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Supporting Information

Dihydrogen Phosphate Selective Anion Receptor Based on Acylhydrazone and Pyrazole

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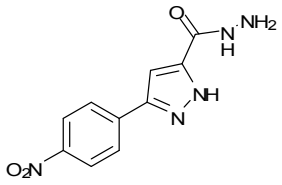
Contents



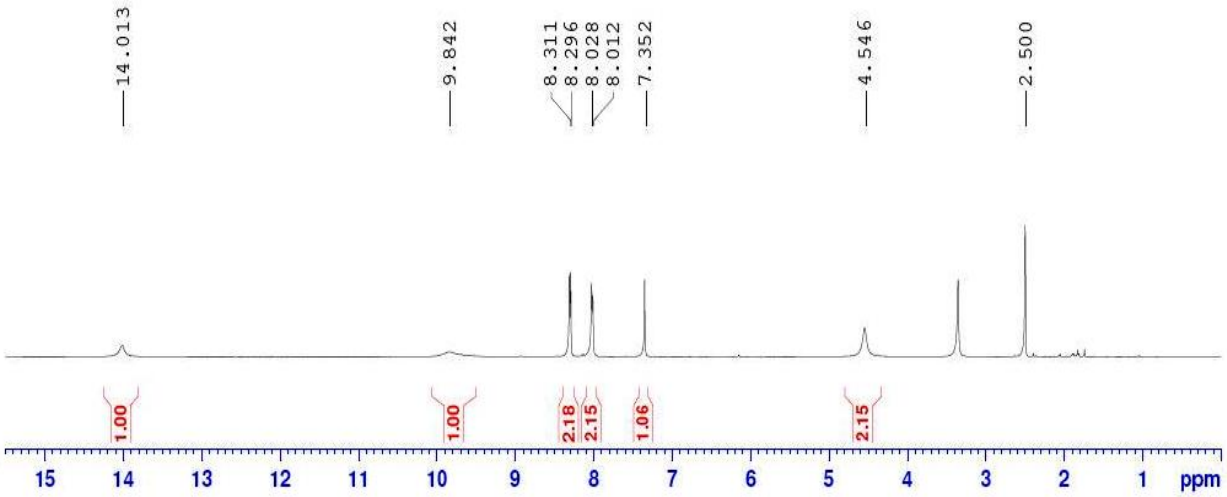


Fig. S1. ^{1}H NMR spectrum of 3-(4-nitrophenyl)-1*H*-pyrazole-5-carbohydrazide

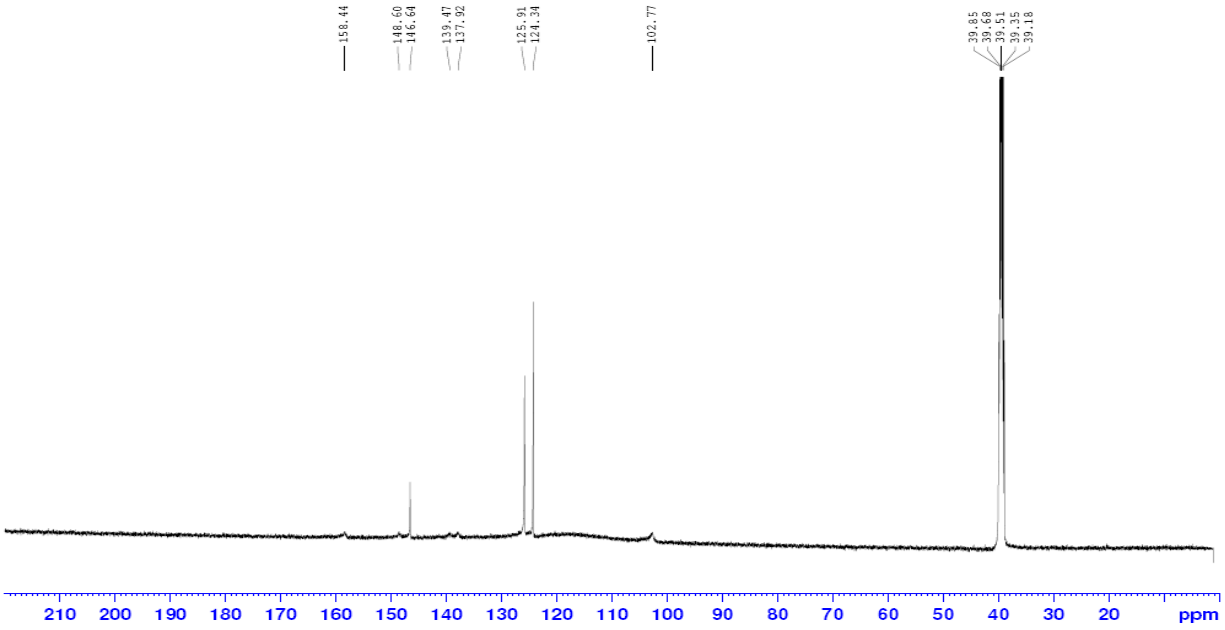
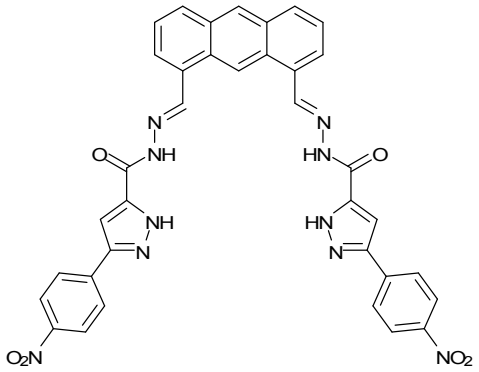


Fig. S2. ^{13}C NMR spectrum of 3-(4-nitrophenyl)-1*H*-pyrazole-5-carbohydrazide



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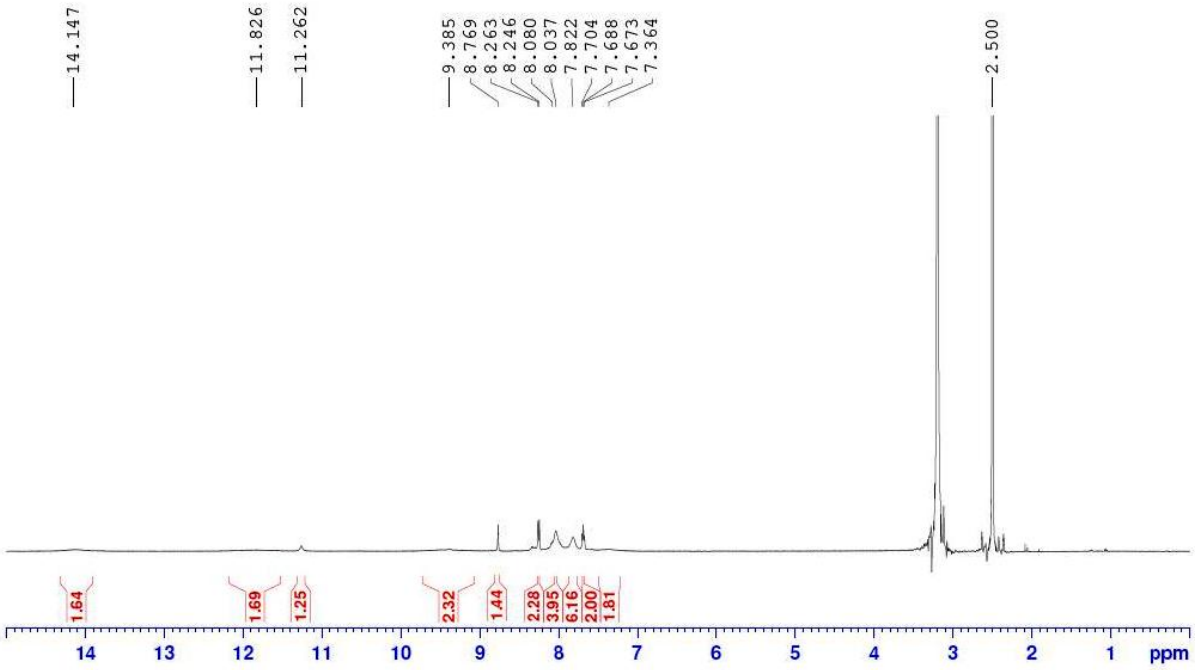


Fig. S3. ^{1}H NMR spectrum of compound **1**

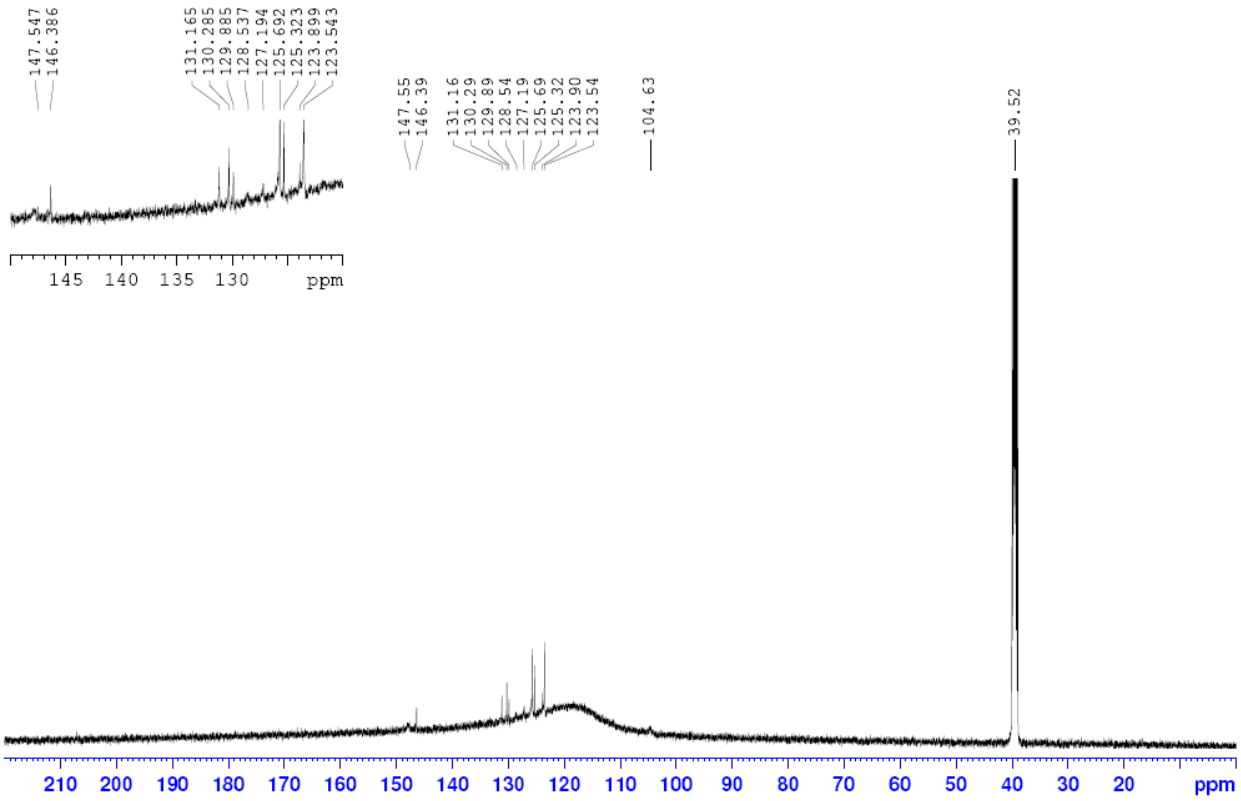
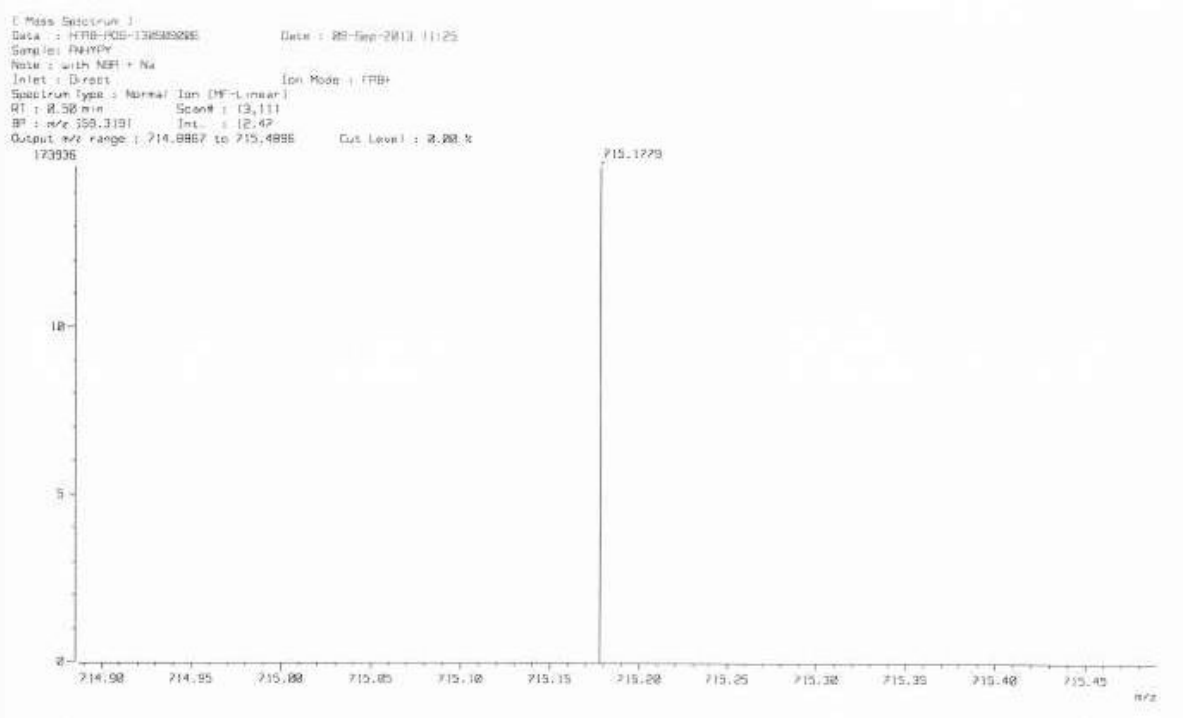


Fig. S4. ^{13}C NMR spectrum of compound **1**.



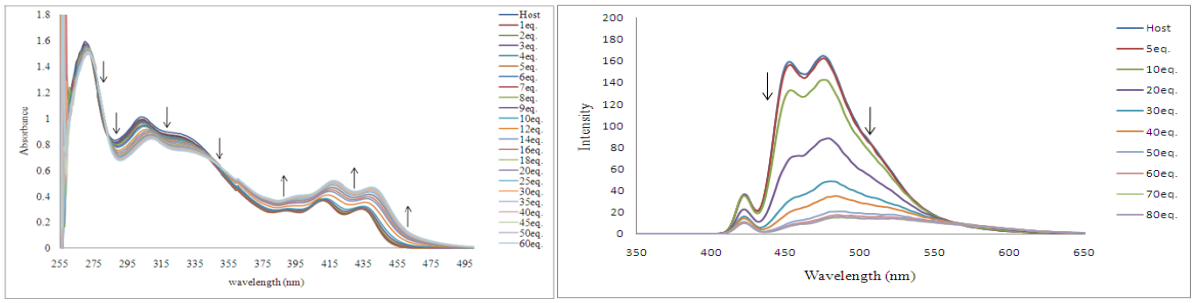
[Elemental Composition] Page: 1
Data : HFAB-POS-130909006 Date : 09-Sep-2013 11:25
Sample: ANHYPY
Note : with NBA + Na
Inlet : Direct Ion Mode : FAB+
RT : 0.50 min Scan#: (3,11)
Elements : C 36/0, H 24/0, O 6/0, N 10/0, Na 1/0
Mass Tolerance : 10mmu
Unsaturation (U.S.) : 0.0 - 100.0

Observed m/z	Int%						
715.1779	14.8						
Estimated m/z	Error[ppm]	U.S.	C	H	O	N	Na
715.1778	+0.2	29.5	36	24	6	10	1

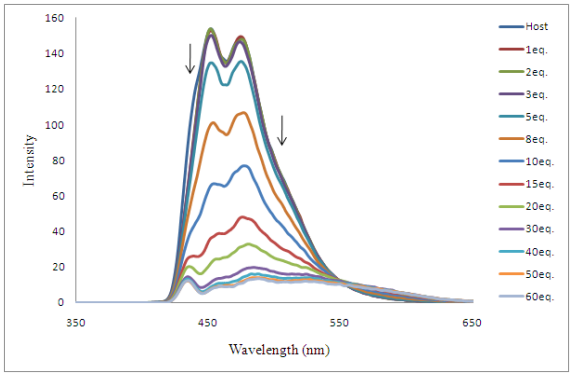
[Theoretical Ion Distribution] Page: 1
Molecular Formula : C36 H24 O6 N10 Na
(m/z 715.1778, MW 715.6397, U.S. 29.5)
Base Peak : 715.1778, Averaged MW : 715.6416(a), 715.6423(w)

m/z	INT.	
715.1778	100.0000	**********
716.1807	44.3025	**********
717.1833	10.7869	******
718.1859	1.8817	*
719.1885	0.2601	
720.1910	0.0300	
721.1934	0.0030	
722.1959	0.0003	

Fig. S5. HRMS(FAB) spectrum of compound **1**.



(a) (b)



(c)

Figure S6. Family of UV-vis spectra(a) and fluorescence spectra(b) recorded over the course of titrating a 20 μM DMSO solution of receptor **1** with increasing amounts of tetrabutylammonium acetate. Family of fluorescence spectra(c) recorded over the course of titrating a 20 μM DMSO solution of receptor **1** with increasing amounts of tetrabutylammonium hydroxide.

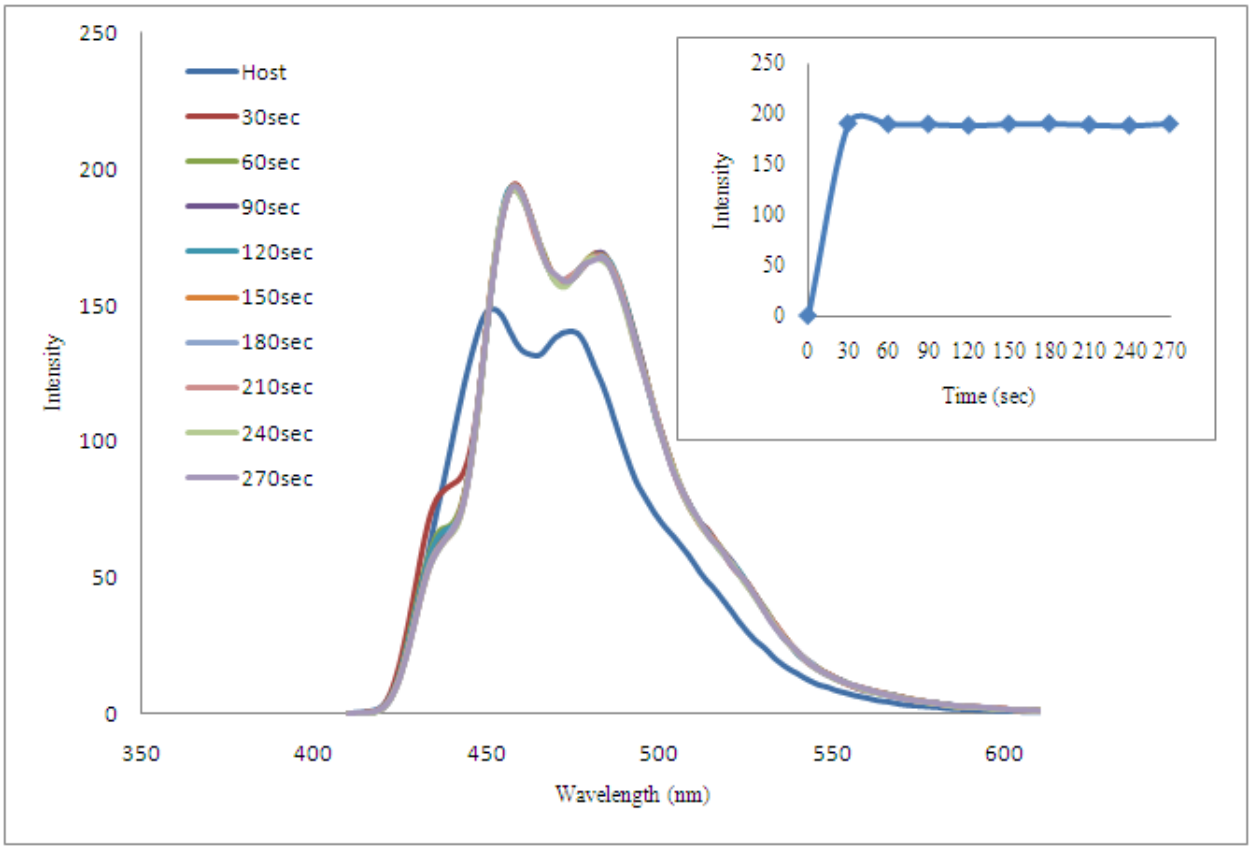
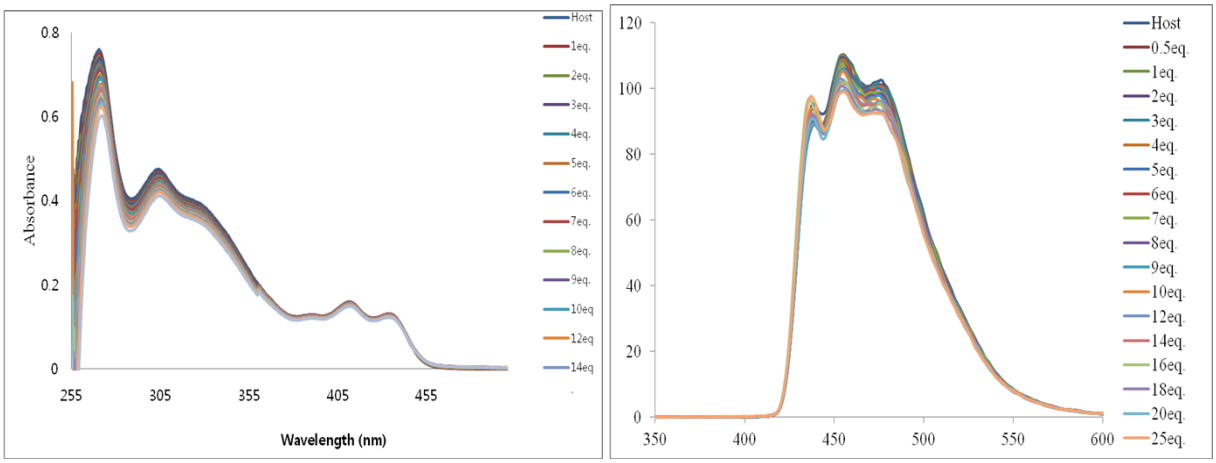


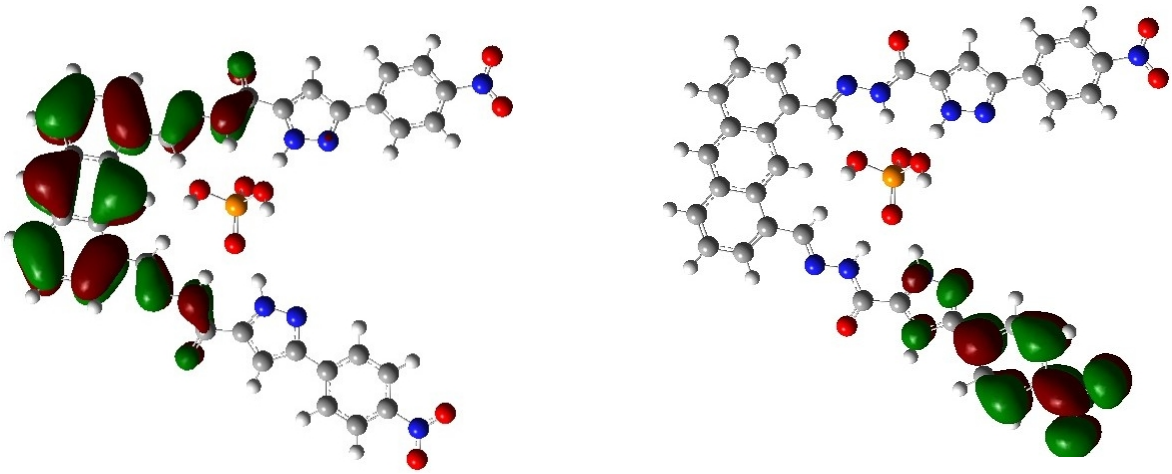
Figure S7. Time dependent fluorescence spectra of receptor **1** (20 μM) upon addition with dihydrogen phosphate(22 eq.) at 25°C. Inset: emission intensity at 460 nm versus binding time.



(a) **(b)**

Figure S8. Family of UV-vis spectra(a) and fluorescence spectra(b) recorded over the course of titrating a 9:1 DMSO : HEPES at pH 7.4 solution of receptor **1** with increasing amounts of tetrabutylammonium dihydrogen phospahte.

a)



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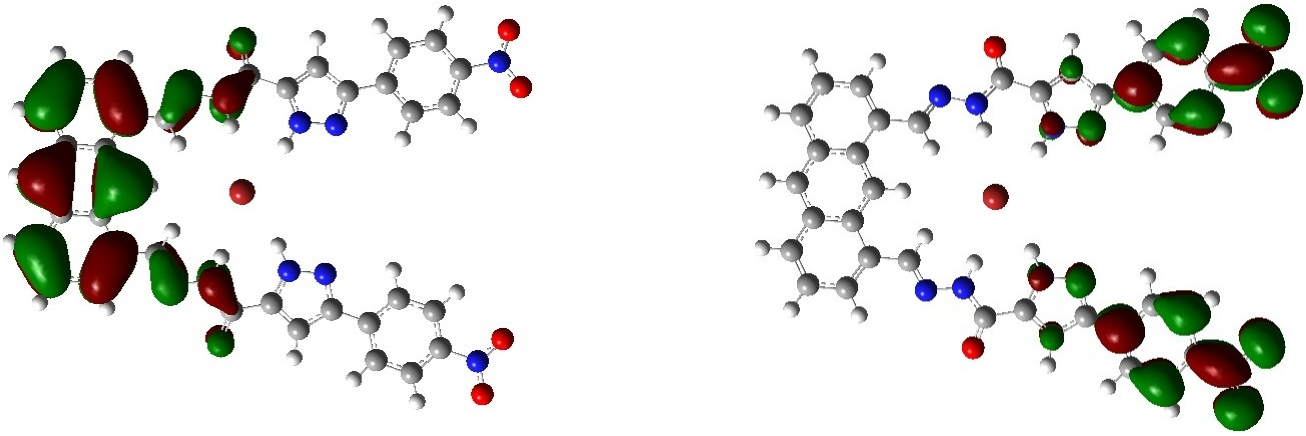
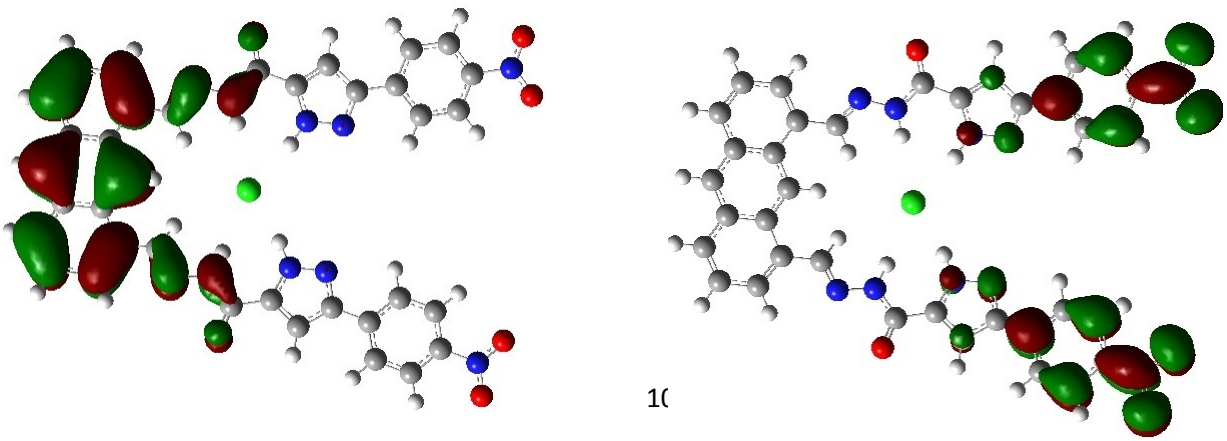


c)



d)

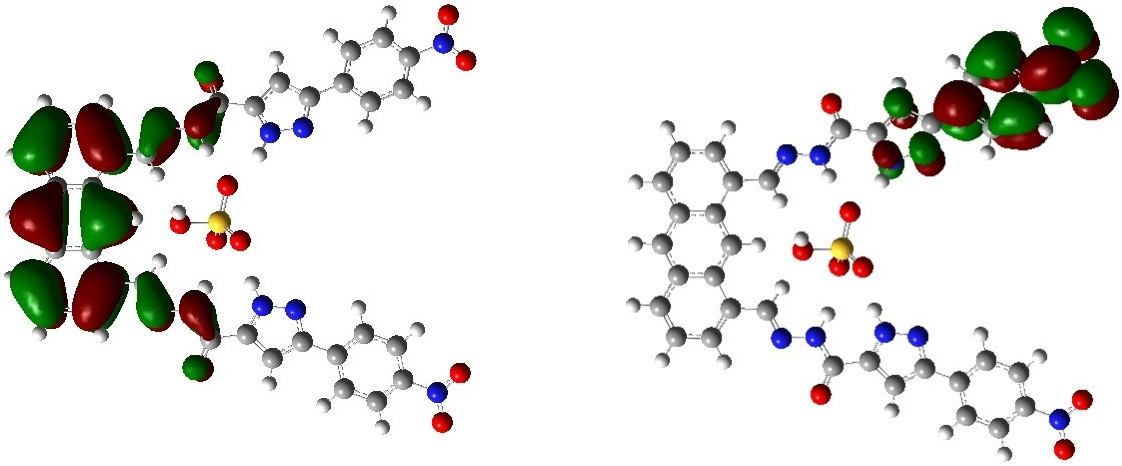


Fig.S9. DFT optimized Host-anion model complexes in DMSO (B3LYP/6-31G*, polarizable continuum model). Molecular orbital distribution plots of HOMO and LUMO states in the ground state. a) HOMO-LUMO diagram for Host…$H_2PO_4^-$ complex b) HOMO-LUMO diagram for Host…Br^- complex c) HOMO-LUMO diagram for Host…Cl^- complex d) HOMO-LUMO diagram for Host…HSO_4^- complex

Binding Energy Calculation Procedure

We have optimized the geometries of monomers (Host and H2PO4-) and complex (Host.H2PO4-) to obtain the binding energy. All the calculations were performed with the Gaussian 09 suit of programs. Geometry optimizations were carried out with the density functional theory (DFT) implemented in Gaussian 09. For DFT calculations, the common B3LYP hybrid functional were used with the 6-31G* basis set. The solvation effect of DMSO was considered using polarizable continuum model (PCM). Geometries were re-optimized in the condensed phase using the same optimization criteria. The electronic binding energies for complex are summarized in Table SI-1. The binding energies concerning solvation energy and basis set superposition error correction (BSSEC) are also listed. For complex structure several geometries have been optimized. Here, we chose the lowest energy structure as representative structure. (See Table S2-S4 for Coordinates of Optimized Geometries.). The binding energy in the gas phase is much larger than the solvent phase binding energy. The large difference may be attributed to the shielding effect by the solvent while DMSO is employed as the solvent in the PCM calculation. It is noteworthy that the reported host.H2PO4-complex shows the highest binding energy compared with the previously reported complexes due to the strong N-H…O type H-bonding along the planarity in the host geometry. In the solvent phase the binding energy has reduced by a large amount comparing with that in the gas phase, showing the significant effect of solvation. For better comparison in the final discussion the manuscript is based on the BSSE corrected binding energy. All geometries of hosts, guest, and complexes optimized in DMSO are also listed below.

Table S1. Binding Energy of host with dihydrogen phosphate anion complex.

Host·$H_2PO_4^-$		
ΔE	ΔE_{DMSO}	ΔE_{BSSEC}
-87.01	-36.96	-24.96

ΔE: electronic binding energy, ΔE_{DMSO}: binding energy in solution, ΔE_{BSSEC}: binding energy in solution after BSSEC (basis set superposition error correction). Units are in kcal/mol.

Coordinates for Optimized Geometries in DMSO (B3LYP/6-31G*, polarizable continuum model)

Table S2. Optimized Structure of host

C	-6.38924200	-3.65674000	-0.39363700
C	-5.63924200	-2.49766100	-0.29767900
C	-6.31446300	-1.22361800	-0.14438800
C	-7.76068400	-1.21832800	-0.12594700
C	-8.47578200	-2.44913500	-0.23256100
C	-7.80449300	-3.63864100	-0.35451500
C	-5.64194200	-0.00000200	0.00001500
C	-8.43716100	0.00001100	-0.00008700
C	-7.76068200	1.21834300	0.12582100
C	-6.31446200	1.22361900	0.14437100
C	-5.63923900	2.49765800	0.29769700
C	-6.38923600	3.65674600	0.39357300
C	-7.80448400	3.63865900	0.35434800
C	-8.47577600	2.44915800	0.23236600
H	-4.56071100	-0.00000500	0.00004400
H	-5.87049100	-4.60168200	-0.51629300
H	-9.56203200	-2.42155700	-0.21561800
H	-8.35055500	-4.57360300	-0.43675400
H	-9.52459900	0.00001700	-0.00013300
H	-5.87048500	4.60168500	0.51625200
H	-8.35054300	4.57362900	0.43652900
H	-9.56202500	2.42159000	0.21533900
C	-4.17666200	-2.57286400	-0.37363300
N	-3.55795300	-3.69496000	-0.24343400
N	-2.20242200	-3.66118700	-0.38897600

C	-1.44886500	-4.78903400	-0.14744500
C	0.00476700	-4.63077000	-0.40184700
H	0.94349000	-6.13555600	0.89132600
H	0.13494800	-3.10879100	-1.90783300
C	3.94297400	-6.24781500	0.69289500
C	5.26532800	-6.60398500	0.92531600
C	6.27779800	-5.88946400	0.28363500
C	5.99267100	-4.83117200	-0.58232400
C	4.66733400	-4.48561300	-0.80458300
C	3.62199900	-5.18604500	-0.17217100
H	3.15534700	-6.80493200	1.18847700
H	6.80026400	-4.29559300	-1.06516700
H	4.42851000	-3.66555300	-1.47193200
O	-1.91249900	-5.85066700	0.25029700
H	-3.61744400	-1.65332600	-0.56669000
H	5.51692100	-7.42052400	1.59009000
N	7.66986200	-6.25725000	0.52435100
O	8.55211100	-5.61168200	-0.04956800
O	7.90201500	-7.19705900	1.29080000
H	-1.74410300	-2.76252600	-0.53279900
C	1.04500600	-5.34992400	0.15858900
C	2.22225500	-4.81119200	-0.41455300
N	0.58781100	-3.73090500	-1.25102000
N	1.92080100	-3.83052400	-1.28588100
C	-4.17666400	2.57284900	0.37376900
N	-3.55793000	3.69492200	0.24350000
N	-2.20240600	3.66115400	0.38913200
C	-1.44883400	4.78897200	0.14749500
C	0.00479100	4.63077900	0.40197800

C	2.22227700	4.81125700	0.41468000
H	0.94349100	6.13542100	-0.89137800
H	0.13499900	3.10911300	1.90828100
C	1.04501900	5.34989900	-0.15852400
N	0.58785000	3.73110700	1.25134700
N	1.92083800	3.83073600	1.28618000
C	3.94297900	6.24770400	-0.69302100
C	3.62201700	5.18607900	0.17222700
C	4.66736200	4.48575900	0.80474900
C	5.99269300	4.83128400	0.58241400
C	6.27781000	5.88943200	-0.28372500
C	5.26533000	6.60384100	-0.92551400
H	3.15534600	6.80473200	-1.18869400
H	4.42854900	3.66581400	1.47224200
H	6.80029400	4.29578800	1.06533800
H	5.51691000	7.42027200	-1.59042700
O	-1.91246300	5.85055800	-0.25037900
H	-1.74411100	2.76250000	0.53307600
H	-3.61747300	1.65330900	0.56690200
N	7.66986900	6.25717700	-0.52451400
O	7.90200600	7.19691900	-1.29104300
O	8.55211300	5.61163200	0.04943400

Table S3. Optimized Structure of $H_2PO_4^-$

O	-1.27229800	0.46286100	-0.79407200
O	0.10983000	0.78370100	1.35006800
O	-0.15881000	-1.58689100	0.19546200
O	1.30225500	0.21028500	-0.84910300
P	-0.00757200	-0.09466800	0.12961100
H	-1.41877300	1.39838500	-0.57987900
H	1.68453800	1.06197800	-0.58311000

Table S4. Optimized Structure of host-$H_2PO_4^-$ complex

C	-6.10058700	-3.88260400	-0.09121600
C	-5.40513300	-2.68763800	-0.06181100
C	-6.13715800	-1.43913600	-0.14415200
C	-7.57936500	-1.49247900	-0.22994300
C	-8.23801700	-2.75955700	-0.24874200
C	-7.51412100	-3.92280800	-0.19043600
C	-5.51210400	-0.18353200	-0.17036100
C	-8.30102900	-0.29608400	-0.31243100
C	-7.67246000	0.95520800	-0.32379500
C	-6.22949700	1.02054000	-0.24905100
C	-5.59817300	2.32650300	-0.27373300
C	-6.38821800	3.45802600	-0.37483200
C	-7.80008200	3.38013800	-0.45256700
C	-8.42948700	2.16147000	-0.42391100
H	-4.43256000	-0.14673100	-0.14817300
H	-5.54255300	-4.81033500	-0.01839900
H	-9.32283200	-2.78115800	-0.31187600
H	-8.01792700	-4.88489800	-0.20444300
H	-9.38563900	-0.33977500	-0.38106600
H	-5.90425100	4.42920900	-0.38488800
H	-8.37920800	4.29588500	-0.52785300
H	-9.51284200	2.09266900	-0.47783400
C	-3.94308800	-2.69244200	0.07388600
N	-3.25191000	-3.73441100	-0.24206100
N	-1.90513800	-3.64707300	-0.03465200
C	-1.10050200	-4.70556400	-0.37970300
C	0.35588700	-4.52076200	-0.14783100

H	1.20202700	-6.42517400	-0.84369300
H	0.55901100	-2.54373900	0.69078500
C	4.20338000	-6.61615000	-0.58336900
C	5.50454700	-7.09627100	-0.65172300
C	6.55207200	-6.26730300	-0.24586000
C	6.31927700	-4.97238400	0.22508700
C	5.01454700	-4.50569200	0.28743500
C	3.93421200	-5.31637500	-0.11463300
H	3.38954000	-7.26114600	-0.89675600
H	7.15179800	-4.35211400	0.53247600
H	4.81654300	-3.50320200	0.64903500
O	-1.51925800	-5.75827700	-0.85713100
H	-3.45559400	-1.79883600	0.47023300
H	5.71453500	-8.09552900	-1.01162500
N	7.92054200	-6.76457000	-0.31531900
O	8.83411300	-6.01718700	0.04941000
O	8.10686300	-7.91125100	-0.73582300
H	-1.51867800	-2.78280200	0.37366800
C	1.35399800	-5.44295800	-0.42389600
C	2.55871500	-4.81012900	-0.04402200
N	0.98753000	-3.42233000	0.36439100
N	2.31057700	-3.57374400	0.43692100
C	-4.14048500	2.44785100	-0.17731100
N	-3.54105000	3.57347200	-0.37607100
N	-2.18196800	3.54142200	-0.23424200
C	-1.44723000	4.68585600	-0.41219400
C	0.02389400	4.53481600	-0.26057800
C	2.21412300	4.90349500	-0.15251000
H	0.76529100	6.57737600	-0.58589800

H	0.33376400	2.44023800	0.15483100
C	0.97202400	5.53988100	-0.37376200
N	0.71718900	3.38890200	0.01284000
N	2.03456800	3.58650400	0.08183700
C	3.76425700	6.84726300	-0.42504700
C	3.56329900	5.48026500	-0.15509900
C	4.68665600	4.67201700	0.11105200
C	5.96702100	5.20564700	0.10757100
C	6.13172500	6.56636900	-0.16487800
C	5.04018500	7.39498900	-0.43182700
H	2.91660200	7.49091100	-0.63427400
H	4.54147800	3.61842700	0.32037700
H	6.83228800	4.58750100	0.31142400
H	5.19743500	8.44573800	-0.64002400
O	-1.93253000	5.78455800	-0.67727800
H	-1.73035700	2.63890000	-0.01798100
H	-3.56385800	1.56293100	0.08967000
N	7.47408800	7.13420400	-0.17054100
O	7.59988400	8.33888600	-0.41425700
O	8.42747500	6.38576400	0.06881500
O	-2.43469300	0.30382600	1.95932800
O	-0.65056100	-1.37199800	1.19460300
O	-0.78690000	1.08418000	0.24523100
O	0.05451300	0.65468200	2.59467800
P	-0.90950300	0.10952900	1.39622700
H	-2.65599900	-0.36283300	2.63206700
H	0.36379100	-0.07933600	3.15164200

Table S5. Optimized Structure of host-Br^- complex

C	-6.38793100	3.67266100	-0.02737700
C	-5.66060600	2.49853300	0.01064200
C	-6.36151900	1.23018100	-0.01231700
C	-7.80556700	1.22764000	-0.03755800
C	-8.49853500	2.47552300	-0.06712000
C	-7.80486400	3.65989400	-0.07146900
C	-5.69248200	-0.00000300	-0.02294400
C	-8.48121800	-0.00000400	-0.05198800
C	-7.80556500	-1.22764800	-0.03757400
C	-6.36151800	-1.23018700	-0.01233100
C	-5.66060400	-2.49853900	0.01061300
C	-6.38792700	-3.67266700	-0.02742200
C	-7.80486000	-3.65990100	-0.07151600
C	-8.49853200	-2.47553200	-0.06715200
H	-4.61457500	-0.00000200	-0.07627500
H	-5.85119700	4.61601100	-0.00912900
H	-9.58597500	2.46763500	-0.08831700
H	-8.34098300	4.60520800	-0.09639700
H	-9.56936500	-0.00000400	-0.08506000
H	-5.85119100	-4.61601600	-0.00918600
H	-8.34097700	-4.60521500	-0.09645700
H	-9.58597200	-2.46764500	-0.08834900
C	-4.19930000	2.50657400	0.09810500
N	-3.49458600	3.56813100	-0.10044500
N	-2.14964800	3.37291800	0.01608700
C	-1.26318500	4.41004200	-0.16423700
C	0.17702400	4.03440900	-0.08012600
H	1.14381900	5.98659300	-0.27277600

H	0.27014500	1.88033500	0.15901000
C	4.17392200	5.87929900	-0.15138400
C	5.50782500	6.26468900	-0.15057000
C	6.49392600	5.28512300	-0.02729800
C	6.16496900	3.93252600	0.09342800
C	4.82837600	3.56097100	0.09105700
C	3.80804500	4.52546400	-0.03063800
H	3.40445300	6.63883800	-0.24581400
H	6.95582800	3.19835400	0.18655200
H	4.54901800	2.51740400	0.18396900
O	-1.58749500	5.57111700	-0.36909600
H	-3.69703000	1.57144600	0.34725100
H	5.79766500	7.30405700	-0.24279400
N	7.89944100	5.68494500	-0.02486200
O	8.75330700	4.80138300	0.08691100
O	8.16054300	6.88686200	-0.13448800
H	-1.81925300	2.41416500	0.17696600
C	1.23964100	4.91901200	-0.14968900
C	2.39929500	4.12100900	-0.02823500
N	0.73509800	2.79201200	0.07285500
N	2.06775700	2.82192500	0.10605800
C	-4.19929700	-2.50657900	0.09807900
N	-3.49458100	-3.56812900	-0.10049600
N	-2.14964400	-3.37291800	0.01604600
C	-1.26317900	-4.41003700	-0.16429900
C	0.17702900	-4.03440300	-0.08018700
C	2.39929900	-4.12100400	-0.02826400
H	1.14382700	-5.98658400	-0.27285600
H	0.27014700	-1.88033200	0.15898200

C	1.23964800	-4.91900300	-0.14976000
N	0.73510100	-2.79200700	0.07281300
N	2.06776100	-2.82191500	0.10598700
C	4.17392600	-5.87929700	-0.15136300
C	3.80804800	-4.52546100	-0.03063100
C	4.82837800	-3.56096800	0.09107400
C	6.16497100	-3.93252500	0.09347400
C	6.49392900	-5.28512300	-0.02723700
C	5.50782800	-6.26468800	-0.15052100
H	3.40445800	-6.63883600	-0.24580200
H	4.54902000	-2.51739900	0.18397100
H	6.95582900	-3.19835300	0.18660700
H	5.79766900	-7.30405800	-0.24273200
O	-1.58748800	-5.57110600	-0.36918900
H	-1.81925000	-2.41416700	0.17694600
H	-3.69703100	-1.57145500	0.34724800
N	7.89944300	-5.68494600	-0.02477200
O	8.16054600	-6.88686400	-0.13439600
O	8.75330800	-4.80138500	0.08700600
Br	-1.26286200	-0.00000200	0.41611300

Table S6. Optimized Structure of host-Cl^- complex

C	6.47256400	-3.67016600	-0.01847400
C	5.75061800	-2.49287600	-0.04993500
C	6.45943800	-1.22951500	-0.02937900
C	7.90298900	-1.22838800	-0.01721800
C	8.59026300	-2.47972200	0.00574300
C	7.89048000	-3.66098900	0.01523600
C	5.79294100	0.00000300	-0.00761200
C	8.57913500	0.00000600	-0.00808800
C	7.90298600	1.22839800	-0.01719900
C	6.45943500	1.22952300	-0.02936000
C	5.75061200	2.49288200	-0.04989500
C	6.47255600	3.67017300	-0.01841800
C	7.89047200	3.66099900	0.01529000
C	8.59025800	2.47973300	0.00577900
H	4.71689000	0.00000100	0.05995000
H	5.93326000	-4.61215500	-0.03487800
H	9.67786200	-2.47813300	0.01786800
H	8.42329400	-4.60829400	0.03524800
H	9.66751100	0.00000700	0.01640500
H	5.93325000	4.61216100	-0.03480700
H	8.42328400	4.60830500	0.03531500
H	9.67785700	2.47814600	0.01790300
C	4.28903500	-2.48268500	-0.13178800
N	3.56336700	-3.52690700	0.07850300
N	2.22326200	-3.30033900	-0.03135000
C	1.31487200	-4.31979600	0.14817800
C	-0.11470600	-3.90884400	0.07659200
H	-1.13709100	-5.83741300	0.22447000

H	-0.14000300	-1.74843100	-0.10808900
C	-4.16187300	-5.63924000	0.10814400
C	-5.50620200	-5.98613300	0.09823600
C	-6.46378700	-4.97640900	-0.00536000
C	-6.09594500	-3.63157200	-0.09765600
C	-4.74923500	-3.29858600	-0.08651300
C	-3.75699100	-4.29420900	0.01590800
H	-3.41475900	-6.42247500	0.18736800
H	-6.86526100	-2.87318200	-0.17616300
H	-4.43968600	-2.26182600	-0.15747200
O	1.61623700	-5.48929000	0.33903000
H	3.80196800	-1.54180100	-0.38974300
H	-5.82592800	-7.01845300	0.16843200
N	-7.87992800	-5.33584100	-0.01759100
O	-8.70824400	-4.42622100	-0.11127200
O	-8.17537700	-6.53200400	0.06609200
H	1.91196900	-2.33269400	-0.17760900
C	-1.20162700	-4.76486500	0.12639200
C	-2.33732900	-3.93083200	0.02315400
N	-0.63540000	-2.64789100	-0.04828000
N	-1.96788800	-2.63880400	-0.08123600
C	4.28902900	2.48268800	-0.13174400
N	3.56336000	3.52690800	0.07855100
N	2.22325400	3.30033800	-0.03129300
C	1.31486300	4.31979200	0.14824500
C	-0.11471300	3.90884200	0.07663100
C	-2.33733600	3.93083000	0.02316200
H	-1.13710200	5.83741000	0.22449800
H	-0.14000700	1.74842900	-0.10806100

C	-1.20163500	4.76486300	0.12641700
N	-0.63540500	2.64788900	-0.04825500
N	-1.96789300	2.63880100	-0.08122700
C	-4.16188200	5.63923600	0.10813900
C	-3.75699800	4.29420600	0.01589900
C	-4.74924000	3.29858200	-0.08654300
C	-6.09595000	3.63156900	-0.09770100
C	-6.46379100	4.97640400	-0.00540100
C	-5.50621100	5.98612800	0.09821500
H	-3.41477000	6.42247100	0.18738000
H	-4.43969100	2.26182300	-0.15750500
H	-6.86526500	2.87317800	-0.17622500
H	-5.82593900	7.01844900	0.16841300
O	1.61622700	5.48928900	0.33907700
H	1.91196300	2.33269400	-0.17756200
H	3.80196300	1.54180200	-0.38969200
N	-7.87993400	5.33583500	-0.01764800
O	-8.17538400	6.53200300	0.06600500
O	-8.70824900	4.42621500	-0.11137000
Cl	1.30427200	-0.00000400	-0.27291800

Table S7. Optimized Structure of host-HSO_4^- complex

C	5.64045800	-4.40212700	-0.21281300
C	5.06780400	-3.14600500	-0.13416800
C	5.91822900	-1.97351700	-0.19115500
C	7.34773300	-2.16434100	-0.29834100
C	7.87658300	-3.48813400	-0.36495100
C	7.04114300	-4.57483200	-0.33257700
C	5.42072500	-0.66202200	-0.16935200
C	8.18146600	-1.04140200	-0.34138300
C	7.68092200	0.26508600	-0.30638300
C	6.25083100	0.46780100	-0.23602100
C	5.74508600	1.82666600	-0.22883900
C	6.63881500	2.88154900	-0.25634800
C	8.03795500	2.66885700	-0.30509700
C	8.54953300	1.39681900	-0.33812700
H	4.35290500	-0.51649100	-0.09668900
H	4.98710200	-5.26761000	-0.17394900
H	8.95397500	-3.61407800	-0.44512800
H	7.44806300	-5.58131000	-0.38699500
H	9.25796100	-1.18920400	-0.40823900
H	6.24123800	3.89130800	-0.24911600
H	8.70388700	3.52775200	-0.32826500
H	9.62274600	1.22738900	-0.38873700
C	3.61166800	-3.01664900	0.01267800
N	2.83930700	-4.01784500	-0.23468000
N	1.50625300	-3.81967400	-0.05252900
C	0.62924900	-4.85551800	-0.30414500
C	-0.81733600	-4.54704100	-0.12411500

H	-1.72629800	-6.47937000	-0.59778600
H	-0.96457100	-2.47350300	0.46022100
C	-4.75456500	-6.49581000	-0.41560600
C	-6.07452000	-6.92588100	-0.44274400
C	-7.08556200	-6.02391800	-0.10912500
C	-6.79530200	-4.70484800	0.24808100
C	-5.47228900	-4.28799600	0.27116000
C	-4.42736400	-5.17409800	-0.05908600
H	-3.96578300	-7.19460900	-0.67512600
H	-7.60505000	-4.03130200	0.50053800
H	-5.22345300	-3.26888800	0.54538200
O	0.97355600	-5.97609300	-0.65116900
H	3.20418500	-2.06449700	0.35865000
H	-6.33441100	-7.94111200	-0.71589200
N	-8.47677000	-6.47087100	-0.13368000
O	-9.35276100	-5.65571400	0.16729500
O	-8.70401300	-7.64148400	-0.45360500
H	1.17578400	-2.89376100	0.24263200
C	-1.85274800	-5.44868100	-0.30544200
C	-3.03295400	-4.72328000	-0.02847200
N	-1.40972200	-3.36718100	0.23865200
N	-2.73908700	-3.45058300	0.30331400
C	4.30096600	2.08274400	-0.20993700
N	3.84163900	3.27096200	-0.01392500
N	2.48409400	3.39304700	-0.01604000
C	1.91276500	4.64354100	0.09156000
C	0.42575600	4.65675100	0.17835500
C	-1.70812900	5.27730700	0.12016700
H	-0.04807000	6.68856200	-0.48519600

H	-0.17872800	2.72352200	0.96603700
C	-0.39282100	5.72981900	-0.12970000
N	-0.40826200	3.65127800	0.58764300
N	-1.69419300	4.00682700	0.56786500
C	-3.01663700	7.31847800	-0.49671200
C	-2.97990300	5.98761700	-0.03957600
C	-4.19835800	5.34702100	0.26333600
C	-5.40845900	6.00929700	0.11751400
C	-5.40951100	7.33030700	-0.33780900
C	-4.22096600	7.99271500	-0.64755500
H	-2.09060500	7.83117200	-0.73658500
H	-4.17294300	4.32127300	0.61386300
H	-6.34945700	5.52493900	0.34789000
H	-4.25730300	9.01659900	-0.99856500
O	2.54164500	5.69188400	0.10011900
H	1.91638600	2.55376000	-0.18095900
H	3.61966600	1.25026000	-0.37607500
N	-6.67975100	8.03498900	-0.49288400
O	-6.65041500	9.20157400	-0.89681600
O	-7.71738200	7.42900700	-0.21170600
O	2.31250200	0.01048300	1.75816100
O	0.36262100	-1.26890100	0.89364900
O	0.02755500	1.04291900	1.74084300
O	1.30884300	0.67262400	-0.36484100
S	0.86840000	0.13140400	0.93509600
H	2.09501900	-0.16794900	2.69132900

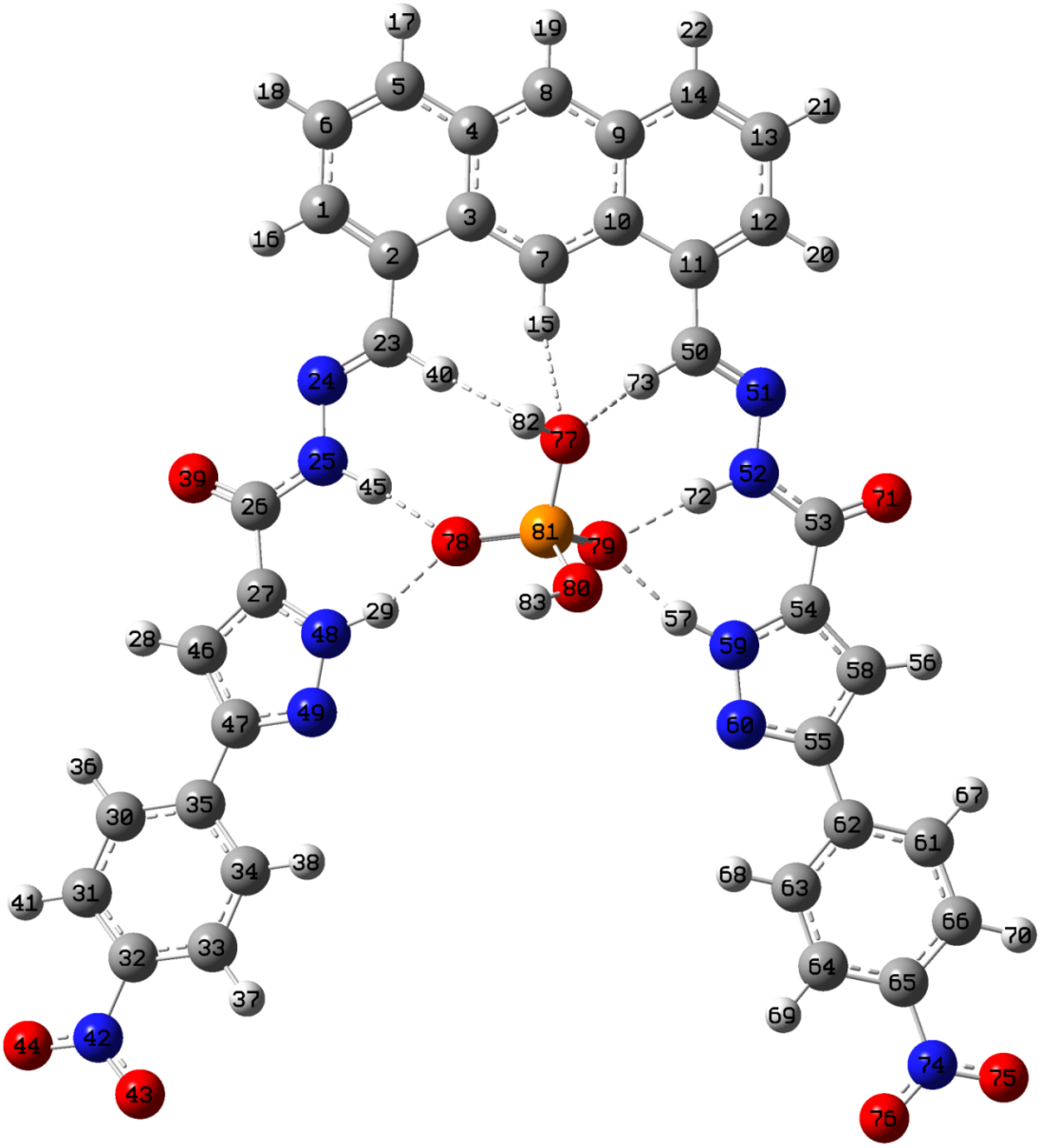


Figure S9. Optimized bindimg mode between receptor 1 and dihydrogen phosphate