Supporting Information

# Solution and solid state studies of urea derivatives of DITIPIRAM acting as powerful anion receptors

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**Contents**

# 1. Crystal Data

Diffractometer and data collection

The X-ray measurements of **6**@(DMSO·H2O) and **6**@(Cl)TBA were performed at 100(2) K on a Bruker D8 Venture Photon100 diffractometer equipped with a TRIUMPH monochromator and a MoKα fine focus sealed tube (λ = 0.71073 Å) using Bruker APEX2 program [1]. Data were corrected for absorption effects using the multi-scan method (SADABS) [2]. The structure was solved and refined using SHELXTL Software Package [3].
All non-hydrogen atoms were refined anisotropically. Most of hydrogen atoms were placed in calculated positions and refined within the riding model. Position and temperature factors of four hydrogen atoms engaged in hydrogen bonds were refined. The temperature factors of all other hydrogen atoms were not refined and were set to be either 1.2 or 1.5 times larger than Ueq of the corresponding heavy atom. The atomic scattering factors were taken from the International Tables [4]. Thermal ellipsoids parameters are presented at 50% probability level.

**Table S1.** Crystal data and structure refinement details for **6**@(DMSO·H2O) and **6**@(Cl)TBA.

| Compound | **6**@(DMSO·H2O) | **6**@(Cl)TBA |
|---|---|---|
| Empirical formula | $C_{28}H_{29}F_2N_5O_4S_3$ | $C_{42}H_{57}ClF_2N_6O_2S_2$ |
| Formula weight | 633.74 | 815.50 |
| CCDC No. | 2063422 | 2063423 |
| Wavelength | 1.54184 | 1.54184 |
| Crystal system | monoclinic | monoclinic |
| Space group | P $2_1$/n | P $2_1$ |
| Unit cell dimensions | a = 10.2142(5) Å<br>b = 22.3169(11) Å<br>c = 12.6528(6) Å<br>β = 90.0136(12)° | a = 8.4288(4) Å<br>b = 28.6479(13) Å<br>c = 17.9789(8) Å<br>β = 99.7682(13)° |
| Volume | 2884.2 Å$^3$ | 4278.4 Å$^3$ |
| Z | 4 | 4 |
| Density Calc. | 1.459 g/cm$^3$ | 1.266 g/cm$^3$ |
| F(000) | 1320 | 1736 |
| Crystal size | 0.104 × 0.273 × 0.559 mm | 0.034 x 0.246 x 0.296 mm |
| Index ranges | -12 ≤ h ≤ 12<br>-26 ≤ k ≤ 26<br>-15 ≤ l ≤ 15 | -10 ≤ h ≤ 10<br>-34 ≤ k ≤ 34<br>-21 ≤ l ≤ 21 |
| Reflections collected (all / independent) | 38247/5095 | 70952/15117 |
| Absorption correction | multi-scan | multi-scan |
| Restraints / parameters | 5095/407 | 15117/1098 |
| Goodness-of-fit on $F^2$ | 1.040 | 1.028 |

Thermal ellipsoid plots (ORTEP) for reported crystal structures with the thermal ellipsoids shown at a 50% probability level

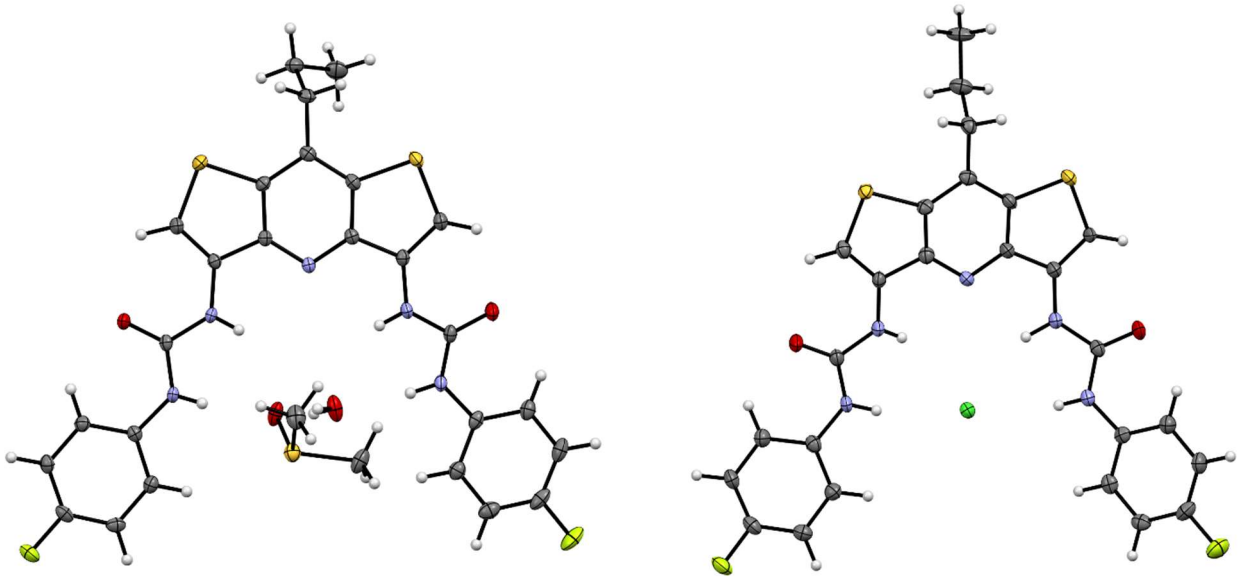
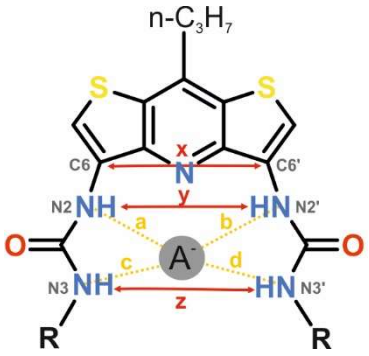


**Figure S1**. Thermal ellipsoid plot (ORTEP) diagram for structures **6**@(DMSO·H2O) (left) and **6**@(Cl)TBA (right).

## 2. Computational studies




**a-d** - hydrogen bonds
**x**, **y**, **z** - distances between given atoms
**R** = Alk, aryl

**Table S2.** Relevant geometrical descriptors, hydrogen bond lengths, and calculated Gibbs free energies of energy-optimized complexes of receptors **2-7** with anions[a]

| Structure | Descriptors (Å) | | | Hydrogen bond lengths (Å) | | | | $\Delta(\Delta G^0)$[b] |
|---|---|---|---|---|---|---|---|---|
| | x | y | z | a | b | c | d | |
| **2**@$Cl^-$ | 4.88 | 4.96 | 6.81 | 3.45 | 3.44 | 3.43 | 3.42 | -28.3 |
| **3**@$Cl^-$ | 4.87 | 4.95 | 6.71 | 3.43 | 3.44 | 3.36 | 3.37 | -31.4 |
| **4**@$Cl^-$ | 4.87 | 4.94 | 6.67 | 3.42 | 3.42 | 3.34 | 3.35 | **-39.3** |
| **5**@$Cl^-$ | 4.87 | 4.94 | 6.68 | 3.43 | 3.43 | 3.36 | 3.35 | -34.5 |
| **6**@$Cl^-$ | 4.87 | 4.94 | 6.70 | 3.43 | 3.43 | 3.36 | 3.36 | -31.4 |
| **6**@$Cl^-$[a] | 4.82 | 4.87 | 6.54 | 3.39 | 3.46 | 3.29 | 3.30 | - |
| **7**@$Cl^-$ | 4.87 | 4.94 | 6.68 | 3.46 | 3.45 | 3.35 | 3.36 | -31.8 |
| **2**@$MeCO_2^-$ | 4.92 | 5.14 | 7.30 | 2.86 | 2.86 | 2.85 | 2.87 | -52.1 |
| **3**@$MeCO_2^-$ | 4.96 | 5.32 | 7.65 | 2.83 | 2.82 | 2.75 | 2.75 | -73.7 |
| **4**@$MeCO_2^-$ | 4.96 | 5.31 | 7.62 | 2.82 | 2.81 | 2.73 | 2.73 | -72.4 |
| **5**@$MeCO_2^-$ | 4.92 | 5.16 | 7.27 | 2.86 | 2.85 | 2.80 | 2.78 | **-75.6** |
| **6**@$MeCO_2^-$ | 4.96 | 5.31 | 7.64 | 2.83 | 2.83 | 2.74 | 2.74 | -65.1 |
| **7**@$MeCO_2^-$ | 4.92 | 5.16 | 7.28 | 2.86 | 2.85 | 2.80 | 2.82 | -70.9 |
| **2**@$PhCO_2^-$ | 4.91 | 5.10 | 7.19 | 2.92 | 2.92 | 2.93 | 2.89 | -48.4 |
| **3**@$PhCO_2^-$ | 4.93 | 5.18 | 7.30 | 2.80 | 2.85 | 2.80 | 2.82 | -60.2 |
| **4**@$PhCO_2^-$ | 4.93 | 5.17 | 7.26 | 2.87 | 2.83 | 2.78 | 2.81 | **-65.3** |
| **5**@$PhCO_2^-$ | 4.93 | 5.18 | 7.29 | 2.88 | 2.84 | 2.78 | 2.81 | -61.8 |
| **6**@$PhCO_2^-$ | 4.91 | 5.12 | 7.19 | 2.86 | 2.90 | 2.83 | 2.83 | -60.6 |
| **7**@$PhCO_2^-$ | 4.92 | 5.14 | 7.25 | 2.87 | 2.87 | 2.83 | 2.85 | -64.7 |

[a] The structures were found using conformational search analysis; the final geometry optimization (without constrains) and energy calculations was calculated at DFT/M06-2X/6-31G(d)/C-PCM:DMSO level of theory using Spartan'18 Parallel Suite. [b] Free binding energy $\Delta(\Delta G^0) = \Delta G^0_{complex} - (\Delta G^0_{receptor} + \Delta G^0_{anion})$ in kJ/mol.

## 3. Copies of $^{1}H$ and $^{13}C$ NMR spectra

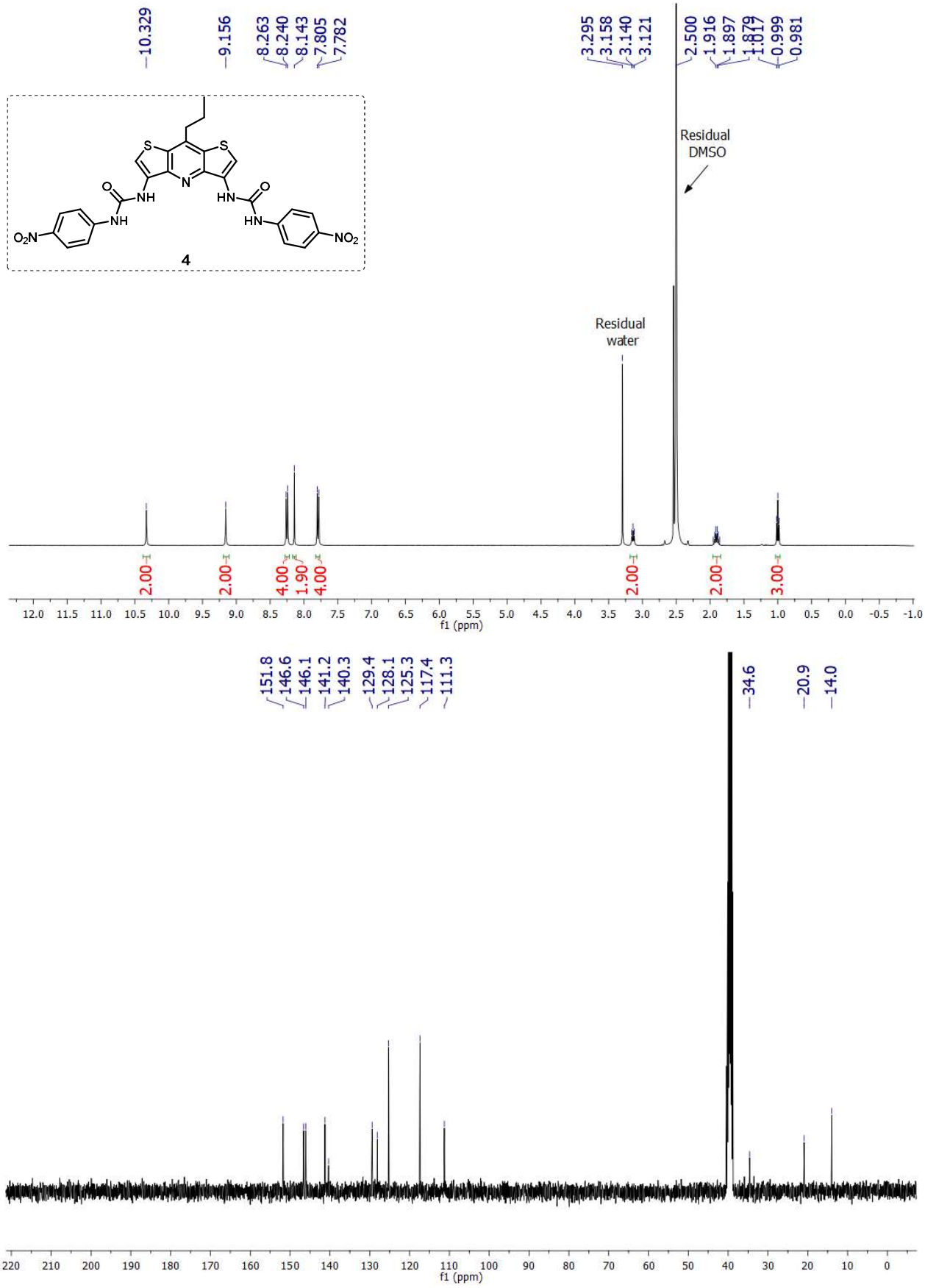



**Figure S2.** $^{1}H$ NMR (400 MHz) and $^{13}C$ NMR (100 MHz) spectra of compound **4** in DMSO-$d_6$.

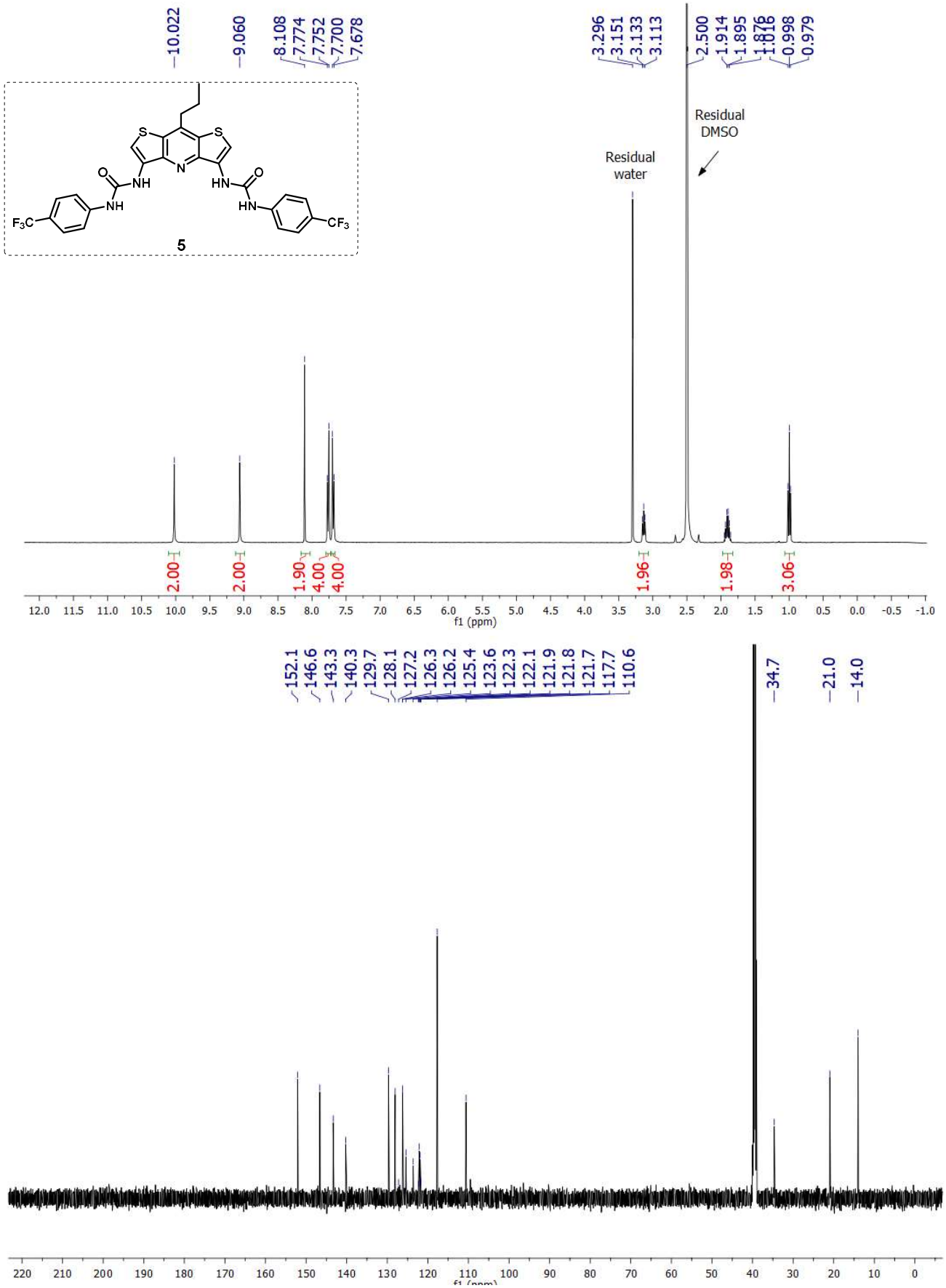



**Figure S3.** $^{1}$H NMR (400 MHz) and $^{13}$C NMR (100 MHz) spectra of compound **5** in DMSO-$d_6$.

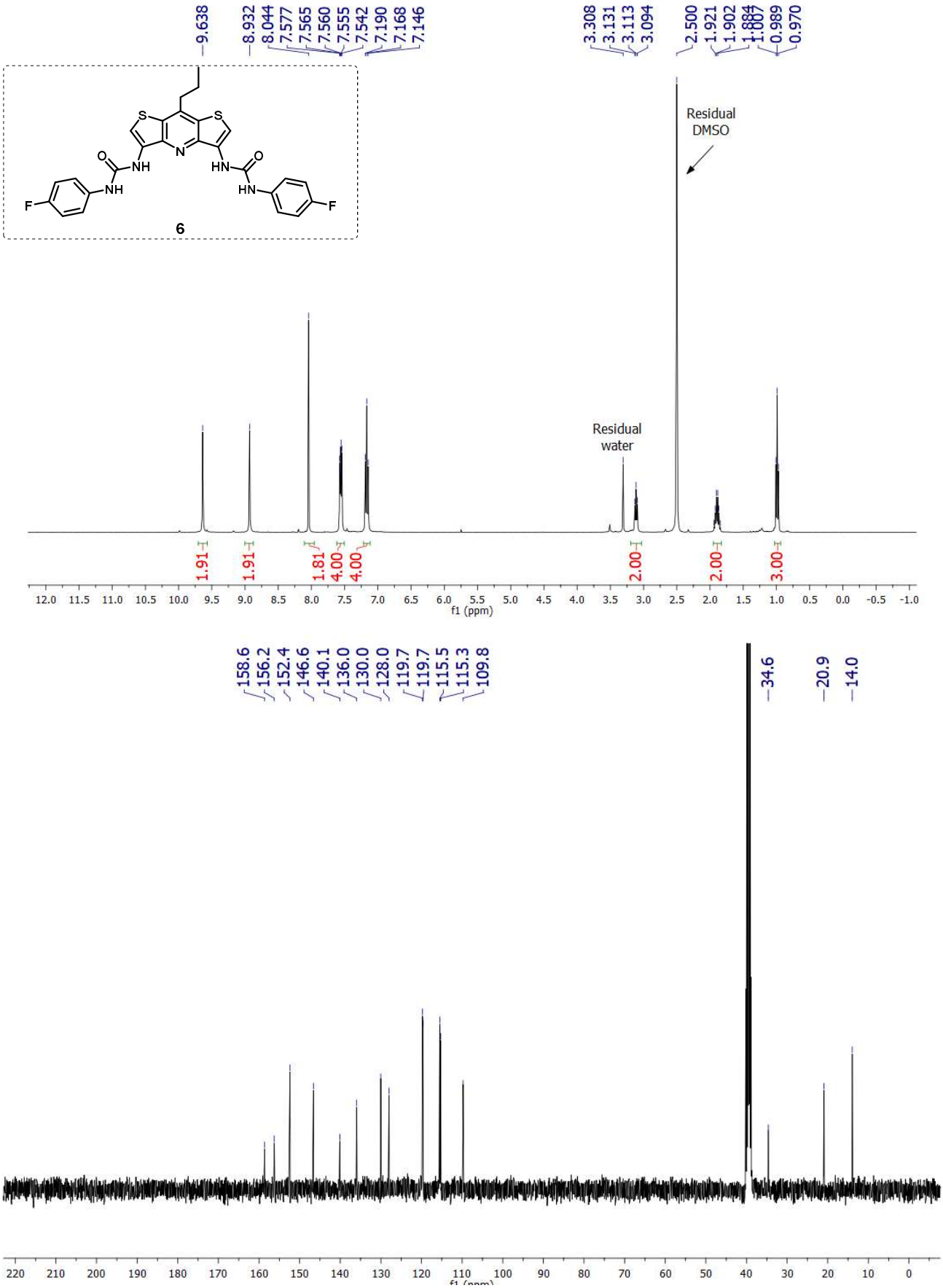



**Figure S4.** $^{1}$H NMR (400 MHz) and $^{13}$C NMR (100 MHz) spectra of compound **6** in DMSO-$d_6$.

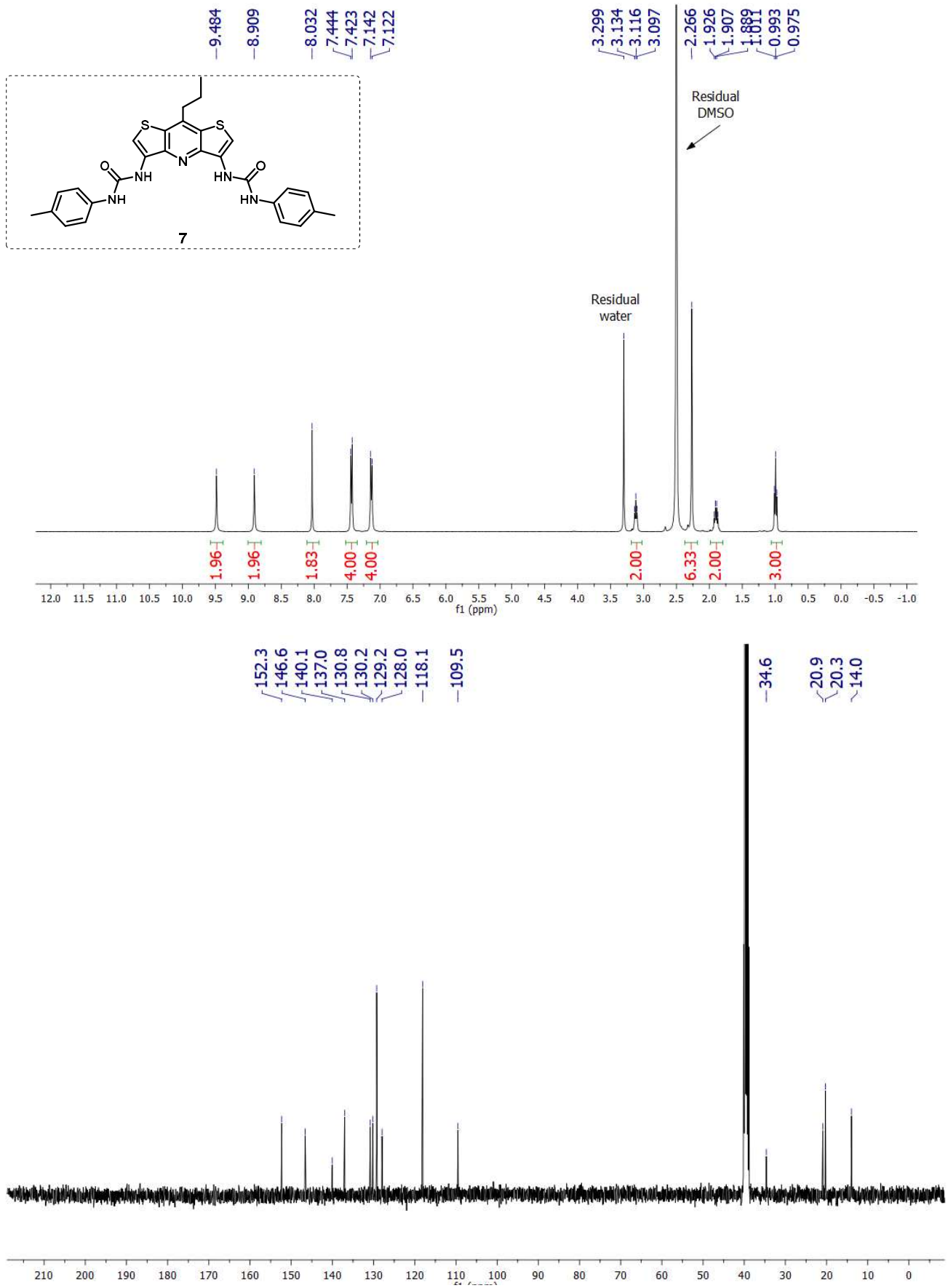



**Figure S5.** $^{1}$H NMR (400 MHz) and $^{13}$C NMR (100 MHz) spectra of compound **7** in DMSO-$d_6$.

## 4. Titration experiments

As the source of anions, commercially available tetrabutylammonium salts were used. The host solution was titrated in a NMR tube with the solution of the respective TBA salt in receptor aliquots (details are given in Table S3 and S4). The binding constants were calculated from the changes in chemical shifts of ligand protons which were shifted during titration. Nonlinear curve fitting was carried out with HypNMR 2008 [5] (Version 4.0.71) program with fitting to the appropriate global binding model (see Table S3 and S4).

**Table. S3.** Titration details and global stability constants $K_a$ ($M^{-1}$) for Receptors **5-7** with various anions in DMSO-$d_6$ + 0.5% $H_2O$[a]

| Entry | Receptor | Anion | $C_{Host}$ [M] | $C_{Guest}$ [M] | $K_a$ [$M^{-1}$] |
|---|---|---|---|---|---|
| 1 | **5** | $Cl^-$ | 0.01021 | 0.11190 | 3400±80 |
| 2 | | $MeCO_2^-$ | | 0.11144 | >10000 [b] |
| 3 | | $PhCO_2^-$ | | 0.08957 | >10000 [b] |
| 4 | | $H_2PO_4^-$ | | 0.13135 | - [c] |
| 5 | **6** | $Cl^-$ | 0.01039 | 0.12261 | 4650±250 |
| 6 | | $MeCO_2^-$ | | 0.09386 | > 10000 [b] |
| 7 | | $PhCO_2^-$ | | 0.09747 | > 10000 [b] |
| 8 | | $H_2PO_4^-$ | | 0.09582 | - [c] |
| 9 | **7** | $Cl^-$ | 0.01011 | 0.12144 | 2500±50 |
| 10 | | $MeCO_2^-$ | | 0.09195 | > 10000 [b] |
| 11 | | $H_2PO_4^-$ | | 0.12078 | - [c] |

[a] Values determined by $^1$H NMR titration experments at *T* = 303K using HypNMR 2008 software [5], errors < 10%, TBA salts as the source of anions. [b] Stability constants above the limit of the $^1$H NMR titration technique ($\geq 10000$). [c] Not determined.

**Tab. S4.** Titration details and global stability constants $K_a$ ($M^{-1}$) for Receptors **5-7** with various anions in DMSO-$d_6$ + 10% $CD_3OH$ [a]

| Entry | Receptor | Anion | $C_{Host}$ [M] | $C_{Guest}$ [M] | $K_a$ [$M^{-1}$] |
|---|---|---|---|---|---|
| 1 | **5** | $Cl^-$ | 0.01024 | 0.10714 | 1040±20 |
| 2 | | $MeCO_2^-$ | | 0.09991 | 6300±300 |
| 3 | | $PhCO_2^-$ | | 0.09874 | 2400±80 |
| 4 | | $H_2PO_4^-$ | | 0.14096 | - [b] |
| 5 | **6** | $Cl^-$ | 0.01023 | 0.12818 | 1250±20 |
| 6 | | $MeCO_2^-$ | | 0.09904 | 6400±300 |
| 7 | | $PhCO_2^-$ | | 0.10073 | 2050±40 |
| 8 | | $H_2PO_4^-$ | | 0.09361 | - [b] |
| 9 | **7** | $Cl^-$ | 0.01003 | 0.13525 | 915±10 |
| 10 | | $MeCO_2^-$ | | 0.09795 | 2950±150 |
| 11 | | $H_2PO_4^-$ | | 0.10495 | - [b] |

[a] Values determined by $^1$H NMR titration experments at *T* = 303K using HypNMR 2008 software [5], errors < 10%, TBA salts as the source of anions. [b] Not determined.

**Figure S6.** Labeling of the selected proton peaks of the receptors **5-7**.

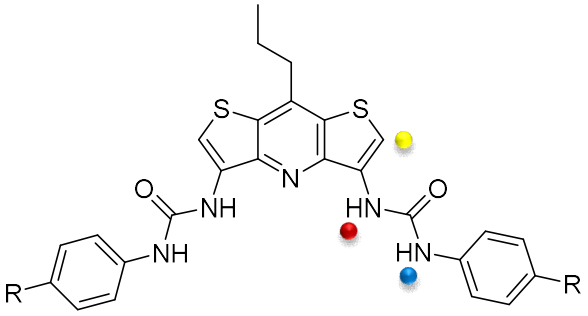
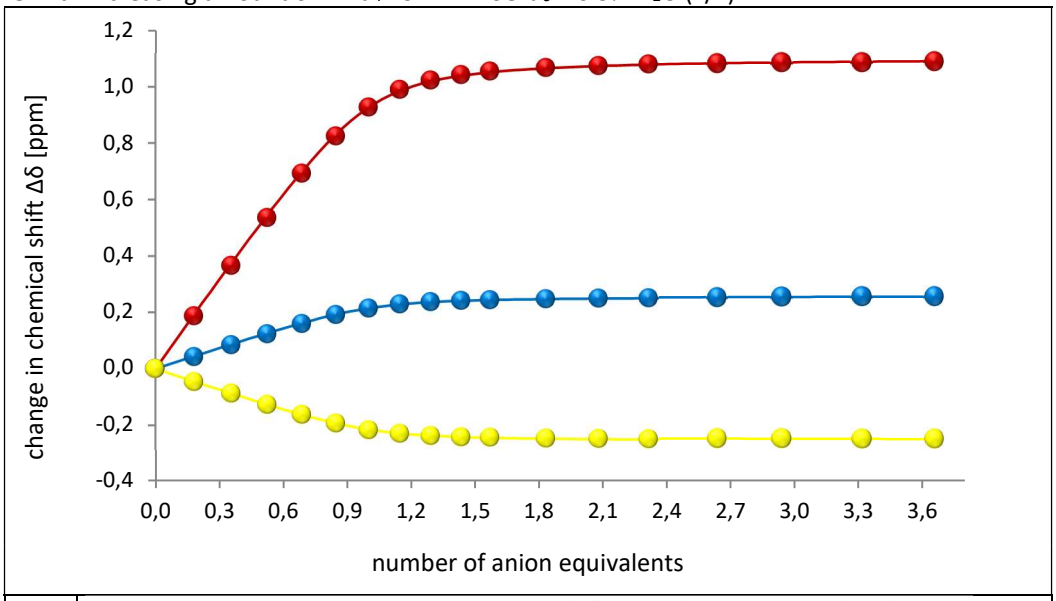


**Table S4.** Corresponding experimental chemical shift changes (symbols) and calculated binding isotherms (lines) assuming 1:1 binding model; Stacked plots from $^{1}$H NMR titrations of Receptor **5** with increasing amount of n-$Bu_4NCl$ in DMSO-$d_6$ + 0.5% $H_2O$ (v/v).



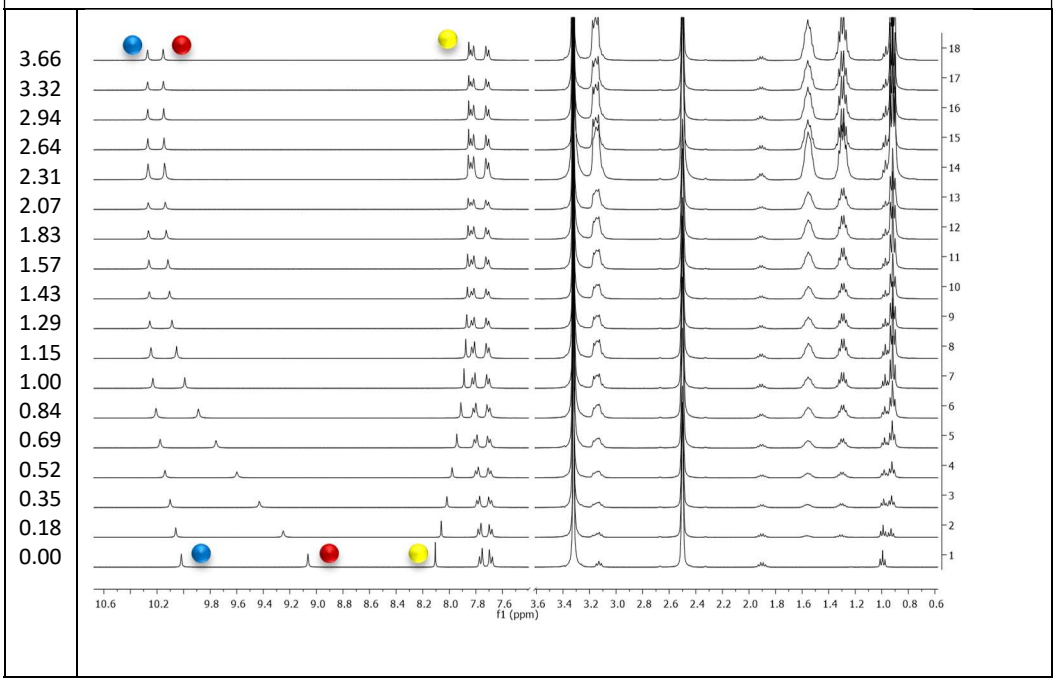



**Table S5.** Corresponding experimental chemical shift changes (symbols) and calculated binding isotherms (lines) assuming 1:1 binding model; Stacked plots from $^{1}$H NMR titrations of Receptor **5** with increasing amount of n-Bu4NCO$_2$Me in DMSO-$d_6$ + 0.5% $H_2O$ (v/v).

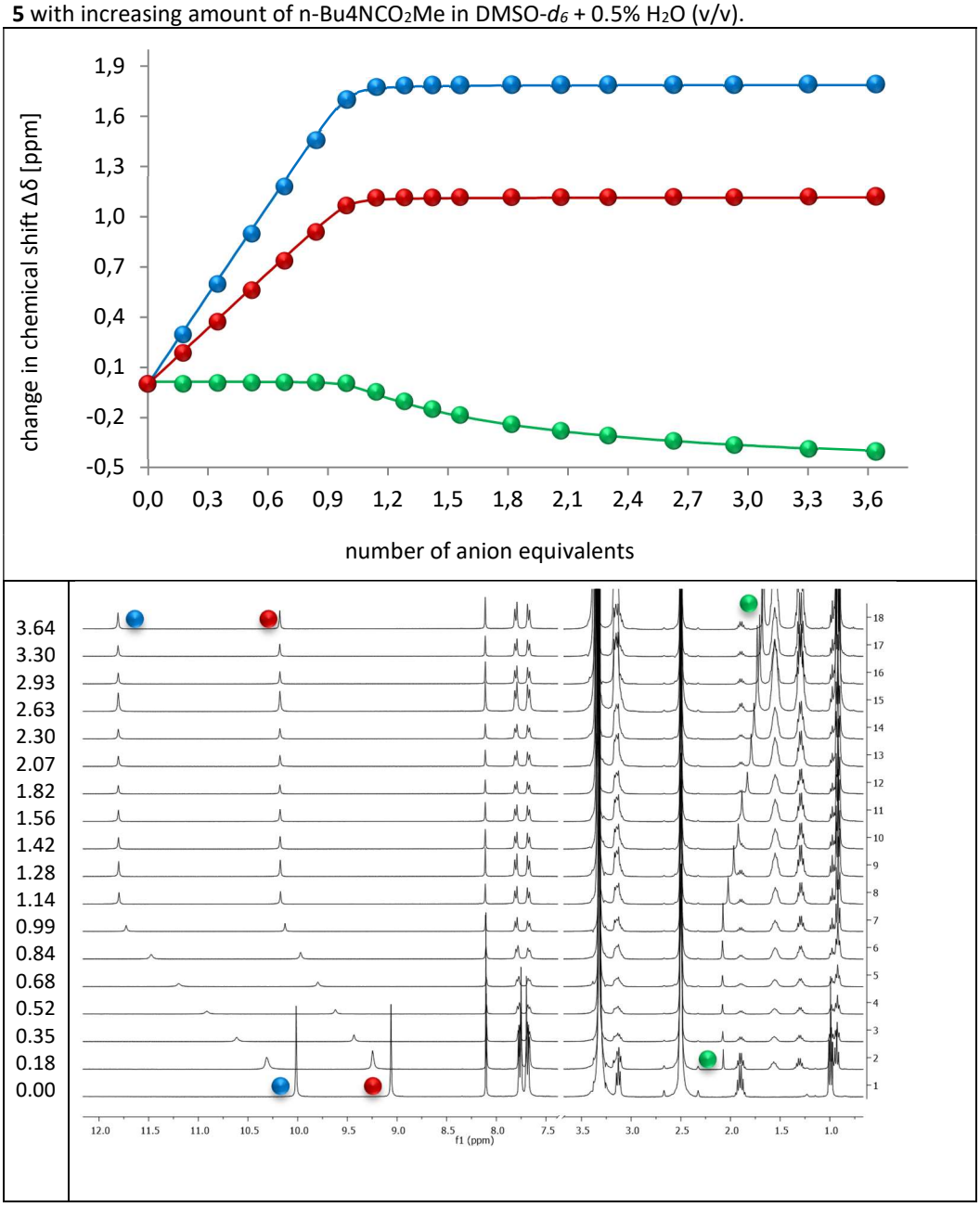


**Table S6.** Corresponding experimental chemical shift changes (symbols) and calculated binding isotherms (lines) assuming 1:1 binding model; Stacked plots from $^{1}$H NMR titrations of Receptor **5** with increasing amount of n-$Bu_4NCO_2Ph$ in DMSO-$d_6$ + 0.5% $H_2O$ (v/v).

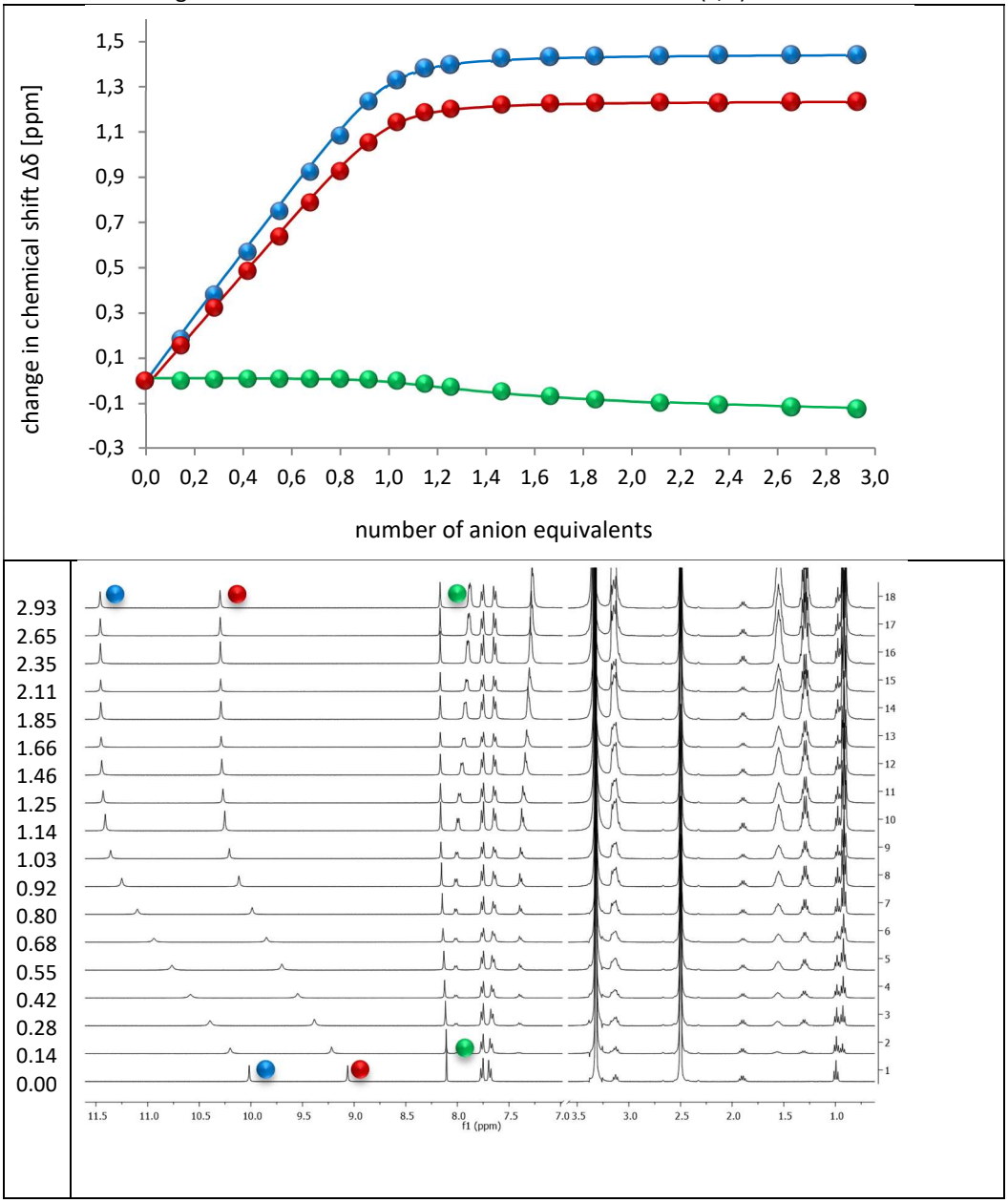


**Table S7.** Corresponding experimental chemical shift changes (symbols) and calculated binding isotherms (lines) assuming 1:1 binding model; Stacked plots from $^{1}$H NMR titrations of Receptor **5** with increasing amount of n-$Bu_4NH_2PO_4$ in DMSO-$d_6$ + 0.5% $H_2O$ (v/v).

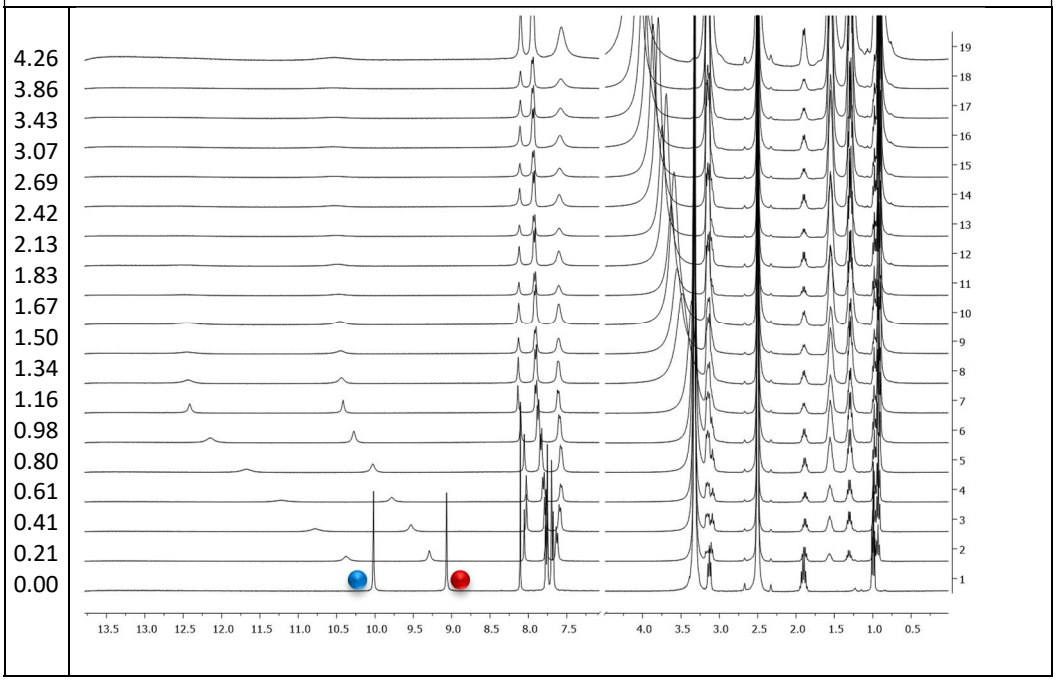
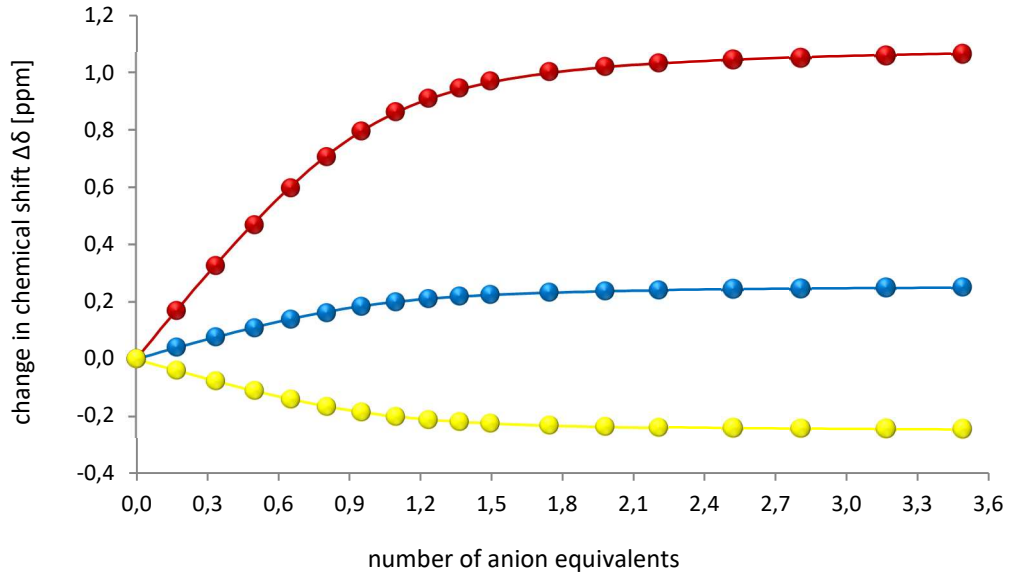
| |
|---|
| Fitting failed due to a complex binding model |
|  |

**Table S8.** Corresponding experimental chemical shift changes (symbols) and calculated binding isotherms (lines) assuming 1:1 binding model; Stacked plots from $^{1}$H NMR titrations of Receptor **5** with increasing amount of n-$Bu_4NCl$ in DMSO-$d_6$ + 10% $CD_3OH$ (v/v).



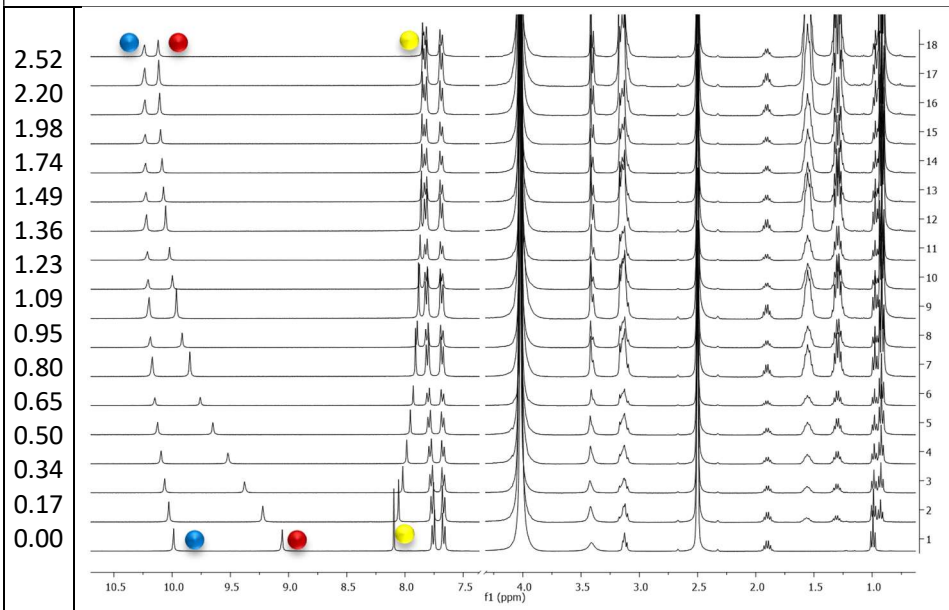
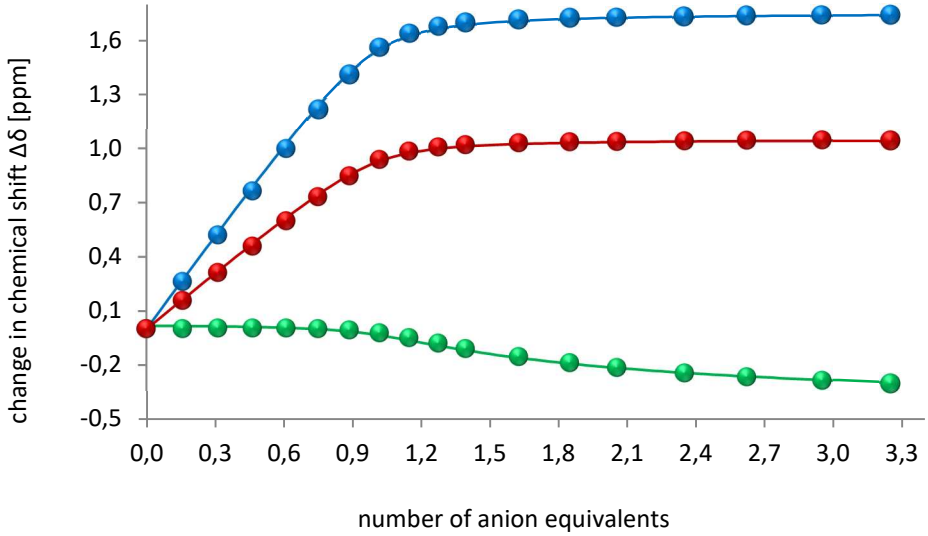



**Table S9.** Corresponding experimental chemical shift changes (symbols) and calculated binding isotherms (lines) assuming 1:1 binding model; Stacked plots from $^{1}$H NMR titrations of Receptor **5** with increasing amount of n-Bu4NCO$_2$Me in DMSO-$d_6$ + 10% CD$_3$OH (v/v).



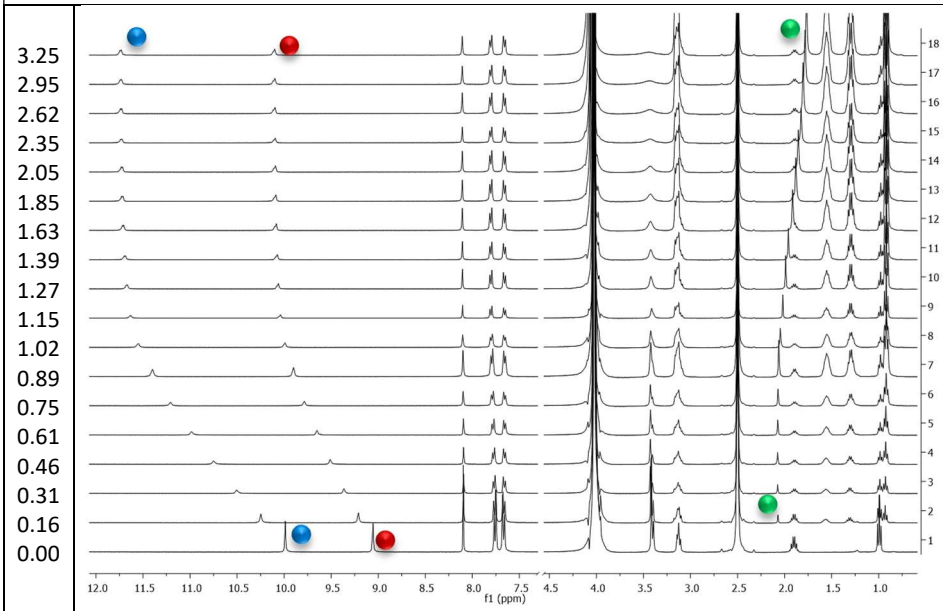



**Table S10.** Corresponding experimental chemical shift changes (symbols) and calculated binding isotherms (lines) assuming 1:1 binding model; Stacked plots from $^{1}$H NMR titrations of Receptor **5** with increasing amount of n-$Bu_4NCO_2Ph$ in DMSO-$d_6$ + 10% $CD_3OH$ (v/v).

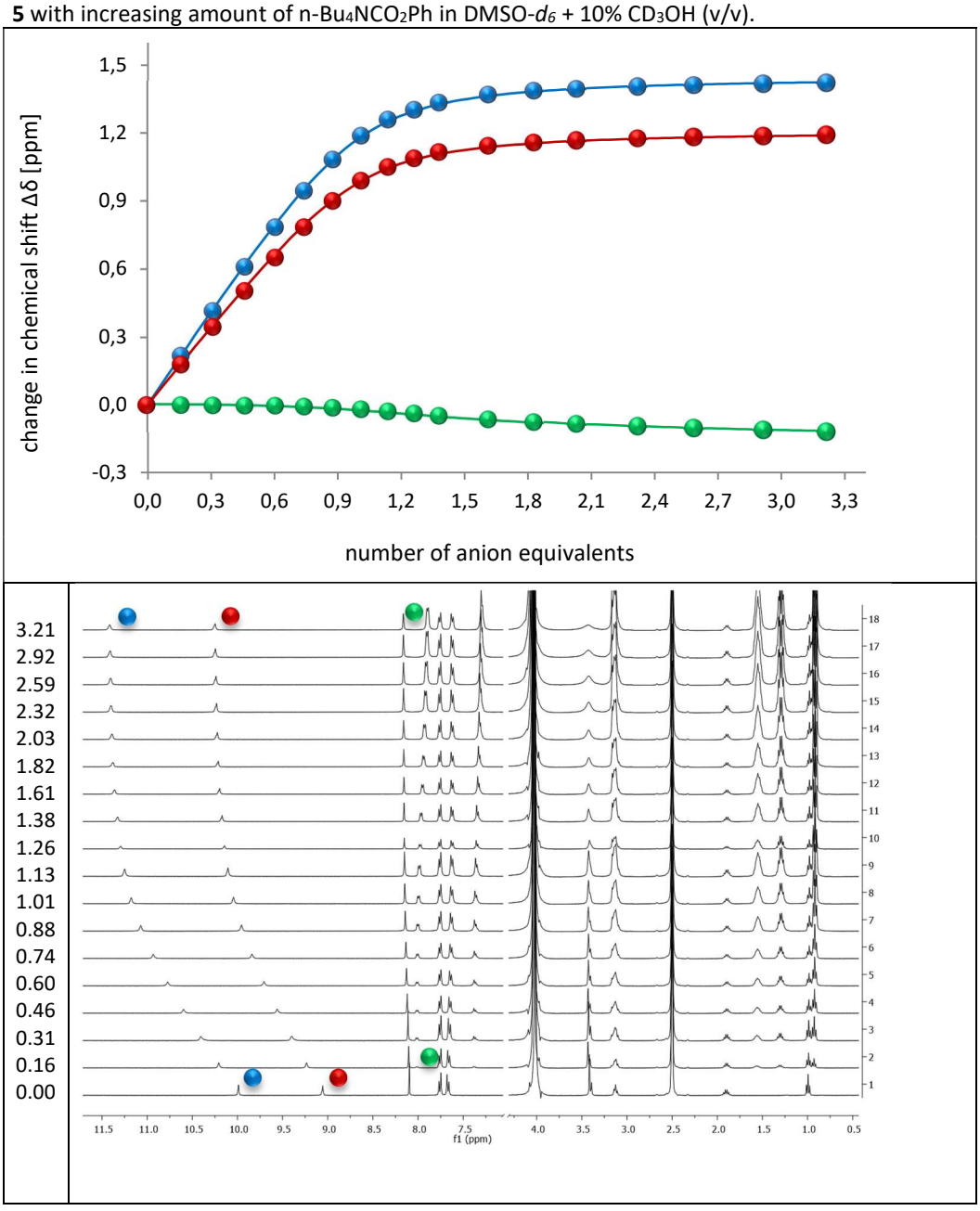


**Table S11.** Corresponding experimental chemical shift changes (symbols) and calculated binding isotherms (lines) assuming 1:1 binding model; Stacked plots from $^{1}$H NMR titrations of Receptor **5** with increasing amount of n-$Bu_4NH_2PO_4$ in DMSO-$d_6$ + 10% $CD_3OH$ (v/v).

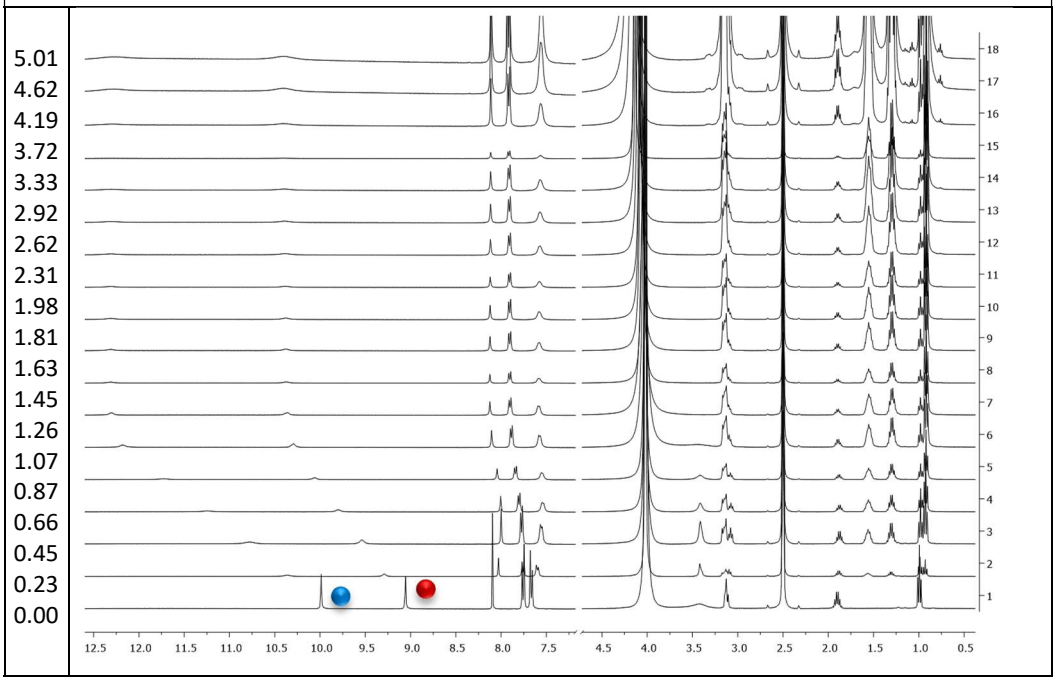
| |
|---|
| Fitting failed due to a complex binding model |
|  |

**Table S12.** Corresponding experimental chemical shift changes (symbols) and calculated binding isotherms (lines) assuming 1:1 binding model; Stacked plots from $^{1}$H NMR titrations of Receptor **6** with increasing amount of n-$Bu_4NCl$ in DMSO-$d_6$ + 0.5% $H_2O$ (v/v).

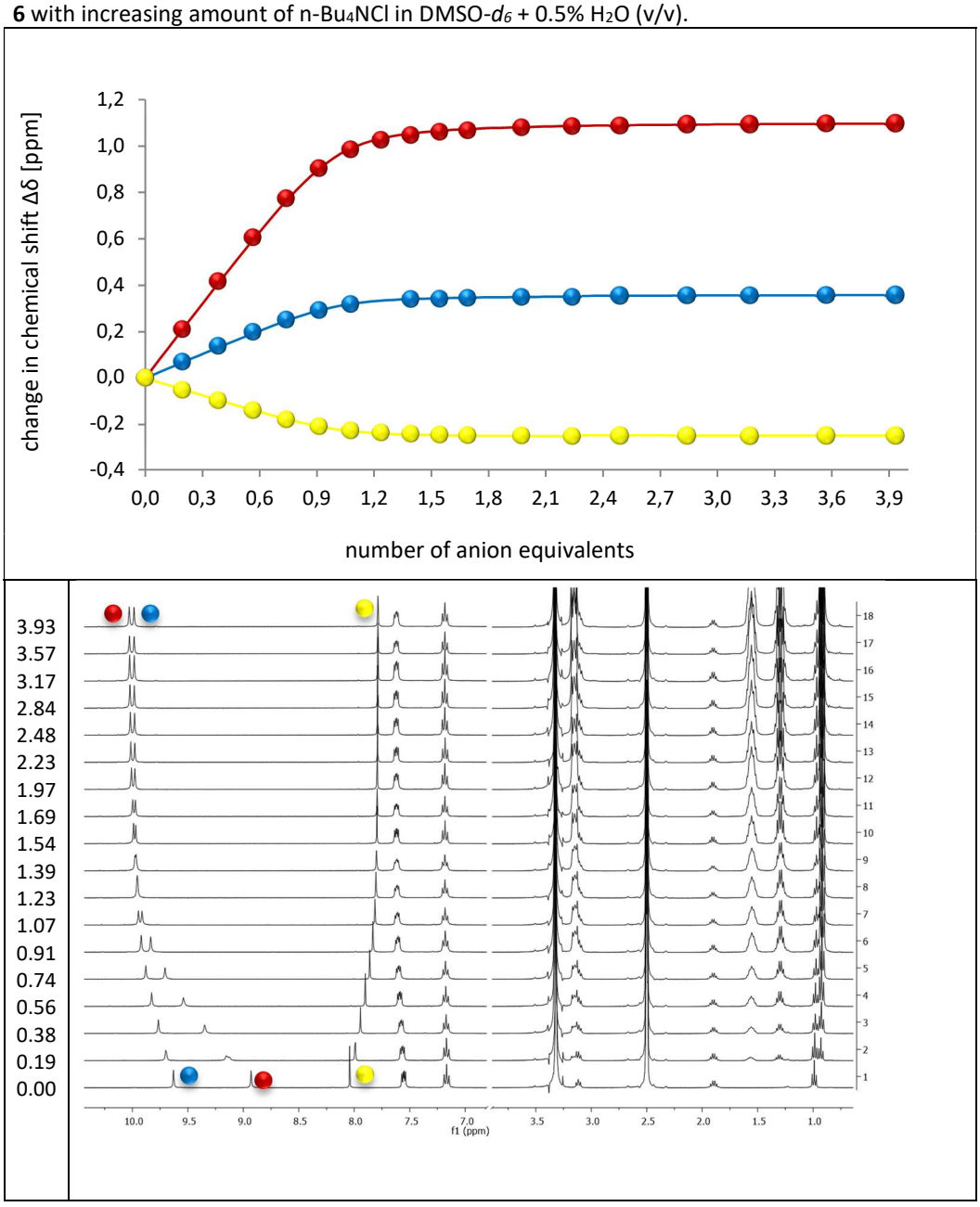


**Table S13.** Corresponding experimental chemical shift changes (symbols) and calculated binding isotherms (lines) assuming 1:1 binding model; Stacked plots from $^{1}$H NMR titrations of Receptor **6** with increasing amount of n-Bu4NCO$_2$Me in DMSO-$d_6$ + 0.5% $H_2O$ (v/v).

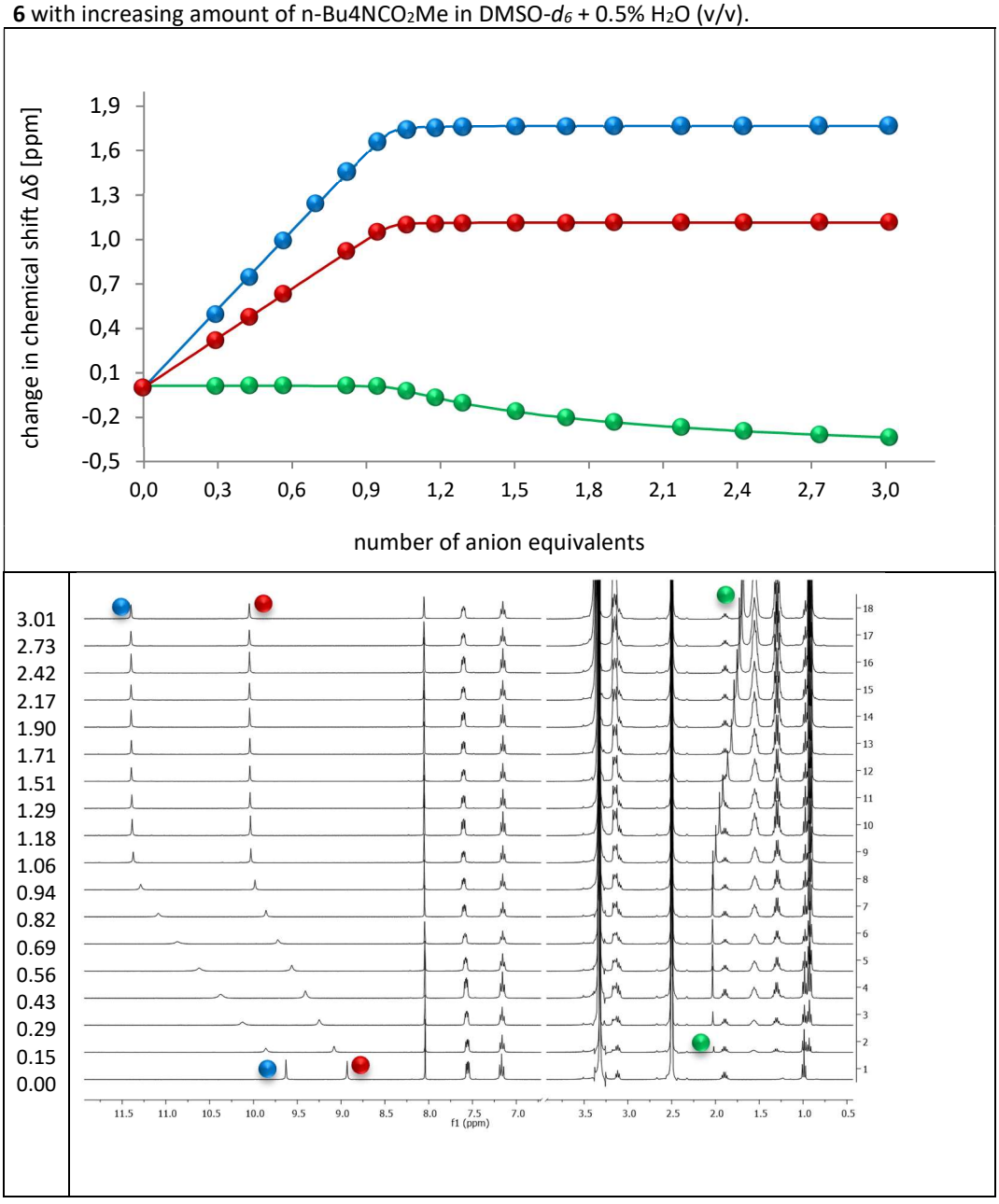
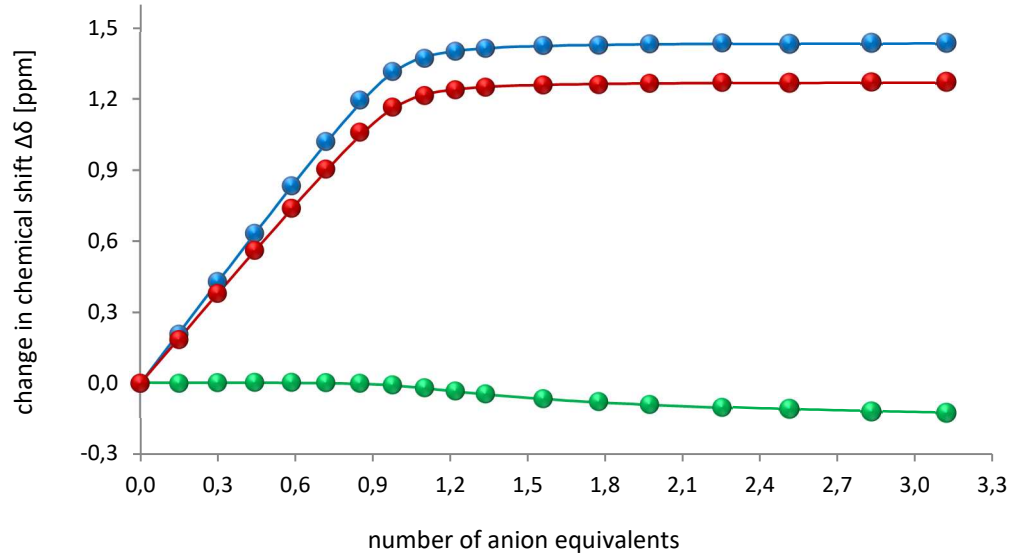


**Table S14.** Corresponding experimental chemical shift changes (symbols) and calculated binding isotherms (lines) assuming 1:1 binding model; Stacked plots from $^{1}$H NMR titrations of Receptor **6** with increasing amount of n-$Bu_4NCO_2Ph$ in DMSO-$d_6$ + 0.5% $H_2O$ (v/v).



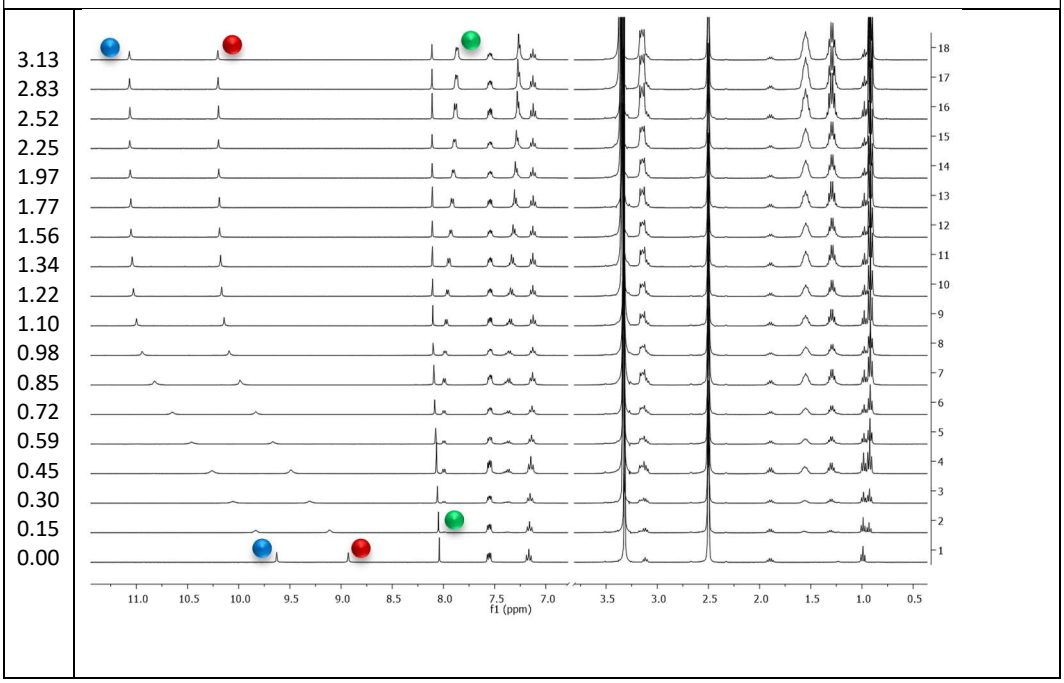



**Table S15.** Corresponding experimental chemical shift changes (symbols) and calculated binding isotherms (lines) assuming 1:1 binding model; Stacked plots from $^{1}$H NMR titrations of Receptor **6** with increasing amount of n-$Bu_4NH_2PO_4$ in DMSO-$d_6$ + 0.5% $H_2O$ (v/v).

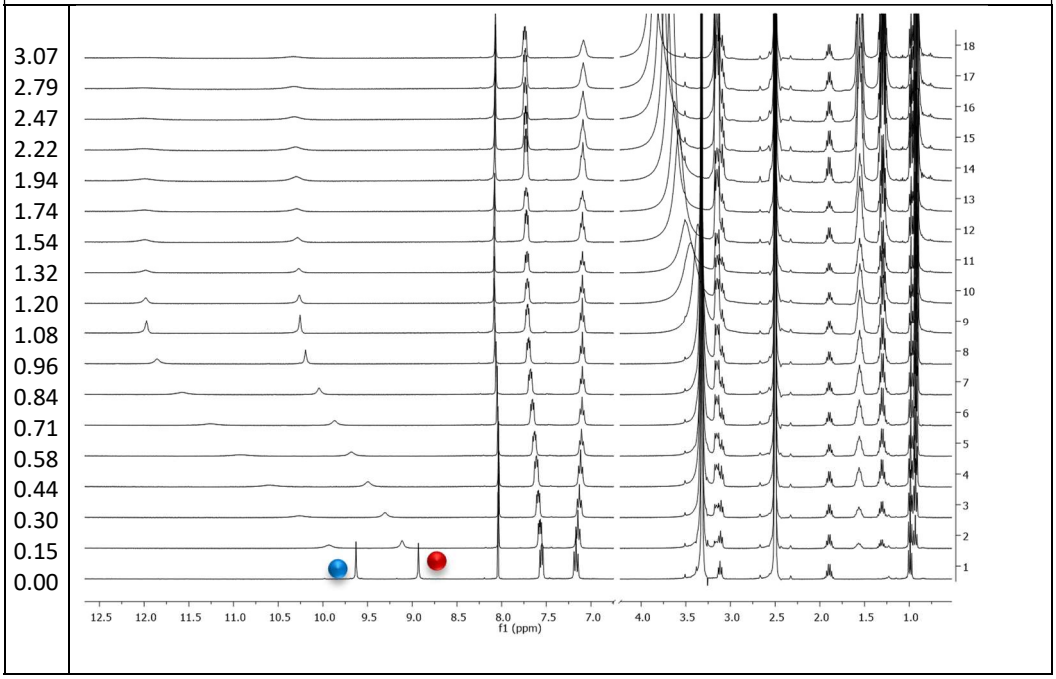
| |
|---|
| Fitting failed due to a complex binding model |
|  |

**Table S16.** Corresponding experimental chemical shift changes (symbols) and calculated binding isotherms (lines) assuming 1:1 binding model; Stacked plots from $^{1}$H NMR titrations of Receptor **6** with increasing amount of n-$Bu_4NCl$ in DMSO-$d_6$ + 10% $CD_3OH$ (v/v).

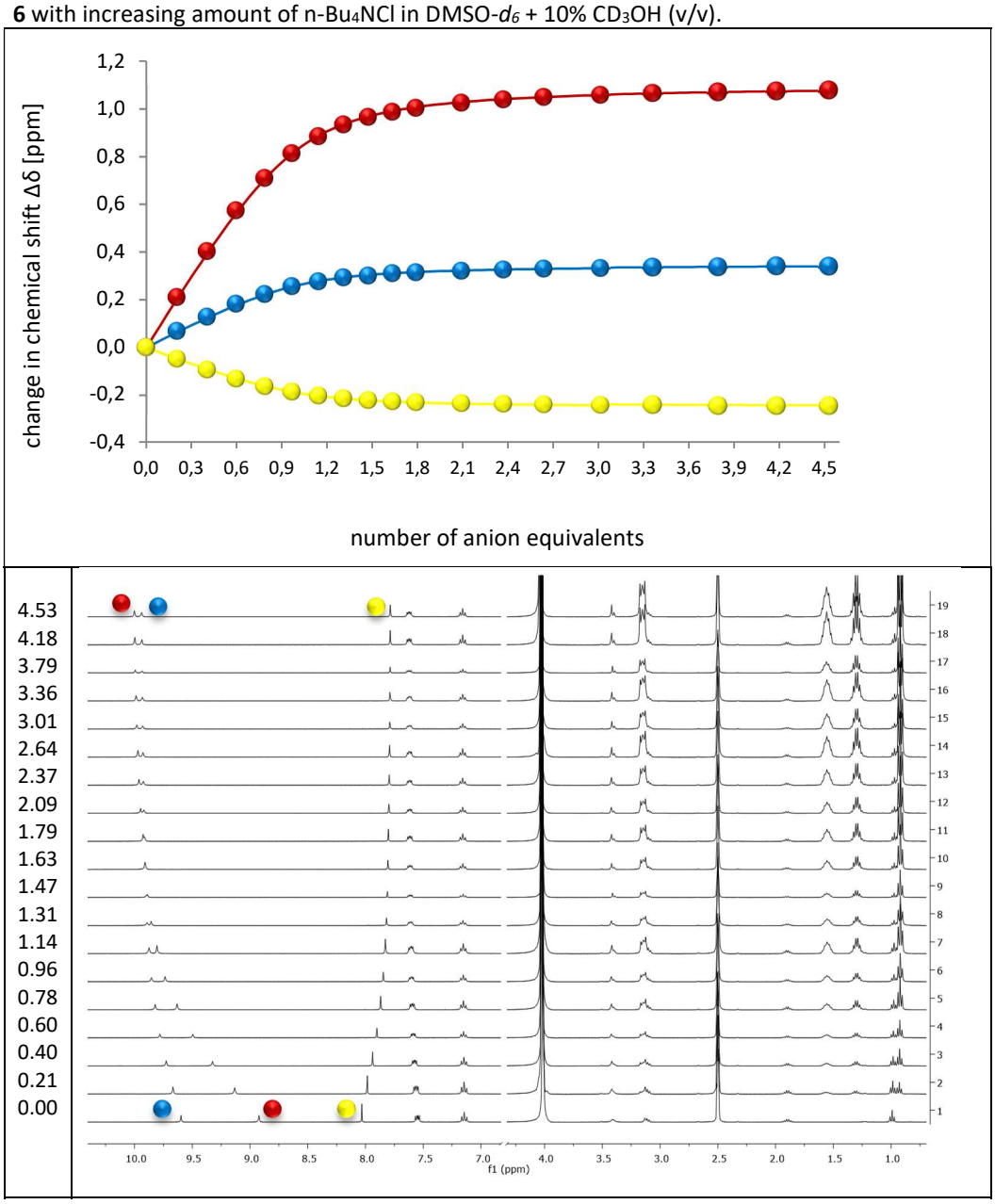
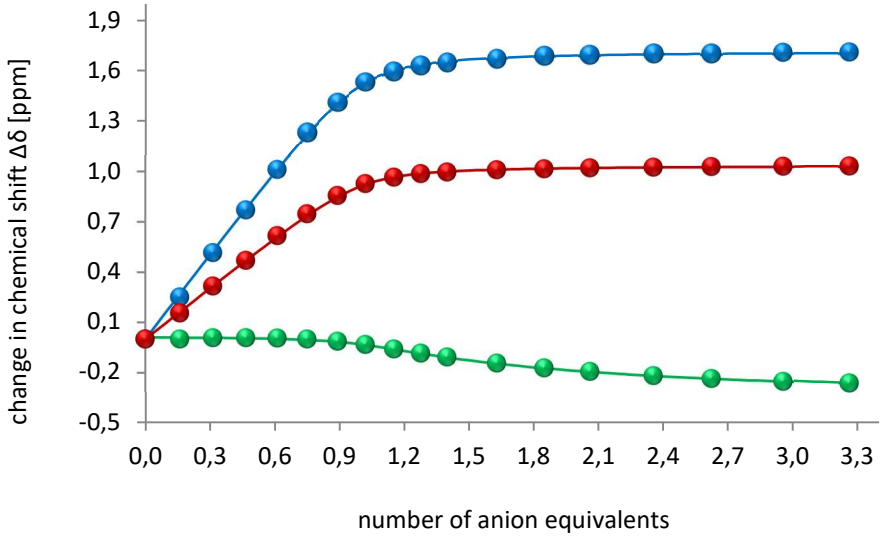


**Table S17.** Corresponding experimental chemical shift changes (symbols) and calculated binding isotherms (lines) assuming 1:1 binding model; Stacked plots from $^{1}$H NMR titrations of Receptor **6** with increasing amount of n-Bu4NCO$_2$Me in DMSO-*d*$_6$ + 10% CD$_3$OH (v/v).



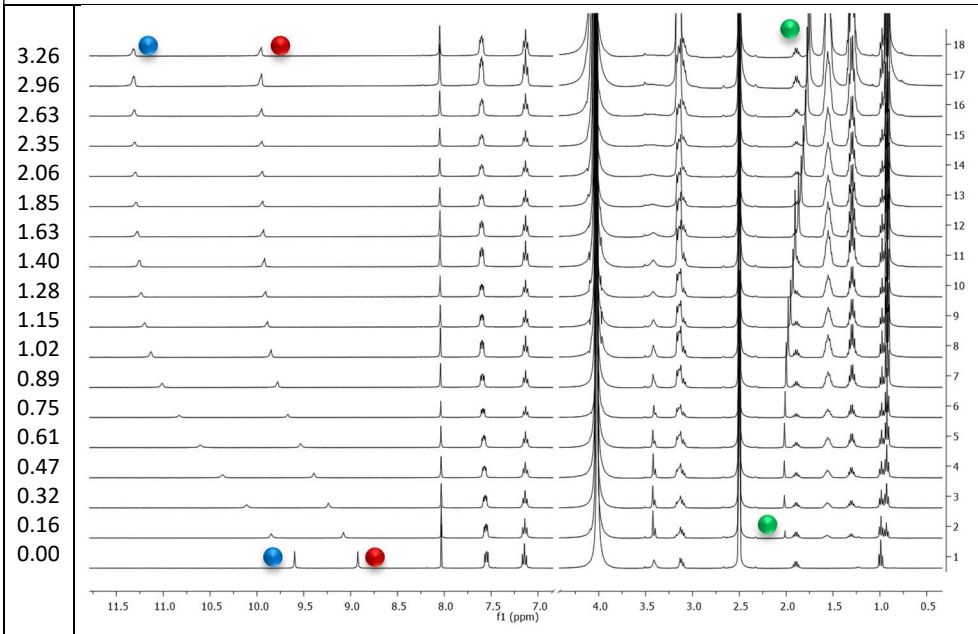
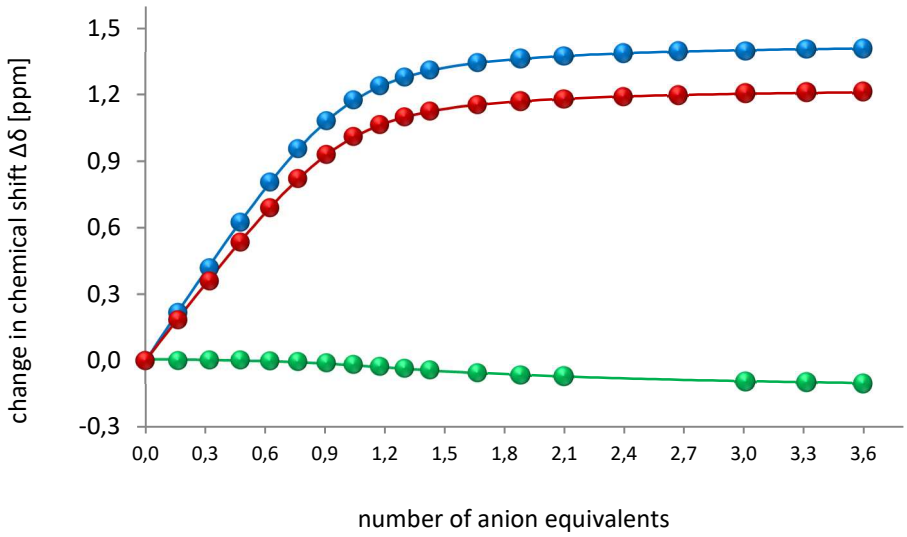



**Table S18.** Corresponding experimental chemical shift changes (symbols) and calculated binding isotherms (lines) assuming 1:1 binding model; Stacked plots from $^{1}$H NMR titrations of Receptor **6** with increasing amount of n-$Bu_4NCO_2Ph$ in DMSO-$d_6$ + 10% $CD_3OH$ (v/v).



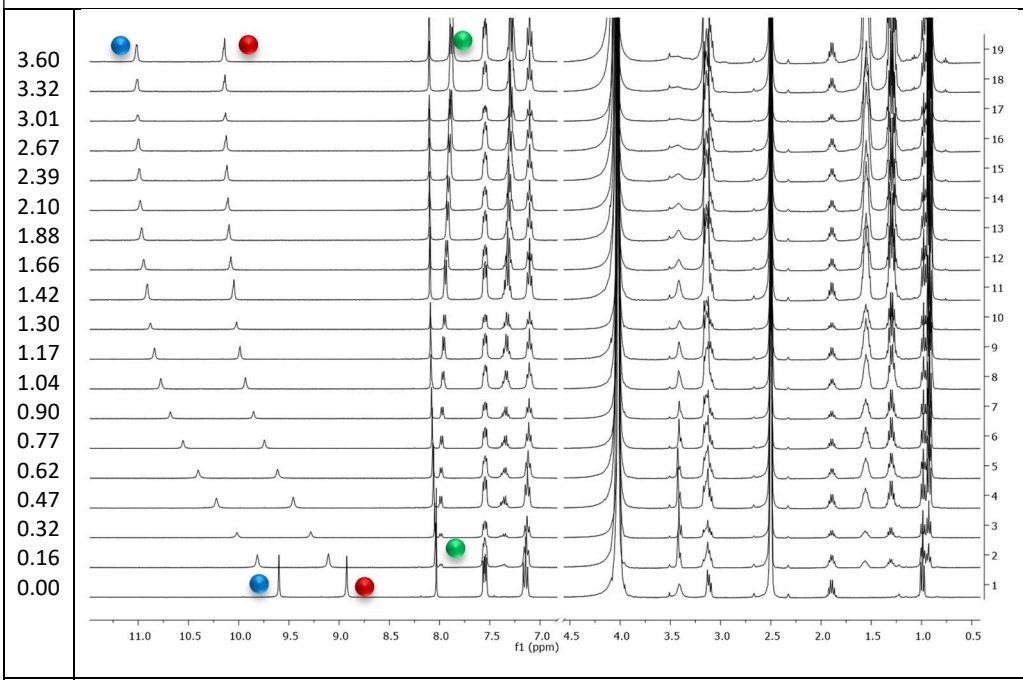



**Table S19.** Corresponding experimental chemical shift changes (symbols) and calculated binding isotherms (lines) assuming 1:1 binding model; Stacked plots from $^{1}$H NMR titrations of Receptor **6** with increasing amount of n-$Bu_4NH_2PO_4$ in DMSO-$d_6$ + 10% $CD_3OH$ (v/v).

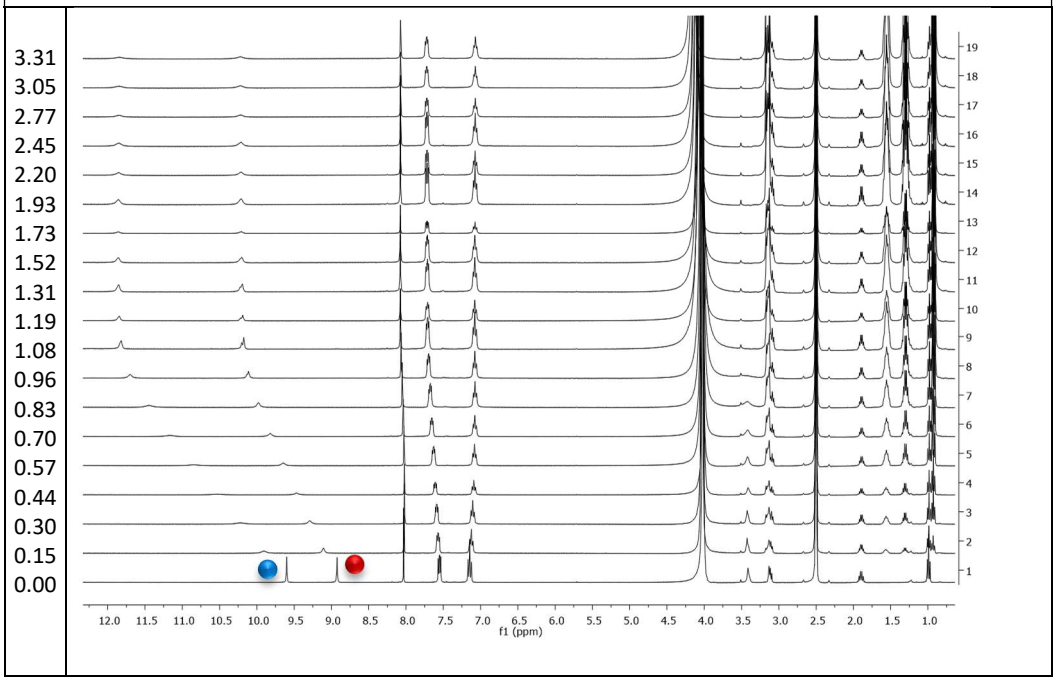
| |
|---|
| Fitting failed due to a complex binding model |
|  |

**Table S20.** Corresponding experimental chemical shift changes (symbols) and calculated binding isotherms (lines) assuming 1:1 binding model; Stacked plots from $^{1}$H NMR titrations of Receptor **7** with increasing amount of n-$Bu_4NCl$ in DMSO-$d_6$ + 0.5% $H_2O$ (v/v).

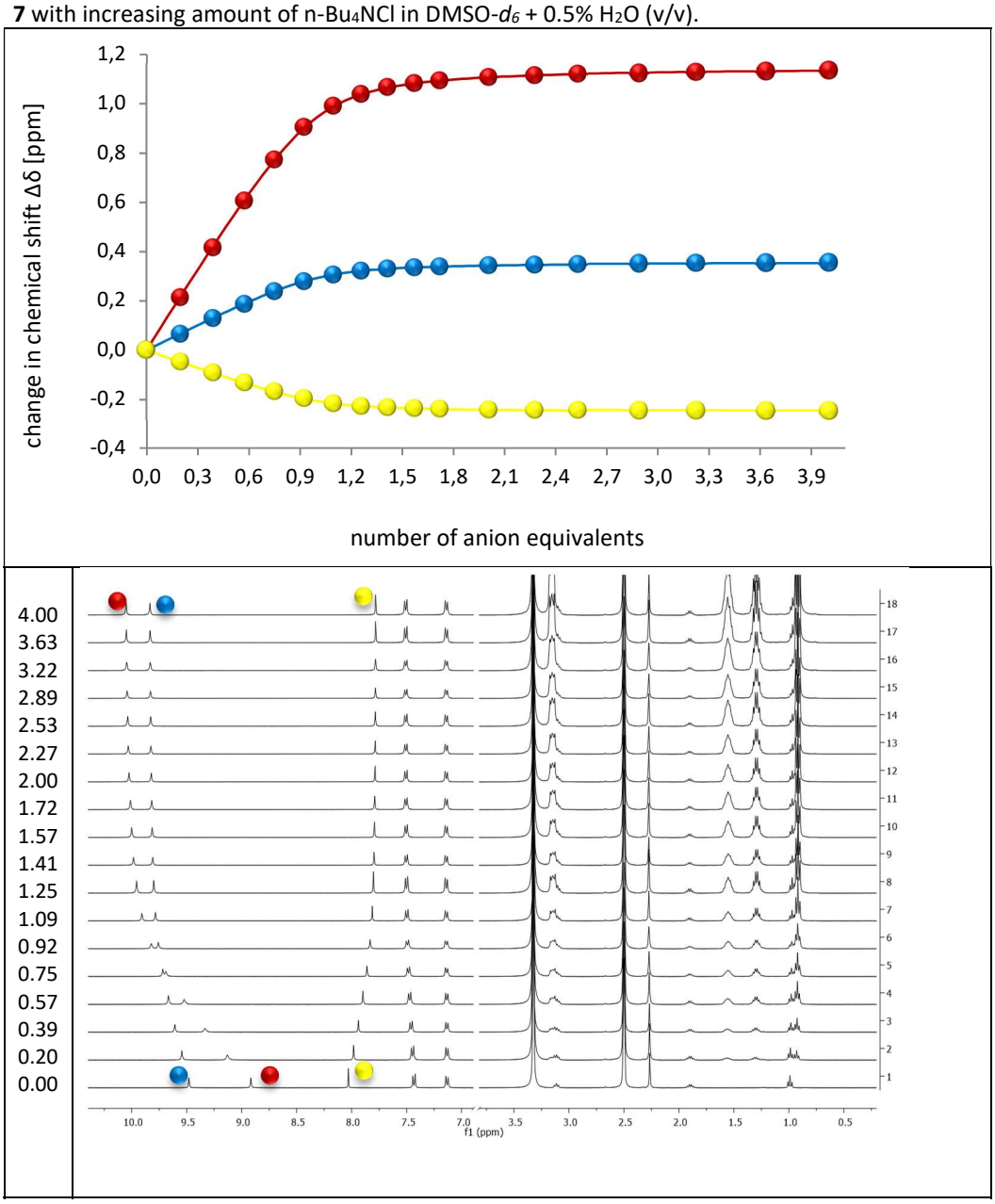
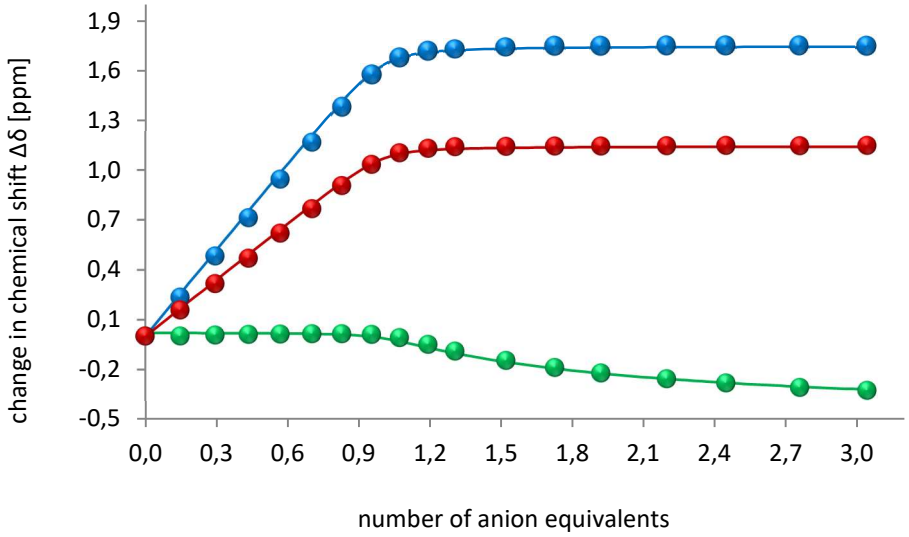


**Table S21.** Corresponding experimental chemical shift changes (symbols) and calculated binding isotherms (lines) assuming 1:1 binding model; Stacked plots from $^{1}$H NMR titrations of Receptor **7** with increasing amount of n-Bu4NCO$_2$Me in DMSO-$d_6$ + 0.5% $H_2O$ (v/v).



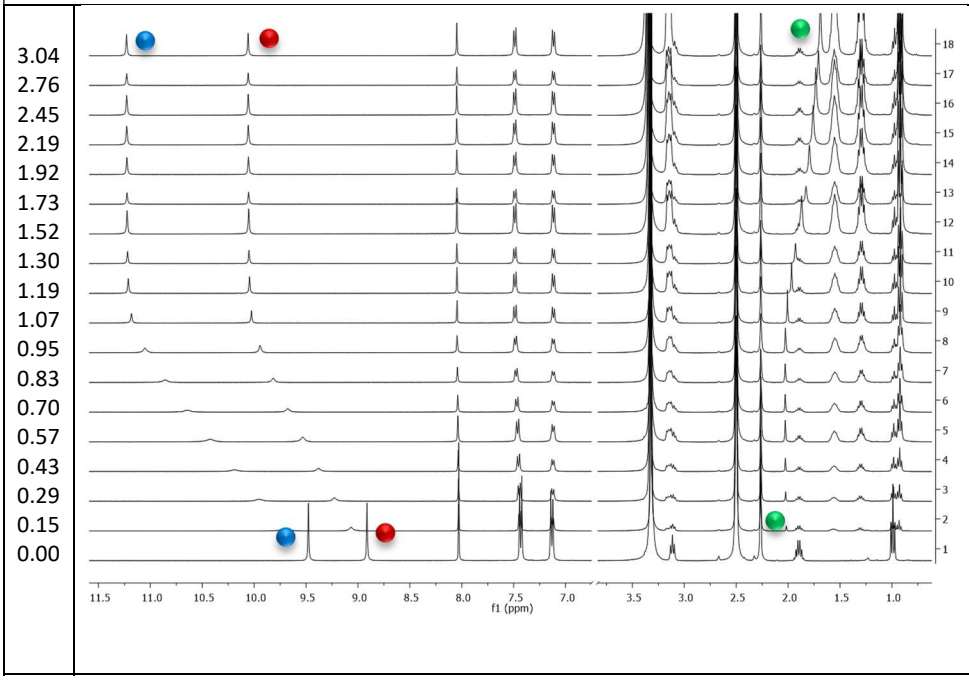



**Table S22.** Corresponding experimental chemical shift changes (symbols) and calculated binding isotherms (lines) assuming 1:1 binding model; Stacked plots from $^{1}$H NMR titrations of Receptor **7** with increasing amount of n-$Bu_4NH_2PO_4$ in DMSO-$d_6$ + 0.5% $H_2O$ (v/v).

Fitting failed due to a complex binding model

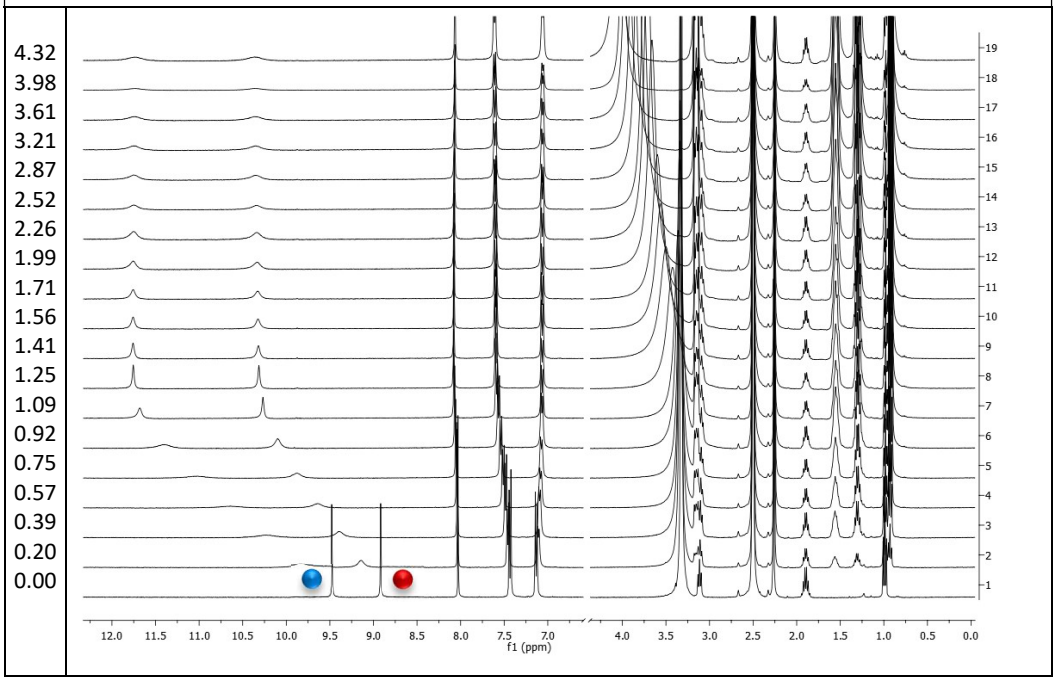
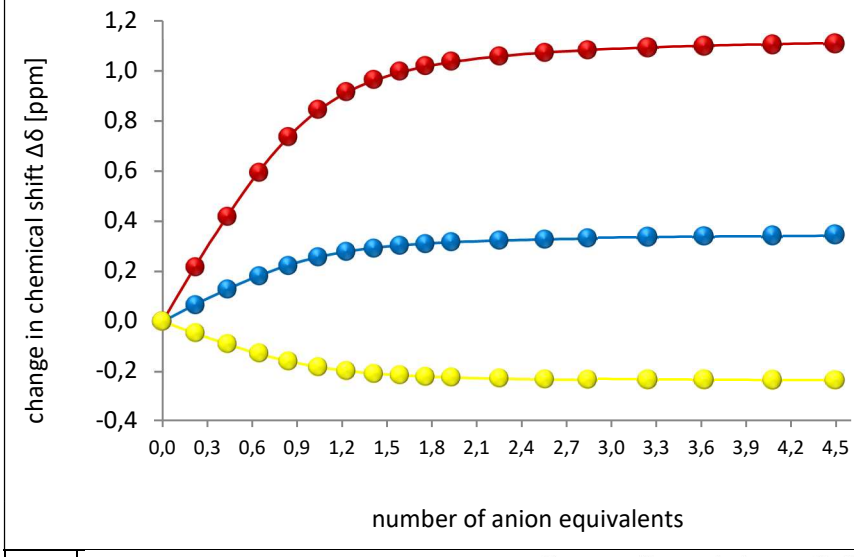


**Table S23.** Corresponding experimental chemical shift changes (symbols) and calculated binding isotherms (lines) assuming 1:1 binding model; Stacked plots from $^{1}$H NMR titrations of Receptor **7** with increasing amount of n-$Bu_4NCl$ in DMSO-$d_6$ + 10% $CD_3OH$ (v/v).



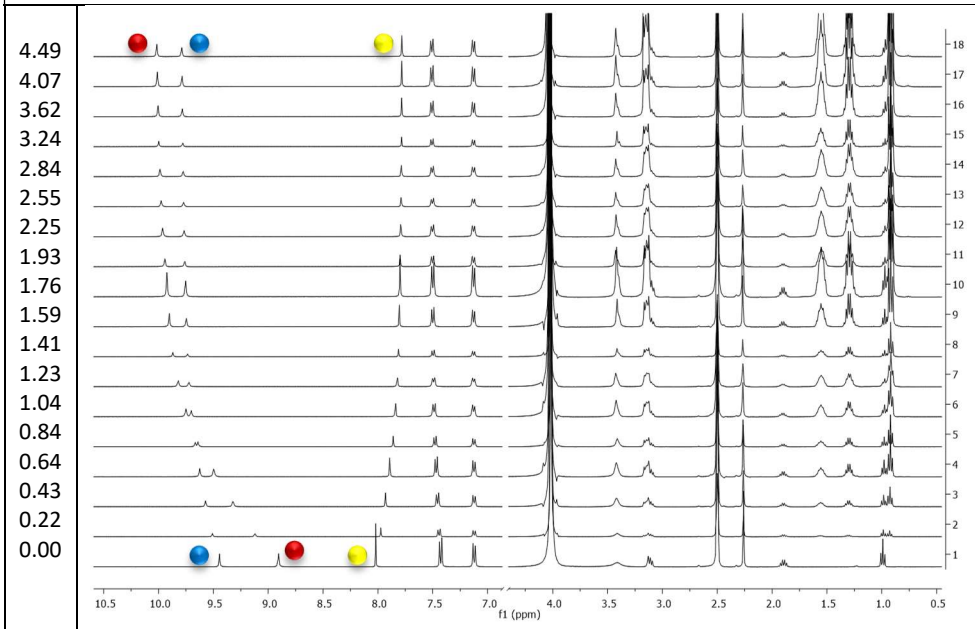



**Table S24.** Corresponding experimental chemical shift changes (symbols) and calculated binding isotherms (lines) assuming 1:1 binding model; Stacked plots from $^{1}$H NMR titrations of Receptor **7** with increasing amount of n-Bu4NCO$_2$Me in DMSO-*d*$_6$ + 10% CD$_3$OH (v/v).

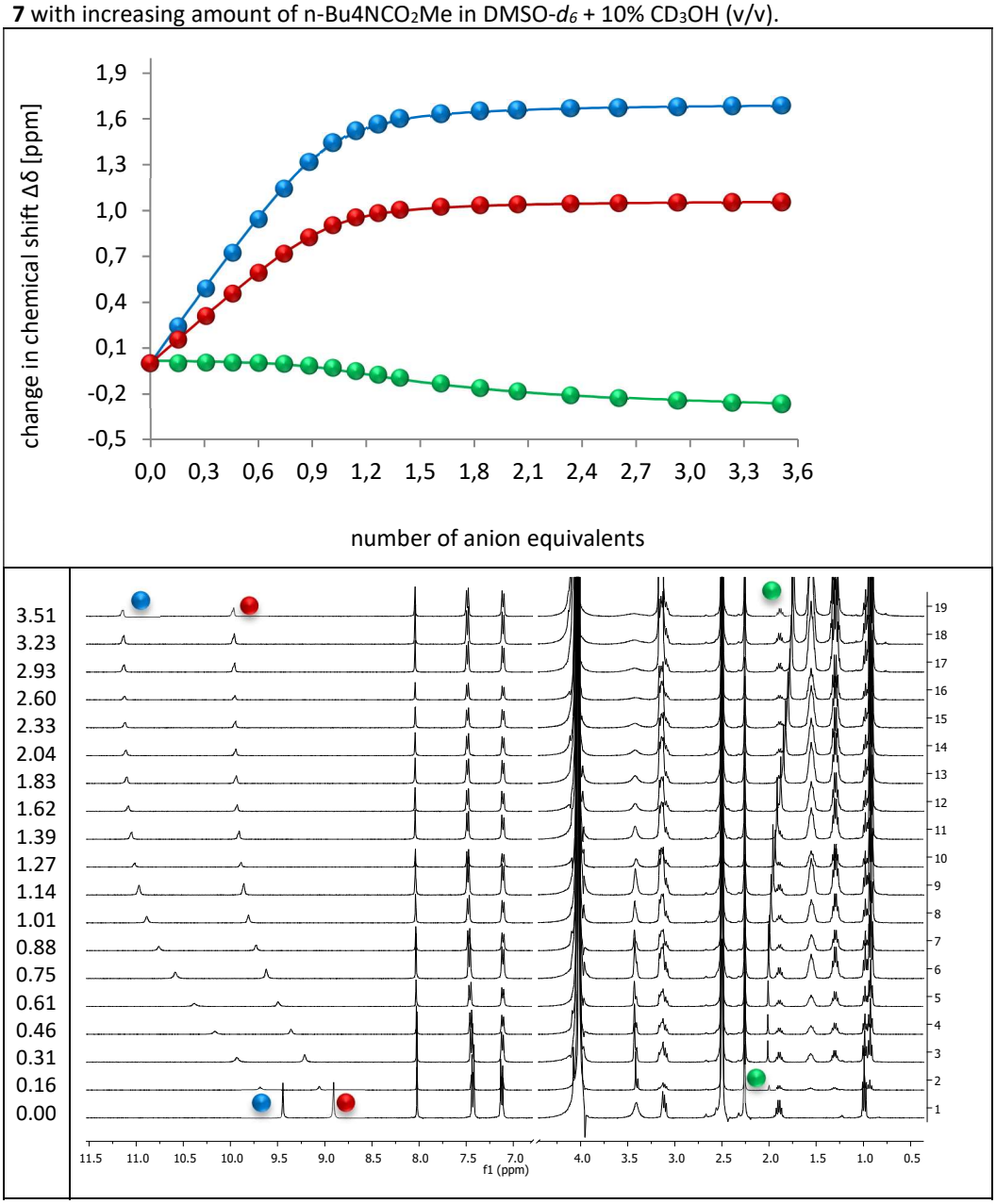
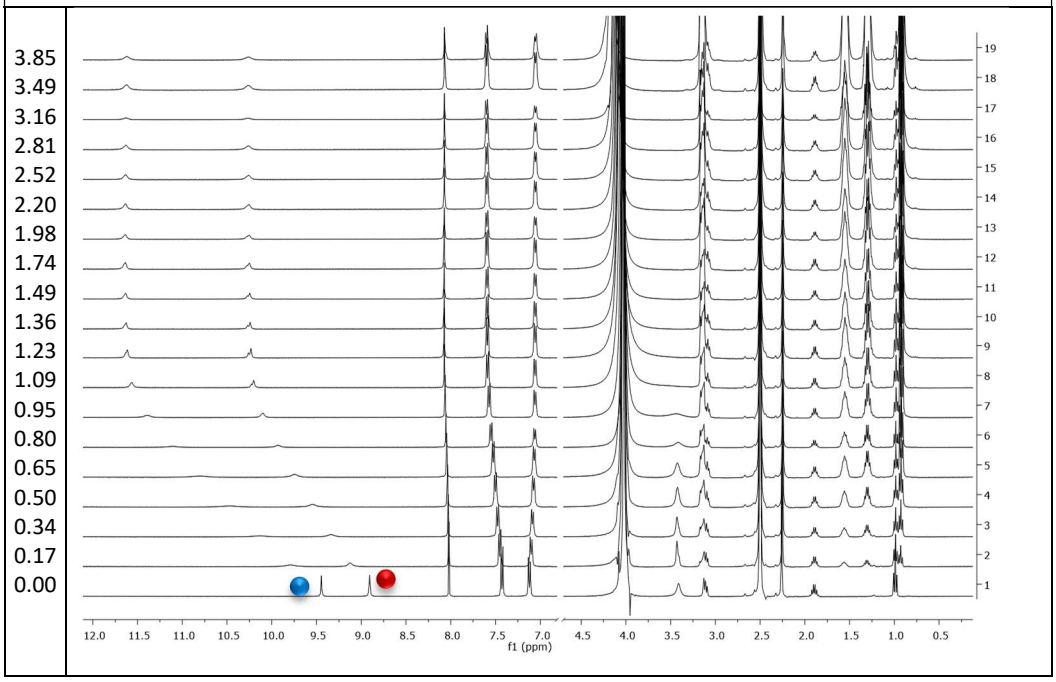


**Table S25.** Corresponding experimental chemical shift changes (symbols) and calculated binding isotherms (lines) assuming 1:1 binding model; Stacked plots from $^{1}$H NMR titrations of Receptor **7** with increasing amount of n-$Bu_4NH_2PO_4$ in DMSO-$d_6$ + 10% $CD_3OH$ (v/v).

| |
|---|
| Fitting failed due to a complex binding model |
|  |

## 6. Cartesian coordinates of calculated structures

**Table S26**. Cartesian coordinates of the studied structures; all values in Hartrees (@298.15K); energies for $Cl^-$, $MeCO_2^-$, and $PhCO_2^-$ are -460.351275, -228.487930, and -420.111546, respectively.

| Receptor **2** $\Delta G^0$ = -2076.65198 au | | | | Receptor **3** $\Delta G^0$ = -2224.28751 au | | | | Receptor **4** $\Delta G^0$ = -2633.15986 au | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| C | -0.104806 | -0.001085 | -4.315002 | C | -0.405838 | 0.425268 | -4.177602 | C | -0.417267 | 0.468169 | -4.602083 |
| N | -0.610128 | -0.000846 | -1.471477 | N | -0.261372 | 0.157942 | -1.305093 | N | -0.274284 | 0.198180 | -1.728911 |
| C | -0.236170 | -1.172094 | -3.567365 | C | -0.590361 | -0.791121 | -3.517794 | C | -0.617221 | -0.745640 | -3.942211 |
| C | -0.237881 | 1.170016 | -3.567763 | C | -0.141844 | 1.500615 | -3.327276 | C | -0.139353 | 1.539526 | -3.751417 |
| C | -0.485842 | 1.126143 | -2.174801 | C | -0.081307 | 1.325771 | -1.924230 | C | -0.081079 | 1.363586 | -2.348371 |
| C | -0.483943 | -1.127906 | -2.174349 | C | -0.510464 | -0.878063 | -2.107576 | C | -0.536355 | -0.833901 | -2.532244 |
| S | -0.137609 | -2.816578 | -4.136557 | S | -0.927226 | -2.350001 | -4.223462 | S | -0.975459 | -2.299301 | -4.648245 |
| S | -0.140964 | 2.814323 | -4.137688 | S | 0.150152 | 3.163883 | -3.763890 | S | 0.173913 | 3.198937 | -4.188186 |
| C | -0.425619 | -3.433696 | -2.521103 | C | -0.962985 | -3.103045 | -2.641586 | C | -1.017262 | -3.053142 | -3.068440 |
| H | -0.455766 | -4.501137 | -2.367338 | H | -1.154322 | -4.162737 | -2.572380 | H | -1.221316 | -4.110609 | -3.000061 |
| C | -0.589869 | -2.454721 | -1.593073 | C | -0.730132 | -2.230246 | -1.626991 | C | -0.770649 | -2.183779 | -2.054561 |
| C | -0.430612 | 3.431788 | -2.522665 | C | 0.345269 | 3.613234 | -2.082133 | C | 0.372741 | 3.646334 | -2.507899 |
| H | -0.462152 | 4.499245 | -2.369268 | H | 0.559068 | 4.642350 | -1.839052 | H | 0.597945 | 4.673183 | -2.265148 |
| C | -0.594038 | 2.453033 | -1.594268 | C | 0.199229 | 2.567770 | -1.227244 | C | 0.213075 | 2.602816 | -1.653505 |
| C | 0.214845 | -0.000545 | -5.782163 | C | -0.425338 | 0.553377 | -5.673714 | C | -0.433186 | 0.595392 | -6.098086 |
| H | -0.234790 | 0.880727 | -6.256570 | H | -0.791078 | 1.548908 | -5.954405 | H | -0.782352 | 1.596301 | -6.380669 |
| H | -0.231725 | -0.882921 | -6.257295 | H | -1.127291 | -0.175686 | -6.097268 | H | -1.145846 | -0.123007 | -6.521877 |
| C | 1.732623 | 0.002489 | -6.033176 | C | 0.970180 | 0.332412 | -6.282760 | C | 0.960118 | 0.350291 | -6.702747 |
| H | 2.176688 | -0.880776 | -5.558067 | H | 1.332138 | -0.663271 | -5.999144 | H | 1.306056 | -0.649285 | -6.412609 |
| H | 2.174438 | 0.881903 | -5.548917 | H | 1.668771 | 1.060779 | -5.853368 | H | 1.668543 | 1.070194 | -6.275242 |
| C | 2.051049 | 0.010921 | -7.525701 | C | 0.941741 | 0.466597 | -7.802891 | C | 0.937993 | 0.476287 | -8.223582 |
| H | 3.131731 | 0.011192 | -7.697606 | H | 1.936546 | 0.309924 | -8.230649 | H | 1.931523 | 0.300684 | -8.646902 |
| H | 1.630052 | 0.900409 | -8.007417 | H | 0.598042 | 1.464149 | -8.098232 | H | 0.611816 | 1.477550 | -8.526014 |
| H | 1.628726 | -0.871938 | -8.018308 | H | 0.261548 | -0.269477 | -8.245524 | H | 0.247348 | -0.251315 | -8.663926 |
| N | -0.832528 | -2.542716 | -0.227663 | N | -0.671221 | -2.440204 | -0.253117 | N | -0.706930 | -2.399144 | -0.680152 |
| H | -0.927547 | -1.651740 | 0.251053 | H | -0.489866 | -1.606020 | 0.298741 | H | -0.506305 | -1.569824 | -0.127136 |
| N | -0.838917 | 2.541645 | -0.229218 | N | 0.275917 | 2.521360 | 0.160801 | N | 0.285324 | 2.559916 | -0.263338 |
| H | -0.933473 | 1.650984 | 0.250197 | H | 0.123325 | 1.602021 | 0.565998 | H | 0.119344 | 1.643820 | 0.145062 |
| C | -1.003884 | -3.718346 | 0.472045 | C | -0.820839 | -3.662586 | 0.358348 | C | -0.862129 | -3.619182 | -0.078673 |
| C | -1.003494 | 3.717955 | 0.471091 | C | 0.512470 | 3.609975 | 0.966931 | C | 0.524898 | 3.647698 | 0.533092 |
| O | -0.931359 | -4.819932 | -0.080576 | O | -1.047958 | -4.687195 | -0.281525 | O | -1.111344 | -4.640049 | -0.710325 |
| O | -0.923790 | 4.819390 | -0.080862 | O | 0.698379 | 4.733603 | 0.504821 | O | 0.725186 | 4.768134 | 0.077229 |
| C | -1.317703 | -4.712863 | 2.687262 | C | -0.778182 | -4.676277 | 2.639961 | C | -0.791268 | -4.634529 | 2.193595 |
| H | -1.912765 | -4.426502 | 3.559600 | C | -0.917433 | -6.666800 | 4.619477 | C | -0.913104 | -6.615970 | 4.131667 |
| H | -1.847947 | -5.520413 | 2.174142 | C | -1.143654 | -5.984710 | 2.295511 | C | -1.146302 | -5.947719 | 1.835054 |
| C | 0.068233 | -5.185037 | 3.123147 | C | -0.485375 | -4.374899 | 3.979750 | C | -0.502502 | -4.338443 | 3.541157 |
| H | 0.582444 | -4.361638 | 3.637072 | C | -0.556185 | -5.360737 | 4.957182 | C | -0.560968 | -5.321025 | 4.510718 |
| H | 0.659180 | -5.428007 | 2.230155 | C | -1.207453 | -6.963309 | 3.289470 | C | -1.205577 | -6.934352 | 2.809268 |
| C | -0.004407 | -6.402862 | 4.042544 | H | -1.374574 | -6.234258 | 1.269894 | H | -1.372737 | -6.192354 | 0.808155 |
| H | -0.615964 | -6.157381 | 4.921004 | H | -0.202192 | -3.360358 | 4.250411 | H | -0.228960 | -3.325074 | 3.820853 |
| H | -0.520823 | -7.218794 | 3.519960 | H | -0.325782 | -5.104152 | 5.987255 | H | -0.336404 | -5.090984 | 5.545570 |
| C | 1.377336 | -6.873719 | 4.493075 | H | -1.492086 | -7.973483 | 3.007973 | H | -1.478639 | -7.948017 | 2.539796 |
| H | 1.898908 | -6.080254 | 5.040161 | H | -0.972755 | -7.438147 | 5.381579 | C | 0.710513 | 4.227764 | 2.946938 |
| H | 1.994836 | -7.146950 | 3.629990 | C | 0.720372 | 4.187815 | 3.387222 | C | 1.064034 | 5.820552 | 5.191230 |
| H | 1.308811 | -7.747265 | 5.149131 | C | 1.097403 | 5.780008 | 5.672458 | C | 0.589692 | 3.681469 | 4.240736 |

| | | | |
|---|---|---|---|
| C | -1.314143 | 4.713756 | 2.686175 |
| H | -1.908013 | 4.428764 | 3.559756 |
| H | -1.843410 | 5.522743 | 2.174273 |
| C | 0.073813 | 5.182576 | 3.119338 |
| H | 0.587095 | 4.357858 | 3.632057 |
| H | 0.663543 | 5.424363 | 2.225259 |
| C | 0.005772 | 6.400418 | 4.039010 |
| H | -0.604664 | 6.156137 | 4.918596 |
| H | -0.509757 | 7.217639 | 3.517556 |
| C | 1.389635 | 6.867827 | 4.486716 |
| H | 1.910187 | 6.073136 | 5.032954 |
| H | 1.324732 | 7.741768 | 5.142624 |
| H | 2.006027 | 7.139084 | 3.622220 |
| N | -1.282569 | -3.563773 | 1.793342 |
| H | -1.179720 | -2.647163 | 2.211972 |
| N | -1.283484 | 3.564487 | 1.792251 |
| H | -1.188430 | 2.646879 | 2.210529 |

| | | | |
|---|---|---|---|
| C | 0.603979 | 3.634396 | 4.672417 |
| C | 1.029884 | 5.548041 | 3.251935 |
| C | 1.213444 | 6.326554 | 4.396306 |
| C | 0.791566 | 4.423450 | 5.801008 |
| H | 0.364968 | 2.578855 | 4.780185 |
| H | 1.126093 | 5.990715 | 2.270944 |
| H | 1.452327 | 7.379818 | 4.276572 |
| H | 0.696040 | 3.973136 | 6.784910 |
| H | 1.243089 | 6.398021 | 6.553205 |
| N | -0.691806 | -3.611948 | 1.723065 |
| H | -0.470651 | -2.711221 | 2.133832 |
| N | 0.518527 | 3.310330 | 2.305399 |
| H | 0.327103 | 2.348875 | 2.565344 |

| | | | |
|---|---|---|---|
| C | 1.017521 | 5.592671 | 2.799211 |
| C | 1.192546 | 6.383967 | 3.925662 |
| C | 0.764469 | 4.469375 | 5.362013 |
| H | 0.354513 | 2.627364 | 4.357804 |
| H | 1.117373 | 6.028072 | 1.816322 |
| H | 1.428333 | 7.436487 | 3.818593 |
| H | 0.669006 | 4.046553 | 6.355242 |
| N | -0.707579 | -3.576231 | 1.294015 |
| H | -0.472135 | -2.678299 | 1.704479 |
| N | 0.515602 | 3.352050 | 1.883061 |
| H | 0.315396 | 2.392293 | 2.145019 |
| N | 1.244242 | 6.660097 | 6.363707 |
| O | 1.121711 | 6.148774 | 7.469132 |
| O | 1.508839 | 7.843304 | 6.197701 |
| N | -0.975210 | -7.657694 | 5.143227 |
| O | -1.297133 | -8.786686 | 4.797806 |
| O | -0.702757 | -7.362234 | 6.299444 |

| Receptor **5** $\Delta G^0$ = -2898.17201 au | | | | Receptor **6** $\Delta G^0$ = -2422.71753 au | | | | Receptor **7** $\Delta G^0$ = -2302.83125 au | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| C | -0.420198 | 0.480790 | -4.803589 | C | -0.413275 | 0.427067 | -4.179725 | C | -0.420548 | 0.478890 | -4.810129 |
| N | -0.295492 | 0.217532 | -1.929363 | N | -0.262611 | 0.157004 | -1.307990 | N | -0.285943 | 0.214346 | -1.937448 |
| C | -0.607067 | -0.734831 | -4.143314 | C | -0.569210 | -0.794527 | -3.522433 | C | -0.610460 | -0.736305 | -4.149856 |
| C | -0.164899 | 1.557678 | -3.952834 | C | -0.175699 | 1.506844 | -3.327412 | C | -0.157392 | 1.554666 | -3.960296 |
| C | -0.113967 | 1.384817 | -2.549083 | C | -0.110359 | 1.330103 | -1.924637 | C | -0.101236 | 1.381205 | -2.556982 |
| C | -0.536765 | -0.819751 | -2.732579 | C | -0.487939 | -0.882616 | -2.112685 | C | -0.535231 | -0.821819 | -2.739543 |
| S | -0.935180 | -2.295030 | -4.850020 | S | -0.869350 | -2.359156 | -4.232249 | S | -0.946541 | -2.295423 | -4.855042 |
| S | 0.126759 | 3.220595 | -4.390262 | S | 0.074041 | 3.177137 | -3.760402 | S | 0.139563 | 3.216654 | -4.397632 |
| C | -0.980328 | -3.046559 | -3.268493 | C | -0.888237 | -3.116330 | -2.652215 | C | -0.987317 | -3.047124 | -3.272371 |
| H | -1.169602 | -4.106702 | -3.199877 | H | -1.055545 | -4.180279 | -2.585742 | H | -1.180686 | -4.106461 | -3.203053 |
| C | -0.756124 | -2.172148 | -2.253562 | C | -0.676980 | -2.240664 | -1.635550 | C | -0.756016 | -2.173636 | -2.258193 |
| C | 0.309371 | 3.673091 | -2.708821 | C | 0.261954 | 3.627230 | -2.078331 | C | 0.329650 | 3.667606 | -2.715643 |
| H | 0.519732 | 4.703093 | -2.466267 | H | 0.452196 | 4.660646 | -1.833521 | H | 0.544921 | 4.696472 | -2.473177 |
| C | 0.159456 | 2.628763 | -1.853416 | C | 0.142719 | 2.576811 | -1.225462 | C | 0.179049 | 2.623440 | -1.859904 |
| C | -0.426226 | 0.604358 | -6.300004 | C | -0.430513 | 0.552652 | -5.675815 | C | -0.430118 | 0.603956 | -6.306438 |
| H | -0.784611 | 1.600399 | -6.588082 | H | -0.806359 | 1.542880 | -5.961441 | H | -0.798693 | 1.596839 | -6.592922 |
| H | -1.127457 | -0.123305 | -6.727165 | H | -1.122370 | -0.186099 | -6.099363 | H | -1.124368 | -0.130098 | -6.733751 |
| C | 0.974188 | 0.373547 | -6.893789 | C | 0.970039 | 0.343498 | -6.277228 | C | 0.971908 | 0.387354 | -6.901988 |
| H | 1.329334 | -0.621250 | -6.598395 | H | 1.341924 | -0.645606 | -5.983127 | H | 1.335773 | -0.604954 | -6.608748 |
| H | 1.671099 | 1.102677 | -6.462940 | H | 1.657976 | 1.083261 | -5.850181 | H | 1.663083 | 1.121407 | -6.470437 |
| C | 0.961756 | 0.495115 | -8.415101 | C | 0.947810 | 0.463646 | -7.798465 | C | 0.957471 | 0.512030 | -8.422965 |
| H | 1.959980 | 0.328479 | -8.830987 | H | 1.946235 | 0.311888 | -8.219434 | H | 1.956852 | 0.355033 | -8.839761 |
| H | 0.627439 | 1.492091 | -8.722781 | H | 0.596702 | 1.455072 | -8.105342 | H | 0.614416 | 1.506787 | -8.728165 |
| H | 0.281730 | -0.240806 | -8.858221 | H | 0.276774 | -0.282945 | -8.237386 | H | 0.283518 | -0.228535 | -8.867399 |
| N | -0.703412 | -2.383045 | -0.878688 | N | -0.614260 | -2.452033 | -0.262091 | N | -0.698679 | -2.381855 | -0.884425 |
| H | -0.520738 | -1.549787 | -0.325568 | H | -0.447777 | -1.615654 | 0.291306 | H | -0.504443 | -1.549340 | -0.334752 |
| N | 0.226767 | 2.587406 | -0.463673 | N | 0.224993 | 2.529700 | 0.162347 | N | 0.252126 | 2.577689 | -0.471752 |
| H | 0.071800 | 1.669568 | -0.055424 | H | 0.100380 | 1.605737 | 0.566477 | H | 0.086109 | 1.660975 | -0.065940 |
| C | -0.851404 | -3.604709 | -0.272602 | C | -0.770298 | -3.673116 | 0.349057 | C | -0.842499 | -3.605086 | -0.271331 |
| C | 0.466719 | 3.676614 | 0.335356 | C | 0.465059 | 3.617812 | 0.967264 | C | 0.481927 | 3.667637 | 0.336289 |
| O | -1.080352 | -4.629235 | -0.908900 | O | -0.993554 | -4.698908 | -0.290382 | O | -1.079918 | -4.628068 | -0.910720 |
| O | 0.660668 | 4.797650 | -0.125591 | O | 0.631389 | 4.745140 | 0.506672 | O | 0.673855 | 4.790448 | -0.126394 |
| C | -0.801223 | -4.620380 | 2.002748 | C | -0.764162 | -4.686455 | 2.628493 | C | -0.788280 | -4.621234 | 2.009039 |
| C | -0.939559 | -6.613572 | 3.959725 | C | -0.968158 | -6.648481 | 4.574911 | C | -0.927533 | -6.626928 | 4.004219 |
| C | -1.162740 | -5.928951 | 1.648878 | C | -1.160250 | -5.984343 | 2.278562 | C | -1.139334 | -5.934003 | 1.668092 |
| C | -0.512248 | -4.325895 | 3.346927 | C | -0.471389 | -4.396001 | 3.970176 | C | -0.512984 | -4.321345 | 3.350528 |
| C | -0.579465 | -5.312630 | 4.317201 | C | -0.573583 | -5.374473 | 4.951931 | C | -0.584763 | -5.309337 | 4.326367 |
| C | -1.226137 | -6.913950 | 2.630614 | C | -1.260319 | -6.969605 | 3.262053 | C | -1.203432 | -6.909132 | 2.663953 |
| H | -1.393641 | -6.174508 | 0.622888 | H | -1.390497 | -6.227894 | 1.251561 | H | -1.362246 | -6.191114 | 0.642365 |
| H | -0.235317 | -3.313114 | 3.627128 | H | -0.163227 | -3.391544 | 4.248839 | H | -0.244398 | -3.304773 | 3.628877 |
| H | -0.353674 | -5.066285 | 5.350383 | H | -0.350859 | -5.153972 | 5.990918 | H | -0.369044 | -5.047177 | 5.359707 |
| H | -1.508713 | -7.923223 | 2.346461 | H | -1.566939 | -7.978782 | 3.005252 | H | -1.480965 | -7.922190 | 2.379602 |
| C | 0.675225 | 4.261447 | 2.748904 | C | 0.715861 | 4.197007 | 3.380542 | C | 0.674590 | 4.250774 | 2.756460 |
| C | 1.065150 | 5.862202 | 5.008912 | C | 1.132688 | 5.774351 | 5.620955 | C | 1.054812 | 5.855955 | 5.059100 |
| C | 0.573193 | 3.713710 | 4.041176 | C | 0.609763 | 3.651467 | 4.669545 | C | 0.560553 | 3.702839 | 4.042507 |
| C | 0.977043 | 5.622634 | 2.602890 | C | 1.036259 | 5.553578 | 3.234788 | C | 0.977368 | 5.611870 | 2.626688 |
| C | 1.170307 | 6.411162 | 3.735385 | C | 1.243966 | 6.344092 | 4.365993 | C | 1.160042 | 6.387974 | 3.772331 |
| C | 0.767115 | 4.504989 | 5.159918 | C | 0.818809 | 4.435851 | 5.797201 | C | 0.747499 | 4.494830 | 5.168943 |
| H | 0.338402 | 2.659307 | 4.160292 | H | 0.361911 | 2.600000 | 4.790103 | H | 0.320010 | 2.648145 | 4.156475 |
| H | 1.060296 | 6.062610 | 1.620133 | H | 1.124614 | 5.992428 | 2.251525 | H | 1.066277 | 6.061490 | 1.647992 |

| | | | |
|---|---|---|---|
| H | 1.403168 | 7.463741 | 3.609002 |
| H | 0.683650 | 4.066354 | 6.150517 |
| N | -0.716498 | -3.557065 | 1.096878 |
| H | -0.490991 | -2.657723 | 1.508927 |
| N | 0.465562 | 3.382270 | 1.680343 |
| H | 0.272166 | 2.422140 | 1.944734 |
| C | -0.960818 | -7.690954 | 4.996271 |
| C | 1.297074 | 6.690295 | 6.232043 |
| F | -1.327125 | -7.231961 | 6.209491 |
| F | 0.254030 | -8.265975 | 5.168513 |
| F | -1.805241 | -8.692741 | 4.684587 |
| F | 2.449337 | 6.363662 | 6.863165 |
| F | 0.319970 | 6.528492 | 7.151154 |
| F | 1.368723 | 8.006808 | 5.967847 |

| | | | |
|---|---|---|---|
| H | 1.492688 | 7.396172 | 4.267720 |
| H | 0.738726 | 4.018139 | 6.795687 |
| N | -0.651632 | -3.622114 | 1.714206 |
| H | -0.429456 | -2.723058 | 2.127642 |
| N | 0.497556 | 3.315952 | 2.304451 |
| H | 0.317719 | 2.353373 | 2.568293 |
| F | -1.075615 | -7.609780 | 5.527483 |
| F | 1.339671 | 6.547898 | 6.716658 |

| | | | |
|---|---|---|---|
| H | 1.390685 | 7.444356 | 3.650361 |
| H | 0.649094 | 4.043319 | 6.153677 |
| N | -0.699165 | -3.556536 | 1.090335 |
| H | -0.479940 | -2.655548 | 1.501339 |
| N | 0.471172 | 3.371692 | 1.673843 |
| H | 0.279400 | 2.410595 | 1.934615 |
| C | -0.976270 | -7.706711 | 5.055853 |
| H | -0.061364 | -8.310376 | 5.040593 |
| H | -1.818607 | -8.384643 | 4.887279 |
| H | -1.074236 | -7.276850 | 6.056698 |
| C | 1.290015 | 6.706701 | 6.281722 |
| H | 2.350687 | 6.708820 | 6.558932 |
| H | 0.725822 | 6.329141 | 7.139513 |
| H | 0.994402 | 7.744665 | 6.102861 |

| Anion complex **2**@$Cl^-$<br>$\Delta G^0$ = -2537.01404 au | | | | Anion complex **3**@$Cl^-$<br>$\Delta G^0$ = -2684.65076 au | | | | Anion complex **4**@$Cl^-$<br>$\Delta G^0$ = -3093.52609 au | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| C | -0.205518 | 0.004661 | -4.465160 | C | -0.404673 | 0.011450 | -4.318619 | C | -0.367869 | 0.007425 | -4.764501 |
| N | -0.659027 | -0.018595 | -1.618240 | N | -0.263329 | 0.007144 | -1.437639 | N | -0.246885 | 0.006166 | -1.881835 |
| C | -0.339221 | -1.174769 | -3.727467 | C | -0.373248 | -1.163340 | -3.561158 | C | -0.335507 | -1.166654 | -4.005303 |
| C | -0.308298 | 1.171803 | -3.703088 | C | -0.359973 | 1.183985 | -3.558378 | C | -0.336173 | 1.180852 | -4.004398 |
| C | -0.530683 | 1.111197 | -2.308710 | C | -0.291358 | 1.131972 | -2.147587 | C | -0.276887 | 1.129269 | -2.593594 |
| C | -0.560478 | -1.137027 | -2.331826 | C | -0.303224 | -1.115407 | -2.150571 | C | -0.276036 | -1.116408 | -2.594389 |
| S | -0.268930 | -2.824136 | -4.293552 | S | -0.405835 | -2.818919 | -4.117210 | S | -0.359540 | -2.824044 | -4.556940 |
| S | -0.197480 | 2.830073 | -4.236043 | S | -0.374818 | 2.840995 | -4.109810 | S | -0.360722 | 2.838874 | -4.554396 |
| C | -0.530875 | -3.439362 | -2.667334 | C | -0.327937 | -3.420953 | -2.468295 | C | -0.292234 | -3.422512 | -2.907648 |
| H | -0.563576 | -4.507023 | -2.512342 | H | -0.323459 | -4.487528 | -2.301585 | H | -0.287136 | -4.488964 | -2.738914 |
| C | -0.669275 | -2.456182 | -1.739852 | C | -0.280027 | -2.429877 | -1.541098 | C | -0.253242 | -2.429052 | -1.983449 |
| C | -0.445357 | 3.418564 | -2.597866 | C | -0.292317 | 3.438134 | -2.459644 | C | -0.293857 | 3.435724 | -2.904323 |
| H | -0.453959 | 4.483455 | -2.421896 | H | -0.277599 | 4.504234 | -2.290369 | H | -0.288653 | 4.502007 | -2.734305 |
| C | -0.606326 | 2.420548 | -1.690135 | C | -0.255020 | 2.444531 | -1.534713 | C | -0.254543 | 2.441222 | -1.981310 |
| C | 0.092256 | 0.017658 | -5.936870 | C | -0.413907 | 0.010608 | -5.820156 | C | -0.369784 | 0.007413 | -6.266058 |
| H | -0.355338 | 0.908241 | -6.395678 | H | -0.929139 | 0.906195 | -6.188649 | H | -0.899786 | 0.893996 | -6.635415 |
| H | -0.368882 | -0.855794 | -6.414698 | H | -0.978066 | -0.856627 | -6.185284 | H | -0.917454 | -0.868923 | -6.634278 |
| C | 1.606254 | 0.009410 | -6.208221 | C | 1.013655 | -0.030925 | -6.392317 | C | 1.059607 | -0.007161 | -6.834640 |
| H | 2.046923 | -0.886099 | -5.753304 | H | 1.522137 | -0.928589 | -6.020021 | H | 1.586503 | -0.892524 | -6.458651 |
| H | 2.063558 | 0.876023 | -5.715045 | H | 1.574776 | 0.833503 | -6.016831 | H | 1.602464 | 0.869954 | -6.461968 |
| C | 1.905934 | 0.039185 | -7.704239 | C | 1.004301 | -0.028866 | -7.918565 | C | 1.052839 | -0.010888 | -8.360855 |
| H | 2.984217 | 0.026210 | -7.890117 | H | 2.022297 | -0.063142 | -8.318443 | H | 2.072086 | -0.023906 | -8.758703 |
| H | 1.492616 | 0.943207 | -8.165061 | H | 0.518243 | 0.874776 | -8.302803 | H | 0.547353 | 0.880119 | -8.749437 |
| H | 1.463882 | -0.828419 | -8.206548 | H | 0.457877 | -0.896567 | -8.304704 | H | 0.526797 | -0.892144 | -8.744299 |
| N | -0.889240 | -2.508499 | -0.370791 | N | -0.213416 | -2.467744 | -0.154618 | N | -0.196121 | -2.463760 | -0.594687 |
| H | -0.952259 | -1.604553 | 0.104805 | H | -0.186217 | -1.555027 | 0.308115 | H | -0.167690 | -1.549702 | -0.132853 |
| N | -0.820369 | 2.450375 | -0.319538 | N | -0.189850 | 2.479391 | -0.148107 | N | -0.196109 | 2.473296 | -0.592581 |
| H | -0.893014 | 1.538697 | 0.139163 | H | -0.171801 | 1.566025 | 0.313927 | H | -0.168098 | 1.558013 | -0.133521 |
| C | -1.017263 | -3.661643 | 0.372123 | C | -0.175269 | -3.612310 | 0.603834 | C | -0.178987 | -3.603032 | 0.161018 |
| C | -0.950522 | 3.591332 | 0.442247 | C | -0.155419 | 3.622543 | 0.612746 | C | -0.182296 | 3.610359 | 0.166455 |
| O | -0.909726 | -4.783375 | -0.136169 | O | -0.206099 | -4.735773 | 0.101579 | O | -0.217616 | -4.729139 | -0.326493 |
| O | -0.860947 | 4.721928 | -0.050266 | O | -0.180528 | 4.747156 | 0.112690 | O | -0.224781 | 4.737769 | -0.317736 |
| C | -1.259111 | -4.534535 | 2.649322 | C | -0.035330 | -4.268561 | 3.007701 | C | -0.074926 | -4.239677 | 2.563493 |
| H | -1.904463 | -4.251103 | 3.486805 | C | 0.097459 | -5.942591 | 5.262619 | C | 0.010401 | -5.892633 | 4.791052 |
| H | -1.697561 | -5.419090 | 2.177983 | C | -0.125618 | -5.659370 | 2.856650 | C | -0.162368 | -5.635838 | 2.407234 |
| C | 0.148852 | -4.847814 | 3.153437 | C | 0.120869 | -3.726300 | 4.294315 | C | 0.053380 | -3.694095 | 3.857960 |
| H | 0.568858 | -3.946925 | 3.621472 | C | 0.185441 | -4.555985 | 5.407568 | C | 0.096544 | -4.511651 | 4.970416 |
| H | 0.789246 | -5.092858 | 2.295434 | C | -0.057474 | -6.478487 | 3.985624 | C | -0.119096 | -6.456762 | 3.524975 |
| C | 0.157043 | -6.002839 | 4.152695 | H | -0.248107 | -6.092622 | 1.873937 | H | -0.263577 | -6.069199 | 1.423140 |
| H | -0.514085 | -5.762500 | 4.988103 | H | 0.190657 | -2.647271 | 4.412444 | H | 0.120067 | -2.616336 | 3.978150 |
| H | -0.253455 | -6.899741 | 3.670280 | H | 0.306199 | -4.114312 | 6.392723 | H | 0.196932 | -4.089793 | 5.963607 |
| C | 1.556921 | -6.300350 | 4.686685 | H | -0.129278 | -7.554770 | 3.853840 | H | -0.186661 | -7.532673 | 3.412674 |
| H | 1.969161 | -5.425825 | 5.202724 | H | 0.147704 | -6.592012 | 6.131316 | C | -0.074277 | 4.238483 | 2.571104 |
| H | 2.238357 | -6.557454 | 3.867768 | C | -0.040836 | 4.272409 | 3.020003 | C | 0.024109 | 5.884092 | 4.803936 |
| H | 1.547410 | -7.136291 | 5.393325 | C | 0.057844 | 5.937847 | 5.283315 | C | 0.065552 | 3.688786 | 3.862797 |
| C | -1.215709 | 4.438844 | 2.725893 | C | 0.115395 | 3.726468 | 4.305031 | C | -0.168929 | 5.634827 | 2.420703 |
| H | -1.801170 | 4.097494 | 3.585139 | C | -0.148274 | 5.662719 | 2.874729 | C | -0.118374 | 6.452116 | 3.540954 |
| H | -1.743005 | 5.289481 | 2.282885 | C | -0.096747 | 6.477486 | 4.007813 | C | 0.114677 | 4.502693 | 4.977757 |
| C | 0.180763 | 4.865216 | 3.176190 | C | 0.162846 | 4.551733 | 5.422454 | H | 0.137309 | 2.610837 | 3.978649 |
| H | 0.694238 | 4.000737 | 3.618528 | H | 0.198150 | 2.647877 | 4.418584 | H | -0.279862 | 6.070983 | 1.438863 |

| | | | |
|---|---|---|---|
| H | 0.761553 | 5.169506 | 2.295239 |
| C | 0.131196 | 6.010693 | 4.184997 |
| H | -0.464143 | 5.701022 | 5.054352 |
| H | -0.393028 | 6.864554 | 3.735565 |
| C | 1.522557 | 6.444198 | 4.642946 |
| H | 2.053034 | 5.610035 | 5.115968 |
| H | 1.468721 | 7.263923 | 5.366382 |
| H | 2.123502 | 6.783255 | 3.791604 |
| N | -1.294771 | -3.447571 | 1.684346 |
| H | -1.246813 | -2.490909 | 2.032892 |
| N | -1.204550 | 3.357146 | 1.754546 |
| H | -1.164156 | 2.396349 | 2.091274 |
| Cl | -1.054472 | -0.053734 | 2.036936 |

| | | | |
|---|---|---|---|
| H | -0.271222 | 6.098966 | 1.893368 |
| H | -0.181622 | 7.553265 | 3.880307 |
| H | 0.283869 | 4.107002 | 6.406164 |
| H | 0.095027 | 6.583722 | 6.155242 |
| N | -0.100506 | -3.350616 | 1.947467 |
| H | -0.067349 | -2.365147 | 2.215453 |
| N | -0.090021 | 3.357894 | 1.956105 |
| H | -0.056817 | 2.371490 | 2.220998 |
| Cl | -0.093020 | 0.008119 | 2.228510 |

| | | | |
|---|---|---|---|
| H | -0.189683 | 7.528292 | 3.432966 |
| H | 0.224834 | 4.078216 | 5.968824 |
| N | -0.112650 | -3.333095 | 1.514450 |
| H | -0.070878 | -2.344904 | 1.778022 |
| N | -0.112987 | 3.335778 | 1.518931 |
| H | -0.066229 | 2.346182 | 1.777444 |
| N | 0.082584 | 6.749506 | 5.968128 |
| O | 0.202291 | 6.233225 | 7.072164 |
| O | 0.012827 | 7.960297 | 5.799793 |
| N | 0.059039 | -6.762055 | 5.952536 |
| O | -0.013891 | -7.971980 | 5.779453 |
| O | 0.173339 | -6.249920 | 7.059050 |
| Cl | -0.059136 | 0.002649 | 1.770782 |

| Anion complex **5**@$Cl^-$ $\Delta G^0$ = -3358.53642 au | | | | Anion complex **6**@$Cl^-$ $\Delta G^0$ = -2883.08076 au | | | | Anion complex **7**@$Cl^-$ $\Delta G^0$ = -2763.19463 au | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| C | -0.555740 | 0.143647 | -4.948201 | C | -0.380311 | 0.019405 | -4.324972 | C | -0.391445 | 0.003847 | -4.964834 |
| N | -0.359662 | 0.062704 | -2.071415 | N | -0.224127 | 0.012436 | -1.445004 | N | -0.241672 | 0.007555 | -2.084732 |
| C | -0.532099 | -1.050899 | -4.221969 | C | -0.334449 | -1.156223 | -3.569192 | C | -0.366800 | -1.168793 | -4.203725 |
| C | -0.475582 | 1.295006 | -4.158740 | C | -0.341223 | 1.191363 | -3.563542 | C | -0.334531 | 1.178594 | -4.208589 |
| C | -0.380352 | 1.205315 | -2.752043 | C | -0.265196 | 1.137565 | -2.153395 | C | -0.262079 | 1.130127 | -2.798385 |
| C | -0.434801 | -1.039843 | -2.811871 | C | -0.257986 | -1.109581 | -2.158867 | C | -0.292981 | -1.116948 | -2.793444 |
| S | -0.610319 | -2.690996 | -4.816685 | S | -0.359180 | -2.811072 | -4.126510 | S | -0.413954 | -2.826255 | -4.753070 |
| S | -0.469535 | 2.966298 | -4.666943 | S | -0.374737 | 2.849571 | -4.111572 | S | -0.339909 | 2.834602 | -4.764016 |
| C | -0.511670 | -3.335488 | -3.185791 | C | -0.269278 | -3.414504 | -2.478790 | C | -0.338869 | -3.422715 | -3.101762 |
| H | -0.525989 | -4.405911 | -3.046035 | H | -0.257635 | -4.481311 | -2.313734 | H | -0.344609 | -4.488721 | -2.931576 |
| C | -0.426261 | -2.369235 | -2.236060 | C | -0.222980 | -2.424453 | -1.550635 | C | -0.281367 | -2.428967 | -2.178096 |
| C | -0.342569 | 3.518672 | -3.004065 | C | -0.290884 | 3.444093 | -2.460190 | C | -0.248216 | 3.435319 | -3.114917 |
| H | -0.302136 | 4.579686 | -2.808529 | H | -0.286564 | 4.510014 | -2.288973 | H | -0.225922 | 4.501747 | -2.948307 |
| C | -0.304932 | 2.500223 | -2.106999 | C | -0.239452 | 2.448967 | -1.537750 | C | -0.214298 | 2.443519 | -2.188154 |
| C | -0.596423 | 0.189368 | -6.448569 | C | -0.401556 | 0.020818 | -5.826369 | C | -0.411741 | 0.001777 | -6.466218 |
| H | -1.134391 | 1.088429 | -6.774349 | H | -0.922583 | 0.915677 | -6.188375 | H | -0.950647 | 0.886045 | -6.828626 |
| H | -1.155350 | -0.673755 | -6.830540 | H | -0.966919 | -0.847168 | -6.187948 | H | -0.960068 | -0.877239 | -6.826827 |
| C | 0.817349 | 0.193198 | -7.054244 | C | 1.020445 | -0.015542 | -6.411711 | C | 1.009689 | -0.007235 | -7.053457 |
| H | 1.350057 | -0.708350 | -6.728313 | H | 1.536095 | -0.911243 | -6.044532 | H | 1.542654 | -0.893259 | -6.687521 |
| H | 1.373853 | 1.052730 | -6.661228 | H | 1.581982 | 0.850895 | -6.041630 | H | 1.556067 | 0.869422 | -6.685037 |
| C | 0.770289 | 0.252741 | -8.578611 | C | 0.996418 | -0.013301 | -7.937786 | C | 0.982129 | -0.004534 | -8.579527 |
| H | 1.778393 | 0.254730 | -9.004193 | H | 2.010544 | -0.045096 | -8.347537 | H | 1.995609 | -0.014550 | -8.991968 |
| H | 0.257002 | 1.160188 | -8.915629 | H | 0.504331 | 0.889069 | -8.317232 | H | 0.470127 | 0.887615 | -8.956842 |
| H | 0.231410 | -0.610434 | -8.984759 | H | 0.448494 | -0.882362 | -8.318611 | H | 0.451355 | -0.884347 | -8.959800 |
| N | -0.333618 | -2.443207 | -0.851587 | N | -0.149389 | -2.463346 | -0.164280 | N | -0.217002 | -2.460374 | -0.791264 |
| H | -0.274368 | -1.543105 | -0.366811 | H | -0.119550 | -1.551404 | 0.300295 | H | -0.184011 | -1.545067 | -0.334135 |
| N | -0.206132 | 2.495096 | -0.720783 | N | -0.168687 | 2.478798 | -0.151045 | N | -0.143473 | 2.476965 | -0.802163 |
| H | -0.198266 | 1.568448 | -0.284859 | H | -0.133994 | 1.563513 | 0.306446 | H | -0.139976 | 1.562350 | -0.342689 |
| C | -0.328893 | -3.603786 | -0.122601 | C | -0.128564 | -3.607954 | 0.593945 | C | -0.180540 | -3.602097 | -0.026838 |
| C | -0.089393 | 3.612200 | 0.064527 | C | -0.165652 | 3.617381 | 0.616335 | C | -0.122368 | 3.617762 | -0.035432 |
| O | -0.406400 | -4.714674 | -0.642831 | O | -0.170723 | -4.731715 | 0.093110 | O | -0.203945 | -4.727729 | -0.525737 |
| O | -0.078396 | 4.751045 | -0.397883 | O | -0.215981 | 4.744635 | 0.124282 | O | -0.146631 | 4.744468 | -0.531435 |
| C | -0.189270 | -4.310304 | 2.262746 | C | -0.017806 | -4.270165 | 2.995590 | C | -0.044731 | -4.254541 | 2.376338 |
| C | -0.089328 | -6.030999 | 4.465829 | C | 0.059460 | -5.928458 | 5.215582 | C | 0.084488 | -5.938620 | 4.650627 |
| C | -0.314952 | -5.696898 | 2.078149 | C | -0.135526 | -5.658384 | 2.840100 | C | -0.141933 | -5.643928 | 2.232995 |
| C | -0.017220 | -3.802387 | 3.562307 | C | 0.139417 | -3.734829 | 4.284443 | C | 0.112731 | -3.716130 | 3.663063 |
| C | 0.030718 | -4.653450 | 4.655289 | C | 0.177798 | -4.559964 | 5.401923 | C | 0.173329 | -4.546471 | 4.775273 |
| C | -0.264354 | -6.543123 | 3.181260 | C | -0.095052 | -6.489620 | 3.960978 | C | -0.076509 | -6.459217 | 3.365036 |
| H | -0.447801 | -6.105576 | 1.086778 | H | -0.258109 | -6.088707 | 1.856364 | H | -0.271536 | -6.083202 | 1.253564 |
| H | 0.082279 | -2.729764 | 3.707204 | H | 0.231111 | -2.658823 | 4.409631 | H | 0.183204 | -2.637381 | 3.785250 |
| H | 0.166861 | -4.242256 | 5.650673 | H | 0.297592 | -4.150570 | 6.399890 | H | 0.291766 | -4.101626 | 5.760972 |
| H | -0.360816 | -7.614655 | 3.029597 | H | -0.185426 | -7.566190 | 3.855544 | H | -0.157996 | -7.536233 | 3.233323 |
| C | 0.176496 | 4.184407 | 2.473568 | C | -0.078825 | 4.260238 | 3.024179 | C | -0.065795 | 4.256380 | 2.375088 |
| C | 0.518547 | 5.776483 | 4.746955 | C | -0.031098 | 5.901375 | 5.257167 | C | -0.045258 | 5.929053 | 4.660727 |
| C | 0.324828 | 3.596749 | 3.744667 | C | 0.071281 | 3.715707 | 4.309985 | C | -0.192097 | 3.715194 | 3.664135 |
| C | 0.197973 | 5.581549 | 2.356485 | C | -0.204877 | 5.648726 | 2.878336 | C | 0.071383 | 5.642384 | 2.234486 |
| C | 0.371386 | 6.365842 | 3.495250 | C | -0.179346 | 6.471423 | 4.005875 | C | 0.076811 | 6.452673 | 3.372320 |
| C | 0.494700 | 4.383926 | 4.869587 | C | 0.095070 | 4.532385 | 5.434079 | C | -0.181090 | 4.540062 | 4.781788 |
| H | 0.305399 | 2.513768 | 3.837061 | H | 0.169138 | 2.639430 | 4.427720 | H | -0.303841 | 2.639540 | 3.782230 |
| H | 0.080677 | 6.049749 | 1.389842 | H | -0.322462 | 6.085795 | 1.896929 | H | 0.169580 | 6.083766 | 1.252124 |

| | | | |
|---|---|---|---|
| H | 0.388004 | 7.446404 | 3.393306 |
| H | 0.609773 | 3.915209 | 5.843136 |
| N | -0.227065 | -3.372314 | 1.230168 |
| H | -0.159170 | -2.392791 | 1.517684 |
| N | 0.012216 | 3.305510 | 1.402397 |
| H | 0.001263 | 2.312144 | 1.643991 |
| C | -0.080738 | -6.962328 | 5.635165 |
| C | 0.738457 | 6.602243 | 5.973061 |
| F | 0.495462 | -6.421045 | 6.724902 |
| F | 0.577102 | -8.110958 | 5.373555 |
| F | -1.328199 | -7.332152 | 6.013345 |
| F | 0.539606 | 7.915722 | 5.764538 |
| F | -0.077257 | 6.239597 | 6.987448 |
| F | 1.997695 | 6.478529 | 6.456432 |
| Cl | -0.098347 | -0.046870 | 1.586231 |

| | | | |
|---|---|---|---|
| H | -0.276138 | 7.548183 | 3.908254 |
| H | 0.209971 | 4.116494 | 6.429952 |
| N | -0.056497 | -3.347975 | 1.937547 |
| H | -0.013249 | -2.363319 | 2.208394 |
| N | -0.101302 | 3.346750 | 1.958255 |
| H | -0.050044 | 2.360508 | 2.221531 |
| F | 0.094672 | -6.743168 | 6.302420 |
| F | -0.009327 | 6.707738 | 6.350474 |
| Cl | 0.018864 | -0.002506 | 2.214628 |

| | | | |
|---|---|---|---|
| H | 0.180280 | 7.527970 | 3.242526 |
| H | -0.285039 | 4.094122 | 5.768709 |
| N | -0.107117 | -3.336435 | 1.313818 |
| H | -0.091668 | -2.349990 | 1.581241 |
| N | -0.077767 | 3.345231 | 1.305329 |
| H | -0.086884 | 2.355703 | 1.561821 |
| C | 0.184808 | -6.838143 | 5.857134 |
| H | 1.231709 | -7.062022 | 6.093577 |
| H | -0.325401 | -7.789914 | 5.682625 |
| H | -0.257199 | -6.365672 | 6.739545 |
| C | -0.008083 | 6.816953 | 5.879565 |
| H | 0.993122 | 6.829179 | 6.326146 |
| H | -0.704407 | 6.464109 | 6.646445 |
| H | -0.269467 | 7.847666 | 5.623512 |
| Cl | -0.109971 | 0.006655 | 1.617788 |

| Anion complex **2**@$MeCO_2^-$ $\Delta G^0$ = -2305.15974 au | | | | Anion complex **3**@$MeCO_2^-$ $\Delta G^0$ = -2452.80352 au | | | | Anion complex **4**@$MeCO_2^-$ $\Delta G^0$ = -2861.67536 au | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| C | -0.339870 | -0.120307 | -4.617647 | C | -0.373303 | 0.016088 | -4.479691 | C | -4.833354 | 0.010629 | 0.294817 |
| N | -0.119962 | -0.528868 | -1.768956 | N | -0.240906 | 0.011714 | -1.592334 | N | -1.943946 | 0.007946 | 0.189861 |
| C | 0.884545 | -0.265417 | -3.964945 | C | -0.349736 | -1.153121 | -3.723895 | C | -4.076396 | -1.158078 | 0.273291 |
| C | -1.448413 | -0.189966 | -3.773572 | C | -0.326133 | 1.182777 | -3.721879 | C | -4.074917 | 1.177698 | 0.259064 |
| C | -1.298434 | -0.378918 | -2.377883 | C | -0.262072 | 1.145641 | -2.304531 | C | -2.657268 | 1.140946 | 0.208587 |
| C | 0.949907 | -0.477704 | -2.565844 | C | -0.282282 | -1.120526 | -2.306689 | C | -2.658809 | -1.123931 | 0.220521 |
| S | 2.476377 | -0.227014 | -4.673139 | S | -0.383325 | -2.779421 | -4.338118 | S | -4.687923 | -2.786045 | 0.302882 |
| S | -3.129926 | -0.072380 | -4.218498 | S | -0.326973 | 2.810970 | -4.332413 | S | -4.684309 | 2.806796 | 0.266395 |
| C | 3.217105 | -0.514308 | -3.110709 | C | -0.306875 | -3.422309 | -2.718024 | C | -3.067377 | -3.426623 | 0.243972 |
| H | 4.291823 | -0.581198 | -3.048471 | H | -0.301405 | -4.491817 | -2.586161 | H | -2.934031 | -4.496098 | 0.242393 |
| C | 2.318462 | -0.635568 | -2.096723 | C | -0.260473 | -2.469428 | -1.746899 | C | -2.098626 | -2.471544 | 0.205757 |
| C | -3.621506 | -0.256026 | -2.546500 | C | -0.244469 | 3.448598 | -2.710275 | C | -3.062606 | 3.444314 | 0.203924 |
| H | -4.673428 | -0.241969 | -2.308297 | H | -0.220904 | 4.517537 | -2.575428 | H | -2.927589 | 4.513519 | 0.190120 |
| C | -2.578314 | -0.399334 | -1.685469 | C | -0.219282 | 2.492608 | -1.741586 | C | -2.095202 | 2.487447 | 0.180745 |
| C | -0.451968 | 0.152041 | -6.090325 | C | -0.375670 | 0.016469 | -5.981347 | C | -6.334951 | 0.011126 | 0.289568 |
| H | -1.391550 | -0.265721 | -6.472867 | H | -0.873324 | 0.921433 | -6.351037 | H | -6.705882 | 0.909456 | 0.798299 |
| H | 0.363139 | -0.354016 | -6.622754 | H | -0.954756 | -0.839241 | -6.350583 | H | -6.706567 | -0.851925 | 0.856001 |
| C | -0.403150 | 1.658983 | -6.395136 | C | 1.053322 | -0.049975 | -6.547557 | C | -6.897850 | -0.034840 | -1.141384 |
| H | 0.538087 | 2.072128 | -6.012826 | H | 1.545671 | -0.954415 | -6.170037 | H | -6.521605 | -0.932688 | -1.646481 |
| H | -1.214930 | 2.160361 | -5.854129 | H | 1.627099 | 0.806483 | -6.172933 | H | -6.520920 | 0.829019 | -1.702305 |
| C | -0.524455 | 1.931086 | -7.891904 | C | 1.050558 | -0.053314 | -8.073546 | C | -8.424023 | -0.034951 | -1.140843 |
| H | -0.484653 | 3.004449 | -8.101149 | H | 2.069774 | -0.101572 | -8.468830 | H | -8.818102 | -0.071134 | -2.161002 |
| H | -1.472189 | 1.543955 | -8.282031 | H | 0.577447 | 0.854874 | -8.463262 | H | -8.812422 | 0.868667 | -0.658115 |
| H | 0.289908 | 1.447181 | -8.442359 | H | 0.495228 | -0.915616 | -8.459017 | H | -8.811921 | -0.902490 | -0.595528 |
| N | 2.529889 | -0.893688 | -0.749688 | N | -0.197174 | -2.649301 | -0.368786 | N | -0.717808 | -2.648537 | 0.157557 |
| H | 1.702549 | -1.061813 | -0.165171 | H | -0.198980 | -1.812990 | 0.226046 | H | -0.126729 | -1.808887 | 0.129255 |
| N | -2.580039 | -0.542848 | -0.304846 | N | -0.159834 | 2.665703 | -0.362630 | N | -0.713911 | 2.660910 | 0.137645 |
| H | -1.675579 | -0.472667 | 0.177884 | H | -0.184592 | 1.826214 | 0.227259 | H | -0.125058 | 1.819260 | 0.126473 |
| C | 3.774609 | -1.062339 | -0.174246 | C | -0.139225 | -3.887920 | 0.237156 | C | -0.111786 | -3.880830 | 0.142279 |
| C | -3.718654 | -0.638748 | 0.469000 | C | -0.114463 | 3.901140 | 0.250501 | C | -0.104203 | 3.891333 | 0.124175 |
| O | 4.823312 | -0.876652 | -0.807043 | O | -0.132815 | -4.939296 | -0.405897 | O | -0.739030 | -4.937972 | 0.165303 |
| O | -4.851519 | -0.694136 | -0.027312 | O | -0.088720 | 4.955242 | -0.387735 | O | -0.728751 | 4.950330 | 0.131903 |
| C | 4.957269 | -1.561825 | 1.912337 | C | -0.024597 | -4.888494 | 2.512850 | C | 2.166799 | -4.859305 | 0.081012 |
| H | 4.750709 | -2.258832 | 2.730620 | C | 0.103322 | -6.870319 | 4.508926 | C | 4.142329 | -6.815886 | 0.042677 |
| H | 5.741156 | -2.005360 | 1.289603 | C | 0.018353 | -6.245074 | 2.158464 | C | 1.811756 | -6.222855 | 0.075036 |
| C | 5.433553 | -0.222418 | 2.473633 | C | -0.003566 | -4.538833 | 3.874773 | C | 3.534242 | -4.505367 | 0.065304 |
| H | 4.637250 | 0.207872 | 3.096227 | C | 0.060388 | -5.518069 | 4.858406 | C | 4.519793 | -5.471686 | 0.046412 |
| H | 5.602656 | 0.472963 | 1.640664 | C | 0.081735 | -7.216774 | 3.159674 | C | 2.802395 | -7.193753 | 0.056048 |
| C | 6.712636 | -0.365644 | 3.295601 | H | 0.003432 | -6.536011 | 1.117887 | H | 0.772621 | -6.515664 | 0.085031 |
| H | 6.536269 | -1.071891 | 4.117995 | H | -0.037048 | -3.487572 | 4.152427 | H | 3.810324 | -3.454582 | 0.068910 |
| H | 7.497718 | -0.807626 | 2.667636 | H | 0.076029 | -5.220861 | 5.903264 | H | 5.567101 | -5.193544 | 0.035400 |
| C | 7.196220 | 0.969448 | 3.858889 | H | 0.114623 | -8.263145 | 2.868073 | H | 2.532999 | -8.243622 | 0.051544 |
| H | 6.434785 | 1.416653 | 4.508061 | H | 0.153772 | -7.637297 | 5.275862 | C | 2.178268 | 4.862056 | 0.083221 |
| H | 7.405035 | 1.679375 | 3.050509 | C | -0.040068 | 4.890415 | 2.532637 | C | 4.160254 | 6.812062 | 0.047208 |
| H | 8.111799 | 0.848535 | 4.446629 | C | 0.068974 | 6.863550 | 4.538419 | C | 3.544596 | 4.503520 | 0.074133 |
| C | -4.575196 | -0.658026 | 2.760741 | C | -0.024887 | 4.534520 | 3.892999 | C | 1.827689 | 6.226745 | 0.072577 |
| H | -4.209813 | -1.093137 | 3.696490 | C | -0.001009 | 6.248919 | 2.184770 | C | 2.821526 | 7.194358 | 0.054613 |
| H | -5.383678 | -1.297537 | 2.393119 | C | 0.053470 | 7.216180 | 3.190668 | C | 4.533320 | 5.466627 | 0.056337 |
| C | -5.098604 | 0.756334 | 3.009782 | C | 0.029360 | 5.509522 | 4.881407 | H | 3.817218 | 3.451784 | 0.081628 |
| H | -4.277338 | 1.380665 | 3.387462 | H | -0.055136 | 3.481830 | 4.165547 | H | 0.789452 | 6.522831 | 0.078457 |

| | | | |
|---|---|---|---|
| H | -5.419854 | 1.189790 | 2.053488 |
| C | -6.260188 | 0.774687 | 4.001281 |
| H | -5.937705 | 0.316488 | 4.945749 |
| H | -7.075391 | 0.149679 | 3.613203 |
| C | -6.777149 | 2.187650 | 4.265690 |
| H | -5.985601 | 2.819185 | 4.684752 |
| H | -7.614369 | 2.183278 | 4.971062 |
| H | -7.121173 | 2.655230 | 3.336069 |
| N | 3.743633 | -1.455828 | 1.121441 |
| H | 2.833620 | -1.574227 | 1.568548 |
| N | -3.481760 | -0.710661 | 1.804566 |
| H | -2.535609 | -0.498566 | 2.124315 |
| C | 0.194794 | -0.920645 | 2.237997 |
| O | -0.676131 | -0.122890 | 1.789949 |
| O | 0.933645 | -1.648547 | 1.519191 |
| C | 0.358522 | -0.989061 | 3.751001 |
| H | 1.065079 | -1.767086 | 4.045112 |
| H | -0.613523 | -1.176194 | 4.218038 |
| H | 0.715556 | -0.020413 | 4.116110 |
| H | -0.012205 | 6.544293 | 1.145416 |
| H | 0.083613 | 8.264033 | 2.904191 |
| H | 0.040421 | 5.207635 | 5.924996 |
| H | 0.112175 | 7.627056 | 5.309270 |
| N | -0.086347 | -3.822718 | 1.603948 |
| H | -0.108552 | -2.883828 | 2.015276 |
| N | -0.095673 | 3.829279 | 1.617924 |
| H | -0.130168 | 2.887886 | 2.023467 |
| C | -0.213117 | 0.004910 | 2.594576 |
| O | -0.227280 | 1.112089 | 1.993638 |
| O | -0.193097 | -1.108889 | 2.006432 |
| C | -0.183972 | 0.016278 | 4.115205 |
| H | -0.604749 | -0.905492 | 4.521921 |
| H | -0.720168 | 0.883083 | 4.507542 |
| H | 0.860562 | 0.088669 | 4.439304 |
| H | 2.555620 | 8.245102 | 0.046619 |
| H | 5.579747 | 5.185065 | 0.049956 |
| N | 1.266290 | -3.807658 | 0.099686 |
| H | 1.670250 | -2.862239 | 0.093534 |
| N | 1.274117 | 3.813653 | 0.102342 |
| H | 1.674801 | 2.866711 | 0.106708 |
| N | 5.190559 | 7.832544 | 0.030153 |
| O | 6.363028 | 7.477119 | 0.024314 |
| O | 4.848802 | 9.008953 | 0.022244 |
| N | 5.169137 | -7.839889 | 0.024879 |
| O | 4.823349 | -9.015137 | 0.022012 |
| O | 6.342772 | -7.488456 | 0.013937 |
| C | 2.231633 | 0.003109 | 0.123287 |
| O | 1.634385 | 1.112478 | 0.109617 |
| O | 1.637583 | -1.106901 | 0.078813 |
| C | 3.751044 | 0.008433 | 0.159761 |
| H | 4.136030 | -0.917931 | 0.590393 |
| H | 4.121664 | 0.869507 | 0.720008 |
| H | 4.120376 | 0.088991 | -0.868939 |

| Anion complex **5**@$MeCO_2^-$ $\Delta G^0$ = -3126.68875 au | | | | Anion complex **6**@$MeCO_2^-$ $\Delta G^0$ = -2651.23024 au | | | | Anion complex **7**@$MeCO_2^-$ $\Delta G^0$ = -2531.34619 au | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| C | 0.304191 | 5.047339 | -0.513036 | C | -0.337808 | 0.007427 | -4.489798 | C | -5.072786 | 0.007519 | 0.337291 |
| N | 0.212561 | 2.172507 | -0.250424 | N | -0.250747 | 0.005018 | -1.600732 | N | -2.186549 | 0.005166 | 0.228703 |
| C | 0.532675 | 4.387859 | 0.694677 | C | -0.325199 | -1.161315 | -3.733027 | C | -4.314459 | -1.162657 | 0.336346 |
| C | 0.023936 | 4.196236 | -1.581780 | C | -0.304690 | 1.174674 | -3.731704 | C | -4.314152 | 1.176556 | 0.278251 |
| C | 0.001131 | 2.789840 | -1.415496 | C | -0.263539 | 1.138774 | -2.313661 | C | -2.898916 | 1.135020 | 0.237325 |
| C | 0.465811 | 2.976049 | 0.785751 | C | -0.279113 | -1.127512 | -2.315134 | C | -2.899985 | -1.122757 | 0.270496 |
| S | 0.910305 | 5.105963 | 2.236659 | S | -0.352437 | -2.788897 | -4.345444 | S | -4.900678 | -2.802902 | 0.407087 |
| S | -0.335326 | 4.645838 | -3.227679 | S | -0.299875 | 2.802848 | -4.342736 | S | -4.902440 | 2.816104 | 0.242794 |
| C | 0.960394 | 3.530775 | 2.998423 | C | -0.298933 | -3.429790 | -2.723544 | C | -3.266744 | -3.426426 | 0.332051 |
| H | 1.172079 | 3.470511 | 4.054408 | H | -0.296246 | -4.499111 | -2.590136 | H | -3.116221 | -4.494286 | 0.344367 |
| C | 0.704327 | 2.506041 | 2.141569 | C | -0.264469 | -2.475532 | -1.753516 | C | -2.317080 | -2.455847 | 0.258745 |
| C | -0.493107 | 2.965489 | -3.689593 | C | -0.245005 | 3.441337 | -2.720066 | C | -3.267656 | 3.438005 | 0.188553 |
| H | -0.728911 | 2.728360 | -4.715063 | H | -0.225725 | 4.510345 | -2.585512 | H | -3.119157 | 4.505679 | 0.154786 |
| C | -0.284909 | 2.098517 | -2.662996 | C | -0.233781 | 2.485866 | -1.750608 | C | -2.315197 | 2.467363 | 0.200461 |
| C | 0.294706 | 6.543941 | -0.636203 | C | -0.318094 | 0.008046 | -5.991297 | C | -6.574241 | 0.009386 | 0.337420 |
| H | 0.624441 | 6.834260 | -1.641583 | H | -0.825892 | 0.904789 | -6.367327 | H | -6.940661 | 0.900034 | 0.863194 |
| H | 1.011539 | 6.977222 | 0.072424 | H | -0.877288 | -0.856995 | -6.369036 | H | -6.944354 | -0.862662 | 0.890559 |
| C | -1.103323 | 7.126767 | -0.367782 | C | 1.118925 | -0.033451 | -6.539532 | C | -7.145986 | -0.012608 | -1.089976 |
| H | -1.427808 | 6.829742 | 0.637042 | H | 1.622134 | -0.930153 | -6.158000 | H | -6.780046 | -0.906714 | -1.609116 |
| H | -1.817026 | 6.688990 | -1.076227 | H | 1.673600 | 0.831620 | -6.156372 | H | -6.766926 | 0.855447 | -1.642617 |
| C | -1.108163 | 8.647921 | -0.491525 | C | 1.135150 | -0.033039 | -8.065544 | C | -8.672280 | -0.000259 | -1.078686 |
| H | -2.104696 | 9.055182 | -0.295721 | H | 2.159738 | -0.066826 | -8.448239 | H | -9.074204 | -0.023816 | -2.096161 |
| H | -0.806639 | 8.957267 | -1.498399 | H | 0.654870 | 0.869604 | -8.459168 | H | -9.049225 | 0.902100 | -0.584761 |
| H | -0.410560 | 9.098267 | 0.223201 | H | 0.596158 | -0.901635 | -8.459780 | H | -9.063553 | -0.869271 | -0.538278 |
| N | 0.625728 | 1.140660 | 2.391885 | N | -0.216602 | -2.651126 | -0.374056 | N | -0.935941 | -2.572099 | 0.165942 |
| H | 0.316301 | 0.539215 | 1.618617 | H | -0.206270 | -1.810872 | 0.214935 | H | -0.402881 | -1.707531 | 0.013070 |
| N | -0.291168 | 0.707595 | -2.664513 | N | -0.199540 | 2.659871 | -0.370551 | N | -0.930573 | 2.587415 | 0.195728 |
| H | 0.039230 | 0.234481 | -1.813451 | H | -0.237674 | 1.820836 | 0.219363 | H | -0.381186 | 1.732917 | 0.352572 |
| C | 0.819617 | 0.570782 | 3.626763 | C | -0.167005 | -3.886542 | 0.237975 | C | -0.256124 | -3.769860 | 0.185119 |
| C | -0.596792 | -0.057885 | -3.762577 | C | -0.147059 | 3.894290 | 0.243148 | C | -0.261844 | 3.787019 | 0.097604 |
| O | 1.169757 | 1.219044 | 4.612429 | O | -0.167490 | -4.941755 | -0.399381 | O | -0.826393 | -4.850506 | 0.349019 |
| O | -0.993616 | 0.422632 | -4.823632 | O | -0.095096 | 4.948906 | -0.393185 | O | -0.846316 | 4.857869 | -0.080337 |
| C | 0.667777 | -1.659802 | 4.710236 | C | -0.048103 | -4.881786 | 2.513805 | C | 2.069778 | -4.629490 | -0.029276 |
| C | 0.781481 | -3.578338 | 6.746750 | C | 0.110425 | -6.834777 | 4.480424 | C | 4.194826 | -6.503300 | -0.135843 |
| C | 1.177130 | -1.320142 | 5.972849 | C | 0.006022 | -6.237789 | 2.159065 | C | 1.851178 | -5.969167 | 0.316627 |
| C | 0.218698 | -2.976447 | 4.484430 | C | -0.025829 | -4.532419 | 3.875390 | C | 3.360077 | -4.236943 | -0.421064 |
| C | 0.275984 | -3.925259 | 5.489660 | C | 0.054465 | -5.504017 | 4.865311 | C | 4.398561 | -5.158074 | -0.468957 |
| C | 1.229309 | -2.281981 | 6.979658 | C | 0.086101 | -7.216367 | 3.151892 | C | 2.909058 | -6.879046 | 0.257202 |
| H | 1.528558 | -0.316918 | 6.165956 | H | -0.011190 | -6.530714 | 1.119385 | H | 0.870123 | -6.297150 | 0.631355 |
| H | -0.178407 | -3.243624 | 3.508420 | H | -0.069283 | -3.483369 | 4.157543 | H | 3.542009 | -3.197290 | -0.685514 |
| H | -0.075566 | -4.935664 | 5.298139 | H | 0.074374 | -5.236043 | 5.916857 | H | 5.388424 | -4.823747 | -0.773057 |
| H | 1.626098 | -2.006624 | 7.951819 | H | 0.131048 | -8.268742 | 2.889171 | H | 2.718759 | -7.914443 | 0.532696 |
| C | -0.618416 | -2.453221 | -4.433274 | C | -0.074099 | 4.886521 | 2.522161 | C | 2.064196 | 4.670278 | 0.143398 |
| C | -0.954341 | -4.698374 | -6.071978 | C | 0.097902 | 6.834170 | 4.492904 | C | 4.175100 | 6.558160 | 0.005446 |
| C | -0.226934 | -3.731551 | -3.991184 | C | -0.062000 | 4.534501 | 3.883233 | C | 3.373870 | 4.317702 | 0.508464 |
| C | -1.188737 | -2.316349 | -5.709059 | C | -0.004579 | 6.242514 | 2.170128 | C | 1.817415 | 5.978326 | -0.291377 |
| C | -1.351941 | -3.439597 | -6.515311 | C | 0.083144 | 7.218356 | 3.164985 | C | 2.868535 | 6.896503 | -0.350684 |
| C | -0.393550 | -4.842733 | -4.799656 | C | 0.024501 | 5.503518 | 4.875213 | C | 4.404715 | 5.245931 | 0.438610 |
| H | 0.213715 | -3.841398 | -3.003471 | H | -0.118433 | 3.485446 | 4.163376 | H | 3.575771 | 3.305285 | 0.851781 |
| H | -1.497778 | -1.344503 | -6.065750 | H | -0.016147 | 6.537320 | 1.130901 | H | 0.818493 | 6.277293 | -0.577621 |

| | | | |
|---|---|---|---|
| H | -1.793062 | -3.321416 | -7.500465 |
| H | -0.081837 | -5.820246 | -4.442865 |
| N | 0.579693 | -0.783711 | 3.630233 |
| H | 0.236917 | -1.179905 | 2.744324 |
| N | -0.409626 | -1.403024 | -3.541261 |
| H | -0.001073 | -1.654676 | -2.634944 |
| C | 0.849823 | -4.627025 | 7.808430 |
| C | -1.178571 | -5.907813 | -6.919578 |
| F | 1.717390 | -5.618981 | 7.496839 |
| F | -0.340672 | -5.237606 | 8.005539 |
| F | 1.237043 | -4.142861 | 9.002084 |
| F | -2.328531 | -6.554017 | -6.607806 |
| F | -0.195791 | -6.822307 | -6.781683 |
| F | -1.260371 | -5.616930 | -8.232327 |
| C | 0.372956 | -1.838202 | 0.128966 |
| O | 0.729536 | -1.362712 | -0.982886 |
| O | -0.259162 | -1.185830 | 1.008519 |
| C | 0.734236 | -3.278905 | 0.456986 |
| H | 1.456527 | -3.282715 | 1.281510 |
| H | 1.169574 | -3.789734 | -0.403521 |
| H | -0.154761 | -3.816263 | 0.799503 |
| H | 0.139819 | 8.270726 | 2.904409 |
| H | 0.036346 | 5.233575 | 5.926378 |
| N | -0.118755 | -3.816547 | 1.604133 |
| H | -0.132651 | -2.876248 | 2.013429 |
| N | -0.157356 | 3.824216 | 1.610235 |
| H | -0.208411 | 2.884678 | 2.018376 |
| F | 0.196391 | -7.792283 | 5.441068 |
| F | 0.190592 | 7.789015 | 5.455631 |
| C | -0.259329 | 0.005043 | 2.586948 |
| O | -0.309449 | 1.113777 | 1.990744 |
| O | -0.181576 | -1.103491 | 1.993780 |
| C | -0.256758 | 0.008291 | 4.107611 |
| H | -0.677074 | -0.919654 | 4.500715 |
| H | -0.806594 | 0.867966 | 4.496279 |
| H | 0.781491 | 0.084908 | 4.450186 |
| H | 2.654740 | 7.908728 | -0.688076 |
| H | 5.408522 | 4.944174 | 0.730912 |
| N | 1.092922 | -3.621415 | 0.008608 |
| H | 1.417894 | -2.668110 | -0.190069 |
| N | 1.095056 | 3.656996 | 0.225658 |
| H | 1.438895 | 2.721244 | 0.463986 |
| C | 5.317786 | -7.506256 | -0.223121 |
| H | 5.443126 | -7.867660 | -1.250643 |
| H | 5.119461 | -8.374885 | 0.411399 |
| H | 6.269092 | -7.062702 | 0.086352 |
| C | 5.304264 | 7.553320 | -0.092901 |
| H | 5.906009 | 7.376836 | -0.992101 |
| H | 5.975010 | 7.477375 | 0.768711 |
| H | 4.923202 | 8.577270 | -0.143388 |
| C | 1.861871 | -0.023899 | 0.240697 |
| O | 1.288164 | 0.917600 | 0.854553 |
| O | 1.262806 | -0.867478 | -0.484471 |
| C | 3.365535 | -0.185207 | 0.406221 |
| H | 3.548072 | -0.995948 | 1.121522 |
| H | 3.825448 | 0.727586 | 0.788961 |
| H | 3.825991 | -0.471799 | -0.542546 |

| Anion complex **2**@$PhCO_2^-$ $\Delta G^0$ = -2496.78196 au | | | | Anion complex **3**@$PhCO_2^-$ $\Delta G^0$ = -2644.42200 au | | | | Anion complex **4**@$PhCO_2^-$ $\Delta G^0$ = -3053.29626 au | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| C | -0.226776 | 0.029890 | -5.189450 | C | -0.456410 | 0.057753 | -5.004475 | C | -5.291164 | 0.058997 | 0.084948 |
| N | -0.679385 | 0.021555 | -2.338859 | N | -0.113963 | 0.089955 | -2.135325 | N | -2.404112 | 0.089805 | -0.052082 |
| C | -0.324047 | -1.143504 | -4.440784 | C | -0.448345 | -1.100591 | -4.228045 | C | -4.516020 | -1.099048 | 0.140349 |
| C | -0.365143 | 1.198668 | -4.438572 | C | -0.276569 | 1.231961 | -4.275178 | C | -4.550050 | 1.232266 | -0.048698 |
| C | -0.570278 | 1.152027 | -3.038088 | C | -0.120983 | 1.208417 | -2.866583 | C | -3.134332 | 1.207502 | -0.103808 |
| C | -0.564074 | -1.103086 | -3.046292 | C | -0.266541 | -1.044866 | -2.823759 | C | -3.102718 | -1.043143 | 0.057981 |
| S | -0.177854 | -2.786913 | -5.005727 | S | -0.612589 | -2.741319 | -4.786101 | S | -5.081976 | -2.741518 | 0.273285 |
| S | -0.319450 | 2.843502 | -5.012160 | S | -0.186350 | 2.855141 | -4.899999 | S | -5.164838 | 2.855864 | -0.195340 |
| C | -0.465783 | -3.407214 | -3.390237 | C | -0.421578 | -3.350911 | -3.157677 | C | -3.443853 | -3.348631 | 0.203889 |
| H | -0.474583 | -4.475077 | -3.232656 | H | -0.443551 | -4.416931 | -2.995926 | H | -3.282240 | -4.414267 | 0.246387 |
| C | -0.666250 | -2.431048 | -2.466049 | C | -0.246851 | -2.373086 | -2.228080 | C | -2.507342 | -2.369733 | 0.090210 |
| C | -0.550821 | 3.456379 | -3.385375 | C | 0.043918 | 3.498620 | -3.289618 | C | -3.542644 | 3.496569 | -0.315426 |
| H | -0.587560 | 4.523493 | -3.231657 | H | 0.161768 | 4.563749 | -3.166469 | H | -3.409766 | 4.561107 | -0.430501 |
| C | -0.656468 | 2.477566 | -2.446561 | C | 0.050036 | 2.546092 | -2.319174 | C | -2.576699 | 2.542962 | -0.243773 |
| C | 0.065989 | 0.037176 | -6.662326 | C | -0.571072 | 0.036653 | -6.501900 | C | -6.792654 | 0.038744 | 0.087738 |
| H | -0.434642 | 0.892721 | -7.133214 | H | -1.060865 | 0.955562 | -6.847308 | H | -7.173451 | 0.960477 | 0.544868 |
| H | -0.345981 | -0.868616 | -7.124476 | H | -1.208858 | -0.800576 | -6.812066 | H | -7.150568 | -0.795050 | 0.704326 |
| C | 1.576351 | 0.110669 | -6.942201 | C | 0.806085 | -0.092811 | -7.174951 | C | -7.359544 | -0.097895 | -1.336008 |
| H | 2.072673 | -0.736456 | -6.452764 | H | 1.290881 | -1.012599 | -6.825878 | H | -6.972451 | -1.018643 | -1.789043 |
| H | 1.981483 | 1.023582 | -6.488830 | H | 1.440787 | 0.743123 | -6.856411 | H | -6.996553 | 0.736527 | -1.948298 |
| C | 1.868114 | 0.095032 | -8.440315 | C | 0.685026 | -0.108303 | -8.696352 | C | -8.885502 | -0.118489 | -1.329705 |
| H | 2.943545 | 0.156623 | -8.633042 | H | 1.667744 | -0.199850 | -9.168716 | H | -9.281624 | -0.216261 | -2.345009 |
| H | 1.384269 | 0.941905 | -8.939634 | H | 0.218745 | 0.814941 | -9.057936 | H | -9.284940 | 0.805171 | -0.896561 |
| H | 1.492905 | -0.826576 | -8.899005 | H | 0.068300 | -0.950673 | -9.028813 | H | -9.260271 | -0.959744 | -0.736180 |
| N | -0.964762 | -2.525712 | -1.114601 | N | -0.044165 | -2.485893 | -0.857704 | N | -1.124167 | -2.479967 | -0.011766 |
| H | -1.241596 | -1.658608 | -0.644050 | H | 0.039978 | -1.615014 | -0.323699 | H | -0.590585 | -1.605294 | -0.052521 |
| N | -0.816961 | 2.571721 | -1.070392 | N | 0.187653 | 2.691520 | -0.943869 | N | -1.193201 | 2.687011 | -0.275880 |
| H | -0.707476 | 1.709975 | -0.522865 | H | -0.055943 | 1.885117 | -0.356483 | H | -0.629083 | 1.883664 | 0.028924 |
| C | -0.951155 | -3.692648 | -0.378730 | C | 0.155125 | -3.681676 | -0.203307 | C | -0.457758 | -3.669805 | -0.154052 |
| C | -0.941911 | 3.759604 | -0.378119 | C | 0.492065 | 3.879947 | -0.319362 | C | -0.550269 | 3.869506 | -0.528752 |
| O | -0.536511 | -4.761490 | -0.842548 | O | 0.090287 | -4.769223 | -0.777626 | O | -1.023346 | -4.760418 | -0.138824 |
| O | -1.034187 | 4.851924 | -0.952777 | O | 0.756203 | 4.909941 | -0.940618 | O | -1.133577 | 4.898885 | -0.860143 |
| C | -1.191020 | -4.548863 | 1.908275 | C | 0.688613 | -4.525397 | 2.074644 | C | 1.865622 | -4.479457 | -0.495006 |
| H | -1.926596 | -4.385527 | 2.703171 | C | 1.206116 | -6.388122 | 4.116781 | C | 3.948342 | -6.287802 | -0.825239 |
| H | -1.371296 | -5.543408 | 1.488073 | C | 0.375247 | -5.879536 | 1.888585 | C | 1.613454 | -5.864252 | -0.441012 |
| C | 0.222927 | -4.460258 | 2.481475 | C | 1.261870 | -4.115931 | 3.290225 | C | 3.183468 | -4.026954 | -0.723870 |
| H | 0.412168 | -3.426053 | 2.799527 | C | 1.512021 | -5.038058 | 4.300812 | C | 4.223437 | -4.921072 | -0.885388 |
| H | 0.947775 | -4.691550 | 1.688799 | C | 0.641079 | -6.794234 | 2.908736 | C | 2.657715 | -6.762166 | -0.607567 |
| C | 0.427249 | -5.398926 | 3.667828 | H | -0.071285 | -6.210269 | 0.960829 | H | 0.611399 | -6.228673 | -0.268705 |
| H | -0.312423 | -5.157490 | 4.443900 | H | 1.512733 | -3.066810 | 3.432877 | H | 3.378524 | -2.959176 | -0.778998 |
| H | 0.229077 | -6.433511 | 3.356610 | H | 1.953855 | -4.697777 | 5.233242 | H | 5.233488 | -4.569287 | -1.060225 |
| C | 1.834434 | -5.292761 | 4.252795 | H | 0.393499 | -7.840490 | 2.750436 | H | 2.469751 | -7.828933 | -0.564036 |
| H | 2.032704 | -4.270061 | 4.595754 | H | 1.404217 | -7.110370 | 4.902990 | C | 1.774653 | 4.747176 | -0.581479 |
| H | 2.589180 | -5.545501 | 3.499239 | C | 0.720985 | 4.787939 | 1.988688 | C | 3.834435 | 6.577111 | -0.930161 |
| H | 1.968034 | -5.967346 | 5.104669 | C | 1.177293 | 6.674720 | 4.024762 | C | 3.106448 | 4.400549 | -0.266712 |
| C | -0.985786 | 4.772512 | 1.849685 | C | 0.431269 | 4.481358 | 3.329222 | C | 1.497540 | 6.034571 | -1.080804 |
| H | -1.413708 | 4.456991 | 2.806592 | C | 1.248859 | 6.048763 | 1.675198 | C | 2.530674 | 6.944380 | -1.251968 |
| H | -1.652996 | 5.527332 | 1.421957 | C | 1.467399 | 6.976599 | 2.695429 | C | 4.134702 | 5.306315 | -0.437660 |
| C | 0.405255 | 5.367472 | 2.067027 | C | 0.658593 | 5.415033 | 4.333788 | H | 3.321017 | 3.406180 | 0.115704 |
| H | 1.063470 | 4.595297 | 2.488208 | H | 0.027100 | 3.501433 | 3.574199 | H | 0.484616 | 6.315085 | -1.329490 |

| | | | |
|---|---|---|---|
| H | 0.825706 | 5.653165 | 1.093621 |
| C | 0.374938 | 6.581649 | 2.993421 |
| H | -0.056595 | 6.288763 | 3.959876 |
| H | -0.294597 | 7.342118 | 2.569994 |
| C | 1.763022 | 7.181762 | 3.210412 |
| H | 2.439814 | 6.444350 | 3.656962 |
| H | 1.725490 | 8.051342 | 3.874390 |
| H | 2.200064 | 7.502623 | 2.257919 |
| N | -1.450728 | -3.555480 | 0.877411 |
| H | -1.690794 | -2.608431 | 1.172779 |
| N | -0.987970 | 3.615221 | 0.970684 |
| H | -0.750475 | 2.700563 | 1.354719 |
| C | -0.957891 | -0.138210 | 1.594824 |
| O | -0.255284 | 0.833190 | 1.208976 |
| O | -1.898952 | -0.664075 | 0.937663 |
| C | -0.637914 | -0.755956 | 2.944426 |
| C | -0.014685 | -2.003002 | 5.373163 |
| C | -1.584181 | -1.556776 | 3.592290 |
| C | 0.618848 | -0.571088 | 3.529937 |
| C | 0.933190 | -1.200672 | 4.734213 |
| C | -1.278860 | -2.172324 | 4.804910 |
| H | -2.562082 | -1.697797 | 3.138886 |
| H | 1.350305 | 0.054114 | 3.025870 |
| H | 1.918485 | -1.069615 | 5.172961 |
| H | -2.021083 | -2.793332 | 5.299441 |
| H | 0.232107 | -2.497515 | 6.309025 |
| H | 1.483099 | 6.299129 | 0.650052 |
| H | 1.875612 | 7.950111 | 2.437136 |
| H | 0.426651 | 5.155265 | 5.362897 |
| H | 1.353072 | 7.405801 | 4.808048 |
| N | 0.434935 | -3.520282 | 1.128433 |
| H | 0.487266 | -2.551192 | 1.460368 |
| N | 0.477526 | 3.776653 | 1.048319 |
| H | 0.133969 | 2.887015 | 1.418743 |
| C | -0.559272 | 0.131356 | 1.865834 |
| O | -0.753754 | 1.256832 | 1.335097 |
| O | 0.230532 | -0.744575 | 1.419812 |
| C | -1.335065 | -0.179424 | 3.131905 |
| C | -2.757546 | -0.727174 | 5.482521 |
| C | -1.375261 | -1.477516 | 3.648414 |
| C | -2.021085 | 0.841803 | 3.797642 |
| C | -2.723766 | 0.571695 | 4.971246 |
| C | -2.085643 | -1.753544 | 4.815949 |
| H | -0.856724 | -2.277912 | 3.130973 |
| H | -1.995950 | 1.847486 | 3.388817 |
| H | -3.246516 | 1.372972 | 5.485951 |
| H | -2.114130 | -2.767907 | 5.204584 |
| H | -3.307379 | -0.939611 | 6.395225 |
| H | 2.323481 | 7.936720 | -1.635807 |
| H | 5.155680 | 5.037452 | -0.193406 |
| N | 0.901076 | -3.498684 | -0.330491 |
| H | 1.232151 | -2.525310 | -0.306450 |
| N | 0.820045 | 3.764923 | -0.379005 |
| H | 1.155565 | 2.871532 | -0.005968 |
| N | 4.907632 | 7.536851 | -1.111823 |
| O | 6.048945 | 7.195747 | -0.826860 |
| O | 4.630316 | 8.649683 | -1.541199 |
| N | 5.034676 | -7.235348 | -0.993756 |
| O | 4.776538 | -8.432100 | -0.966016 |
| O | 6.167584 | -6.799541 | -1.156648 |
| C | 1.486555 | 0.123745 | 0.797855 |
| O | 0.961420 | 1.265117 | 0.884734 |
| O | 1.168848 | -0.747297 | -0.057230 |
| C | 2.576586 | -0.210714 | 1.794947 |
| C | 4.599618 | -0.806987 | 3.636326 |
| C | 2.921821 | -1.538883 | 2.059791 |
| C | 3.244357 | 0.817635 | 2.467750 |
| C | 4.258658 | 0.522190 | 3.377147 |
| C | 3.924671 | -1.838316 | 2.980744 |
| H | 2.391018 | -2.341904 | 1.557833 |
| H | 2.965135 | 1.848001 | 2.267748 |
| H | 4.780989 | 1.327152 | 3.886380 |
| H | 4.178210 | -2.874565 | 3.186428 |
| H | 5.386438 | -1.037847 | 4.349055 |

| Anion complex **5**@$PhCO_2^-$ $\Delta G^0$ = -3318.30710 au | | | | Anion complex **6**@$PhCO_2^-$ $\Delta G^0$ = -2842.85217 au | | | | Anion complex **7**@$PhCO_2^-$ $\Delta G^0$ = -2722.96742 au | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| C | -5.437059 | 0.052398 | 0.011546 | C | -0.029354 | 0.031410 | 5.146066 | C | -0.084082 | -0.008666 | 5.607436 |
| N | -2.548046 | 0.077894 | -0.077443 | N | -0.126533 | 0.080752 | 2.261322 | N | -0.100936 | 0.001161 | 2.719269 |
| C | -4.665982 | -1.108310 | 0.059624 | C | 0.054950 | 1.210378 | 4.404545 | C | -0.087432 | 1.164442 | 4.852644 |
| C | -4.690782 | 1.225856 | -0.090426 | C | -0.164384 | -1.121205 | 4.371371 | C | -0.086482 | -1.176462 | 4.844283 |
| C | -3.274335 | 1.198828 | -0.123737 | C | -0.191512 | -1.055588 | 2.957332 | C | -0.107535 | -1.129633 | 3.428775 |
| C | -3.251182 | -1.055073 | 0.002953 | C | -0.012230 | 1.192592 | 2.990141 | C | -0.084202 | 1.126959 | 3.436741 |
| S | -5.238761 | -2.751174 | 0.156836 | S | 0.252199 | 2.834489 | 5.005976 | S | -0.098073 | 2.804492 | 5.442135 |
| S | -5.300851 | 2.852736 | -0.218016 | S | -0.300526 | -2.767514 | 4.928290 | S | -0.064909 | -2.820536 | 5.422733 |
| C | -3.600894 | -3.361478 | 0.104271 | C | 0.219832 | 3.480336 | 3.378292 | C | -0.076369 | 3.429762 | 3.807370 |
| H | -3.442224 | -4.427996 | 0.131221 | H | 0.315429 | 4.545849 | 3.238822 | H | -0.072412 | 4.498258 | 3.659661 |
| C | -2.659211 | -2.384011 | 0.025128 | C | 0.067871 | 2.527391 | 2.420574 | C | -0.064932 | 2.459741 | 2.854723 |
| C | -3.675597 | 3.491537 | -0.302931 | C | -0.368686 | -3.358100 | 3.280250 | C | -0.109253 | -3.434763 | 3.784292 |
| H | -3.539374 | 4.557437 | -0.398864 | H | -0.453836 | -4.420179 | 3.111475 | H | -0.113907 | -4.502262 | 3.629519 |
| C | -2.711495 | 2.535569 | -0.234036 | C | -0.293281 | -2.371477 | 2.348136 | C | -0.136363 | -2.458627 | 2.838309 |
| C | -6.938442 | 0.037604 | -0.008186 | C | 0.088475 | -0.001109 | 6.642838 | C | -0.019959 | -0.014332 | 7.107697 |
| H | -7.322462 | 0.948374 | 0.468144 | H | -0.497860 | -0.838124 | 7.041822 | H | -0.544172 | -0.896322 | 7.496254 |
| H | -7.307952 | -0.810901 | 0.580804 | H | -0.335736 | 0.917503 | 7.067069 | H | -0.541456 | 0.866289 | 7.502880 |
| C | -7.486589 | -0.059377 | -1.442381 | C | 1.552752 | -0.142973 | 7.092347 | C | 1.431820 | -0.017492 | 7.616400 |
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| H | -7.111037 | 0.788121 | -2.028644 | H | 1.971209 | -1.062447 | 6.665204 | H | 1.950285 | -0.897954 | 7.217881 |
| C | -9.012669 | -0.071354 | -1.456353 | C | 1.671027 | -0.170860 | 8.613669 | C | 1.488477 | -0.021679 | 9.141509 |
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| H | -9.412461 | 0.844467 | -1.007070 | H | 1.104654 | -1.010120 | 9.032362 | H | 0.983424 | -0.905648 | 9.546438 |
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| H | 1.503769 | 1.190830 | -5.509914 |
| H | -0.288239 | -0.040447 | -6.714193 |

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