Supporting Information

Synthesis of *para*-linked Azacalix[n]pyridine[n]pyrazines and their uranyl ions binding property

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1. General Information

All commercially available reagents were used as received. TLC analysis was performed on pre-coated, glass-backed silica gel plates and visualized with UV light. Flash column chromatography was performed on silica gel (100-200). Anhydrous 1,4-dioxane was dried by 4 Å molecular sieve. ^{1}H NMR and ^{13}C NMR spectra were recorded using 400 MHz spectrometers. Chemical shifts are reported in ppm versus tetramethylsilane with either tetramethylsilane or the residual solvent resonance used as an internal standard. Mass analysis was performed at analysis and testing center, Sichuan University.

2. Experimental Procedures and Characterization of Products.

Synthesis of 3. A mixture of 2,5-dibromopyrazine **1** (2.38g, 10mmol), 30% aqueous methylamine solution (20mL), copper powder (64 mg, 1 mmol), and a stirring bar was sealed in a 75 mL screwed tube. The reaction mixture was kept stirring at 100 °C for 12 h. After the reaction was completed, the reaction mixture was cooled to room temperature and ethyl acetate (20 mL) was added to extract the target product. The organic layer was separated and the aqueous layer was extracted by ethyl acetate (3 × 50 mL). The combined extracts were dried by anhydrous Na_2SO_4 and the solvent was removed under reduced pressure to give crude product that was purified by silica gel column chromatography (eluent: petroleum ether/ethyl acetate) to give the pure product.

3 (1.0 g, 73%): yellow solid, mp 100-102 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.50 (s, 2H), 4.01 (s, 2H), 2.89 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 149.5, 126.8, 29.9; IR (KBr, cm^{-1}) ν 3265, 1550, 1465, 1373, 1282, 1192, 1120, 1011, 858; HRMS-ESI calcd. for $C_6H_{11}N_4$: $[M+H]^+$ 139.0978. Found: 139.0979.

Synthesis of 4. Under argon protection, a solution of *N*^{2},*N*^{5}-dimethylpyrazine -2,5-diamine **3** (1.38g, 10mmol) and NaH (1.44 g, 60 mmol) in dry 1,4-dioxane (150 mL) was heated at reflux for 3h, then 2, 6-dibromopyridine **2** (7.14g, 30mmol) was added slowly. The reaction mixture was kept stirring at 110 °C for another 6 h. After cooling down to room temperature, the reaction was quenched at 0 °C by adding water (5 mL). After removal of 1,4-dioxane using a rotary evaporator, the crude product was added 150 mL H_2O and was extracted with DCM (3 × 100 mL). The combined organic layer was dried over anhydrous Na_2SO_4. After filtration, the filtrate was concentrated and the residue was was column chromatographed with silica gel (100-200 mesh) using a mixture of dichloromethane and acetone (v : v = 50 : 1) as an eluent to give product **4**.

4 (2.1 g, 45%): white solid, mp 200-201 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.52 (s, 2H), 7.39(t, *J* = 8.0 Hz, 2H), 7.01(d, *J* = 8.0 Hz, 2H), 6.97 (d, *J* = 8.0 Hz, 2H), 6.36 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 156.73, 147.87, 139.79, 139.55, 136.02, 119.82, 109.61, 36.00; IR (KBr, cm^{-1}) ν 3433, 1591, 1472, 1412, 1353, 1088, 765; HRMS-ESI calcd. for $C_{16}H_{15}N_6Br_2$: $[M+H]^+$ 448.97195. Found: 448.97250.

Synthesis of azacalix[n]pyridine[n]pyrazines 5 (n = 2) and **6** (n = 4).

Under argon protection, a mixture of trimer **4** (1 mmol), diamine **3** (1 mmol), $Pd_2(dba)_3$ (138 mg, 0.15 mmol), dppp (123 mg, 0.3 mmol), and sodium tert-butoxide

(288 mg, 3 mmol) in anhydrous 1,4-dioxane (250 mL) was warmed (or heated at reflux) for a period of time. When **3** or **4** was consumed, as monitored by TLC, the reaction was quenched by cooling down to room temperature and the mixture was filtered through a Celite pad. After removal of the solvent, the residue was dissolved in dichloromethane (45 mL) and washed with brine (3 × 15 mL), the aqueous phase was re-extracted with dichloromethane (3 × 20 mL), and the combined organic phase was dried over anhydrous sodium sulfate. Basic aluminium oxide column chromatography, with elution with a mixture of dichloromethane and acetone (v : v = 8 : 1) gave pure products **5** and **6**.

5 (75 mg, 35% at refux temperature): white solid, mp > 300 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.21 (s, 4H), 7.60(t, *J* = 8.0 Hz, 2H), 7.39(d, *J* = 8.0 Hz, 4H), 3.45 (s, 12H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 156.18, 149.12, 140.11, 137.99, 101.24, 36.92; IR (KBr, cm^{-1}) ν 3434, 1581, 1448, 1360, 1166; HRMS-ESI calcd. for $C_{22}H_{23}N_{10}$: $[M+H]^+$ 427.21017. Found: 427.21017.

6 (53 mg, 25% at 80 °C): white solid, mp > 300 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.27 (s, 8H), 7.27(t, *J* = 8.0 Hz, 4H), 6.39(d, *J* = 8.0 Hz, 8H), 3.46 (s, 24H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 155.38, 148.38, 139.07, 138.02, 100.99, 35.57; IR (KBr, cm^{-1}) ν 3430, 1577, 1464, 1415, 1249; HRMS-ESI calcd. for $C_{44}H_{45}N_{20}$: $[M+H]^+$ 853.41266. Found: 853.41306.

3. ^{1}H NMR titration spectra

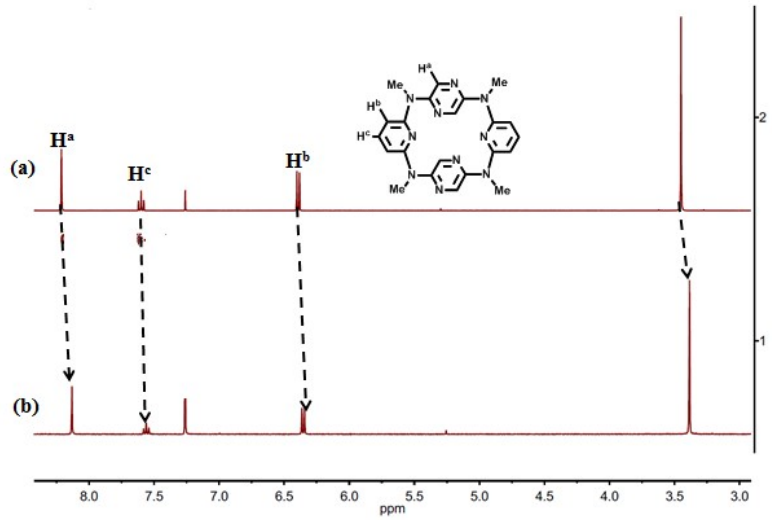


Figure S1. Partial ^{1}H NMR spectra in $CDCl_3/CD_3CN$ (v/v, 3/1). (a) 10.0 mM **5**; (b) 10.0 mM **5** + 10.0 mM $UO_2(NO_3)_2$.

4. Uv-vis titration data

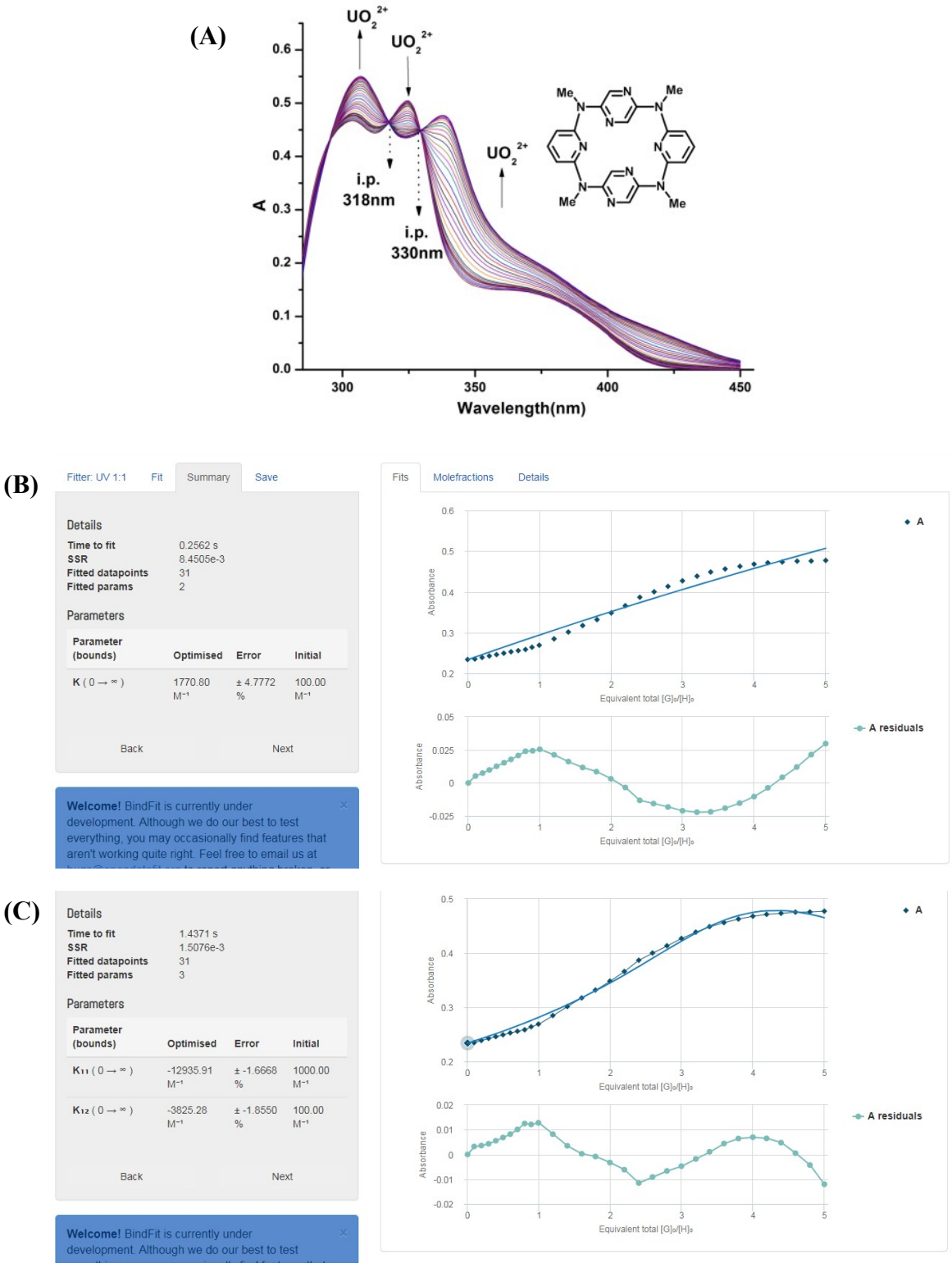


Figure S2. (A) UV-vis titration spectra of **5** (0.02 mM) with addition of 0-5.0 equiv of $UO_2(NO_3)_2$ in 9:1 dichloromethane/acetonitrile. (B) and (C) screenshots taken from the summary window of the website supramolecular.org. The titration data fitted to 1:1 binding model (B) and 1:2 binding model (C).

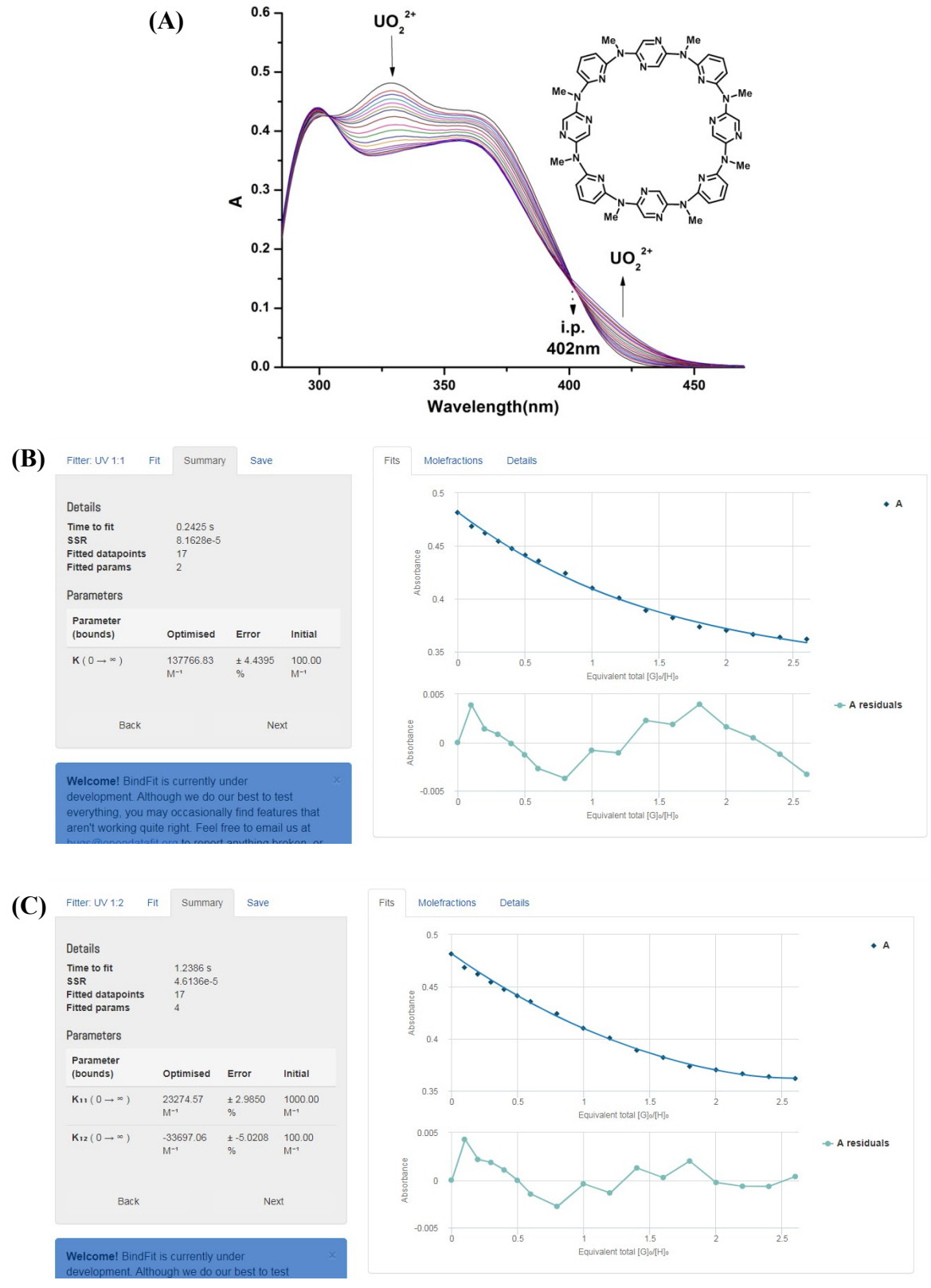


Figure S3. UV-vis titration spectra of **6** (0.02 mM) with addition of 0-2.6 equiv of $UO_2(NO_3)_2$ in 9:1 dichloromethane/acetonitrile. (B) and (C) are screenshots taken from the summary window of the website supramolecular.org. The titration data fitted to 1:1 binding model (B) and 1:2 binding model (C).

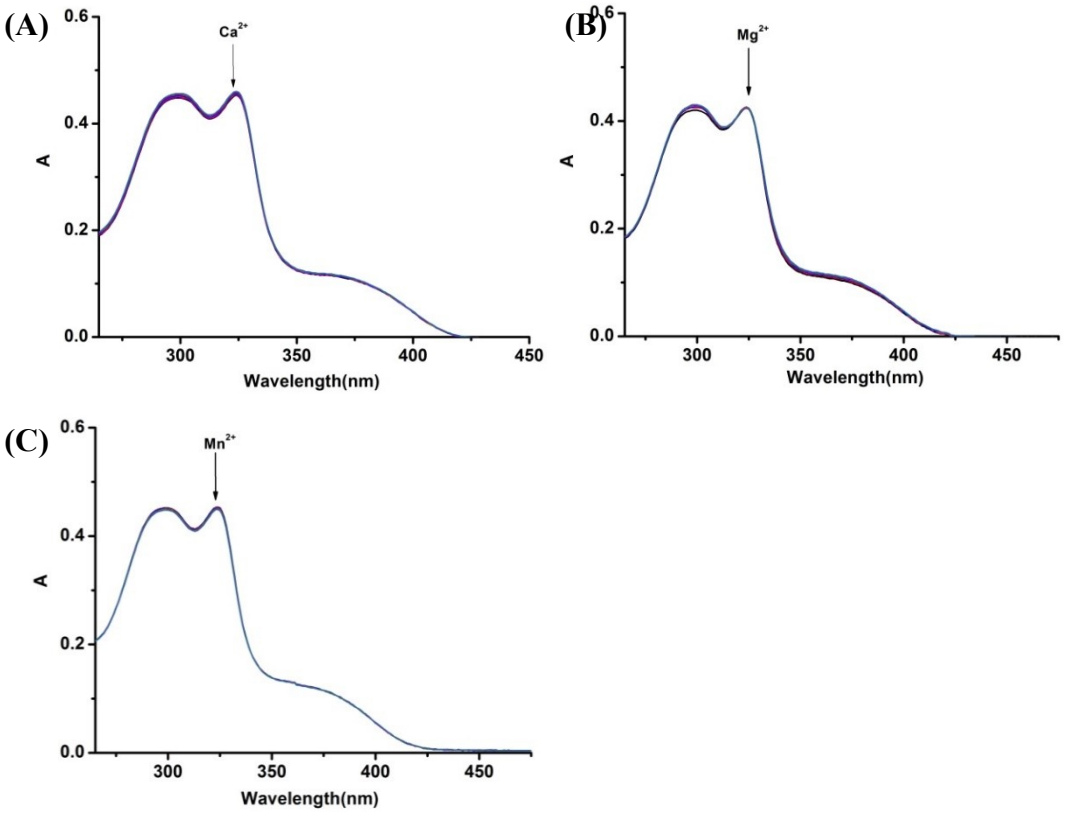


Figure S4. UV-vis titration spectra of **5** (0.02 mM) with addition of 0-1.0 equiv of (A) $CaCl_2$ (B) $MgCl_2$ and (C) $MnCl_2$ in 9:1 dichloromethane/acetonitrile.

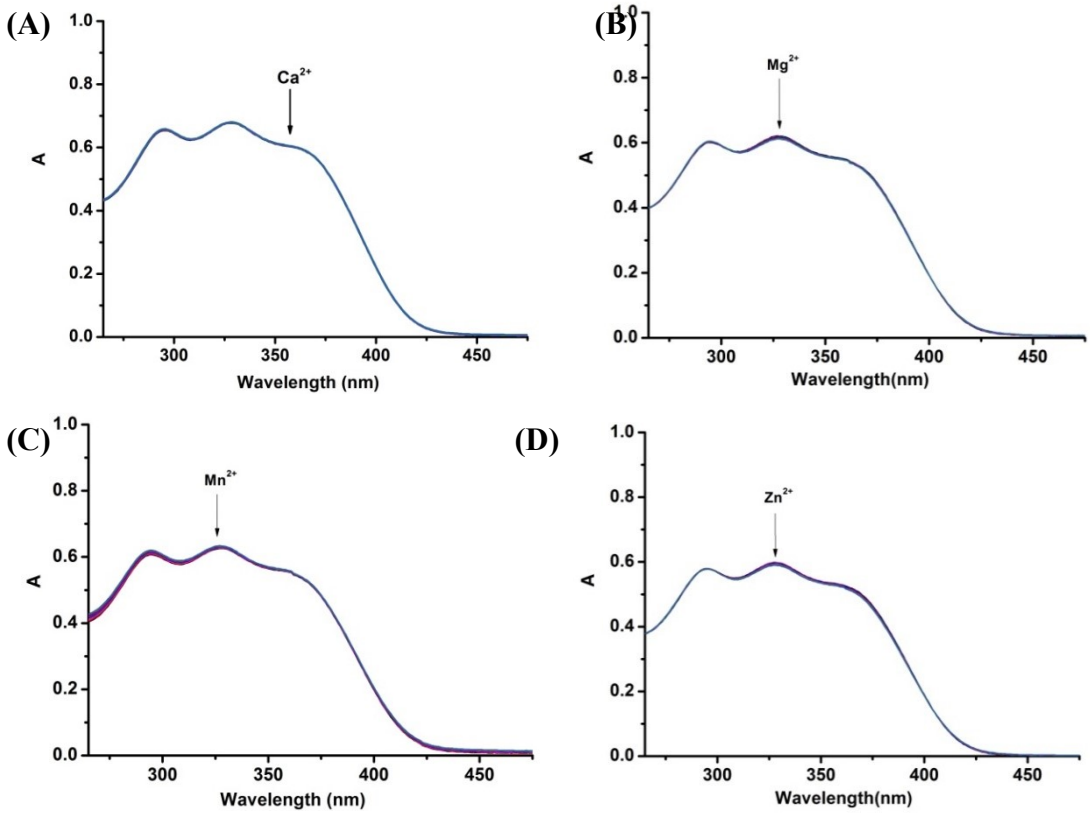
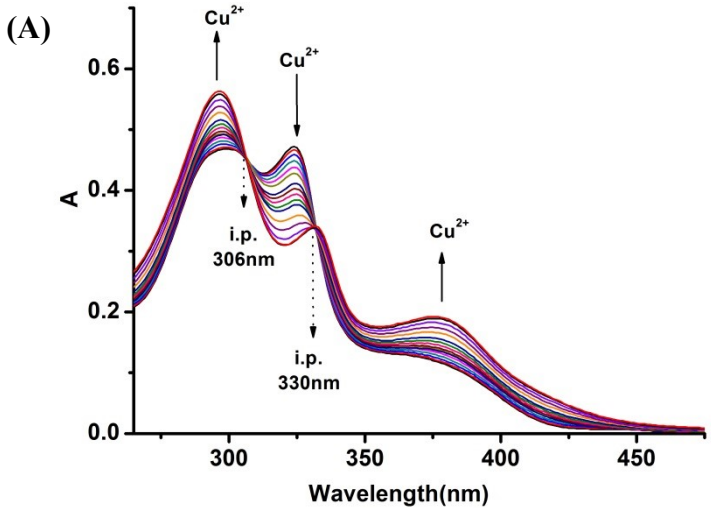
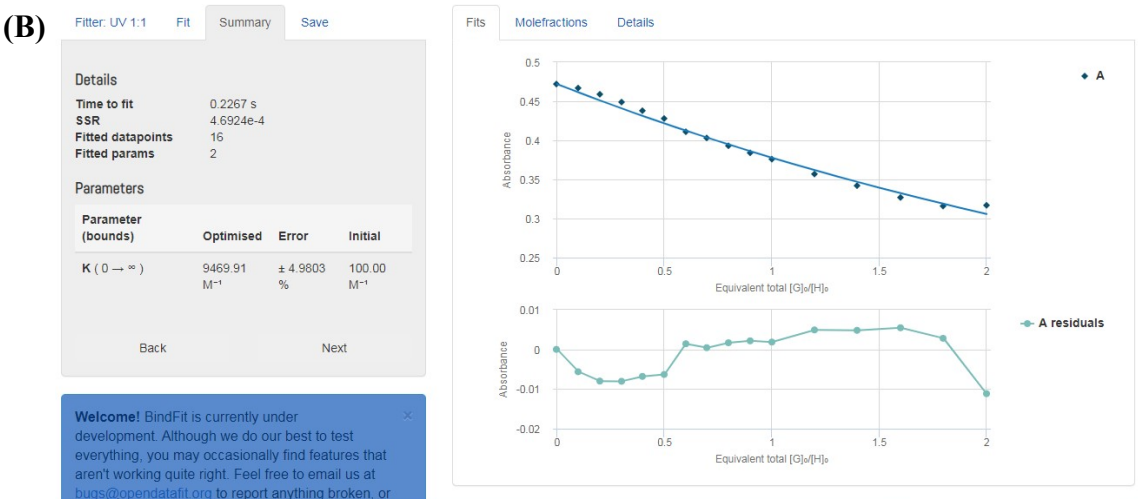


Figure S5. UV-vis titration spectra of **6** (0.02 mM) with addition of 0-1.0 equiv of (A) $CaCl_2$, (B) $MgCl_2$, (C) $MnCl_2$ and (D) $ZnCl_2$ in 9:1 dichloromethane/acetonitrile.





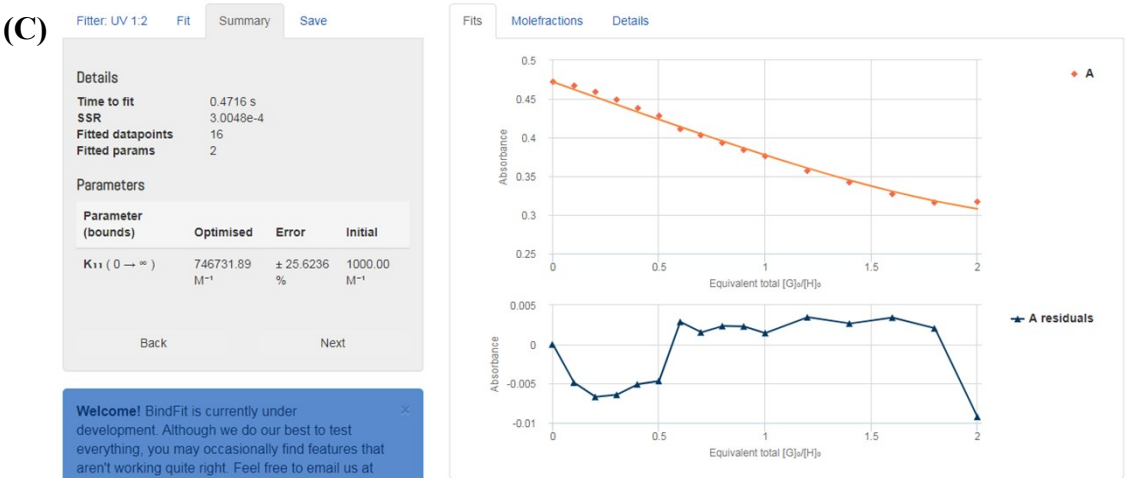


Figure S6. (A) UV-vis titration spectra of **5** (0.02 mM) with addition of 0-3.0 equiv of $CuCl_2$ in 9:1 dichloromethane/acetonitrile. (B) and (C) screenshots taken from the

summary window of the website supramolecular.org. The titration data fitted to 1:1 binding model (B) and 1:2 binding model (C).

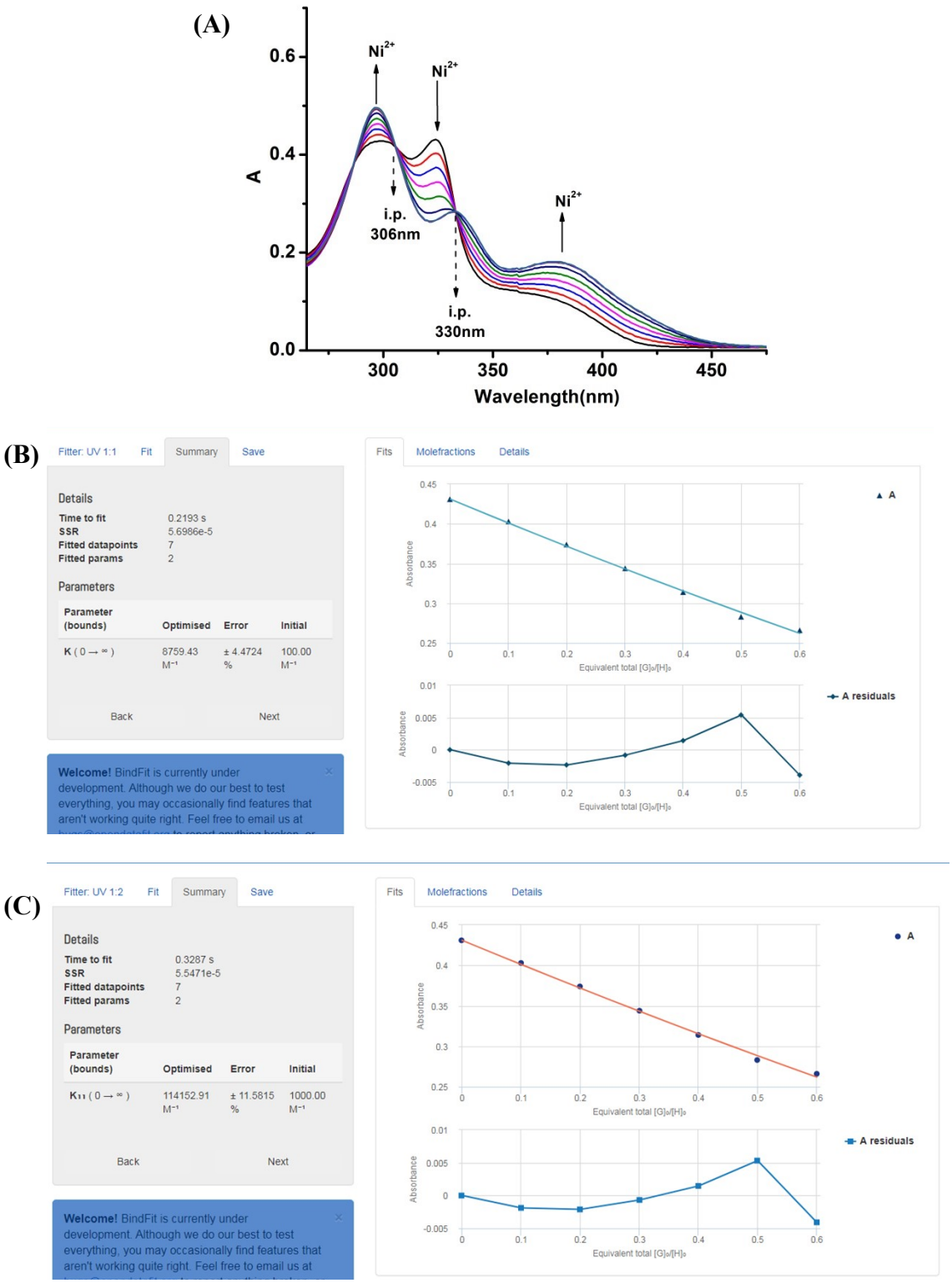


Figure S7. (A) UV-vis titration spectra of **5** (0.02 mM) with addition of 0-3.0 equiv of $NiCl_2$ in 9:1 dichloromethane/acetonitrile. (B) and (C) screenshots taken from the summary window of the website supramolecular.org. The titration data fitted to 1:1 binding model (B) and 1:2 binding model (C).

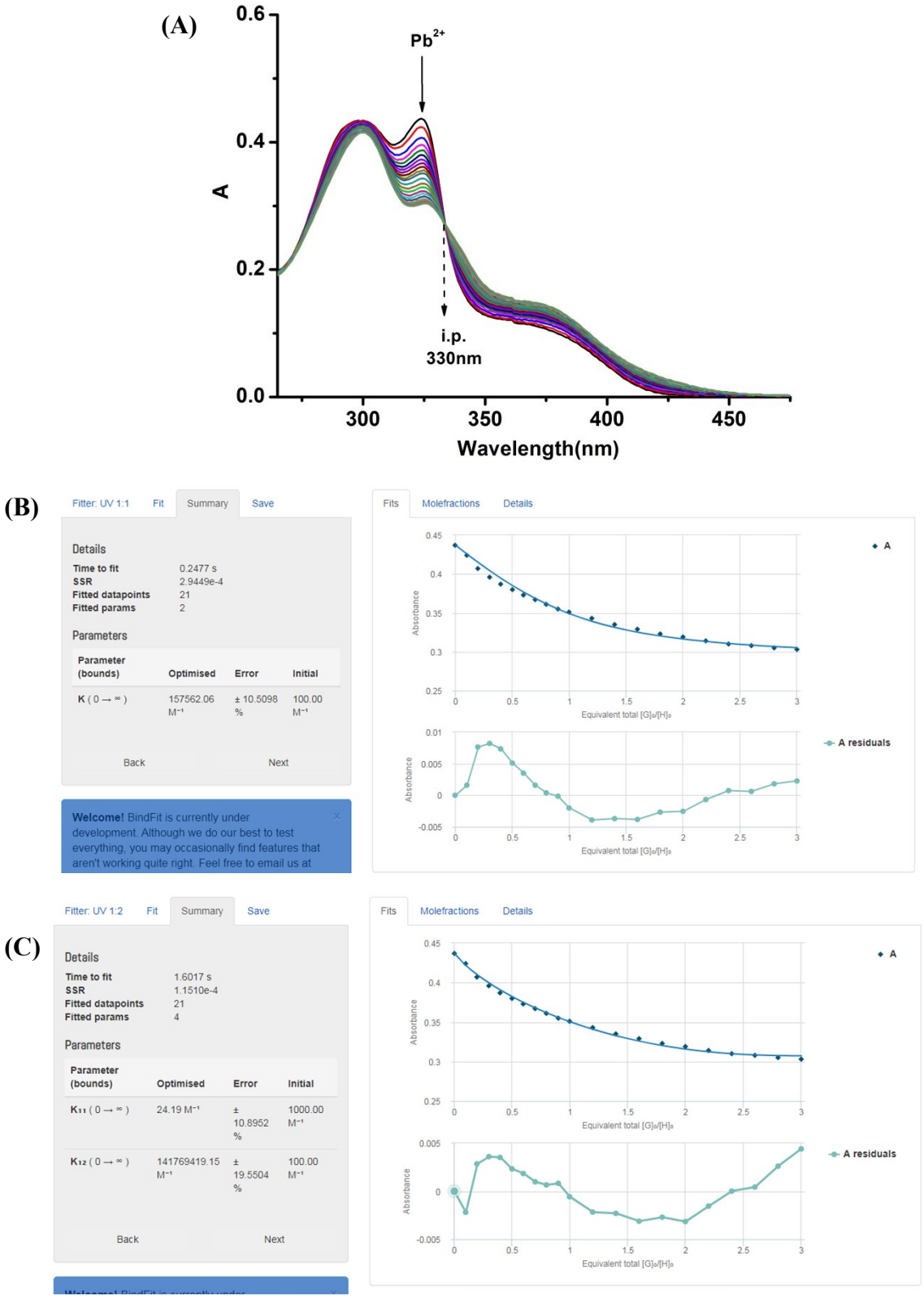


Figure S8. (A) UV-vis titration spectra of **5** (0.02 mM) with addition of 0-3.0 equiv of $PbCl_2$ in 9:1 dichloromethane/acetonitrile. (B) and (C) screenshots taken from the summary window of the website supramolecular.org. The titration data fitted to 1:1 binding model (B) and 1:2 binding model (C).

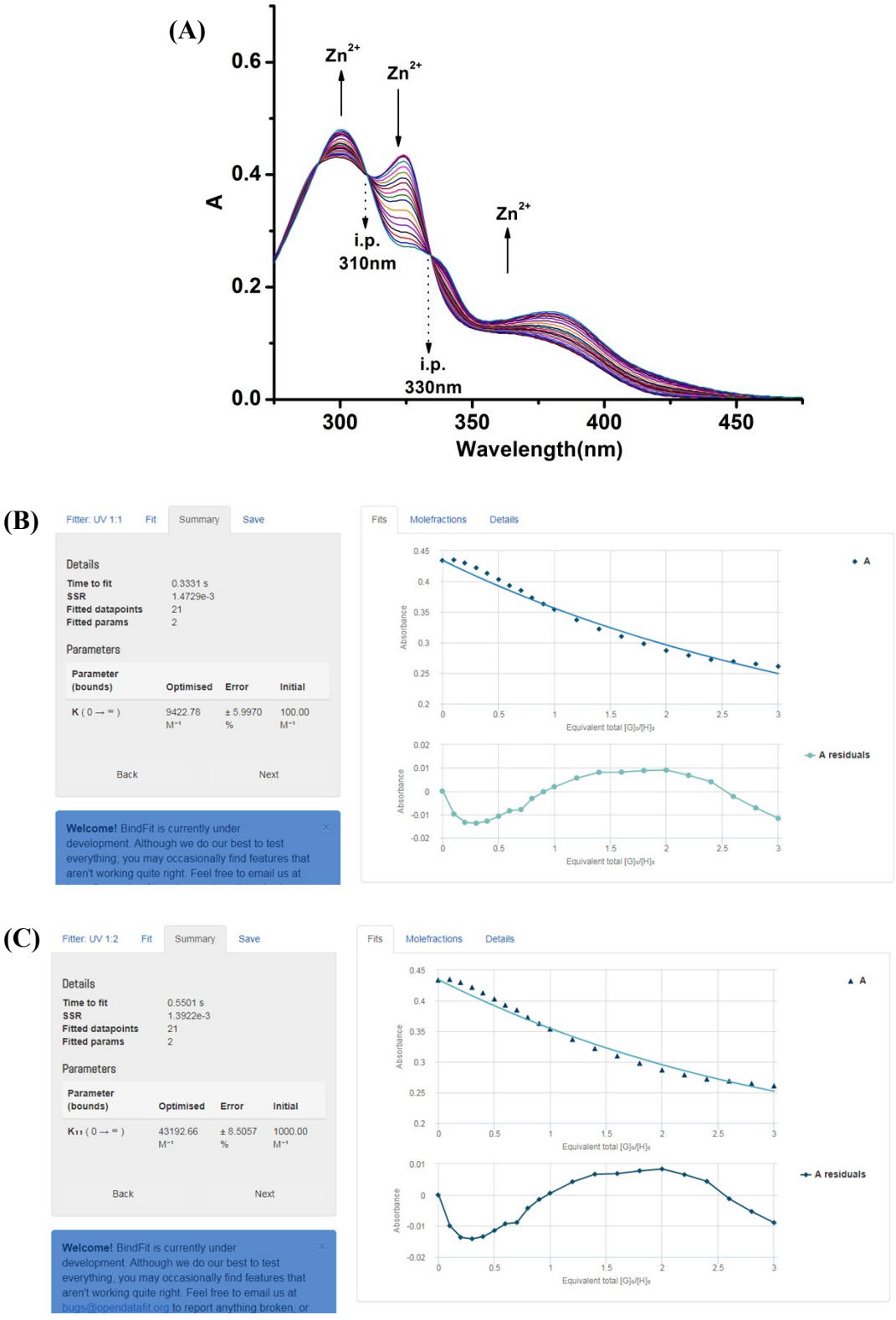


Figure S9. (A) UV-vis titration spectra of **5** (0.02 mM) with addition of 0-3.0 equiv of $ZnCl_2$ in 9:1 dichloromethane/acetonitrile. (B) and (C) screenshots taken from the summary window of the website supramolecular.org. The titration data fitted to 1:1 binding model (B) and 1:2 binding model (C).

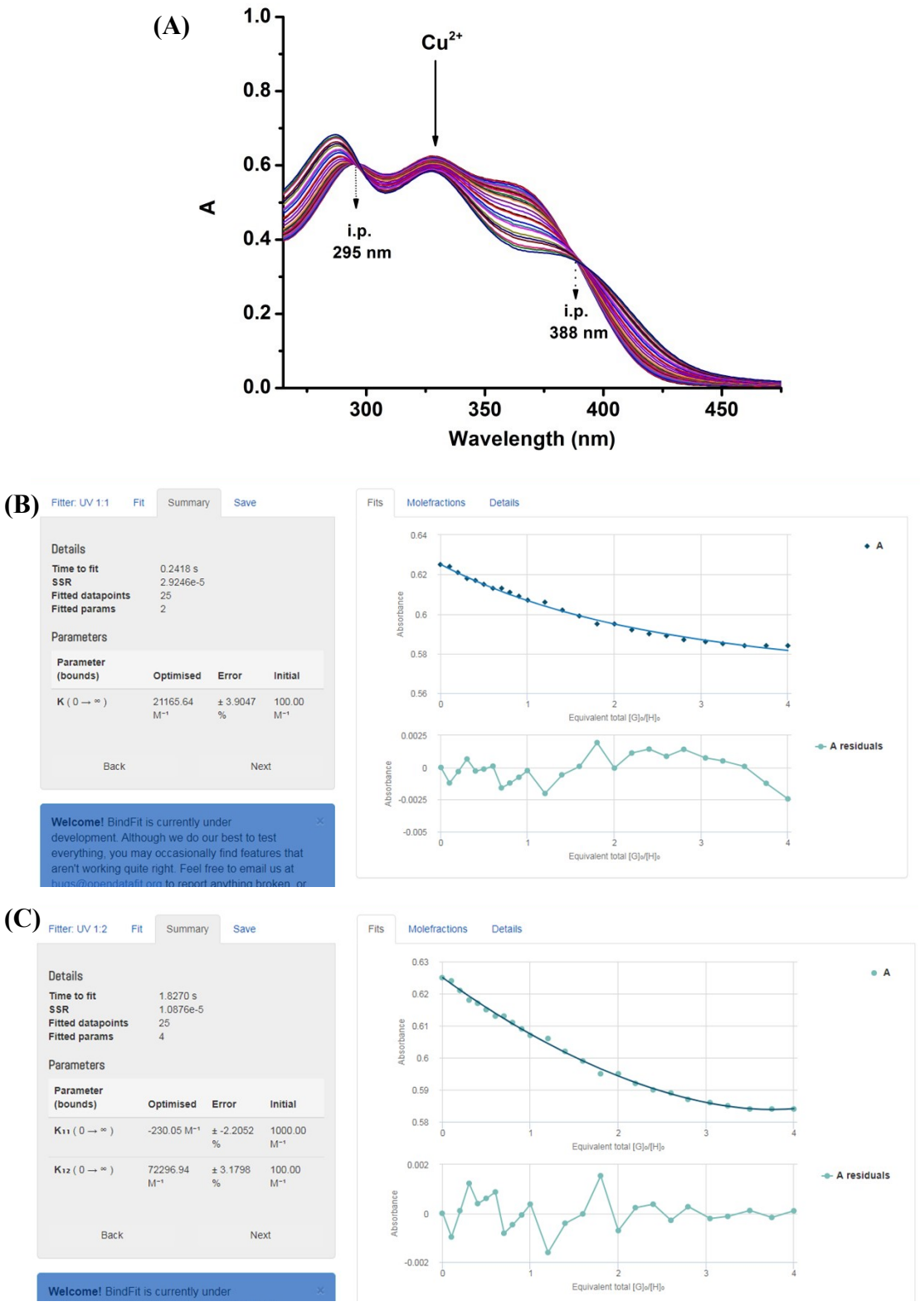


Figure S10. (A) UV-vis titration spectra of **6** (0.02 mM) with addition of 0-4.0 equiv of $CuCl_2$ in 9:1 dichloromethane/acetonitrile. (B) and (C) screenshots taken from the summary window of the website supramolecular.org. The titration data fitted to 1:1 binding model (B) and 1:2 binding model (C).

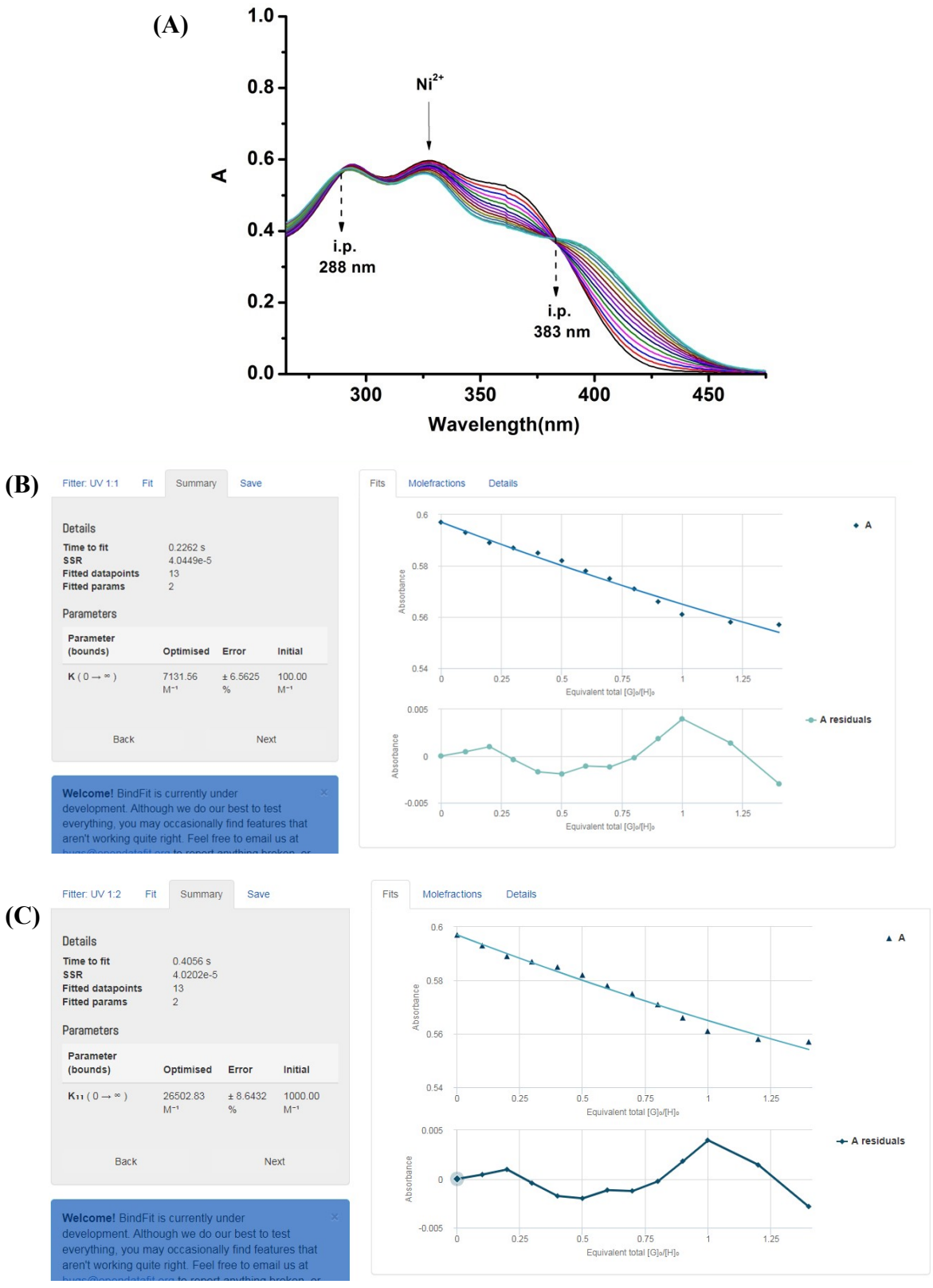


Figure S11. (A) UV-vis titration spectra of **6** (0.02 mM) with addition of 0-1.4 equiv of $NiCl_2$ in 9:1 dichloromethane/acetonitrile. (B) and (C) screenshots taken from the summary window of the website supramolecular.org. The titration data fitted to 1:1 binding model (B) and 1:2 binding model (C).

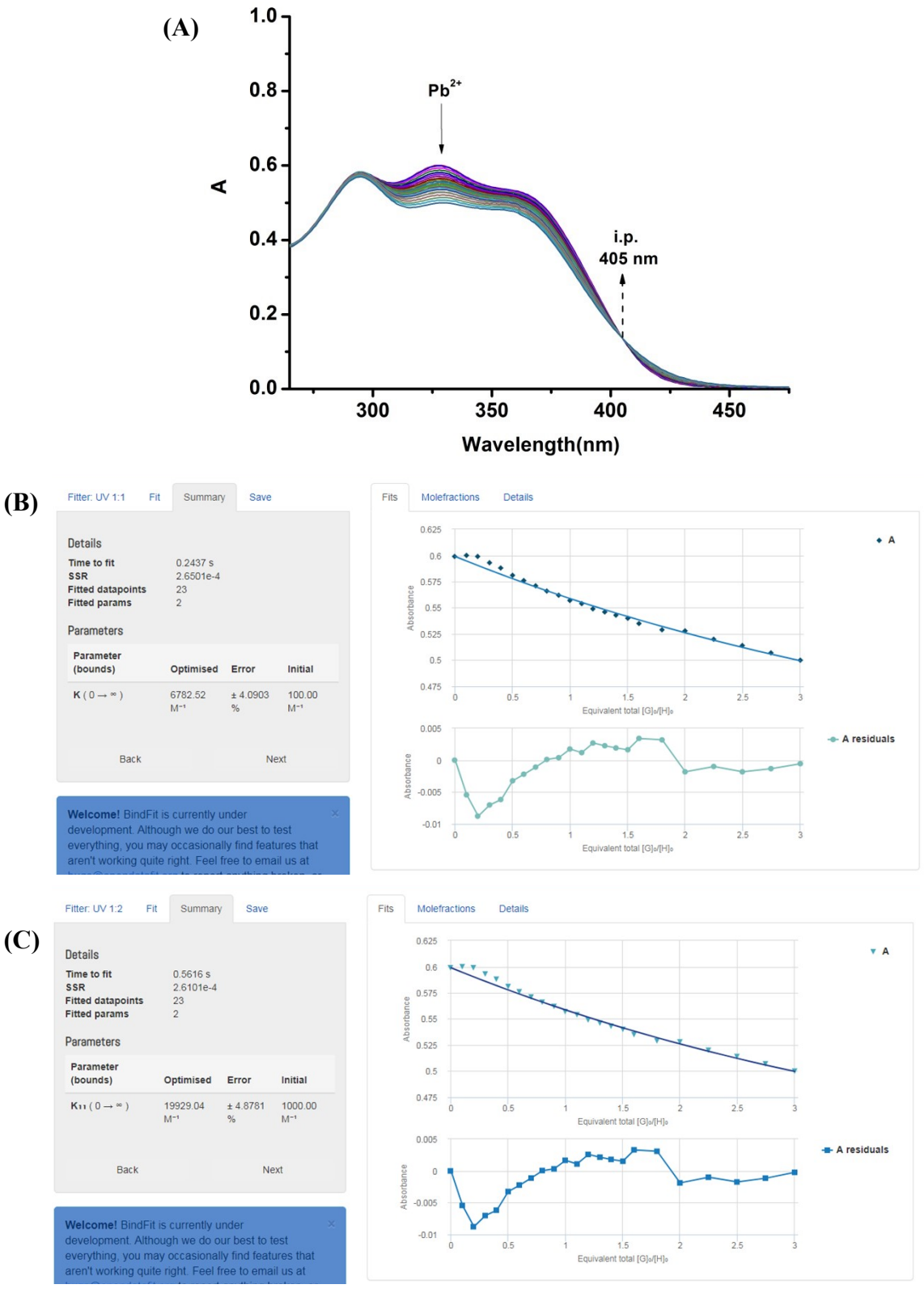


Figure S12. (A) UV-vis titration spectra of **6** (0.02 mM) with addition of 0-3.0 equiv of $PbCl_2$ in 9:1 dichloromethane/acetonitrile. (B) and (C) screenshots taken from the summary window of the website supramolecular.org. The titration data fitted to 1:1 binding model (B) and 1:2 binding model (C).

Table S1. The calculated binding constants (K^{11}) between **5**, **6** and metal ions.

Ion	K^{11} (M^{-1}) [a]	
	5	**6**
UO_2^{2+}	(1.77± 0.05)× 10^3	(1.38± 0.05)× 10^5
Mg^{2+}	/	/
Ca^{2+}	/	/
Mn^{2+}	/	/
Ni^{2+}	(8.76± 0.04)× 10^3	(7.13± 0.06)× 10^3
Cu^{2+}	(9.47± 0.05)× 10^3	(2.12± 0.04)× 10^4
Zn^{2+}	(9.42± 0.06)× 10^3	/
Pb^{2+}	(1.58± 0.11)× 10^5	(6.78± 0.04)× 10^3

[a] The binding constants were calculated from the 1:1 binding data. The 1:2 binding model was ignored because of the large errors associated with the fitting of the binding model.

5. Crystal data and structure refinement for X-ray structure

Structure of 6

Empirical formula	C_{44} H_{45} $N_{20}Cl$	
Formula weight	895.45	
Temperature	297 K	
Wavelength	1.54184 Å	
Space group	P 41 21 2	
Unit cell dimensions	a = 12.00341(12) Å	a= 90°.
	b = 12.00341(12) Å	b= 90°.
	c = 64.3711(14) Å	g = 90°.
Volume	9274.7(3) $Å^3$	
Z	8	
Density (calculated)	1.283 Mg/m^3	
F(000)	3752	
Completeness to theta = 26.000°	99.9 %	
Absorption correction	spherical harmonics	

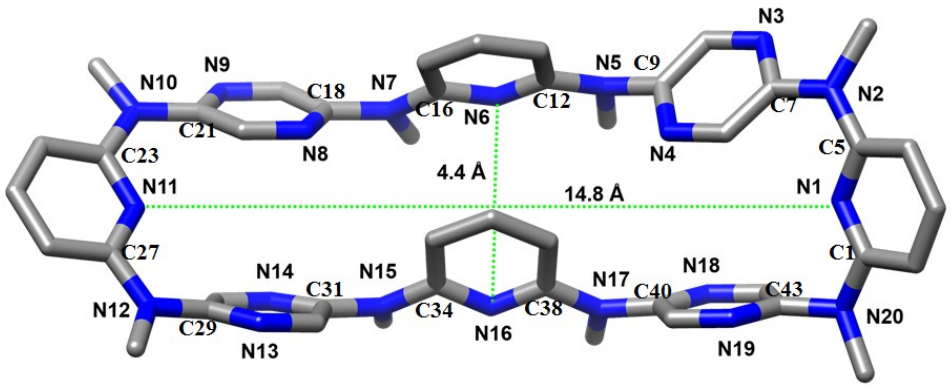


Figure S13. X-ray molecular structure of **6** with top view. Selected bond lengths [Å]: N(2)-C(5), 1.409; N(2)-C(7), 1.382; N(5)-C(9), 1.417; N(5)-C(12), 1.383; N(7)-C(16), 1.385; N(7)-C(18), 1.409; N(10)-C(21), 1.408; N(10)-C(23), 1.386; N(12)-C(27), 1.389; N(12)-C(29), 1.414; N(15)-C(31), 1.391; N(15)-C(34), 1.403; N(17)-C(38), 1.390; N(17)-C(40), 1.397; N(20)-C(43), 1.424; N(20)-C(1)1.407. Selected angles (deg): C(5)-N(2)-C(7), 121.95; C(9)-N(5)-C(12), 120.29; C(16)-N(7)-C(18), 124.60; C(21)-N(10)-C(23), 122.71; C(27)-N(12)-C(29), 119.08; C(31)-N(15)-C(34), 121.79; C(38)-N(17)-C(40), 123.36; C(43)-N(20)-C(1), 117.89.

6. Copies of ^{1}H , ^{13}C NMR spectra and HRMS spectra

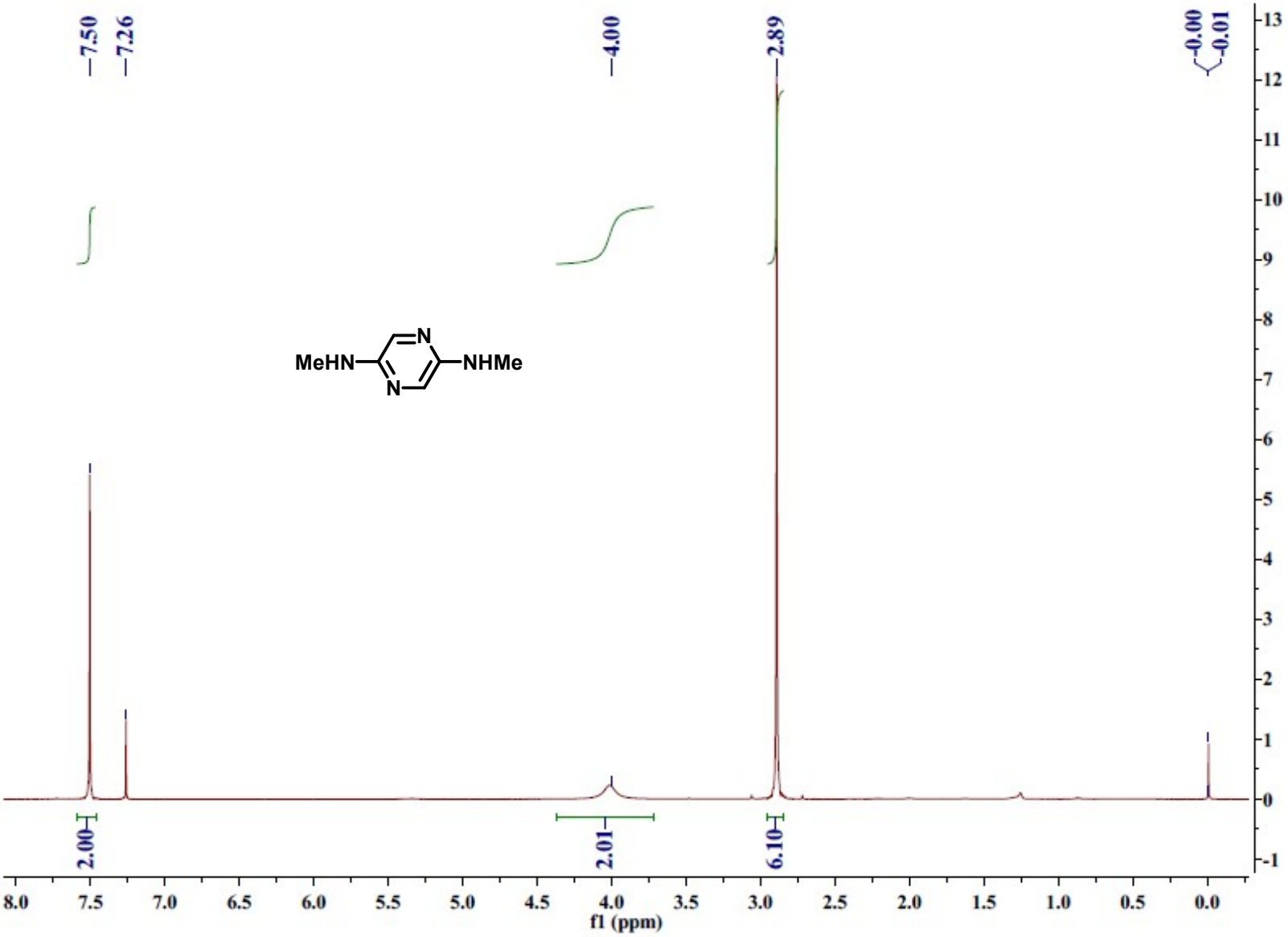


Figure S14. [1] H NMR spectrum of **3**

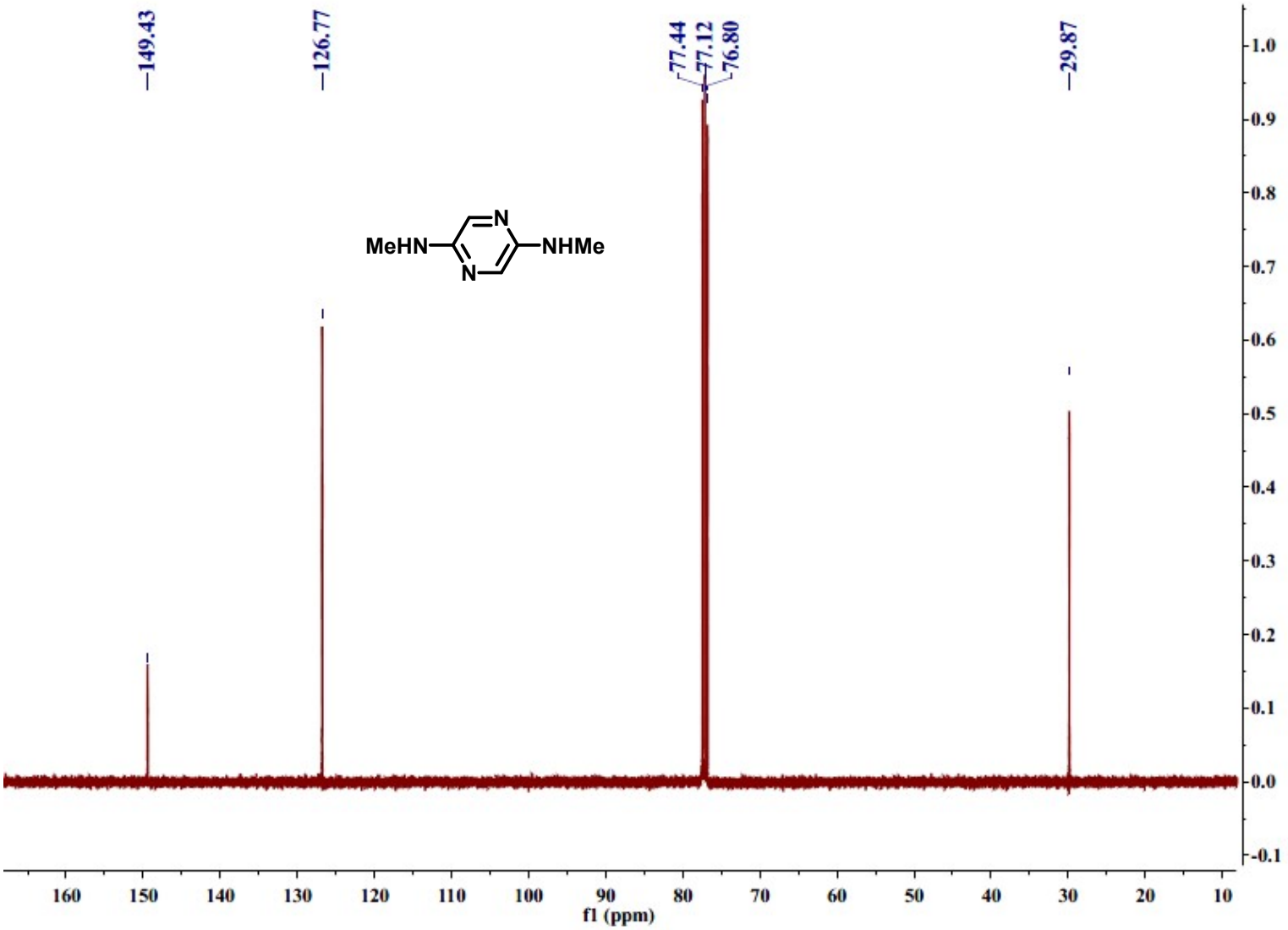


Figure S15. [13] C NMR spectrum of **3**

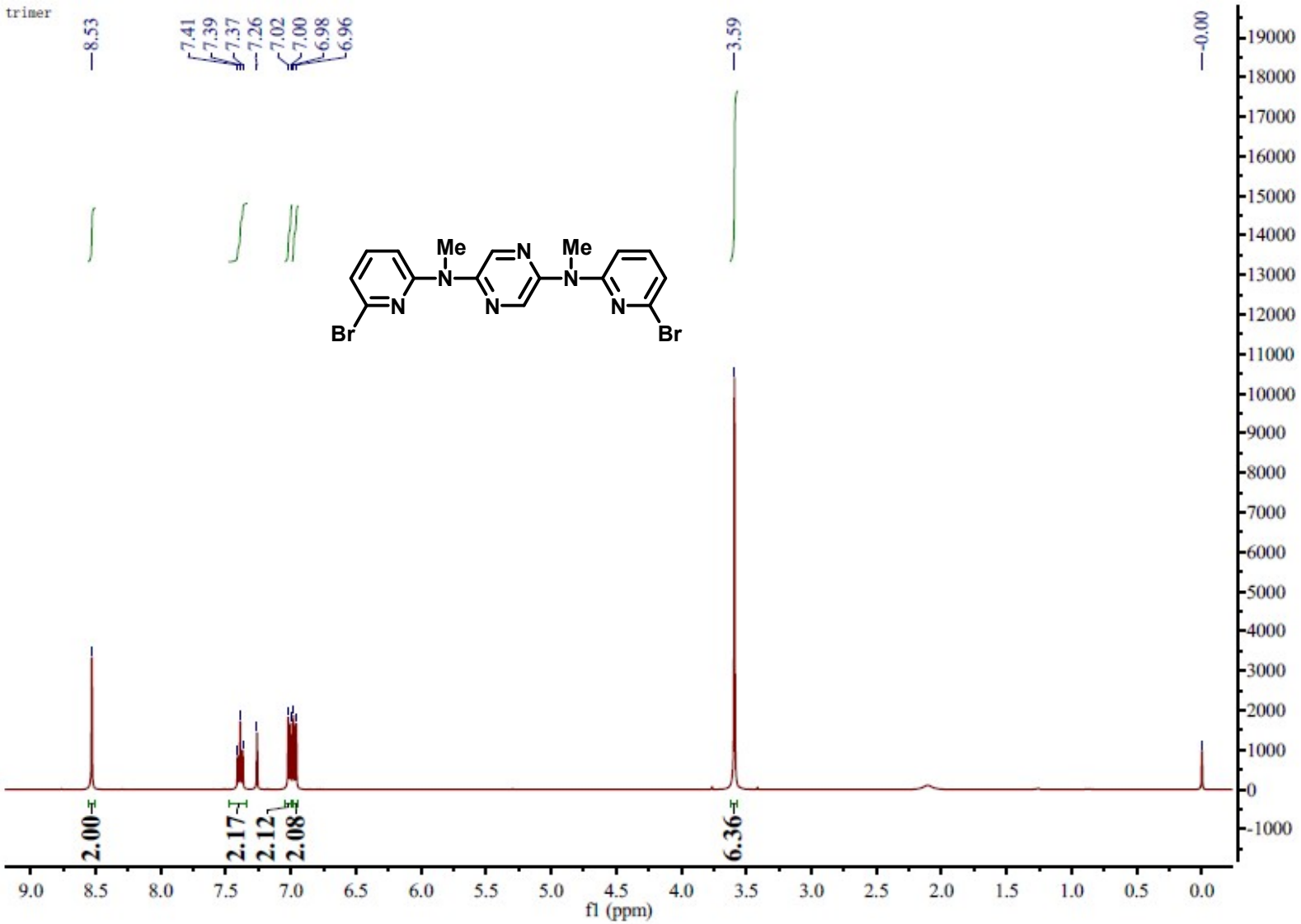


Figure S16. [1] H NMR spectrum of **4**

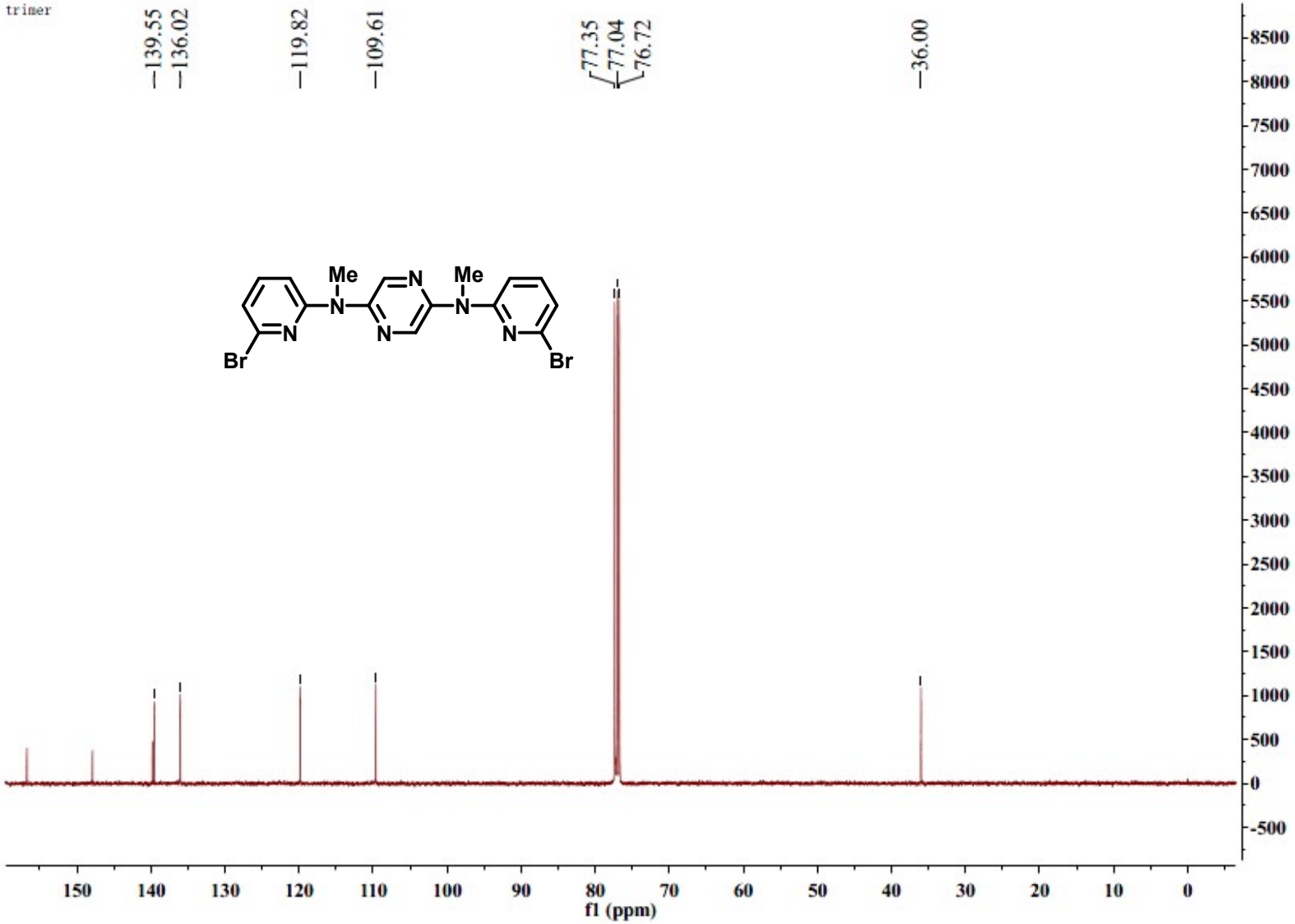


Figure S17. ^{13}C NMR spectrum of **4**

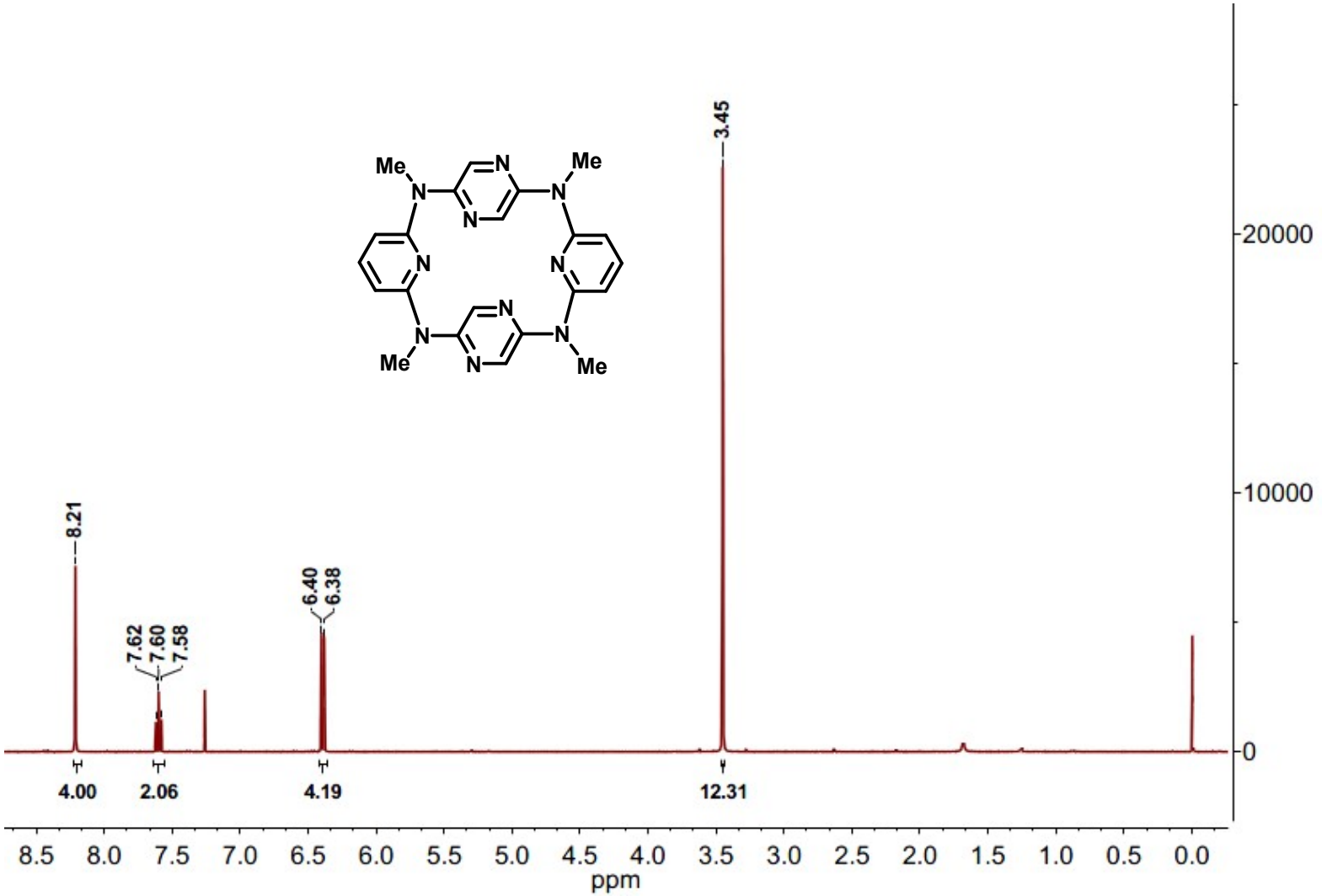


Figure S18. [1] H NMR spectrum of **5**

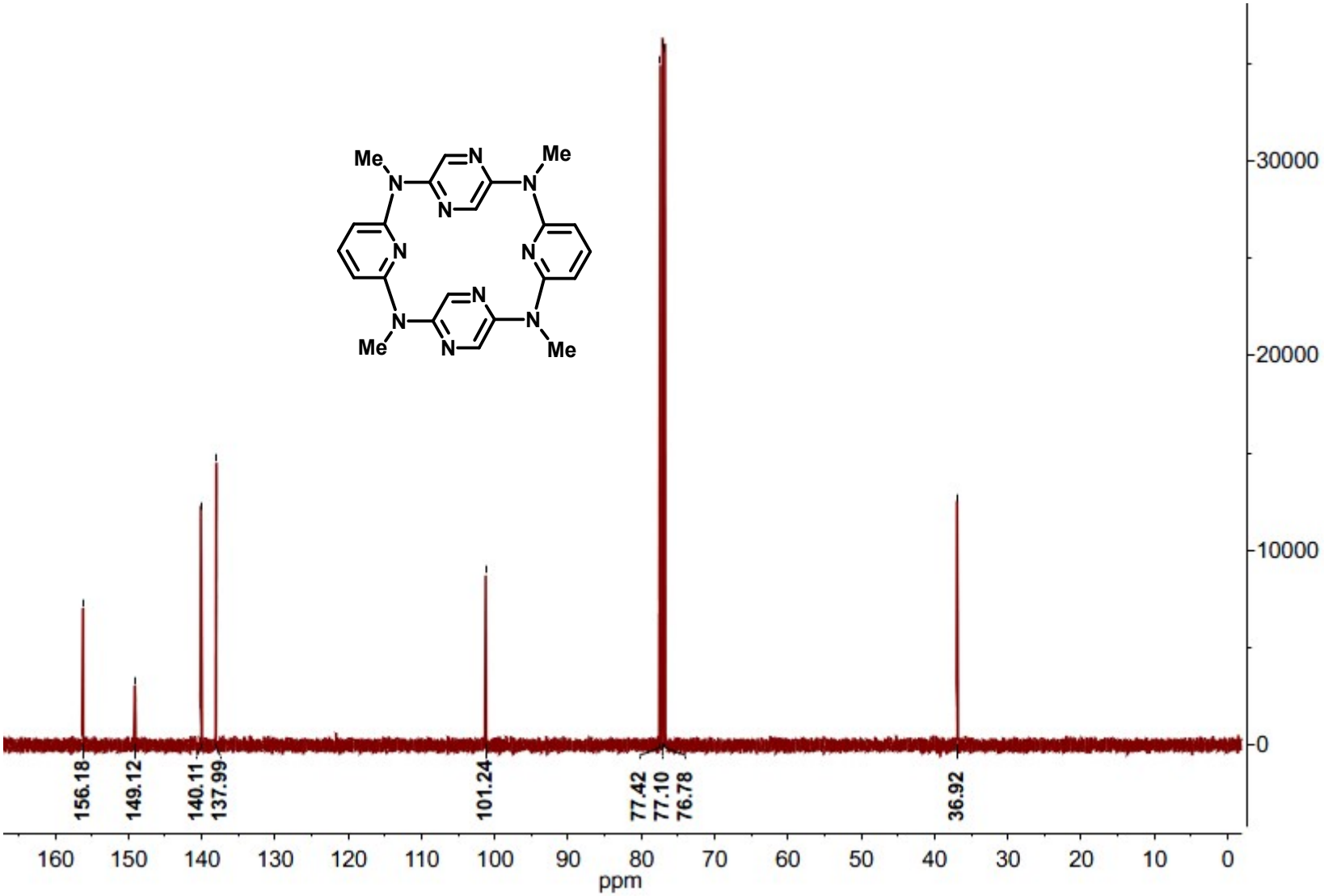


Figure S19. ^{13}C NMR spectrum of **5**

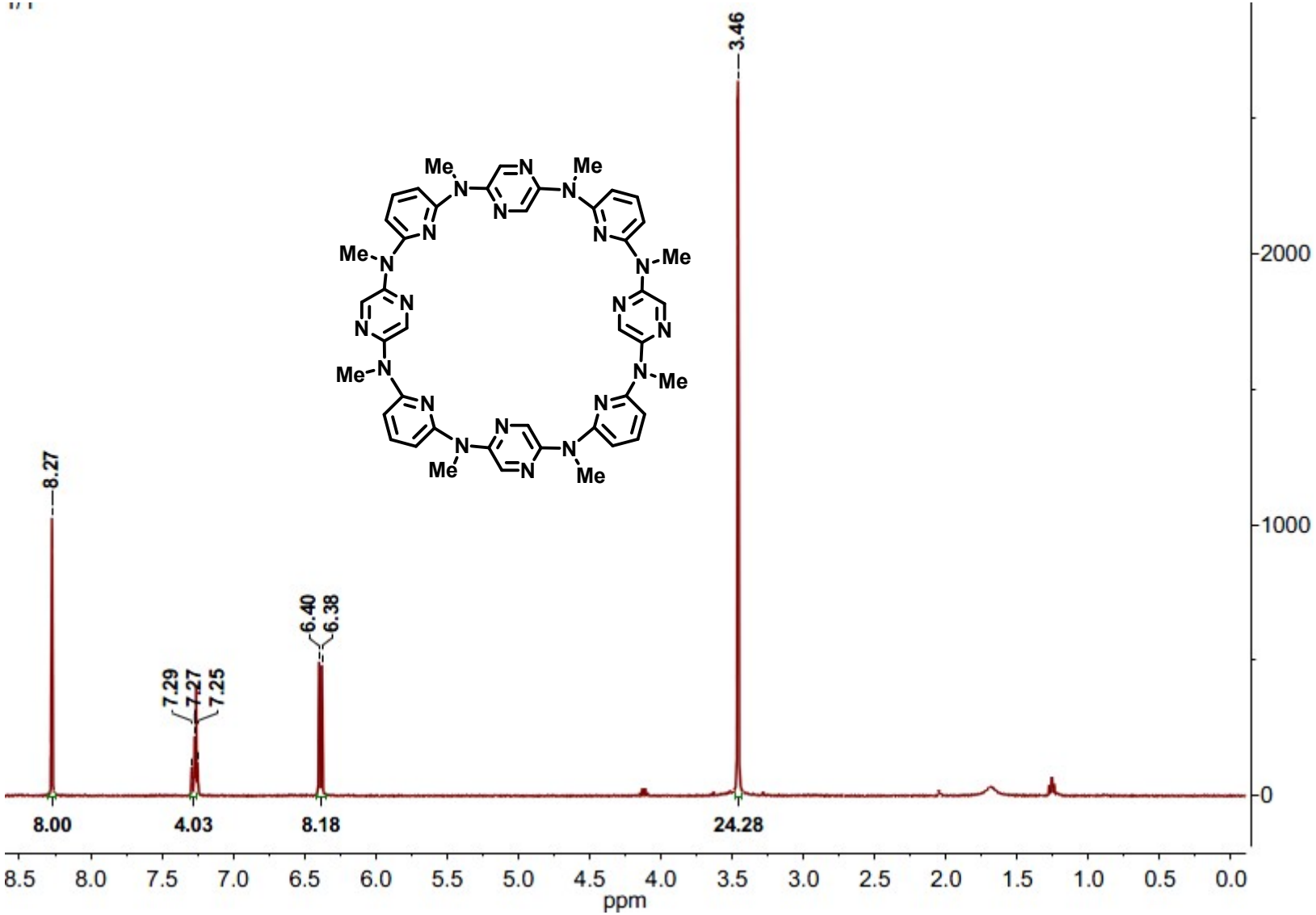


Figure S20. [1] H NMR spectrum of **6**

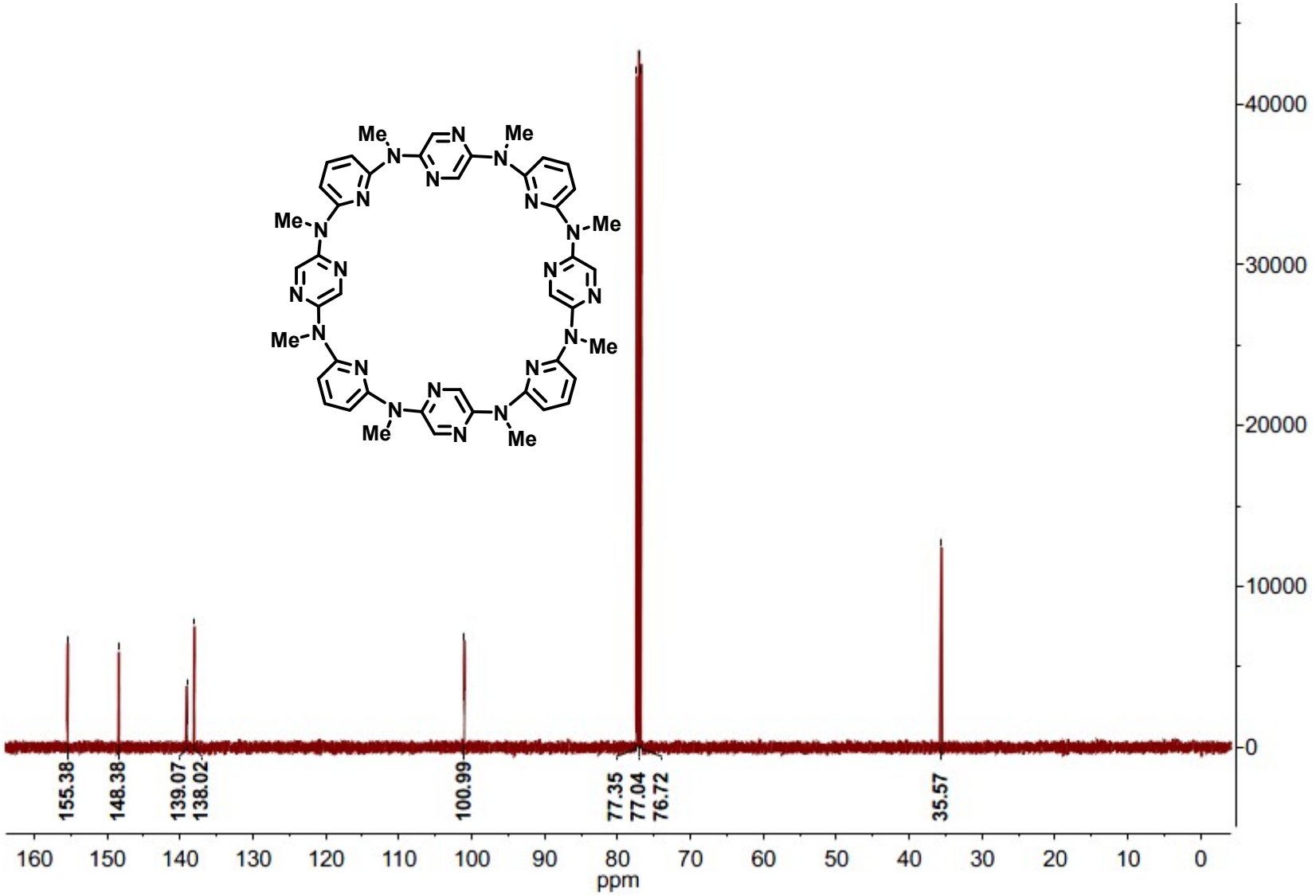


Figure S21. ^{13}C NMR spectrum of **6**

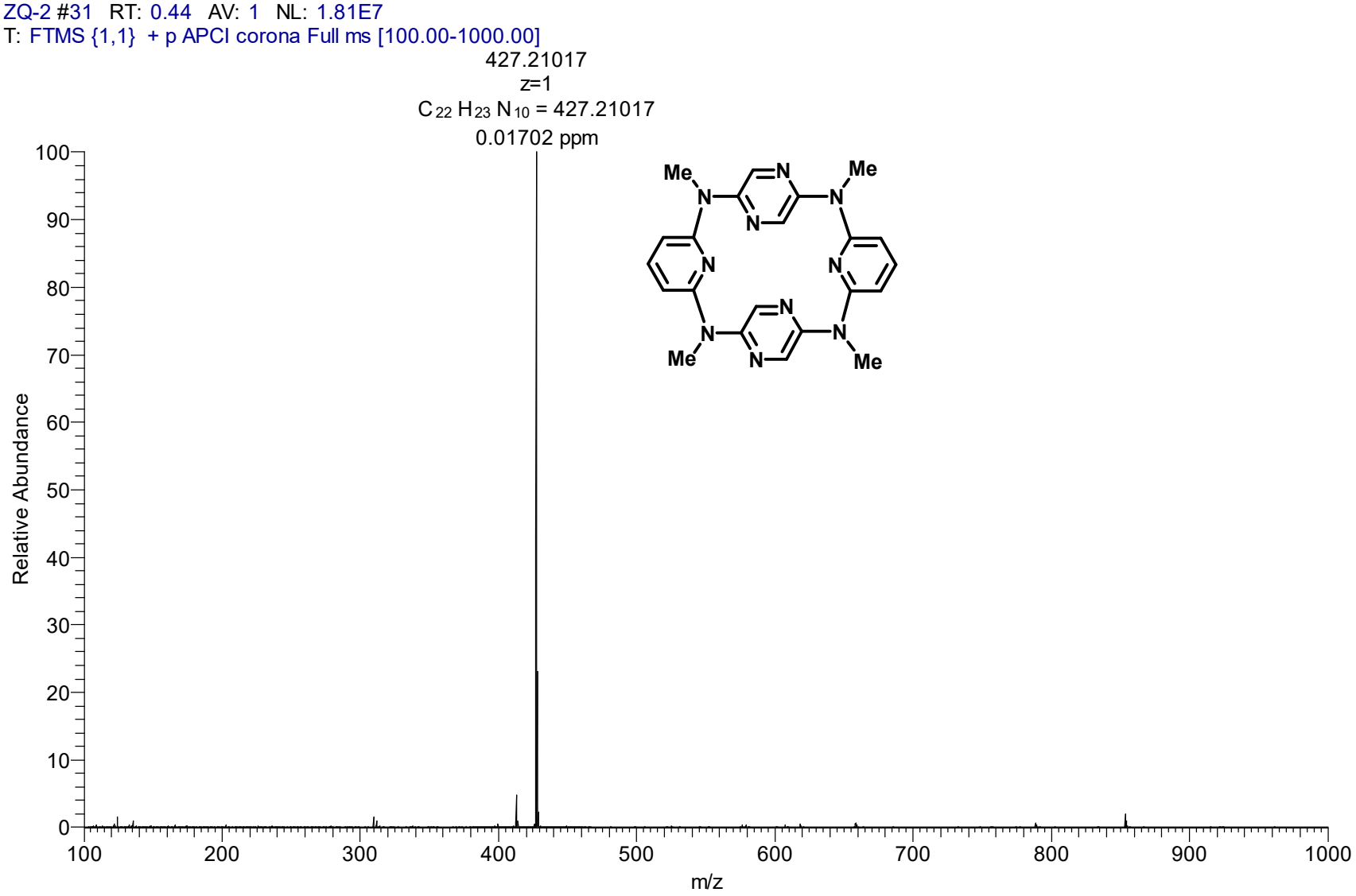


Figure S22. Mass spectrum of **5**

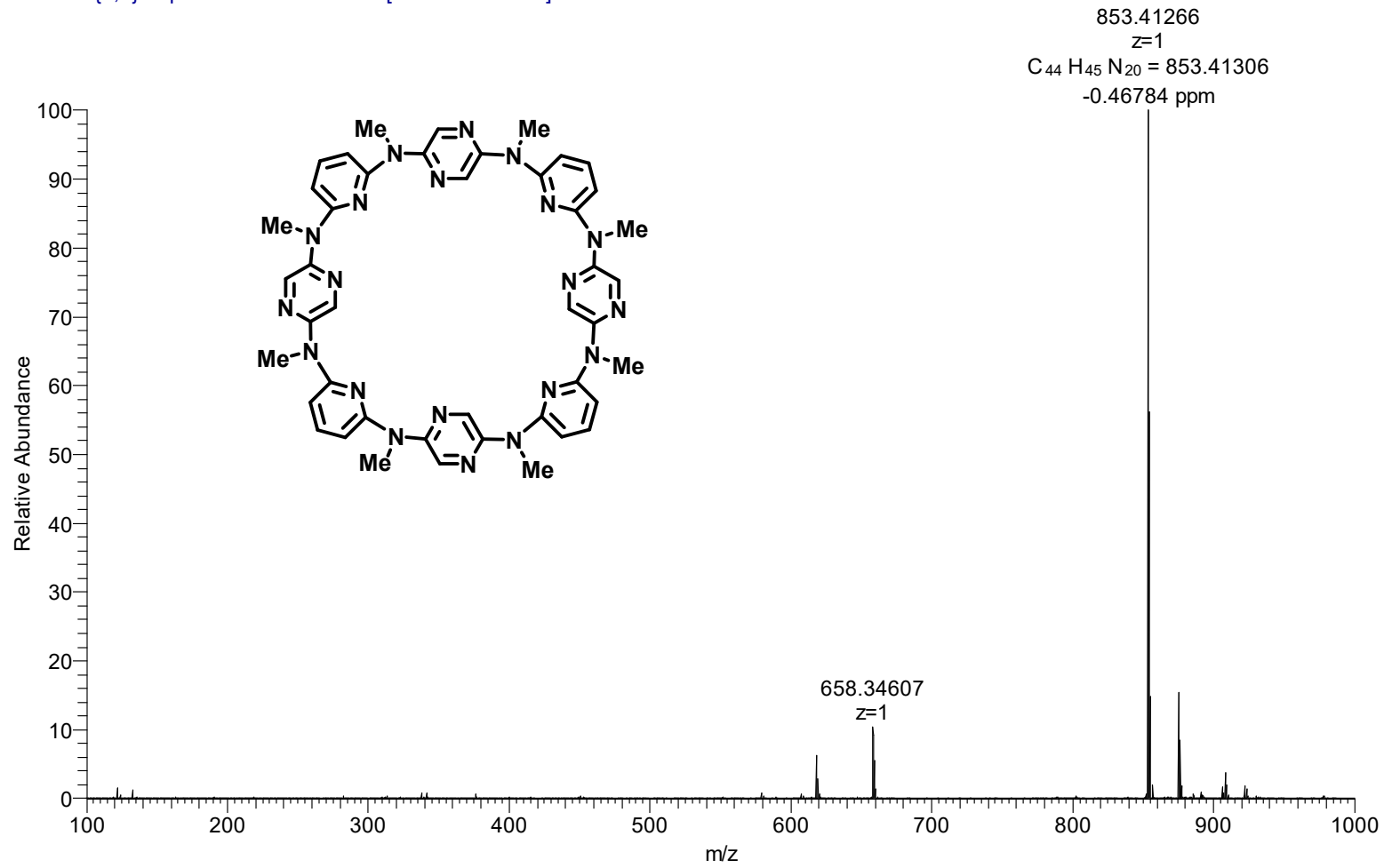


Figure S23. Mass spectrum of **6**

7. The DFT computational results

The quantum chemical calculations were carried out with the Gaussian 09 software package[1] using the B3LYP functional.[2, 3] For carbon, nitrogen, oxygen and hydrogen atoms, the 6-31G (d) basis set was used. For uranium, the Stuttgart RSC 1997 effective core potential (ECP) was used.[4-6] Thus, the ground-state geometry was fully optimized by density functional theory (DFT) at the level of B3LYP/6-31G(d), SDD-MWB60. The optimized structures by DFT methods were below.

5:

N	-2.83958800	0.02222300	0.06140300
C	-3.52692100	-1.09075000	-0.22359700
C	-4.91242200	-1.06588300	-0.49511700
H	-5.46921000	-1.96516700	-0.72357300
C	-4.83901500	1.33627500	-0.19064500
H	-5.32921500	2.30147600	-0.19883500
C	-3.46025900	1.20477600	0.05911400
C	-1.40336100	-2.29326300	-0.06691100
C	-0.77154000	-3.01899600	0.94226600
H	-1.34745100	-3.59021800	1.66809600
C	-1.27791900	2.31621800	0.22149300
C	-0.63789300	1.61844800	-0.83109500
H	-1.20999300	1.05274800	-1.55635300
N	2.83958800	-0.02222200	0.06143700
C	3.46025800	-1.20477600	0.05916200
C	4.83901700	-1.33627600	-0.19058000
H	5.32921700	-2.30147700	-0.19875900
C	4.91242800	1.06588000	-0.49506500
H	5.46921800	1.96516300	-0.72352000
C	3.52692400	1.09074900	-0.22356100
C	1.27791600	-2.31621700	0.22152100
C	0.63790300	-1.61845400	-0.83107800

H	1.21001200	-1.05275900	-1.55633400
C	1.40336200	2.29326200	-0.06690700
C	0.77152800	3.01900200	0.94225800
H	1.34743100	3.59022900	1.66809100
N	0.67846200	1.62261200	-0.97584600
N	-0.55877600	3.04536600	1.07728400
N	-0.67845000	-1.62261800	-0.97584600
N	0.55876300	-3.04536000	1.07730800
C	5.54809900	-0.17029000	-0.46499000
C	-5.54809300	0.17028800	-0.46505600
H	6.61347000	-0.22811500	-0.67378100
H	-6.61346200	0.22811100	-0.67386000
N	2.81845800	2.28715400	-0.18519800
N	2.67571200	-2.32823700	0.36068500
N	-2.67571600	2.32823900	0.36063900
N	-2.81845600	-2.28715500	-0.18521900
C	-3.32196200	3.51470600	0.91695200
H	-4.05177000	3.22669900	1.68006200
H	-2.55571100	4.13421900	1.37970500
H	-3.83632300	4.09589700	0.13913600
C	3.52210600	3.55266600	-0.35038700
H	2.80748900	4.36858000	-0.23875200
H	4.31260200	3.67545200	0.40071500
H	3.97658100	3.63563100	-1.34792300
C	3.32195100	-3.51470000	0.91701300
H	4.05175200	-3.22668900	1.68012900
H	2.55569500	-4.13420900	1.37976200
H	3.83631900	-4.09589700	0.13920700
C	-3.52210200	-3.55266700	-0.35040900
H	-4.31260700	-3.67545100	0.40068400
H	-3.97656600	-3.63563700	-1.34795000

H	-2.80748600	-4.36858100	-0.23876300

6:

N	4.64023700	-2.41604800	1.12469100
N	0.00044300	-2.55878600	1.39171900
N	7.34499300	-0.25222200	-0.89814300
N	-2.28348700	-2.42799100	1.79319400
N	3.89654700	1.70036000	-0.15933900
C	-3.58513500	-2.36841000	1.29995900
N	4.61921800	-2.82800100	-1.63373600
C	5.75159400	-2.33189700	0.39779700
H	6.67622500	-2.13070000	0.93012500
C	-1.15952900	-1.97300500	1.07025700
N	-3.77209000	1.50467000	-0.22100300
C	1.12873600	-2.14172100	0.79914000
N	2.31794500	-2.76728300	1.22645500
C	3.49452200	-2.67452500	0.47526000
C	5.74601800	-2.48625400	-0.99676700
C	3.51061000	-2.93600600	-0.90797800
H	2.60408000	-3.23546400	-1.42761700
N	6.92675600	-2.37245700	-1.76551700
C	6.22123400	1.99775000	0.35073700
N	-0.02256000	2.65976600	1.11823900
C	1.13943700	-1.11460900	-0.15910200
H	2.06385200	-0.73515600	-0.57612500
N	-7.38718100	-0.16653000	-0.80198800
C	-3.87952400	-2.38417800	-0.08952500
H	-3.08581500	-2.44167200	-0.82703700
C	7.79393400	-1.29226400	-1.61320100
N	7.58834500	1.88284500	0.01954900

N	-7.46518400	-2.38179600	-0.11202400
C	3.59932000	2.32029700	0.99626300
C	-6.11791800	-2.31667000	0.35082100
C	-0.07487600	-0.51576400	-0.47475200
H	-0.09669100	0.32181300	-1.16476500
C	-1.25260500	-0.92647600	0.13954900
H	-2.17877100	-0.39304300	-0.03911600
N	-5.12274300	-2.36288100	-0.54826500
C	1.18336400	2.68521500	0.53056200
C	8.11133300	0.83258100	-0.74174400
C	-3.55998000	2.66871400	0.42019400
N	2.26173600	2.44035100	1.40110600
C	5.17519600	1.55271600	-0.48685200
H	5.38343700	1.05981600	-1.42808600
N	-4.58921100	-2.35605800	2.18909800
C	1.33936900	2.97476000	-0.83683000
H	2.31075300	2.97948500	-1.30672100
N	5.92441800	2.64722400	1.48102200
C	-2.04137300	-3.03735700	3.10517400
H	-1.57595700	-4.02217500	2.99416800
H	-2.99577400	-3.12563100	3.61977000
H	-1.36777900	-2.40517100	3.68934300
C	9.07301400	-1.29922900	-2.20547200
H	9.44016300	-2.15250800	-2.76074100
C	-1.12544100	2.89295900	0.39622000
C	-4.95439100	1.30830500	-0.78944100
H	-5.10678400	0.36744600	-1.30253800
C	0.18275800	3.22870000	-1.57054100
H	0.26862900	3.46421100	-2.62865100
C	-5.98509400	2.28159500	-0.71770600
N	-2.33026300	2.88143500	1.10066100

C	4.64222400	2.81952800	1.79487800
H	4.43930200	3.38116400	2.70311600
N	-7.23567600	2.11492000	-1.32760900
C	9.40193400	0.92450400	-1.30279800
H	10.01312100	1.81002000	-1.19256900
C	-7.85076700	0.86356800	-1.51596800
N	-5.75420200	3.45243400	-0.11321700
C	-5.83626700	-2.32082100	1.71453300
H	-6.64278200	-2.29849600	2.44495800
C	-7.97194300	-1.36851600	-0.91919100
C	-4.55448000	3.64265500	0.44178100
H	-4.37559800	4.60241700	0.92200700
C	9.86132500	-0.16696300	-2.03288600
H	10.85284400	-0.13268200	-2.47722600
C	-8.94621500	0.74573100	-2.39276900
H	-9.30302600	1.58009600	-2.98101900
C	-1.07441800	3.18868000	-0.97935100
H	-1.97391600	3.38887600	-1.54823600
C	2.43796500	-3.16681900	2.63038300
H	2.75849900	-2.33062800	3.26471200
H	3.17966800	-3.96338900	2.71436600
H	1.46614900	-3.52852200	2.96239700
C	-2.30915100	2.53604000	2.52401400
H	-1.57542700	3.15406900	3.04450000
H	-2.05140700	1.48070700	2.68653700
H	-3.30255800	2.72711700	2.93696000
C	1.98141700	2.37109600	2.83818300
H	2.79967600	1.84348900	3.33108700
H	1.05240500	1.82447500	2.99340000
H	1.86902100	3.36674000	3.28847100
C	7.15451500	-3.33254900	-2.84195400

H	6.24483000	-3.91594600	-2.97624800
H	7.98713000	-4.00998300	-2.60792900
H	7.37564100	-2.81640300	-3.78250400
C	8.50916700	2.90191600	0.52349300
H	7.98975000	3.48607700	1.27960100
H	8.84739900	3.56784700	-0.28176000
H	9.38436800	2.43105900	0.98230600
C	-9.07665500	-1.58692400	-1.76835500
H	-9.53404000	-2.56169900	-1.87284200
C	-8.06947200	-3.71025300	-0.15774900
H	-7.91576000	-4.21156400	-1.12537500
H	-9.14460300	-3.64802400	0.04056700
H	-7.61510400	-4.32448700	0.62174300
C	-9.54738700	-0.50406000	-2.49960700
H	-10.38814900	-0.63780600	-3.17552700
C	-7.99029200	3.31250800	-1.70485300
H	-7.50264300	4.17733000	-1.26204800
H	-9.01545000	3.24964000	-1.32709000
H	-8.02164500	3.43230000	-2.79545700

[5+UO_2^{2+}]

N	-2.58428900	-0.11053000	0.04935700
C	-3.14937700	-1.33222800	-0.18576900
N	-2.39930400	-2.52815600	0.08073400
N	-2.84755300	2.29010100	0.22158800
N	2.82819800	-2.28205900	-0.07142200
N	2.46161300	2.58190500	-0.07759000
C	3.69724400	-3.35548100	0.48439600
H	4.21704100	-2.98256600	1.36775200
H	3.06853300	-4.19451900	0.76705700

H	4.41977300	-3.69103500	-0.26549700
C	-3.00361700	-3.50193200	1.02557400
H	-2.32660100	-3.67096500	1.86804900
H	-3.92760300	-3.08203300	1.41692300
H	-3.22531500	-4.44976600	0.52660900
C	-3.77650500	3.44129500	0.10679000
H	-4.59648400	3.32574400	0.82002100
H	-3.25299400	4.35348900	0.38480900
H	-4.17057000	3.54230500	-0.90814400
C	3.13749400	3.68475800	-0.81727000
H	3.80930500	4.23680100	-0.15338900
H	3.69801400	3.26468700	-1.65265700
H	2.37876000	4.36363200	-1.19575000
C	-3.37670000	0.99942800	0.01379900
C	-4.75201400	0.88466300	-0.27646800
H	-5.40038900	1.74689800	-0.27653000
C	-5.28532600	-0.35280900	-0.59294400
H	-6.33401500	-0.43563300	-0.86015900
C	-4.47776100	-1.48784000	-0.55432000
H	-4.87039700	-2.46907000	-0.79220700
C	3.37030700	-0.97240400	-0.11518800
C	3.19456000	1.36638800	0.05528400
C	4.76937400	-0.87598300	-0.15156400
H	5.37679700	-1.75604600	-0.30582000
C	5.37249900	0.35802700	0.02839100
H	6.45455100	0.43884400	0.05496300
C	4.58139000	1.49051700	0.16390400
H	5.03323400	2.45979700	0.32474000
N	2.57592000	0.14460400	-0.03924200
U	-0.04247400	-0.02823600	0.02764900
O	0.09333600	-1.02500100	1.48144400

O	-0.11775000	0.97479600	-1.42500300
C	-1.52041100	2.61416900	0.51720000
C	-0.85725800	3.72751000	-0.15338200
H	-1.40786000	4.52863300	-0.63857800
C	0.56367300	2.08059600	1.41775000
C	1.18243300	2.79129600	0.37905500
H	1.09869800	1.58826800	2.22576700
C	-1.14858300	-2.78403500	-0.39586200
C	-0.31380700	-3.86482500	0.13825800
C	0.78600500	-1.99413800	-1.44542300
H	-0.72773800	-4.78860600	0.53239700
C	1.54688400	-2.62961700	-0.46089900
H	1.20371000	-1.44388300	-2.28357500
N	-0.59039400	-2.01090600	-1.32784000
N	0.97209300	-3.71912000	0.14192700
N	0.43688700	3.75924100	-0.23794500
N	-0.80439400	1.93067800	1.39759100

[6+UO_2^{2+}]

N	-2.43107500	4.45059200	-0.34847700
N	2.05859000	4.06948700	0.74077400
N	-6.02274300	0.56066100	-0.43470700
N	4.38973300	3.98658800	0.86834400
N	-4.41917900	-2.74590100	0.13952900
C	5.55071800	3.19596800	0.72220300
N	-2.41243800	1.76174700	-1.00601600
C	-3.50565000	3.87833800	-0.91396100
H	-4.35649200	4.52353800	-1.10292100
C	3.16471000	3.40626800	1.15842400
N	4.03614200	-1.58863300	0.69290600

C	0.84793900	3.57094400	1.03353600
N	-0.26898200	4.30525600	0.50765900
C	-1.32628700	3.68814400	-0.08646600
C	-3.52403600	2.52255900	-1.22531300
C	-1.31908000	2.30763000	-0.47054000
H	-0.45538300	1.67549100	-0.33033400
N	-4.59293600	1.75400200	-1.83025300
N	-0.41174500	-2.85103200	1.29963300
C	0.65360300	2.42172000	1.80593100
H	-0.33661200	2.10264000	2.10717800
N	7.97034700	-1.21254900	-0.40199600
C	5.53052900	1.99303100	-0.00235600
H	4.62648200	1.63438400	-0.48124100
C	-5.88545600	1.69559500	-1.17309500
N	-7.34335900	-0.78757500	1.05787700
N	8.92118400	0.87194900	0.26087800
C	-3.98274400	-3.10456900	1.36744600
C	7.78807000	1.65544900	0.41644900
C	1.80043900	1.72537100	2.22186600
H	1.70198000	0.83537500	2.83255400
C	3.06222700	2.19416300	1.89080600
H	3.94838300	1.67215900	2.22322200
N	6.62573700	1.24116700	-0.14763200
C	-1.60438600	-2.97844100	0.70778200
C	-7.20439500	0.32616300	0.22406400
C	3.14374800	-2.59677800	0.57270000
N	-2.65259600	-3.38086200	1.59148600
H	-6.03330100	-2.08685500	-1.02744500
N	6.71357100	3.65174800	1.23271200
C	-1.79245400	-2.73168400	-0.68389300
H	-2.63688600	-3.15451600	-1.20997500

N	-6.06037400	-2.35577100	2.30669800
C	4.47400600	5.43634600	0.59884300
H	4.15969800	5.66546000	-0.42474800
H	5.50874700	5.74089800	0.75244100
H	3.83022900	5.97782600	1.29321900
C	-6.89009100	2.63520100	-1.33206500
H	-6.74874100	3.51380700	-1.94747700
C	0.69807600	-2.53207900	0.57566400
C	5.26213700	-1.73628100	0.16526400
H	5.95401500	-0.91269500	0.24405100
C	-0.62886900	-2.37103000	-1.42598800
H	-0.72140700	-2.22742500	-2.49842200
C	5.63285900	-2.94863600	-0.49650600
N	1.88383600	-2.48024800	1.24852000
C	-4.95391600	-3.07272700	2.43615300
H	-4.79736400	-3.56919700	3.38335400
N	6.88553200	-3.23163900	-1.03674900
C	-8.27095900	1.24600700	0.09209500
H	-9.21573600	1.05745600	0.57935600
C	7.95339600	-2.30996400	-1.18203300
N	4.70742100	-3.93575100	-0.62691000
C	7.82017600	2.90947900	1.08795800
H	8.72865200	3.32806100	1.49810000
C	8.95004100	-0.30217500	-0.54835000
C	3.48596600	-3.77009000	-0.10092200
H	2.78652900	-4.59261700	-0.21312200
C	-8.10887000	2.38907100	-0.67939400
H	-8.93042300	3.08865000	-0.78012700
C	8.97628600	-2.56320500	-2.12215700
H	8.95981700	-3.43120900	-2.76407400
C	0.60366200	-2.24772600	-0.82247200

H	1.48436400	-1.97148100	-1.38571600
C	-0.26244600	5.78415400	0.62081500
H	-0.94664600	6.10829100	1.40994500
H	-0.58170500	6.23052200	-0.32129600
H	0.75702000	6.08664600	0.84783500
C	1.92375500	-2.49708800	2.72632000
H	1.95585700	-3.52331800	3.10896400
H	1.03782200	-2.00268100	3.12318100
H	2.82463900	-1.96634100	3.03779400
C	-2.27613200	-3.92624500	2.92135000
H	-2.36529100	-3.16525500	3.70302700
H	-1.24055700	-4.24608200	2.87298200
H	-2.91100300	-4.78329000	3.15465100
C	-4.66167500	1.87551300	-3.33014000
H	-3.66856400	1.68388000	-3.73800900
H	-4.98978300	2.87678600	-3.62827000
H	-5.35215700	1.12480300	-3.71557800
C	-8.47386000	-0.84794500	2.01988700
H	-8.28233700	-1.66867400	2.70714100
H	-9.41628500	-1.02732200	1.49421200
H	-8.53649000	0.07932200	2.59401200
C	10.00929900	-0.48225400	-1.45247000
H	10.78122800	0.26723500	-1.56844400
C	10.19101500	1.34093700	0.85108900
H	10.58051900	2.23027000	0.34109500
H	10.92772000	0.54238000	0.78536100
H	10.04627200	1.57519100	1.90999100
C	10.01118500	-1.63690800	-2.23622300
H	10.80290300	-1.80091000	-2.95827700
C	7.10628200	-4.59997600	-1.56898600
H	6.40115500	-5.27625800	-1.09588700

H	8.12664000	-4.90935300	-1.33978400
H	6.94121800	-4.63970700	-2.65126100
U	-3.62532900	-0.48078700	-0.80201700
O	-3.84406100	-0.99746700	-2.49317500
O	-3.34449200	-0.10495300	0.92063100
C	-5.66036900	-2.19226900	-0.01378100
C	-6.36623200	-1.78278000	1.10792600

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