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# Supplementary Information

For

## Anion Binding with Biphenyl-bis-Urea Derivatives: Solution and Solid-State Studies.

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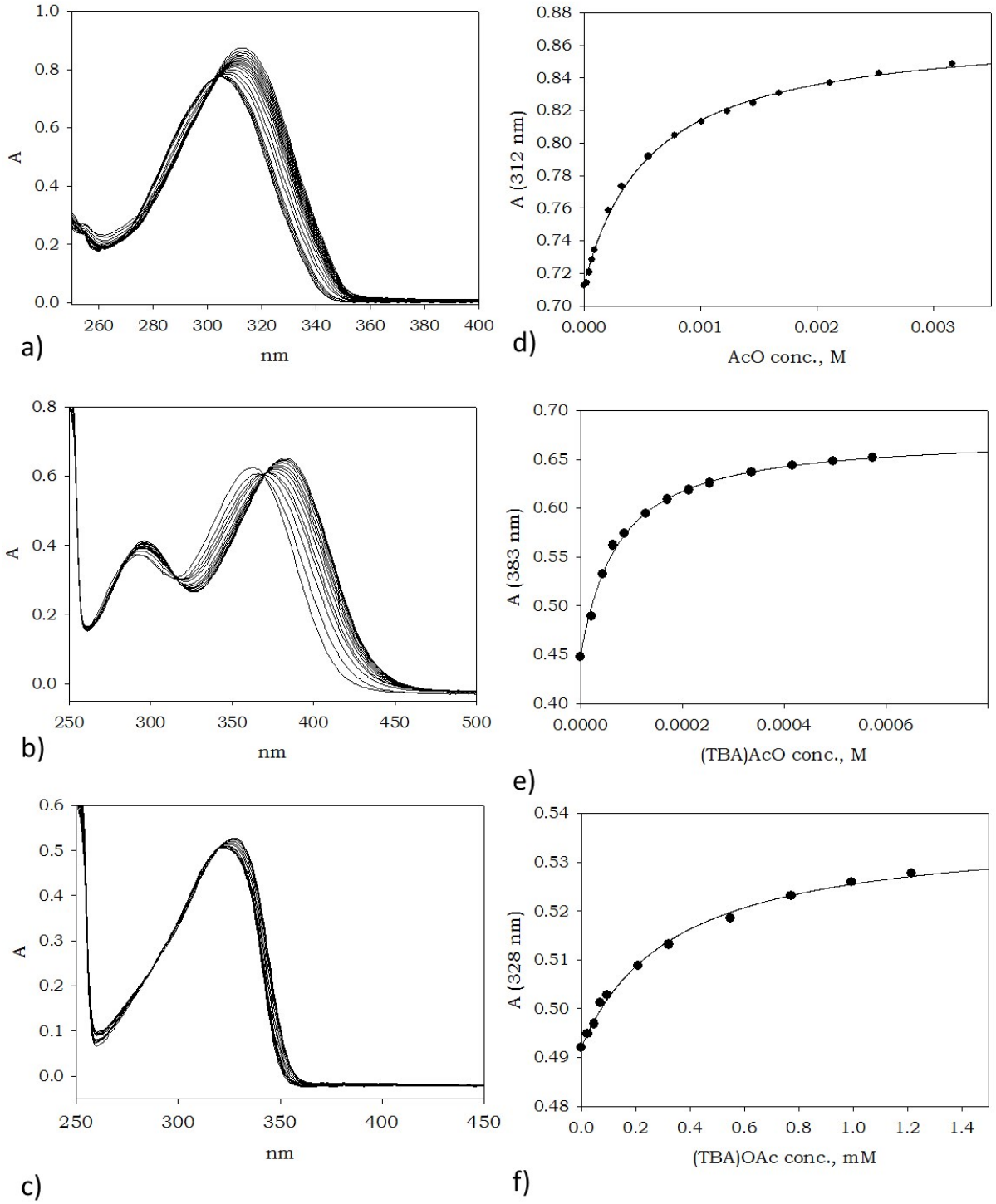



**Figure S1.** Family of spectra obtained by addition of increasing aliquots of (TBA)AcO to a 1.66 x $10^{-5}$ M solution of **1** (a), **2** (b) and **3** (c) in DMSO at 298 K. Relative Abs vs. concentration plots d-f) where lines represent best fit to a 1:1 binding isotherm.

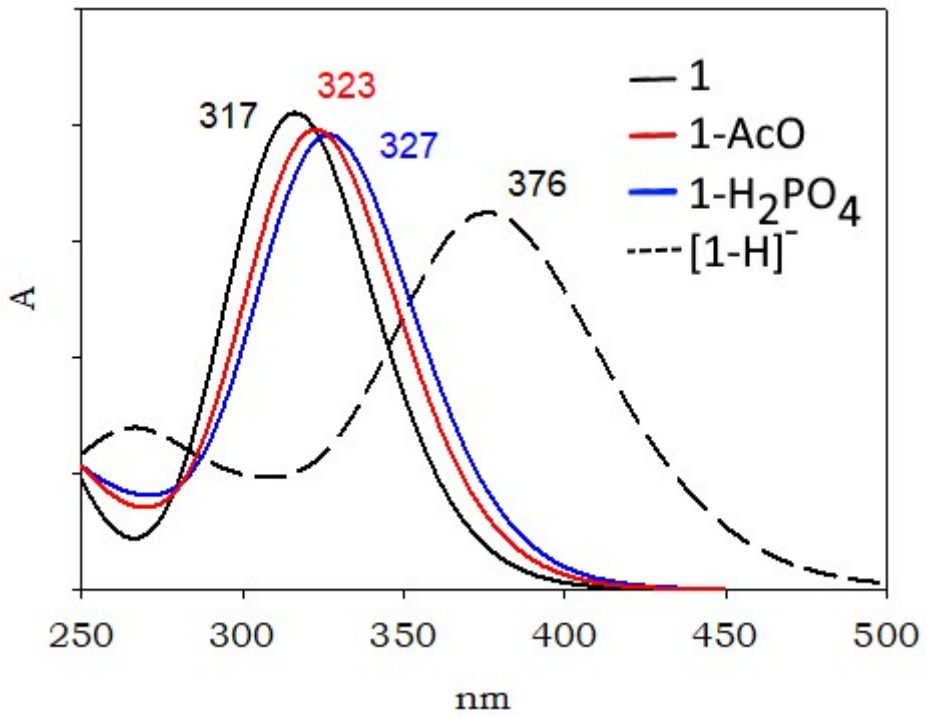



**Figure S2.** Theoretical UV spectra calculated at B3LYP/6-311+G(d,p) level of theory for receptor **1**, its deprotonated form [**1**-H]$^-$, and its acetate and phosphate complexes, **1**-AcO and **1**-$H_2PO_4$.

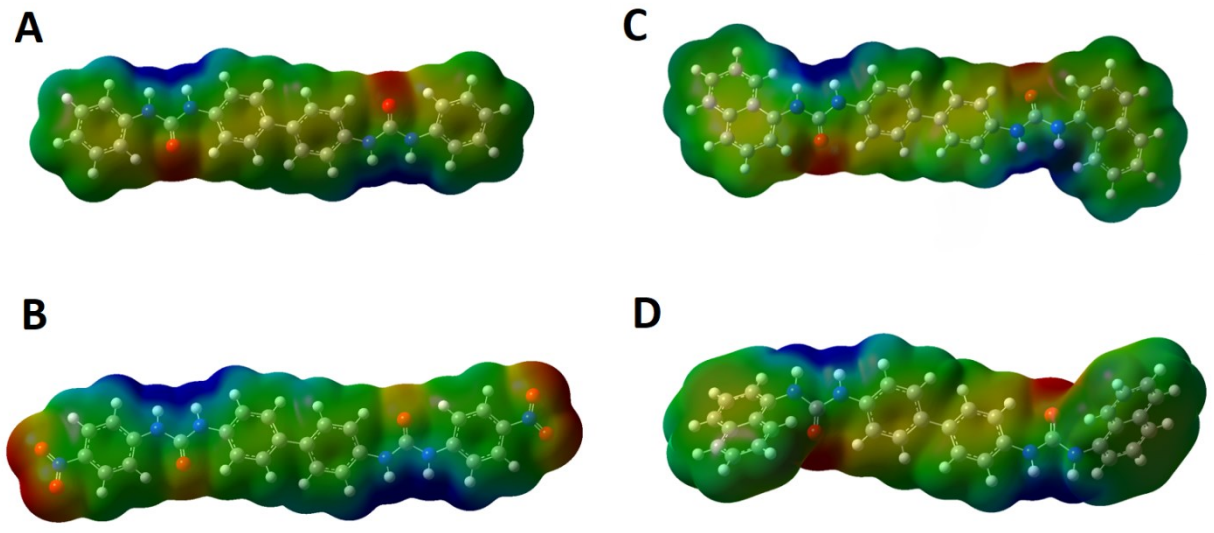



**Figure S3.** Electrostatic Potential Surface (EPS) calculated at B3LYP/6-311+G(d,p) level of theory for receptor **1** (A), **2** (B), **3** *conf. A* (C) and **3** *conf. B* (D).

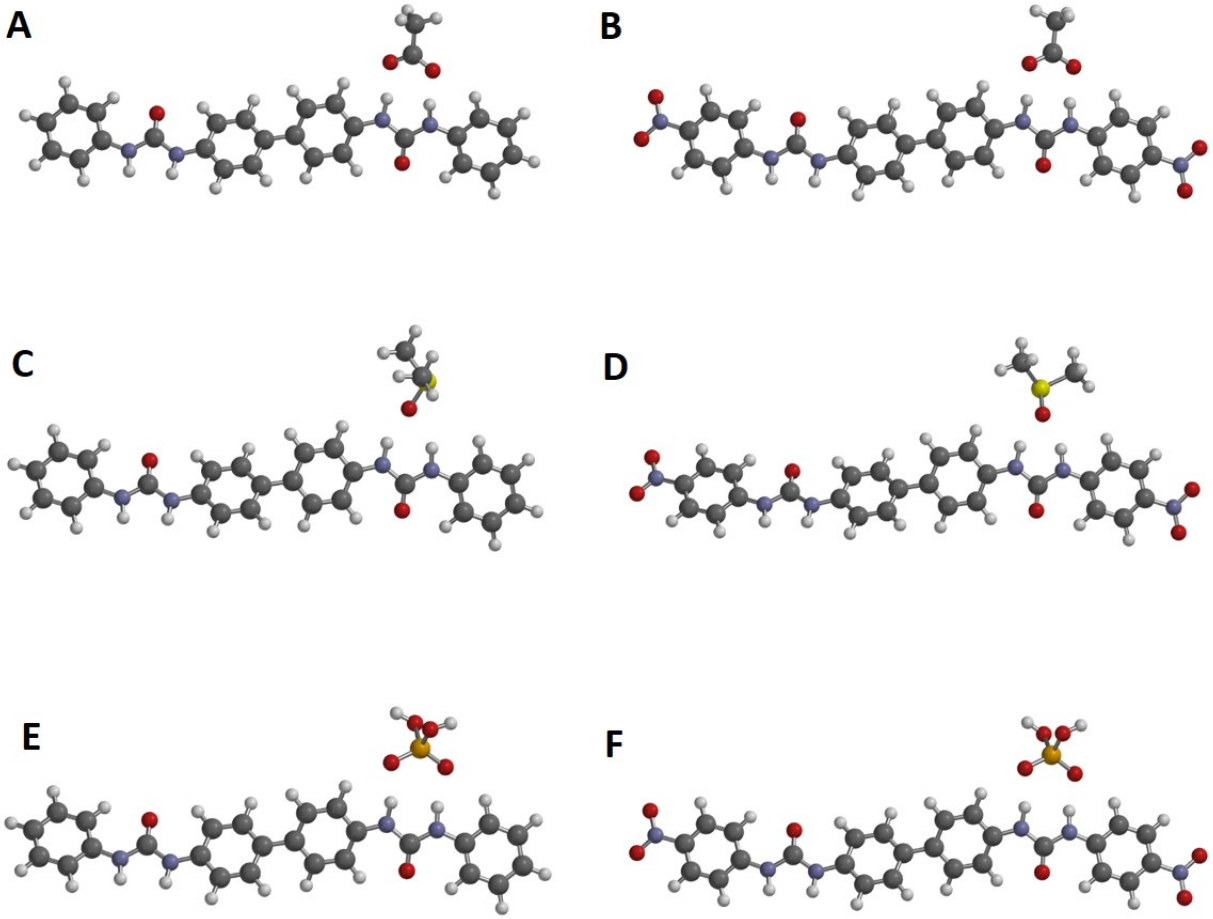



**Figure S4.** Representation of the optimized geometries calculated at B3LYP/6-311+G(d,p) (DMSO solution between acetate (A and B), dimethylsulfoxide (C and D) and phosphate (E and F), and receptors **1** (left) and **2** (right).

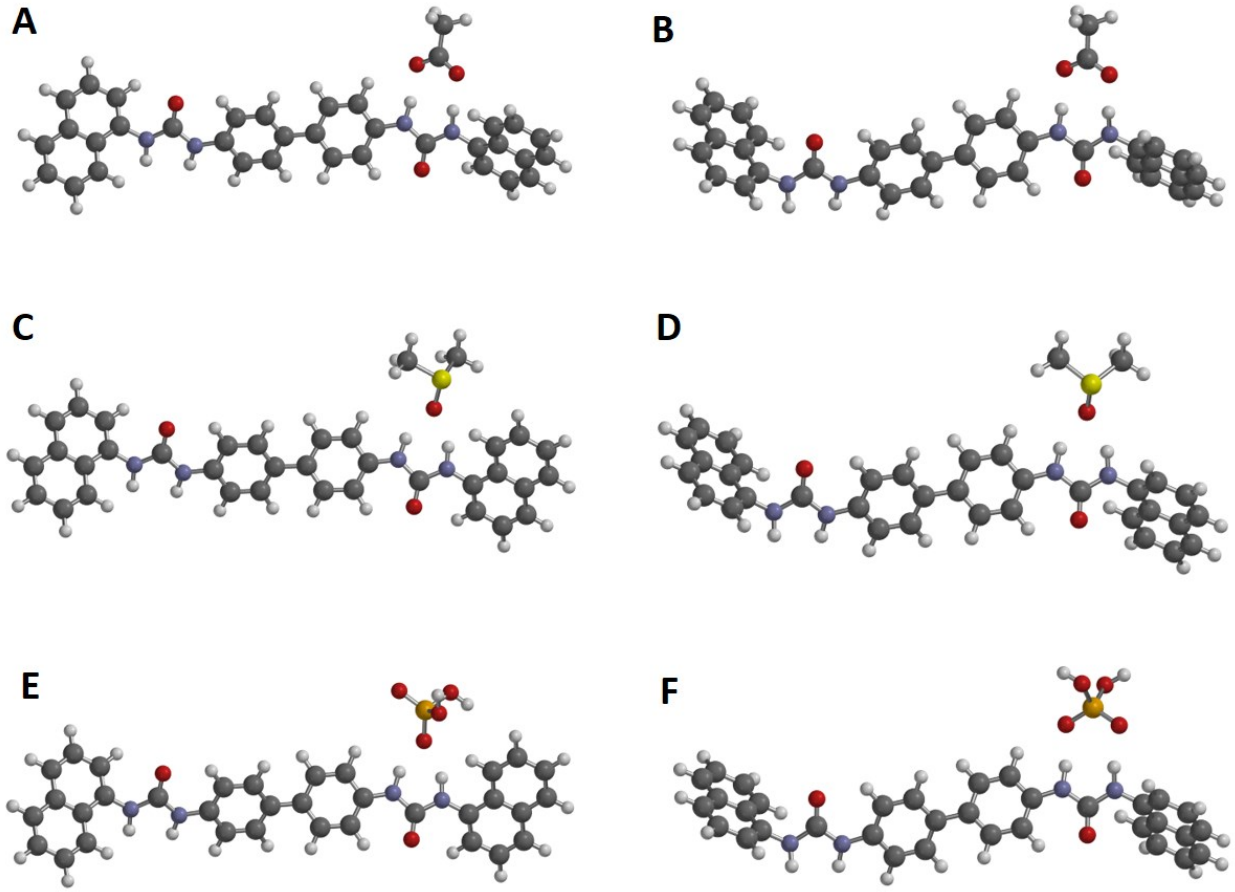
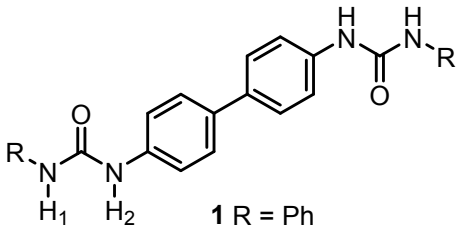



**Figure S5.** Optimized geometry in DMSO solution between involved guests: acetate (A and B), dimethylsulfoxide (C and D) and phosphate (E and F), and receptors **3a** (left) and **3b** (right).

**Table S1**. Calculated partial charges on ureic N-H bonds for **1-3**. Calculations were performed at B3LYP/6-311+G(d,p) level of theory.

| Receptor | N-$H_1$ Charge (atomic unit) | N-$H_2$ Charge (atomic unit) | Averaged (atomic unit) |
|---|---|---|---|
| **1** | 0.254 | 0.254 | 0.254 |
| **2** | 0.262 | 0.258 | 0.260 |
| **3A** | 0.250 | 0.253 | 0.252 |
| **3B** | 0.249 | 0.252 | 0.251 |

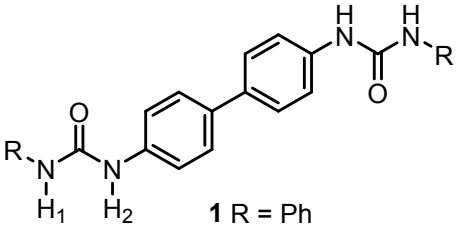



**1** R = Ph
**2** R = p$NO_2$-Ph
**3** R = Naph

**Table S2.** Calculated hydrogen bond distance (NH…O) for receptors **1-3** and acetate, dimethylsolfoxide and phosphate. Calculations were performed at B3LYP/6-311+G(d,p) level of theory.

| | HB lenght (Å) | | | | | |
|---|---|---|---|---|---|---|
| **Receptor** | **Acetate** | | **Phosphate** | | **DMSO** | |
| | **$H_1$…O** | **$H_2$…O** | **$H_1$…O** | **$H_2$…O** | **$H_1$…O** | **$H_2$…O** |
| **1** | 1.814 | 1.817 | 1.893 | 1.892 | 1.889* | 1.930* |
| **2** | 1.754 | 1.796 | 1.836 | 1.874 | 1.850* | 1.934* |
| **3a** | 1.807 | 1.812 | 1.908* | 1.843* | 1.907* | 1.925* |
| **3b** | 1.797 | 1.813 | 1.870 | 1.880 | 1.940* | 1.934* |

* two bifurcate hydrogen bonds are observed.




**1** R = Ph
**2** R = p$NO_2$-Ph
**3** R = Naph

**Single crystal X-ray diffraction**

Suitable single crystals for X-ray analysis of receptors **1** and **2**, as well as complexes [**1**-((TBA)$H_2PO_4$)$_2$], [**1**-((TBA)$NO_3$)$_2$], [**1**-((TBA)Br)$_2$], [**1**-((TBA)I)$_2$-DMSO], [**2**-((TBA)Br)$_2$], [**2**-((TBA)AcO)$_2$] and [**3**-((TBA)AcO)$_2$] were obtained by slow evaporation from dimethyl sulfoxide solutions. Suitable single crystals for X-ray analysis of [**1**-((TBA)AcO)$_2$-$H_2O$], [(**2**)$_2$-(TBA)$_2$$HPO_4$)] and [**3**-((TBA)Br)$_2$] were obtained by slow evaporation from *N*,*N*-dimethylformamide solutions. Crystallisations were performed by dissolving the receptor (0.1 mmol) in solvent (2 mL) followed by addition of the anion salt (0.4 mmol) and allowing the solution to slowly evaporate.

Data for receptors and complexes [**1**-((TBA)$H_2PO_4$)$_2$], [**1**-((TBA)I)$_2$-DMSO] and [**2**-((TBA)AcO)$_2$] were collected at 295 K on Oxford Diffraction Xcalibur Nova R diffractometer with Ruby detector using mirror-monochromatized $CuK_\alpha$ radiation ($\lambda$ = 1.54184 Å). Data for [**1**-((TBA)AcO)$_2$-$H_2O$], [**1**-((TBA)$NO_3$)$_2$], [**2**-((TBA)Br)$_2$], [**2$_2$**-(TBA)$_2$$HPO_4$)], [**3**-((TBA)Br)$_2$] and [**3**-((TBA)AcO)$_2$] were collected at 295 K on Oxford Diffraction Xcalibur2 diffractometer with a Sapphire 3 CCD detector using graphite-monochromatized $MoK_\alpha$ radiation ($\lambda$ = 0.71073 Å). The *CrysAlisPro*[1] program was used for the data collection and processing. The intensities for [**1**-((TBA)$NO_3$)$_2$] and [**3**-((TBA)Br)$_2$] were corrected for absorption using analytical and numerical absorption correction methods, respectively.[1] The intensities for all other structures were corrected for absorption using the multi-scan absorption correction method.[1] Data for [**1**-((TBA)Br)$_2$] were collected at 170 K on a Bruker-Nonius Kappa Apex II diffractometer using graphite-monochromated $MoK_\alpha$ radiation ($\lambda$ = 0.71073 Å). COLLECT[2] software was used for the data collection and DENZO-SMN[3] for the data processing. The intensities were corrected for absorption using the multi-scan absorption correction method.[4] The structures were solved using direct methods with *SIR–2004*[5] and *SIR–2014*[6], or by dual-space algorithm using SHELXT[7], and refined by full-matrix least-squares calculations based on $F^2$ using *SHELXL*[8] program integrated in the *Olex*2[9] or *WinGX*[10] program package. Hydrogen atoms of water molecule in [**1**-((TBA)Br)$_2$] were found in the Fourier map. All other hydrogen atoms in this complex and all hydrogen atoms in receptors and other complexes were included in calculated positions, with *SHELXL*[8] defaults. Details of crystal data, data collection and refinement parameters of all structures are given in Tables S3 and Table S4.

Four carbon atoms of biphenyl moiety in receptor **1** were disordered over two sites and have been refined with fixed occupancy ratio of 51/49 %. Geometric restraint was used in the refinement of some C–C phenyl ring distances. Two butyl group carbon atoms of tetrabutylammonium cation A in [**1**-((TBA)Br)$_2$] were disordered over two sites and were refined with fixed occupancy ratio of 51/49 %. All atoms of four butyl groups of tetrabutylammonium cation B in the same structure were severely disordered over two sites and were refined with fixed occupancy ratio of 52/48 %, 55/45 % and 63/37 %. Geometric restraints and restraint on anisotropic displacement parameters were applied in their refinement, as well as in the refinement of water molecule. In addition, restraint on anisotropic displacement parameters was also applied in the refinement of some carbon atoms in bis-urea molecule. All atoms of dihydrogenphosphate anion in [**1**-((TBA)$H_2PO_4$)$_2$], as well as the O1, O3 and O4 atoms of hydrogenphosphate anion in [(**2**)$_2$-(TBA)$_2$$HPO_4$)] were disordered over two sites and were refined with fixed occupancy ratio of 55/45 % and 51/49 %, respectively. Geometric restraint on C–C distances in tetrabutylammonium cations and P–O distances in dihydrogenphosphate and hydrogenphosphate anions were applied in the refinement of these two structures. Restraint on anisotropic displacement parameters of some carbon atoms in tetrabutylammonium cation in [**1**-((TBA)$H_2PO_4$)$_2$] and [(**2**)$_2$-(TBA)$_2$$HPO_4$)], some oxygen atoms of dihydrogenphosphate and hydrogenphosphate anions, and one nitro group oxygen atom in [(**2**)$_2$-(TBA)$_2$$HPO_4$)] was also applied in the refinement. Checkcif A level Alert for [(**2**)$_2$-(TBA)$_2$$HPO_4$)] indicated that there are 75 missing reflections in [(**2**)$_2$-(TBA)$_2$$HPO_4$)] below $\theta_{min}$ (4.211$^o$). Due to very weakly diffracting crystal detector distance was set to lower limit. Reflections were not omitted from the final least-squares refinement. Two terminal carbon atoms of tetrabutyl groups in [**3**-((TBA)AcO)$_2$] were disordered over two sites and were refined with fixed occupancy ratio of 65/35 and 52/48 %. Geometric restraint on C–C distances in tetrabutylammonium cation, as well as restraint on anisotropic displacement parameters on some carbon atoms in tetrabutylammonium cation and two atoms in naphthalene ring was applied in the refinement. Restraint on anisotropic displacement parameters was also applied in the refinement of one carbon atom in tetrabutylammonium cation and one oxygen atom in acetate anion of [**1**-((TBA)AcO)$_2$-$H_2O$].Geometric restraint on C–C distances in tetrabutylammonium cation was applied also in the refinement of [**1**-((TBA)I)$_2$-DMSO], [**1**-((TBA)$NO_3$)$_2$], [**2**-((TBA)Br)$_2$], [**2**-((TBA)AcO)$_2$] and [**3**-((TBA)Br)$_2$]. The structures of receptor **2**, as well as complexes [**1**-((TBA)$H_2PO_4$)$_2$] and [**2**-((TBA)AcO)$_2$] contains solvent-accessible voids with a small amount of solvent molecule(s) used

for recrystallization. As they could not be modelled satisfactorily, data were treated with the SQUEEZE routine in PLATON[11], or with the *Solvent Mask* routine in *Olex*2[9]. PLATON[11] and Mercury[12] programs were used for structure analysis and drawing preparation. CCDC 2015334-2015345 contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/structures.

**Table S3.** X-ray crystallographic data for receptor **1** and its complexes described in this paper.

| | **1** | [**1**-((TBA)Br)$_2$] | [**1**-((TBA)I)$_2$] -DMSO | [**1**-((TBA)NO$_3$)$_2$] | [**1**-((TBA)AcO)$_2$] -H$_2$O | [**1**-((TBA)H$_2$PO$_4$)$_2$] |
|---|---|---|---|---|---|---|
| Formula | $C_{26}H_{22}N_4O_2$ | $C_{58}H_{96}Br_2N_6O_3$ | $C_{60}H_{100}I_2N_6O_3$ | $C_{58}H_{94}N_8O_8$ | $C_{62}H_{102}N_6O_7$ | $C_{58}H_{99}N_6O_{10.50}P_2$ |
| Formula weight | 422.47 | 1085.22 | 1239.31 | 1031.41 | 1043.49 | 1110.37 |
| Crystal system | monoclinic | monoclinic | triclinic | monoclinic | monoclinic | monoclinic |
| Space group | *C* 2/c | *P* 2$_1$/c | *P* 1 | *P* 2$_1$/c | *P* 2$_1$ | *I* 2/a |
| Unit cell dimensions | | | | | | |
| $a$ / Å | 13.1438(2) | 16.5304(6) | 9.8525(2) | 15.0086(13) | 10.0943(7) | 18.2621(5) |
| $b$ / Å | 4.63066(7) | 18.1277(4) | 9.8769(2) | 9.8413(5) | 16.7406(10) | 14.8485(4) |
| $c$ / Å | 35.1361(7) | 19.8203(8) | 17.3039(4) | 20.6682(16) | 18.7190(12) | 24.8790(9) |
| $\alpha$ / ° | 90 | 90 | 85.666(2) | 90 | 90 | 90 |
| $\beta$ / ° | 99.9688(17) | 92.4926(14) | 86.551(2) | 99.841(8) | 91.772(6) | 90.576(3) |
| $\gamma$ / ° | 90 | 90 | 76.335(2) | 90 | 90 | 90 |
| $V$ / Å$^3$ | 2106.25(6) | 5933.7(3) | 1629.98(6) | 3007.9(4) | 3161.7(4) | 6746.0(4) |
| $Z$ | 4 | 4 | 1 | 2 | 2 | 4 |
| $D_{calc.}$ / g cm$^{-3}$ | 1.332 | 1.215 | 1.263 | 1.139 | 1.096 | 1.093 |
| Absorption coef. $\mu$ / mm$^{-1}$ | 0.694 | 1.412 | 8.207 | 0.076 | 0.071 | 1.024 |
| $\theta$ range / ° | 5.112 - 67.973 | 1.668 - 24.999 | 4.617 - 67.989 | 4.216 - 25.998 | 4.329 - 25.997 | 3.466 - 67.996 |
| Collected reflections No. | 8324 | 28501 | 15717 | 15814 | 13957 | 23142 |
| Independent refl. No. / $R_{Int.}$ | 1927/0.0245 | 10211/0.0668 | 7966/0.0263 | 5886/0.0270 | 10473/0.0272 | 6002/0.0286 |
| Reflections No. $I \geq 2\sigma(I)$ | 1742 | 4085 | 7908 | 3210 | 6486 | 4908 |
| Data[a]/Restraints/Parameters | 1927/2/181 | 10211/255/803 | 7966/8/660 | 5886/7/338 | 10473/13/689 | 6002/42/407 |
| Flack parameter, $x$ | --- | --- | 0.274(4) | --- | -0.3(8) | --- |
| Goodness-of-fit on $F^2$, $S$ | 1.044 | 1.019 | 1.064 | 1.027 | 1.017 | 1.590 |
| $R$ [$I \geq 2\sigma(I)$] / $R$ [all data] | 0.0445/0.0491 | 0.0892/0.2217 | 0.0254/0.0256 | 0.0777/0.1354 | 0.0652/0.1075 | 0.1039/0.1115 |
| $wR$ [$I \geq 2\sigma(I)$] / $wR$ [all data] | 0.1253/0.1318 | 0.2057/0.2792 | 0.0680/0.0691 | 0.2218/0.2708 | 0.1625/0.1991 | 0.3457/0.3711 |
| Max./min. el. density / e Å$^{-3}$ | 0.132/-0.179 | 0.728/-0.814 | 0.390/-0.467 | 0.616/-0.328 | 0.384/-0.232 | 0.829/-0.363 |

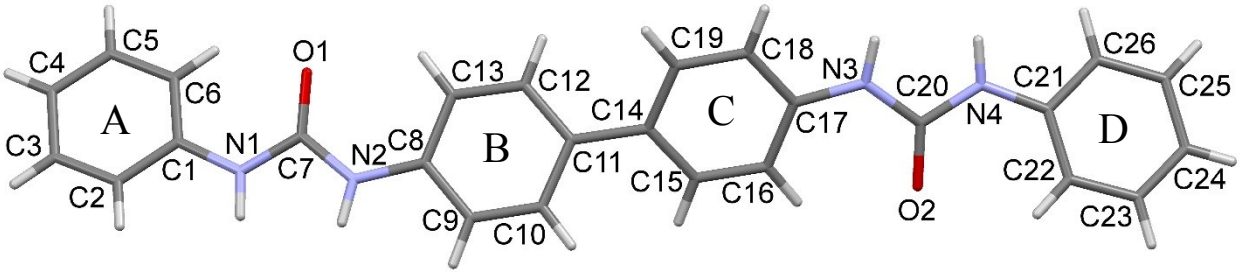
[a] Equal to independent reflections.

**Table S4.** X-ray crystallographic data for **2** and complexes of **2** and **3** described in this paper.

| | **2** | [**2**-((TBA)Br)$_2$] | [**2**-((TBA)AcO)$_2$] | [(**2**)$_2$-(TBA)$_2$HPO$_4$)] | [**3**-((TBA)Br)$_2$] | [**3**-((TBA)AcO)$_2$] |
|---|---|---|---|---|---|---|
| Formula | $C_{26}H_{20}N_6O_6$ | $C_{58}H_{92}Br_2N_8O_6$ | $C_{62}H_{98}N_8O_{10}$ | $C_{84}H_{113}N_{14}O_{16}P$ | $C_{66}H_{98}Br_2N_6O_2$ | $C_{70}H_{104}N_6O_6$ |
| Formula weight | 512.48 | 1157.21 | 1115.48 | 1605.85 | 1167.32 | 1125.59 |
| Crystal system | monoclinic | triclinic | monoclinic | triclinic | monoclinic | monoclinic |
| Space group | *C* 2/c | *P* -1 | *C* 2/c | *P* -1 | *P* 2/c | *P* $2_1$/c |
| Unit cell dimensions | | | | | | |
| *a* / Å | 25.2125(6) | 7.9775(4) | 12.1290(3) | 13.8036(8) | 21.451(2) | 10.0860(14) |
| *b* / Å | 8.18205(12) | 10.0854(5) | 14.2416(3) | 18.2461(10) | 8.7308(7) | 17.874(3) |
| *c* / Å | 47.2764(7) | 20.0463(10) | 38.0026(10) | 18.3745(9) | 17.3855(11) | 19.228(4) |
| $\alpha$ / ° | 90 | 101.107(4) | 90 | 81.787(4) | 90 | 90 |
| $\beta$ / ° | 91.9897(17) | 96.410(4) | 90.258(2) | 83.628(4) | 92.489(7) | 99.871(15) |
| $\gamma$ / ° | 90 | 93.701(4) | 90 | 70.879(5) | 90 | 90 |
| *V* / Å$^3$ | 9746.8(3) | 1566.61(14) | 6564.4(3) | 4317.5(4) | 3252.9(5) | 3415.0(10) |
| *Z* | 12 | 1 | 4 | 2 | 2 | 2 |
| $D_{calc.}$ / g cm$^{-3}$ | 1.048 | 1.227 | 1.129 | 1.235 | 1.192 | 1.095 |
| Absorption coef. $\mu$ / mm$^{-1}$ | 0.642 | 1.345 | 0.613 | 0.104 | 1.291 | 0.069 |
| $\theta$ range / ° | 3.508 - [illegible] | 4.272 - 25.997 | 4.789 - 67.992 | 4.211 - 25.999 | 4.303 - 25.999 | 4.362 - 25.999 |
| Collected reflections No. | 17506 | 14947 | 15369 | 39563 | 13652 | 19409 |
| Independent refl. No. / $R_{Int.}$ | 8582/0.0166 | 6138/0.0291 | 5956/0.0184 | 16919/0.0394 | 6364/0.0265 | 6697/0.0405 |
| Reflections No. $I \geq 2\sigma(I)$ | 7302 | 4615 | 3994 | 8741 | 4311 | 3064 |
| Data[a]/Restraints/Parameters | 8582/0/514 | 6138/2/338 | 5956/3/366 | 16919/71/1071 | 6364/5/347 | 6697/38/395 |
| Flack parameter, *x* | --- | --- | --- | --- | --- | --- |
| Goodness-of-fit on $F^2$, *S* | 1.064 | 1.014 | 1.309 | 1.023 | 1.015 | 1.012 |
| *R* [$I \geq 2\sigma(I)$] / *R* [all data] | 0.0839/0.09 | 0.0427/0.0678 | 0.0893/0.1057 | 0.0915/0.1649 | 0.0491/0.0810 | 0.0814/0.1640 |
| *wR* [$I \geq 2\sigma(I)$] / *wR* [all data] | 0.2263/0.23 | 0.0956/0.1073 | 0.3183/0.3548 | 0.2562/0.3163 | 0.1254/0.1471 | 0.2284/0.2996 |
| Max./min. el. density / e Å$^{-3}$ | 0.356/- | 0.397-0.358 | 0.492/-0.235 | 1.052/-1.122 | 0.602/-0.274 | 0.301/-0.316 |

[a] Equal to independent reflections.

**Table S5.** Dihedral and torsion angles (°) in bis-urea receptors **1**-**3**.




**Scheme S1.** Numbering scheme of rings and $\tau$ torsion angle in receptors **1** and **2**

| | **Ur1** [a] **/ ring A**<br>**Ur2** [b] **/ ring D** | **Ur1** [a] **/ ring B**<br>**Ur2** [b] **/ ring C** | $\tau$ [c] |
|---|---|---|---|
| **1** [d] | 56.14(8)<br>--- | 66.95(12)<br>--- | 6.4(3)<br>--- |
| [**1**-((TBA)Br)$_2$] | 6.2(6)<br>7.0(5) | 12.9(5)<br>28.6(4) | 17.6(12)<br>17.7(12) |
| [**1**-((TBA)I)$_2$]-DMSO | 5.9(3)<br>3.7(3) | 15.8(2)<br>17.0(2) | 11.1(6)<br>10.3(6) |
| [**1**-((TBA)NO$_3$)$_2$] | 15.55(19)<br>--- | 15.67(18)<br>--- | –1.2(5)<br>--- |
| [**1**-((TBA)AcO)$_2$]-H$_2$O | 21.0(3)<br>20.7(3) | 10.4(3)<br>12.1(2) | 28.2(7)<br>28.6(7) |
| [**1**-((TBA)H$_2$PO$_4$)$_2$] | 5.96(15)<br>--- | 37.64(15)<br>--- | 0.1(4)<br>--- |
| **2** | 4.9(2)<br>4.47(18)<br>2.09(19)<br>--- | 13.42(19)<br>19.00(19)<br>25.97(18)<br>--- | 16.9(5)<br>15.4(5)<br>0.5(5)<br>--- |
| [**2**-((TBA)Br)$_2$] | 2.94(15)<br>--- | 25.57(15)<br>--- | 0.5(4)<br>--- |
| [**2**-((TBA)AcO)$_2$] | 13.3(2)<br>--- | 27.40(17)<br>--- | 36.4(4)<br>--- |
| [(**2**)$_2$-(TBA)$_2$HPO$_4$)] | 30.1(2)<br>20.9(3)<br>2.1(2)<br>8.5(2) | 3.6(2)<br>6.4(2)<br>8.8(2)<br>8.4(2) | –29.1(7)<br>–31.5(7)<br>–25.7(6)<br>–25.8(6) |
| [**3**-((TBA)Br)$_2$] [e] | 21.9(2)<br>--- | 18.88(16)<br>--- | –36.6(4)<br>--- |
| [**3**-((TBA)AcO)$_2$] [e] | 24.24(19)<br>--- | 13.35(17)<br>--- | –1.1(4)<br>--- |

[a] the N1/C7/N2/O1 atoms; [b] the N3/C20/N4/O2 atoms;
[c] the C10–C11–C14– C15 and C12–C11–C14–C19 torsion angles
[d] data for only major component of disordered C8–C13 phenyl ring are given
[e] the numbering of atoms in A and B rings in **3** is C1–C5/C10 and C12–C17, respectively.

**Table S6.** Hydrogen-bonding receptor–anion geometries for co-crystal salts and co-crystal salt solvates of **1**.

| | **D–H···A** | **H···A / Å** | **D···A / Å** | **D–H···A / °** | **rs vdW or rs vdW/i [a]/ %** |
|---|---|---|---|---|---|
| [**1**-((TBA)Br)$_2$] | N1–H1···Br2 | 2.62 | 3.463(8) | 160 | 17.1 |
| | N2–H2···Br2 | 2.49 | 3.356(7) | 167 | 21.2 |
| | N3–H3···Br1 | 2.45 | 3.315(7) | 166 | 22.5 |
| | N4–H4···Br1 | 2.65 | 3.479(7) | 157 | 16.1 |
| [**1**-((TBA)I)$_2$]-DMSO | N1–H1···I1 | 2.73 | 3.576(4) | 169 | 19.7 |
| | N2–H2···I1 | 2.80 | 3.637(4) | 165 | 17.6 |
| | N3–H3···I2 | 2.84 | 3.658(4) | 159 | 16.5 |
| | N4–H4···I2 | 2.70 | 3.552(4) | 170 | 20.6 |
| [**1**-((TBA)NO$_3$)$_2$] | N1–H1···O2 | 2.32 | 3.022(4) | 139 | 14.7 |
| | N1–H1···O4 | 2.63 | 3.382(4) | 147 | 3.3 |
| | N2–H2···O4 | 2.06 | 2.905(3) | 169 | 24.3 |
| | C2–H2A···O2 | 2.65 | 3.394(5) | 138 | 2.6 |
| [**1**-((TBA)AcO)$_2$]-H$_2$O | N1–H1N···O1A | 2.01 | 2.858(6) | 168 | 26.1 |
| | N1–H1N···O2A | 2.70 | 3.397(7) | 139 | 0.7 |
| | N2–H2N···O2A | 2.00 | 2.792(7) | 153 | 26.5 |
| | N3–H3N···O2B | 1.95 | 2.791(5) | 164 | 28.3 |
| | N4–H4N···O1B | 1.98 | 2.819(5) | 165 | 27.2 |
| | C2–H2···O1A | 2.67 | 3.367(8) | 133 | 1.8 |
| | C9–H9···O2A | 2.67 | 3.386(8) | 134 | 1.8 |
| | C18–H18···O2B | 2.64 | 3.344(5) | 133 | 2.9 |
| | C26–H26···O1B | 2.53 | 3.256(7) | 135 | 7.0 |
| [**1**-((TBA)H$_2$PO$_4$)$_2$] [b] | N1–H1···O5 | 2.18 | 2.960(6) | 151 | 19.9 |
| | N2–H2···O4 | 1.92 | 2.775(7) | 175 | 31.9 |
| | C2–H2A···O5 | 2.55 | 3.281(6) | 136 | 6.3 |

[a] reduction of the sum of the van der Waals radii of H and O atoms (rs vdW) or reduction of the sum of the van der Waals radii of H atom and ionic radii of $I^-$ or $Br^-$ ions (rs vdW/i)

[b] data for only major component of disordered dihydrogen phosphate anion atoms are given

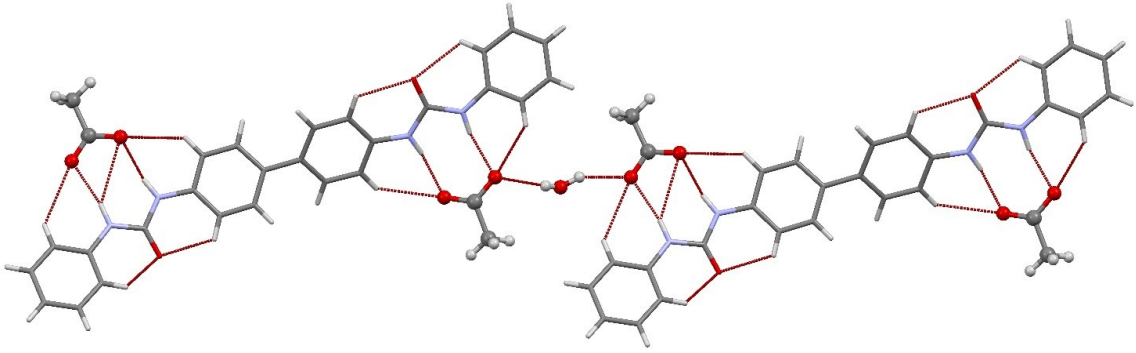
**Table S7.** Hydrogen-bonding receptor–anion geometries for co-crystal salts of **2** and **3**.

| | **D–H···A** | **H···A / Å** | **D···A / Å** | **D–H···A / °** | **rs vdW or rs vdW/i [a]/ %** |
|---|---|---|---|---|---|
| [**2**-((TBA)Br)$_2$] | N1–H1···Br1 | 2.42 | 3.273(2) | 169 | 23.4 |
| | N2–H2···Br1 | 2.64 | 3.436(2) | 155 | 16.5 |
| [**2**-((TBA)AcO)$_2$] | N1–H1···O4 | 1.87 | 2.705(6) | 164 | 31.3 |
| | N1–H1···O5 | 2.70 | 3.419(4) | 142 | 0.7 |
| | N2–H2···O5 | 1.96 | 2.815(4) | 174 | 27.9 |
| | C6–H6···O4 | 2.43 | 3.127(6) | 132 | 10.7 |
| [(**2**)$_2$-(TBA)$_2$HPO$_4$)] | N1A–H1A···O2 [c] | 1.92 | 2.711(4) | 152 | 29.4 |
| | N2A–H2A···O2 [c] | 2.16 | 2.946(5) | 152 | 21.0 |
| | N3A–H3A···O3 | 2.30 | 3.151(11) | 171 | 15.4 |
| | N4A–H4A···O4 | 2.15 | 2.972(8) | 159 | 21.0 |
| | N1B–H1B···O3 [c] | 2.65 | 3.415(10) | 149 | 2.6 |
| | N1B–H1B···O4 [c] | 2.54 | 3.292(8) | 147 | 6.6 |
| | N2B–H2B···O4 [c] | 2.00 | 2.858(8) | 176 | 26.5 |
| | N3B–H3B···O1 | 2.52 | 3.283(7) | 148 | 7.4 |
| | N3B–H3B···O3 | 2.29 | 3.062(11) | 150 | 15.8 |
| | N4B–H4B···O1 | 1.92 | 2.777(5) | 178 | 29.4 |
| | C26–H26A···O4 | 2.25 | 3.073(9) | 147 | 17.3 |
| | C18B–H18B···O3 | 2.36 | 3.137(10) | 140 | 13.2 |
| [**3**-((TBA)Br)$_2$] | N1–H1···Br1 | 2.62 | 3.437(3) | 158 | 17.1 |
| | N2–H2···Br1 | 2.44 | 3.279(2) | 166 | 22.8 |
| | C9–H9···Br1 | 2.96 | 3.849(3) | 159 | 6.3 |
| [**3**-((TBA)AcO)$_2$] | N1–H1···O2 | 2.05 | 2.874(5) | 160 | 24.6 |
| | N2–H2···O2 | 2.16 | 2.923(5) | 149 | 20.6 |
| | N2–H2···O3 | 2.67 | 3.445(6) | 151 | 1.8 |
| | C9–H9···O2 | 2.44 | 3.325(6) | 160 | 10.3 |

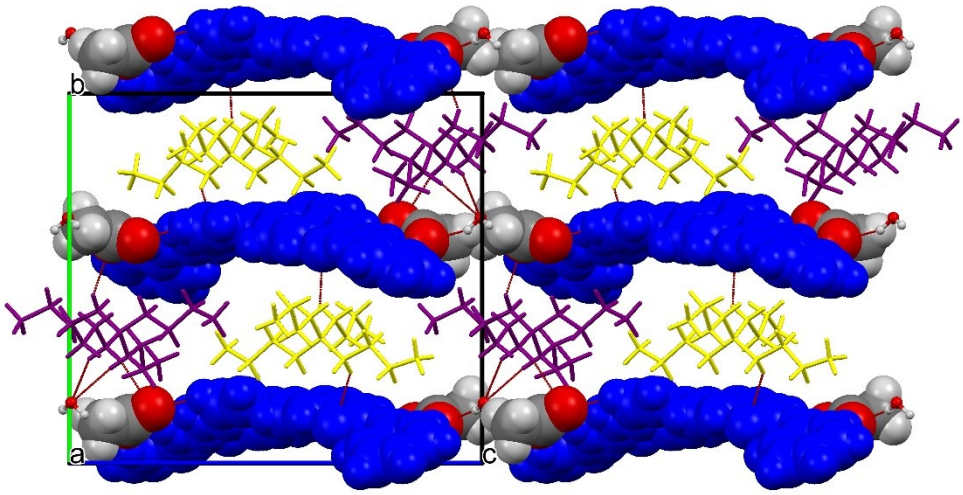
[a] reduction of the sum of the van der Waals radii of H and O atoms (rs vdW) or reduction of the sum of the van der Waals radii of H atom and ionic radii of $I^-$ or $Br^-$ ions (rs vdW/i)

[b] data for only major component of disordered hydrogen phosphate anion atoms are given

[c] symmetry code: –1+x, y, z

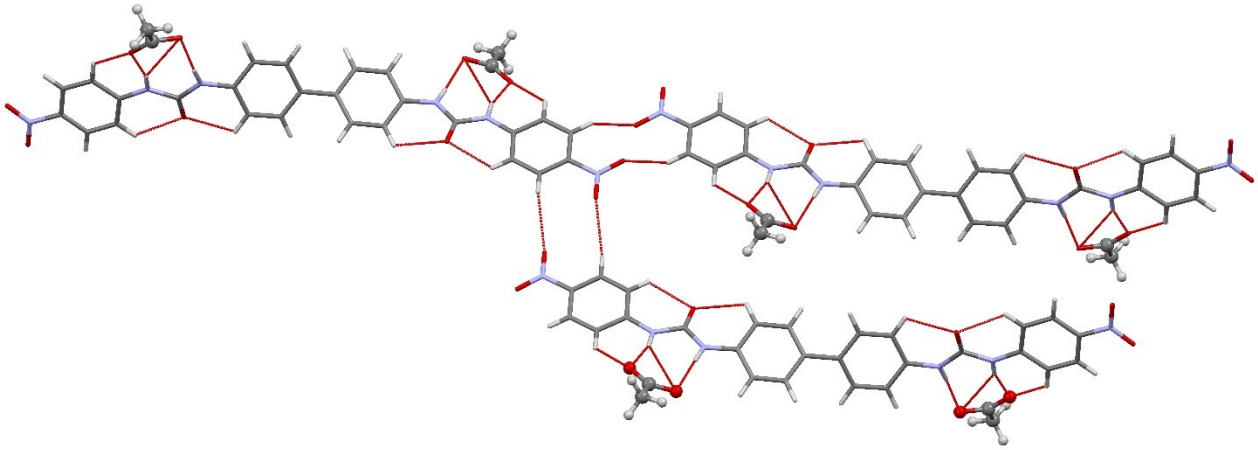


(a)

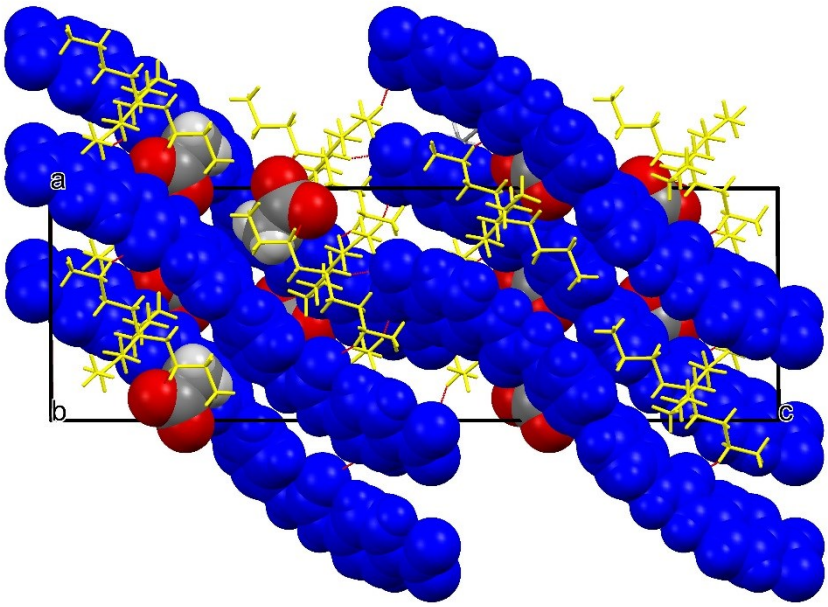



(b)

**Figure S6.** (a) Part of the crystal structure of [**1**-((TBA)OAc)$_2$]-$H_2O$, showing position of water molecules which link neighbouring receptors via acetates. (b) A crystal packing diagram of [**1**-((TBA)OAc)$_2$]-$H_2O$, viewed along the *a* axis, showing three-dimensional network built of receptor molecules, acetates, cations and water molecules.

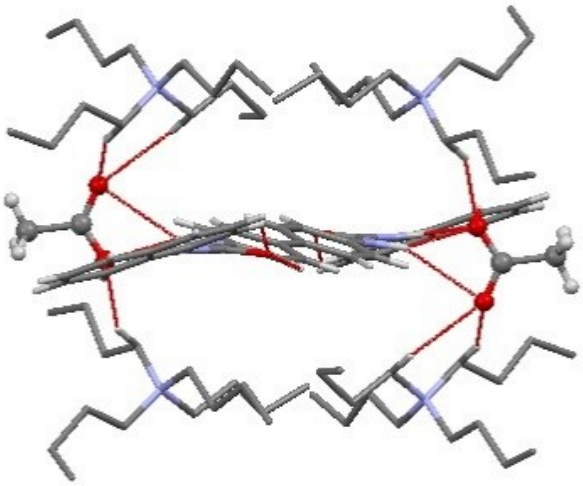


(a)




(b)

**Figure S7.** (a) Part of the crystal structure of [**2**-((TBA)OAc)$_2$], showing $C_{Ar}$–H···O hydrogen bonds that linked neighbouring receptor molecules. (b) A crystal packing diagram of [**2**-((TBA)OAc)$_2$], viewed along the *b* axis, showing three-dimensional network formed between mutually parallel receptor-acetates sheets and TBA cations.



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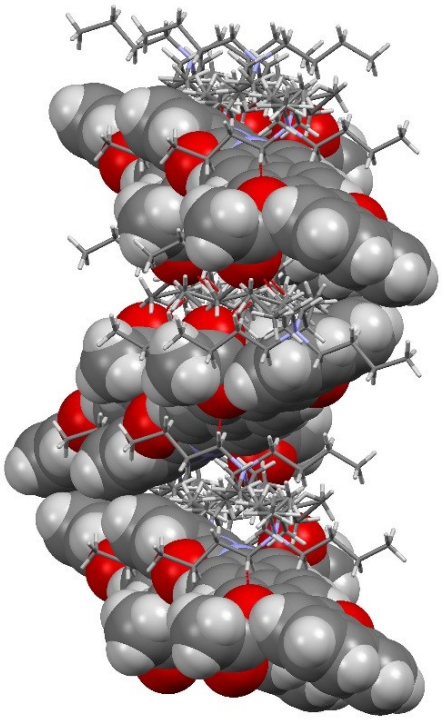
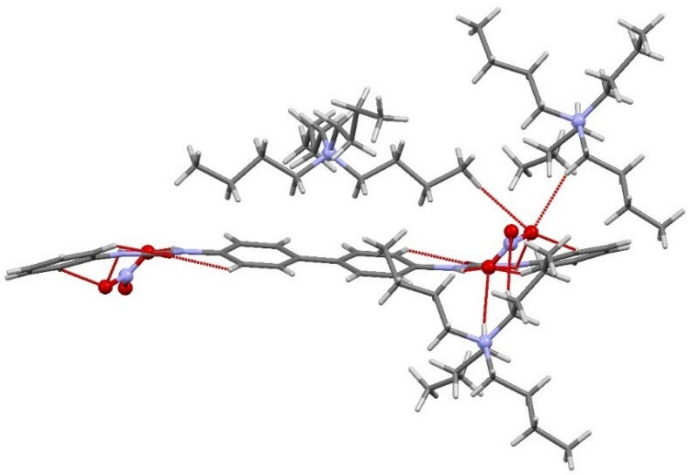
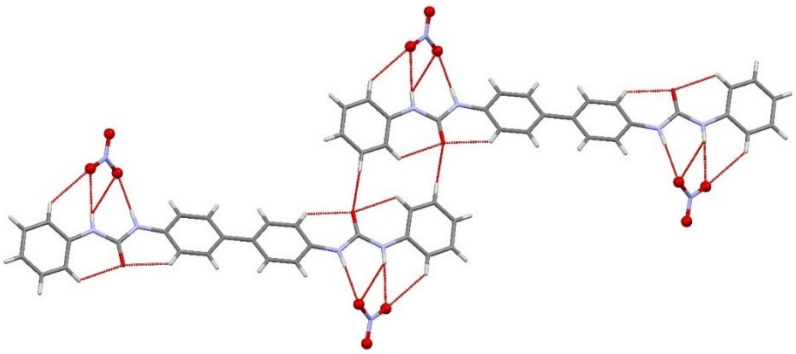


(b)

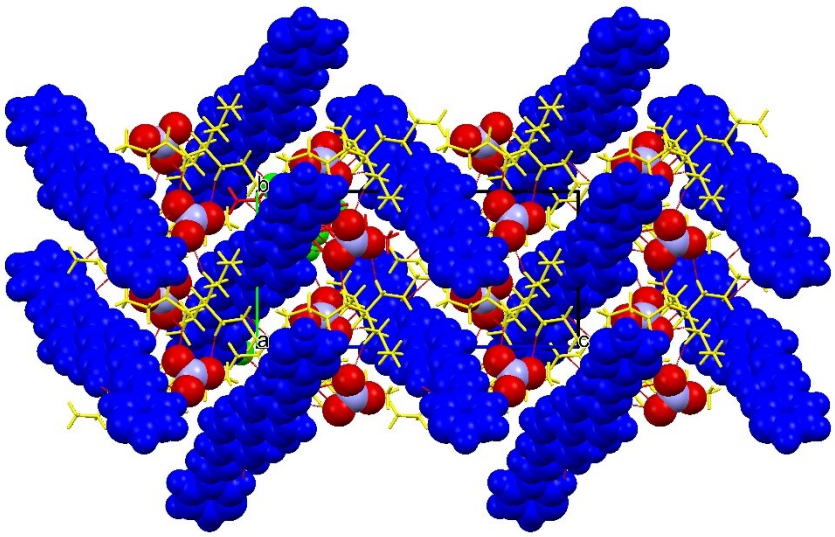
**Figure S8.** (a) Part of the crystal structure of [**3**-((TBA)OAc)$_2$], showing four TBA cations perpendicularly positioned with respect to the receptor-anion aggregates. Hydrogen atoms not included in hydrogen bods have been omitted for clarity. (b) Part of the crystal structure of [**3**-((TBA)OAc)$_2$], showing two-dimensional network formed between neighbouring receptor molecules, acetates and TBA cations. Only major component of disordered butyl group carbon atoms is presented.



(a)

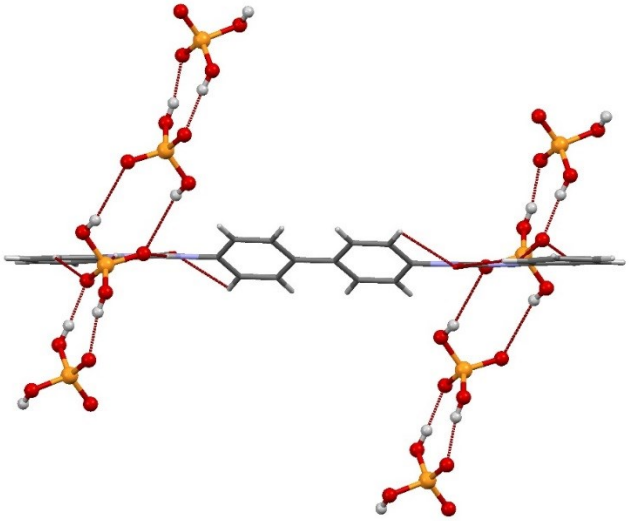


(b)

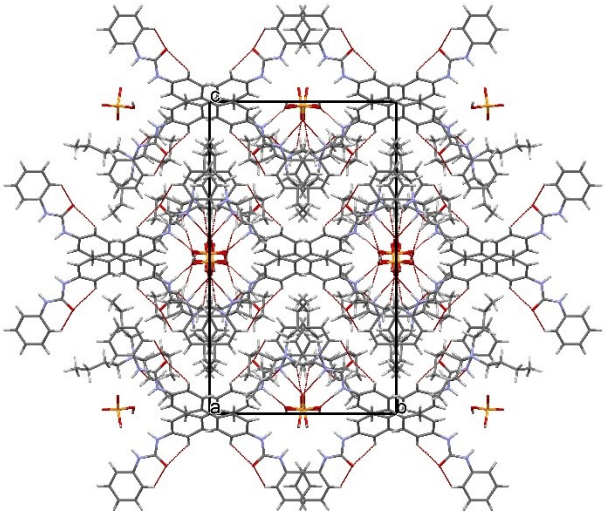


(c)

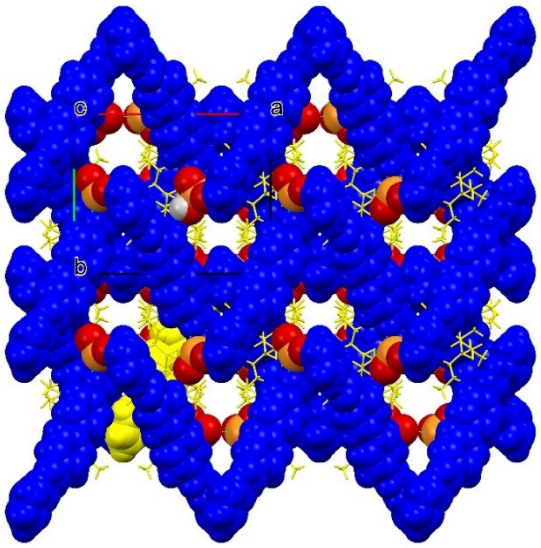
**Figure S9.** Part of the crystal structure of [**1**-((TBA)$NO_3$)$_2$], showing position of nitrates with respect to the urea moiety atoms due to the presence of C–H···O hydrogen bonds (a), and one C–H···O hydrogen bond that links neighbouring receptor molecules. (c) A crystal packing diagram of [**1**-((TBA)$NO_3$)$_2$], viewed along the *a* axis, showing three-dimensional network built of receptor molecules, nitrates and cations.



(a)

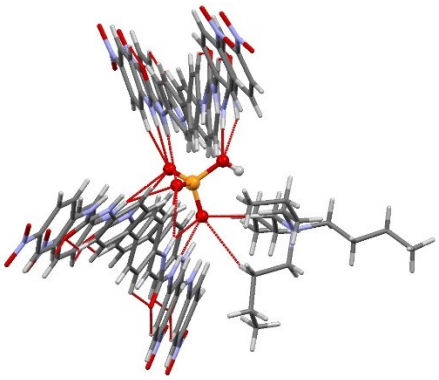



(b)

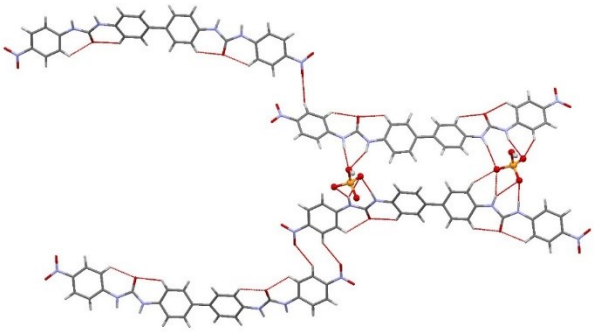



(c)

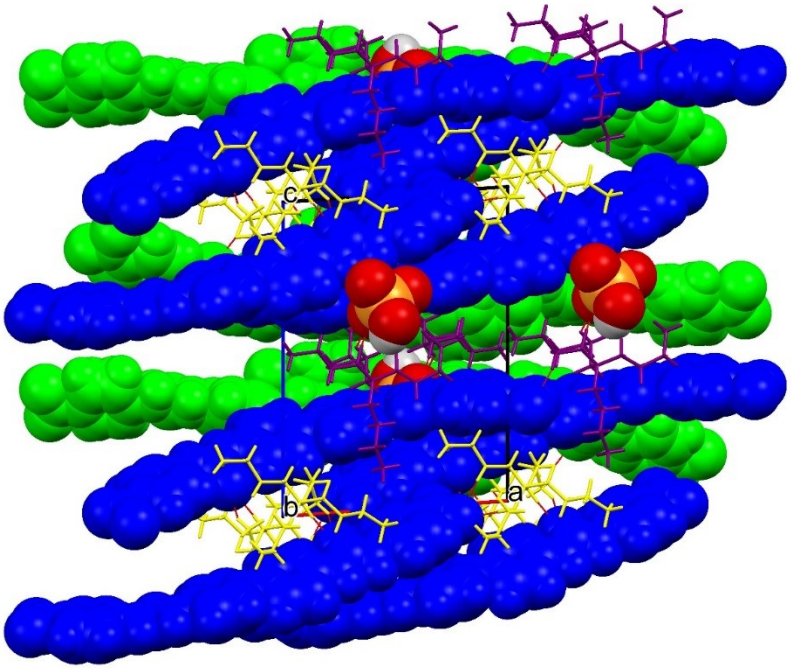
**Figure S10.** (a) Part of the crystal structure of [**1**-((TBA)$H_2PO_4$)$_2$], showing infinite chains and clusters of dihydrogen phosphate anions formed by O–H···O hydrogen bonds. (b) A crystal packing diagram of [**1**-((TBA)$H_2PO_4$)$_2$], viewed along the *a* and *c* axis, showing arrangement of dihydrogen phosphate anions along the *a* axis (b), and zig-zag arrangement of receptor molecules and hydrophobic channels (c). Only major component of disordered dihydrogen phosphate anion atoms is presented in all figures.



(a)

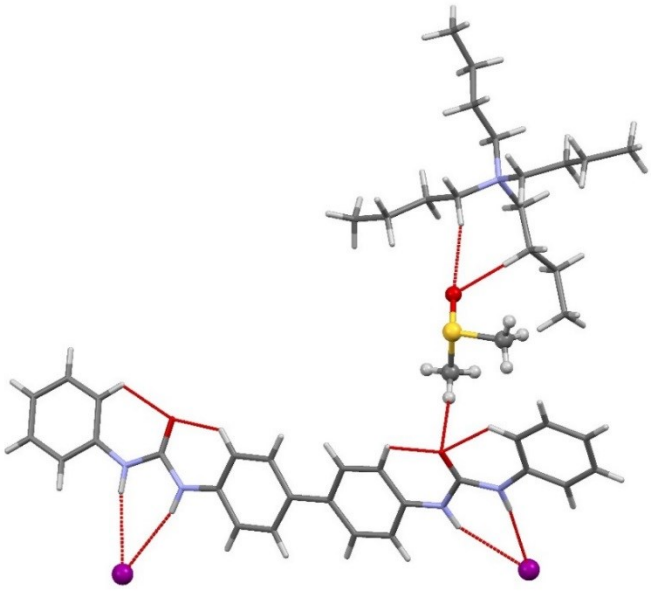


(b)

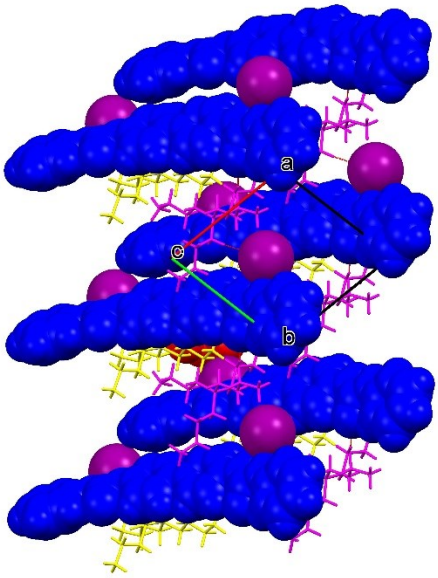



(c)

**Figure S11.** Part of the crystal structure of [(**2**)$_2$-(TBA)$_2$HPO$_4$)], showing position of hydrogen phosphate anion between two pairs of receptor molecules and one TBA cation (a) and two $C_{Ar}$–H···$O_{NO2}$ hydrogen bonds that link neighbouring receptor molecules (b).(c) A crystal packing diagram of [(**2**)$_2$-(TBA)$_2$HPO$_4$)], viewed along the *b* axis, showing position of TBA cations which link receptor-anion aggregates into three-dimensional network. Only major component of disordered oxygen atoms in hydrogen phosphate anion is presented in both figures.



(a)

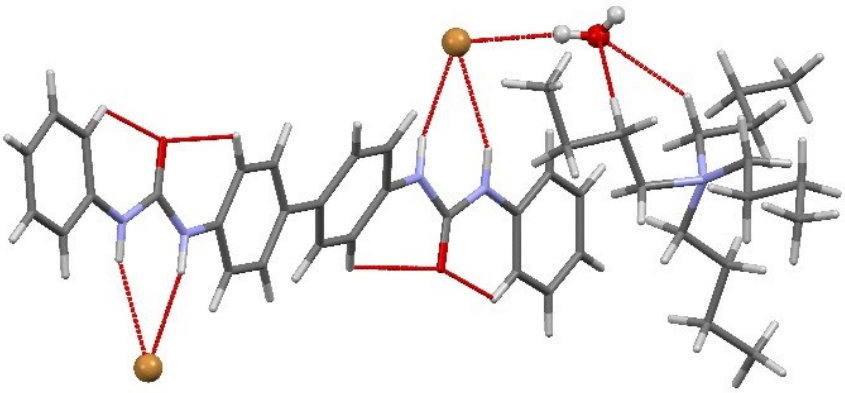



(b)

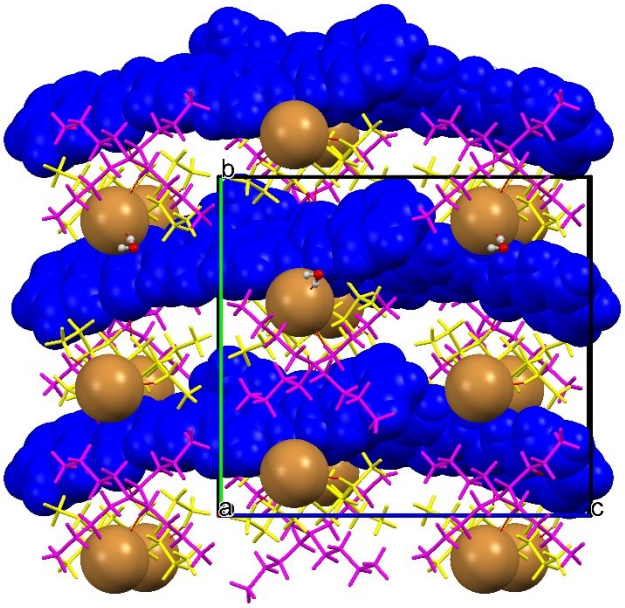
**Figure S12.** (a) Part of the crystal structure of [**1**-((TBA)I)$_2$-DMSO], showing entrapment of DMSO molecule by C–H···O and C–H···O hydrogen bonds. (b) A crystal packing diagram of [**1**-((TBA)I)$_2$-DMSO], viewed along the *c* axis, showing two-dimensional network built of receptor molecules, cations, anions and DMSO molecules.

**Packing description of the complexes [1-((TBA)Br)$_2$], [2-((TBA)Br)$_2$], [3-((TBA)Br)$_2$]**

Briefly, compared to [**1**-((TBA)Br)$_2$], hydrogen-bonding pattern in [**2**-((TBA)Br)$_2$] is different mainly due to the lack of water in the lattice, and thus the packing is quite symmetric (Figure S14). Besides N-H···O hydrogen bonds receptor **2** is hydrogen-bonded to bromide with one additional $C_{Ar}$-H···Br hydrogen bond (Fig. S14a), so that bromide is situated between two receptor molecules and form receptor-Br-receptor layers. TBA cations are bonded to the layers by $C_{TBA}$-H···Br hydrogen bonds, so that bromides are encapsulated in pairs within centrosymmetric pockets delimited by two receptors and four TBA cations (Figure S14a). Cations are additionally linked to receptors by $C_{TBA}$-H···$O_{NO2}$ hydrogen bonds, and overall structure consists of alternating anionic receptor-Br-receptor mutually parallel layers and TBA cations between them, so forming three-dimensional network (Figure S14b). Identically as in [**2**-((TBA)Br)$_2$], bromides in [**3**-((TBA)Br)$_2$] are situated between two receptor molecules and mutually linked by one $C_{Ar}$-H···O(=C) hydrogen bond, so virtually forming sheets. Due to the fact that receptor molecule is extremely bent, bromides are not displaced in the receptor's plane (Figure S15a). TBA cations, occupying the interstitial regions, are hydrogen-bonded to the bromides, but also to receptor molecules by $C_{TBA}$-H···Br, $C_{TBA}$-H···O(=C) HBs and $C_{TBA}$-H···$N_{urea}$ HB hydrogen bonds, so linking hydrogen-bonded sheets into two-dimensional network (Figure S15b), completely different network compared to structures of [**1**-((TBA)Br)$_2$] and [**2**-((TBA)Br)$_2$].

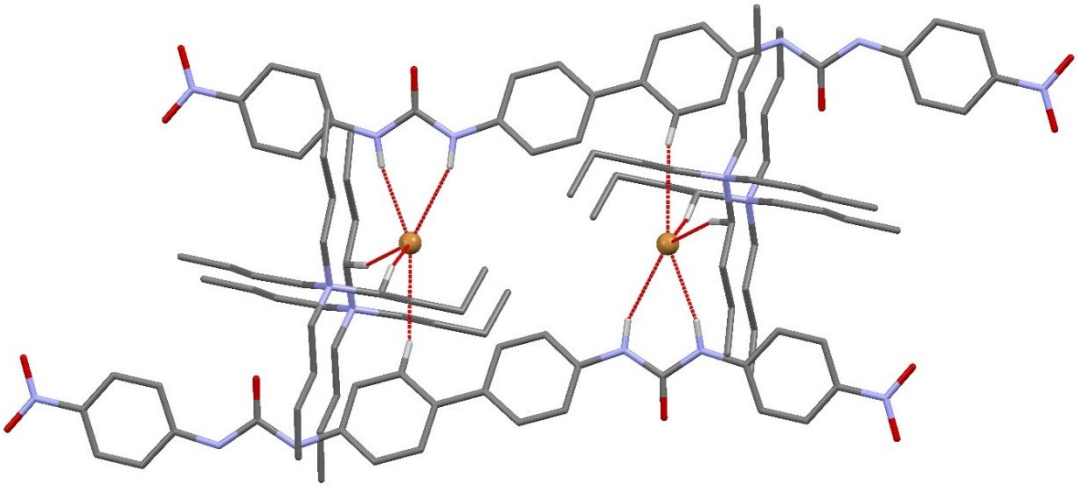


(a)

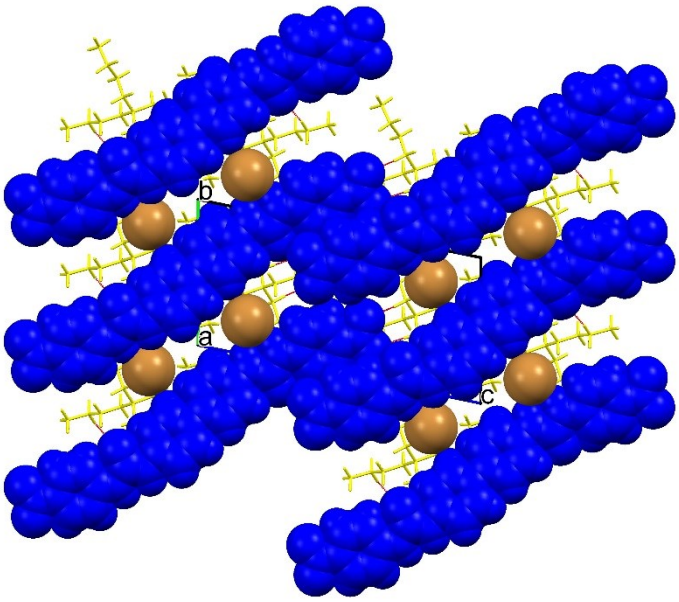



(b)

**Figure S13.** (a) Part of the crystal structure of [**1**-((TBA)Br)$_2$], showing entrapment of water molecule by O–H···Br and C–H···O hydrogen bonds. (b) A crystal packing diagram of [**1**-((TBA)Br)$_2$], viewed along the *a* axis, showing three-dimensional network built of receptor molecules, cations, anions and water molecules. Only major component of disordered butyl group carbon atoms is presented.

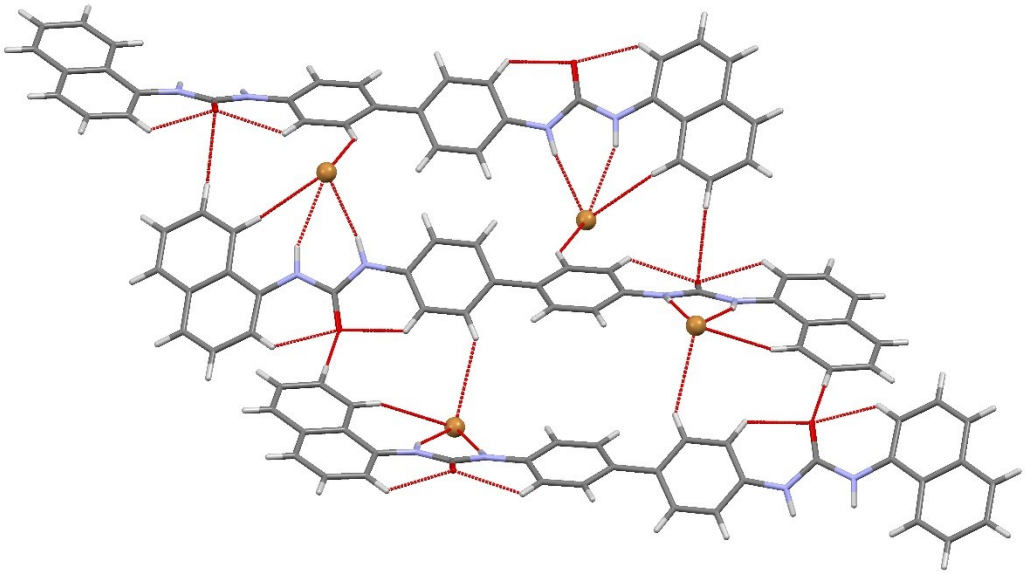


(a)

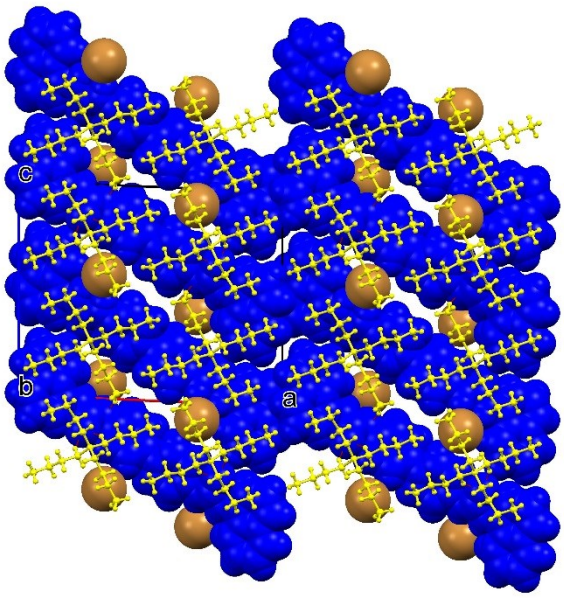



(b)

**Figure S14.** (a) Part of the crystal structure of [**2**-((TBA)Br)$_2$], showing position of bromide between two receptor molecules and four TBA cations and bonded to them by N–H···Br and C–H···Br hydrogen bonds. Hydrogen atoms not included in hydrogen bods have been omitted for clarity. (b) A crystal packing diagram of [**2**-((TBA)Br)$_2$], viewed along the *a* axis, showing receptor–bromide–receptor interactions and position of TBA cations.



(a)




(b)

**Figure S15.** (a) Part of the crystal structure of [**3**-((TBA)Br)$_2$], showing position of bromide anions between mutually linked receptor molecules by $C_{Ar}$–H···O bond. (b) A crystal packing diagram of [**3**-((TBA)Br)$_2$], viewed along the *b* axis, showing two-dimensional network formed by hydrogen-bonded sheets of receptor molecules and bromides and TBA cations.

**Computational Details.** Ab initio and density functional calculations were performed using the Gaussian09 program package.[13] Optimization of all involved system was performed at B3LYP/6-311+G(d,p) level of theory. Solvent environment effects were described by using the polarizable continuum model (PCM) with the integral equation formalism variant for dimethyl sulfoxide (DMSO, 46.83) as implicit solvent. Frequencies were calculated and checked to make sure that all frequencies were positive. The geometry-optimized structures were used in the TD-DFT calculations, with B3LYP functional and the same basis-set and solvent effects as in the geometry optimization. Adiabatic approximation of time dependent DFT was used to solve for 50 singlet excited states. Zero-point energy (ZPE) was included in each result.

**Cartesian coordinates for complex between receptor 1 and acetate.**

| | | | |
|---|---|---|---|
| H | -0.04600000 | 1.79700000 | 0.22200000 |
| C | 0.55900000 | 0.90100000 | 0.13800000 |
| C | 2.16700000 | -1.36500000 | -0.01900000 |
| C | -0.06000000 | -0.36100000 | 0.13100000 |
| C | 1.93700000 | 1.03500000 | 0.07000000 |
| C | 2.77300000 | -0.09600000 | -0.01100000 |
| C | 0.78200000 | -1.47900000 | 0.05200000 |
| H | 2.39300000 | 2.01800000 | 0.08900000 |
| H | 0.34900000 | -2.47200000 | 0.01900000 |
| H | 2.78500000 | -2.24500000 | -0.09500000 |
| C | -1.53400000 | -0.50100000 | 0.20500000 |
| C | -4.36100000 | -0.76200000 | 0.34500000 |
| C | -2.39300000 | 0.43200000 | -0.39500000 |
| C | -2.13700000 | -1.57600000 | 0.87900000 |
| C | -3.51600000 | -1.70700000 | 0.94800000 |
| C | -3.77900000 | 0.31800000 | -0.33400000 |
| H | -1.97400000 | 1.26600000 | -0.94600000 |
| H | -1.51900000 | -2.31300000 | 1.37900000 |
| H | -3.94600000 | -2.54600000 | 1.48500000 |
| H | -4.40800000 | 1.05100000 | -0.81100000 |
| N | -5.74700000 | -0.97700000 | 0.45700000 |
| H | -5.99800000 | -1.81800000 | 0.95400000 |
| N | 4.15000000 | 0.13900000 | -0.06800000 |
| H | 4.41500000 | 1.14300000 | -0.12400000 |
| C | -6.77900000 | -0.16500000 | 0.02100000 |
| C | 5.16300000 | -0.79800000 | -0.12200000 |
| N | 6.40800000 | -0.20700000 | -0.04600000 |
| H | 6.44800000 | 0.80200000 | 0.19300000 |
| N | -8.02200000 | -0.71000000 | 0.28600000 |
| H | -8.04500000 | -1.63000000 | 0.70100000 |
| C | -9.29200000 | -0.17200000 | 0.00300000 |
| C | -11.90500000 | 0.74700000 | -0.48100000 |
| C | -10.40300000 | -0.98300000 | 0.28900000 |

| | | | |
|---|---|---|---|
| C | -9.50200000 | 1.10800000 | -0.52900000 |
| C | -10.80300000 | 1.55100000 | -0.76400000 |
| C | -11.69300000 | -0.52600000 | 0.04900000 |
| H | -10.25000000 | -1.97600000 | 0.70000000 |
| H | -8.65700000 | 1.73800000 | -0.75400000 |
| H | -10.95000000 | 2.54300000 | -1.17600000 |
| H | -12.53500000 | -1.17000000 | 0.27800000 |
| H | -12.91100000 | 1.10400000 | -0.66800000 |
| C | 7.65800000 | -0.82900000 | -0.16300000 |
| C | 10.26500000 | -1.88600000 | -0.38800000 |
| C | 7.85400000 | -2.19500000 | -0.43000000 |
| C | 8.79100000 | -0.00300000 | -0.01200000 |
| C | 10.07200000 | -0.52900000 | -0.12300000 |
| C | 9.14700000 | -2.70400000 | -0.53900000 |
| H | 6.99700000 | -2.84000000 | -0.54200000 |
| H | 8.64200000 | 1.05100000 | 0.19200000 |
| H | 10.92600000 | 0.12900000 | -0.00100000 |
| H | 9.27600000 | -3.76200000 | -0.74500000 |
| H | 11.26500000 | -2.29500000 | -0.47400000 |
| O | -6.61000000 | 0.91200000 | -0.53500000 |
| O | 4.97700000 | -2.01100000 | -0.22500000 |
| C | 5.76600000 | 3.26500000 | 0.26000000 |
| O | 4.67200000 | 2.88300000 | -0.24200000 |
| C | 5.95300000 | 4.77300000 | 0.44400000 |
| H | 6.99300000 | 5.02400000 | 0.65400000 |
| H | 5.33500000 | 5.11100000 | 1.28100000 |
| H | 5.61300000 | 5.30700000 | -0.44600000 |
| O | 6.69800000 | 2.50500000 | 0.63700000 |

**Cartesian coordinates for complex between receptor 1 and DMSO.**

| | | | |
|---|---|---|---|
| H | -0.05500000 | 1.80600000 | 0.17600000 |
| C | 0.55200000 | 0.90800000 | 0.12700000 |
| C | 2.16600000 | -1.35700000 | 0.05900000 |
| C | -0.06500000 | -0.35400000 | 0.15600000 |
| C | 1.93100000 | 1.04200000 | 0.06600000 |
| C | 2.77000000 | -0.08900000 | 0.03000000 |
| C | 0.77900000 | -1.47200000 | 0.12000000 |
| H | 2.38100000 | 2.02800000 | 0.05700000 |
| H | 0.34900000 | -2.46800000 | 0.11900000 |
| H | 2.78200000 | -2.24200000 | 0.02100000 |
| C | -1.54000000 | -0.49400000 | 0.22200000 |
| C | -4.36700000 | -0.75400000 | 0.34800000 |
| C | -2.39400000 | 0.41000000 | -0.42600000 |
| C | -2.14700000 | -1.54000000 | 0.93800000 |
| C | -3.52700000 | -1.66900000 | 1.00100000 |
| C | -3.78100000 | 0.29500000 | -0.37300000 |
| H | -1.97200000 | 1.22000000 | -1.01000000 |
| H | -1.53300000 | -2.25400000 | 1.47400000 |
| H | -3.96000000 | -2.48400000 | 1.57200000 |
| H | -4.40500000 | 1.00700000 | -0.89000000 |
| N | -5.75600000 | -0.97000000 | 0.45400000 |
| H | -6.00800000 | -1.80600000 | 0.96200000 |
| N | 4.15100000 | 0.14900000 | -0.02000000 |
| H | 4.41400000 | 1.15100000 | -0.02100000 |
| C | -6.78700000 | -0.16500000 | 0.01000000 |
| C | 5.16100000 | -0.78800000 | -0.10700000 |
| N | 6.41500000 | -0.21400000 | -0.07400000 |
| H | 6.47800000 | 0.80600000 | 0.09100000 |
| N | -8.03100000 | -0.71300000 | 0.26300000 |
| H | -8.05300000 | -1.63500000 | 0.67400000 |
| C | -9.30300000 | -0.17600000 | -0.01800000 |
| C | -11.92100000 | 0.73800000 | -0.49100000 |
| C | -10.41100000 | -0.99600000 | 0.25600000 |
| C | -9.51900000 | 1.11100000 | -0.53200000 |
| C | -10.82300000 | 1.55100000 | -0.76300000 |
| C | -11.70300000 | -0.54200000 | 0.02100000 |
| H | -10.25400000 | -1.99400000 | 0.65400000 |
| H | -8.67800000 | 1.75000000 | -0.74800000 |
| H | -10.97300000 | 2.54900000 | -1.16100000 |
| H | -12.54200000 | -1.19300000 | 0.24000000 |
| H | -12.92800000 | 1.09200000 | -0.67500000 |
| C | 7.65600000 | -0.86100000 | -0.19000000 |
| C | 10.24300000 | -1.96900000 | -0.41100000 |
| C | 7.82600000 | -2.23300000 | -0.44600000 |
| C | 8.80400000 | -0.05600000 | -0.04800000 |
| C | 10.07600000 | -0.60600000 | -0.15800000 |
| C | 9.11000000 | -2.76800000 | -0.55300000 |
| H | 6.95900000 | -2.86500000 | -0.55500000 |
| H | 8.67900000 | 1.00300000 | 0.14800000 |

| | | | |
|---|---|---|---|
| H | 10.94200000 | 0.03700000 | -0.04400000 |
| H | 9.21900000 | -3.82900000 | -0.75100000 |
| H | 11.23500000 | -2.39700000 | -0.49600000 |
| O | -6.61800000 | 0.91300000 | -0.54800000 |
| O | 4.96300000 | -2.00100000 | -0.20400000 |
| S | 6.40300000 | 3.90100000 | 0.11500000 |
| C | 5.51200000 | 5.35000000 | -0.53000000 |
| H | 4.47900000 | 5.31700000 | -0.18300000 |
| H | 6.01800000 | 6.25100000 | -0.18300000 |
| H | 5.55900000 | 5.29000000 | -1.61600000 |
| C | 6.09900000 | 4.16100000 | 1.89000000 |
| H | 6.51800000 | 3.30000000 | 2.41000000 |
| H | 6.61700000 | 5.07000000 | 2.19800000 |
| H | 5.02700000 | 4.23800000 | 2.06700000 |
| O | 5.54000000 | 2.68200000 | -0.28900000 |

**Cartesian coordinates for complex between receptor 1 and phosphate.**

| | | | |
|---|---|---|---|
| H | -0.39500000 | 1.50400000 | 0.65100000 |
| C | 0.18100000 | 0.62000000 | 0.39800000 |
| C | 1.71200000 | -1.62600000 | -0.19200000 |
| C | -0.48100000 | -0.59300000 | 0.14600000 |
| C | 1.56400000 | 0.71700000 | 0.36100000 |
| C | 2.36000000 | -0.40700000 | 0.06800000 |
| C | 0.32400000 | -1.70300000 | -0.15000000 |
| H | 2.05300000 | 1.66200000 | 0.56500000 |
| H | -0.14300000 | -2.65500000 | -0.37700000 |
| H | 2.29900000 | -2.50000000 | -0.42600000 |
| C | -1.95900000 | -0.69600000 | 0.19100000 |
| C | -4.79300000 | -0.88700000 | 0.27600000 |
| C | -2.78300000 | 0.36000000 | -0.22400000 |
| C | -2.60000000 | -1.85700000 | 0.65400000 |
| C | -3.98300000 | -1.95400000 | 0.69400000 |
| C | -4.17200000 | 0.28200000 | -0.18700000 |
| H | -2.33300000 | 1.26800000 | -0.60900000 |
| H | -2.00900000 | -2.69400000 | 1.00800000 |
| H | -4.44400000 | -2.86400000 | 1.06500000 |
| H | -4.77500000 | 1.11000000 | -0.52200000 |
| N | -6.18600000 | -1.06900000 | 0.35700000 |
| H | -6.46500000 | -1.96600000 | 0.72600000 |
| N | 3.74900000 | -0.21200000 | 0.03900000 |
| H | 4.03800000 | 0.75800000 | 0.22000000 |
| C | -7.19000000 | -0.19400000 | -0.01500000 |
| C | 4.72300000 | -1.18500000 | -0.09400000 |
| N | 5.99900000 | -0.65900000 | -0.14700000 |
| H | 6.11200000 | 0.36100000 | -0.20700000 |
| N | -8.45100000 | -0.71200000 | 0.22200000 |
| H | -8.50400000 | -1.61900000 | 0.66200000 |
| C | -9.70100000 | -0.11200000 | -0.01900000 |
| C | -12.28200000 | 0.92500000 | -0.43600000 |
| C | -10.83600000 | -0.80800000 | 0.43000000 |
| C | -9.87100000 | 1.11200000 | -0.68200000 |
| C | -11.15600000 | 1.61500000 | -0.88000000 |
| C | -12.11000000 | -0.29400000 | 0.22100000 |
| H | -10.71400000 | -1.75500000 | 0.94500000 |
| H | -9.00700000 | 1.65500000 | -1.02900000 |
| H | -11.27100000 | 2.56300000 | -1.39400000 |
| H | -12.97000000 | -0.84900000 | 0.57700000 |
| H | -13.27500000 | 1.32700000 | -0.59700000 |
| C | 7.20900000 | -1.37200000 | -0.21300000 |
| C | 9.73700000 | -2.61600000 | -0.33600000 |
| C | 7.31900000 | -2.77100000 | -0.14400000 |
| C | 8.38500000 | -0.60800000 | -0.34200000 |
| C | 9.62800000 | -1.22600000 | -0.40300000 |
| C | 8.57500000 | -3.37300000 | -0.20600000 |
| H | 6.42700000 | -3.36900000 | -0.05000000 |
| H | 8.30000000 | 0.47100000 | -0.39200000 |

| | | | |
|---|---|---|---|
| H | 10.51800000 | -0.61400000 | -0.50300000 |
| H | 8.63800000 | -4.45500000 | -0.15200000 |
| H | 10.70700000 | -3.09600000 | -0.38400000 |
| O | -6.98600000 | 0.91100000 | -0.49900000 |
| O | 4.47700000 | -2.38800000 | -0.15800000 |
| O | 4.23000000 | 2.56100000 | 0.58200000 |
| O | 6.62900000 | 2.14000000 | -0.34900000 |
| O | 5.40100000 | 4.23900000 | -0.98900000 |
| P | 5.57900000 | 3.08800000 | 0.16800000 |
| O | 6.15600000 | 3.91600000 | 1.46100000 |
| H | 4.60600000 | 4.76400000 | -0.84000000 |
| H | 7.09700000 | 4.10600000 | 1.36400000 |

**Cartesian coordinates for complex between receptor 2 and acetate.**

| | | | |
|---|---|---|---|
| H | -0.04966300 | 1.77690500 | 0.67932500 |
| C | 0.61058800 | 0.96004400 | 0.41073800 |
| C | 2.36093000 | -1.11163900 | -0.21635100 |
| C | 0.07469700 | -0.30674100 | 0.12350800 |
| C | 1.97810800 | 1.19177100 | 0.38871400 |
| C | 2.88125100 | 0.15921000 | 0.07572000 |
| C | 0.98518900 | -1.32587300 | -0.18988700 |
| H | 2.36571400 | 2.17668700 | 0.62077400 |
| H | 0.61704300 | -2.31401400 | -0.44274900 |
| H | 3.02894200 | -1.92006400 | -0.46705700 |
| C | -1.38703000 | -0.55259900 | 0.15135100 |
| C | -4.18691600 | -1.01320200 | 0.21000400 |
| C | -2.30442000 | 0.43272300 | -0.24132700 |
| C | -1.91543100 | -1.78388700 | 0.57376200 |
| C | -3.28372500 | -2.01212800 | 0.60329200 |
| C | -3.68051600 | 0.22067900 | -0.21753900 |
| H | -1.94213100 | 1.39018900 | -0.59778500 |
| H | -1.25056100 | -2.57181400 | 0.90769400 |
| H | -3.65766400 | -2.97149900 | 0.94609600 |
| H | -4.35456400 | 1.00052100 | -0.53406800 |
| N | -5.56025000 | -1.33481000 | 0.26291700 |
| H | -5.75201900 | -2.29133600 | 0.52553200 |
| N | 4.24599900 | 0.49249900 | 0.06241000 |
| H | 4.44769000 | 1.49683600 | 0.23014300 |
| C | -6.63658000 | -0.50532900 | 0.05447200 |
| C | 5.30709300 | -0.36714400 | -0.06936400 |
| N | 6.52585500 | 0.30901100 | -0.09483400 |
| H | 6.50536900 | 1.35037000 | -0.13460500 |
| N | -7.85383900 | -1.17084900 | 0.20477200 |
| H | -7.81586700 | -2.15482900 | 0.43067800 |
| C | -9.14071700 | -0.66055200 | 0.06964200 |
| C | -11.78464900 | 0.18601600 | -0.15905000 |
| C | -10.20679100 | -1.56656000 | 0.25651900 |
| C | -9.42973500 | 0.68383600 | -0.23517600 |
| C | -10.74680400 | 1.09849800 | -0.34760900 |
| C | -11.51833100 | -1.15169900 | 0.14425100 |
| H | -9.99537500 | -2.60363600 | 0.49077400 |
| H | -8.62549700 | 1.38580100 | -0.38045600 |
| H | -10.97306700 | 2.12942300 | -0.58116800 |
| H | -12.33142200 | -1.84898300 | 0.28780200 |
| C | 7.79122400 | -0.24534700 | -0.11892000 |
| C | 10.43187300 | -1.16801200 | -0.15550000 |
| C | 8.06871000 | -1.62958300 | -0.04414000 |
| C | 8.87854900 | 0.65956300 | -0.21127900 |
| C | 10.18069800 | 0.20754400 | -0.22956100 |
| C | 9.37707400 | -2.07936500 | -0.06217000 |
| H | 7.25518800 | -2.33252400 | 0.02431900 |
| H | 8.66987000 | 1.72076900 | -0.26507200 |
| H | 11.00438100 | 0.90400600 | -0.30046200 |

| | | | |
|---|---|---|---|
| H | 9.58799000 | -3.13815800 | -0.00349700 |
| O | -6.55107300 | 0.68008300 | -0.23193200 |
| O | 5.20872000 | -1.58968800 | -0.15794300 |
| N | -13.16234600 | 0.63097100 | -0.27918000 |
| O | -14.06276800 | -0.19380700 | -0.10798500 |
| O | -13.37752100 | 1.81484500 | -0.54749600 |
| N | 11.79428100 | -1.64891900 | -0.17468000 |
| O | 11.99555700 | -2.86653000 | -0.10540700 |
| O | 12.71239600 | -0.82559500 | -0.25941100 |
| H | 6.51612100 | 5.48251800 | 1.18041300 |
| C | 5.88045400 | 5.26810000 | 0.31549600 |
| H | 6.38551600 | 5.66637300 | -0.56688500 |
| H | 4.92332000 | 5.77093000 | 0.45475900 |
| C | 5.70587100 | 3.75673900 | 0.19405700 |
| O | 6.69038200 | 3.09099400 | -0.24196700 |
| O | 4.60540800 | 3.24967400 | 0.55010800 |

**Cartesian coordinates for complex between receptor 2 and DMSO.**

| | | | |
|---|---|---|---|
| H | -1.53814800 | -2.57814100 | 1.40556300 |
| C | -2.17824700 | -1.81640100 | 0.97617500 |
| C | -3.87918100 | 0.13245400 | -0.05915100 |
| C | -1.61182200 | -0.66726600 | 0.40019600 |
| C | -3.55292400 | -1.99323700 | 1.03359300 |
| C | -4.42409500 | -1.02256200 | 0.51616700 |
| C | -2.49669300 | 0.29297100 | -0.11026700 |
| H | -3.95707800 | -2.88957500 | 1.49283800 |
| H | -2.10389900 | 1.18645600 | -0.58205000 |
| H | -4.52870200 | 0.88886900 | -0.46976600 |
| C | -0.14234200 | -0.48078400 | 0.33565500 |
| C | 2.67430100 | -0.13184500 | 0.21243100 |
| C | 0.72510400 | -1.56292900 | 0.13002800 |
| C | 0.44205900 | 0.78866600 | 0.47820900 |
| C | 1.81695800 | 0.96223100 | 0.41813300 |
| C | 2.10729500 | -1.40644000 | 0.06793700 |
| H | 0.31671700 | -2.55783200 | -0.00737800 |
| H | -0.18386600 | 1.65457000 | 0.66045100 |
| H | 2.23702600 | 1.95453700 | 0.54200600 |
| H | 2.74330600 | -2.26107900 | -0.09978000 |
| N | 4.05169000 | 0.13960700 | 0.16612700 |
| H | 4.32021400 | 1.11908900 | 0.28939600 |
| N | -5.80609500 | -1.28725700 | 0.61768200 |
| H | -6.02712400 | -2.16095700 | 1.07374600 |
| C | 5.08548300 | -0.74617900 | -0.01359900 |
| C | -6.85714800 | -0.52465800 | 0.16632100 |
| N | -8.09152400 | -1.12093000 | 0.42682100 |
| H | -8.08034000 | -2.02097700 | 0.88614500 |
| N | 6.31924300 | -0.09339500 | 0.00358400 |
| H | 6.28126700 | 0.91984200 | 0.13881400 |
| C | 7.58134300 | -0.64609100 | -0.12535100 |
| C | 10.20168000 | -1.57839800 | -0.36586900 |
| C | 8.67837200 | 0.24199600 | -0.03908200 |
| C | 7.83319100 | -2.01862400 | -0.33583900 |
| C | 9.13490400 | -2.47461800 | -0.45393400 |
| C | 9.97457600 | -0.21412700 | -0.15763500 |
| H | 8.49712600 | 1.29708900 | 0.12619200 |
| H | 7.00791100 | -2.70801600 | -0.40372200 |
| H | 9.32948800 | -3.52572400 | -0.61541000 |
| H | 10.80852400 | 0.47005300 | -0.08977400 |
| C | -9.36281200 | -0.64327400 | 0.12551000 |
| C | -11.97975200 | 0.15603300 | -0.39508400 |
| C | -9.61468000 | 0.59938600 | -0.48769900 |
| C | -10.45186200 | -1.47258600 | 0.46927500 |
| C | -11.75035200 | -1.08048700 | 0.21374500 |
| C | -10.91855800 | 0.99101500 | -0.74416800 |
| H | -8.79250900 | 1.24184800 | -0.75588300 |
| H | -10.26875300 | -2.43224700 | 0.93906500 |
| H | -12.58133900 | -1.71875700 | 0.47829600 |

| | | | |
|---|---|---|---|
| H | -11.11643000 | 1.94418400 | -1.21412800 |
| O | 4.95712300 | -1.95524600 | -0.16993800 |
| O | -6.73753000 | 0.55216600 | -0.39990800 |
| N | 11.56030400 | -2.06594900 | -0.49077300 |
| O | 12.48742900 | -1.25433000 | -0.41526500 |
| O | 11.74088900 | -3.27402600 | -0.66792600 |
| N | -13.34347500 | 0.57635900 | -0.66824500 |
| O | -13.52553100 | 1.66999800 | -1.20723000 |
| O | -14.26533000 | -0.17788900 | -0.34975100 |
| S | 5.38032000 | 3.95097900 | -0.22795600 |
| C | 4.59769500 | 5.08085400 | 0.96243700 |
| H | 5.15277100 | 5.05266100 | 1.90001900 |
| H | 4.59331400 | 6.08346800 | 0.53352200 |
| H | 3.57619600 | 4.73178100 | 1.10488100 |
| C | 7.05858400 | 4.64969000 | -0.19987100 |
| H | 7.67025500 | 4.03916500 | -0.86210900 |
| H | 7.01040200 | 5.67243600 | -0.57554000 |
| H | 7.44013700 | 4.62031100 | 0.82086800 |
| O | 5.48431700 | 2.59351500 | 0.51440500 |

**Cartesian coordinates for complex between receptor 2 and phosphate.**

| | | | |
|---|---|---|---|
| H | -0.34388000 | 1.52501400 | 0.75885900 |
| C | 0.29730100 | 0.71058600 | 0.44112000 |
| C | 1.99877200 | -1.35940000 | -0.31374000 |
| C | -0.26687600 | -0.52645100 | 0.08755500 |
| C | 1.66970700 | 0.91389800 | 0.42363400 |
| C | 2.54614700 | -0.11909000 | 0.04750800 |
| C | 0.61899700 | -1.54570900 | -0.28963200 |
| H | 2.08239400 | 1.87541200 | 0.70502700 |
| H | 0.22784100 | -2.50958100 | -0.59574200 |
| H | 2.64674900 | -2.16711500 | -0.61441100 |
| C | -1.73330500 | -0.74331700 | 0.11252300 |
| C | -4.54100600 | -1.15046200 | 0.16313500 |
| C | -2.63207800 | 0.27881000 | -0.22486800 |
| C | -2.28407600 | -1.98345000 | 0.47603600 |
| C | -3.65646100 | -2.18541500 | 0.50185100 |
| C | -4.01212800 | 0.09324900 | -0.20450100 |
| H | -2.25171100 | 1.24546700 | -0.53460500 |
| H | -1.63345700 | -2.80002000 | 0.76638100 |
| H | -4.04862400 | -3.15276000 | 0.79867100 |
| H | -4.67191800 | 0.90105800 | -0.47818800 |
| N | -5.91979300 | -1.44817000 | 0.20711300 |
| H | -6.12846700 | -2.41231800 | 0.42494200 |
| N | 3.92100300 | 0.18471500 | 0.03679500 |
| H | 4.13352600 | 1.17269500 | 0.22813600 |
| C | -6.98174800 | -0.59159800 | 0.03890100 |
| C | 4.95942100 | -0.70493900 | -0.08860900 |
| N | 6.20320400 | -0.07601400 | -0.13946500 |
| H | 6.23263700 | 0.94950700 | -0.23821700 |
| N | -8.20966100 | -1.24205000 | 0.16646500 |
| H | -8.18739500 | -2.23451500 | 0.35399700 |
| C | -9.48828600 | -0.70483800 | 0.06141400 |
| C | -12.11845000 | 0.19535700 | -0.11246100 |
| C | -10.56851400 | -1.60050100 | 0.21376200 |
| C | -9.75586100 | 0.65649700 | -0.18120400 |
| C | -11.06626200 | 1.09785800 | -0.26644900 |
| C | -11.87340200 | -1.15903400 | 0.12845800 |
| H | -10.37312500 | -2.65046300 | 0.39983000 |
| H | -8.94051700 | 1.35063900 | -0.29984800 |
| H | -11.27629600 | 2.14193200 | -0.45176400 |
| H | -12.69755700 | -1.84823100 | 0.24554900 |
| C | 7.44950300 | -0.68149600 | -0.13260600 |
| C | 10.04839500 | -1.70808000 | -0.11153000 |
| C | 7.66900100 | -2.06927700 | 0.01081400 |
| C | 8.56991900 | 0.17475100 | -0.26309800 |
| C | 9.85344100 | -0.32940000 | -0.25327900 |
| C | 8.95886000 | -2.57140600 | 0.02068900 |
| H | 6.82843100 | -2.73579500 | 0.10818400 |
| H | 8.40127900 | 1.23935500 | -0.36772600 |
| H | 10.70458200 | 0.32936000 | -0.35373300 |

| | | | |
|---|---|---|---|
| H | 9.12688700 | -3.63361400 | 0.13164900 |
| O | -6.87629800 | 0.60321700 | -0.19726700 |
| O | 4.82108000 | -1.92363700 | -0.15298100 |
| N | -13.48897500 | 0.66861200 | -0.20330600 |
| O | -14.40246500 | -0.14822000 | -0.06673600 |
| O | -13.68520900 | 1.86748200 | -0.41321600 |
| N | 11.39230900 | -2.24381300 | -0.10108300 |
| O | 11.54352500 | -3.46394200 | 0.01967300 |
| O | 12.34186700 | -1.46148700 | -0.21276300 |
| O | 6.58331300 | 2.73707800 | -0.48066600 |
| O | 4.23756200 | 2.99122200 | 0.61915600 |
| O | 6.10864600 | 4.50418500 | 1.35817600 |
| P | 5.51048700 | 3.62167700 | 0.10955500 |
| O | 5.18385400 | 4.75416700 | -1.03321300 |
| H | 6.98121700 | 4.87189800 | 1.16831500 |
| H | 4.43040600 | 5.31057900 | -0.79808300 |

**Cartesian coordinates for complex between receptor 3a and acetate.**

| | | | |
|---|---|---|---|
| O | 5.09057900 | -1.91061500 | -0.47743500 |
| N | 6.56721800 | -0.15805300 | -0.25887500 |
| H | 6.65341500 | 0.84907700 | -0.03459700 |
| N | 4.31262000 | 0.26021700 | -0.40123300 |
| H | 4.60460900 | 1.25069300 | -0.48349700 |
| C | 7.75647100 | -0.90656600 | -0.39583000 |
| C | 7.91913100 | -1.80769700 | -1.43161100 |
| H | 7.11321900 | -1.95333800 | -2.13819600 |
| C | 9.11828400 | -2.53462500 | -1.58326100 |
| H | 9.20970300 | -3.23273000 | -2.40800000 |
| C | 10.16642600 | -2.35162500 | -0.71277900 |
| H | 11.09299800 | -2.90187200 | -0.83567000 |
| C | 10.04564200 | -1.43631400 | 0.36457100 |
| C | 11.10779900 | -1.23601100 | 1.28812700 |
| H | 12.03159000 | -1.78605100 | 1.14158300 |
| C | 10.97342400 | -0.37190800 | 2.34838000 |
| H | 11.79189900 | -0.23167500 | 3.04556400 |
| C | 9.76102800 | 0.33240100 | 2.53597200 |
| H | 9.65611300 | 1.00432900 | 3.38049100 |
| C | 8.71503800 | 0.17021800 | 1.65647200 |
| H | 7.79885500 | 0.72522400 | 1.80642400 |
| C | 8.82299100 | -0.70747100 | 0.54357700 |
| C | 5.30338000 | -0.69930500 | -0.39059900 |
| C | 2.92643600 | 0.05213400 | -0.41640700 |
| C | 2.11130400 | 1.18654500 | -0.59388700 |
| H | 2.58134700 | 2.15387800 | -0.72870600 |
| C | 0.72816200 | 1.07787500 | -0.60721000 |
| H | 0.13916100 | 1.97357500 | -0.77037500 |
| C | 0.08495600 | -0.16099400 | -0.44538400 |
| C | 0.90705000 | -1.28244400 | -0.26407500 |
| H | 0.45636600 | -2.25685900 | -0.10984800 |
| C | 2.29672500 | -1.19228900 | -0.24781800 |
| H | 2.89505700 | -2.07770500 | -0.10224700 |
| O | -6.43028200 | 1.35821800 | 0.12534200 |
| N | -7.88804000 | -0.34680000 | -0.38354500 |
| H | -7.94361100 | -1.33589700 | -0.57262400 |
| N | -5.62106200 | -0.67557800 | -0.58696300 |
| H | -5.90320000 | -1.56847400 | -0.96568400 |
| C | -9.11845600 | 0.32181300 | -0.19866000 |
| C | -9.29284800 | 1.63408900 | -0.59142300 |
| H | -8.46427000 | 2.17600000 | -1.02390200 |
| C | -10.54315500 | 2.27066900 | -0.44038200 |
| H | -10.64667700 | 3.30268300 | -0.75559700 |
| C | -11.62129700 | 1.59286800 | 0.07448500 |
| H | -12.58603600 | 2.07791100 | 0.17386900 |
| C | -11.48453900 | 0.24154700 | 0.48575400 |
| C | -12.58260200 | -0.48132400 | 1.02503600 |
| H | -13.54294800 | 0.01770500 | 1.09981200 |
| C | -12.43959000 | -1.78084600 | 1.44889400 |

| | | | |
|---|---|---|---|
| H | -13.28694200 | -2.31857100 | 1.85855200 |
| C | -11.17956800 | -2.41563700 | 1.36264400 |
| H | -11.06440500 | -3.43326400 | 1.71773200 |
| C | -10.09555400 | -1.74723800 | 0.84062900 |
| H | -9.13856400 | -2.25361300 | 0.81169500 |
| C | -10.21219900 | -0.40973500 | 0.37339800 |
| C | -6.62639200 | 0.20933300 | -0.25155500 |
| C | -4.22660200 | -0.48331700 | -0.52537400 |
| C | -3.41632900 | -1.50506300 | -1.04457100 |
| H | -3.87619400 | -2.38433600 | -1.48440700 |
| C | -2.03281100 | -1.40038800 | -1.01634500 |
| H | -1.44293300 | -2.20002100 | -1.44918200 |
| C | -1.39304100 | -0.27555000 | -0.46918100 |
| C | -2.21754700 | 0.73364100 | 0.04925700 |
| H | -1.76905400 | 1.61000300 | 0.50342600 |
| C | -3.60736100 | 0.64532500 | 0.02796800 |
| H | -4.20830300 | 1.43977200 | 0.44127400 |
| H | 5.80211000 | 5.42415300 | -0.90826000 |
| C | 6.26055000 | 4.89497200 | -0.07133300 |
| H | 5.79992800 | 5.26635900 | 0.85015500 |
| H | 7.32768400 | 5.11645200 | -0.02752300 |
| C | 6.00991700 | 3.39047300 | -0.17041100 |
| O | 4.92464500 | 3.01122300 | -0.69671600 |
| O | 6.88693200 | 2.61401700 | 0.30376600 |

**Cartesian coordinates for complex between receptor 3a and DMSO.**

| | | | |
|---|---|---|---|
| O | 4.78155500 | -2.42789500 | -0.16449200 |
| N | 6.31843700 | -0.70873900 | -0.20889000 |
| H | 6.39162500 | 0.30889500 | -0.22041400 |
| N | 4.08132600 | -0.23624400 | -0.33831900 |
| H | 4.43495800 | 0.71834700 | -0.40158100 |
| C | 7.51423400 | -1.45338000 | -0.19336900 |
| C | 7.63374100 | -2.66186800 | -0.85474000 |
| H | 6.78003600 | -3.06877300 | -1.37647500 |
| C | 8.85723100 | -3.36481400 | -0.86142800 |
| H | 8.91455700 | -4.30955600 | -1.39042600 |
| C | 9.96710200 | -2.85849600 | -0.22963000 |
| H | 10.91040800 | -3.39308300 | -0.24883700 |
| C | 9.88894800 | -1.62192100 | 0.46220600 |
| C | 11.01764500 | -1.07800300 | 1.13309200 |
| H | 11.95595200 | -1.62093400 | 1.08883300 |
| C | 10.93081900 | 0.10417800 | 1.82880600 |
| H | 11.80092000 | 0.50455000 | 2.33661100 |
| C | 9.69898600 | 0.79476900 | 1.89340300 |
| H | 9.62793900 | 1.71620800 | 2.46005300 |
| C | 8.58785400 | 0.30102900 | 1.24828900 |
| H | 7.65294500 | 0.84063900 | 1.32703900 |
| C | 8.64570000 | -0.90894300 | 0.50470800 |
| C | 5.03700500 | -1.22812500 | -0.23472800 |
| C | 2.68584900 | -0.37523300 | -0.37379300 |
| C | 1.93045700 | 0.79528500 | -0.56246000 |
| H | 2.43959600 | 1.74441400 | -0.68970800 |
| C | 0.54437300 | 0.75291300 | -0.60432100 |
| H | 0.00144300 | 1.67578200 | -0.77382700 |
| C | -0.15700300 | -0.45588900 | -0.46158700 |
| C | 0.60826300 | -1.61579200 | -0.27426100 |
| H | 0.11007000 | -2.56911300 | -0.13690600 |
| C | 1.99982700 | -1.59087500 | -0.22905700 |
| H | 2.55488500 | -2.50255100 | -0.07503000 |
| O | -6.60982400 | 1.31174700 | 0.13916200 |
| N | -8.12950600 | -0.31049000 | -0.45156000 |
| H | -8.22355100 | -1.28713300 | -0.68565900 |
| N | -5.87639300 | -0.71225500 | -0.67651000 |
| H | -6.19252900 | -1.57736800 | -1.09083800 |
| C | -9.33223700 | 0.39420000 | -0.21955500 |
| C | -9.46692000 | 1.72220400 | -0.57181300 |
| H | -8.62921900 | 2.24559500 | -1.00997100 |
| C | -10.68885700 | 2.39945400 | -0.37283500 |
| H | -10.76176800 | 3.44316300 | -0.65644500 |
| C | -11.77895500 | 1.74609500 | 0.14862800 |
| H | -12.72261500 | 2.26267100 | 0.28479200 |
| C | -11.68297900 | 0.37930100 | 0.51818900 |
| C | -12.79415800 | -0.31901100 | 1.06293300 |
| H | -13.73370800 | 0.21167300 | 1.17476700 |
| C | -12.68888700 | -1.63465000 | 1.44623000 |

| | | | |
|---|---|---|---|
| H | -13.54568200 | -2.15340000 | 1.86067900 |
| C | -11.45518400 | -2.31157700 | 1.31187700 |
| H | -11.36949400 | -3.34264300 | 1.63511700 |
| C | -10.35957500 | -1.66770500 | 0.78335800 |
| H | -9.42223600 | -2.20620100 | 0.71626500 |
| C | -10.43829100 | -0.31383200 | 0.35722000 |
| C | -6.84840400 | 0.19121100 | -0.29430300 |
| C | -4.47638200 | -0.58277200 | -0.59643900 |
| C | -3.70631800 | -1.63162600 | -1.12340300 |
| H | -4.19952800 | -2.48366700 | -1.58027100 |
| C | -2.32014000 | -1.58884100 | -1.07929800 |
| H | -1.76119500 | -2.40773300 | -1.51711100 |
| C | -1.63828000 | -0.50170700 | -0.50789100 |
| C | -2.42211500 | 0.53629300 | 0.01585200 |
| H | -1.94004200 | 1.38527600 | 0.48731800 |
| C | -3.81410600 | 0.51010700 | -0.02127200 |
| H | -4.38437700 | 1.32401700 | 0.39745000 |
| C | 6.83516800 | 4.47083200 | -1.14168200 |
| H | 6.14306800 | 4.49227100 | -1.98354600 |
| H | 7.00944100 | 5.47189500 | -0.74520900 |
| H | 7.78065700 | 4.01284400 | -1.42824100 |
| C | 4.55733500 | 4.32621900 | 0.40347600 |
| H | 3.98391000 | 3.77308600 | 1.14566800 |
| H | 4.77605100 | 5.32869600 | 0.77297300 |
| H | 4.02886500 | 4.36345800 | -0.54910300 |
| O | 5.76656500 | 2.09878500 | -0.49698600 |
| S | 6.13092000 | 3.44109300 | 0.18219400 |

**Cartesian coordinates for complex between receptor 3 conf. A and phosphate.**

| | | | |
|---|---|---|---|
| O | 4.61962000 | -2.58454100 | -0.01463600 |
| N | 6.16762900 | -0.88050700 | -0.20736600 |
| H | 6.23233600 | 0.13385800 | -0.30522900 |
| N | 3.93831700 | -0.40587300 | -0.36376900 |
| H | 4.31115700 | 0.54136500 | -0.48487000 |
| C | 7.36551400 | -1.61244600 | -0.12997700 |
| C | 7.47008700 | -2.91021700 | -0.59952600 |
| H | 6.59941000 | -3.39600100 | -1.01342300 |
| C | 8.69878900 | -3.60186100 | -0.54808600 |
| H | 8.74212500 | -4.61737900 | -0.92596200 |
| C | 9.82920300 | -3.00256900 | -0.04826600 |
| H | 10.77533200 | -3.53185800 | -0.02211200 |
| C | 9.76790200 | -1.67336100 | 0.44528400 |
| C | 10.91935900 | -1.03097500 | 0.97584300 |
| H | 11.85828100 | -1.57480800 | 0.97907100 |
| C | 10.85378400 | 0.24611700 | 1.47956600 |
| H | 11.74131500 | 0.72131400 | 1.88192500 |
| C | 9.62143800 | 0.93826500 | 1.48335600 |
| H | 9.56728100 | 1.93836100 | 1.89834000 |
| C | 8.48704800 | 0.35002500 | 0.97049000 |
| H | 7.55739700 | 0.90363400 | 1.00022200 |
| C | 8.52239000 | -0.96302200 | 0.42621200 |
| C | 4.88249200 | -1.39531000 | -0.18409700 |
| C | 2.54287600 | -0.52704500 | -0.37342500 |
| C | 1.80080200 | 0.65590400 | -0.54222100 |
| H | 2.32258400 | 1.59964300 | -0.66000400 |
| C | 0.41419500 | 0.63144500 | -0.57387700 |
| H | -0.11806100 | 1.56307600 | -0.72895500 |
| C | -0.30203300 | -0.56967200 | -0.43719400 |
| C | 0.44933600 | -1.74119300 | -0.26609900 |
| H | -0.06038500 | -2.68922600 | -0.13392600 |
| C | 1.84152200 | -1.73497700 | -0.23353500 |
| H | 2.38628300 | -2.65507600 | -0.09209700 |
| O | -6.72840100 | 1.28523100 | 0.19034000 |
| N | -8.27297000 | -0.29829000 | -0.43902900 |
| H | -8.38451400 | -1.26865000 | -0.69097500 |
| N | -6.02556900 | -0.74276200 | -0.64198400 |
| H | -6.35401200 | -1.59736900 | -1.06831700 |
| C | -9.46353700 | 0.42982300 | -0.21723600 |
| C | -9.56386800 | 1.76451200 | -0.55562600 |
| H | -8.70827300 | 2.27456100 | -0.97447400 |
| C | -10.77376400 | 2.46595200 | -0.36724200 |
| H | -10.81950100 | 3.51426000 | -0.63935700 |
| C | -11.88582000 | 1.83067000 | 0.12964600 |
| H | -12.81996000 | 2.36627900 | 0.25766000 |
| C | -11.82538400 | 0.45784200 | 0.48400600 |
| C | -12.95979800 | -0.22238800 | 1.00314800 |
| H | -13.88922700 | 0.32738500 | 1.10716300 |
| C | -12.88909600 | -1.54450000 | 1.37186000 |

| | | | |
|---|---|---|---|
| H | -13.76329800 | -2.04920700 | 1.76686300 |
| C | -11.66846400 | -2.24669800 | 1.24804100 |
| H | -11.61024700 | -3.28317600 | 1.55989500 |
| C | -10.55105500 | -1.62073300 | 0.74422900 |
| H | -9.62455500 | -2.17854000 | 0.68470200 |
| C | -10.59370800 | -0.26046100 | 0.33366700 |
| C | -6.98376600 | 0.17521900 | -0.26036100 |
| C | -4.62353100 | -0.63550200 | -0.55962400 |
| C | -3.86952800 | -1.69172900 | -1.09485700 |
| H | -4.37559700 | -2.53318800 | -1.55727300 |
| C | -2.48278500 | -1.66894700 | -1.05333800 |
| H | -1.93650400 | -2.49227300 | -1.49872200 |
| C | -1.78402800 | -0.59565200 | -0.47605500 |
| C | -2.55224200 | 0.44888900 | 0.05795900 |
| H | -2.05725800 | 1.28747400 | 0.53459600 |
| C | -3.94462800 | 0.44285100 | 0.02341500 |
| H | -4.50238000 | 1.26179200 | 0.44917600 |
| O | 4.53825100 | 4.29041000 | -0.36320100 |
| O | 5.56235800 | 1.88120700 | -0.66060300 |
| O | 6.97384700 | 4.01057400 | -0.94684100 |
| P | 5.67347300 | 3.32326800 | -0.20634900 |
| O | 6.14163900 | 3.22540200 | 1.37076000 |
| H | 7.71725900 | 3.39881300 | -1.02084800 |
| H | 6.10233000 | 4.08215400 | 1.81415900 |

**Cartesian coordinates for complex between receptor 3 conf. B and acetate.**

| | | | |
|---|---|---|---|
| O | -6.55931200 | 0.46490700 | 0.48489700 |
| N | -7.78903800 | -1.47039700 | 0.37885700 |
| H | -7.73534900 | -2.45466000 | 0.60159700 |
| N | -5.49293100 | -1.55810900 | 0.20285300 |
| H | -5.66575400 | -2.53070700 | -0.00817300 |
| C | -9.05151000 | -0.85339000 | 0.63018800 |
| C | -9.69907000 | -1.10014500 | 1.82105900 |
| H | -9.22076200 | -1.72638800 | 2.56574300 |
| C | -10.96870800 | -0.53930800 | 2.08505100 |
| H | -11.45590900 | -0.75026200 | 3.02986200 |
| C | -11.56966600 | 0.27935800 | 1.16014100 |
| H | -12.53766500 | 0.72418700 | 1.36376800 |
| C | -10.93809500 | 0.55037300 | -0.08245600 |
| C | -11.55263800 | 1.37576400 | -1.06303700 |
| H | -12.51411500 | 1.82392100 | -0.83587500 |
| C | -10.94990600 | 1.59847400 | -2.27777800 |
| H | -11.43019400 | 2.22834100 | -3.01787600 |
| C | -9.70300400 | 0.99679500 | -2.57096600 |
| H | -9.24161700 | 1.16424700 | -3.53761500 |
| C | -9.07524000 | 0.20113100 | -1.64129000 |
| H | -8.12408200 | -0.25759400 | -1.87731500 |
| C | -9.66289400 | -0.03670800 | -0.37056500 |
| C | -6.60187500 | -0.75433400 | 0.37256300 |
| C | -4.13404400 | -1.18609100 | 0.19683200 |
| C | -3.20077500 | -2.16320300 | -0.18201500 |
| H | -3.54485400 | -3.14891400 | -0.47881800 |
| C | -1.84147100 | -1.88231600 | -0.19462400 |
| H | -1.15470000 | -2.65692000 | -0.51563500 |
| C | -1.34979300 | -0.61769200 | 0.16957000 |
| C | -2.29631300 | 0.34609400 | 0.54768100 |
| H | -1.96320300 | 1.32950100 | 0.85976200 |
| C | -3.66337600 | 0.08126500 | 0.56481500 |
| H | -4.36057200 | 0.84725600 | 0.86604200 |
| O | 5.30614600 | -1.36467300 | 0.53797500 |
| N | 6.52510600 | 0.56878700 | 0.29453200 |
| H | 6.47787800 | 1.59964500 | 0.39744400 |
| N | 4.24049000 | 0.63807700 | 0.09586800 |
| H | 4.40999900 | 1.63202000 | -0.13891200 |
| C | 7.78580700 | -0.02587900 | 0.56533200 |
| C | 8.47334300 | 0.34130700 | 1.70428200 |
| H | 8.01385500 | 1.04028000 | 2.39362000 |
| C | 9.75222300 | -0.18771300 | 1.98854400 |
| H | 10.26446100 | 0.12025300 | 2.89303200 |
| C | 10.33277100 | -1.09664800 | 1.13761300 |
| H | 11.30796100 | -1.51704000 | 1.35879700 |
| C | 9.66740100 | -1.49239500 | -0.05299200 |
| C | 10.25974700 | -2.40968000 | -0.96365900 |
| H | 11.22889800 | -2.83158400 | -0.71868000 |
| C | 9.62813900 | -2.75134900 | -2.13549200 |

| | | | |
|---|---|---|---|
| H | 10.09278300 | -3.44969000 | -2.82245600 |
| C | 8.37235600 | -2.18201600 | -2.45462900 |
| H | 7.88801700 | -2.44193700 | -3.38923500 |
| C | 7.76550100 | -1.30114900 | -1.58982000 |
| H | 6.80683300 | -0.86861400 | -1.84362900 |
| C | 8.38170400 | -0.93964800 | -0.36237600 |
| C | 5.34850100 | -0.14956400 | 0.33012900 |
| C | 2.89333700 | 0.25646700 | 0.12900500 |
| C | 1.94274300 | 1.24147200 | -0.20124200 |
| H | 2.28776300 | 2.23209600 | -0.47512100 |
| C | 0.58482600 | 0.95778600 | -0.18777700 |
| H | -0.11115100 | 1.73970000 | -0.47054700 |
| C | 0.10202200 | -0.31682300 | 0.15502100 |
| C | 1.05816200 | -1.28874200 | 0.48298000 |
| H | 0.73338400 | -2.28115600 | 0.77628600 |
| C | 2.42525700 | -1.02262000 | 0.47306600 |
| H | 3.13096600 | -1.79469900 | 0.73606900 |
| H | 5.16718800 | 5.84141300 | -1.07944200 |
| C | 5.62875100 | 5.49545300 | -0.15310400 |
| H | 5.05886900 | 5.91948800 | 0.68031300 |
| H | 6.65293200 | 5.86429000 | -0.08490700 |
| C | 5.57930000 | 3.97089000 | -0.05366800 |
| O | 4.57516700 | 3.38497300 | -0.55123700 |
| O | 6.52945700 | 3.38775800 | 0.54197000 |

**Cartesian coordinates for complex between receptor 3 conf. B and DMSO.**

| | | | |
|---|---|---|---|
| O | -5.08100600 | -1.67329700 | -0.64159600 |
| N | -6.33581000 | 0.18692900 | -0.14545600 |
| H | -6.27577500 | 1.20082100 | -0.03990100 |
| N | -4.05016900 | 0.31624700 | -0.07079500 |
| H | -4.26274700 | 1.28962600 | 0.14779500 |
| C | -7.60329300 | -0.37173600 | -0.47290200 |
| C | -8.30050500 | 0.12734800 | -1.55275900 |
| H | -7.84974300 | 0.90544200 | -2.15826400 |
| C | -9.58103600 | -0.36905100 | -1.88498000 |
| H | -10.10453800 | 0.04257000 | -2.74021300 |
| C | -10.14841800 | -1.37499700 | -1.14119900 |
| H | -11.12527700 | -1.76916800 | -1.39992300 |
| C | -9.46866500 | -1.90986300 | -0.01497400 |
| C | -10.04700200 | -2.93402000 | 0.78353900 |
| H | -11.01832100 | -3.32639600 | 0.50135600 |
| C | -9.39794400 | -3.41495800 | 1.89530000 |
| H | -9.85132600 | -4.19435200 | 2.49722500 |
| C | -8.13812500 | -2.88600500 | 2.26435700 |
| H | -7.63966100 | -3.25953000 | 3.15177900 |
| C | -7.54454900 | -1.90280400 | 1.50761100 |
| H | -6.58215800 | -1.50280300 | 1.79817400 |
| C | -8.18053500 | -1.39415400 | 0.34408800 |
| C | -5.14610400 | -0.48890800 | -0.31754700 |
| C | -2.69085500 | -0.02383600 | -0.11045000 |
| C | -1.76756300 | 0.98280900 | 0.22218700 |
| H | -2.12905700 | 1.96553300 | 0.50564500 |
| C | -0.40281700 | 0.73330100 | 0.21140600 |
| H | 0.27300900 | 1.53111100 | 0.49759900 |
| C | 0.10964400 | -0.52904200 | -0.13159900 |
| C | -0.82196900 | -1.52366800 | -0.46222600 |
| H | -0.47282800 | -2.50757800 | -0.75535100 |
| C | -2.19481200 | -1.29047200 | -0.45541500 |
| H | -2.88195700 | -2.07743800 | -0.72352600 |
| O | 6.75104800 | 0.39909400 | -0.49238400 |
| N | 8.02363400 | -1.50546400 | -0.34600000 |
| H | 7.99124600 | -2.49673000 | -0.53992500 |
| N | 5.73054000 | -1.64002900 | -0.16089200 |
| H | 5.92508800 | -2.60551600 | 0.06368800 |
| C | 9.27139800 | -0.86761400 | -0.61936400 |
| C | 9.91494200 | -1.12469100 | -1.81014000 |
| H | 9.44419500 | -1.77553400 | -2.53833900 |
| C | 11.17051000 | -0.54286000 | -2.09523800 |
| H | 11.65510900 | -0.76258100 | -3.03938100 |
| C | 11.76092500 | 0.30657500 | -1.19151900 |
| H | 12.71787300 | 0.76722400 | -1.41155200 |
| C | 11.13299800 | 0.58948800 | 0.05026500 |
| C | 11.73704300 | 1.44741900 | 1.00917800 |
| H | 12.68724200 | 1.91080100 | 0.76573300 |
| C | 11.13841200 | 1.68231700 | 2.22365900 |

| | | | |
|---|---|---|---|
| H | 11.61066000 | 2.33703500 | 2.94717100 |
| C | 9.90650200 | 1.06095400 | 2.53839600 |
| H | 9.44860700 | 1.23857100 | 3.50489600 |
| C | 9.28900400 | 0.23341900 | 1.62989100 |
| H | 8.34937400 | -0.24017100 | 1.88223100 |
| C | 9.87260300 | -0.01820700 | 0.35998400 |
| C | 6.82137100 | -0.81602000 | -0.35241700 |
| C | 4.36407800 | -1.29930700 | -0.16114400 |
| C | 3.45277800 | -2.29640300 | 0.21976700 |
| H | 3.81913500 | -3.27251600 | 0.52125700 |
| C | 2.08748600 | -2.04728900 | 0.22817000 |
| H | 1.41805200 | -2.83639800 | 0.55046100 |
| C | 1.56822800 | -0.79574600 | -0.14220000 |
| C | 2.49227700 | 0.18864600 | -0.52173400 |
| H | 2.13697600 | 1.16287700 | -0.83815300 |
| C | 3.86512700 | -0.04436900 | -0.53489900 |
| H | 4.54533400 | 0.73616700 | -0.83743300 |
| S | -5.50055900 | 4.18503500 | -0.39522000 |
| C | -6.85659200 | 5.10928300 | 0.39017100 |
| H | -6.67546100 | 5.16603500 | 1.46360600 |
| H | -6.90393500 | 6.10280800 | -0.05714300 |
| H | -7.77443700 | 4.56203500 | 0.18022600 |
| C | -4.10969600 | 5.20412000 | 0.18401600 |
| H | -3.19768200 | 4.73219700 | -0.17809800 |
| H | -4.20947200 | 6.20083900 | -0.24719000 |
| H | -4.12244000 | 5.24061000 | 1.27341600 |
| O | -5.40036500 | 2.85821700 | 0.39672800 |

**Cartesian coordinates for complex between receptor 3 conf. B and phosphate.**

| | | | |
|---|---|---|---|
| O | 6.87674100 | 0.40278800 | -0.48080700 |
| N | 8.15475500 | -1.49908000 | -0.34421700 |
| H | 8.12640100 | -2.48823700 | -0.54929300 |
| N | 5.86124500 | -1.64242000 | -0.17250300 |
| H | 6.05805400 | -2.60965600 | 0.04236300 |
| C | 9.40172300 | -0.85449600 | -0.60437600 |
| C | 10.05419900 | -1.09957200 | -1.79286900 |
| H | 9.59093300 | -1.74645000 | -2.52937300 |
| C | 11.30921500 | -0.51045400 | -2.06514200 |
| H | 11.80077400 | -0.72070200 | -3.00785000 |
| C | 11.89024200 | 0.33429900 | -1.15100800 |
| H | 12.84660600 | 0.80071600 | -1.36121800 |
| C | 11.25311200 | 0.60476700 | 0.08886000 |
| C | 11.84741200 | 1.45752700 | 1.05842500 |
| H | 12.79715700 | 1.92684700 | 0.82473200 |
| C | 11.24005200 | 1.68026800 | 2.27086100 |
| H | 11.70484300 | 2.33125400 | 3.00253200 |
| C | 10.00882800 | 1.05123600 | 2.57277400 |
| H | 9.54399600 | 1.21924800 | 3.53767600 |
| C | 9.40062300 | 0.22845400 | 1.65374400 |
| H | 8.46141200 | -0.25101900 | 1.89630100 |
| C | 9.99326900 | -0.01051500 | 0.38558400 |
| C | 6.94992400 | -0.81332500 | -0.35105900 |
| C | 4.49302600 | -1.30738300 | -0.17836400 |
| C | 3.58339300 | -2.31468100 | 0.17864400 |
| H | 3.95203000 | -3.29415300 | 0.46622700 |
| C | 2.21688100 | -2.07170900 | 0.18103100 |
| H | 1.54859600 | -2.86905900 | 0.48493300 |
| C | 1.69421800 | -0.81653900 | -0.17235600 |
| C | 2.61712300 | 0.17799800 | -0.52798600 |
| H | 2.25979700 | 1.15588100 | -0.83047800 |
| C | 3.99120900 | -0.04851000 | -0.53435500 |
| H | 4.67012700 | 0.74015500 | -0.81819300 |
| O | -4.92472400 | -1.76460000 | -0.53491200 |
| N | -6.22047100 | 0.11869400 | -0.35818400 |
| H | -6.24344900 | 1.13836900 | -0.48255300 |
| N | -3.93080800 | 0.28035700 | -0.14197300 |
| H | -4.11762600 | 1.26147300 | 0.09669700 |
| C | -7.44981000 | -0.55473200 | -0.60688000 |
| C | -8.12218500 | -0.32021300 | -1.78756000 |
| H | -7.67915100 | 0.34013500 | -2.52408500 |
| C | -9.36639400 | -0.93574500 | -2.05263200 |
| H | -9.87000200 | -0.73218500 | -2.99076100 |
| C | -9.92330900 | -1.79648400 | -1.13830400 |
| H | -10.87127300 | -2.28245100 | -1.34287400 |
| C | -9.26996400 | -2.05713700 | 0.09543400 |
| C | -9.83820200 | -2.92460800 | 1.06788400 |
| H | -10.78024200 | -3.41281200 | 0.84106300 |
| C | -9.21638200 | -3.13806200 | 2.27485700 |

| | | | |
|---|---|---|---|
| H | -9.66184800 | -3.80027200 | 3.00864800 |
| C | -7.99599700 | -2.48409600 | 2.56816400 |
| H | -7.51976800 | -2.64436700 | 3.52894500 |
| C | -7.41345900 | -1.64660200 | 1.64551700 |
| H | -6.48254800 | -1.14698900 | 1.87958400 |
| C | -8.02062100 | -1.41643600 | 0.38255500 |
| C | -5.01264000 | -0.54731000 | -0.36327600 |
| C | -2.57007100 | -0.06327600 | -0.16330000 |
| C | -1.65306500 | 0.94333800 | 0.19218800 |
| H | -2.03034800 | 1.91903300 | 0.47627200 |
| C | -0.28744300 | 0.69827500 | 0.18793600 |
| H | 0.38324600 | 1.49491300 | 0.48999900 |
| C | 0.23441500 | -0.55650300 | -0.16955000 |
| C | -0.68995400 | -1.54946800 | -0.52399300 |
| H | -0.33414100 | -2.52711600 | -0.83034200 |
| C | -2.06414500 | -1.32216700 | -0.52445300 |
| H | -2.74418600 | -2.10982500 | -0.80748800 |
| O | -4.24231400 | 3.07419300 | 0.55266400 |
| O | -6.55500100 | 2.97556400 | -0.65422900 |
| O | -6.05236500 | 4.68715300 | 1.22791200 |
| P | -5.45490900 | 3.77868100 | -0.00538000 |
| O | -5.00541600 | 4.90390300 | -1.11698100 |
| H | -6.90032000 | 5.09351200 | 1.00813500 |
| H | -4.22517000 | 5.40183500 | -0.84192900 |

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