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SUPPORTING INFORMATION

Anion directed conformational diversities of an arene based hexa-amide receptor and recognition of $[F_4(H_2O)_6]^{4-}$ cluster

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Table of contents

1.	Material , Instrumentation & Various conformers	2
2.	Experimental Section	2-6
3.	^{1}H, ^{13}C, HRMS &^{19}F spectra of **L**	7-8
4.	^{1}H &^{13}C spectra of complex **1**	9
5.	^{1}H &^{13}C spectra of complex **2**	10
6.	^{1}H &^{13}C spectra of complex **3**	11
7.	Crystallographic tables of complex **1**, **2**, **3** and **L**	12
8.	H-bonding tables of complex **1**, **2**, **3** and **L**	13-14
9.	ITC titration profile	15
10.	Tables for binding constants & binding energies	16
11.	^{1}H NMRtitration profiles of **L** with acetate	17
12.	^{1}H NMRtitration profiles of **L** with fluoride	18
13.	Crystal images	19
14.	DFT optimised structures	20-23
15.	Cartesian coordinates of the optimised structures	24-43

Materials: All reagents, tetrabutylammonium salts, and solventsfor syntheses were purchased fromcommercial sources andused as received. Freshly dried tetrahydrofuran was used for each reaction. The solvents used for crystallization were all of HPLC grade.

Instrumentation:^{1}H NMR spectra were recorded with a 300 MHz Bruker DPX-300. ^{13}C NMR spectra were obtained at75.47 MHz.HRMS experimentswere carried out on a Waters QtoF Model YA 263 massspectrometer in positive ESI mode. Elemental analyses for thesynthesized ligand and complexes were carried out with aPerkin-Elmer 2500 series II elemental analyzer. ITC experiments were performed in VP-ITC instrument.

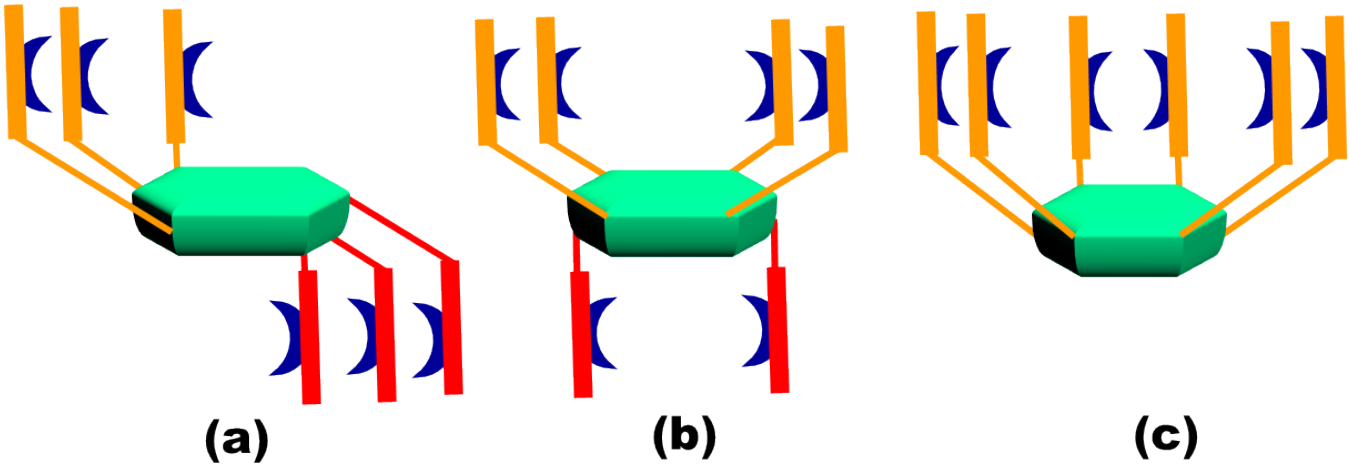

Fig. 1S: Various conformers obtained from hexapodal receptors; (a) *aaabbb[**A**]*, (b) *aabaab[**B**]*, (c) *aaaaaa[**C**]*.

EXPERIMENTAL SECTION

General Synthetic procedure forL:

Hexakis(aminomethyl)benzene (0.303 g, 1.2 mmol) and 1 ml triethylamine were dissolved in 100 ml dry tetrahydrofuran and stirred at 0 ºC for 20 minutes under N_2atmosphere. 2-(trifuromethyl) benzoyl chloride (7.80 mmol, 6.5 eq) were added from a dropping funnel to the reaction mass under N_2atmosphere with constant stirring. Formation of off-white precipitate was observed immediately. The temperature of the reaction was gradually brought to room temperature, and the reaction was stirred continuously for 24 hrs. Subsequently, the reaction mixture was filtered and the solid was washed with THF and water. The precipitate was further washed with diethyl ether and dried in air. ^{1}H NMR, 300 MHz (DMSO-d_6) δ ppm: 4.73-4.75 (d, 12H, -CH_2), 7.38-7.40 (d, 6H, -CH), 7.59-7.62 (m, 12H, -CH), 7.75-7.78 (d, 6H, -CH), 8.69-8.72 (b, 6H, -NH); ^{13}C NMR, 75 MHz (DMSO-d_6) δ ppm: 121.85, 126.31, 128.57, 129.81, 132.05, 135.99, 137.11, 166.66. Yield: 92%. ^{1}H decoupled ^{19}F NMR 500 MHz (DMSO-d_6) δ ppm: -60.374 (-CF_3), -165.00 (C_6F_6). HRMS (ESI): *m/z* 1308.1714 [**M**+Na]$^+$, 1286.2754 [**M**+H]$^+$. Elemental analysis: Calcd. For **L**: C, 56.08; H, 3.29; N, 6.54. Found: C, 55.84; H, 3.21; N, 6.37.

Synthesis and characterization data of Complexes 1-3.

The complexes (**1**-**3**) were crystallized in a glass beaker by adding 4 equivalents of tetrabutylammonium salt at room temperature. The details of the crystallization processes and characterization data are enlisted below.

Complex 1:

Empirical formula: [**L**$(CH_3COO)_2(TBA)_2$], Solvent of crystallization: acetone-dioxane (1:1, v/v) binary solvent mixture. ^{1}H NMR, 300 MHz (DMSO-d_6) δ ppm: 0.93 (t, 24H, -$NCH_2CH_2CH_2CH_3$), 1.12 (s, 6H, -$OOCCH_3$), 1.29-1.32 (m, 16H, - $NCH_2CH_2CH_2CH_3$), 1.56 (m, 16H, - $NCH_2CH_2CH_2CH_3$), 3.14-3.19 (t, 16H, - $NCH_2CH_2CH_2CH_3$), 4.62 (s, 12H, -CH_2), 7.18-7.21 (d, 6H, -CH), 7.30-7.33 (t, 6H, -CH), 7.53-7.55 (t, 6H, -CH), 7.69-7.72 (d, 6H, -CH), 9.32 (b, 6H, -NH); ^{13}C NMR, 75 MHz (DMSO-d_6) δ ppm: 13.47, 19.19, 23.04, 24.49, 57.48, 121.84, 126.18, 128.68, 129.61, 131.69, 135.84, 136.57, 166.23, 173.37. Yield: 50%. ^{1}H decoupled ^{19}F NMR 500 MHz (DMSO-d_6) δ ppm: -60.31 (-CF_3), -165.02 (C_6F_6).Elemental analysis: Calcd. For complex **1**: C, 59.59; H, 6.54; N, 5.35. Found: C, 60.38; H, 6.58; N, 6.37.

Complex 2:

Empirical formula: [**L**(NO_3)(TBA)], Solvent of crystallization: acetone/dioxane (1:1, v/v) binary solvent mixture. ^{1}H NMR, 300 MHz (DMSO-d_6) δ ppm: 0.94 -0.96 (t, 12H, -$NCH_2CH_2CH_2CH_3$), 1.29-1.32 (m, 8H, -$NCH_2CH_2CH_2CH_3$), 1.57 (m, 8H, - $NCH_2CH_2CH_2CH_3$), 3.14-3.19 (t, 8H, - $NCH_2CH_2CH_2CH_3$), 4.73-4.75 (m, 12H, -CH_2), 7.38-7.40 (d, 6H, -CH), 7.58-7.62 (m, 12H, -CH), 7.75-7.77 (d, 6H, -CH), 8.69-8.70 (b, 6H, -NH); ^{13}C NMR, 75 MHz (DMSO-d_6) δ ppm: 13.49, 19.21, 23.05, 57.50, 121.86, 126.31, 128.58, 129.81, 132.05, 135.97, 137.11, 166.67. Yield: 70%. Elemental analysis: Calcd. For complex **2**: C, 56.19; H, 4.84; N, 6.90. Found: C, 55.87; H, 4.77; N, 6.64.

Complex 3:

Empirical formula: $[(\mathbf{L})_2(F)_4(H_2O)_6(TBA)_4(C_4H_8O_2)_3]$, Solvent of crystallization: acetone/dioxane (1:1, v/v) binary solvent mixture. ^{1}H NMR, 300 MHz (DMSO-d_6) δ ppm: 0.90-0.95 (t, 24H, -$NCH_2CH_2CH_2CH_3$), 1.29-1.32 (m, 16H, -$NCH_2CH_2CH_2CH_3$), 1.56 (m, 16H, -$NCH_2CH_2CH_2CH_3$), 3.13-3.19 (t, 16H, -$NCH_2CH_2CH_2CH_3$), 4.60 (s, 12H, -CH_2), 7.31(m, 12H, -CH), 7.52-7.54 (m, 6H, -CH), 7.66-7.68 (m, 6H, -CH), 10.31 (b, 6H, -NH); ^{13}C NMR, 75 MHz (DMSO-d_6) δ ppm: 14.06, 19.79, 23.64, 58.09, 122.53, 126.15, 126.53, 126.58, 126.90, 127.32, 129.64, 132.09, 137.13, 166.92. Yield: 70%. Elemental analysis: Calcd. For complex **3**: C, 58.04; H, 6.46; N, 5.21. Found: C, 58.18; H, 6.37; N, 5.42.

Single crystal X-ray crystallographic details.

The crystallographic details of complexes **1**-**3** and **L** are given in Table 1S. In each case, a crystal of suitable size is collected from the mother liquor and is dipped in paratone oil. Then it is mounted on the tip of a glass fibre and cemented using epoxy resin. Intensity data for all crystals are collected using MoKα (λ = 0.7107 Å) radiation on a Bruker SMART APEX diffractometer equipped with a CCD area detector at 120 K. The data integration and reduction are processed with SAINT[R1Sa] software. An empirical absorption correction is applied to the collected reflections with SADABS.[R1Sb]The structures are solved by direct methods using SHELXTL[R2S]and are refined on F2 by the full-matrix least-squares technique using the SHELXL-97[R3S] program package. Graphics are generated using PLATON-97[R4S]and MERCURY 3.1[R5S].

Structural details of free Ligand (**L**):

The disordered dioxane molecule (containing atoms O4A-C40-C5A-O3A-C37-C4A-C4B) has been removed from the revised structure by SQUEEZE treatment. Other two dioxane molecules (containing atoms O2A-C7A-C36-O1A-C6A-C35 & O10-C43A-C42A-O10-C43A-C42A) are not showing any disorder; hence these are kept as it is. A detail of the SQUEEZE treatment has been mentioned in the modified .cif under "_refine_special_details" section. Volume squeezed during refinement was 362 Å^3. (CCDC 996875).

Structural details of complex 1:

The disordered dioxane molecule (containing atoms O6-C50-C52-O7-C51-C49) and a discrete oxygen molecule O8 has been removed from the revised structure by SQUEEZE treatment. A detail of the SQUEEZE treatment has been mentioned in the modified .cif under "_refine_special_details" section. Volume squeezed during refinement was 377 Å^3. (CCDC944132).

Structural details of complex 2:

The crystal data (CCDC 944135) of nitrate complex can't be improved further as because the crystal is very scarcely obtained. The crystal takes almost 3 months to grow inside the fridge and can be obtained

only after several trials. However, we have collected the data several times before submitting it to the current journal. The coverage reported here is the optimum and can't be improved further. We have tried our best to develop a chemically sensible model for the disordered nitrate in the revised cif file. The oxygen atoms O7A, O7B, O8, O9A and O9B are the parts of the disordered nitrate. The nitrate shows rotational disorder. The nitrate consisting of N7A-O9A-O8-O7A flips to the position N7B-O9B-O8-O7B keeping O8 in pivotal position. Here O9A and O9B have been assigned with occupancy 0.5. In this way the thermal parameter of the respective oxygen centers namely O9A (0.143980) and O9B (0.185690) have been reduced to 0.081500 and 0.060080. Part treatment has been performed in the revised structure for the disordered atoms. Disorder and Part treatment are also performed for the disordered –CF3 group.

Structural details of complex 3:

The crystal is plate shaped and highly solvent losing in nature. The crystal takes almost 2 – 3 months to grow in fridge and can be obtained after several trials. The crystal turns into opaque immediate after cementing it on the epoxy resin and losses its crystalline nature. However, we have collected the data several times before submitting it to the current journal. To the best of our effort this is the best data which we could produce after several trails. The 'Theta (max)' value which we report herein is the optimum obtained by our efforts. Disorder treatment have been performed on oxygen atoms O16 and O17 (by FVAR command) and by virtue of this treatment (CDC 996874). The residual electron density can't be reduced to <1 as it contains some disordered atoms which can't be modeled properly. We have tried to develop most sensible network through refinements. For instance, we have assigned F16 (Thermal parameter: 0.043060) as oxygen and O15 (Thermal parameter: 0.148240) as fluoride and then refined the structure in XShell. The thermal parameters of the newly assigned fluoride (Thermal parameter: 0.208700) and oxygen (Thermal parameter: 0.186720) become quite high with respect to previously assigned atoms. Hydrogen has been assigned to O14 by increasing the Q peaks in the XShell program. Hence it can't be fluoride. Increase in thermal parameter is also observed by assigning O11 as oxygen and F16 as oxygen. Hence fluorides and oxygens are unambiguously assigned to the network.

Isothermal titration calorimetric studies.

The solution-state binding affinity of the receptor (**L)** with acetate is performed by ITC experiments. In a typical ITC experiment, a solution of the acetate as its tetrabutylammonium salt in DMSO is titrated into a solution of receptor at 298 K. A clear exothermic titration profile is obtained upon titration with CH_3COO^- and subsequent fitting to a 1:2 binding profile has provided access to the association constants (K1, K2), enthalpy change (ΔH1, ΔH2), entropy change (TΔS1, TΔS2), and free energy change (ΔG1, ΔG2) of the binding processes. The titration data is fitted in a sequential site model (ligand in cell) with number of binding sites two. The molar ratio of this titration curve has shown saturation beyond 2 equivalents of guest. The ITC profiles of the fluoride showed fitting in 1:2 (sequential sites) model with high Chi^2/DoF values for which we have not included those parameters in this manuscript. Blank titration is carried out with acetate that is subtracted from the titration data in order to obtain accurate thermodynamic parameters of binding. The software used for ITC analysis is

Origin 7.0. The upper panel of the VP-ITC output figure shows the heat pulses which are observed experimentally in each titration step with respect to time. The lower panel reports the respective time integrals translating as the heat absorbed or evolved for each aliquot and its coherence to a 1:2, sequential binding model. During each titration, a solution of concentration 0.75 mM (approximately) is placed in the cell at 298 K temperature. This solution is then titrated with 35 injections of 8 μL each of a 14.45 mMTBAAcO solution prepared in DMSO. An initial delay of 240s is allowed before each titration. Interval of 180s is allowed between each injection and the stirring speed is set at 329 rpm.

^{1}H-NMR titration studies.

^{1}H NMR titrations with the receptor (**L**) with both tetrabutylammonium acetate and fluoride are carried out in a 300 MHz NMR instrument. The receptor is dissolved in 0.45 ml of DMSO-d_6 at room temperature. The stock anion concentration is maintained almost 10 times more concentrated with respect to receptor concentration. During each titration, 10 μL aliquot of anion prepared in DMSO-d_6 is added and shaken well before recording the NMR data. In the case of titration with acetate, the amide -NH peak is monitored and is used to calculate binding constant values from WINEQNMR2 software[R6S]. The JOB's plot of NMR titrations with both acetate and fluoride show 1:2 (Host : Guest) binding pattern and thus 1: 2 fitting model is chosen in WINEQNMR2 to calculate the binding constants (K1, K2) values. Similarly for fluoride, the same fitting model is chosen as it also showed 1:2 binding pattern in JOB's plot analysis. Aromatic –CH protons are monitored in case of fluoride titrations to calculate the stepwise biding constants. The binding constant values calculated from NMR titrations which are in good resemblance with the value calculated from ITC studies.

DFT Calculation studies

In order to further understand the detailed energetics of the various conformers, density functional theory (DFT) calculations are carried out on 3 complexes. Molecular geometries (including the empty ligand) are completely optimized without constraints at the M06-2X/6-31G(d,p) level of theory, which has previously been shown to accurately predict the binding energies of ions in large molecular systems.[1h, 1i & 9b] From the DFT-optimized geometries, we have obtained binding energies from the equation $E_{binding} = E_{anion} + E_{ligand} - E_{total\ complex}$, where E_{anion} is the electronic energy of the charged anion, E_{ligand} is the energy of the optimized isolated ligand, and $E_{total\ complex}$ is the total energy of the optimized complex.

^{19}F NMR studies:

^{19}F NMR studies are employed in order to find the coordination environment of the fluoride in the homo dimeric cluster $[F_4(H_2O)_6]^{4-}$ of **L** in complex **1**. Unfortunately, overnight scan (NS= 30000) of the sample could not find any new peak for bound fluoride. This is because, in complex **1**, there are eighteen fluorine atoms present in the ligand back bone and our desired one is too weak to be quantified in NMR. Hence, the ^{19}F spectrum of complex **1** is inconclusive from coordination environment point of view of fluorine.

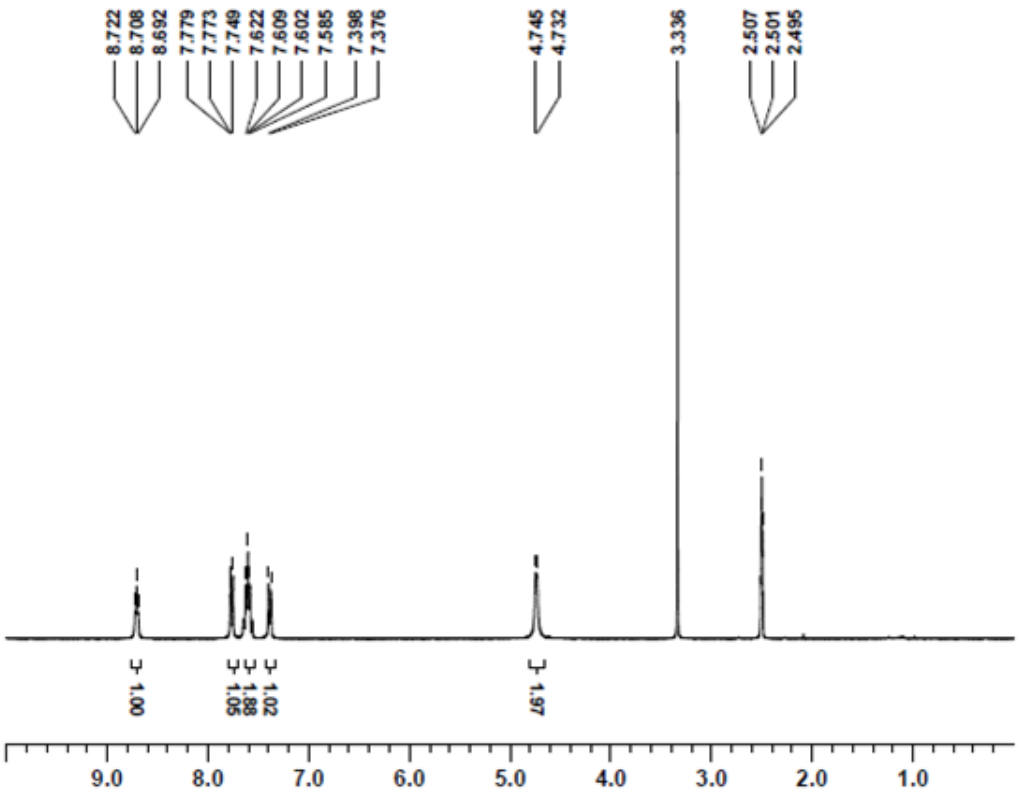

Fig.2S: ^{1}H NMR (300 MHz) spectrum of receptor **L** in DMSO-d_6 at 25°C.

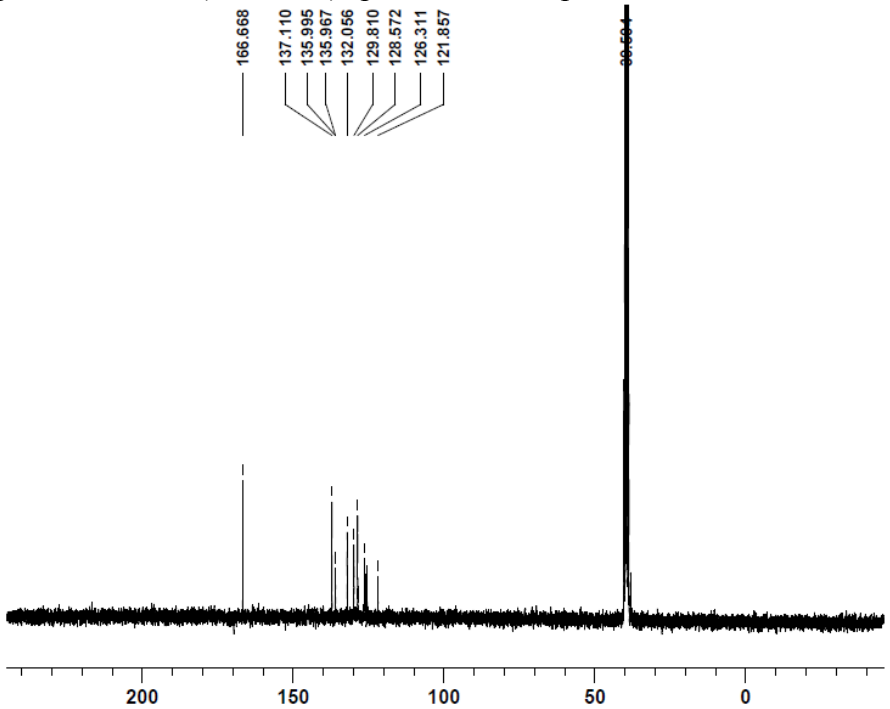

Fig.3S: ^{13}C NMR (75 MHz) spectrum of receptor **L** in DMSO-d_6 at 25°C.

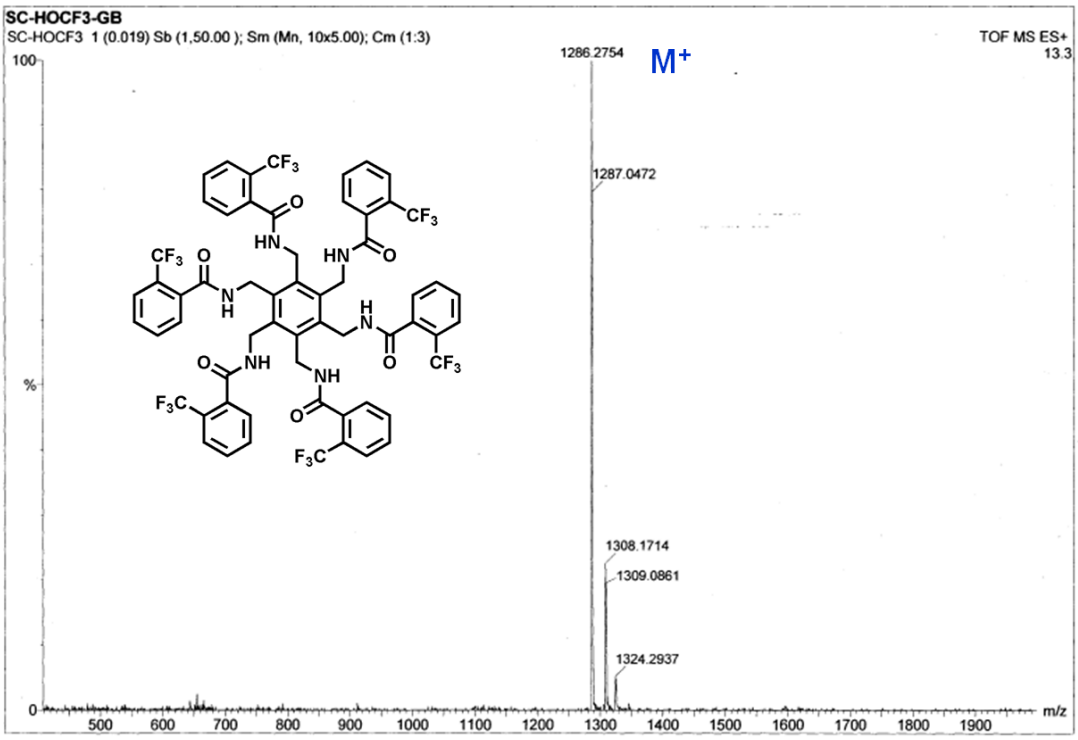

Fig. 4S: HRMS spectrum of **L**.

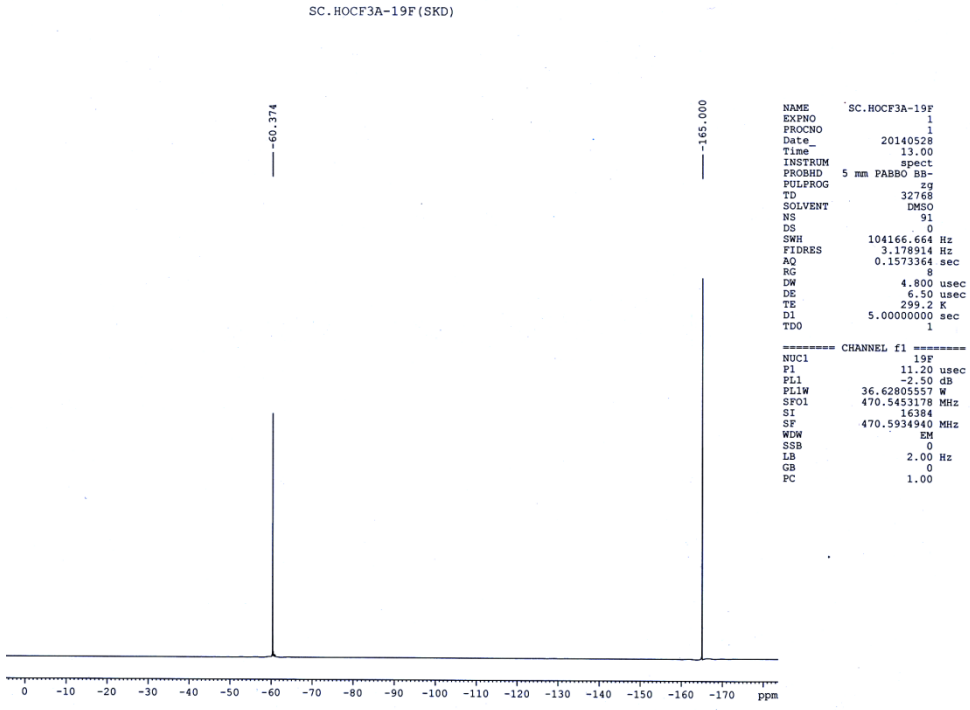

Fig. 5S: ^{19}F-NMR (500 MHz) spectrum of **L**in DMSO-d_6 at 25°C

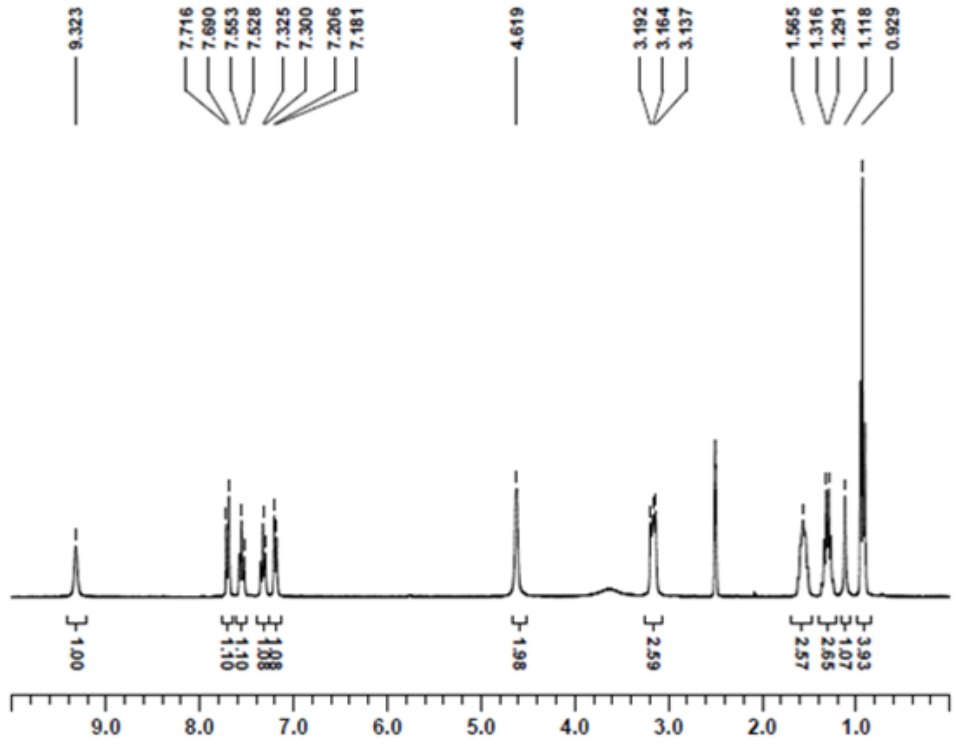

Fig. 6S: ^{1}H NMR (300 MHz) spectrum of **Complex 1** in DMSO-d_6 at 25°C.

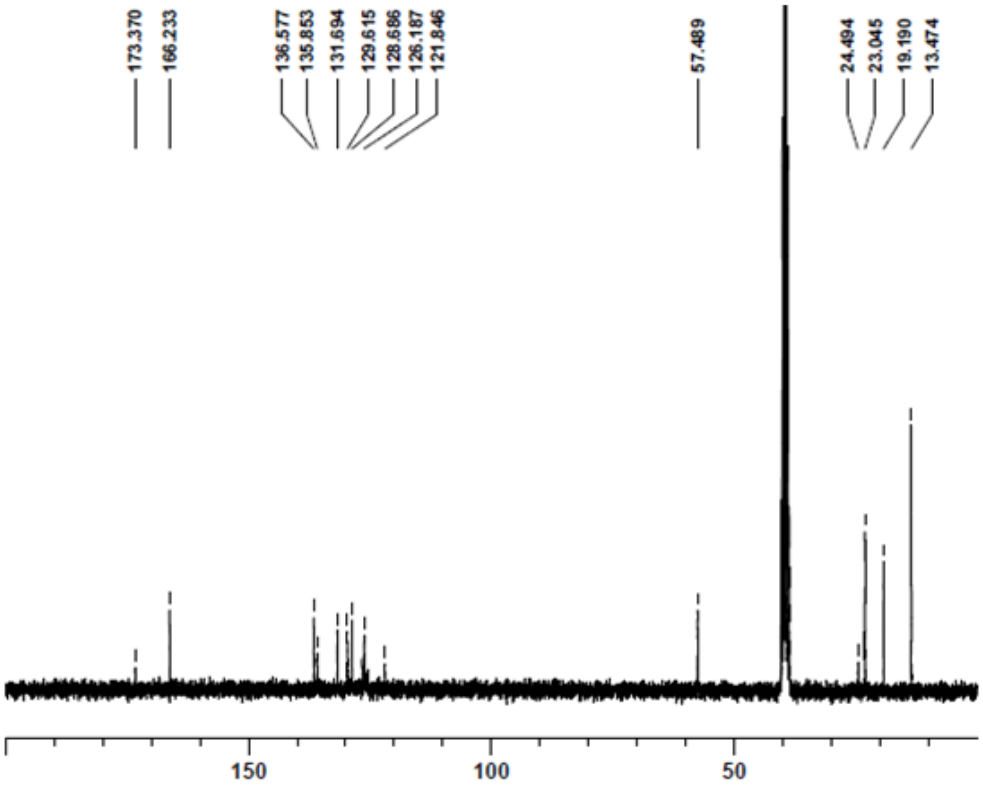

Fig.7S: ^{13}C NMR (75 MHz) spectrum of **Complex 1** in DMSO-d_6 at 25°C.

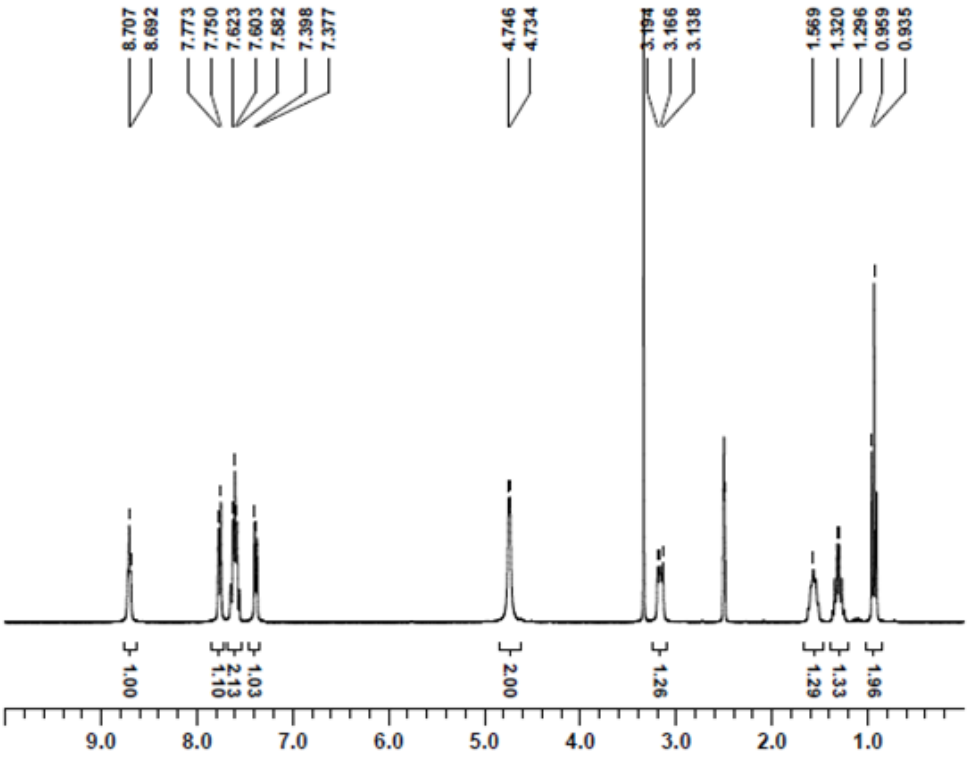

Fig.8S: ^{1}H NMR (300 MHz) spectrum of **Complex 2**in DMSO-d_6 at 25°C.

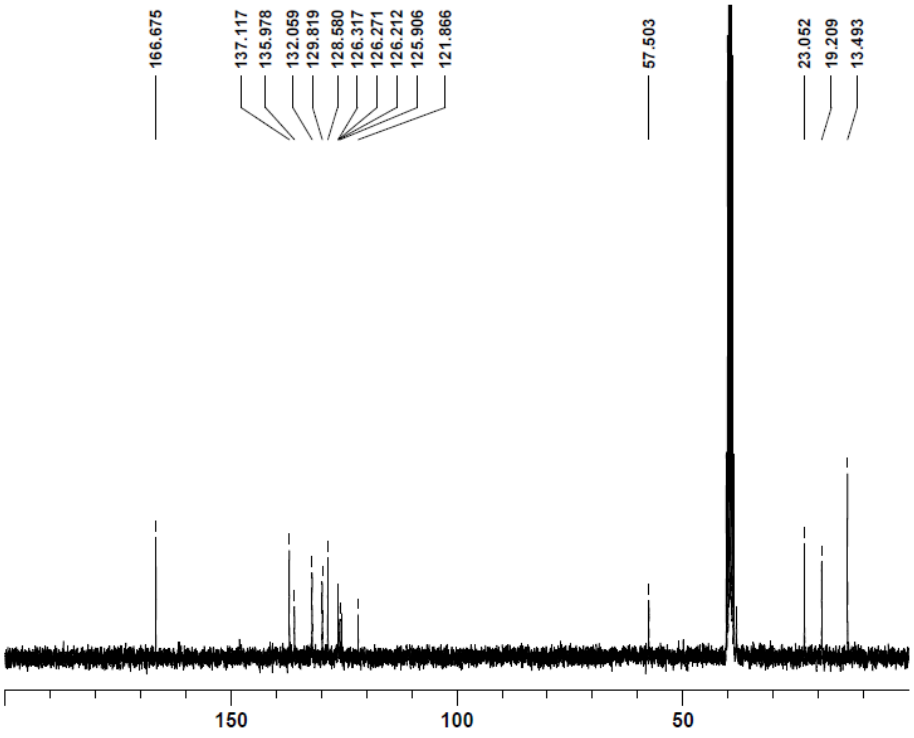

Fig.9S: ^{13}C NMR (75 MHz) spectrum of **Complex 2**in DMSO-d_6 at 25°C.

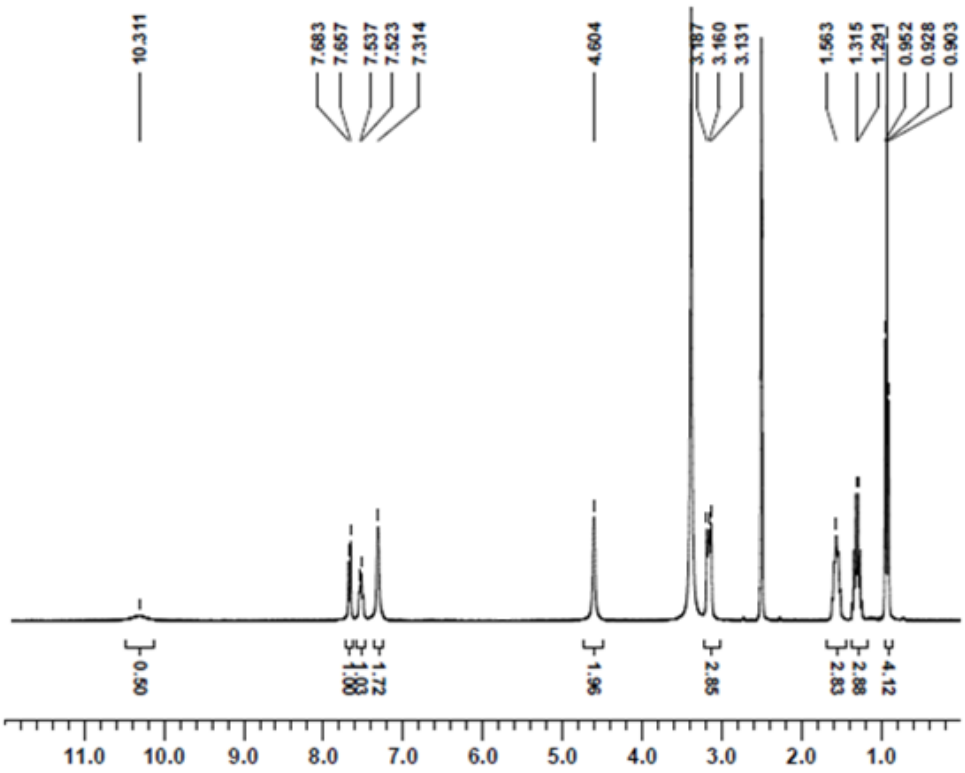

Fig.10S: ^{1}H NMR (300 MHz) spectrum of **Complex 3**in DMSO-d_6 at 25°C.

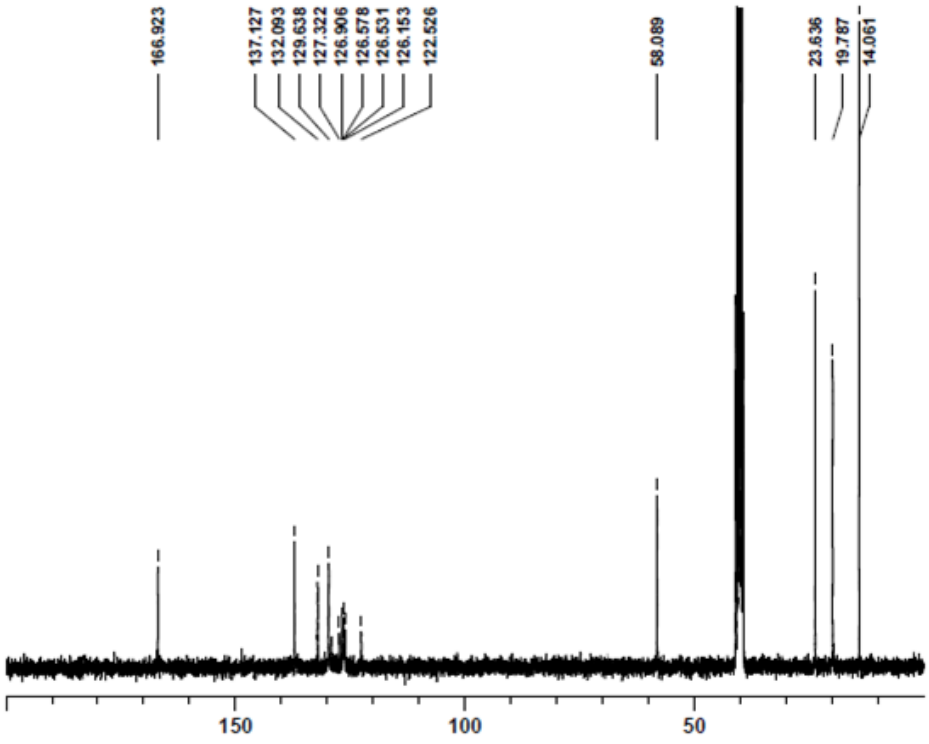

Fig.11S: ^{13}C NMR (75 MHz) spectrum of **Complex 3**in DMSO-d_6 at 25°C.

Table 1S.Crystallographic parameters of the **L** and complexes (**1-3**)

Compound reference	**COMPLEX 1**	**COMPLEX 2**	**COMPLEX 3**	**FREE LIGAND**
hemical formula	$C_{96}H_{120}F_{18}N_8O_{10}$	$C_{76}H_{71}F_{19}N_8O_{10}$	$C_{104}H_{135}F_{20}N_8O_{17}$	$C_{72}H_{66}F_{18}N_6O_{12}$
Formula Mass	1888.00	1617.41	2149.20	1549.31
Crystal system	Monoclinic	Monoclinic	Monoclinic	Triclinic
a/Å	13.026(3)	18.729(3)	19.984(2)	10.968(4)
b/Å	25.015(5)	31.942(3)	21.583(2)	13.856(5)
c/Å	16.358(4)	26.316(3)	31.956(3)	14.250(5)
α/°	90.00	90.00	90.00	76.125(11)
β/°	92.574(4)	101.030(5)	104.776(3)	73.854(11)
γ/°	90.00	90.00	90.00	81.532(12)
Unit cell volume/Å^3	5325(2)	15452(4)	13327(2)	2011.9(13)
Temperature/K	150(2)	150(2)	150(2)	150(2)
Space group	*P2(1)/c*	*C2/c*	*P2(1)/n*	*P***Error!**
No. of formula units per unit cell, *Z*	2	8	4	1
No. of reflections measured	61885	6182	70781	7041
No. of independent reflections	9393	6182	11220	7041
R_{int}	0.0465	0.0000	0.0751	0.0000
Final R_1 values ($I > 2\sigma(I)$)	0.0793	0.0923	0.0999	0.0604
Final $wR(F^2)$ values ($I > 2\sigma(I)$)	0.2323	0.2731	0.2778	0.1978
Final R_1 values (all data)	0.0891	0.1225	0.1200	0.0828
Final $wR(F^2)$ values (all data)	0.2382	0.3043	0.2919	0.2209
Goodness of fit on F^2	1.037	1.207	1.043	0.854
CCDC numbers	944132	944135	996874	996875

H-bonding tables of the free ligand (**L**) and complexes (**1-3**)

Table 2S:**Free receptor (L)**			
D-H···A	**H···A (Å)**	**D···A (Å)**	**∠D-H···A (°)**
N1-H1···O3[1]	2.02	2.8525	163
N2-H2···O10[1]	2.06	2.9221	175
N3-H3A···O1[2]	1.98	2.7752	153
C27-H27B···O2[2]	2.41	3.2279	142
Symmetry codes: (1) 1+x, y, z; (2) x, y, z.			

Table 3S:**Complex 1**			
D-H···A	**H···A (Å)**	**D···A (Å)**	**∠D-H···A (°)**
N1-H1···O2[1]	1.97	2.7901	159
N2-H2···O1[1]	1.92	2.7725	173
N3-H3···O2[1]	1.94	2.7587	159
C5-H5B···O8[1]	2.48	3.3490	148
C18-H18···O1[1]	2.58	3.4506	156
C20-H20···O8[2]	2.19	3.0493	154
C24-H24A···O4[3]	2.49	3.3939	155
C24-H24B···F7[1]	2.45	3.3817	160
C27-H27A···O7[3]	2.46	3.3906	162
C27-H27B···O3[4]	2.57	3.5187	170
C28-H28B···O5[5]	2.46	3.3632	156
C29-H29B···O3[1]	2.46	3.3373	151
C32-H32A···O3[1]	2.44	3.4046	172
C36-H36A···O5[5]	2.51	3.4224	157

C36-H36B···F6[5]	2.36	3.1640	140
C46-H46···F8[2]	2.54	3.1993	128
Symmetry Codes: (1) 1-x,-y,1-z; (2) 2-x,-y,1-z; (3) x, y, z; (4) 1-x,1/2+y,3/2-z; (5) x,1/2-y,-1/2+z.			

Table 4S: **Complex 2**

D-H···A	**H···A (Å)**	**D···A (Å)**	**∠D-H···A (°)**
N1-H1···O8[1]	2.25	3.0500	154
N1-H1···O9B[1]	2.42	3.1830	148
N2-H2···O8[1]	2.10	2.9050	155
N3-H3···O7B[1]	2.16	2.9420	151
N3-H3···O9A[1]	2.01	2.8520	167
N4-H4···O7B[1]	2.21	3.0020	153
N5-H5···O6[2]	1.98	2.8280	168
N6-H6···O4[3]	2.01	2.862	169
Symmetry codes: (1) x, y, z; (2) -x, y, 1/2-z; (3) 1-x, y, 1/2-z			

Table 5S:**Complex 3**

D-H···A	**H···A (Å)**	**D···A (Å)**	**∠D-H···A (°)**
N1-H1···F16[1]	1.81	2.6460	164
N2-H2···F16[1]	1.92	2.7260	156
N3-H3···O14[1]	1.99	2.8330	167
N4-H4···F17[2]	1.86	2.6730	157
N5-H5···F17[2]	1.96	2.7770	159
N6-H6···O11[1]	2.01	2.8190	156
O14-H110···O15[1]	2.08	2.6490	137

O14-H111···F16[1]	1.87	2.6880	154
Symmetry codes: (1) x, y, z; (2) 1+x, y, z.			

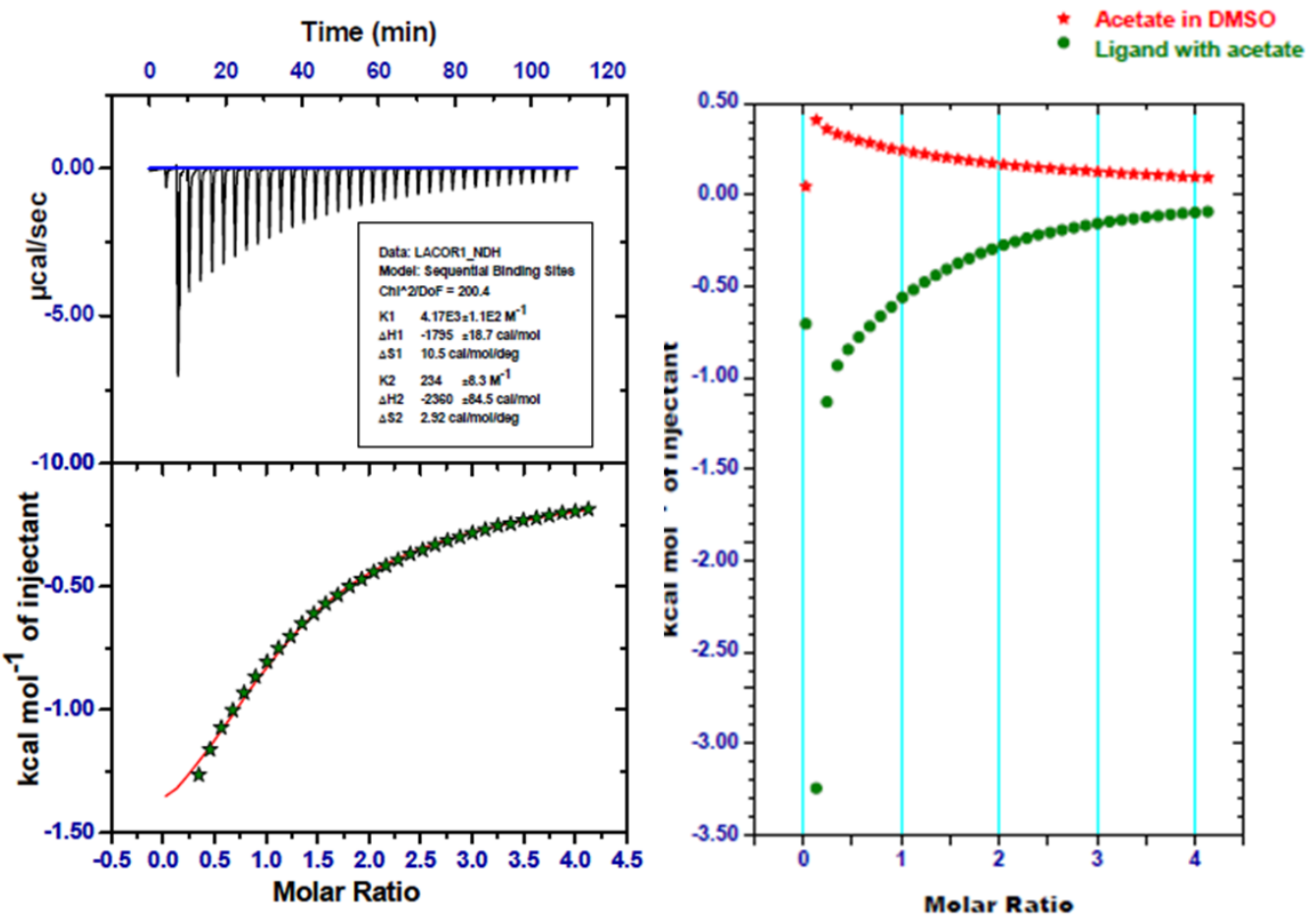

Fig. 12S: ITC titration profile of **L** to TAcO at 298K. Concentrations maintained during experiment are [**L**] = 0.745mM, [TAcO] = 14.45mM. Thermodynamic parameters associated with this titration are, K1 = 4.17E3 ± 1.1E2 M^{-1}, ΔH1 = -1795 ± 18.7cal/mol, ΔS1 = 10.5cal/mol/deg, K2 = 2.34E2 ± 8.3 M^{-1}, ΔH2 = -2360 ± 84.5 cal/mol, ΔS2 = 2.92cal/mol/deg, Chi^2/DOF = 200.4. Initial 3 data points are removed in order to get better fitting. These initial data are premature to affect binding model or parameters.

Table 6S: Thermodynamic parameters associated with acetate binding to **L**in ITC study.

L	**Association Constants (K_1 & K_2) M^{-1} (ITC)& K_T (M^{-2})**	**ΔH (cal/ mol)**	**TΔS (cal/ mol)**	**ΔG (cal/mol)**
L	K_1 = 4.17E3 ± 1.1E2 K_2 = 234 ± 8.3 K_T = (9.76 ± 0.68)E5	ΔH_1 = -1795 ± 18.7 ΔH_2 = -2360 ± 84.5	$T\Delta S_1$ = 3129 $T\Delta S_2$ = 870.16	ΔG_1 = -4924.0 ΔG_2 = -3230.16

Table 7S: Association constant (K_1, K_2) and ΔG values obtained from ^{1}H-NMR titration experiments with TBAAcOand TBAF with **L**in DMSO-d_6.

Anion	**Association Constant (K) M^{-1} (NMR)**	**ΔG (cal/mol) (NMR)**
TBAAcO	K_1 = 1.81E3 ± 43.8 K_2 = 3.30E2 ± 6.98 K_T = 5.97E5 ± 3.05E2	ΔG1 = -4442.4 ΔG2 = -3434.4
TBAF	K_1 = 7.40E3 ± 1.8E2 K_2 = 5.60E3 ± 2.39E2 K_T = 4.14E7 ± 4.30E4	ΔG_1 = -5276.3 ΔG_2 = -5111.3

Table 8S: Binding energies for each of the 3 complexes calculated at the M06-2X/6-31G(d,p) level of theory.

Complex	**$E_{binding}$ (kcal/mol)**
1	77.44
2	71.09
3	136.50

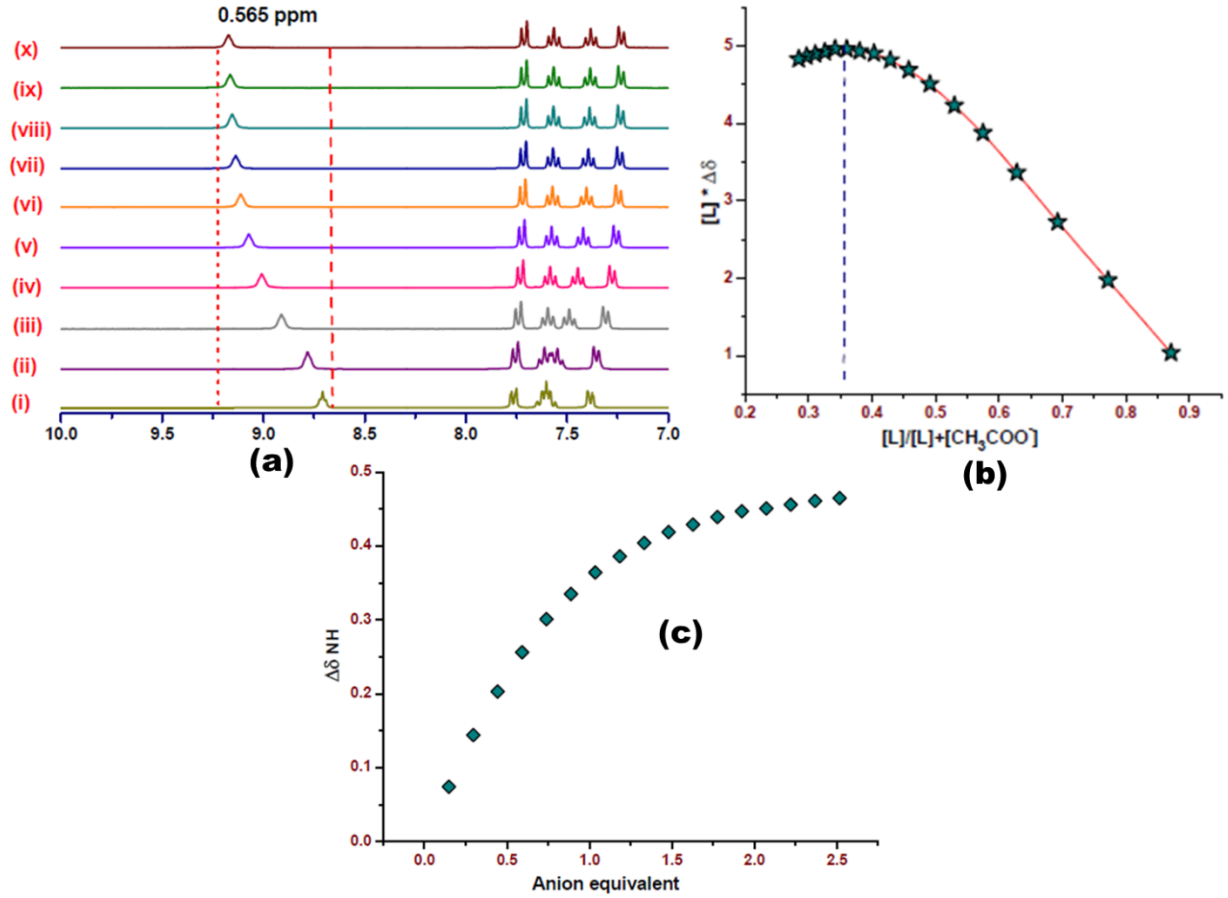

Fig.13S: (a) Partial ^{1}H-NMR (300 MHz) spectral changes of **L** in DMSO-d_6 with added AcO^- in DMSO-d_6 (298K), [**L**] = 14.30mM. The respective ratio of concentrations are [AcO^-]/[**L**]: (i) 0, (ii) 0.15, (iii) 0.49, (iv) 0.74, (v) 1.04, (vi) 1.33, (vii) 1.63, (viii) 1.92, (ix) 2.17, (x) 2.47. (b) Job's plot for **L** with AcO^- in DMSO-d_6 which shows a 1:2 stoichiometry. (c) Anion equivalent plot for titration of **L** with AcO^-.

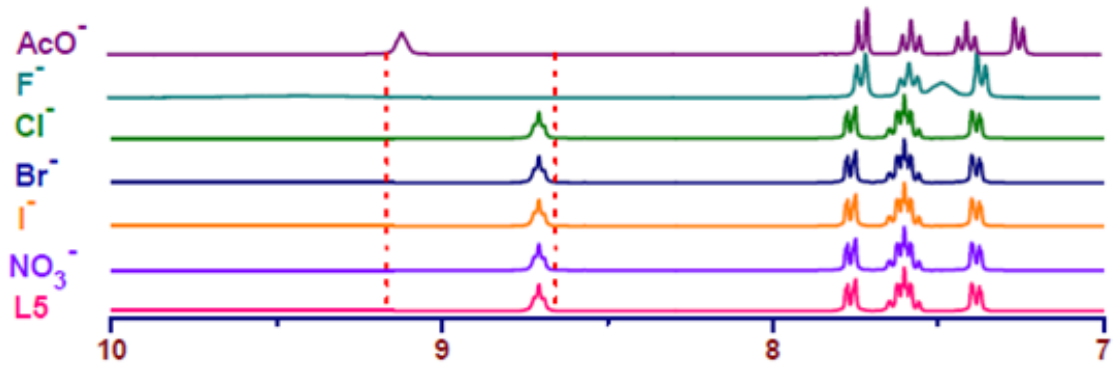

Fig. 14S: Comparative partial^{1}H NMR (300 MHz) spectra of **L**(~ 6mM) in DMSO-d_6 after addition of excess amount (~1 equivalent) of TBA salts of different anions.

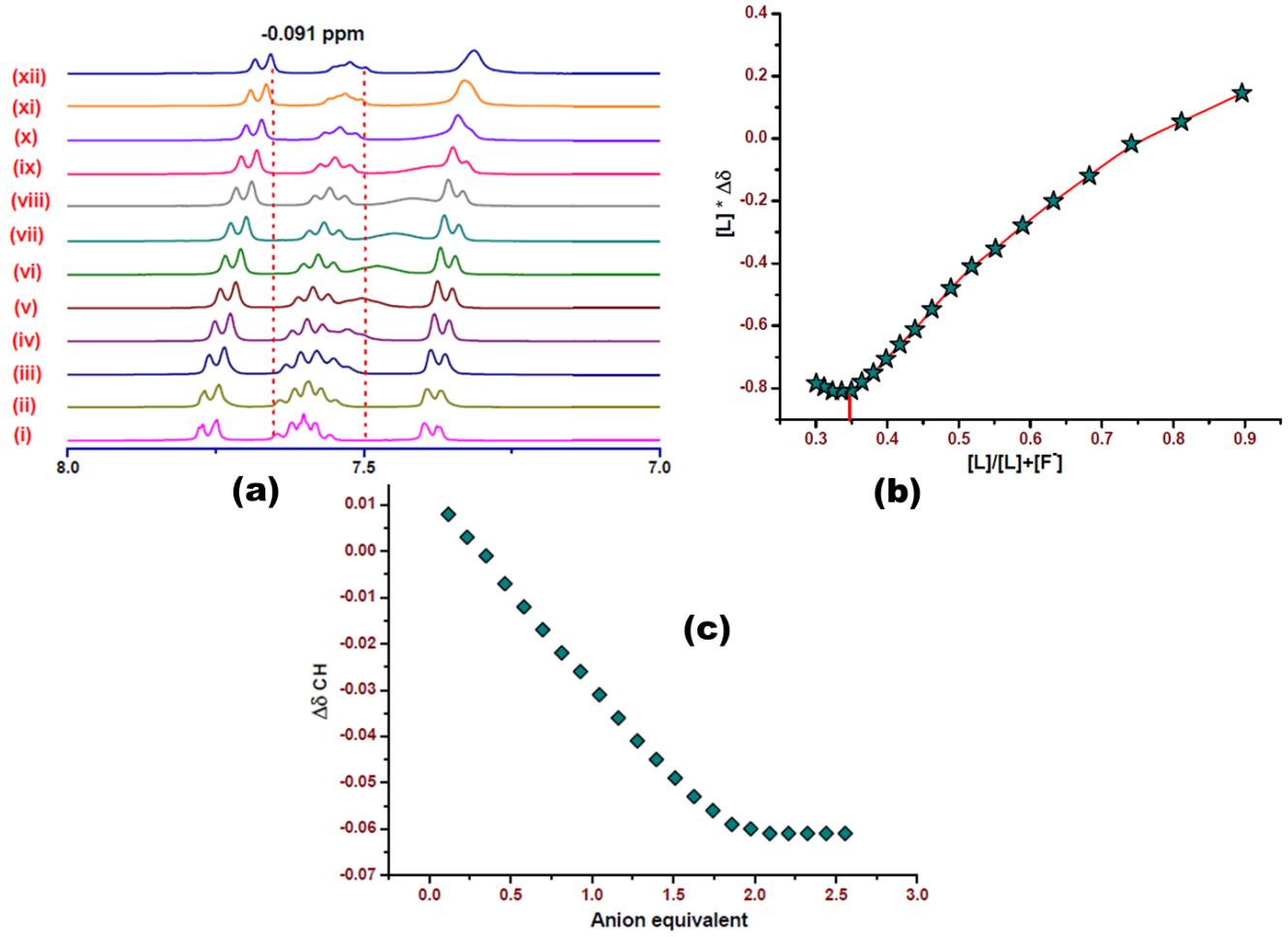

Fig.15S: (a) Partial ^{1}H-NMR (300 MHz) spectral changes of **L** in DMSO-d_6 with added F^{-} in DMSO-d_6 (298K), [**L**] = 10.05mM. The respective ratio of concentrations are [F^{-}]/[**L**]: (i) 0, (ii) 0.20, (iii) 0.46, (iv) 0.70, (v) 0.93, (vi) 1.16, (vii) 1.39, (viii) 1.62, (ix) 1.85, (x) 2.20, (xi) 2.55, (xii) 2.90. (b) Job's plot for **L** with F^{-} in DMSO-d_6 which shows a 1:2 stoichiometry. (c) Anion equivalent plot for titration of **L** with F^{-}.

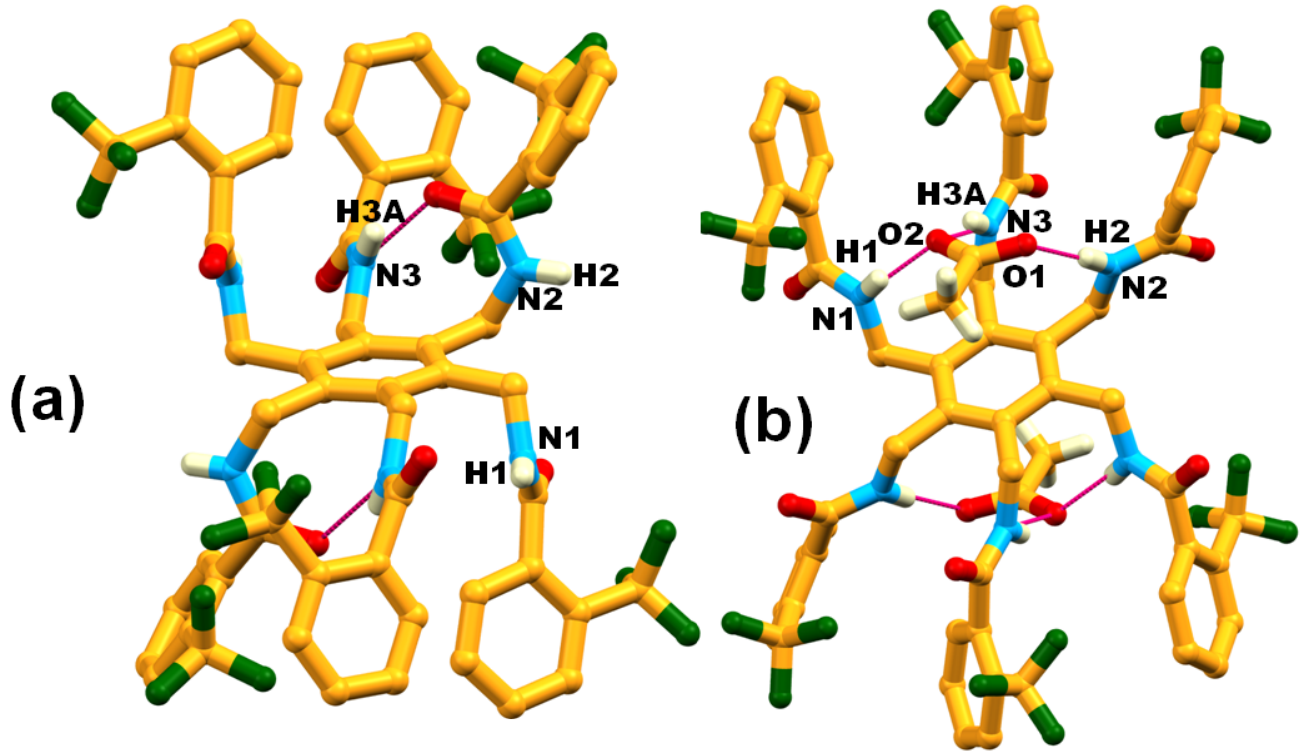

Fig. 16S: (a) Free receptor structure of **L**; (b) Acetate recognition by **L**, in complex **1** in ***A*** conformation.

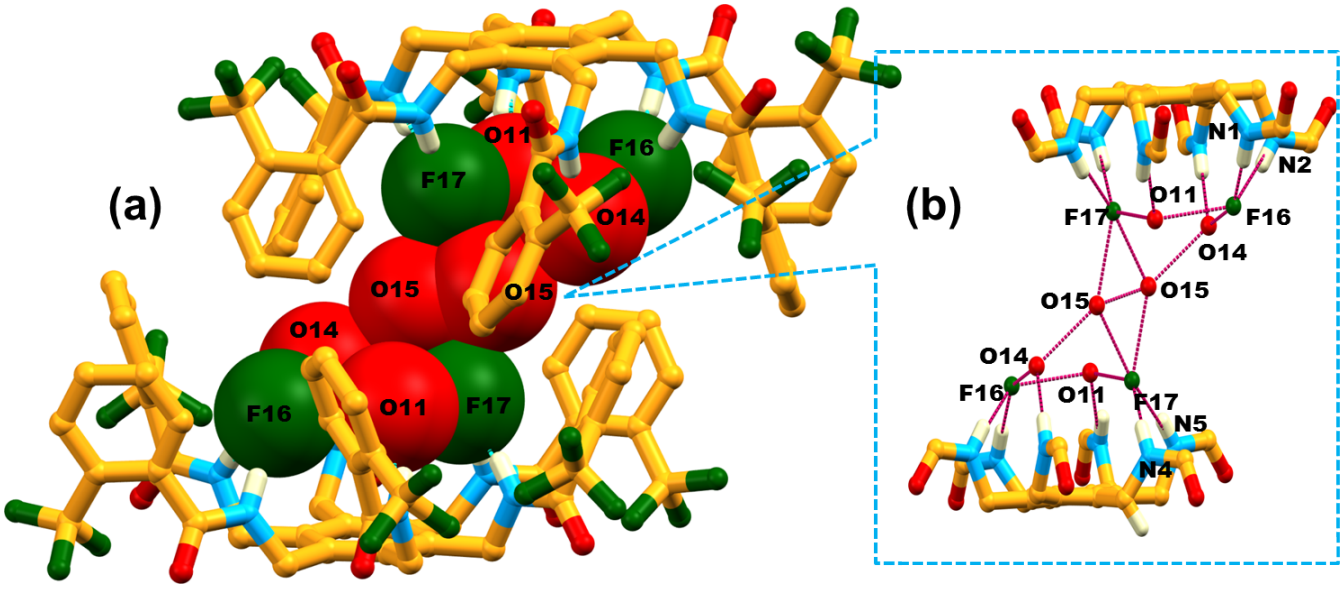

Fig. 17S: (a) Space fill view of $[F_4(H_2O)_6]^{4-}$ cluster inside the dimeric capsular assembly of **L** in complex **3** in ***C*** conformer ; (b) Inset showing discrete $[F_4(H_2O)_6]^{4-}$ cluster in complex **3**.

DFT OPTIMIZED STRUCTURES:

Molecular geometries of the complexes obtained from DFT calculations. Molecular geometries (including the empty ligands) were completely optimized without constraints at the M06-2X/6-31G(d,p) level oftheory.

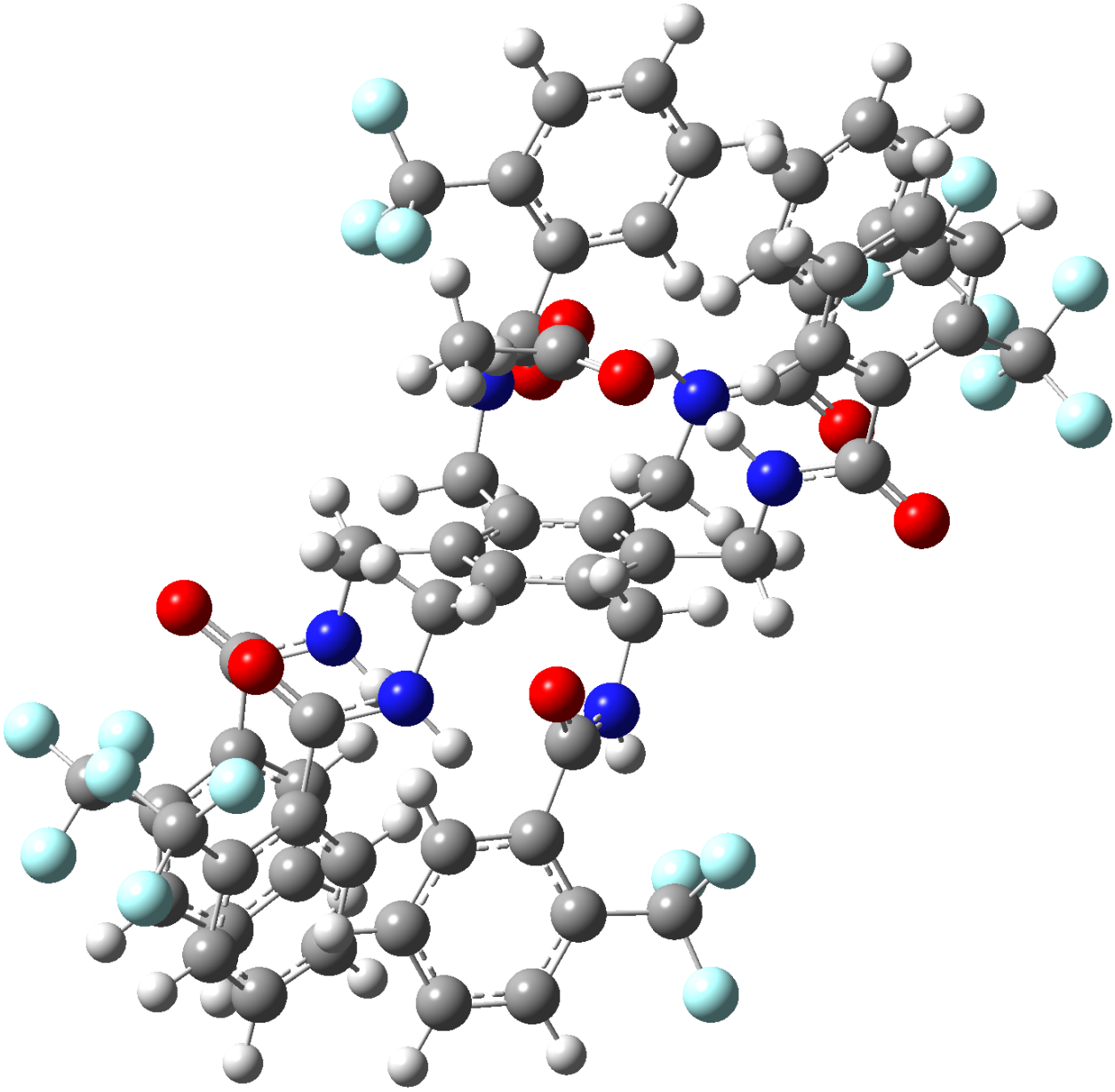

Fig. 18S: DFT optimized structure of complex **1**.

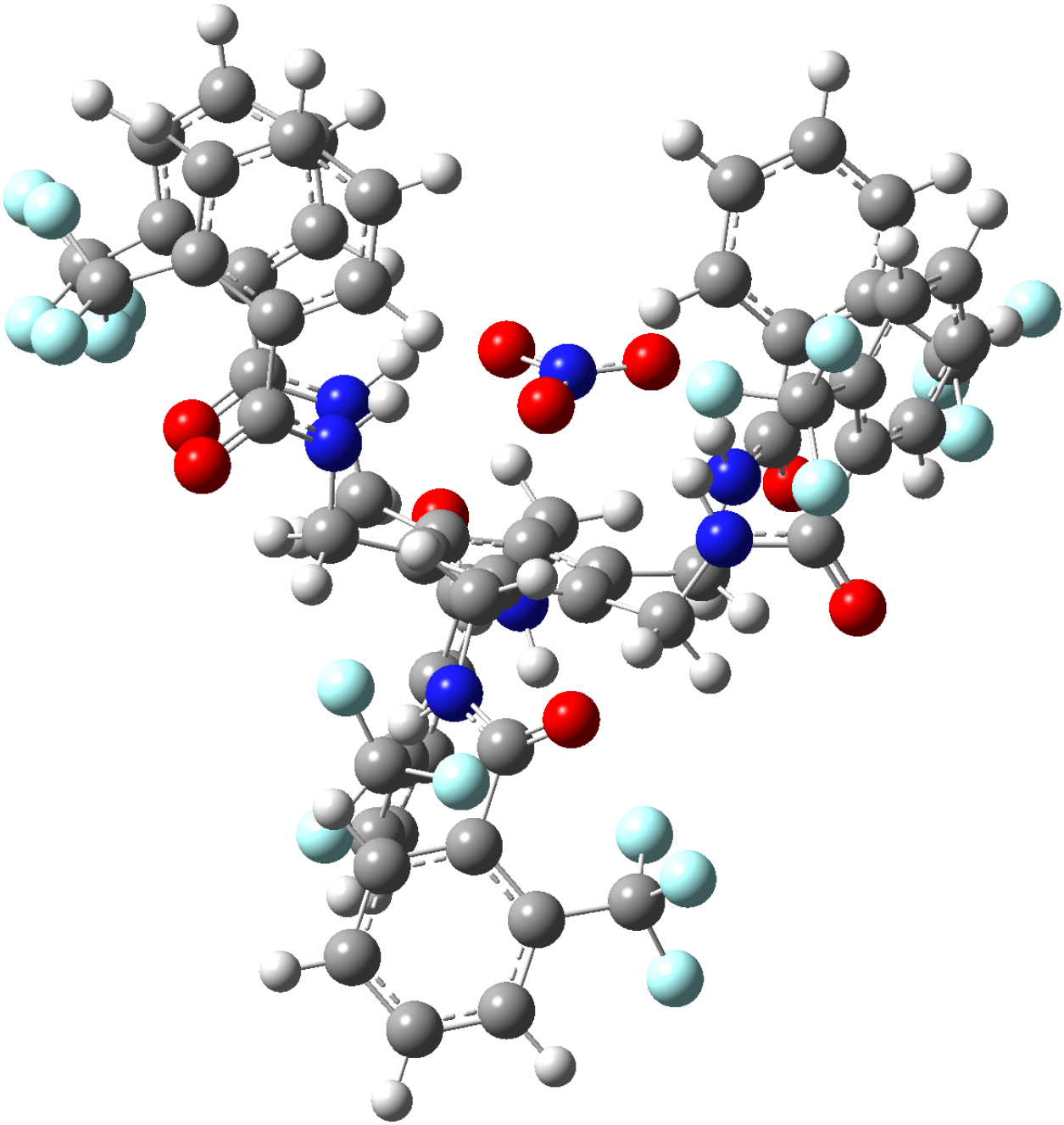

Fig. 19S: DFT optimized structure of complex **2**.

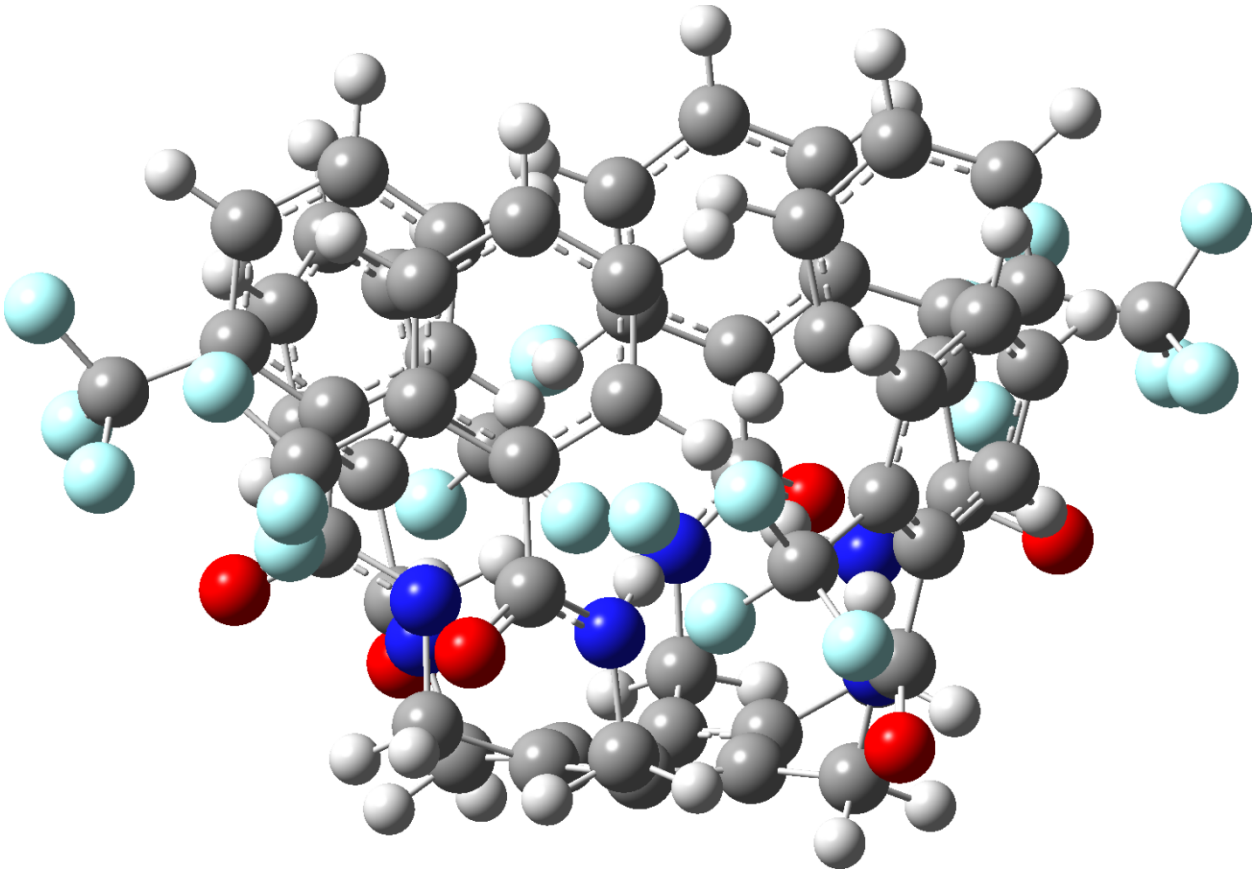

Fig. 20S: DFT optimized structure of complex **3**.

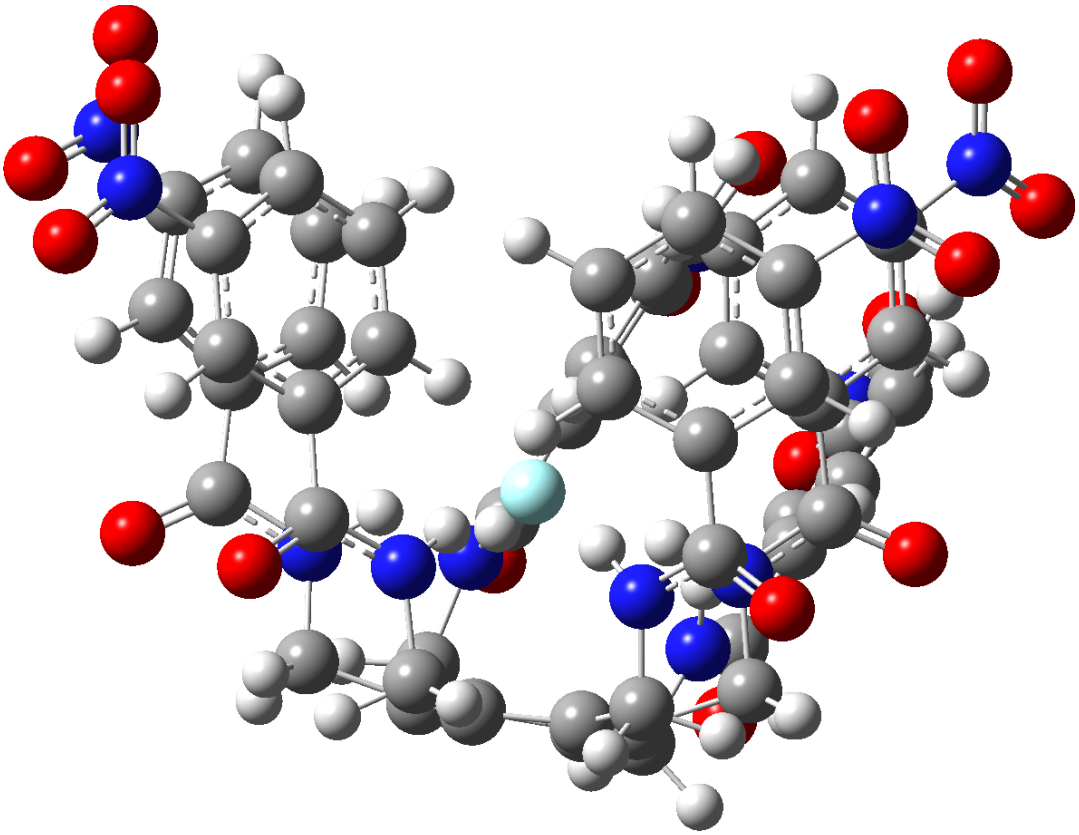

Fig. 21S: DFT optimized structure of previously published[R7S] fluoride complex with *m*-nitrophenyl substituted hexa-amide receptor.

DFT CALCULATION DETAILS:

Table 9S: Cartesian coordinates (Å) and total electronic energy associated with **complex** 1.
Total energy: -5115.68057405 Hartrees.

Complex 1:

O	2.769808	12.365665	0.308037
O	3.550865	10.879524	-1.152729
C	3.295779	11.276512	0.024512
C	3.641500	10.348706	1.171685
H	4.148566	10.828994	1.830248
H	4.161749	9.613264	0.841587
H	2.834200	10.016006	1.570418
F	0.586547	16.456368	13.986850
F	6.883354	17.965023	18.468505
F	0.161275	18.336996	14.927956
F	-1.444838	17.074739	14.290638
F	2.646849	12.575791	10.026325
F	8.771587	17.598053	17.619891
F	1.794773	14.459420	9.479702
F	0.794418	12.642581	8.986188
F	8.454542	19.297572	18.848281
O	5.527340	15.906788	20.679509
O	2.715433	17.131523	15.869226
O	3.419227	14.535216	11.911153
N	2.995749	14.898184	16.057644
H	2.641031	14.143481	16.269593
N	3.563265	12.843451	13.401170
H	3.134959	12.254849	13.859222
N	6.473667	15.090299	18.810859
H	7.185283	14.998994	18.338426
C	5.112393	13.680704	15.972505
C	5.481091	13.472579	17.304010
C	4.376989	14.943961	15.583250
H	4.827432	15.714423	15.965641
H	4.385236	15.039018	14.617468
C	5.413938	12.717626	15.001983
C	2.284986	16.020607	16.163373
C	5.203661	14.533465	18.346597
H	4.655523	15.236637	17.964206
H	4.721994	14.143481	19.093403
C	6.518055	15.737437	19.967674
C	0.918879	15.844501	16.764740
C	5.007140	12.949765	13.561807
H	5.298458	13.830793	13.282368

H	5.442951	12.294873	12.994757
C	-1.460957	16.240488	16.851350
H	-2.235233	16.572437	16.457520
C	8.612308	17.240088	19.917015
C	7.869103	16.195211	20.454650
C	-0.250040	16.377571	16.196056
C	0.817329	15.185106	17.980548
H	1.574030	14.798874	18.359670
C	0.641133	13.324240	13.641881
H	1.070365	13.345503	14.467126
C	-0.404229	15.094551	18.640744
H	-0.453199	14.676301	19.469258
C	2.885729	13.631674	12.564976
C	-1.532841	15.619866	18.073694
H	-2.348638	15.556829	18.516549
C	8.352185	15.537317	21.588750
H	7.862445	14.841400	21.964604
C	1.393576	13.387278	12.493073
C	0.743693	13.268706	11.244583
C	-0.232218	17.052225	14.872395
C	10.267776	16.957669	21.629604
H	11.066655	17.220326	22.026702
C	9.812028	17.613062	20.524919
H	10.306024	18.315983	20.170308
C	-0.649208	13.157890	11.224973
H	-1.089301	13.080344	10.409533
C	-1.380462	13.157890	12.395024
H	-2.309049	13.110362	12.362341
C	8.177314	18.000294	18.727354
C	9.559027	15.919546	22.154166
H	9.886495	15.464273	22.896070
C	-0.742850	13.230434	13.597759
H	-1.234243	13.215425	14.387053
C	1.492895	13.237938	9.965044
F	10.970189	8.558632	18.696142
F	4.673381	7.049977	14.214487
F	11.395461	6.678004	17.755035
F	13.001573	7.940261	18.392353
F	8.909886	12.439209	22.656667
F	2.785149	7.416948	15.063100
F	9.761963	10.555580	23.203290
F	10.762318	12.372419	23.696803
F	3.102194	5.717428	13.834710
O	6.029395	9.108212	12.003482
O	8.841303	7.883477	16.813765
O	8.137508	10.479784	20.771839

N	8.560987	10.116816	16.625347
H	8.915704	10.871519	16.413398
N	7.993471	12.171549	19.281821
H	8.421776	12.760152	18.823769
N	5.083069	9.924701	13.872132
H	4.371452	10.016006	14.344565
C	6.444342	11.334297	16.710487
C	6.075645	11.542421	15.378982
C	7.179746	10.071039	17.099741
H	6.729303	9.300577	16.717350
H	7.171499	9.975982	18.065523
C	6.142797	12.297374	17.681008
C	9.271749	8.994393	16.519618
C	6.353074	10.481535	14.336394
H	6.901212	9.778364	14.718785
H	6.834741	10.871519	13.589588
C	5.038681	9.277563	12.715318
C	10.637856	9.170499	15.918251
C	6.549596	12.065235	19.121184
H	6.258277	11.184207	19.400624
H	6.113785	12.720128	19.688234
C	13.017692	8.774512	15.831641
H	13.791968	8.442563	16.225471
C	2.944428	7.774912	12.765976
C	3.687632	8.819789	12.228341
C	11.806775	8.637429	16.486935
C	10.739407	9.829894	14.702444
H	9.982706	10.216126	14.323321
C	10.915603	11.690760	19.041111
H	10.486371	11.669498	18.215865
C	11.960965	9.920449	14.042247
H	12.009934	10.338700	13.213733
C	8.671007	11.383326	20.118015
C	13.089577	9.395134	14.609297
H	13.905374	9.458172	14.166443
C	3.204550	9.477683	11.094241
H	3.694290	10.173600	10.718387
C	10.163159	11.627722	20.189918
C	10.813042	11.746294	21.438408
C	11.788953	7.962775	17.810596
C	1.288959	8.057332	11.053388
H	0.490081	7.794674	10.656289
C	1.744707	7.401939	12.158073
H	1.250711	6.699017	12.512683
C	12.205943	11.857110	21.458018
H	12.646036	11.934657	22.273459

C	12.937197	11.857110	20.287967
H	13.865784	11.904639	20.320650
C	3.379422	7.014706	13.955637
C	1.997709	9.095454	10.528826
H	1.670241	9.550727	9.786922
C	12.299586	11.784567	19.085233
H	12.790978	11.799576	18.295939
C	10.063840	11.777062	22.717947
N	3.324358	18.392529	11.529579
C	3.055707	19.864161	11.826340
H	3.909105	20.304675	11.966877
H	2.652140	20.262150	11.038680
C	2.024104	17.621567	11.419437
H	2.238357	16.677501	11.347535
H	1.532250	17.743140	12.247951
C	4.101710	17.740638	12.666293
H	3.580485	17.818185	13.481734
H	4.200332	16.795071	12.471829
C	4.087644	18.362261	10.226508
H	3.541300	18.781262	9.543433
H	4.888022	18.901334	10.329459
C	2.179644	20.164592	13.001294
H	2.447980	19.616763	13.754637
H	1.259358	19.946961	12.783952
C	2.279981	21.625718	13.377148
H	2.080555	22.168293	12.597659
H	3.190027	21.820584	13.648417
C	5.481500	18.329491	12.919586
H	6.031583	18.213421	12.128658
H	5.400767	19.281562	13.092806
C	6.149880	17.653086	14.104345
H	5.580772	17.738137	14.883834
H	6.258702	16.707519	13.914784
C	4.495179	16.994691	9.737897
H	3.717125	16.417344	9.688873
H	5.129057	16.599954	10.357240
C	1.107917	17.985035	10.270630
H	1.535374	17.773158	9.425775
H	0.915700	18.936355	10.286971
C	-0.189351	17.187807	10.412801
H	0.026561	16.254747	10.564777
H	-0.677404	17.510500	11.185754
C	7.504166	18.260950	14.403394
H	8.099801	18.093350	13.671295
H	7.860252	17.868215	15.204128
H	7.408703	19.209019	14.527590

C	5.128803	17.122768	8.363577
H	4.501712	17.560530	7.767113
H	5.916469	17.685605	8.430578
C	-1.074511	17.300374	9.182286
H	-1.302367	18.220926	9.035213
H	-1.876497	16.790068	9.317921
H	-0.603759	16.960170	8.417504
C	1.334479	22.010699	14.503077
H	0.426397	21.883122	14.217101
H	1.469938	22.931251	14.735127
H	1.508441	21.457867	15.269494
C	5.522509	15.791970	7.776918
H	6.243300	15.416745	8.288407
H	5.805712	15.914543	6.866696
H	4.769954	15.196613	7.798162
O	7.794837	13.240440	11.530559
O	8.211736	14.093451	8.950237
C	7.827599	14.683805	11.236412
H	6.930079	15.009000	11.063193
H	8.188273	15.171598	11.993024
C	7.076238	12.572539	10.448752
H	6.258510	13.035317	10.210166
H	6.882012	11.644483	10.654655
C	8.194472	12.715125	9.334262
H	9.059235	12.452467	9.685604
H	7.985266	12.154789	8.569480
C	8.662914	14.888928	10.069630
H	8.647955	15.826991	9.822873
H	9.578137	14.648784	10.283703
O	8.778186	12.189810	12.779050

Table 10S: Cartesian coordinates (Å) and total electronic energy associated with **complex2**.
Total energy: -5167.48588849 Hartrees.

Complex 2

F	3.900762	8.394358	3.740165
F	3.849054	8.927789	2.554574
F	3.978317	7.199727	3.649760
F	4.387237	6.538527	3.089252
C	3.039406	5.778308	7.054137
C	4.331765	1.686538	7.495828
H	3.659879	1.060474	7.185869
H	5.166296	1.501274	7.038639
C	0.618108	5.053224	7.302104
H	0.449468	5.969960	7.033473
H	0.105843	4.468686	6.720932
C	2.094699	4.749775	7.144542
C	2.513523	3.414600	7.196201
C	6.309024	3.858594	7.431253
H	6.492127	2.945052	7.154874
H	6.834064	4.449521	6.870745
C	8.298103	4.580483	10.582497
C	4.839746	4.152460	7.224614
C	2.575713	7.222086	7.030890
H	3.296258	7.797042	6.726098
H	1.827383	7.321106	6.421305
C	3.890044	3.114345	7.234946
C	1.466672	2.312601	7.291772
H	1.864288	1.542799	7.730880
H	0.735251	2.622438	7.844531
C	7.929514	4.484657	9.148939
C	0.334555	0.389692	4.269677
C	5.440141	6.583246	7.180703
H	5.031746	7.375408	7.565568
H	6.163036	6.308545	7.767041
C	0.925365	8.656282	10.107227
C	1.096112	0.667588	5.522426
C	9.510228	4.104547	11.070682
C	6.671585	8.260201	4.024293
C	5.172723	0.619675	9.551885
C	4.409020	5.478053	7.118712
C	0.905577	0.086243	3.050507
C	8.038439	8.554068	4.016545
H	8.479169	8.640311	4.830185
C	7.780100	5.433334	12.788368
H	7.198087	5.864551	13.372123

C	9.833184	4.302587	12.382839
H	10.637260	3.979973	12.716044
C	8.749807	8.720166	2.874864
H	9.657236	8.921401	2.908443
C	1.414705	8.605175	8.663338
C	6.804073	8.292143	1.624699
H	6.387832	8.196317	0.800726
C	5.370093	0.881599	11.008690
C	-1.274190	-0.242759	2.068972
H	-1.805444	-0.450382	1.335404
C	5.976629	8.116462	5.370030
C	6.062175	8.126045	2.807707
C	7.422707	5.244876	11.460713
H	6.602863	5.557908	11.150754
C	-1.052378	0.364139	4.342001
H	-1.460938	0.578150	5.150476
C	4.460440	0.613286	11.995391
C	-1.840459	0.041525	3.282976
H	-2.764202	0.015971	3.381130
C	-0.182729	7.959946	10.401688
H	-0.616291	7.506370	9.714613
C	8.117137	8.589204	1.681524
H	8.596585	8.704195	0.893713
C	0.099693	-0.217206	1.957904
H	0.493914	-0.405663	1.136514
C	6.543733	1.472526	11.434883
H	7.195245	1.673761	10.802051
C	8.967576	4.989340	13.230059
H	9.216786	5.139468	14.113440
C	10.453914	3.280443	10.197632
C	6.797251	1.782364	12.757372
H	7.595829	2.184833	13.013088
C	1.562949	9.339841	11.112009
C	3.181030	0.000000	11.737092
C	5.833768	1.478915	13.674332
H	5.996684	1.670567	14.568046
C	-0.710513	7.886480	11.677683
H	-1.462937	7.369019	11.848161
C	4.657992	0.910347	13.335961
H	4.007346	0.725083	13.973959
C	1.035608	9.304705	12.424167
H	1.453180	9.761475	13.116407
C	2.367386	0.105409	2.843868
C	4.583632	7.835373	2.696638
C	-0.118462	8.566844	12.656635
H	-0.485516	8.547679	13.511604

C	-0.947568	4.219538	9.012041
C	2.772120	10.116031	10.856294
F	3.687671	9.534687	10.089147
F	3.442933	10.467393	11.930816
F	2.574361	11.262749	10.285454
F	3.032422	0.916735	3.621348
F	2.918239	-1.124358	3.102167
F	2.743767	0.364139	1.614367
F	9.797881	2.446757	9.412404
F	11.237718	4.043857	9.443400
F	11.290390	2.574525	10.969945
F	4.163425	7.570254	1.614367
F	2.813950	-0.245953	10.536003
F	2.470732	-0.590927	12.594644
C	-1.205958	4.024692	10.481761
C	-0.250341	3.401823	11.238576
H	0.567716	3.178229	10.856294
C	-2.426770	4.353695	11.075848
N	4.508170	1.571546	8.944883
H	4.144180	2.175250	9.438234
N	0.931656	1.887772	6.010610
H	0.484761	2.456340	5.545673
N	0.178168	4.863808	8.694334
H	0.665379	5.180992	9.327165
N	2.172426	7.599002	8.379209
H	2.459458	7.116678	9.030122
N	5.989816	6.918637	5.878878
H	6.344522	6.286186	5.413940
N	6.721254	4.024692	8.823483
H	6.168643	3.823457	9.448566
O	8.750595	4.825159	8.270724
O	-1.720023	3.757337	8.180319
O	5.700643	-0.335391	8.986211
O	1.011071	9.413307	7.841948
O	5.480609	9.097082	5.896959
O	1.750274	-0.207623	6.067436
C	-0.495156	3.104762	12.571397
H	0.147829	2.660769	13.077662
C	-2.626415	4.078993	12.426750
H	-3.426025	4.328141	12.829696
C	-1.703946	3.472095	13.142237
H	-1.864176	3.290026	14.041116
F	-3.018435	5.979542	9.451149
F	-4.268626	4.245092	9.590630
F	-4.307142	5.736783	11.143005
C	-3.496715	5.081972	10.290620

F	3.595326	-1.561964	11.331563
F	2.206540	1.089222	11.471044
C	8.824778	4.446326	18.305628
H	9.278908	5.200158	17.897516
H	8.347848	4.781717	19.080524
C	10.739597	4.216344	19.762432
H	10.996569	5.059613	19.356903
H	10.210084	4.417579	20.547660
C	7.810096	3.903312	17.313761
H	7.319514	3.168646	17.716707
H	8.268438	3.564727	16.528533
C	12.722283	4.222732	21.255399
H	12.171524	4.251480	22.053542
H	12.856469	5.136274	20.960938
C	9.225833	2.239134	19.418895
H	8.721101	1.772781	18.731820
H	9.927826	1.638625	19.718521
C	6.837077	5.011700	16.905649
H	6.400202	5.366256	17.696043
H	7.327437	5.733589	16.484622
C	8.311547	2.507447	20.573490
H	7.589174	3.088791	20.291945
H	8.802887	2.954635	21.281228
C	11.986643	3.488066	20.196374
H	11.744271	2.609661	20.526996
H	12.566945	3.369881	19.429227
C	7.742122	1.197825	21.092670
H	8.319601	0.488713	20.772380
H	7.828631	1.213796	22.061290
C	5.785520	4.484657	15.939612
H	6.214541	4.168431	15.141469
H	5.173305	5.187381	15.717475
H	5.306035	3.762768	16.352890
C	14.035505	3.644582	21.609268
H	13.934347	2.705487	21.782328
H	14.377395	4.078993	22.391913
H	14.648090	3.769156	20.878283
C	6.541011	0.856046	20.826623
H	5.989714	1.641819	20.772380
H	6.208919	0.281090	21.521446
H	6.519226	0.392887	19.987152
C	11.416499	3.951225	16.789414
H	10.769989	4.484657	16.301230
H	11.926528	4.542152	17.362837
C	12.338980	3.258084	15.823377
H	11.833078	2.596885	15.324861

H	13.024176	2.791731	16.324477
C	13.000764	4.197179	14.849591
H	12.347590	4.535764	14.232257
H	13.684880	3.727631	14.366573
H	13.394574	4.931845	15.327444
C	10.698488	2.909916	17.628885
H	11.359438	2.296630	17.985337
H	10.113180	2.398844	17.047713
N	9.875975	3.456124	18.783480
N	3.442560	4.947816	10.414603
O	2.384170	5.481247	10.463680
O	4.328481	4.216344	10.548918
O	2.936152	3.612640	10.399105
O	4.327356	6.017873	10.151138

Table 11S: Cartesian coordinates (Å) and total electronic energy associated with **complex3**.
Total energy: -4987.10774649 Hartrees.

Complex 3

N	-2.979089	0.137798	26.433769
N	-3.167674	3.251181	26.540900
N	-9.220926	-0.415548	26.182777
N	-6.025837	-1.976546	26.384795
N	-9.351317	2.775346	26.703127
N	-6.340347	4.805719	26.914328
O	-1.432699	4.413855	25.466531
O	-1.366069	-1.261717	25.515505
O	-10.997652	-1.065784	24.955364
O	-7.060992	-3.647351	25.175747
O	-10.616458	4.527969	26.035855
O	-5.255099	6.691835	26.176655
F	-13.689361	-0.155023	25.114530
F	-2.193257	-4.726054	28.248872
F	-5.325507	-5.544232	26.237873
F	-12.335582	1.472720	25.601210
F	-14.277263	1.360759	26.531718
F	-9.076467	6.181550	27.756070
F	-0.942886	-3.955245	26.632727
F	-9.888739	7.296856	29.353850
F	-3.037428	-3.360989	26.798014
F	-11.032756	7.060015	27.593843
F	-7.212780	-6.560496	25.812410
F	0.101366	1.976546	25.344096
F	-5.948597	-7.217191	27.437738
F	1.252131	3.838977	25.362461
F	2.060396	1.976546	26.228690
C	-7.483460	1.995924	25.276756
C	-4.820652	1.128224	25.224721
C	-8.322106	-0.363874	24.952303
C	-7.241944	0.656696	25.187991
C	-10.821664	-1.369372	28.365185
C	-11.334117	-0.716982	27.275512
C	-6.425197	2.975584	25.371644
C	-5.836029	0.221769	25.200234
C	-5.099339	2.499749	25.273695
C	-12.814806	-0.966742	29.604842
C	-11.552262	-1.500711	29.623207
C	-13.364222	-0.331577	28.496803
C	-12.666107	-0.185167	27.299999
C	-10.543013	-0.723442	26.081768

C	-13.219723	0.523203	26.170534
C	-5.572347	-1.235879	25.132895
C	-7.142357	-5.255717	27.719339
C	-6.697346	-3.143526	26.299091
C	-7.146499	-3.817446	27.557113
C	-8.416028	-3.479410	29.754825
C	-7.835517	-5.679878	28.897779
C	-6.437336	-6.155713	26.822501
C	-7.759350	-2.973431	28.548838
C	-8.385047	-4.878925	29.861956
C	-4.000817	3.535390	25.285939
C	-5.656166	5.933944	27.101041
C	-0.654838	-0.374639	30.100705
C	-6.715782	4.493520	25.546114
C	-10.694125	3.946632	28.343759
C	-8.888895	2.463146	25.255330
C	-1.144523	-0.083971	28.830439
C	-0.991541	3.546156	27.612209
C	-5.232273	6.228918	28.496803
C	-10.232528	3.798068	26.899023
C	-2.032332	-0.749279	26.498048
C	-3.377787	0.643777	25.077799
C	-1.570787	-1.089469	27.924418
C	-11.117176	2.747356	28.913083
C	-1.467639	-2.495443	28.444768
C	-0.658652	-1.735399	30.617994
C	-10.762416	5.150215	29.063066
C	0.931022	2.755968	26.005246
C	-1.872090	-3.567687	27.465286
C	-11.756910	2.805489	30.278236
C	-4.165730	5.475333	30.617994
C	-11.808623	4.075818	30.884291
C	-1.094207	-2.786111	29.724217
C	0.397703	3.083239	27.434677
C	1.102754	2.947594	28.683517
C	-11.310339	5.193277	30.339454
C	-10.189804	6.366717	28.420281
C	-1.510692	3.767925	28.885535
C	-4.637385	5.139450	29.295693
C	-5.368438	7.484176	29.127345
C	-1.865424	3.722710	26.449074
C	0.604044	3.126301	29.947661
C	-4.242371	6.717672	31.064882
C	-0.809361	3.559074	30.103766
C	-4.935059	7.832978	30.354758
F	-5.153814	9.277708	27.532626

F	-6.423320	9.652347	29.145710
F	-6.875861	8.435846	27.560174
C	-5.974262	8.633931	28.435586
N	-2.336271	7.940633	24.006491
C	-1.469600	8.993499	26.247056
C	-2.236487	7.811447	25.530809
C	-3.123852	9.226034	23.596333
C	-3.016137	6.642314	23.559602
C	-3.037041	6.502362	22.053648
C	-0.168669	7.557381	27.780557
C	-3.999579	5.178206	21.744499
C	-4.603666	9.228187	23.902421
C	-3.969483	4.980120	20.204876
C	-0.911478	8.082737	23.379010
C	2.353582	6.114804	23.210662
C	1.325583	7.184895	22.855599
C	0.085676	6.844705	23.611637
C	-5.023556	10.632008	23.535115
C	-5.272471	11.432961	24.946181
C	-1.365889	8.526276	27.823409
N	8.064964	6.325808	22.779077
C	7.448223	4.986580	23.311671
C	7.874739	6.476525	21.279246
C	9.525978	6.304277	23.238209
C	11.925723	7.264559	23.229027
C	8.435089	5.199737	20.489538
C	10.047637	6.491597	18.818297
C	7.258324	7.533697	23.342279
C	8.734107	5.638969	19.011133
C	5.540829	3.305009	23.486141
C	10.328346	7.454032	22.616851
C	5.941255	4.872465	23.170870
C	6.287975	8.709290	25.252269
C	7.467482	7.705945	24.912511
C	4.105949	3.109076	23.633063
C	11.808756	7.721017	24.661519
C	6.499682	9.142063	26.850049
F	15.721350	19.821439	2.240565
F	0.102115	20.680525	2.292600
O	18.168355	18.861156	1.900807
O	8.228018	1.608366	2.433400
O	8.882510	2.471759	4.964749
C	9.363734	1.259564	4.542348
C	9.486539	1.291860	2.947629
C	7.573840	2.796877	3.045577
C	7.457698	2.796877	4.475008

O	7.661081	16.776955	1.723276
O	6.656697	15.620741	4.092398
C	8.109996	15.472177	3.581231
C	6.133753	16.897529	3.507770
C	6.240819	17.065471	2.200774
C	8.286507	15.726242	2.231382
O	1.952998	12.121953	25.916480
C	3.059005	10.365023	24.820685
C	2.580618	10.132489	27.208172
O	2.706474	9.493018	25.898115
C	1.946912	11.303775	24.673763
C	1.456471	11.325306	26.935754
O	-1.579494	12.085350	24.826807
O	-2.036476	14.804716	24.545206
C	-1.529086	13.017643	26.023611
C	-2.403037	14.098499	25.763436
C	-1.247283	12.664534	23.565724
C	-2.125010	13.958547	23.415741
O	17.114572	0.557653	1.885503
O	5.532442	12.776495	26.262360
O	6.232060	14.281512	24.046282
C	6.796621	13.026255	24.306457
C	4.755824	14.076968	26.100133
C	6.989330	12.759271	25.885872
C	4.614201	14.425770	24.701311
O	-1.942052	12.563339	29.715034
O	1.999348	13.532234	29.806860
O	19.085104	0.312200	0.226505

Table 12S: Cartesian coordinates (Å) and total electronic energy associated with previously published[R7S] fluoride complex with *m*-nitrophenyl substituted hexa-amide receptor .
Total energy: -4192.07545719 Hartrees.

C	7.802253	4.772032	17.388816
C	6.608847	3.847849	16.985952
O	8.881364	4.009446	17.442058
C	7.517770	2.066235	18.105807
C	8.711176	2.990419	18.508671
O	6.438659	2.828822	18.052566
F	-3.290360	8.376757	17.440638
F	7.425072	13.590149	0.476160
O	5.018072	14.184585	1.592821
H	5.839859	14.074740	1.121630
H	4.566046	13.955005	0.869618
O	-0.883645	8.256776	16.162477
H	-0.314607	8.454587	16.788957
H	-1.644311	8.288140	16.575989
O	-3.845903	10.848825	16.552918
H	-3.625394	10.108980	16.930935
H	-3.828158	11.444921	17.179398
O	-1.439277	11.860357	15.566167
O	0.939571	11.032960	17.007249
H	0.766267	10.196094	17.339124
C	-2.480102	5.184497	17.660350
C	-3.678960	5.069054	16.726841
H	-3.636193	4.231844	16.238790
H	-4.501014	5.080078	17.241513
N	-3.666500	6.190662	15.788009
H	-3.472239	6.980686	16.132306
C	-3.704077	6.034549	14.449861
O	-3.849060	4.945416	13.898985
C	-3.475941	7.278212	13.629935
C	-3.656501	8.570292	14.103789
H	-3.975696	8.698670	14.968083
C	-3.373636	9.669953	13.319357
H	-3.501520	10.526909	13.654782
C	-2.897208	9.495286	12.034452
H	-2.690307	10.228770	11.500258
C	-2.739471	8.212869	11.562374
C	-3.023857	7.101315	12.329057
H	-2.915540	6.246708	11.979435
N	-2.199518	8.025536	10.202930
O	-2.126327	6.900292	9.768120
O	-1.799586	9.000045	9.578224
C	-1.183269	5.041128	17.158101

C	-0.985741	4.623150	15.709920
H	-0.365334	3.877870	15.672651
H	-1.833757	4.323914	15.344326
N	-0.469248	5.718857	14.891769
H	-0.591615	6.435083	15.191699
C	0.055897	5.442647	13.695600
O	0.177265	4.295406	13.282088
C	0.478998	6.617447	12.843730
C	0.500155	7.931501	13.282088
H	0.273920	8.131597	14.162355
C	0.859689	8.952547	12.410695
H	0.896908	9.829960	12.715949
C	1.160500	8.667329	11.097394
H	1.371185	9.346639	10.497535
C	1.144371	7.365198	10.694530
C	0.809380	6.334608	11.533978
H	0.805245	5.456510	11.225175
N	1.463583	7.042874	9.285394
O	1.810914	7.972485	8.568402
O	1.374232	5.890274	8.910925
C	-0.069117	5.208606	17.992225
C	1.321646	4.990398	17.431410
H	1.849056	4.494545	18.077412
H	1.257613	4.451631	16.627456
N	2.009947	6.244728	17.115507
H	1.579863	7.138851	17.481102
C	3.197436	6.164069	16.512099
O	3.709828	5.080955	16.238790
C	3.907675	7.460591	16.190872
C	3.318646	8.705520	16.235241
H	2.426491	8.778988	16.489027
C	4.026517	9.851024	15.908690
H	3.615983	10.682235	15.947734
C	5.327838	9.748031	15.532447
H	5.799612	10.514545	15.292859
C	5.944168	8.543629	15.500502
C	5.247247	7.347459	15.832377
H	5.672401	6.520172	15.809305
N	7.328548	8.410071	15.088764
O	7.881118	7.314613	15.138457
O	7.910142	9.425163	14.714296
C	-0.266837	5.555075	19.346345
C	0.931301	5.719639	20.262106
H	0.759579	5.244597	21.090905
H	1.705300	5.311845	19.843269
N	1.239547	7.102797	20.570909

H	1.236142	7.617529	19.965726
C	1.769587	7.478110	21.740457
O	1.916351	6.682402	22.668641
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C	6.592722	3.070221	16.758786
O	8.503961	3.425603	16.641654

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