Supporting Information

Elucidating sensing mechanisms of a pyrene-excimer based calix[4]arene for ratiometric detection of Hg(II) and Ag (I) and chemosensor behaviour as INHIBITION or IMPLICATION logic gates

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I. EXPERIMENTAL INFORMATION

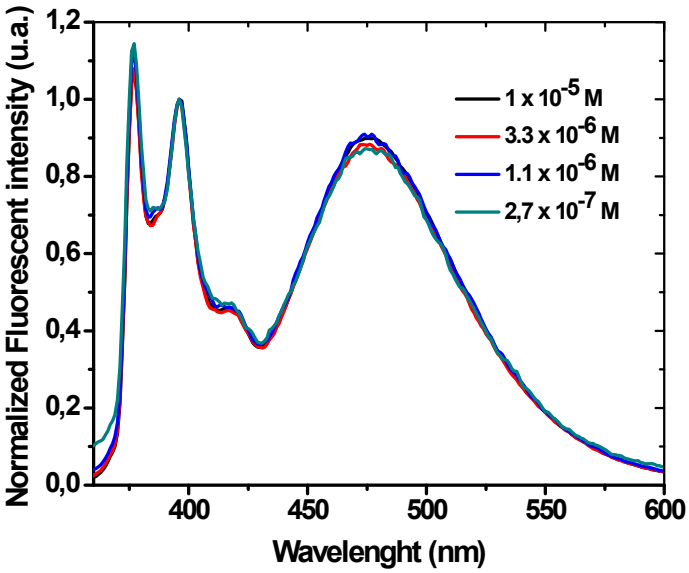


Figure S1. Normalized fluorescence intensities of **2** at different dilutions (CH_3CN/DMSO 99:1).

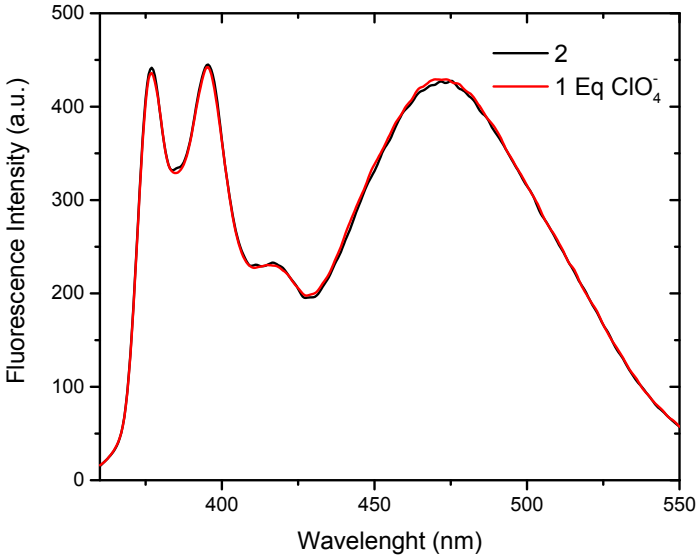


Figure S2. Fluorescence spectra of **2** (1.15 µM in CH_3C/DMSO 99:1) in presence of 2 equilvalents of NBu_4ClO_4.

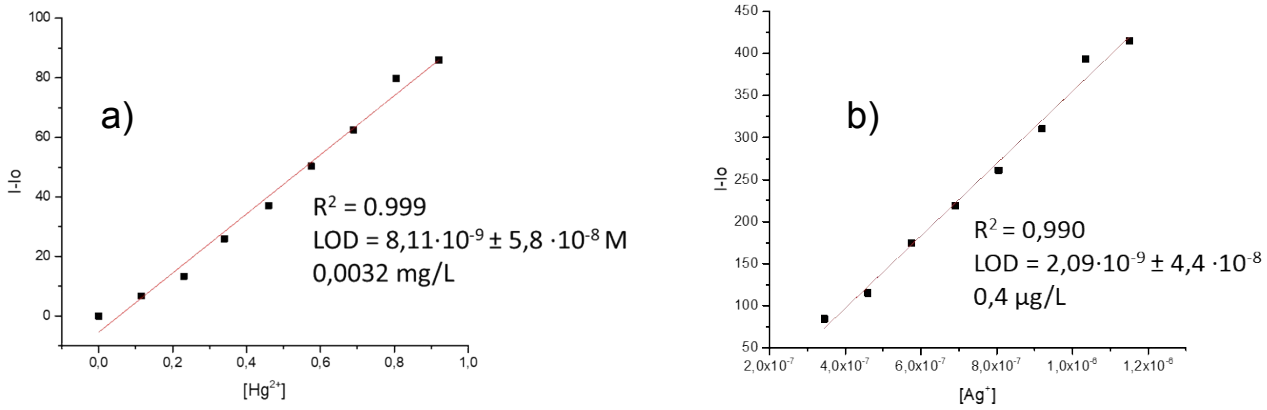


Figure S3. Calibration curve of **2** with Hg^{2+} (a) and Ag+ (b) in (CH_3CN/DMSO 99:1) for LOD determination.

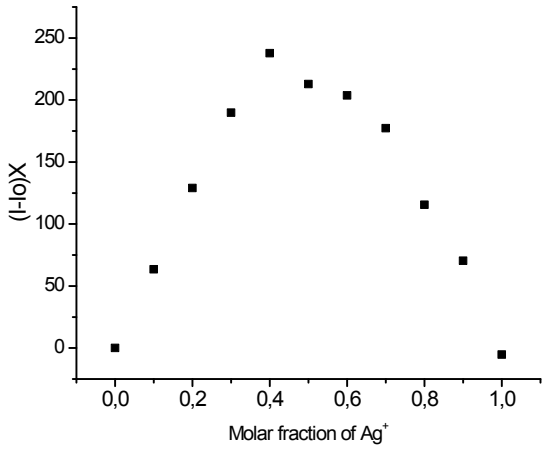


Figure S4. Job Plot for a complex of compound **2** and Ag^+ ion (λ=372 nm, CH_3CN/DMSO 99:1)

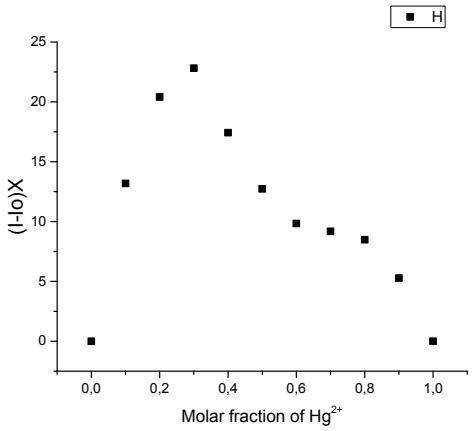


Figure S5. Job Plot for a complex of compound **2** and Hg^{2+} ion (λ=372 nm, CH_3CN/DMSO 99:1)

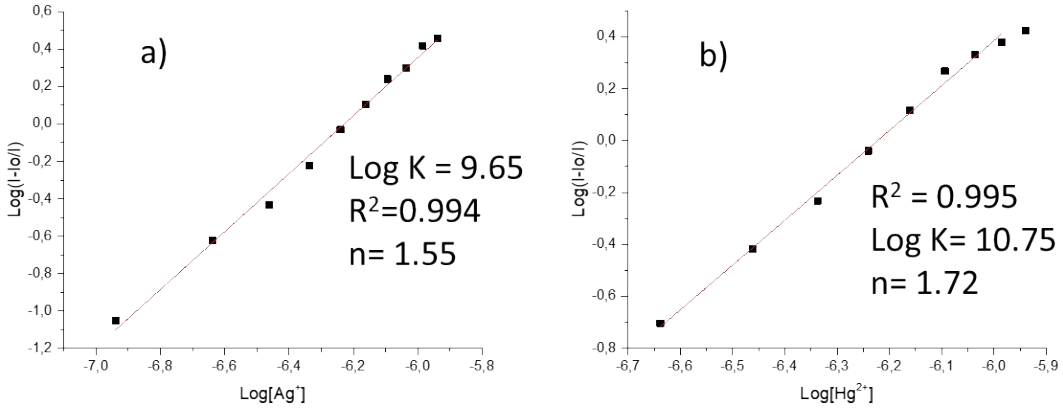


Figure S6. Hill Plots for the complexes 2:Ag^+ (a) and 2:Hg^{2+} (b) in CH_3CN/DMSO (99:1)

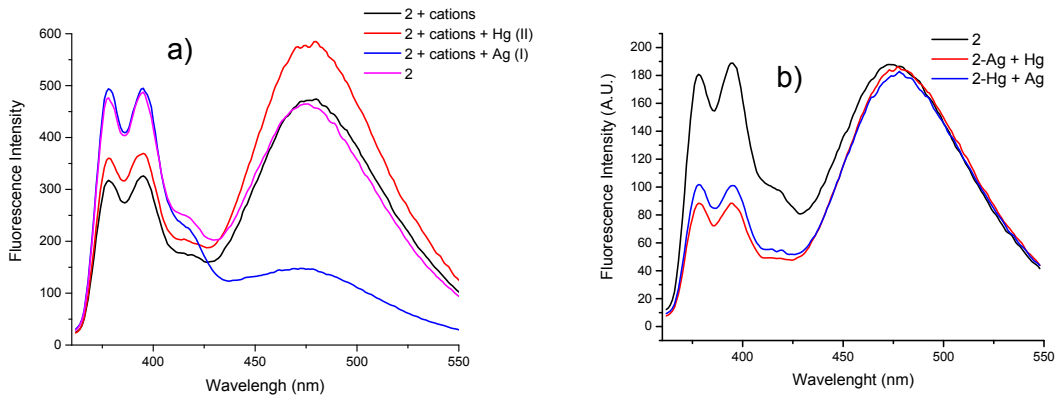


Figure S7. a) Interference studies of **2** in presence of Ag^+, Hg^{2+}, and cation mixture and (b) competitive interferent study of **2** with Ag^+ and Hg^{2+}

Ref	LOD Hg^{2+} (nM)	LOD Ag^{+} (nM)	Solvent
65	70	-	THF
67	100	-	THF/H_2O 9:1
64	36	-	HEPES/CH_3CN 3:7
66	12500	-	MeOH
69	-	68	Acetic/Acetate Buffer
68	-	200	DMF
2[a]	2.09	8.11	CH_3CN

Table S1. Comparative Results for Hg^{2+} and Ag^{+} detection probes. [a]Compound **2** studied in the present work

a) ^{1}H and ^{13}C Spectra

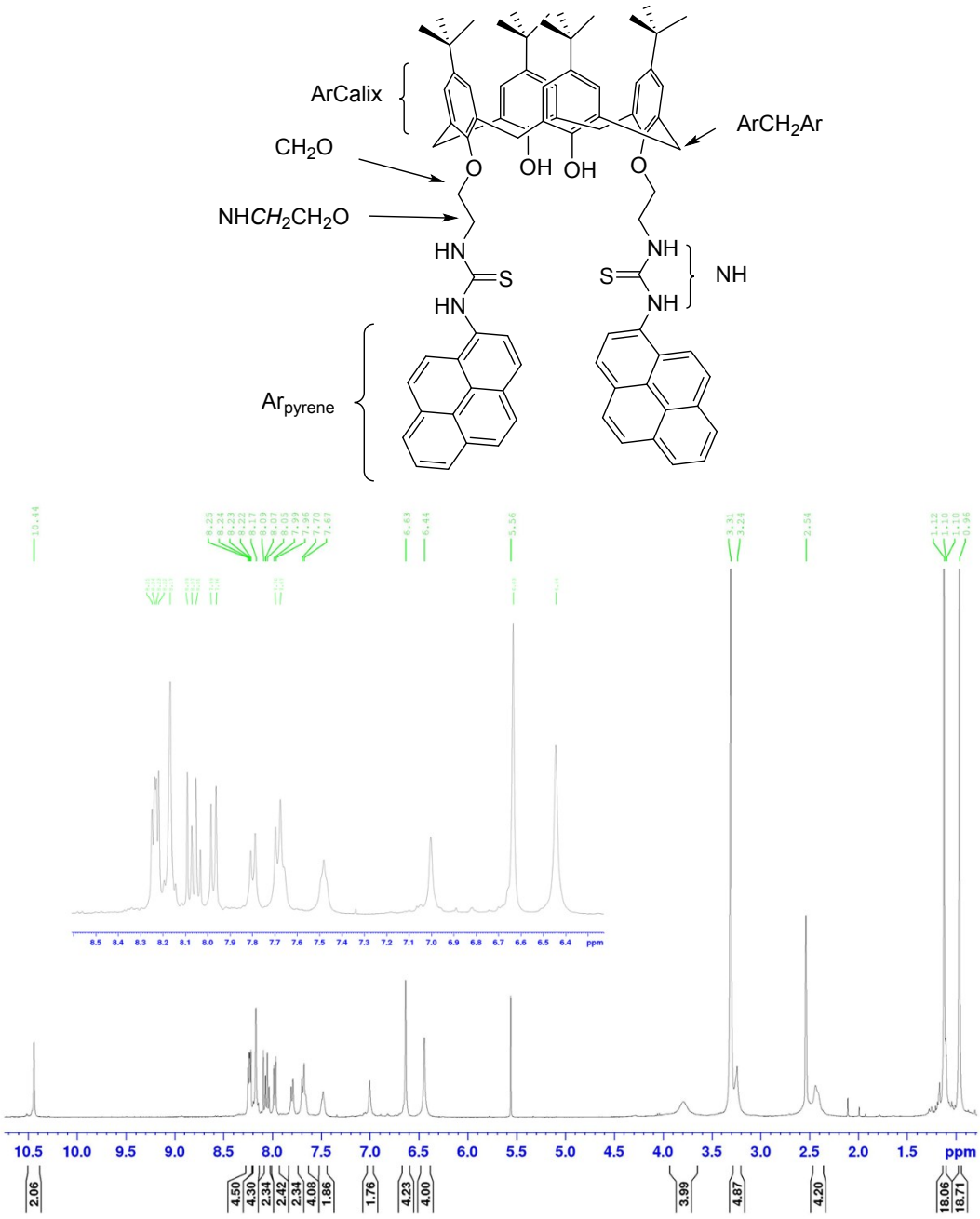


Figure S8. ^{1}H NMR Spectrum (300 MHz, 298 K) of compound **1**.

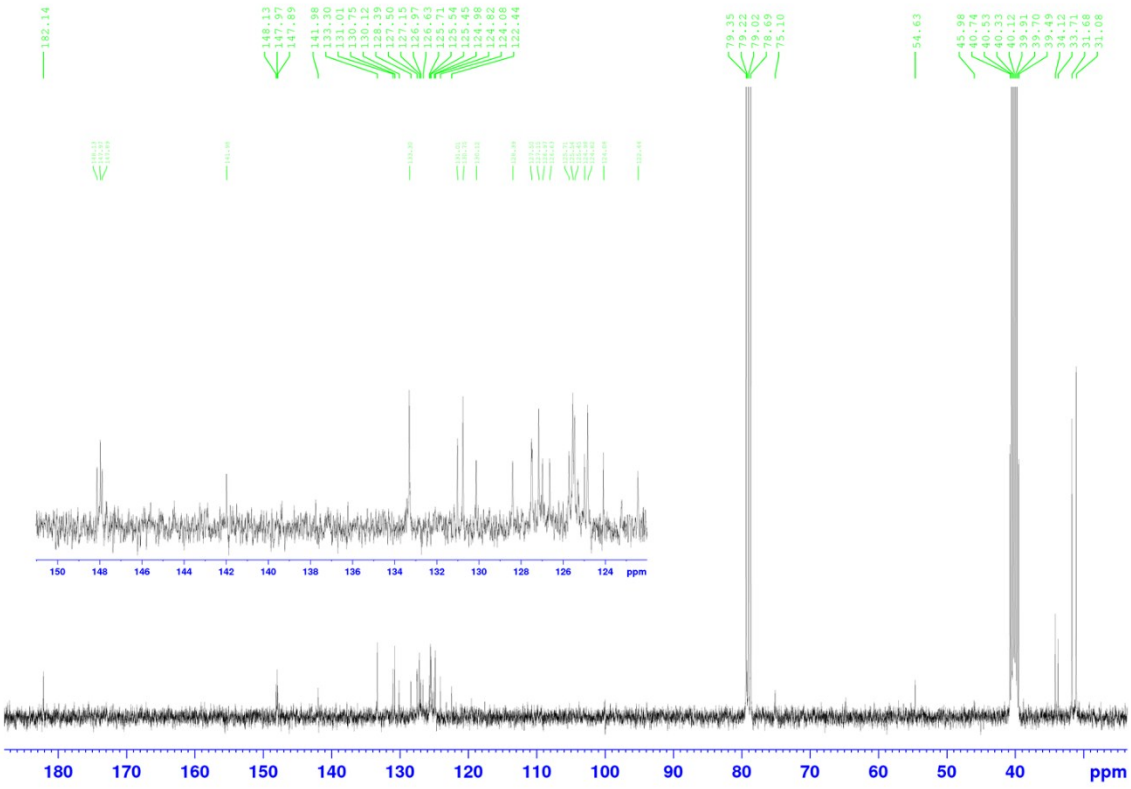


Figure S9. ^{3}C NMR Spectrum (75.5 MHz, 298 K) of compound **1**.

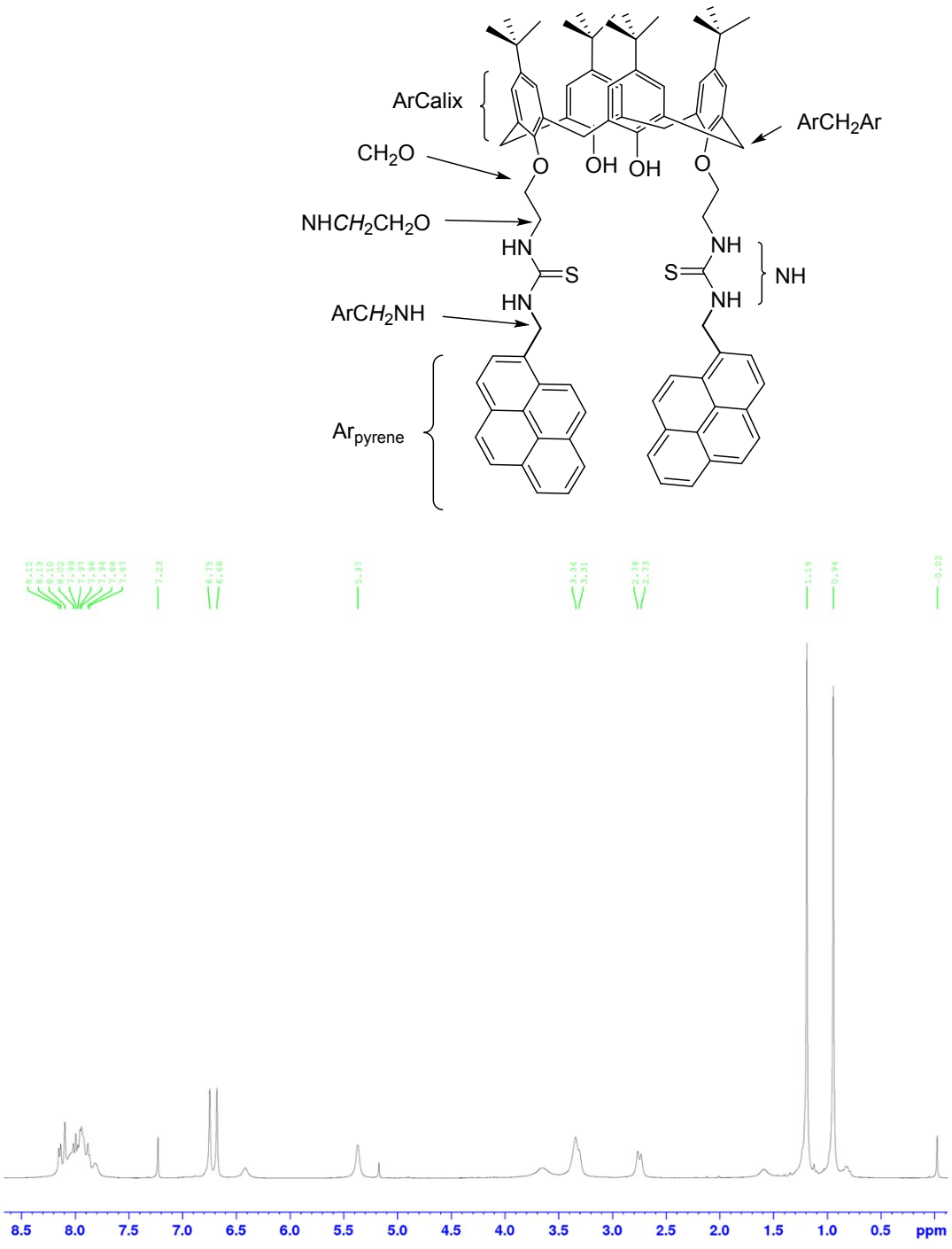


Figure S10. ^{1}H NMR Spectrum (300 MHz, 298 K) of compound **2**.

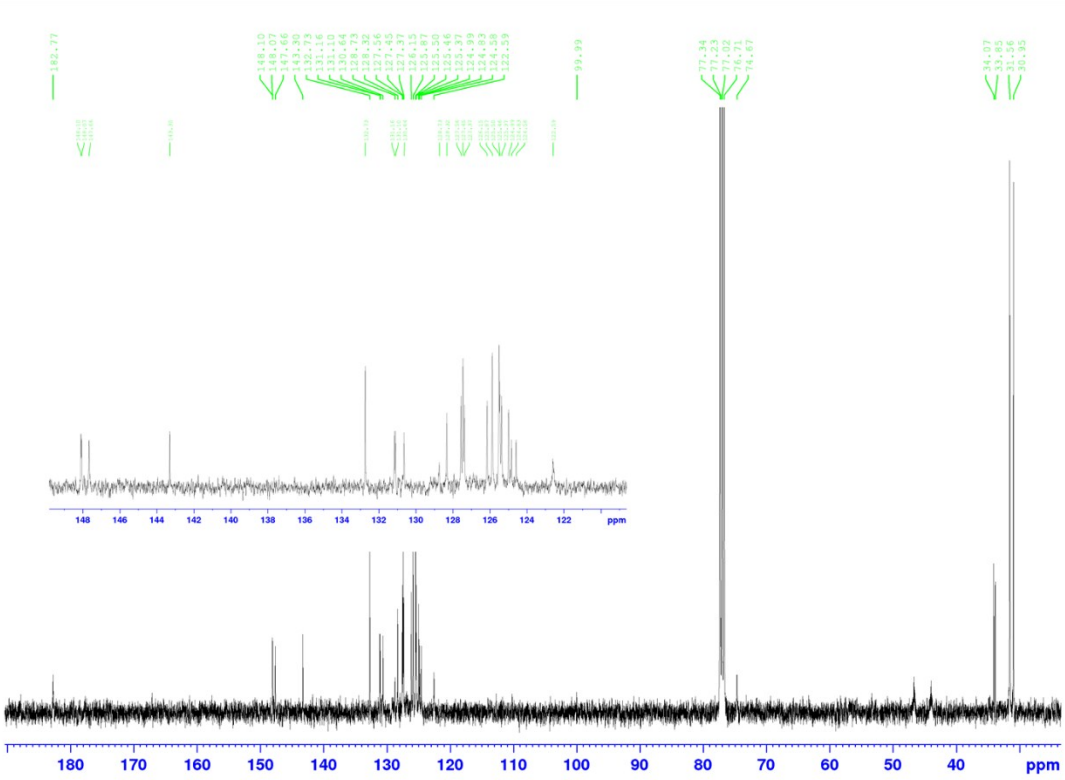


Figure S11. ^{13}C NMR Spectrum (75.5 MHz, 298 K) of compound **2**.

b) Mass Spectra

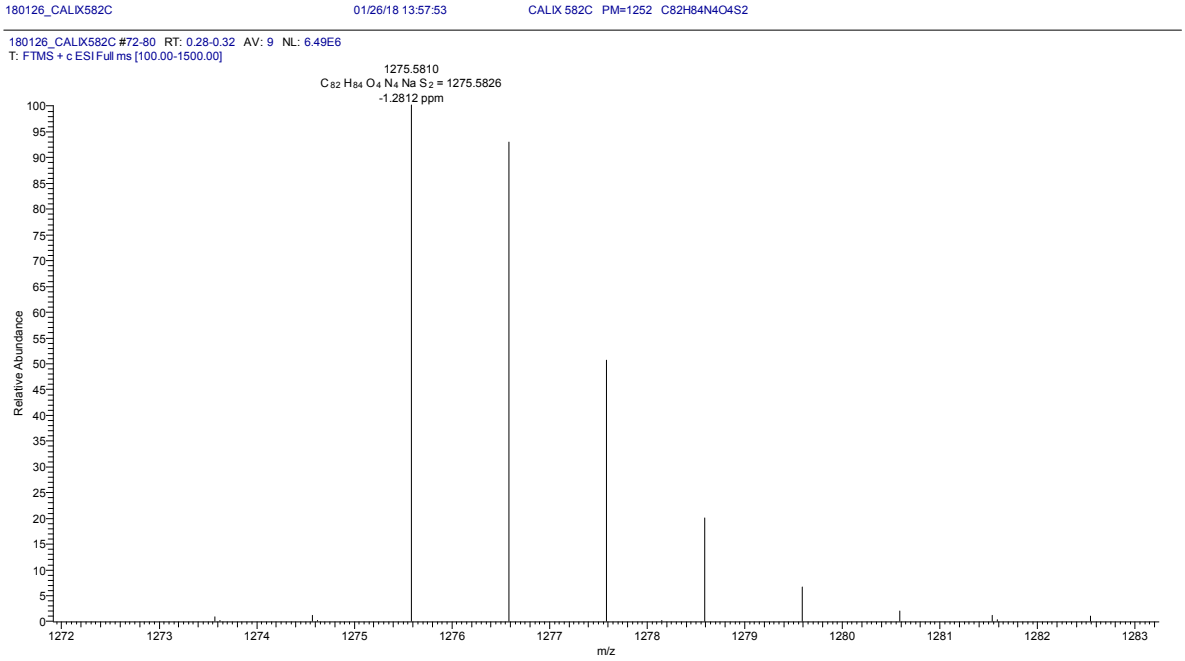


Figure S12. HR2MS (ESI) of compound **1**

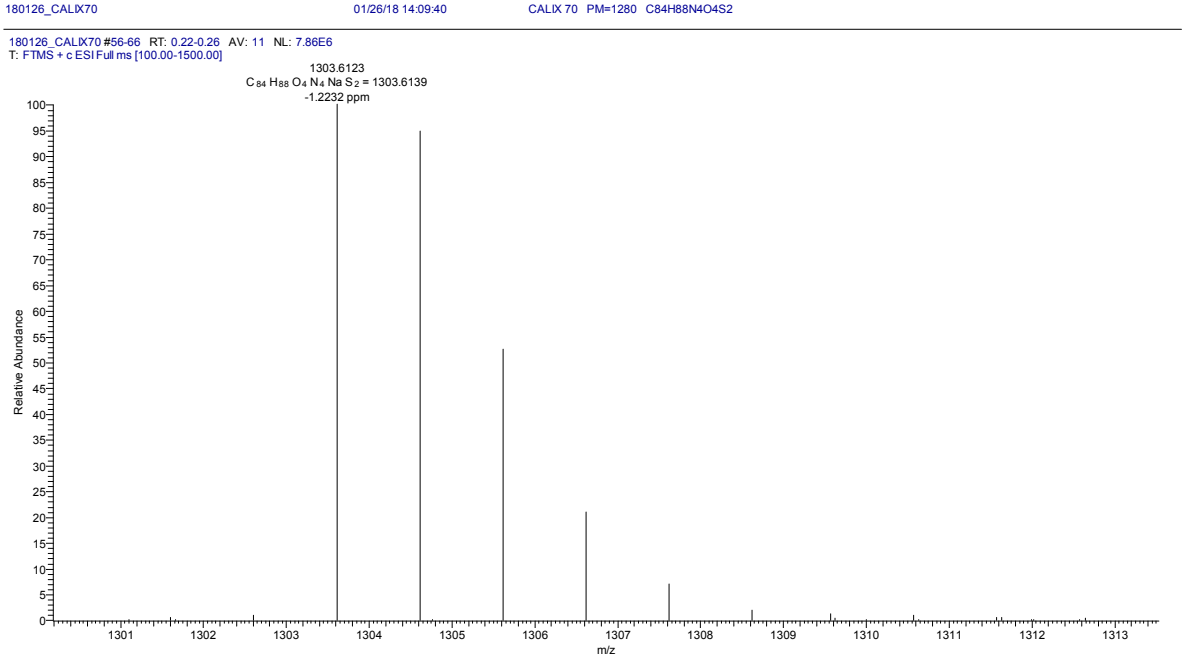
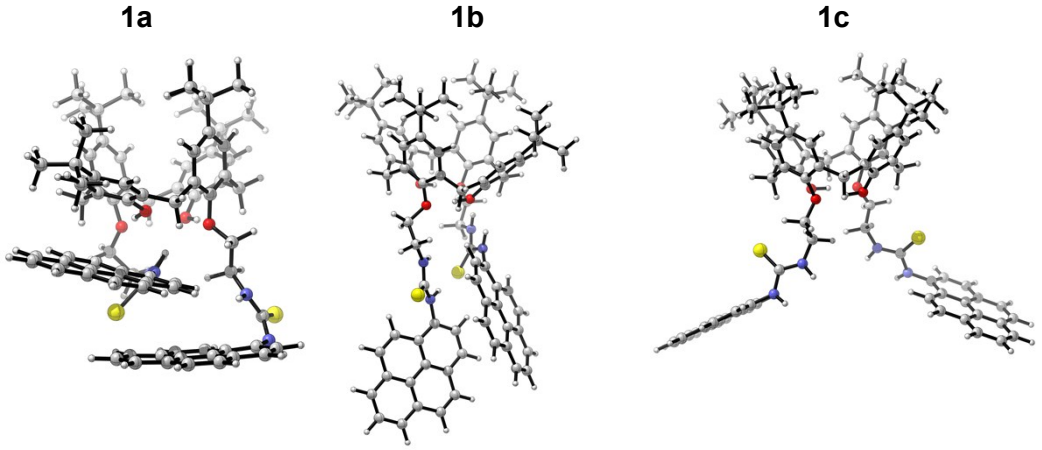


Figure S13. HR-MS (ESI) of compound **2.**

II. Conformational analysis of derivative 1 and Frontier Molecular Orbitals



	1a	1b	1c
ΔG	0.0	4.09	10.91
(% pop)	100	0	0

Figure S14. Highest (H-1 and H) and lowest (L and L+1) molecular orbitals of **2a**.

Frontiers Molecular Orbitals of 2a

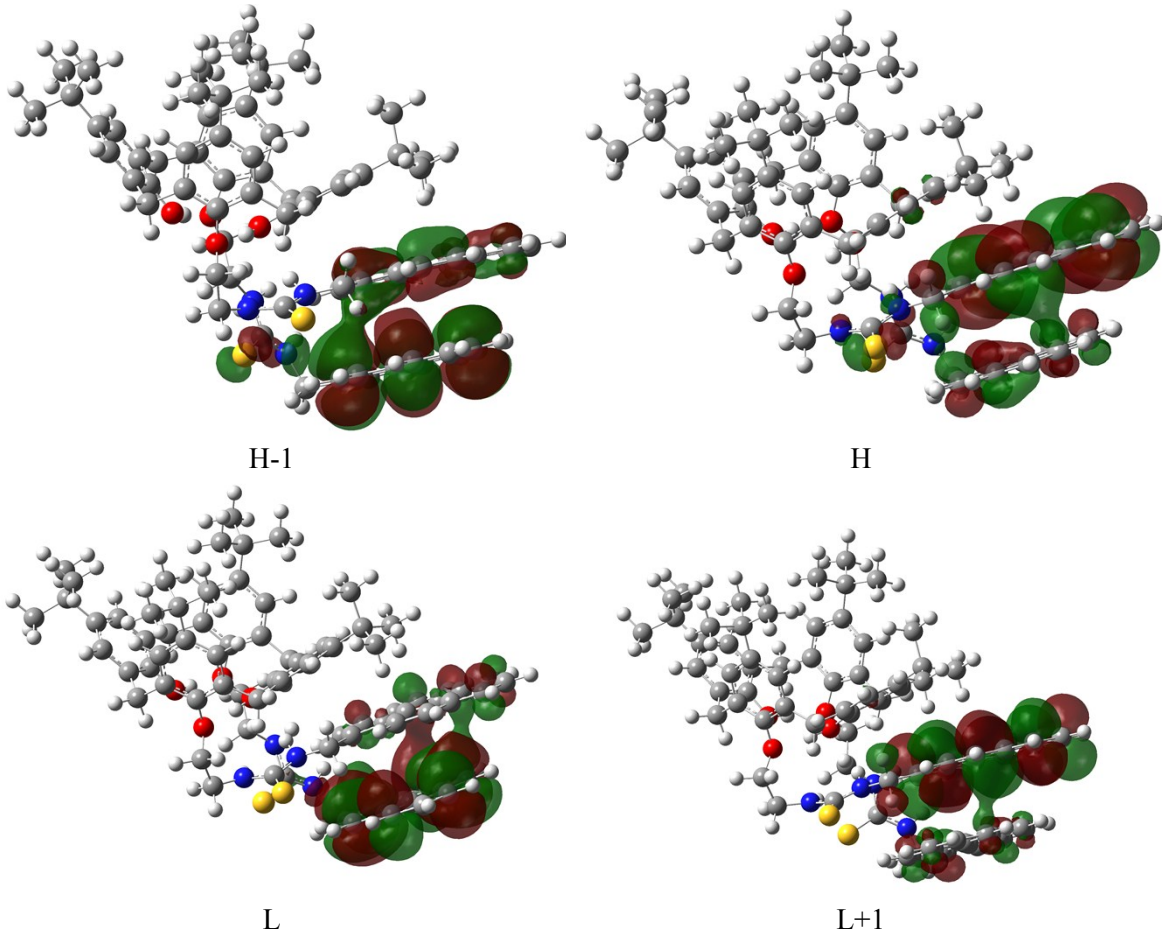


Figure S15. Highest (H-1 and H) and lowest (L and L+1) molecular orbitals of **2a**.

III. Boolean operations for two inputs

Table S2. Table of Boolean Operations for two inputs [1]

Operation N°	Commutative to operation N°	Result for				Entry	Meaning	Logic gate
		A=0 B=0	A=0 B=1	A=1 B=0	A=1 B=1			
0	15	0	0	0	0	’0’ constant	‘0’ constant	ZERO
1	14	0	0	0	1	Conjuction	A and B	AND
2	-	0	0	1	0	Exclusion	A excludes B	INHIBIT
3	12	0	0	1	1	1st variable	A	ID A
4	-	0	1	0	0	Exclusion	B excluding A	INHIBIT
5	10	0	1	0	1	2nd variable	B	ID B
6	9	0	1	1	0	Nonequivalence	Either A or B	XOR
7	8	0	1	1	1	Disjunction	A or B	OR
8	7	1	0	0	0	Nondisjunction	Neither A or B	NOR
9	6	1	0	0	1	Equivalence operation	A equivalent to B	EQU
10	5	1	0	1	0	Negation of variable B	Not B	INV B
11	-	1	0	1	1	Implication	B implies A	IMPLICATION
12	3	1	1	0	0	Negation of variable A	Not A	INV A
13	-	1	1	0	1	Implication	A implies B	IMPLICATION
14	1	1	1	1	0	Nonconjunction	No both A and B	NAND
15	0	1	1	1	1	‘1’ constant	‘1’ constant	ONE