900	-0.4374141800
H	0.0382275600	8.5013738500	1.8510811600
H	-3.8302428400	9.8362006500	-0.9701980000
H	-0.9615644800	10.7489786000	2.1112364100
C	-2.9706505900	2.7262639400	0.1300224900
H	-0.7370100800	2.4281007200	-2.4245267200
C	-3.8310516600	1.6770539100	-0.1994890900
H	-3.1747315700	3.3457181800	1.0070311500
C	-3.5800198100	0.8954488900	-1.3275762900
H	-4.7138904900	1.4901152200	0.4159342900
C	-2.4593343200	1.1613201400	-2.1197831200
H	-4.2734655600	0.1000517100	-1.6110050200
H	2.5642587000	3.4330045800	1.8298909600
C	4.9878834600	5.6305837600	-0.2558172900
H	3.2137979900	6.4583760200	-1.1679386200
C	5.4960125200	4.7172460400	0.6668326900
H	5.6669457000	6.2547780600	-0.8394694800
C	4.6224591400	3.9229378000	1.4102265100
H	6.5742390500	4.6298496600	0.8125814300
C	3.2470220900	4.0368839400	1.2254992100
H	5.0163582800	3.2219340300	2.1488723400
Pb	0.8263284400	-5.2381173100	1.8967372000

Table S11. Atomic coordinates for the DFT optimized (M06-2X/def2-svp/def2-ecp) **6**-Pb^{2+} complex with concave-bound cation.

	x	*y*	*z*
C	-0.3955656300	-2.8923684600	1.7753688300
C	0.6181461100	-3.7779041400	2.2771451800
C	-1.7590716900	-4.7773638500	-0.9291408300
C	-1.2389755600	-4.6636016400	0.3866447000
C	-1.3761702900	-3.3516234500	0.8957817700
C	0.6725679900	-5.1039146500	1.8725768900
C	0.0770711700	-1.5848731200	1.7570863600
C	1.7744170100	-3.0590291400	2.5970392600

C	-0.2407145100	-5.5315076600	0.8632900600
C	-1.9271840600	-2.5272242000	-0.1006154000
C	1.8666824100	-5.8244137800	1.7541032800
C	0.2953563300	-6.5840016600	0.0913124400
H	-1.9334408900	-0.4890951600	-0.8173781600
C	-0.1972400100	0.7044957000	0.8484312300
C	1.4292643800	-1.5626494700	2.4951062300
C	2.9654611800	-3.7969264200	2.6135281200
C	-0.5884702600	-0.6870637100	0.8825593400
H	2.1837607700	-0.9809160600	1.9480151200
H	1.3435681900	-1.0708007500	3.4788120900
H	-1.7535985200	-6.1143758400	-2.6699703300
H	3.9166467000	-3.3066717200	2.8363399800
C	3.0175852400	-5.1654895600	2.1946234400
C	1.5909532900	-7.0254365000	0.8176838000
C	-0.3294175600	-6.8186772100	-1.1685102500
H	2.4208827700	-7.2715039100	0.1399816800
H	1.3794136000	-7.9422532900	1.3969408600
H	4.0004693400	-5.6386000300	2.1297998100
H	-3.5910060600	-3.6193611100	-1.0392878100
C	-2.5101834800	-3.4511507400	-1.1953324200
C	-1.5645477000	-1.1880525500	-0.0630664800
C	-1.3544842300	-5.9199563100	-1.6698948700
H	-2.3959748300	-3.0678903400	-2.2188192900
H	-0.0200978500	-7.6487970300	-1.8101445800
C	-0.6730225400	1.7940426200	0.1270772000
N	0.7901596500	1.1646922400	1.6770183800
N	0.0645476200	2.8214210500	0.5710502700
H	-1.4600885100	1.9334735700	-0.6097888500
C	-0.0368217400	4.2048313700	0.2080537000
N	0.9395094600	2.4196540500	1.5089455300
C	-1.2433386600	4.8818492400	0.4464534700
H	1.8452505200	6.7075739600	-1.0737234500
C	-1.3149208700	6.2288979200	0.0857989700
C	-2.4208314400	4.2134684200	1.0661779800
C	-0.2172727300	6.9075753100	-0.4589931500
H	-2.2526603500	6.7637491000	0.2504957100
C	0.9731071500	6.1966166300	-0.6605258200
C	-0.3117204100	8.3451142000	-0.8120183000
C	1.0818879800	4.8402509700	-0.3502488100
C	2.3541592000	4.1164825300	-0.6192528200
C	-3.6745664400	4.2915553900	0.4471990600
H	-1.3348977000	3.4838024500	2.7891191200

C	-4.7895617600	3.6876005300	1.0285264400
H	-3.7745740500	4.8303323000	-0.4983507000
C	-4.6636368400	3.0028308400	2.2363119700
H	-5.7624786000	3.7622558900	0.5391415500
C	-3.4186523600	2.9259954000	2.8633814600
H	-5.5389235700	2.5425848700	2.6984695600
C	-2.3036857300	3.5263343500	2.2835048100
H	-3.3199052700	2.4136859600	3.8223956200
C	0.3620084500	8.8488227100	-1.9335202700
H	-1.5820616000	8.8541800100	0.8643022800
C	0.2727582400	10.1980067700	-2.2661966200
H	0.9399929100	8.1739589200	-2.5687666100
C	-0.4867119700	11.0639375100	-1.4795884700
H	0.7941661900	10.5744950500	-3.1479822300
C	-1.1586853300	10.5735775100	-0.3599116700
H	-0.5543651200	12.1219776700	-1.7387797400
C	-1.0743120200	9.2233896500	-0.0295172300
H	-1.7460074900	11.2486149400	0.2650678100
C	2.3772001800	2.9738564800	-1.4295046100
H	3.5439721600	5.4868055200	0.5458505600
C	3.5806330100	2.3288237800	-1.7051433600
H	1.4464850800	2.6123476600	-1.8755644900
C	4.7746645300	2.8138777600	-1.1706510200
H	3.5922812400	1.4563007200	-2.3620155800
C	4.7594486100	3.9509028200	-0.3640129600
H	5.7197495100	2.3151686500	-1.3936276900
C	3.5566141200	4.6002866400	-0.0921906300
H	5.6900194200	4.3377584900	0.0549870400
Pb	0.8888209100	-4.4650278800	-1.4636787200

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