

Supporting Information

Benzimidazolium-based chemosensors: Selective recognition of H_2PO_4^- , $\text{HP}_2\text{O}_7^{3-}$, F^- and ATP through fluorescence and gelation studies

Kumaresh Ghosh^{*a}, Debasish Kar^a, Debashis Sahu^b and Bishwajit Ganguly^{*b}

^aDepartment of Chemistry, University of Kalyani, Kalyani-741235, India. Email: ghosh_k2003@yahoo.co.in, Fax: +913325828282; Tel: +913325828750

^bComputation and Simulation Unit, Analytical Discipline and Centralized Instrument Facility, and Academy of Scientific and Innovative Research CSIR-Central Salt and Marine Chemicals Research Institute, Bhavnagar, Gujarat, 364002, India. E-mail: ganguly@csmcni.org

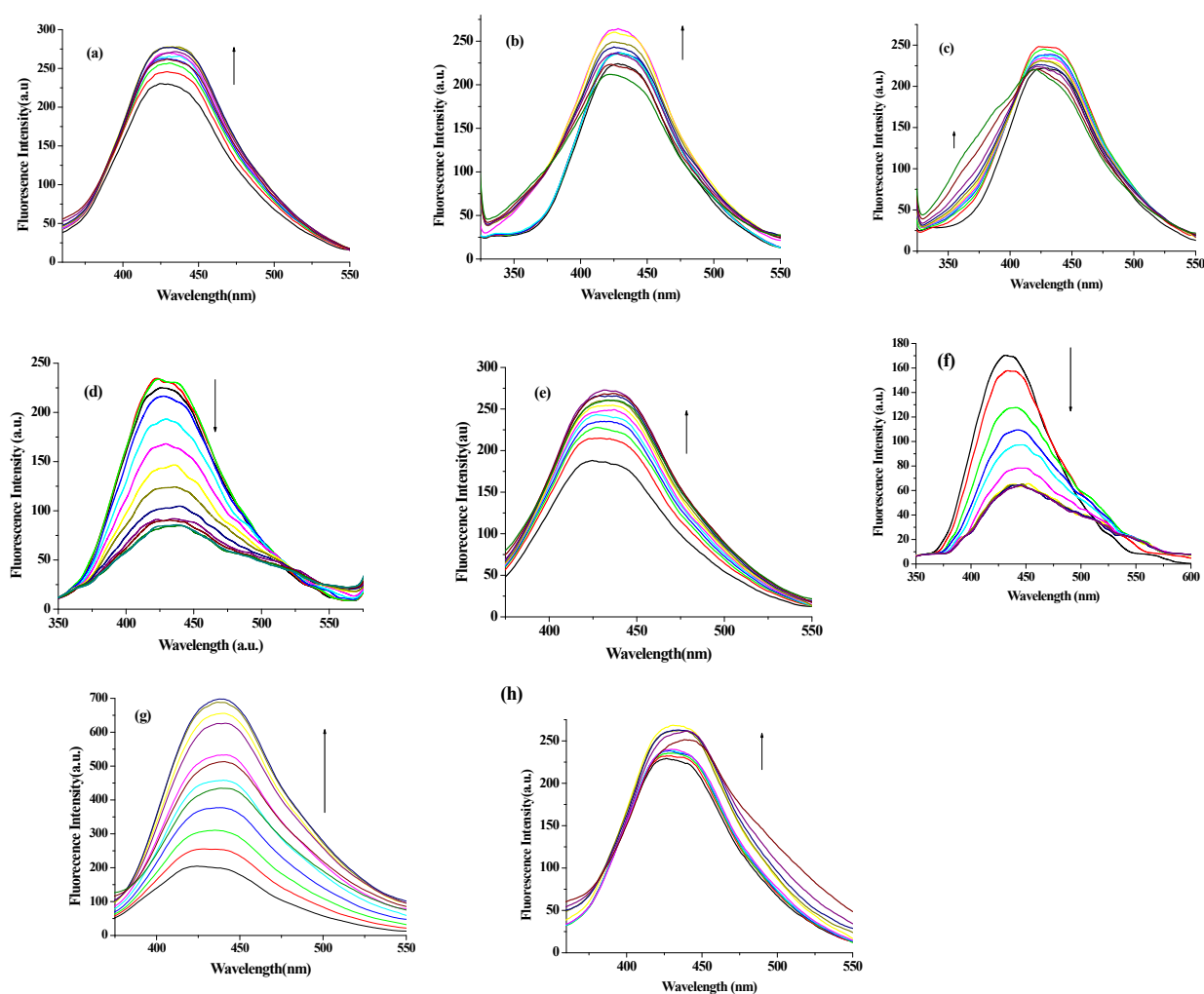


Figure 1S. Change in emission of **1** ($c = 3.16 \times 10^{-5}$ M) upon addition of (a) Cl^- , (b) Br^- , (c) I^- , (d) AcO^- , (e) HSO_4^- , (f) $\text{P}_2\text{O}_7^{4-}$, (g) H_2PO_4^- , (h) F^- (counter cations: tetrabutylammonium ions) in CH_3CN .

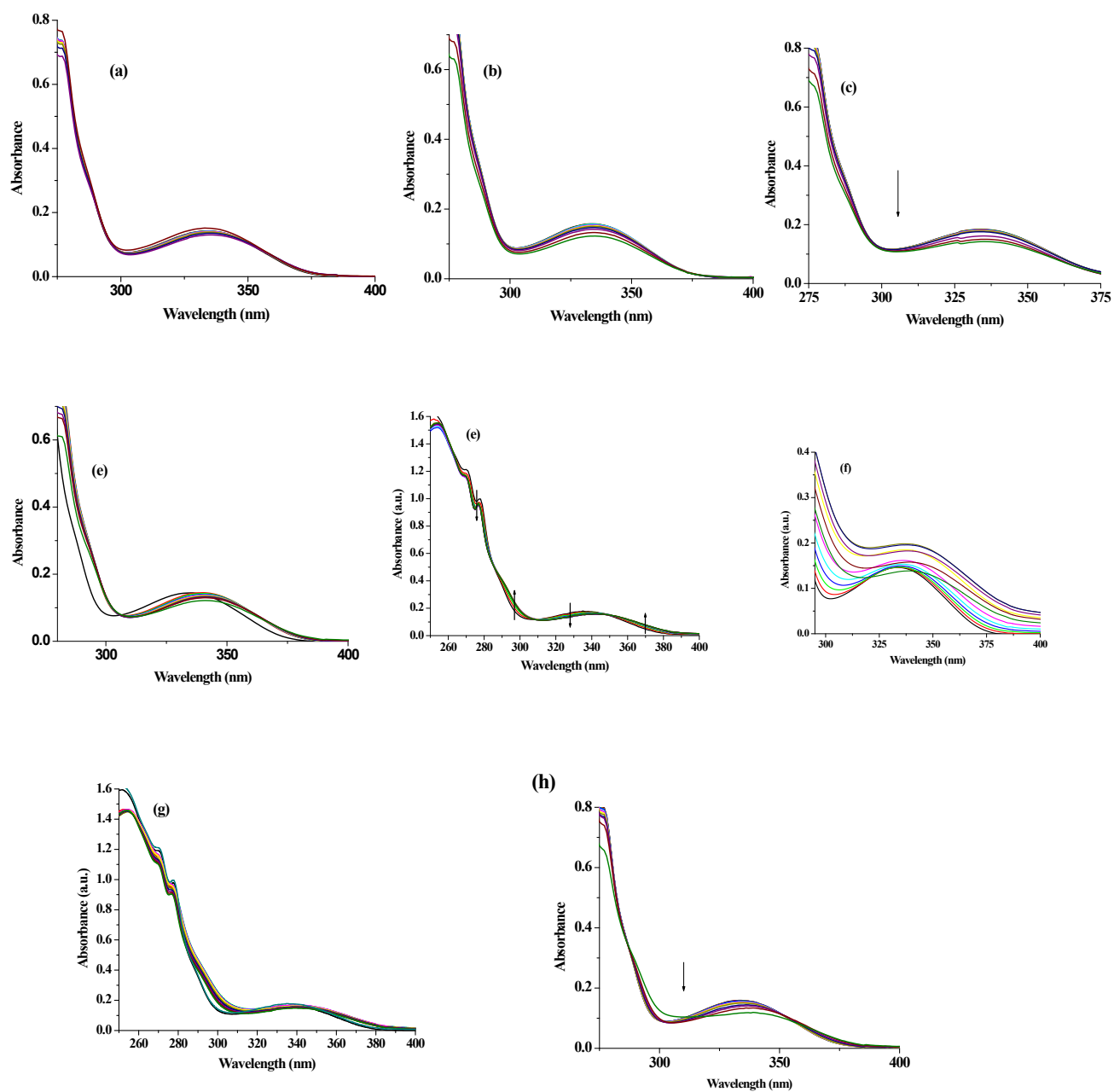


Figure 2S. Change in absorbance of **1** ($c = 3.16 \times 10^{-5} \text{ M}$) upon addition of (a) Cl^- , (b) Br^- , (c) I^- , (d) HSO_4^- , (e) $\text{HP}_2\text{O}_7^{3-}$, (f) H_2PO_4^- , (g) $\text{P}_2\text{O}_7^{4-}$, (h) F^- (counter cations: tetrabutylammonium ions) in CH_3CN .

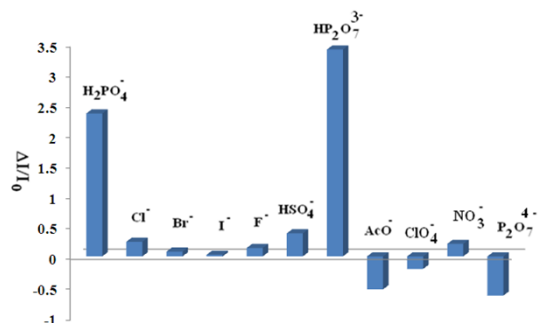


Figure 3S. Change in fluorescence ratio of **1** ($c = 3.16 \times 10^{-5}$ M) at 430 nm upon addition of 2 equiv. amounts of different anionic guests (counter cations: tetrabutylammonium ions) in CH_3CN .

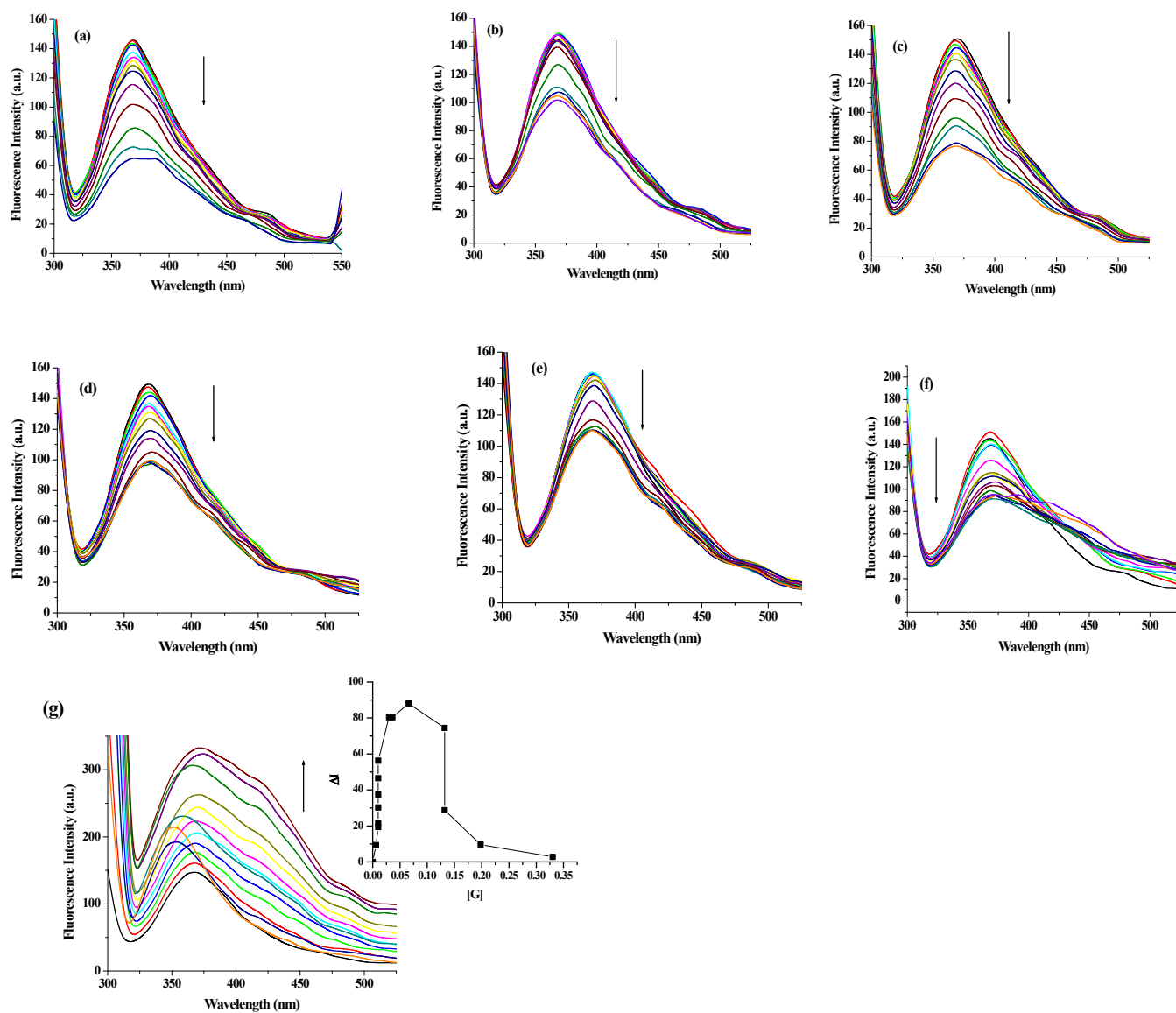


Figure 4S. Change in emission of **2** ($c = 3.27 \times 10^{-5}$ M) upon addition of (a) Cl^- , (b) Br^- , (c) I^- , (d) AcO^- , (e) HSO_4^- , (f) $\text{HP}_2\text{O}_7^{3-}$, (g) H_2PO_4^- (counter cations: tetrabutylammonium ions) in CH_3CN .

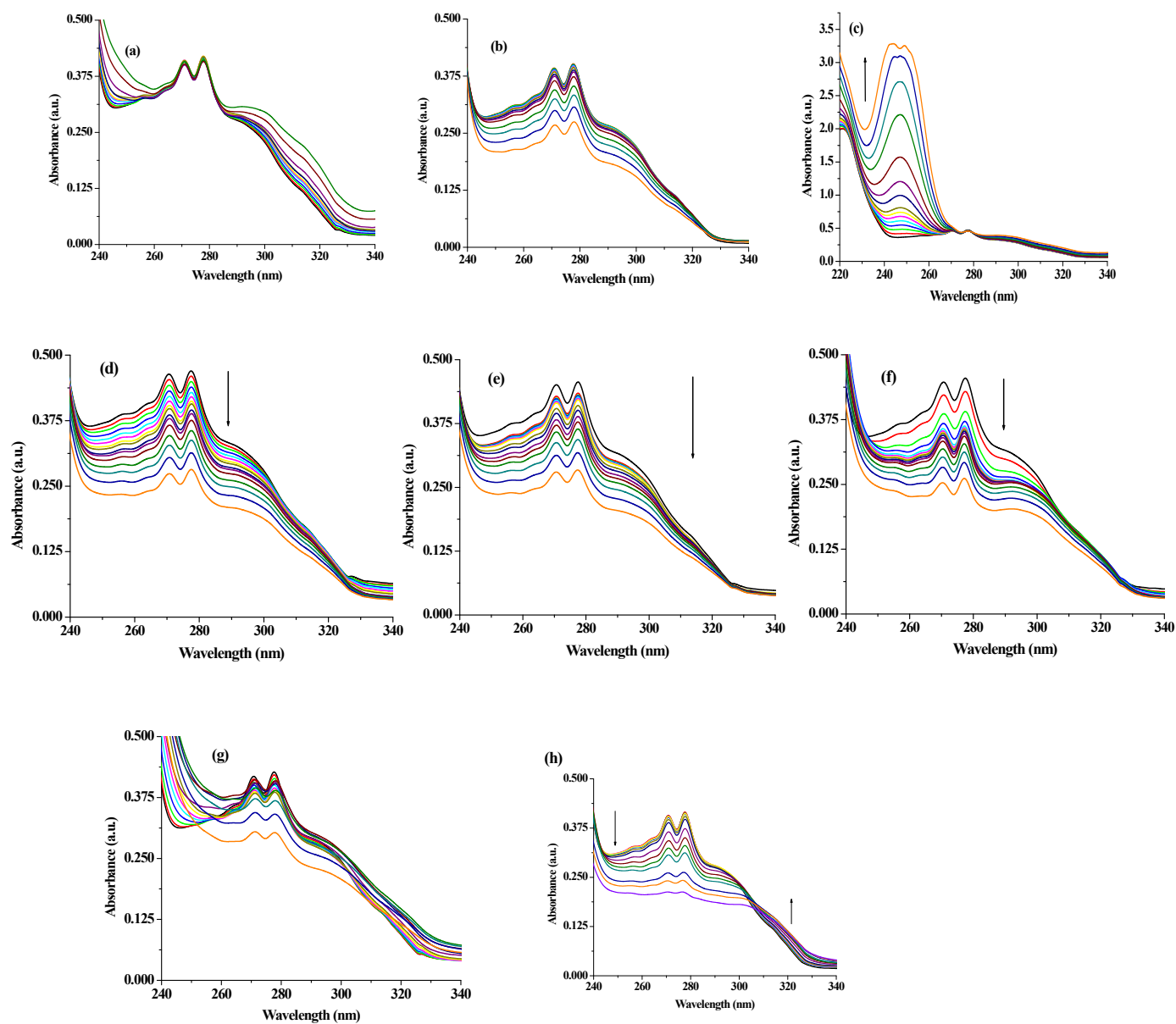


Figure 5S. Change in absorbance of **2** ($c = 3.27 \times 10^{-5}$ M) upon addition of (a) Cl^- , (b) Br^- , (c) I^- , (d) AcO^- , (e) HSO_4^- , (f) $\text{HP}_2\text{O}_7^{3-}$, (g) H_2PO_4^- and (h) F^- (counter cations: tetrabutylammonium ions) in CH_3CN .

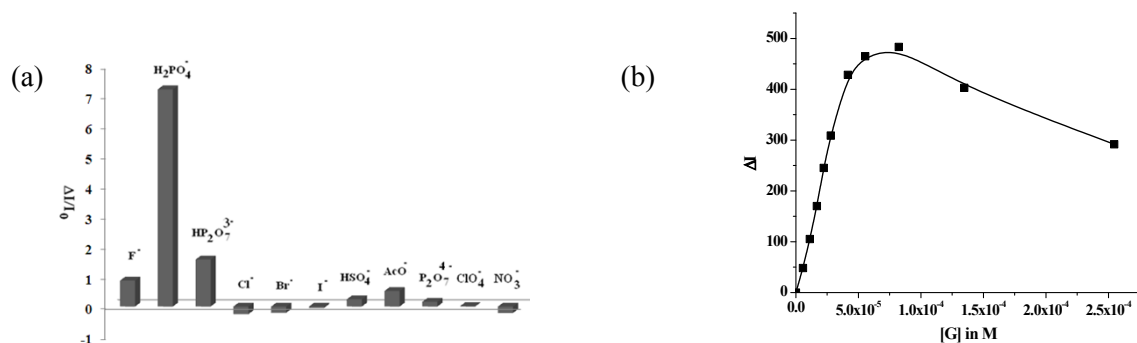


Figure 6S. (a) Change in fluorescence ratio of **2** ($c = 3.27 \times 10^{-5}$ M) at 370 nm upon addition of 2 equiv. amounts of different anionic guests (counter cations: tetrabutylammonium ions) in CH_3CN ; (b) Change in fluorescence of **2** ($c = 3.27 \times 10^{-5}$ M) at 510 nm upon addition of 15 equiv. amounts of tetrabutylammonium dihydrogenphosphate in CH_3CN .

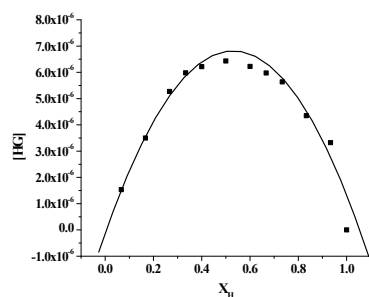


Figure 7S: Job plot of **1** ($c = 3.27 \times 10^{-5}$ M) with $\text{HP}_2\text{O}_7^{3-}$.

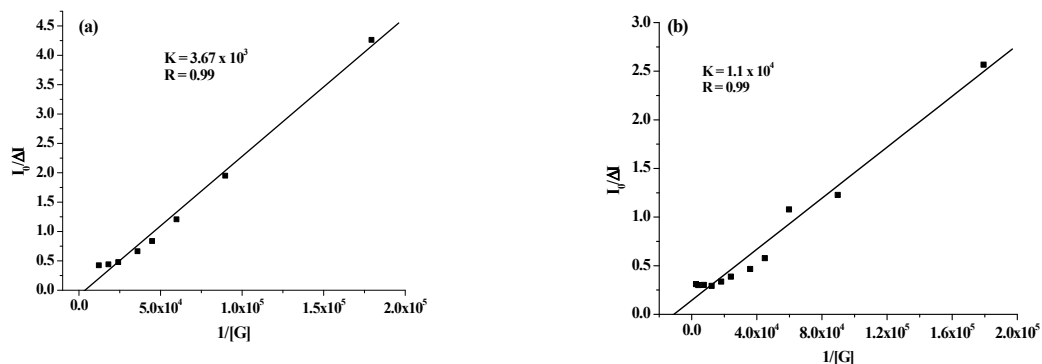


Figure 8S. Benesi-Hilderband plot for (a) H_2PO_4^- and (b) $\text{HP}_2\text{O}_7^{3-}$ with **1** ($c = 3.26 \times 10^{-5}$ M) measured at 430 nm.

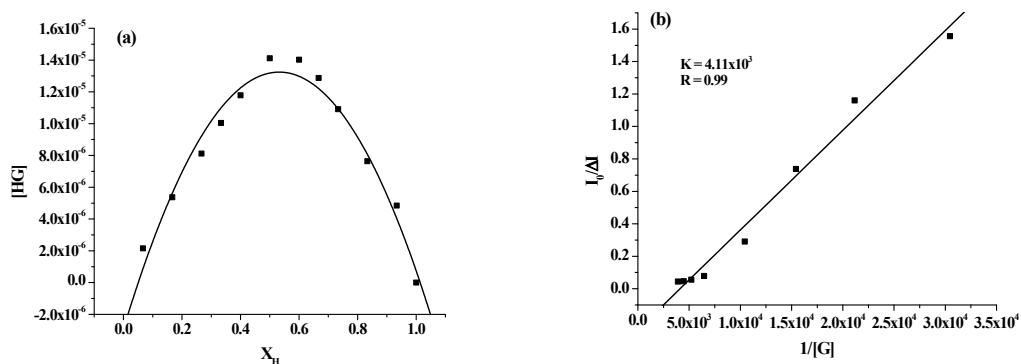


Figure 9S. (a) Job plot of **2** ($c = 3.24 \times 10^{-5}$ M) with and (b) Benesi-Hilderband plot for F^- with **2** ($c = 3.27 \times 10^{-5}$ M) measured at 510 nm.

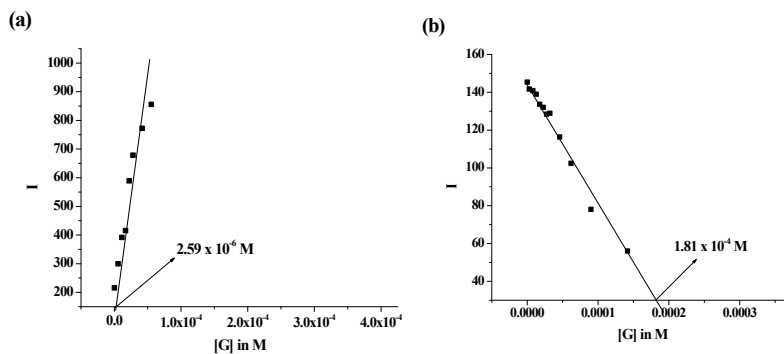


Figure 10S. Plot of detection limit of (a) **1** ($c = 3.16 \times 10^{-5}$ M) with hydrogen pyrophosphate and (b) **2** ($c = 3.27 \times 10^{-5}$ M) with Fluoride and in CH_3CN .

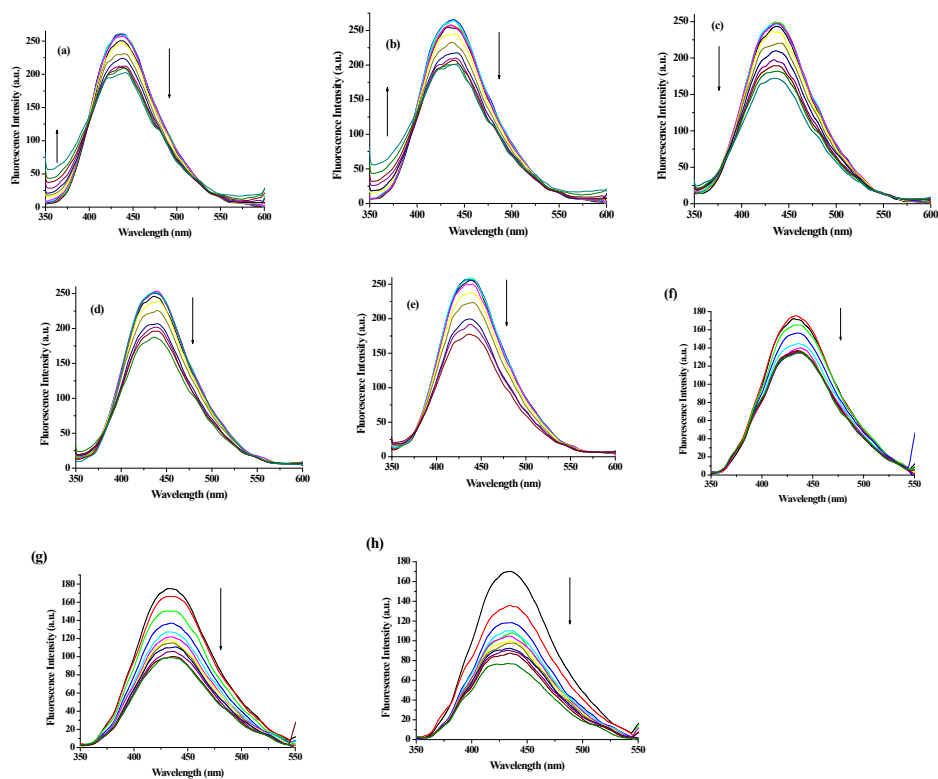


Figure 11S. Change in emission of **1** ($c = 3.26 \times 10^{-5}$ M) upon addition of a) ADP, b) AMP, c) NaH_2PO_4 , (d) Na_2HPO_4 , e) Na_3PO_4 (f) ATP (g) $\text{Na}_4\text{P}_2\text{O}_7$, (h) $(\text{TBA})_3\text{HP}_2\text{O}_7$ in CH_3CN - H_2O (1:1, v/v) at pH 7.3 (10 mM HEPES).

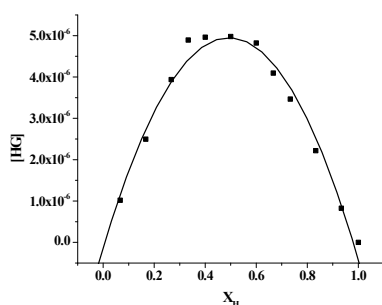


Figure 12S. Job plot of **1** ($c = 3.05 \times 10^{-5}$ M) with $\text{HP}_2\text{O}_7^{3-}$ in CH_3CN : H_2O (1:1 v/v, pH = 7.3 using 10 mM HEPES buffer).

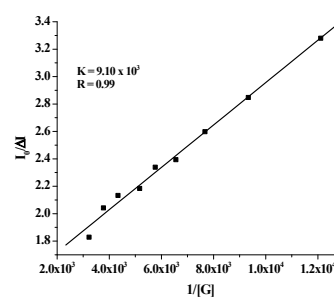


Figure 13S. Benesi-Hilderband plot for $\text{HP}_2\text{O}_7^{3-}$ with **1** ($c = 3.02 \times 10^{-5}$ M) measured at 430 nm.

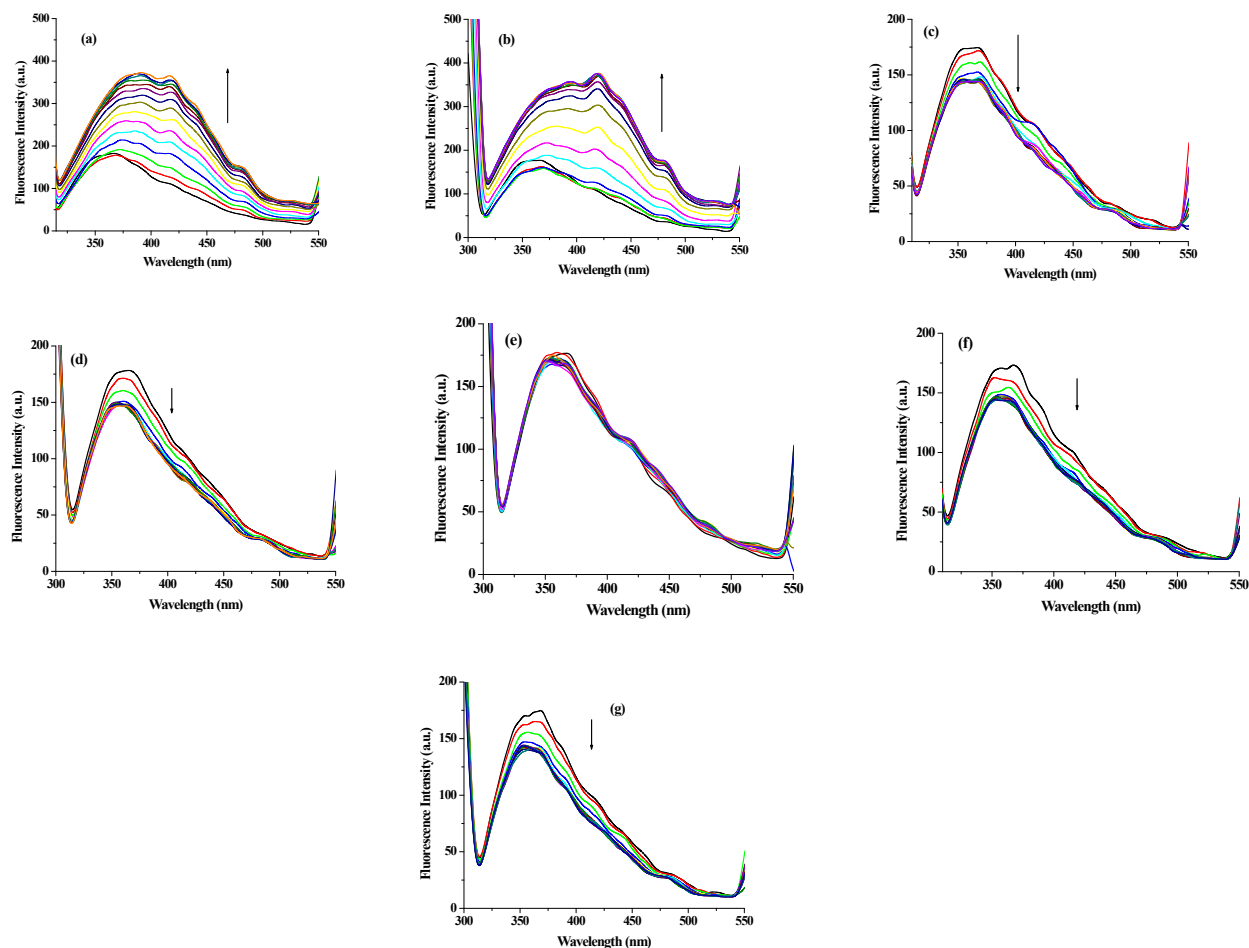


Figure 14S. Change in emission of **2** ($c = 3.26 \times 10^{-5}$ M) upon addition of a) ADP, b) AMP, c) NaH_2PO_4 , (d) Na_2HPO_4 , e) $\text{Na}_4\text{P}_2\text{O}_7$, (f) Na_3PO_4 (g) KF in $\text{CH}_3\text{CN}-\text{H}_2\text{O}$ (1:1, v/v) at pH 7.3 (10 mM HEPES).

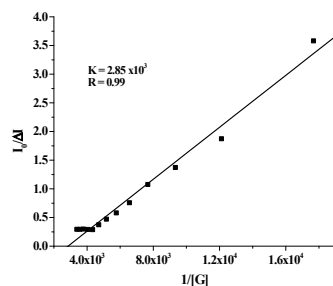


Figure 15S. Benesi-Hilderband plot for ATP with **2** ($c = 3.06 \times 10^{-5}$ M) in $\text{CH}_3\text{CN}-\text{H}_2\text{O}$ (1:1, v/v) at pH 7.3 (10 mM HEPES), measured at 380 nm.

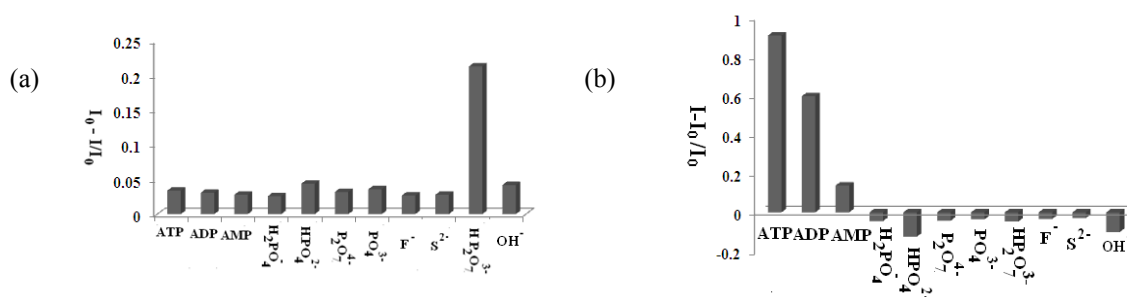


Figure 16S. Change in fluorescence ratio of (a) **1** ($c = 2.23 \times 10^{-5} \text{ M}$) and (b) **2** ($c = 2.25 \times 10^{-5} \text{ M}$) upon addition of 15equiv. amounts of different guests in $\text{CH}_3\text{CN}-\text{H}_2\text{O}$ (1:1, v/v, pH = 6.4).

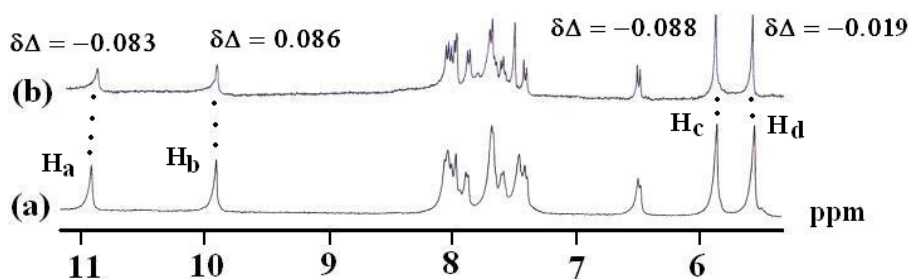


Figure 17S. Partial ^1H NMR (d_6 -DMSO, 400 MHz) of (a) **1** ($c = 3.37 \times 10^{-3} \text{ M}$) and (b) with equiv. amount of tetrabutylammonium pyrophosphate.

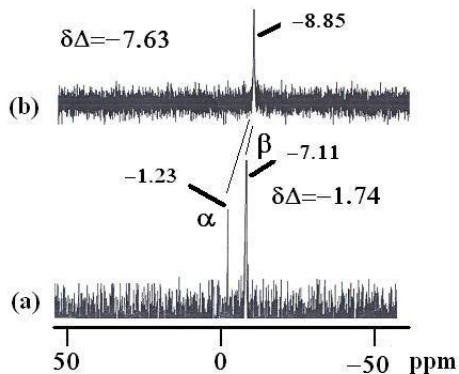


Figure 18S. ^{31}P NMR of (a) tetrabutylammonium hydrogenpyrophosphate ($c = 3.72 \times 10^{-3} \text{ M}$) and with (b) with equiv. amount of receptor **1** ($c = 3.72 \times 10^{-3} \text{ M}$) in d_6 DMSO: D_2O (1:1, v/v).

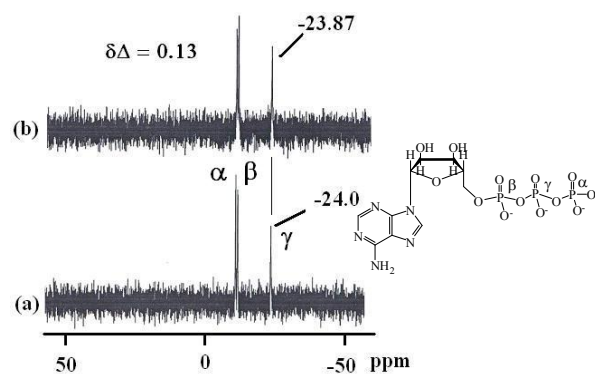


Figure 19S. ^{31}P NMR of (a) ATP ($c = 4.52 \times 10^{-3} \text{ M}$) and with (b) with equiv. amount of receptor **2** ($c = 4.52 \times 10^{-3} \text{ M}$) in d_6 DMSO: D_2O (1:1, v/v).

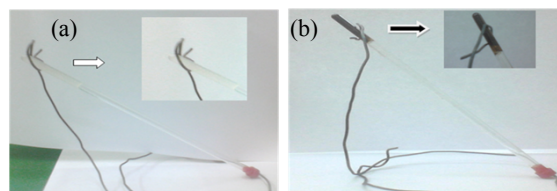


Figure 20S. Formation of gels of (a) **1** upon addition of 1equiv. amount of $(\text{Bu}_4\text{N})_3\text{HP}_2\text{O}_7$ in DMSO and (b) **2** upon addition of 1equiv. amount of $(\text{Bu}_4\text{N})\text{H}_2\text{PO}_4$ in DMSO.

Table 1S. Results of gelation tests for **1** and **2**

Solvent	a
DMSO	G*
DMF	S
Methanol	I
Chloroform	I
Ethanol	S
Acetonitrile	S
n-Hexane	I
Diethyl ether	I

a. S = solution; G = transparent gel; I = insoluble; *mgc = minimum gelatination concentration = 10 mg/mL.

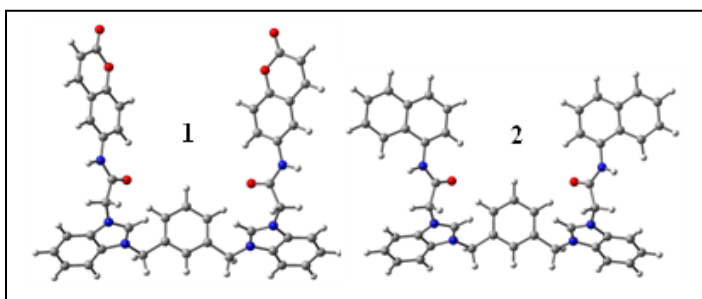


Figure 21S. B3LYP/6-31G(d) calculated optimized structures of the receptor **1** and **2**.

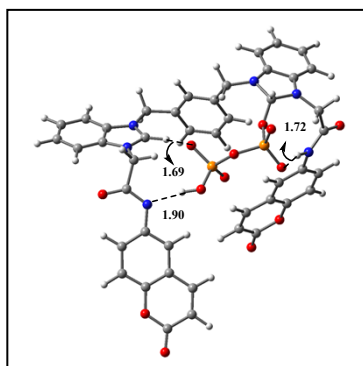


Figure 22S. B3LYP/6-31G(d) optimized structures of the receptor **1** with $\text{P}_2\text{O}_7^{4-}$. All the distances are given in Å.

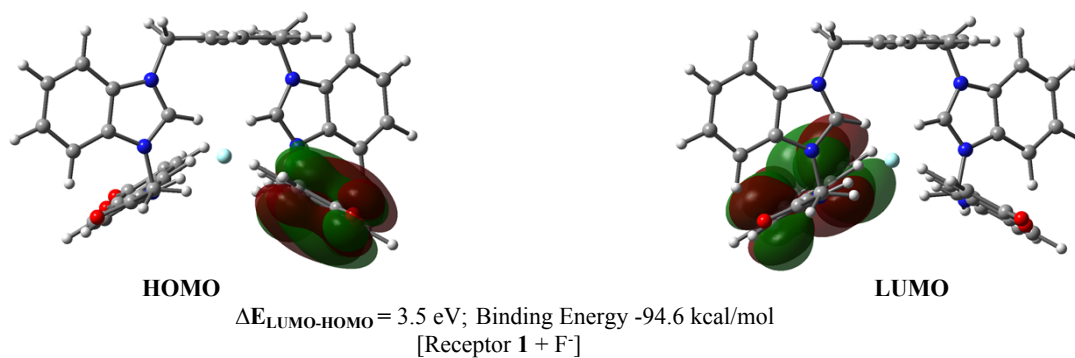


Figure 23S. Frontier molecular orbitals of the B3LYP/6-31G(d) optimized complex of receptor **1** with F^- .

Table 2S: B3LYP/6-31G(d) optimized Cartesian coordinates of the receptors (**1**, **2** and **3**) and their complexes with anions.

Receptor 1 E = -2476.59361554 a.u.				Receptor 1+HP ₂ O ₇ ³⁻ E = -3687.23877220a.u.			
C	1.219928000000	-3.623871000000	-0.919930000000	C	-1.303447000000	-3.898424000000	2.086224000000
C	1.211986000000	-2.368623000000	-1.543484000000	C	-0.758181000000	-2.957630000000	2.965703000000
C	-0.000038000000	-1.740031000000	-1.831642000000	C	0.509751000000	-2.435918000000	2.720975000000
C	-1.212061000000	-2.368472000000	-1.543156000000	C	1.225215000000	-2.818111000000	1.586457000000
C	-1.219990000000	-3.623719000000	-0.919600000000	C	0.697521000000	-3.771871000000	0.712507000000
C	-0.000024000000	-4.229248000000	-0.593318000000	C	-0.551231000000	-4.329915000000	0.990524000000
H	2.143026000000	-1.876409000000	-1.811767000000	H	-1.336824000000	-2.611211000000	3.818907000000
H	-0.000042000000	-0.767934000000	-2.314356000000	H	0.921498000000	-1.681508000000	3.383896000000
H	-2.143113000000	-1.876141000000	-1.811185000000	H	2.160052000000	-2.326653000000	1.345921000000
H	-0.000020000000	-5.206472000000	-0.115251000000	H	-0.978209000000	-5.056544000000	0.299844000000
C	2.498252000000	-4.410937000000	-0.710280000000	C	-2.726448000000	-4.362145000000	2.241909000000
H	2.894078000000	-4.737354000000	-1.678218000000	H	-3.104107000000	-4.146882000000	3.247008000000
H	2.302896000000	-5.310211000000	-0.117433000000	H	-2.822759000000	-5.440776000000	2.069229000000
C	-2.498354000000	-4.510625000000	-0.709605000000	C	1.337631000000	-4.126032000000	-0.617271000000
H	-2.302943000000	-5.309941000000	-0.116839000000	H	0.803282000000	-3.565785000000	-1.392001000000
H	-2.894502000000	-4.736966000000	-1.677438000000	H	1.222836000000	-5.198003000000	-0.823289000000
N	3.603779000000	-3.675081000000	-0.060061000000	N	-3.644987000000	-3.703866000000	1.279416000000
C	3.524278000000	-2.564250000000	0.676564000000	C	-3.328084000000	-2.780285000000	0.353370000000
C	4.945520000000	-4.082648000000	-0.096023000000	C	-5.006067000000	-3.995806000000	1.172529000000
N	4.734649000000	-2.215129000000	1.133852000000	N	-4.423694000000	-2.457123000000	-0.348397000000
H	2.620309000000	-2.008585000000	0.858072000000	H	-2.336925000000	-2.327727000000	0.093647000000
C	5.670792000000	-3.144788000000	0.656960000000	C	-5.509247000000	-3.193725000000	0.133392000000
C	5.566637000000	-5.172766000000	-0.709217000000	C	-5.823947000000	-4.881151000000	1.877381000000
C	7.052451000000	-3.252762000000	0.823140000000	C	-6.853602000000	-3.241192000000	-0.241687000000
C	7.672730000000	-4.333895000000	0.205884000000	C	-7.665107000000	-4.130022000000	0.457639000000
C	6.943727000000	-5.277165000000	-0.545708000000	C	-7.162069000000	-4.935976000000	1.497132000000
H	7.625261000000	-2.539246000000	1.405543000000	H	-7.231226000000	-2.574030000000	-1.007244000000
H	8.745876000000	-4.456222000000	0.308946000000	H	-8.718473000000	-4.194457000000	0.201513000000
H	7.469918000000	-6.107333000000	-1.005128000000	H	-7.833994000000	-5.610511000000	2.019838000000
H	5.012073000000	-5.907935000000	-1.282016000000	H	-5.438448000000	-5.497296000000	2.683049000000
N	-3.603600000000	-2.674651000000	-0.059041000000	N	2.742280000000	-0.376317900000	-0.732597000000
C	-3.523774000000	-2.563780000000	0.677489000000	C	3.142251000000	-2.783438000000	-1.587905000000
C	-4.945380000000	-4.082132000000	-0.094521000000	C	3.831044000000	-4.165656000000	0.026326000000
N	-4.733969000000	-2.214550000000	1.135167000000	N	4.461407000000	-2.572388000000	-1.430622000000
H	-2.619704000000	-2.008171000000	0.858659000000	H	2.559988000000	-2.427952000000	-0.247952000000
C	-5.670332000000	-3.144187000000	0.658662000000	C	4.934471000000	-3.400499000000	-0.404326000000
C	-5.566776000000	-5.172246000000	-0.707440000000	C	3.955031000000	-5.119596000000	1.033077000000
C	-7.051938000000	-3.252068000000	0.825331000000	C	6.196899000000	-3.566021000000	0.161420000000
C	-7.672499000000	-4.333197000000	0.208350000000	C	6.319994000000	-4.530411000000	1.164067000000
C	-6.943816000000	-5.276551000000	-0.543446000000	C	5.222534000000	-5.293105000000	1.592838000000
H	-7.624501000000	-2.538483000000	1.407893000000	H	7.023607000000	-2.938683000000	-0.150430000000
H	-8.745617000000	-4.455453000000	0.311792000000	H	7.289125000000	-4.683583000000	1.630474000000
H	-7.470218000000	-6.106712000000	-1.002637000000	H	5.356834000000	-6.027364000000	2.382367000000
H	-5.012454000000	-5.907477000000	-1.280391000000	H	3.100241000000	-5.694417000000	1.373916000000
C	-5.018277000000	-0.937556000000	1.781411000000	C	5.173161000000	-1.538324000000	-2.197232000000
C	5.019244000000	-0.938225000000	1.780144000000	C	-4.392748000000	-1.525730000000	-1.496108000000
C	-4.699217000000	0.223288000000	0.799699000000	C	5.828974000000	-0.463907000000	-1.301962000000
C	4.699752000000	0.222733000000	0.798715000000	C	-5.277154000000	-0.289500000000	-1.244918000000
N	-5.479855000000	1.317349000000	0.963477000000	N	5.116641000000	0.674015000000	-1.161021000000
N	5.480346000000	1.316834000000	0.962422000000	N	-4.576330000000	0.824171000000	-0.960224000000
H	4.385437000000	-0.835299000000	2.667273000000	H	-3.333839000000	-1.295366000000	-1.662106000000
H	6.057282000000	-0.953684000000	2.116069000000	H	-4.801634000000	-2.056288000000	-2.360709000000
H	-6.056165000000	-0.952972000000	2.117798000000	H	5.983219000000	-2.014170000000	-2.758202000000
H	-4.384083000000	-0.834506000000	2.668248000000	H	4.437631000000	-1.119219000000	-2.889548000000
O	3.773095000000	0.094900000000	0.007099000000	O	-6.508419000000	-0.399834000000	-1.319060000000
O	-3.772891000000	0.095400000000	0.007713000000	O	6.939852000000	-0.701186000000	-0.809237000000
C	-5.381259000000	2.571493000000	0.286264000000	C	4.509998000000	2.820751000000	-0.315713000000
C	-6.555344000000	3.361745000000	0.192525000000	C	4.773359000000	3.988250000000	0.414434000000
C	-4.171943000000	3.020575000000	-0.234635000000	C	5.467459000000	1.802846000000	-0.394994000000
C	-7.870246000000	2.975803000000	0.652438000000	C	3.833959000000	5.072255000000	0.543768000000
C	-6.442072000000	4.630124000000	-0.415143000000	C	6.012711000000	4.129532000000	1.067447000000
C	-4.111631000000	4.276526000000	-0.851411000000	C	6.702788000000	1.961414000000	0.270191000000
H	-3.288843000000	2.401225000000	-0.164854000000	C	4.146908000000	6.176735000000	1.262018000000
C	-8.923793000000	3.812662000000	0.537117000000	H	2.868178000000	4.979889000000	0.052442000000
H	-8.036519000000	1.987412000000	1.074566000000	C	6.968625000000	3.120028000000	0.994898000000
C	-5.232155000000	5.089549000000	-0.940722000000	H	7.435452000000	1.168911000000	0.211417000000

H	-3.165766000000	4.622613000000	-1.256188000000	C	5.434552000000	6.319117000000	1.930439000000
C	-8.790728000000	5.141876000000	-0.057328000000	H	3.463554000000	7.009850000000	1.380683000000
H	-9.920616000000	3.544460000000	0.866975000000	H	7.915610000000	3.251305000000	1.509123000000
H	-5.200314000000	6.068637000000	-1.405476000000	C	-4.142549000000	3.107216000000	-0.415446000000
C	5.381480000000	2.571162000000	0.285617000000	C	-4.557067000000	4.416058000000	-0.130223000000
C	6.555186000000	3.362130000000	0.193019000000	C	-5.085106000000	2.109012000000	-0.685004000000
C	4.172292000000	3.019742000000	-0.236034000000	C	-3.644858000000	5.494447000000	1.551560000000
C	7.869987000000	2.976830000000	0.653774000000	C	-5.932579000000	4.715420000000	-0.117267000000
C	6.441630000000	4.630648000000	-0.414307000000	C	-6.459722000000	2.428623000000	-0.668634000000
C	4.111723000000	4.275876000000	-0.852407000000	C	-4.107780000000	6.737674000000	0.424189000000
H	3.289509000000	2.399851000000	-0.167151000000	H	-2.577740000000	5.285191000000	0.148227000000
C	8.923132000000	3.814339000000	0.539536000000	C	-6.875547000000	3.726096000000	-0.385738000000
H	8.036585000000	1.988401000000	1.075699000000	H	-7.181808000000	1.652045000000	-0.879118000000
C	5.231842000000	5.089575000000	-0.940619000000	C	-5.534211000000	7.040555000000	0.438334000000
H	3.165959000000	4.621549000000	-1.257772000000	H	-3.450261000000	7.571381000000	0.642312000000
C	8.789728000000	5.143689000000	-0.054573000000	H	-7.929800000000	3.983933000000	-0.370656000000
H	9.919860000000	3.546612000000	0.870064000000	H	-3.513846000000	0.760561000000	-0.917176000000
H	5.199793000000	6.068801000000	-1.405065000000	H	4.153968000000	0.757307000000	-1.602536000000
H	6.210792000000	1.256141000000	1.659474000000	O	6.318328000000	5.255440000000	1.791977000000
H	-6.210101000000	1.256735000000	1.660754000000	O	5.795015000000	7.273300000000	2.587951000000
O	-7.509229000000	5.461747000000	-0.526063000000	O	-6.389135000000	5.979191000000	0.157754000000
O	-9.664362000000	5.956813000000	-0.184022000000	O	-6.031787000000	8.121446000000	0.670586000000
O	7.508383000000	5.462927000000	-0.524166000000	H	3.558629000000	2.681751000000	-0.827118000000
O	9.662944000000	5.959201000000	-0.180300000000	H	-3.085316000000	2.850270000000	-0.429332000000
				P	-0.828787000000	-0.081927000000	-0.783287000000
				O	0.047075000000	0.035138000000	0.572413000000
				H	0.953900000000	-0.318809000000	0.322749000000
				O	-1.954019000000	0.941393000000	-0.723850000000
				O	-1.287322000000	-1.531921000000	-1.005696000000
				P	1.822808000000	-0.104406000000	-2.089829000000
				O	1.939825000000	-1.021996000000	-3.308794000000
				O	2.647377000000	1.185273000000	-2.154087000000
				O	2.108044000000	-0.905738000000	-0.762864000000
				O	0.207862000000	0.366351000000	-1.950563000000
Receptor 1+H₂PO₄⁻				Receptor 1+F⁻			
E = -3120.45204546 a.u.				E = -2576.74991039 a.u.			
C	0.785067000000	-4.474194000000	0.746263000000	C	-0.469475000000	-1.106002000000	3.628758000000
C	-0.051720000000	-3.874823000000	1.693591000000	C	-1.812640000000	-1.505861000000	3.635019000000
C	0.497059000000	-3.180624000000	2.772579000000	C	-2.831012000000	-0.555219000000	3.617982000000
C	1.879468000000	-3.083255000000	2.916850000000	C	-2.516433000000	0.804084000000	3.590388000000
C	2.727001000000	-3.680978000000	1.976343000000	C	-1.180729000000	1.221123000000	3.585790000000
C	2.170888000000	-4.373081000000	0.896358000000	C	-0.163213000000	0.258141000000	3.612002000000
H	-1.131648000000	-3.925578000000	1.589217000000	H	-2.063851000000	-2.563274000000	3.659924000000
H	-0.158773000000	-2.715995000000	3.502217000000	H	-3.869125000000	-0.871922000000	3.634506000000
H	2.300064000000	-2.542390000000	3.760790000000	H	-3.314238000000	1.542486000000	3.584658000000
H	2.826241000000	-4.831270000000	0.158220000000	H	0.877431000000	0.576726000000	3.625035000000
C	0.242936000000	-5.273656000000	-0.426285000000	C	0.633659000000	-2.142869000000	3.627821000000
H	0.109401000000	-6.324137000000	-0.152399000000	H	0.413118000000	-2.941393000000	4.339910000000
H	0.945566000000	-5.245960000000	-1.264439000000	H	1.594456000000	-1.701380000000	3.910375000000
C	4.225948000000	-3.569349000000	2.117299000000	C	-0.842295000000	2.693023000000	3.549977000000
H	4.727283000000	-4.453038000000	1.708151000000	H	0.114578000000	2.890036000000	4.044807000000
H	4.506662000000	-3.484810000000	3.171145000000	H	-1.610696000000	3.276493000000	4.065491000000
N	-1.066121000000	-4.803754000000	-0.903067000000	N	0.784470000000	-2.797682000000	2.309105000000
C	-1.317315000000	-3.559063000000	-1.325678000000	C	0.710224000000	-2.171962000000	1.125160000000
C	-2.253714000000	-5.545424000000	-0.971512000000	C	1.033080000000	-4.157687000000	2.077573000000
N	-2.599049000000	-3.446807000000	-1.685352000000	N	0.899150000000	-3.047487000000	0.133149000000
H	-0.615043000000	-2.729194000000	-1.415020000000	H	0.476173000000	-1.121054000000	0.918092000000
C	-3.238064000000	-4.667948000000	-1.456985000000	C	1.078427000000	-4.320044000000	0.681006000000
C	-2.552000000000	-6.873152000000	-0.659302000000	C	1.206100000000	-5.242002000000	2.941419000000
C	-4.559712000000	-5.075595000000	-1.638968000000	C	1.258105000000	-5.570198000000	0.086253000000
C	-4.856862000000	-6.397048000000	-1.323135000000	C	1.423731000000	-6.647530000000	0.948890000000
C	-3.869621000000	-7.279854000000	-0.843577000000	C	1.405017000000	-6.484907000000	2.349498000000
H	-5.323734000000	-4.397938000000	-2.004367000000	H	1.231012000000	-5.694862000000	-0.990411000000
H	-5.872960000000	-6.756683000000	-1.448428000000	H	1.562797000000	-7.640605000000	0.534359000000
H	-4.143316000000	-8.303909000000	-0.611158000000	H	1.542177000000	-7.354657000000	2.983856000000
H	-1.800852000000	-7.563126000000	-0.290181000000	H	1.190220000000	-5.131520000000	0.204210000000
N	4.793855000000	-2.384001000000	1.436740000000	N	-0.750683000000	3.236714000000	2.175544000000
C	4.194034000000	-1.615930000000	0.517252000000	C	-0.673328000000	2.535661000000	1.035015000000
C	6.103725000000	-1.924236000000	1.611690000000	C	-0.655549000000	4.599405000000	1.864155000000
N	5.037228000000	-0.666936000000	0.093012000000	N	-0.552320000000	3.367038000000	-0.005107000000
H	3.188798000000	-1.729507000000	0.110637000000	H	-0.644300000000	1.453259000000	0.902498000000
C	6.258177000000	-0.816538000000	0.760865000000	C	-0.513502000000	4.681129000000	0.468325000000

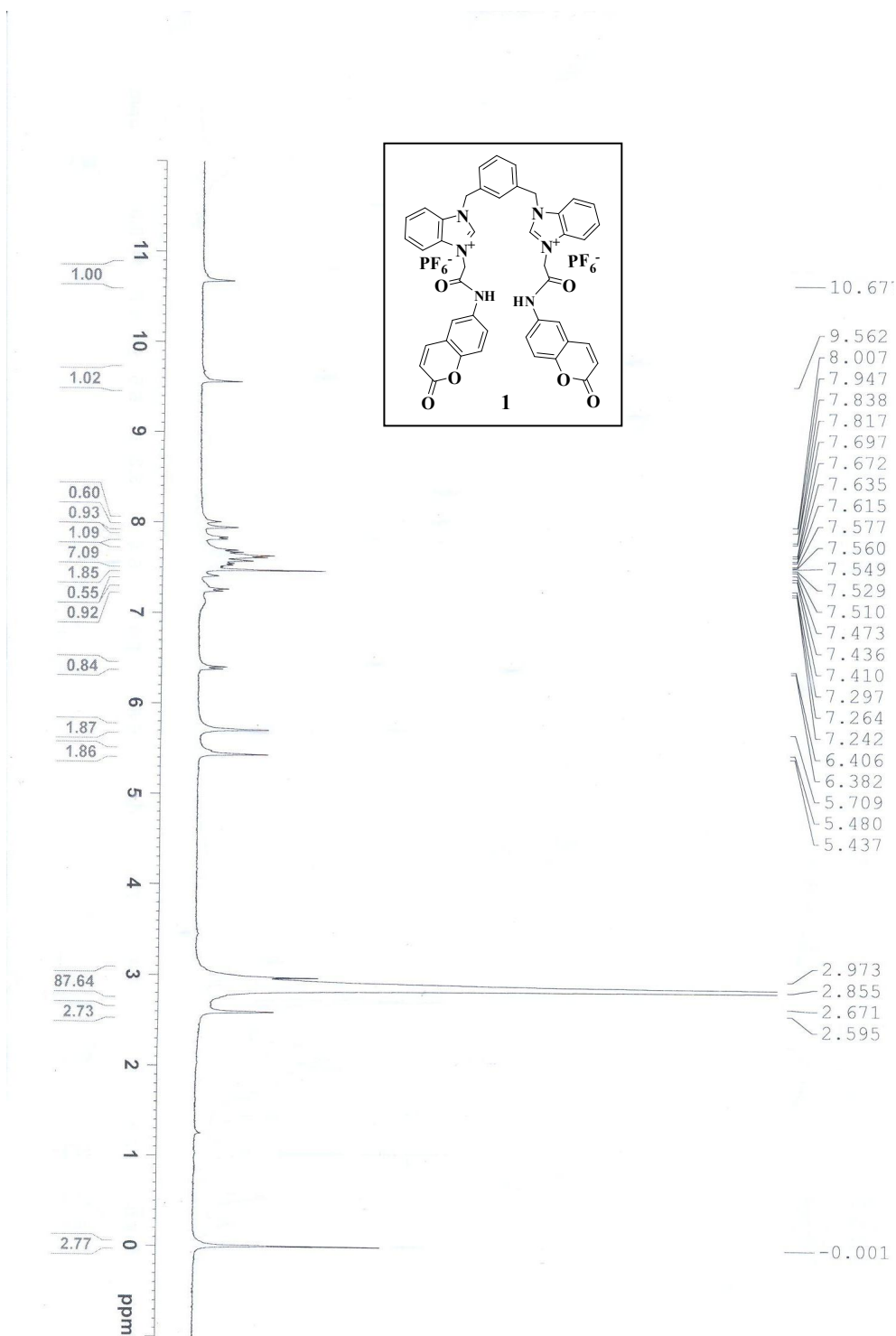
C	7.144710000000	-2.382505000000	2.422613000000	C	-0.671927000000	5.743457000000	2.665200000000
C	7.462649000000	-0.112691000000	0.691359000000	C	-0.358351000000	5.902473000000	-0.189859000000
C	8.500233000000	-0.573496000000	1.493292000000	C	-0.376779000000	7.039995000000	0.609712000000
C	8.346330000000	-1.687536000000	2.343250000000	C	-0.535922000000	6.962617000000	2.008775000000
H	7.560167000000	0.772675000000	0.076818000000	H	-0.189237000000	5.950754000000	-1.259602000000
H	9.452414000000	-0.053210000000	1.472968000000	H	-0.254063000000	8.013345000000	0.145997000000
H	9.184110000000	-2.007304000000	2.954660000000	H	-0.541010000000	7.878511000000	2.590880000000
H	7.029842000000	-3.238783000000	3.078555000000	H	-0.777738000000	5.693008000000	3.743614000000
C	4.685893000000	0.299705000000	-0.956209000000	C	-0.390174000000	2.925686000000	-1.399079000000
C	-3.231979000000	-2.168389000000	-1.972657000000	C	0.792674000000	-2.700847000000	-1.293176000000
C	4.575068000000	1.729314000000	-0.395258000000	C	1.097834000000	2.992237000000	-1.798642000000
C	-3.769788000000	-1.567937000000	-0.651935000000	C	-0.653118000000	-2.931668000000	-1.781014000000
N	3.468862000000	2.395094000000	-0.815308000000	N	1.772003000000	1.859997000000	-1.460450000000
N	-4.677254000000	-0.570436000000	-0.843920000000	N	-1.448334000000	-1.849484000000	-1.566297000000
H	-2.456213000000	-1.509728000000	-2.380901000000	H	1.096297000000	-1.659617000000	-1.396324000000
H	-4.017009000000	-2.320880000000	-2.719014000000	H	1.463862000000	-3.349201000000	-1.855877000000
H	5.486463000000	0.289673000000	-1.703308000000	H	-0.775927000000	1.908691000000	-1.458259000000
H	3.768537000000	-0.070059000000	-1.417517000000	H	-0.959925000000	3.596107000000	-2.043075000000
O	-3.359705000000	-1.972583000000	0.426754000000	O	-0.972262000000	-4.016242000000	-2.251774000000
O	5.465339000000	2.174310000000	0.322250000000	O	1.550264000000	4.006652000000	-2.315398000000
C	2.064951000000	4.275159000000	-1.319995000000	C	3.667898000000	0.467182000000	-0.983434000000
C	1.670123000000	5.611983000000	-1.161858000000	C	5.030416000000	0.143500000000	-1.075653000000
C	3.143231000000	3.758190000000	-0.600838000000	C	3.157348000000	1.613736000000	-1.592919000000
C	0.572419000000	6.216833000000	-1.877474000000	C	5.627109000000	-1.027936000000	-0.470953000000
C	2.383084000000	6.427115000000	-0.263001000000	C	5.881462000000	1.003439000000	-1.794474000000
C	3.847253000000	4.590565000000	0.292733000000	C	4.027738000000	2.461265000000	-2.310079000000
C	0.250644000000	7.513016000000	-1.674785000000	C	6.949694000000	-1.265392000000	-0.598261000000
H	0.011791000000	5.610925000000	-2.585896000000	H	4.992535000000	-1.705710000000	0.090704000000
C	3.465305000000	5.916504000000	0.454571000000	C	5.378541000000	2.153194000000	-2.405397000000
H	4.686230000000	4.190942000000	0.844320000000	H	3.635690000000	3.353176000000	-2.778430000000
C	0.987681000000	8.352623000000	-0.730876000000	C	7.829938000000	-0.366276000000	-1.345367000000
H	-0.564192000000	8.002763000000	-2.195205000000	H	7.433029000000	-2.130280000000	-0.158933000000
H	3.997415000000	6.569681000000	1.137952000000	H	6.058407000000	-2.796364000000	-2.953925000000
C	-6.151187000000	1.264198000000	-0.348828000000	C	-3.471421000000	-0.581403000000	-1.358061000000
C	-6.819901000000	2.118245000000	0.540780000000	C	-4.845538000000	-0.385334000000	-1.562774000000
C	-5.311895000000	0.255940000000	0.122239000000	C	-2.837009000000	-1.740656000000	-1.805433000000
C	-7.703878000000	3.182334000000	0.126197000000	C	-5.566737000000	0.788504000000	-1.133675000000
C	-6.626579000000	1.937866000000	1.923011000000	C	-5.579869000000	-1.386901000000	-2.225107000000
C	-5.131108000000	0.087678000000	1.508721000000	C	-3.589891000000	-2.731204000000	-2.469802000000
C	-8.312288000000	3.964157000000	1.044006000000	C	-6.893109000000	0.904523000000	-1.361304000000
H	-7.871349000000	3.342614000000	-0.936348000000	H	-5.021965000000	1.581650000000	-0.625441000000
C	-5.787662000000	0.928643000000	2.398146000000	C	-4.951880000000	-2.549723000000	-2.673662000000
H	-4.481490000000	-0.695486000000	1.872385000000	H	-3.099197000000	-3.630599000000	-2.814672000000
C	-8.108130000000	3.773542000000	2.480064000000	C	-7.652805000000	-0.144037000000	-2.042959000000
H	-8.982170000000	4.771650000000	0.772433000000	H	-7.467577000000	1.771579000000	-1.056479000000
H	-5.660976000000	0.813452000000	3.469292000000	H	-5.543398000000	-3.302737000000	-3.183441000000
H	-4.905737000000	-0.345702000000	-1.804412000000	F	-0.020311000000	0.128376000000	-0.270919000000
H	2.762904000000	1.862545000000	-1.327313000000	H	-0.995529000000	-1.028755000000	-1.129007000000
O	2.048133000000	7.732914000000	-0.062396000000	H	1.206309000000	1.116291000000	-1.017115000000
O	0.761883000000	9.511069000000	-0.485102000000	O	-6.918503000000	-1.261274000000	-1.133675000000
O	-7.243822000000	2.731012000000	2.840367000000	O	-8.834977000000	-0.123883000000	-2.276322000000
O	-8.608677000000	4.422305000000	3.362595000000	O	7.214762000000	0.750764000000	-1.918130000000
H	1.528934000000	3.643605000000	-2.024333000000	O	9.016244000000	-0.506546000000	-1.503014000000
H	-6.299844000000	1.403126000000	-1.418225000000	H	-2.895529000000	0.179090000000	-0.835685000000
P	1.027743000000	-0.683775000000	-2.245983000000	H	3.006077000000	-0.183519000000	-0.415884000000
O	1.147637000000	0.960664000000	-1.946715000000				
H	0.335034000000	1.236375000000	-1.491917000000				
O	1.746387000000	-0.754935000000	-3.706695000000				
H	1.170410000000	-0.379108000000	-4.392340000000				
O	-0.449055000000	-0.994849000000	-2.320860000000				
O	1.917556000000	-1.431141000000	-1.291135000000				
Receptor 2				Receptor 2+F-			
E = -2254.35461132 a.u.				E = -2354.49160137			
C	1.219866000000	-3.409259000000	-0.938395000000	C	0.607645000000	-1.017395000000	3.352917000000
C	1.212213000000	-2.153506000000	-1.561025000000	C	0.931815000000	-2.382672000000	3.346764000000
C	0.000375000000	-1.525109000000	-1.849797000000	C	-0.059680000000	-3.338454000000	3.153472000000
C	-1.211562000000	-2.153408000000	-1.561172000000	C	-1.385309000000	-2.940853000000	2.961531000000
C	-1.219407000000	-3.409141000000	-0.938525000000	C	-1.727539000000	-1.587088000000	2.987559000000
C	0.000191000000	-4.015785000000	-0.613590000000	C	-0.722623000000	-0.629159000000	3.192089000000
H	2.143425000000	-1.658496000000	-1.823211000000	H	1.964384000000	-2.695761000000	3.479626000000
H	0.000432000000	-0.551416000000	-2.329194000000	H	0.195730000000	-4.393315000000	3.142624000000
H	-2.142697000000	-1.658329000000	-1.823513000000	H	-2.154372000000	-3.690990000000	2.798519000000

H	0.000113000000	-4.992713000000	-0.134837000000	H	-0.979417000000	0.428133000000	3.215902000000
C	2.500994000000	-4.188906000000	-0.718960000000	C	1.705826000000	0.022343000000	3.461420000000
H	2.910092000000	-4.509260000000	-1.683422000000	H	2.353120000000	-0.163998000000	4.321087000000
H	2.306212000000	-5.091444000000	-0.130800000000	H	1.294353000000	1.029892000000	3.568360000000
C	-2.500628000000	-4.188637000000	-0.719184000000	C	-3.175086000000	-1.177490000000	2.851518000000
H	-2.305925000000	-5.091386000000	-0.131325000000	H	-3.503080000000	-0.628978000000	3.741513000000
H	-2.909911000000	-4.508621000000	-1.683698000000	H	-3.813315000000	-2.061640000000	2.756849000000
N	3.590919000000	-3.442774000000	-0.055373000000	N	2.573452000000	-0.013300000000	2.265597000000
C	3.486852000000	-2.335775000000	0.684792000000	C	2.111713000000	0.056021000000	1.007593000000
C	4.940052000000	-3.824898000000	-0.085095000000	C	3.942718000000	-0.307760000000	2.219622000000
N	4.687204000000	-1.966198000000	1.150708000000	N	3.103620000000	-0.168624000000	0.144309000000
H	2.572258000000	-1.796825000000	0.862209000000	H	1.080471000000	0.202186000000	0.658063000000
C	5.642988000000	-2.875803000000	0.675139000000	C	4.275798000000	-0.427274000000	0.857820000000
C	5.585576000000	-4.900277000000	-0.698755000000	C	4.900974000000	-0.488196000000	3.220086000000
C	7.025627000000	-2.956842000000	0.847273000000	C	5.563775000000	-0.763385000000	0.438133000000
C	7.670294000000	-4.023234000000	0.229235000000	C	6.513312000000	-0.946695000000	1.346508000000
C	6.963777000000	-4.978134000000	-0.528820000000	C	6.189031000000	-0.805237000000	2.801273000000
H	7.580727000000	-2.233017000000	1.434051000000	H	5.795764000000	-0.910513000000	-0.610351000000
H	8.745230000000	-4.124253000000	0.336704000000	H	7.528077000000	-1.213147000000	1.159490000000
H	7.508340000000	-5.796260000000	-0.988480000000	H	6.963710000000	-0.954255000000	3.546060000000
H	5.048063000000	-5.644019000000	-1.276752000000	H	4.664236000000	-0.385084000000	4.273813000000
N	-3.590352000000	-3.442570000000	-0.055181000000	N	-3.460660000000	-0.290677000000	1.704730000000
C	-3.486217000000	-2.335348000000	0.684642000000	C	-2.697100000000	-0.051684000000	0.625841000000
C	-4.939370000000	-3.825158000000	-0.084008000000	C	-4.653109000000	0.431760000000	0.599690000000
N	-4.686441000000	-1.966008000000	1.151097000000	N	-3.328438000000	0.791023000000	-0.197996000000
H	-2.571698000000	-1.796606000000	0.861410000000	H	-1.690117000000	-0.407073000000	0.411766000000
C	-5.642192000000	-2.876083000000	0.676342000000	C	-4.557577000000	1.142244000000	0.363028000000
C	-5.584873000000	-4.900908000000	-0.697039000000	C	-5.780965000000	0.528530000000	2.388879000000
C	-7.024704000000	-2.957547000000	0.849285000000	C	-5.565223000000	2.007719000000	-0.067556000000
C	-7.669359000000	-4.024327000000	0.231901000000	C	-6.685675000000	2.104519000000	0.749604000000
C	-6.962954000000	-4.979186000000	-0.526314000000	C	-6.794583000000	1.374746000000	1.951349000000
H	-7.579719000000	-2.233789000000	1.436226000000	H	-5.449809000000	2.603485000000	-0.965051000000
H	-8.744195000000	-4.125692000000	0.340028000000	H	-7.494503000000	2.767521000000	0.460060000000
H	-7.507511000000	-5.797586000000	-0.985485000000	H	-7.689745000000	1.482212000000	2.555505000000
H	-5.047421000000	-5.644605000000	-1.275151000000	H	-5.871386000000	-0.025349000000	3.317043000000
C	-4.940783000000	-0.677538000000	1.788028000000	C	-2.750817000000	1.304090000000	-1.447534000000
C	4.941483000000	-0.677806000000	1.787815000000	C	2.887725000000	-0.293683000000	-1.305135000000
C	-4.593856000000	0.465208000000	0.793390000000	C	-2.212287000000	2.730752000000	-1.222520000000
C	4.594000000000	0.465044000000	0.793518000000	C	2.626243000000	-1.774986000000	-1.644861000000
N	-5.354373000000	1.570842000000	0.936731000000	N	-0.863147000000	2.755029000000	-1.055869000000
N	5.354357000000	1.570798000000	0.936798000000	N	1.299307000000	-2.085037000000	-1.643103000000
H	4.304147000000	-0.584689000000	2.673386000000	H	2.044837000000	0.347366000000	-1.554870000000
H	5.979506000000	-0.665195000000	2.123687000000	H	3.787020000000	0.042153000000	-1.820641000000
H	-5.978723000000	-0.665053000000	2.124154000000	H	-1.966484000000	0.608168000000	-1.738469000000
H	-4.303210000000	-0.584104000000	2.673392000000	H	-3.541365000000	1.339263000000	-2.199014000000
O	3.661733000000	0.305901000000	0.010451000000	O	3.571171000000	-2.531335000000	-1.831268000000
O	-3.661901000000	0.306081000000	0.009960000000	O	-2.984780000000	3.680129000000	-1.181399000000
C	-5.239809000000	2.818067000000	0.248189000000	C	-0.081127000000	3.916248000000	-0.810115000000
C	-6.419069000000	3.626545000000	0.156435000000	C	1.210218000000	3.999083000000	-1.423898000000
C	-4.034681000000	3.242316000000	-0.274568000000	C	-0.533719000000	4.930902000000	0.011044000000
C	-7.698249000000	3.228776000000	0.632336000000	C	1.687572000000	3.039737000000	-2.358196000000
C	-6.294042000000	4.917681000000	-0.457103000000	C	2.044155000000	5.122537000000	-1.108427000000
C	-3.942706000000	4.503642000000	-0.902875000000	C	0.288162000000	6.046327000000	0.288204000000
H	-3.161492000000	2.607820000000	-0.201670000000	H	-1.527957000000	4.871152000000	0.435774000000
C	-8.785675000000	4.070065000000	0.538682000000	C	2.936977000000	3.165266000000	-2.927603000000
H	-7.852613000000	2.234926000000	1.045552000000	H	1.035590000000	2.225945000000	-2.660135000000
C	-7.436186000000	5.758598000000	-0.535174000000	C	3.333806000000	5.207954000000	-1.699566000000
C	-5.040223000000	5.327701000000	-0.981941000000	C	1.554998000000	6.134109000000	-0.240252000000
H	-2.987948000000	4.821405000000	-1.310438000000	H	-0.090415000000	6.832325000000	0.935156000000
C	-8.654656000000	5.351618000000	-0.043231000000	C	3.776325000000	4.251691000000	-2.584778000000
H	-9.754031000000	3.742632000000	0.905426000000	H	3.272241000000	2.438598000000	-3.663191000000
H	-7.328479000000	6.736126000000	-0.997398000000	H	3.962487000000	6.059255000000	-1.450694000000
H	-4.964838000000	6.304388000000	-1.451660000000	H	2.190901000000	6.986642000000	-0.016798000000
H	-9.518842000000	6.005334000000	-0.109040000000	H	4.759047000000	4.339665000000	-3.039088000000
C	5.239374000000	2.818164000000	0.248607000000	C	0.732629000000	-3.371366000000	-1.833956000000
C	6.418320000000	3.627158000000	0.157274000000	C	-0.627322000000	-3.441289000000	-2.288203000000
C	4.034152000000	3.242087000000	-0.274219000000	C	1.442845000000	-4.536033000000	-1.576360000000
C	7.697608000000	3.229775000000	0.633204000000	C	-1.385514000000	-2.296359000000	-2.658135000000
C	6.292846000000	4.918443000000	-0.455867000000	C	-1.243185000000	-4.732022000000	-2.400780000000
C	3.941759000000	4.503572000000	-0.902140000000	C	0.826193000000	-5.793300000000	-1.720052000000
H	3.161221000000	2.607203000000	-0.201666000000	H	2.478463000000	-4.464630000000	-1.272067000000
C	8.784696000000	4.071552000000	0.539978000000	C	-2.690301000000	-2.416645000000	-3.086186000000
H	7.852382000000	2.235846000000	1.046087000000	H	-0.917979000000	-1.318548000000	-2.633543000000

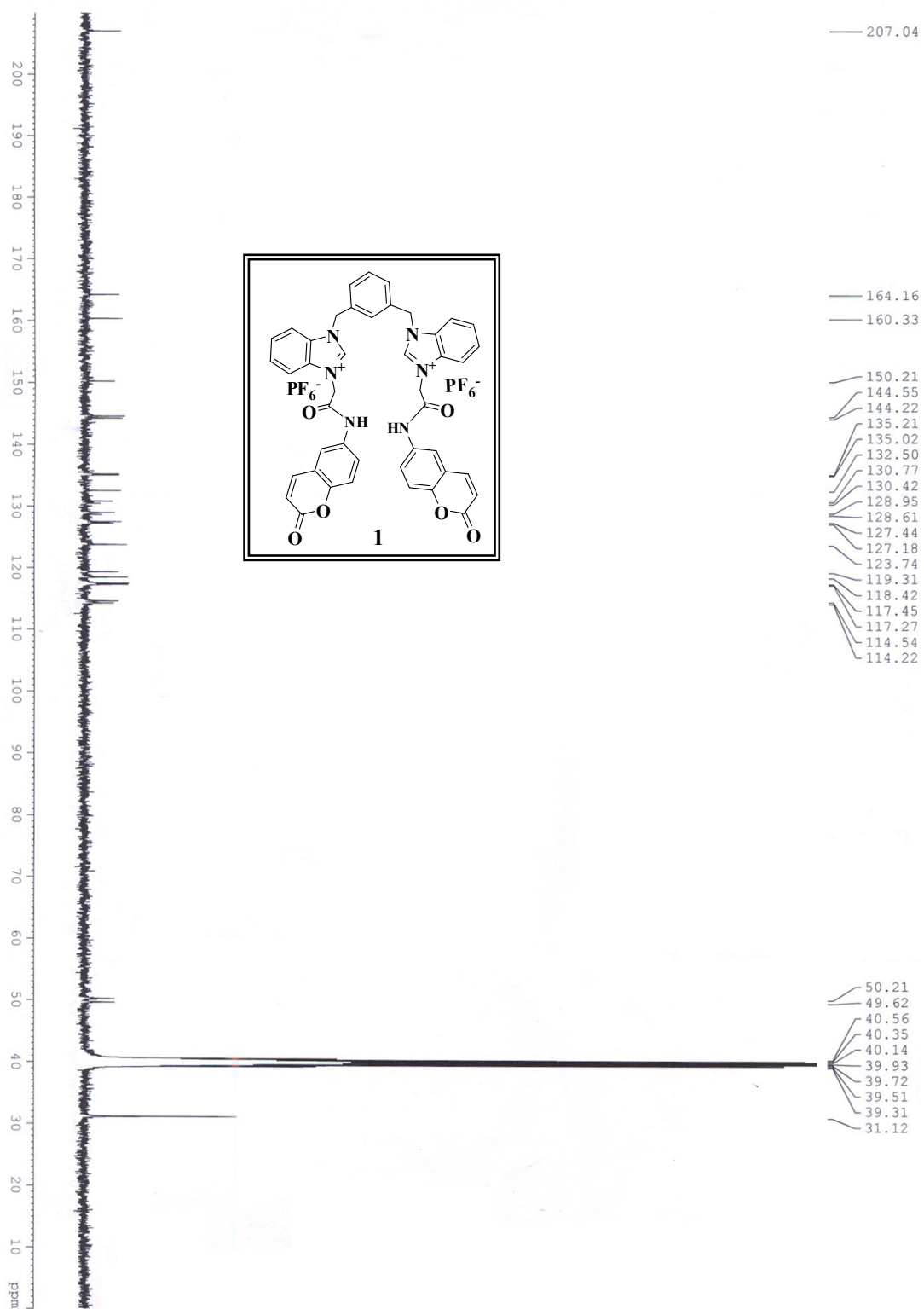
C	7.434645000000	5.759868000000	-0.533495000000	C	-2.595507000000	-4.814797000000	-2.830404000000
C	5.038941000000	5.328116000000	-0.980766000000	C	-0.489396000000	-5.898088000000	-2.105070000000
H	2.986935000000	4.821058000000	-1.309766000000	H	1.408228000000	-6.686830000000	-1.513034000000
C	8.653218000000	5.353245000000	-0.041514000000	C	-3.309219000000	-3.686278000000	-3.161756000000
H	9.753139000000	3.744391000000	0.906732000000	H	-3.243695000000	-1.531746000000	-3.390787000000
H	7.326581000000	6.737503000000	-0.995410000000	H	-3.053764000000	-5.797637000000	-2.908247000000
H	4.963230000000	6.304928000000	-1.450173000000	H	-0.963696000000	-6.870683000000	-2.206054000000
H	9.517135000000	6.007351000000	-0.106976000000	H	-4.337862000000	-3.768529000000	-3.501230000000
H	6.091105000000	1.534762000000	1.629481000000	F	-0.101564000000	0.124550000000	-0.675948000000
H	-6.090742000000	1.534905000000	1.629825000000	H	0.660632000000	-1.320597000000	-1.372215000000
				H	-0.401875000000	1.832226000000	-1.010438000000
Receptor 2+H₂PO₄⁻				Receptor 2+F⁻			
E = -2898.19295993 a.u.				E = -2354.49160137 a.u.			
C	0.308139000000	-4.640358000000	0.323891000000	C	0.607645000000	-1.017395000000	3.352917000000
C	0.784926000000	-5.179612000000	-0.876896000000	C	0.931815000000	-2.382672000000	3.346764000000
C	-0.044287000000	-5.249301000000	-1.996056000000	C	-0.059680000000	-3.338454000000	3.153472000000
C	-1.357846000000	-4.789146000000	-1.920308000000	C	-1.385309000000	-2.940853000000	2.961531000000
C	-1.849328000000	-4.244655000000	-0.727482000000	C	-1.727539000000	-1.587088000000	2.987559000000
C	-1.009165000000	-4.170137000000	0.388727000000	C	-0.722623000000	-0.629159000000	3.192890000000
H	1.804395000000	-5.552447000000	-0.936927000000	H	1.964384000000	-2.695761000000	3.479626000000
H	0.329353000000	-5.675739000000	-2.921857000000	H	0.195730000000	-4.393315000000	3.142624000000
H	-2.004769000000	-4.859471000000	-2.791454000000	H	-2.154372000000	-3.690990000000	2.798519000000
H	-1.381903000000	-3.729973000000	1.310548000000	H	-0.979417000000	0.428133000000	3.215902000000
C	1.203206000000	-4.586997000000	1.542463000000	C	1.705826000000	0.022343000000	3.461420000000
H	1.804783000000	-5.497310000000	1.610571000000	H	2.353120000000	-0.163998000000	4.321087000000
H	0.612807000000	-4.505677000000	2.460779000000	H	1.294353000000	1.029892000000	3.568360000000
C	-3.281720000000	-3.760586000000	-0.639688000000	C	-3.175086000000	-1.177490000000	2.851518000000
H	-3.575933000000	-3.597781000000	0.401014000000	H	-3.503080000000	-0.628978000000	3.741513000000
H	-3.963366000000	-4.498180000000	-1.068837000000	H	-3.813315000000	-2.061640000000	2.756849000000
N	2.162042000000	-3.461850000000	1.515932000000	N	2.573452000000	-0.013300000000	2.265597000000
C	1.958680000000	-2.269771000000	0.942749000000	C	2.111713000000	0.056021000000	1.007593000000
C	3.384459000000	-3.418550000000	2.198501000000	C	3.942718000000	-0.307760000000	2.219622000000
N	2.980575000000	-1.454627000000	1.198711000000	N	3.103620000000	-0.168624000000	0.144309000000
H	1.077743000000	-1.960673000000	0.385300000000	H	1.080471000000	0.202186000000	0.658063000000
C	3.913453000000	-2.135648000000	1.980229000000	C	4.275798000000	-0.427274000000	0.857820000000
C	4.060796000000	-4.366719000000	2.967532000000	C	4.900974000000	-0.488196000000	3.220086000000
C	5.145982000000	-1.750969000000	2.507594000000	C	5.563775000000	-0.763385000000	0.438133000000
C	5.821261000000	-2.696783000000	3.271854000000	C	6.513312000000	-0.946695000000	1.436508000000
C	5.287504000000	-3.980406000000	3.499049000000	C	6.189031000000	-0.805237000000	2.801273000000
H	5.562997000000	-0.766553000000	2.325820000000	H	5.795764000000	-0.910513000000	-0.610351000000
H	6.784088000000	-2.440637000000	3.701896000000	H	7.528077000000	-1.213147000000	1.159490000000
H	5.847230000000	-4.686750000000	4.103644000000	H	6.963710000000	-0.954255000000	3.546620000000
H	3.655669000000	-5.355885000000	3.152055000000	H	4.664236000000	-0.385084000000	4.273813000000
N	-3.515044000000	-2.503155000000	-1.382075000000	N	-3.460660000000	-0.290677000000	1.704730000000
C	-2.755287000000	-1.406808000000	-1.269889000000	C	-2.697100000000	-0.051684000000	0.625841000000
C	-4.592303000000	-2.211975000000	-2.228277000000	C	-4.653109000000	0.431760000000	1.569969000000
N	-3.272385000000	-0.409559000000	-1.993782000000	N	-3.328438000000	0.791023000000	-0.197996000000
H	-1.830661000000	-1.306777000000	-0.691501000000	H	-1.690117000000	-0.407073000000	0.411766000000
C	-4.435744000000	-0.871422000000	-2.626797000000	C	-4.557577000000	1.142244000000	0.363028000000
C	-5.662507000000	-2.987454000000	-2.679373000000	C	-5.780965000000	0.528530000000	2.388879000000
C	-5.335402000000	-0.252615000000	-3.498718000000	C	-5.565223000000	2.007719000000	-0.067556000000
C	-6.393695000000	-1.032272000000	-3.952325000000	C	-6.685675000000	2.104519000000	0.749604000000
C	-6.555932000000	-2.372851000000	-3.550302000000	C	-6.794583000000	1.374746000000	1.951349000000
H	-5.220999000000	0.790005000000	-3.769949000000	H	-5.449809000000	2.603485000000	-0.965051000000
H	-7.119836000000	-0.592006000000	-4.628106000000	H	-7.494503000000	2.767521000000	0.460060000000
H	-7.402225000000	-2.939913000000	-3.924857000000	H	-7.689745000000	1.482212000000	2.555505000000
H	-5.800511000000	-4.017906000000	-2.369813000000	H	-5.871386000000	-0.025349000000	3.317043000000
C	-2.658336000000	0.928154000000	-2.082264000000	C	-2.750817000000	1.304090000000	-1.447534000000
C	3.076726000000	-0.087043000000	0.712309000000	C	2.887725000000	-0.293683000000	-1.305135000000
C	-3.635473000000	2.031608000000	-1.616209000000	C	-2.212287000000	2.730752000000	-1.222520000000
C	4.170206000000	0.009057000000	-0.373892000000	C	2.626243000000	-1.774986000000	-1.644861000000
N	-3.527622000000	2.366632000000	-0.303566000000	N	-0.863147000000	2.755029000000	-1.055869000000
N	4.666963000000	1.271292000000	-0.519663000000	N	1.299307000000	-2.085037000000	-1.643103000000
H	2.102078000000	0.170709000000	0.287629000000	H	2.044837000000	0.347366000000	-1.554870000000
H	3.251030000000	0.573359000000	1.567213000000	H	3.787020000000	0.042153000000	-1.820641000000
H	-1.736388000000	0.886608000000	-1.496593000000	H	-1.966484000000	0.608168000000	-1.738460000000
H	-2.418932000000	1.128683000000	-3.129100000000	H	-3.541365000000	1.339263000000	-2.199014000000
O	4.494658000000	-0.979002000000	-1.014032000000	O	3.571171000000	-2.531335000000	-1.831268000000
O	-4.432613000000	2.506106000000	-2.417471000000	O	-2.984780000000	3.680129000000	-1.181399000000
C	-4.313902000000	3.346812000000	0.370862000000	C	-0.081127000000	3.916248000000	-0.810115000000
C	-4.641376000000	3.119615000000	1.747542000000	C	1.210218000000	3.999083000000	-1.423898000000
C	-4.721431000000	4.501040000000	-0.269462000000	C	-0.533719000000	4.930942000000	0.011044000000

C	-4.316053000000	1.923404000000	2.446414000000	C	1.687572000000	3.039737000000	-2.358196000000
C	-5.350772000000	4.149392000000	2.451941000000	C	2.044155000000	5.122537000000	-1.108427000000
C	-5.447507000000	5.488748000000	0.431894000000	C	0.288162000000	6.046327000000	0.288204000000
H	-4.482036000000	4.647237000000	-1.314502000000	H	-1.527957000000	4.871152000000	0.435774000000
C	-4.642913000000	1.770586000000	3.776854000000	C	2.936977000000	3.165266000000	-2.927603000000
H	-3.828484000000	1.107086000000	1.925179000000	H	1.035590000000	2.225945000000	-2.660135000000
C	-5.660824000000	3.957775000000	3.825485000000	C	3.333806000000	5.207954000000	-1.699566000000
C	-5.743143000000	5.327884000000	1.764795000000	C	1.554998000000	6.134109000000	-0.240252000000
H	-5.756083000000	6.387443000000	-0.093888000000	H	-0.090415000000	6.832325000000	0.935156000000
C	-5.310991000000	2.799720000000	4.480182000000	C	3.776325000000	4.251691000000	-2.584778000000
H	-4.397663000000	0.844056000000	4.290119000000	H	3.272241000000	2.438598000000	-3.663191000000
H	-6.191039000000	4.748184000000	4.350760000000	H	3.962487000000	6.059255000000	-1.450694000000
H	-6.287562000000	6.095278000000	2.308592000000	H	2.190901000000	6.986642000000	-0.016798000000
H	-5.558177000000	2.667038000000	5.529502000000	H	4.759047000000	4.339665000000	-3.039088000000
C	5.606041000000	1.748402000000	-1.474877000000	C	0.732629000000	-3.371366000000	-1.833956000000
C	6.217567000000	3.022211000000	-1.220901000000	C	-0.627322000000	-3.441289000000	-2.288203000000
C	5.911619000000	1.030711000000	-2.615911000000	C	1.442845000000	-4.530633000000	-1.576360000000
C	5.995747000000	3.790818000000	-0.044863000000	C	-1.385514000000	-2.296359000000	-2.658135000000
C	7.111577000000	3.548374000000	-2.212471000000	C	-1.243185000000	-4.732022000000	-2.400780000000
C	6.817548000000	1.556911000000	-3.563461000000	C	0.826193000000	-5.793300000000	-1.720052000000
H	5.456420000000	0.063702000000	-2.777902000000	H	2.478463000000	-4.464692000000	-1.272067000000
C	6.593158000000	5.020142000000	0.130268000000	C	-2.690301000000	-2.416645000000	-3.086186000000
H	5.376451000000	3.406304000000	0.761693000000	H	-0.917979000000	-1.318548000000	-2.633543000000
C	7.706615000000	4.820820000000	-2.000404000000	C	-2.595507000000	-4.814797000000	-2.830404000000
C	7.395362000000	2.789619000000	-3.378340000000	C	-0.489396000000	-5.898088000000	-2.105057000000
H	7.042055000000	0.974036000000	-4.451880000000	H	1.408228000000	-6.686830000000	-1.513034000000
C	7.451748000000	5.547646000000	-0.860749000000	C	-3.309219000000	-3.686278000000	-3.161756000000
H	6.410511000000	5.583289000000	1.041017000000	H	-3.243695000000	-1.531746000000	-3.390787000000
H	8.377209000000	5.209797000000	-2.762347000000	H	-3.053764000000	-5.797637000000	-2.908247000000
H	8.081136000000	3.198238000000	-4.115492000000	H	-0.963696000000	-6.870683000000	-2.206054000000
H	7.915179000000	6.518699000000	-0.713669000000	H	-4.337862000000	-3.768529000000	-3.501230000000
H	4.265431000000	1.980327000000	0.078441000000	F	-0.101564000000	0.124550000000	-0.675948000000
H	-2.769450000000	1.948969000000	0.237631000000	H	0.660632000000	-1.320597000000	-1.372215000000
P	-0.638642000000	-0.099164000000	1.508620000000	H	-0.401875000000	1.832226000000	-1.010438000000
O	-1.238620000000	1.439027000000	1.346733000000				
H	-1.188660000000	1.918280000000	2.191146000000				
O	-1.983627000000	-0.975768000000	1.938009000000				
H	-2.051939000000	-0.993626000000	2.907122000000				
O	0.382148000000	-0.156846000000	2.598491000000				
O	-0.335738000000	-0.539507000000	0.086455000000				

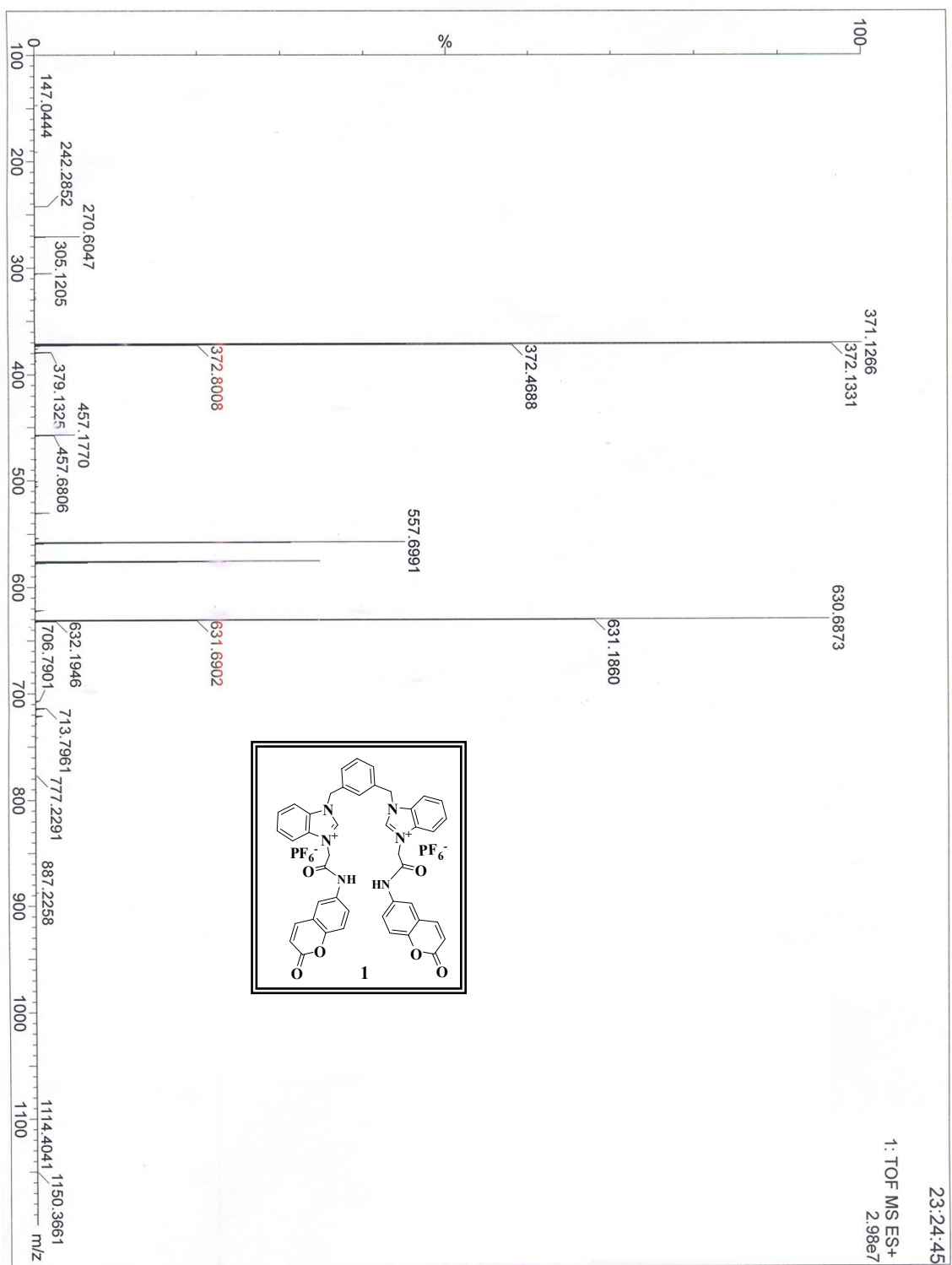
^1H NMR of 1 in CDCl_3 containing d_6 DMSO (400 MHz)



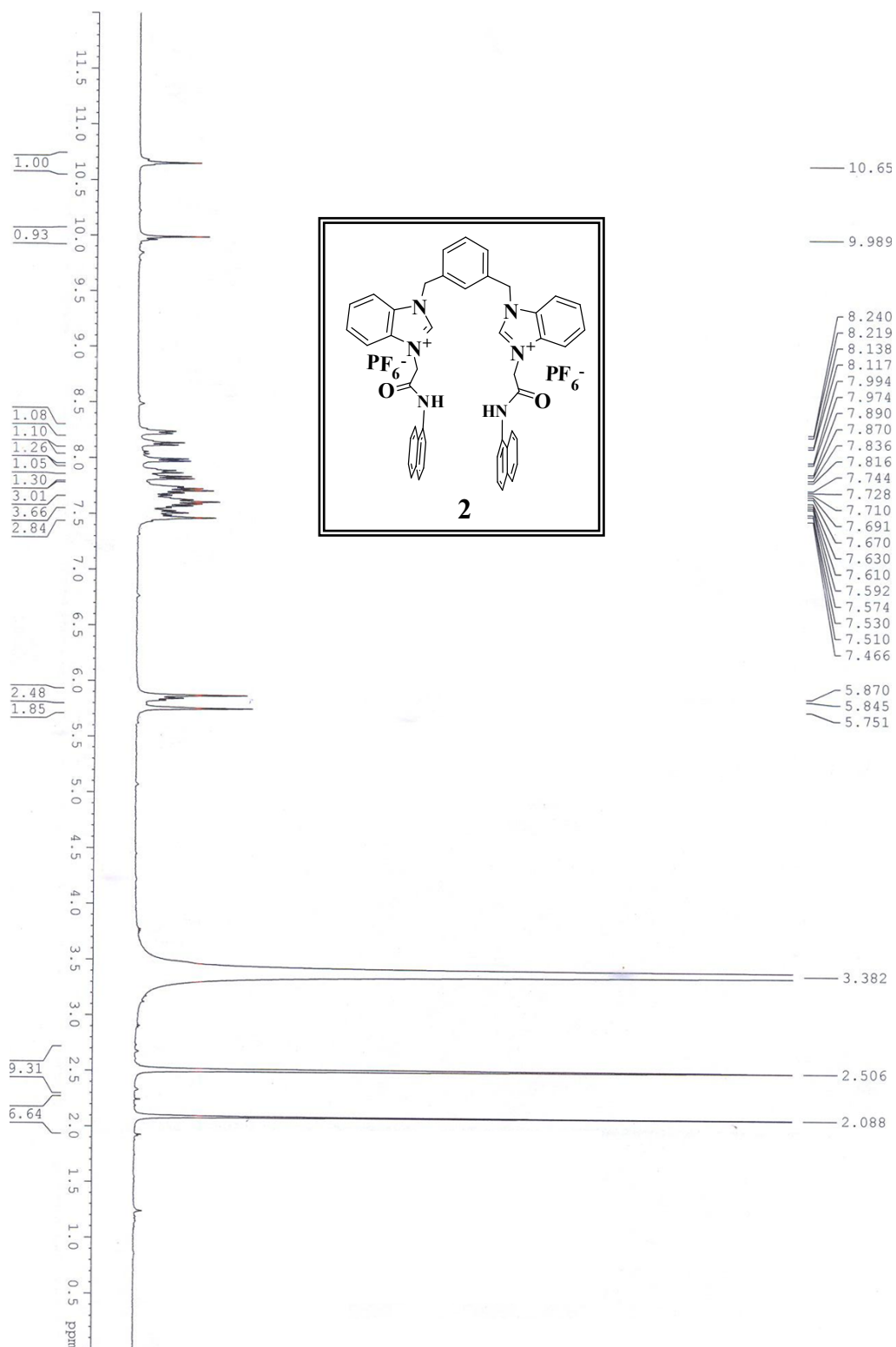
^{13}C NMR of 1 in d_6 DMSO (100 MHz)



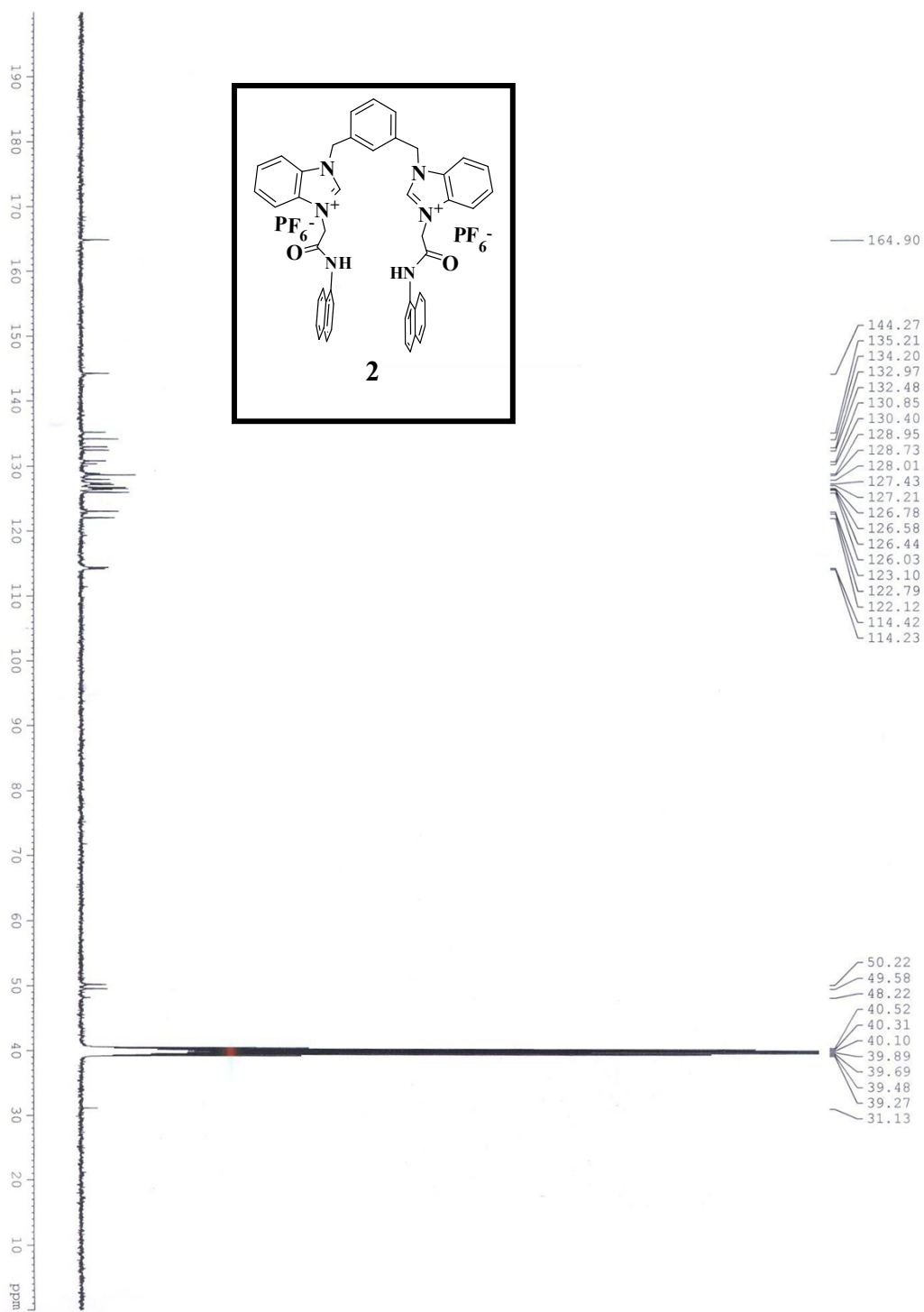
Mass of 1



¹H NMR of 2 in d₆ DMSO (400 MHz)



^{13}C NMR of 2 in d_6 DMSO (100 MHz)



Mass of 2

