Electronic Supplementary Material (ESI) for Chemical Communications

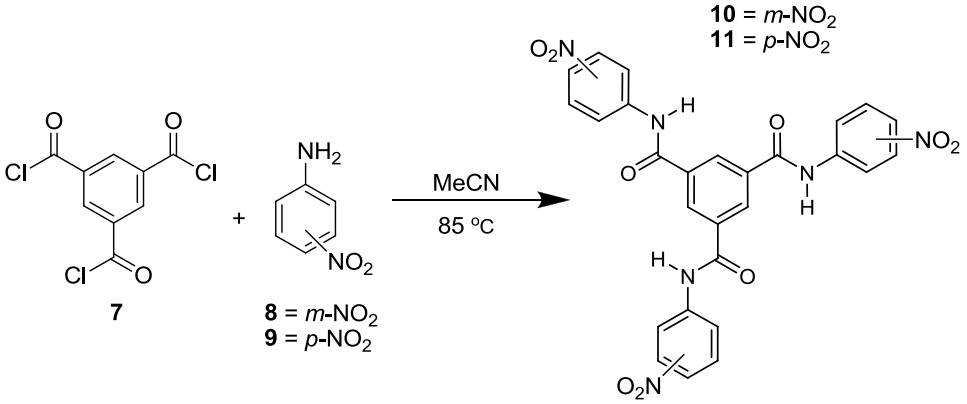
Selective and tuneable recognition of anions using C_{3v}-symmetrical tripodal urea-amide receptor platforms

Cidalia Maria Gomes dos Santos,[a] Elaine M. Boyle,[a] Stefano De Solis,[a,b] Paul E. Kruger[c] and Thorfinnur Gunnlaugsson[a]*

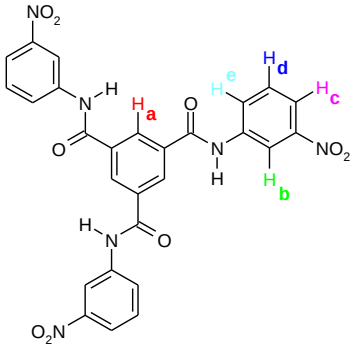
Electronis Suplimentray Informations:

Procedure 1: General experimental procedure for the nitro compounds 10 & 11

The relevant nitroaniline, **8-9**, was dissolved in MeCN and 1,3,5-benzenetricarbonyl trichloride, **7**, was then added. The reaction mixture was then stirred under reflux (85˚C) overnight. The resulting precipitate was then filtered and washed with cold MeCN.



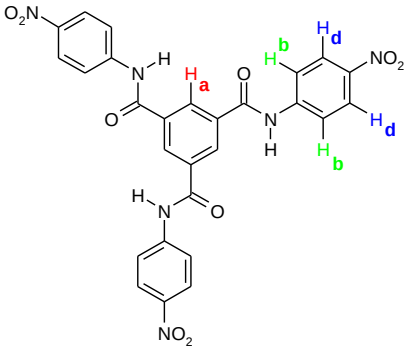
Benzene-1,3,5-tricarboxylic acid tris-[3-nitro-phenyl)-amide] (10)



10 was synthesised according to Procedure 1, using 3-nitroaniline (**8**) (0.314 g, 2.27 mmol) and 1,3,5-benzenetricarbonyl trichloride (**7**) (0.183 g, 0.69 mmol). The product was isolated as an off white solid (0.36 g, 91% yield). m.p. decomposed above 300°C; ^{1}H-NMR (400 MHz, DMSO-d_6) 11.10 (s, 1H, NH), 8.84 (s, 2H, CH_{a+b}), 8.28 (dd, 1H, CH_c, J = 1.00, 1.52 Hz), 8.01 (dd, 1H, CH_e, J = 2.04, 1.52 Hz), 7.70 (t, 1H, CH_d, J = 8.04, 8.52 Hz); ^{13}C-NMR (100 MHz, DMSO-d_6) 164.76, 147.92, 140.07, 134.90, 130.39, 130.23, 126.24, 118.53, 114.48; HRMS (*m/z*) (ES^-) Calculated for $C_{27}H_{17}N_6O_9$ *m/z* = 569.1057 [M - H]$^-$. Found *m/z* = 569.1047; IR υ_{max} (cm^{-1}) 3264, 3087, 1650, 1597, 1523, 1421, 1347, 1325, 1299, 1260, 733.

Benzene-1,3,5-tricarboxylic acid tris-[4-nitro-phenyl)-amide] (11)

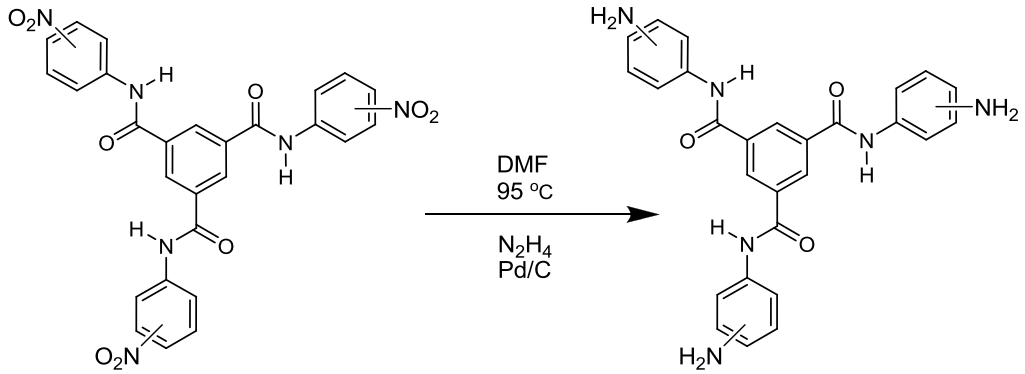
11 was synthesised according to Procedure 1, using 4-nitroaniline (**9**) (0.80 g, 5.79 mmol) and 1,3,5-benzenetricarbonyl trichloride (**7**) (0.465 g, 1.75 mmol). The product was isolated as an off white solid



(0.84 g, 84% yield). m.p. decomposed above 300°C; ^{1}H-NMR (400 MHz, DMSO-d_6) 11.18 (s, 1H, NH), 8.81 (s, 1H, CH_a), 8.31 (d, 2H, CH_d, J = 9.04 Hz), 8.12 (d, 2H, CH_b, J = 9.52 Hz); ^{13}C-NMR (100 MHz, DMSO-d_6) 165.4, 145.5, 143.2, 135.3, 131.2, 125.3, 120.5; HRMS (m/z) (ES^-) Calculated for $C_{27}H_{17}N_6O_9$ m/z = 569.1057 [M - H]$^-$. Found m/z = 569.1050; IR υ_{max} (cm^{-1}) 3393, 3358, 3120, 1696, 1613, 1597, 1544, 1503, 1327, 1305, 1228, 1181, 1110, 849, 737.

<u>Procedure 2:</u> General experimental procedure for the amino compounds 12 & 13

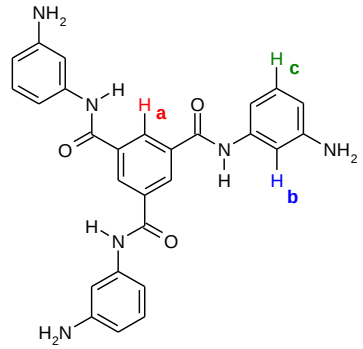
The relevant nitro derivative, **10-11,** was suspended in DMF. To the obtained suspension was added EtOH and the catalyst, 10% Pd/C. Hydrazine monohydrate was subsequently added and the reaction mixture was stirred at 95˚C overnight under an argon atmosphere. The reaction mixture was filtered, through celite while hot, and washed with hot EtOH. The solvent was then removed under reduced pressure to yield brown oil. EtOH was then added and a precipitate was observed within minutes, which was filtered and washed with EtOH to yield the desired product.



10 = *m*-NO_2
11 = *p*-NO_2

12 = *m*-NO_2
13 = *p*-NO_2

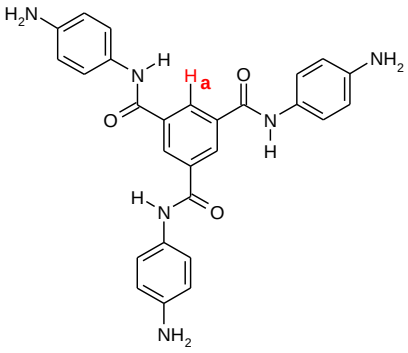
Benzene-1,3,5-tricarboxylic acid tris-[3-amino-phenyl)-amide] (12)



12 was synthesised according to **Procedure 2**, using the tris-nitro compound **10** (0.500 g, 0.876 mmol), and hydrazine monohydrate (1.097 g, 22 mmol). The product was isolated as a white solid (0.383 g, 91% yield). m.p. decomposed above 300°C; ^{1}H-NMR (400 MHz, DMSO-d_6) 10.26 (s, 1H, NH), 8.59 (s, 1H, CH_a), 7.14 (s, 1H, CH_b), 7.00 (t, 1H, CH_c, J = 8.00 Hz, 8.04 Hz), 6.91 (d, 1H, CH, J = 8.04 Hz), 6.34 (d, 1H, CH, J =

8.00 Hz), 5.17 (s, 2H, NH_2); ^{13}C-NMR (100 MHz, DMSO-d_6) 164.8, 149.5, 140.0, 136.1, 129.9, 129.3, 110.4, 108.7, 106.4; HRMS (*m/z*) (ES^+) Calculated for $C_{27}H_{25}N_6O_3$ *m/z* = 481.1988 $[M + H]^+$. Found *m/z* = 481.1981; IR υ_{max} (cm^{-1}) 3323, 1671, 1641, 1611, 1598, 1543, 1493, 1451, 1311, 1252, 681.

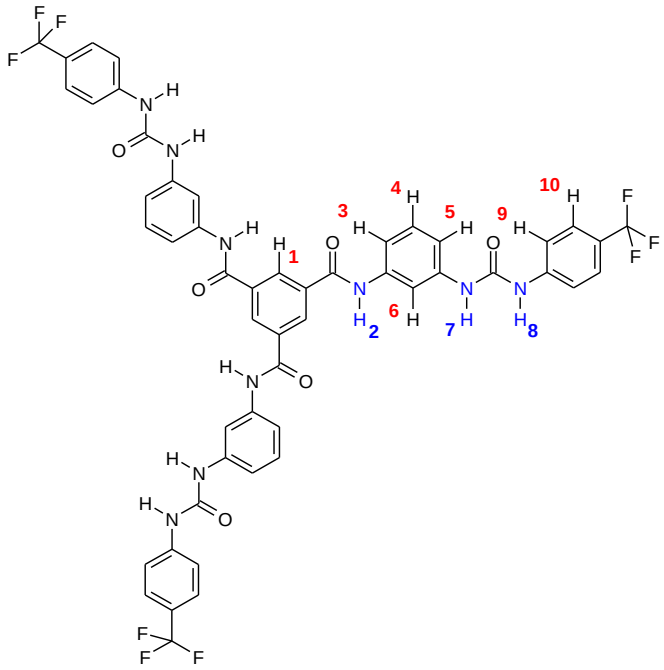
Benzene-1,3,5-tricarboxylic acid tris-[4-amino-phenyl)-amide] (13)



13 was synthesised according to **Procedure 2**, using the tris-nitro compound **11** (0.200 g, 0.351 mmol), and hydrazine monohydrate (0.464 g, 9.28 mmol). The product was isolated as an yellow solid (0.131 g, 78% yield). m.p. 202-206°C; ^{1}H-NMR (400 MHz, DMSO-d_6) 10.17 (s, 1H, NH), 8.57 (s, 1H, CH_a), 7.43 (d, 2H, CH, *J* = 8.76 Hz), 6.57 (d, 2H, CH, *J* = 8.80 Hz), 5.04 (s, 2H, NH_2); ^{13}C-NMR (100 MHz, DMSO-d_6) 163.82, 145.41, 135.72, 128.98, 127.91, 122.11, 113.72. HRMS (*m/z*) (ES^+) Calculated for $C_{27}H_{25}N_6O_3$ *m/z* = 481.1988 $[M + H]^+$. Found *m/z* = 481.1986; IR υ_{max} (cm^{-1}) 3264, 2919, 2851, 1637, 1534, 1511, 1421, 1321, 1255, 1173, 1128, 823.

<u>Procedure 3:</u> General experimental procedure for tripodal urea compounds 1-6

The relevant amine, **12-13**, was suspended in MeCN and stirred at 85˚C for 10 minutes. The desired isocyanate, **14-17**, was then added, and the reaction mixture stirred under reflux (85˚C) overnight under an argon atmosphere. The resulting precipitate was then filtered and washed with cold MeCN.

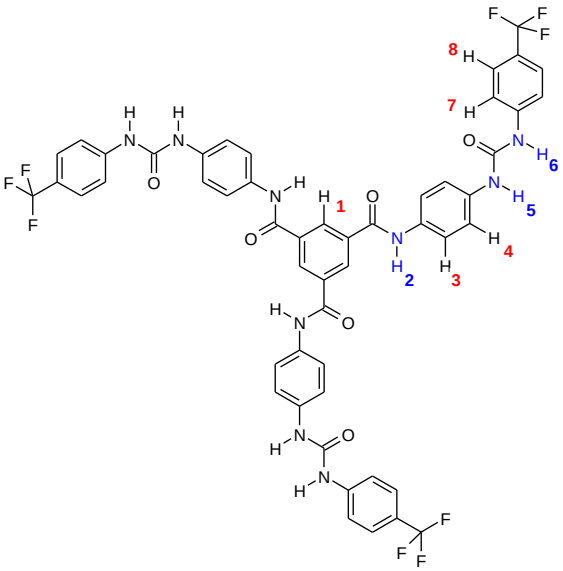


Benzene-1,3,5-tricarboxylic acid tris-({3-[3-(4-trifluoromethyl-phenyl)-ureido]-phenyl}-amide) (1)

1 was synthesised according to **Procedure 3**, using the tris-amine **12** (0.080 g, 0.166 mmol), and trifluoro-p-tolyl isocyanate (0.094 g, 0.504 mmol). The product was isolated as an off white solid (0.157 g, 91% yield). m.p. decomposed above 300°C; ^{1}H-NMR (400 MHz, DMSO-d_6) 10.62 (s, 1H, NH), 9.08 (s, 1H, NH), 8.94 (s, 1H, NH), 8.72 (s, 1H, CH), 8.09 (s, 1H, CH), 7.65 (d,d, 4H, CH, *J* = 8.56 Hz, *J* = 9.00 Hz), 7.49 (d,

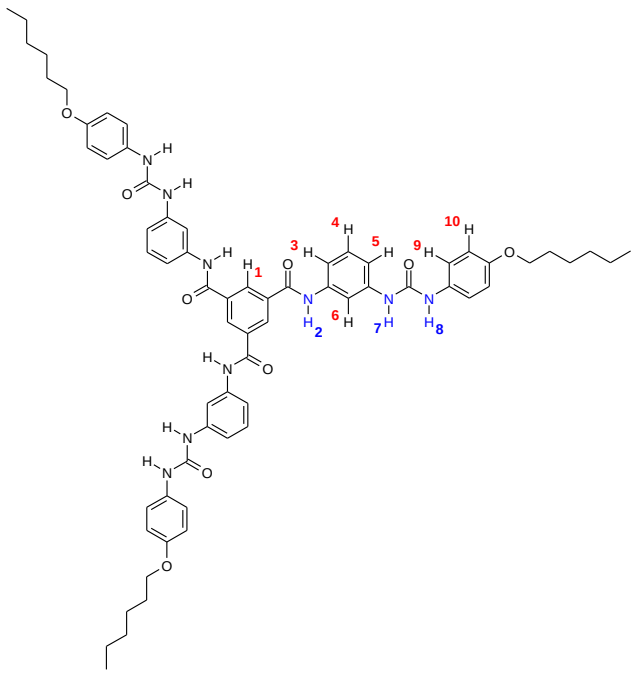
1H, CH, *J* = 8.00 Hz), 7.30 (m, 2H, CH); ^{13}C-NMR (100 MHz, DMSO-d_6) 164.60, 152.20, 143.44, 139.64, 139.42, 135.42, 129.90, 129.08, 128.04, 126.09, 125.90, 121.59, 117.80, 114.40, 114.07, 110.47; ^{19}F-NMR (376 MHz, DMSO-d_6) -60.54 (CF_3); HRMS (*m/z*) (MALDI-ToF) Calculated for $C_{51}H_{36}N_9O_6F_9$ *m/z* = 1040.2567 $[M + H]^+$. Found *m/z* = 1040.2522; IR υ_{max} (cm^{-1}) 3303, 1654, 1602, 1534, 1482, 1414, 1318, 1245, 1209, 1164, 1109, 1068, 840, 773.

Benzene-1,3,5-tricarboxylic acid tris-({4-[3-(4-trifluoromethyl-phenyl)-ureido]-phenyl}-amide) (2)



2 was synthesised according to **Procedure 3**, using the tris-amine **13** (0.073 g, 0.152 mmol), and trifluoro-p-tolyl isocyanate (0.171 g, 0.912 mmol). The product was isolated as a pink solid (0.134 g, 85% yield). m.p. decomposed above 300°C; ^{1}H-NMR (400 MHz, DMSO-d_6) 10.55 (s, 1H, NH), 9.11 (s, 1H, NH), 8.83 (s, 1H, NH), 8.70 (s, 1H, CH), 7.76 (d, 2H, CH, *J* = 8.52 Hz), 7.65 (d + d, 4H, CH, *J* = 8.52 Hz, 9.04 Hz), 7.50 (d, 2H, CH, *J* = 9.04 Hz); ^{13}C-NMR (100 MHz, DMSO-d_6) 164.26, 152.33, 143.54, 135.53, 135.40, 133.56, 129.58, 126.12, 126.08, 125.93, 123.23, 121.83, 121.52, 121.20, 121.12, 118.84, 117.80; ^{19}F-NMR (376 MHz, DMSO-d_6) -60.52 (CF_3); HRMS (*m/z*) (MALDI-ToF) Calculated for $C_{51}H_{36}N_9O_6F_9$ *m/z* = 1041.2645 $[M + H]^+$. Found *m/z* = 1041.2686; IR υ_{max} (cm^{-1}) 3290, 1641, 1602, 1546, 1510, 1407, 1306, 1237, 1161, 1111, 1067, 1015, 831.

Benzene-1,3,5-tricarboxylic acid tris-({3-[3-(4-hexyloxy-phenyl) ureido]-phenyl}-amide) (3)

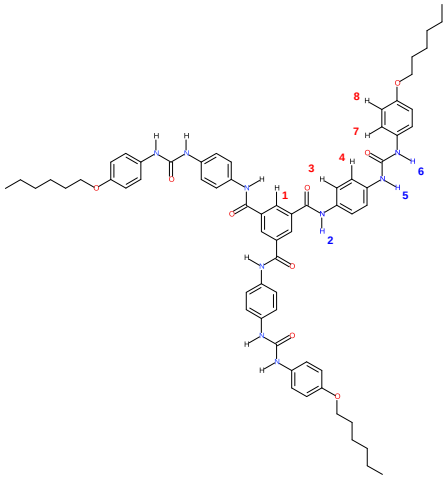


3 was synthesised according to **Procedure 3**, using the tris-amine **12** (0.080 g, 0.166 mmol), and 4-hexyloxyphenyl isocyanate (0.111 g, 0.504 mmol). The product was isolated as an off white solid (0.179 g, 95% yield). m.p. 254-257°C; ^{1}H-NMR (400 MHz, DMSO-d_6) 10.58 (s, 1H, NH), 8.71 (s, 1H, NH), 8.70 (s, 1H, CH), 8.44 (s, 1H, NH), 8.03 (s, 1H, CH), 7.45 (d, 1H, CH, *J* = 7.52 Hz), 7.35 (d, 2H, CH, *J* = 8.52 Hz), 7.26 (m, 2H, CH), 6.85 (d, 2H, CH, *J* = 9.04 Hz), 3.90 (t, 2H, CH_2, *J* = 6.04

Hz, 6.52 Hz), 1.68 (m, 2H, CH_2), 1.40 (t, 2H, CH_2, J = 6.04 Hz, 7.00 Hz), 1.30 (m, 4H, CH_2), 0.88 (t, 3H, CH_3, J = 6.56 Hz, 7.00 Hz); ^{13}C-NMR (100 MHz, DMSO-d_6) 164.57, 153.88, 152.63, 140.25, 139.35, 135.44, 132.58, 129.86, 128.97, 119.91, 114.59, 113.85, 113.76, 110.12, 67.55, 31.05, 28.75, 25.23, 22.10, 13.94; HRMS (m/z) (MALDI-ToF) Calculated for $C_{66}H_{75}N_9O_6$ m/z = 1137.5688 $[M + H]^+$. Found m/z = 1137.5670; IR υ_{max} (cm^{-1}) 3288, 2932, 2858, 1639, 1605, 1551, 1509, 1490, 1447, 1298, 1240, 1034, 831.

Benzene-1,3,5-tricarboxylic acid tris-({4-[3-(4-hexyloxy-phenyl)-ureido]-phenyl}-amide) (4)

4 was synthesised according to **Procedure 3**, using the tris-amine **13** (0.080 g, 0.166 mmol), and 4-hexyloxyphenyl isocyanate (0.111 g, 0.504 mmol). The product was isolated as a white solid (0.168 g, 89% yield). m.p. decomposed above 300°C; ^{1}H-NMR (400 MHz, DMSO-d_6) 10.51 (s, 1H, NH), 8.69 (s, 1H, CH), 8.59 (s, 1H, NH), 8.46 (s, 1H, NH), 7.72 (d, 2H, CH, J = 8.52 Hz), 7.46 (d, 2H, CH, J = 8.52 Hz), 7.35 (d, 2H, CH, J = 9.04 Hz), 6.86 (d, 2H, CH, J = 9.04 Hz), 3.91 (t, 2H, OCH_2, J = 6.52 Hz), 1.69 (m, 2H, CH_2), 1.41 (t, 2H, CH_2, J = 6.04 Hz, 7.52 Hz), 1.31 (t, 2H, CH_2, J = 3.04 Hz, 4.00 Hz), 0.88 (t, 3H, CH_3, J = 6.52 Hz, 7.00 Hz); ^{13}C-NMR (100 MHz, DMSO-d_6) 164.19, 153.84, 152.77, 136.08, 135.56, 133.02, 132.67, 129.50, 121.11, 119.96, 118.36, 114.58, 67.56, 31.05, 28.75, 25.24, 22.11, 13.95; IR υ_{max} (cm^{-1}) 3280, 3044, 2929, 2858, 1638, 1603, 1554, 1507, 1405, 1308, 1211, 1171, 826.

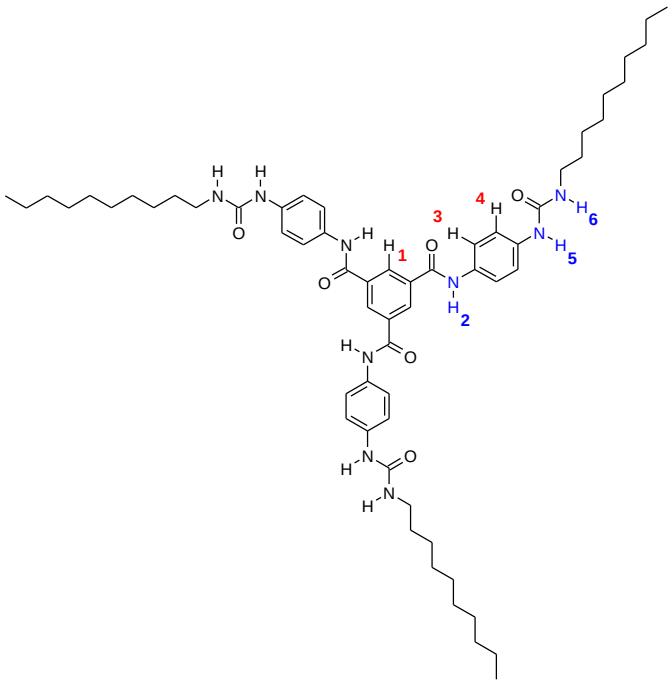


Benzene-1,3,5-tricarboxylic acid tris-({3-[3-(4-octyl-phenyl) ureido]-phenyl}-amide) (5)

5 was synthesised according to **Procedure 3**, using the tris-amine **13** (0.080 g, 0.166 mmol), and 4-octylphenyl isocyanate (0.117 g, 0.504 mmol). The product was isolated as an off white solid (0.178 g, 91% yield). m.p. 235-240°C; ^{1}H-NMR (400 MHz, DMSO-d_6) 10.59 (s, 1H, NH), 8.75 (s, 1H, NH), 8.71 (s,

1H, CH), 8.55 (s, 1H, NH), 8.05 (s, 1H, CH), 7.46 (d, 1H, CH, J = 8.04 Hz), 7.36 (d, 2H, CH, J = 8.04 Hz), 7.27 (m, 2H, CH), 7.08 (d, 2H, CH, J = 8.52 Hz), 1.53 (s, 2H, CH_2), 1.26 (m, 12H, CH_2), 0.85 (t, 3H, CH_3, J = 6.52 Hz, 7.04 Hz); ^{13}C-NMR (150 MHz, DMSO-d_6) 164.58, 152.47, 148.96, 140.15, 139.37, 138.25, 137.28, 135.75, 135.43, 129.87, 128.99, 128.52, 118.21, 117.99, 113.94, 113.78, 110.15, 34.50, 31.30, 31.14, 28.87, 28.71, 28.65, 22.10, 13.97; HRMS (m/z) (MALDI-ToF) Calculated for $C_{72}H_{88}N_9O_6$ m/z = 1174.6858 $[M + H]^+$. Found m/z = 1174.6799; IR υ_{max} (cm^{-1}) 3294, 2922, 2851, 1642, 1604, 1551, 1490, 1447, 1411, 1301, 1241, 781, 686.

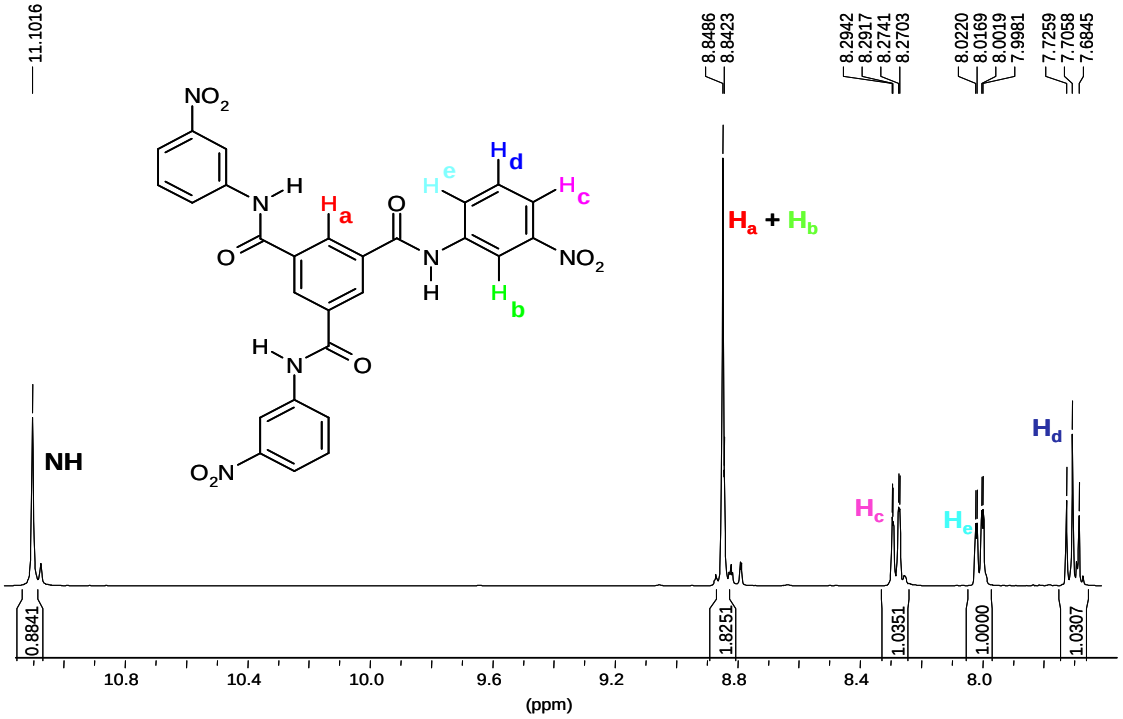
Benzene-1,3,5-tricarboxylic acid tris-({4-[3-decyl-ureido)-phenyl]-amide) (6)



6 was synthesised according to **Procedure 3**, using the tris-amine **13** (0.080 g, 0.166 mmol), and Dodecyl isocyanate (0.107 g, 0.504 mmol). The product was isolated as a white solid (0.123 g, 67% yield). m.p. decomposed above 300°C; ^{1}H-NMR (400 MHz, DMSO-d_6) 10.44 (s, 1H, NH), 8.65 (s, 1H, CH), 8.39 (s, 1H, NH), 7.66 (d, 2H, CH, J = 9.04 Hz), 7.39 (d, 2H, CH, J = 9.04 Hz), 6.10 (s, 1H, NH-CH_2), 3.08 (2H, CH_2-NH), 1.42 (2H, CH_2), 1.25 (18H, CH_2), 0.85 (t, 3H, CH_3, J = 3.52 Hz, 3.52 Hz); ^{13}C-NMR (150 MHz, DMSO-d_6) 164.43, 155.56, 137.18, 135.88, 132.71, 129.70, 121.38, 118.10, 39.52, 31.61, 30.10, 29.36, 29.33, 29.10, 29.03, 26.71, 22.41, 14.27; IR υ_{max} (cm^{-1}) 3326, 2921, 2851, 1638, 1607, 1598, 1510, 1405, 1305, 1231, 832, 720.

Figure S1: A) ^{1}H-NMR of **10** (400 MHz, DMSO-d_6). **B)** ^{13}C-NMR of **10** (100 MHz, DMSO-d_6).

A)



B)

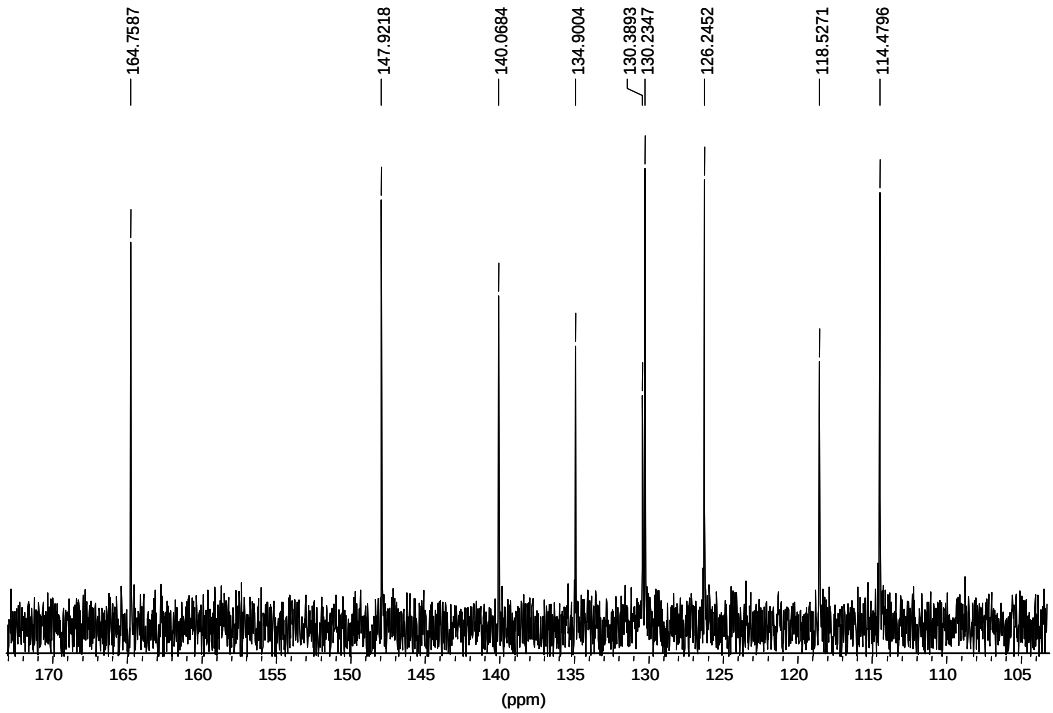
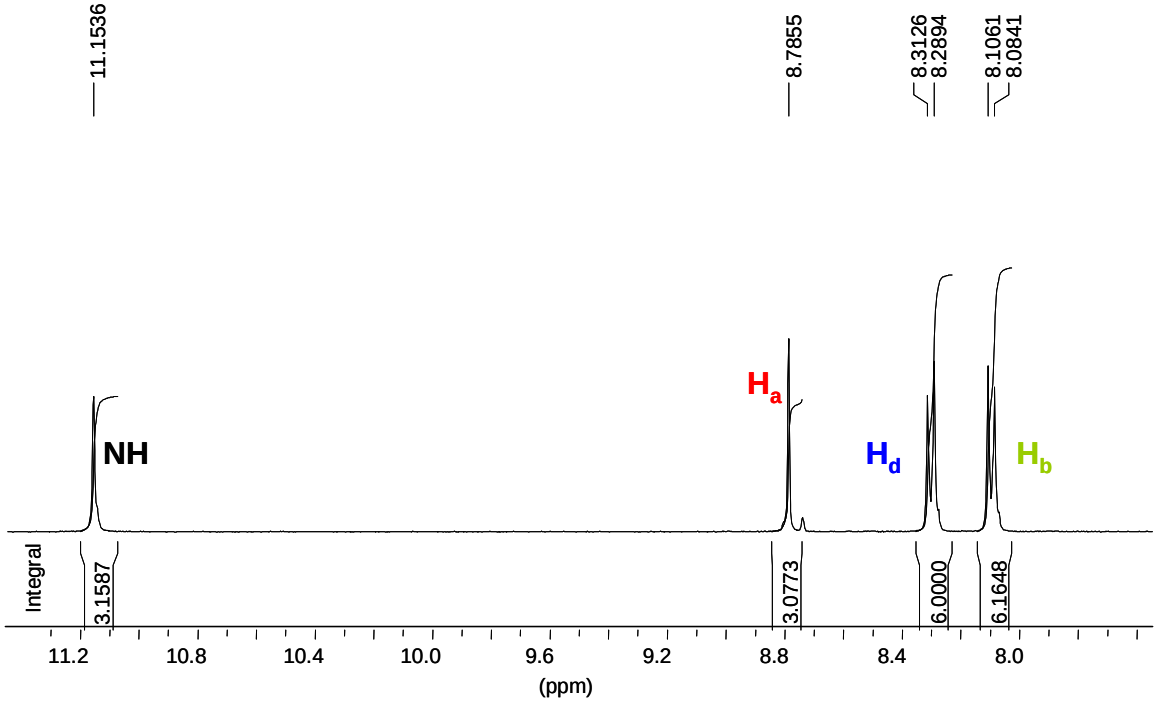


Figure S2: **A)** ^{1}H-NMR of **11** (400 MHz, DMSO-d_6). **B)** ^{13}C-NMR of **11** (100 MHz, DMSO-d_6).

A)



B)

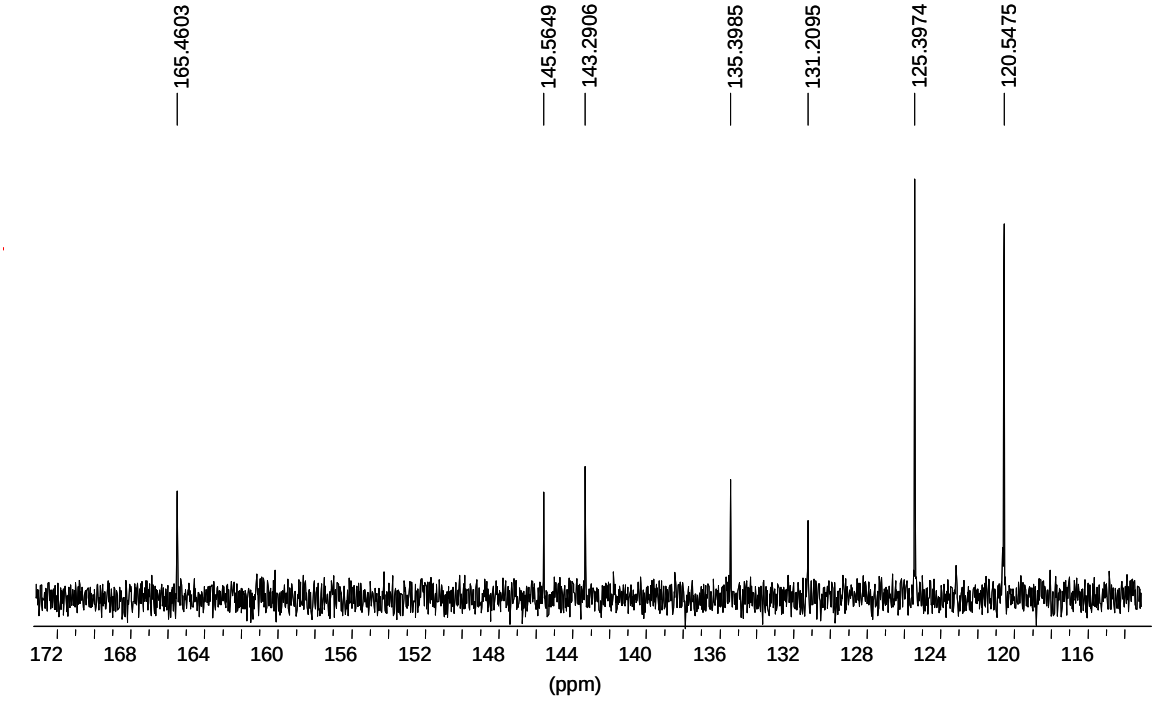
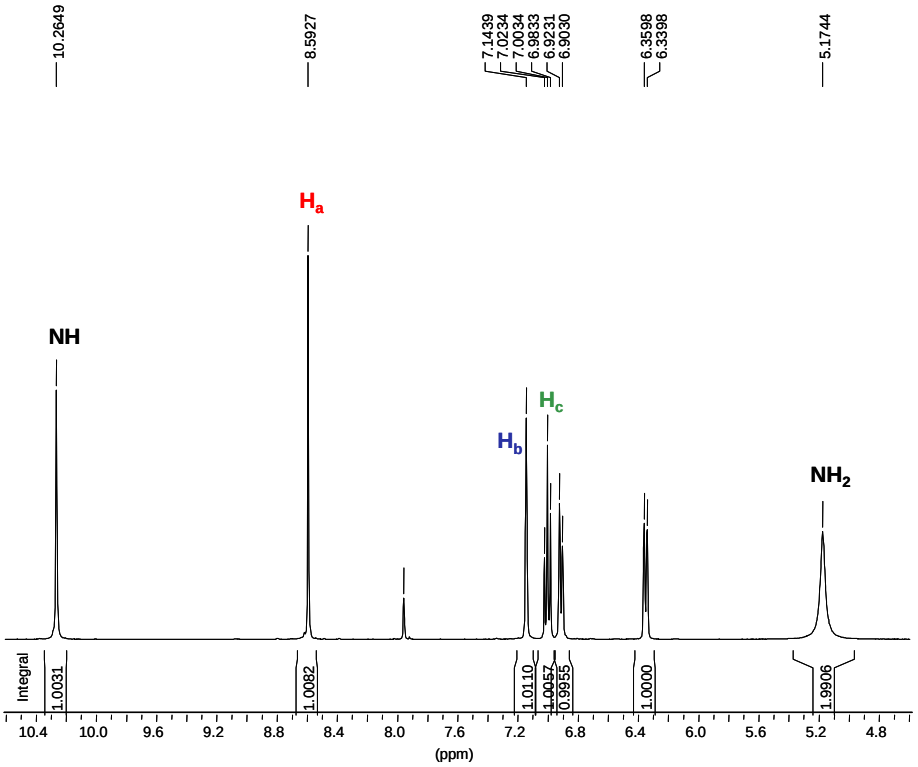


Figure S3: A) ^{1}H-NMR of **12** (400 MHz, DMSO-d_6). **B)** ^{13}C-NMR of **12** (100 MHz, DMSO-d_6).

A)



B)

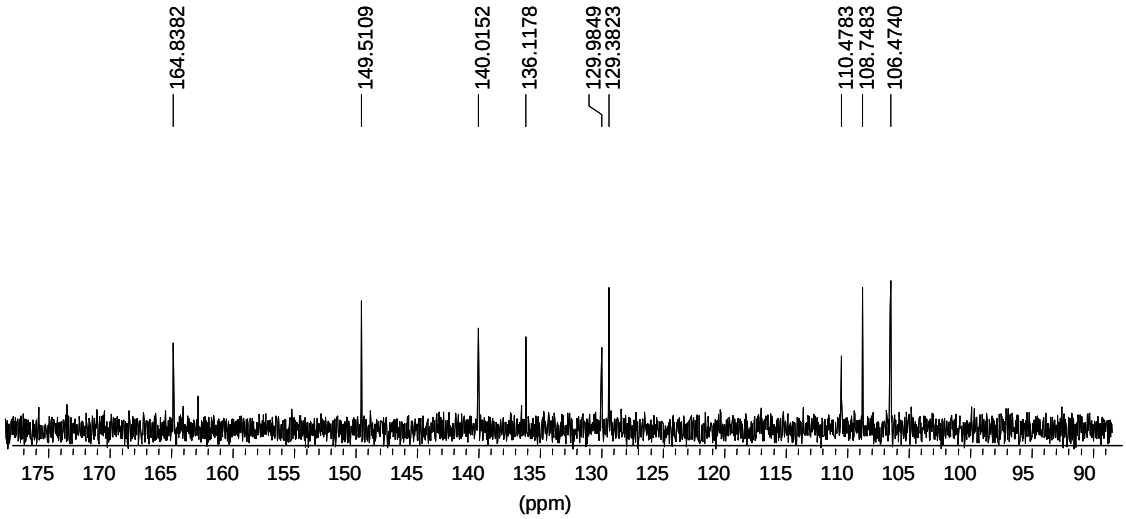
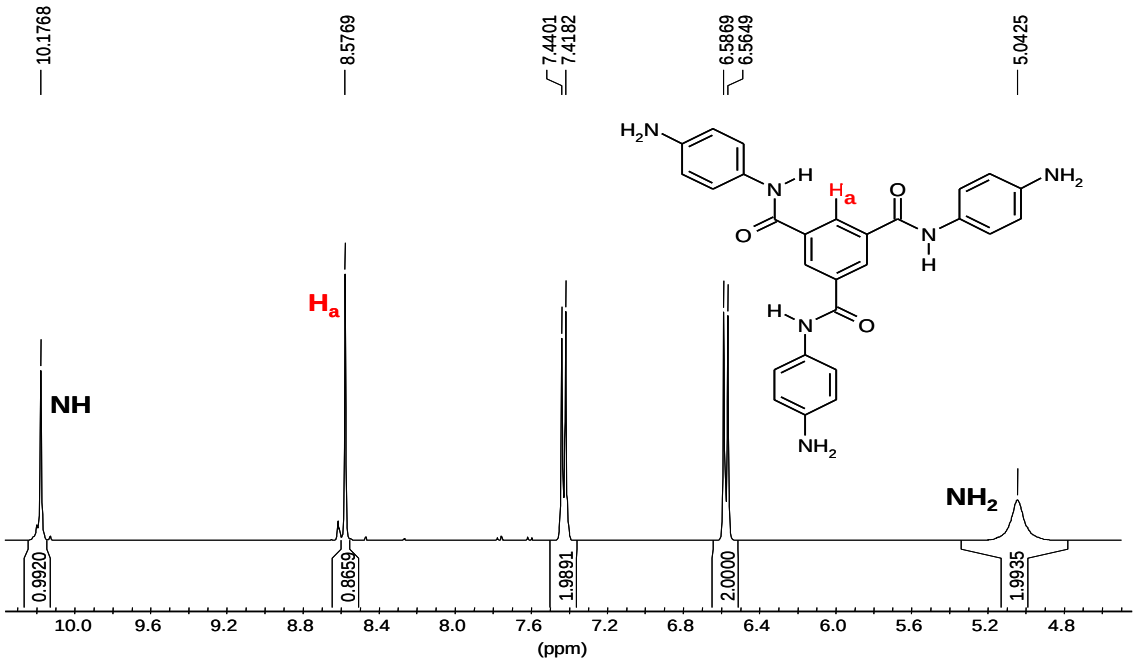


Figure S4: A) ^{1}H-NMR of **13** (400 MHz, DMSO-d_6). **B)** ^{13}C-NMR of **13** (100 MHz, DMSO-d_6.

A)



B)

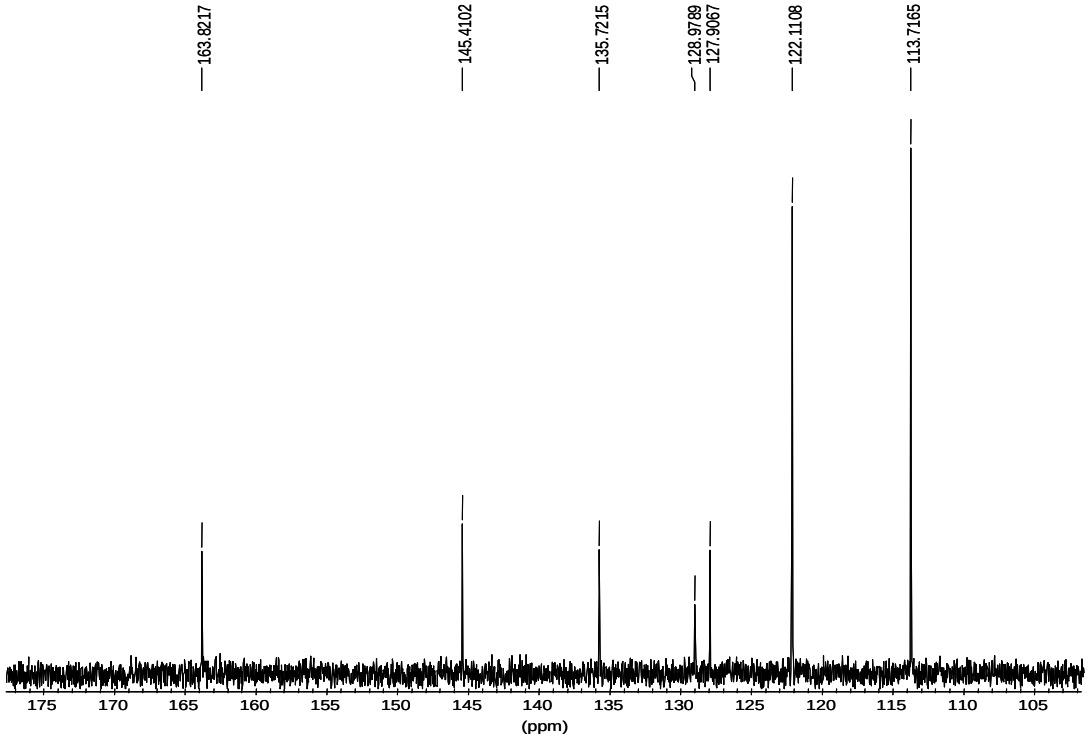
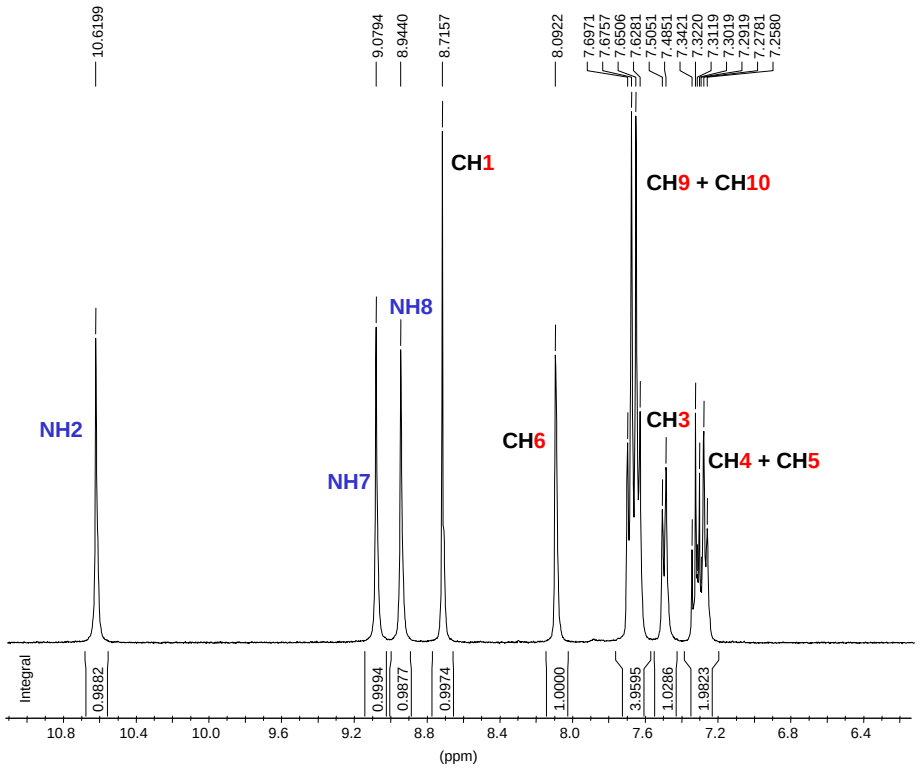
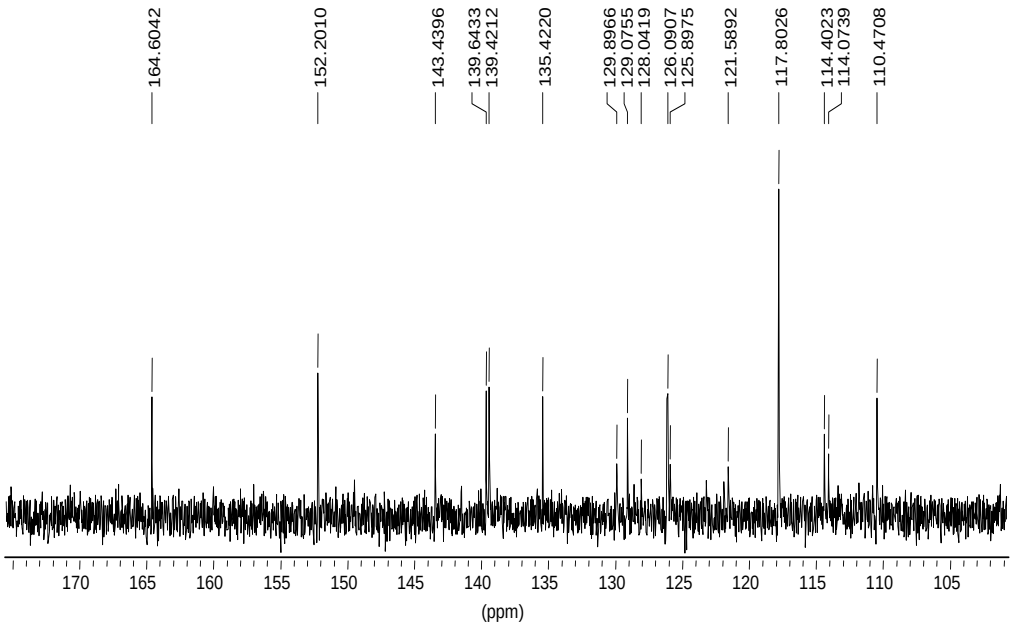


Figure S5: A) ^{1}H-NMR of **1** (400 MHz, DMSO-d_6). **B)** ^{13}C-NMR of **1** (100 MHz, DMSO-d_6). **C)** ^{13}C-NMR and ^{14}C-NMR of **1** (100 MHz, DMSO-d_6). **D)** ^{19}F-NMR of **1** (376 MHz, DMSO-d_6).

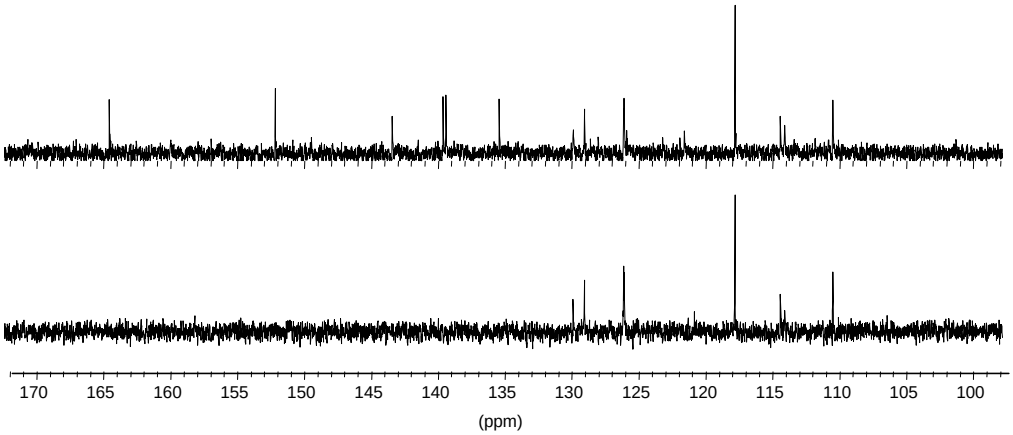
A)



B)



C)


170
165
160
155
150
145
140
135
130
125
120
115
110
105
100
(ppm)

D)

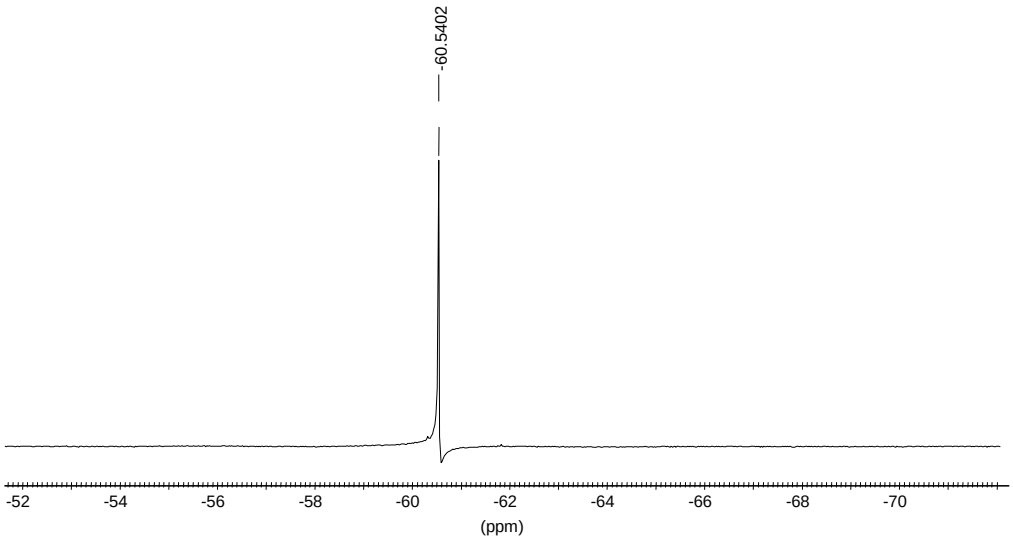
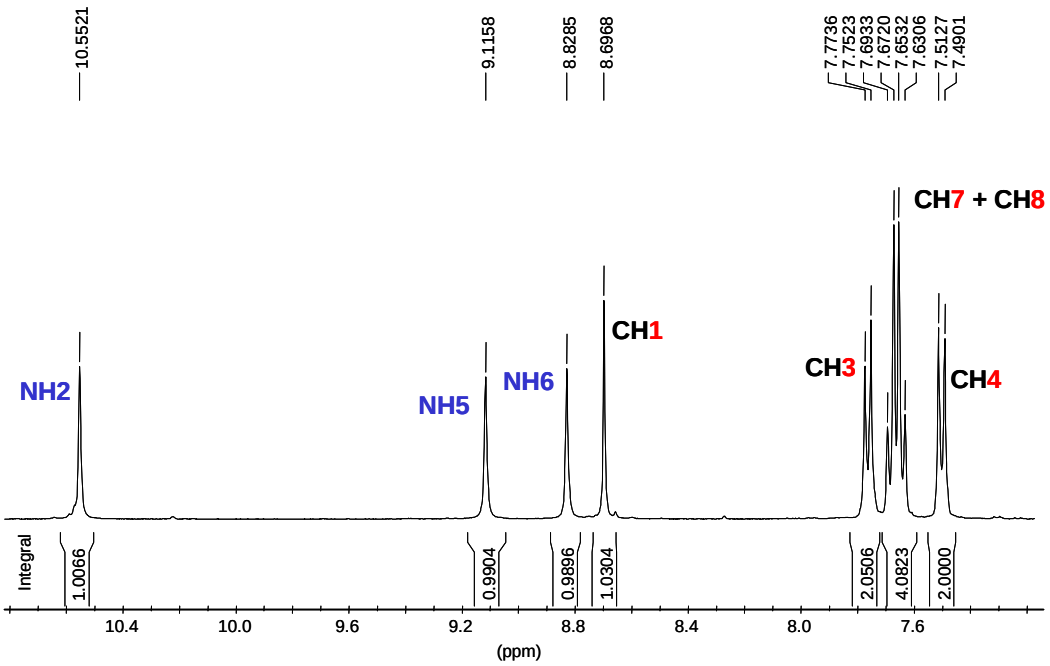
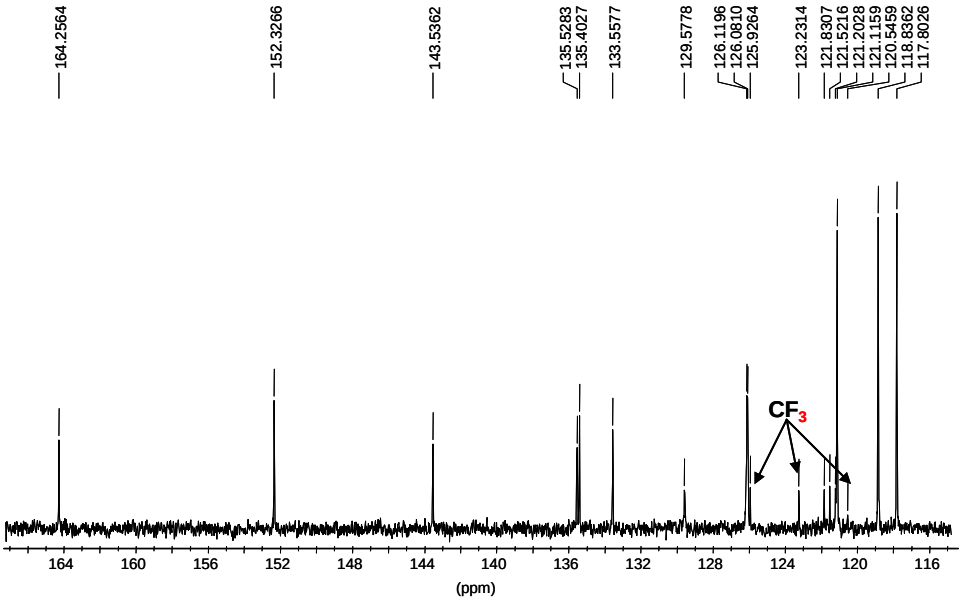

-60.5402
-52
-54
-56
-58
-60
-62
-64
-66
-68
-70
(ppm)

Figure S6: A) ^{1}H-NMR of **2** (400 MHz, DMSO-d_6). **B)** ^{13}C-NMR of **2** (100 MHz, DMSO-d_6). **C)** ^{14}C-NMR of **2** (100 MHz, DMSO-d_6). **D)** ^{19}F-NMR of **2** (100 MHz, DMSO-d_6).

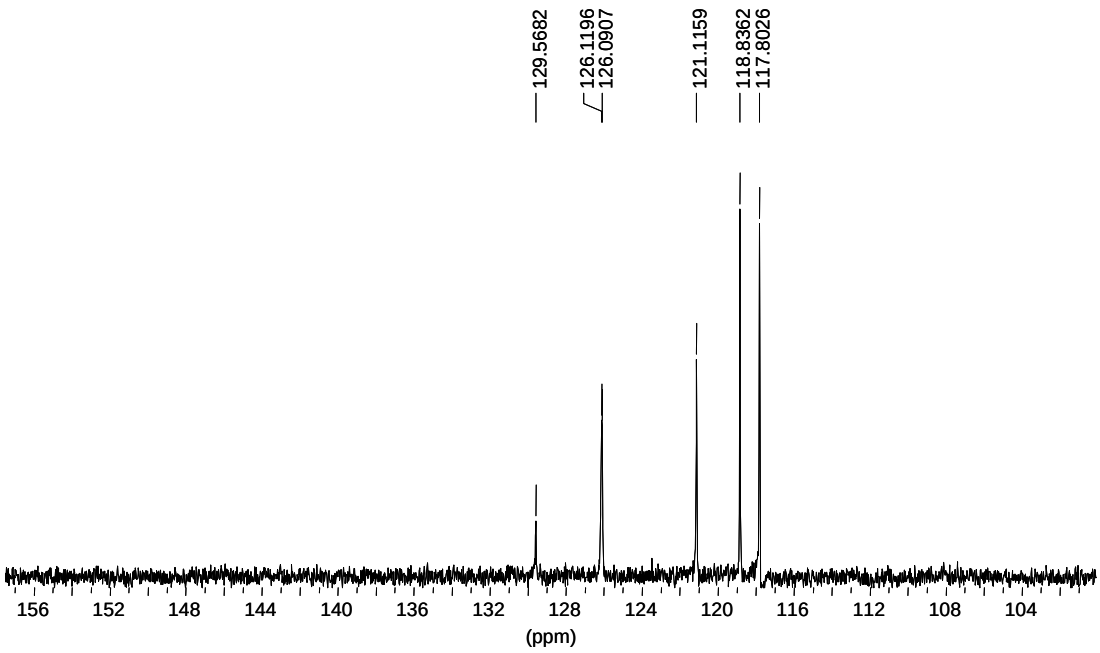
A)



B)



C)


129.5682
126.1196
126.0907
121.1159
118.8362
117.8026
156
152
148
144
140
136
132
128
124
120
116
112
108
104
(ppm)

D)

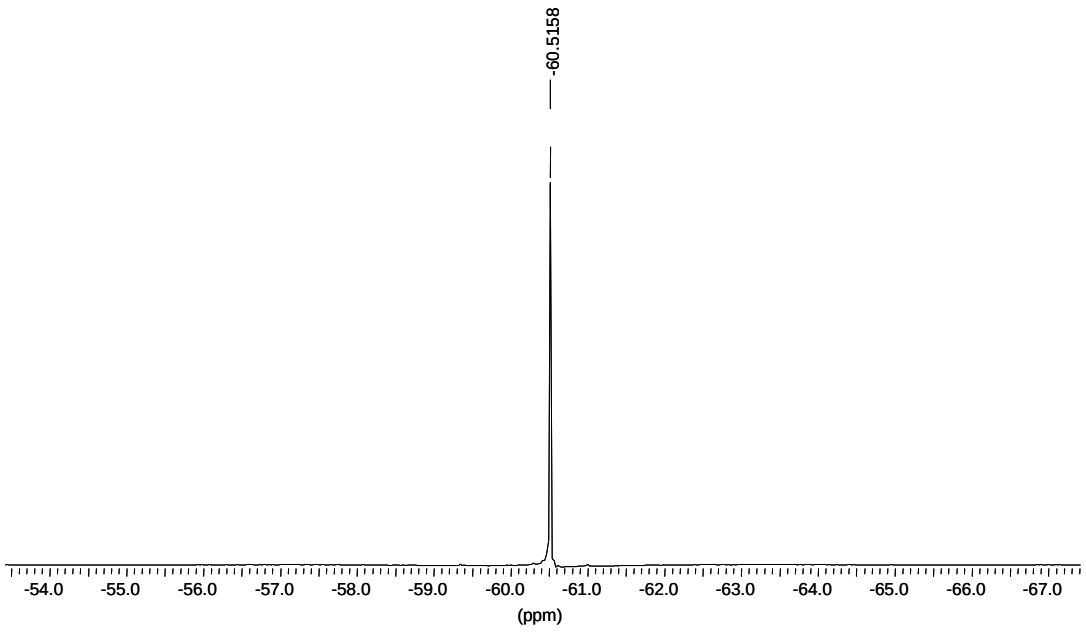
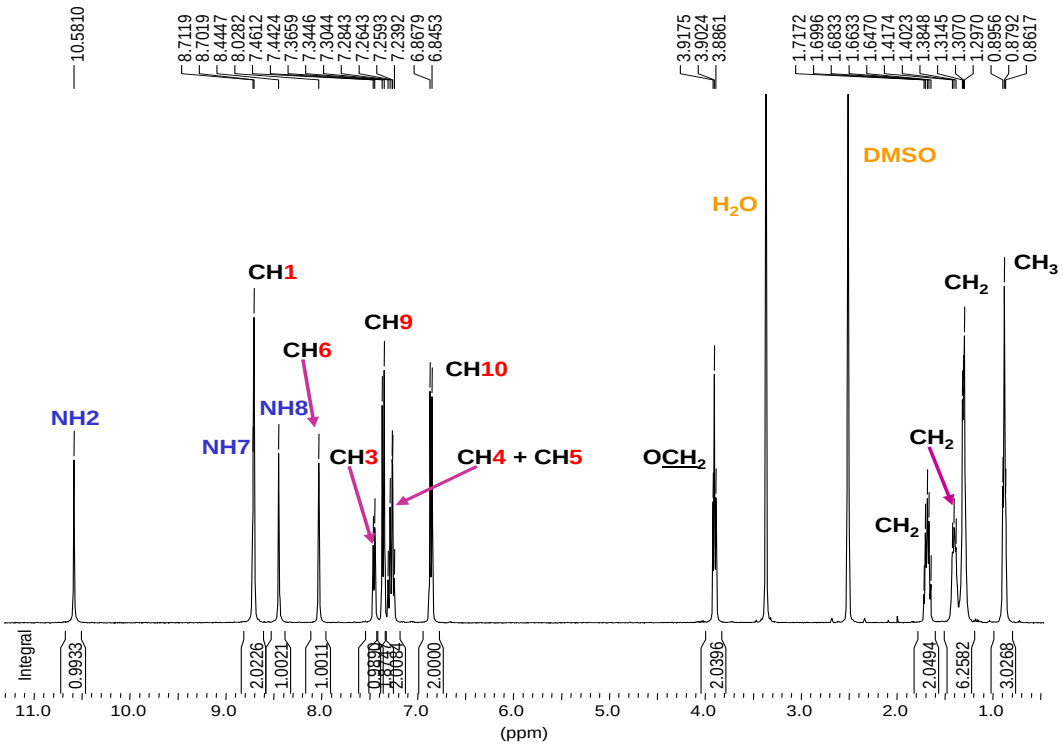
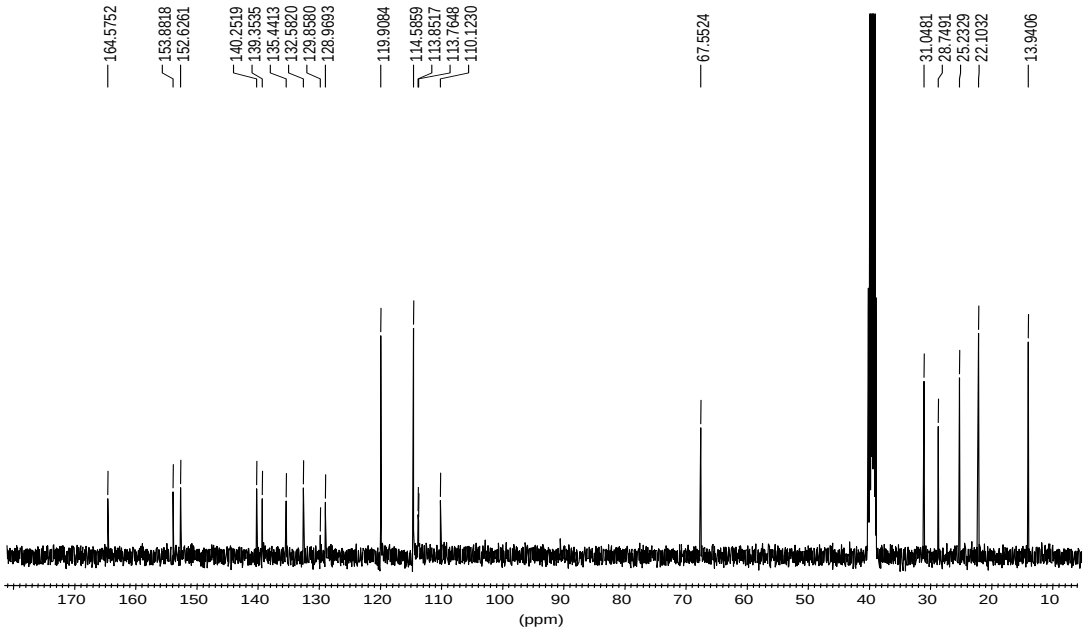

-60.5158
-54.0
-55.0
-56.0
-57.0
-58.0
-59.0
-60.0
-61.0
-62.0
-63.0
-64.0
-65.0
-66.0
-67.0
(ppm)

Figure S7: **A)** ^{1}H-NMR of **3** (400 MHz, DMSO-d_6). **B)** ^{13}C-NMR of **3** (100 MHz, DMSO-d_6). **C)** ^{14}C-NMR of **3** (100 MHz, DMSO-d_6).

A)



B)



C)

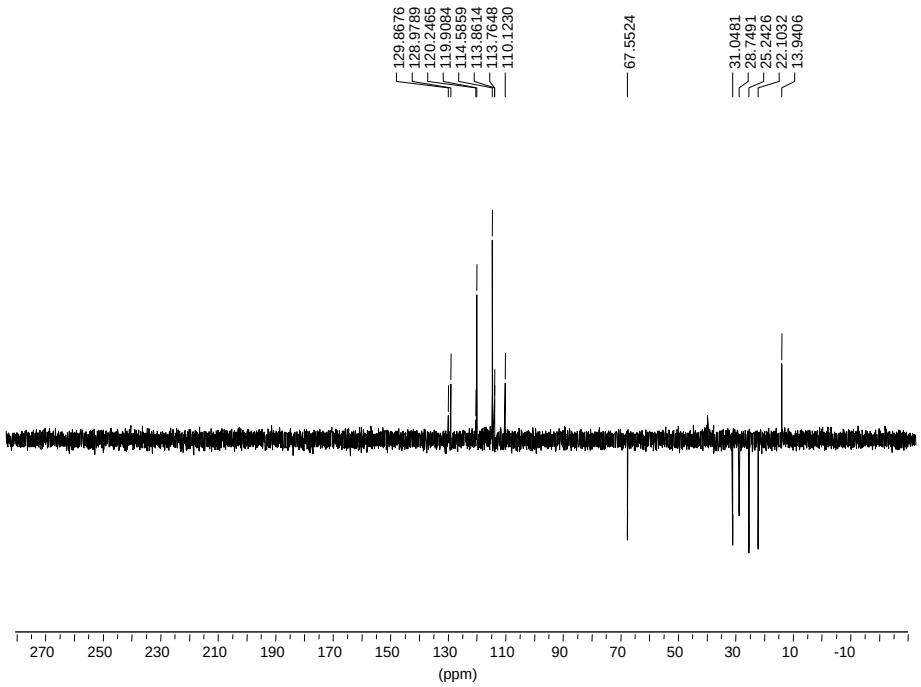
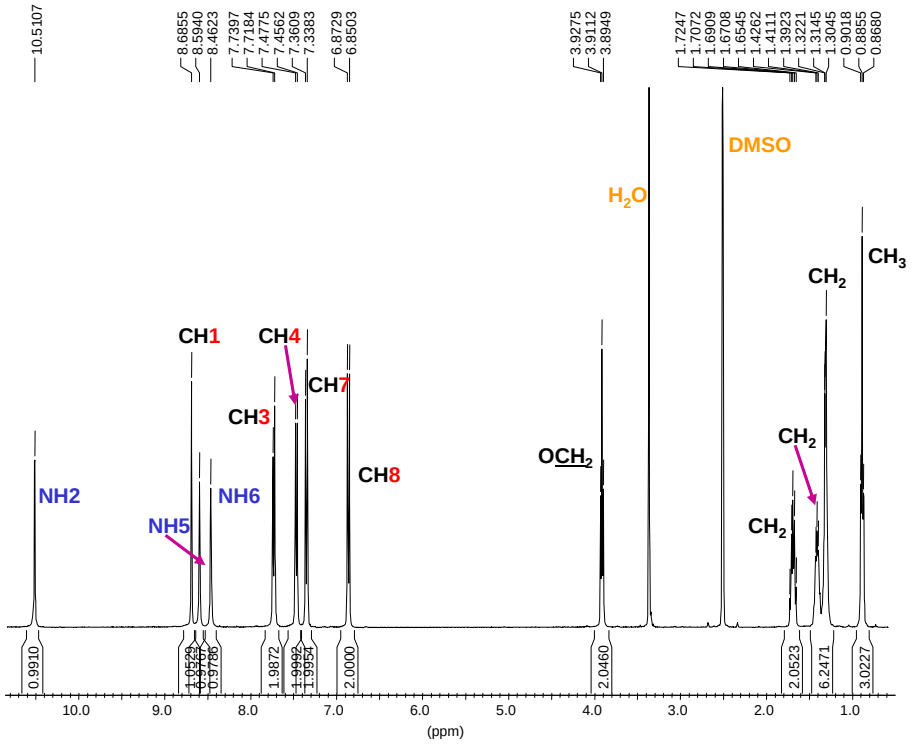
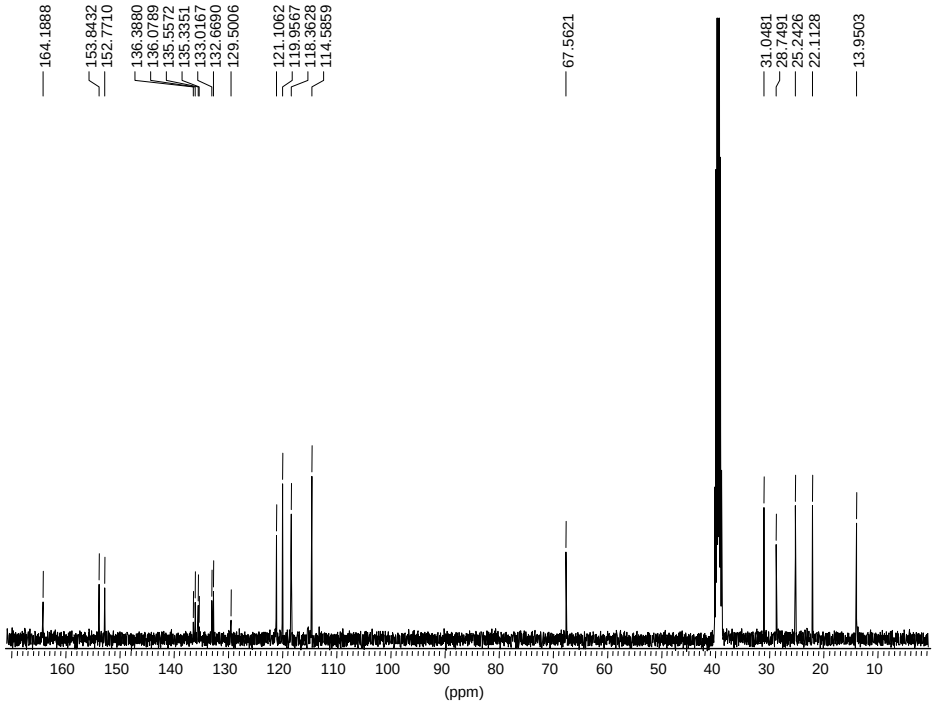


Figure S8: **A)** ^{1}H-NMR of **4** (400 MHz, DMSO-d_6). **B)** ^{13}C-NMR of **4** (100 MHz, DMSO-d_6). **C)** ^{14}C-NMR of **4** (100 MHz, DMSO-d_6).

A)



B)


164.1888
153.8432
152.7710
136.3880
136.0789
135.5572
135.3351
133.0167
132.6690
129.5006
121.1062
119.9567
118.3628
114.5859
67.5621
31.0481
28.7491
25.2426
22.1128
13.9503
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
(ppm)

C)

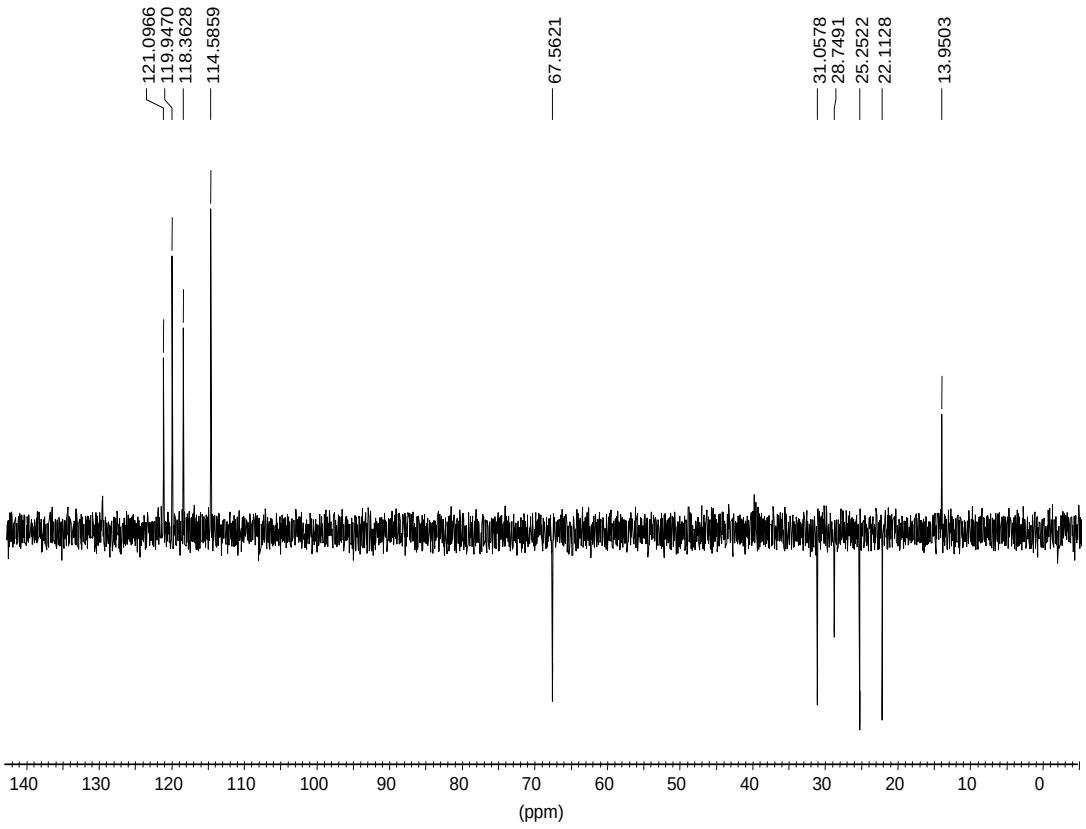
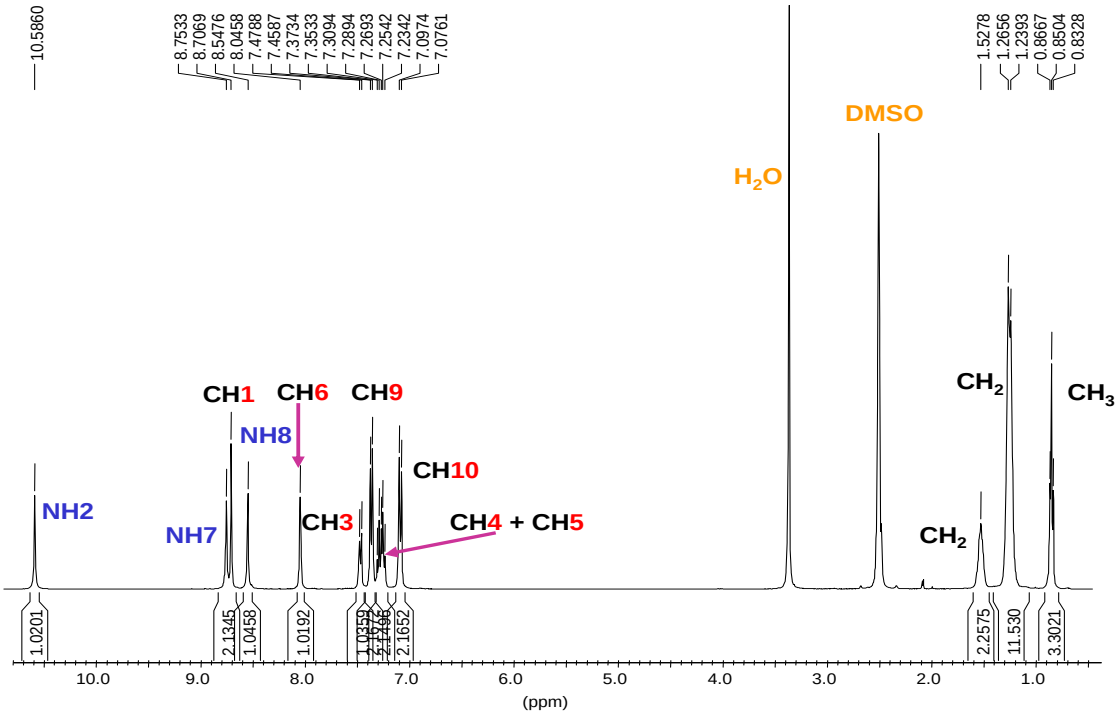
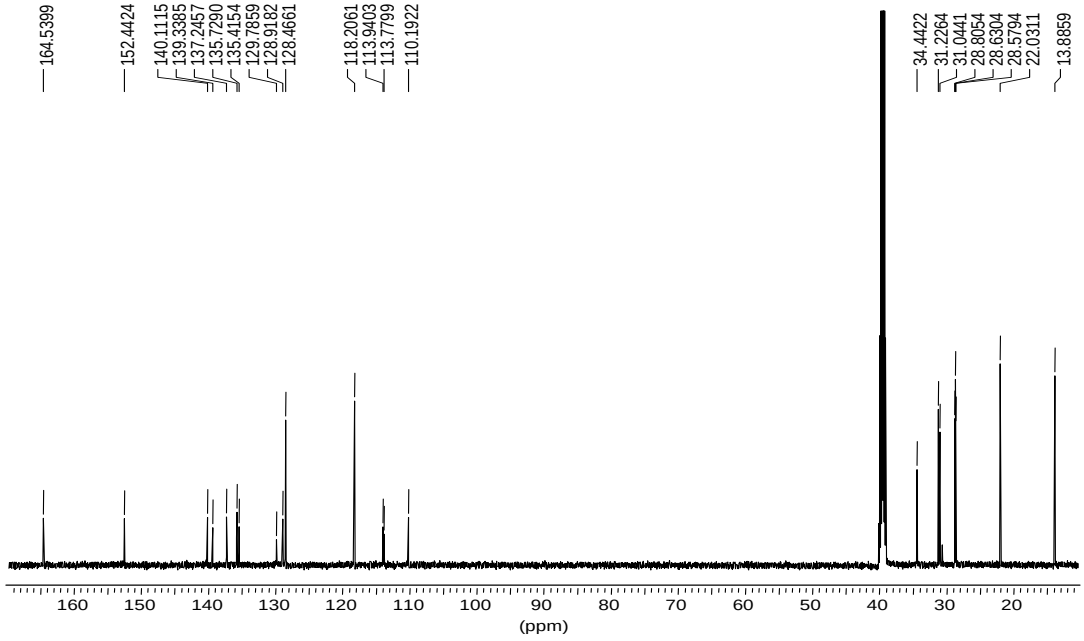

121.0966
119.9470
118.3628
114.5859
67.5621
31.0578
28.7491
25.2522
22.1128
13.9503
140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
(ppm)

Figure S9: A) ^{1}H-NMR of **5** (400 MHz, DMSO-d_6). **B)** ^{13}C-NMR of **5** (150 MHz, DMSO-d_6). **C)** ^{14}C-NMR of **5** (150 MHz, DMSO-d_6).

A)



B)



C)

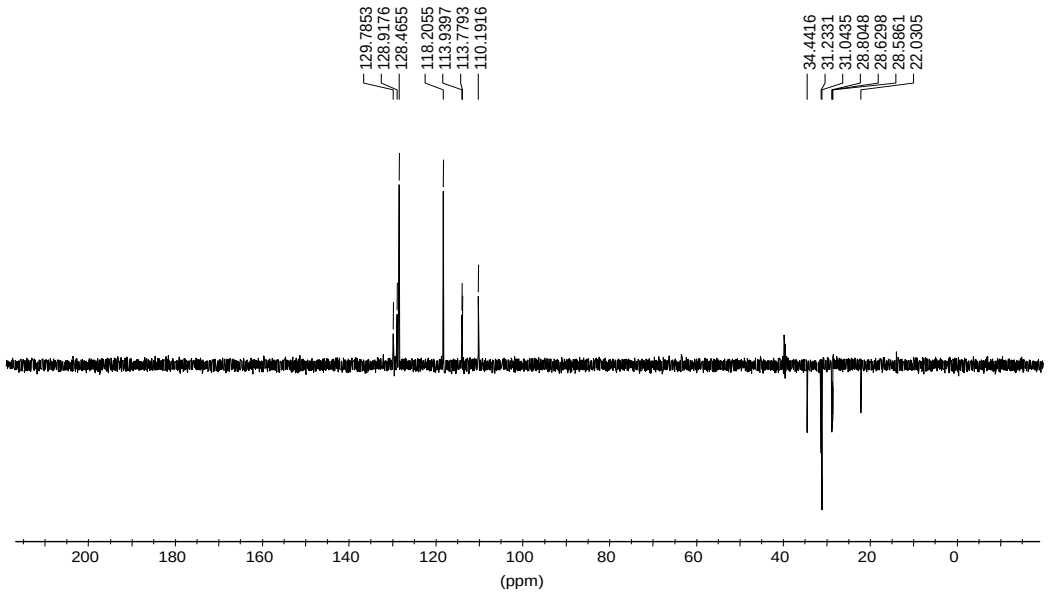
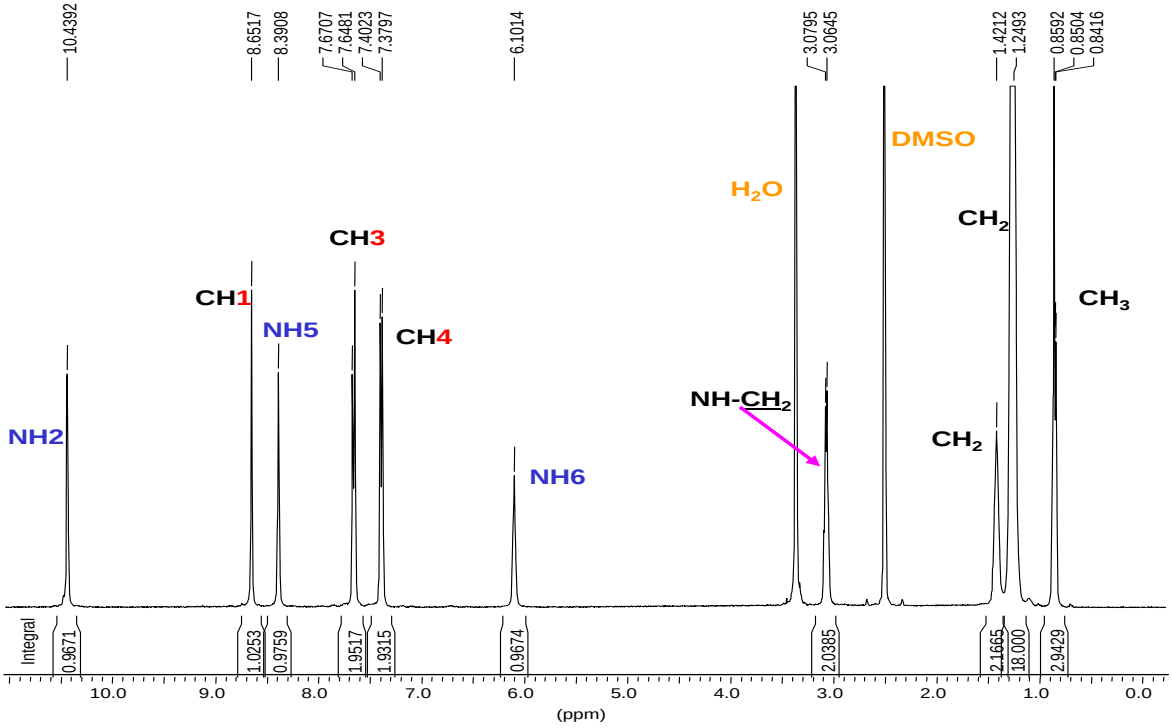
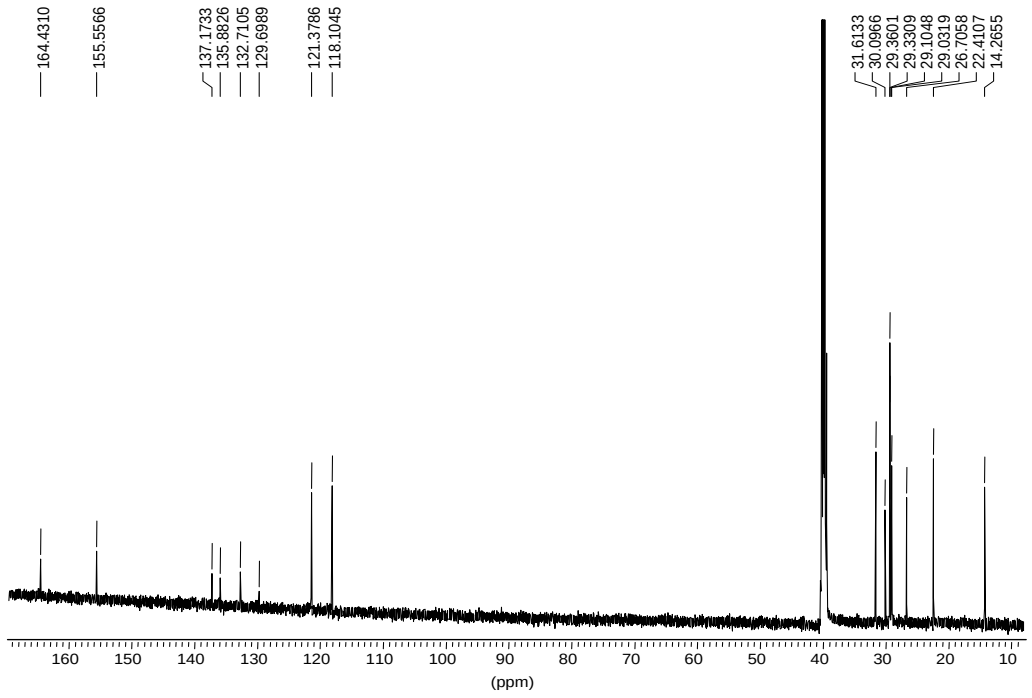


Figure S10: **A)** ^{1}H-NMR of **6** (400 MHz, DMSO-d_6). **B)** ^{13}C-NMR of **6** (150 MHz, DMSO-d_6). **C)** ^{14}C-NMR of **6** (150 MHz, DMSO-d_6).

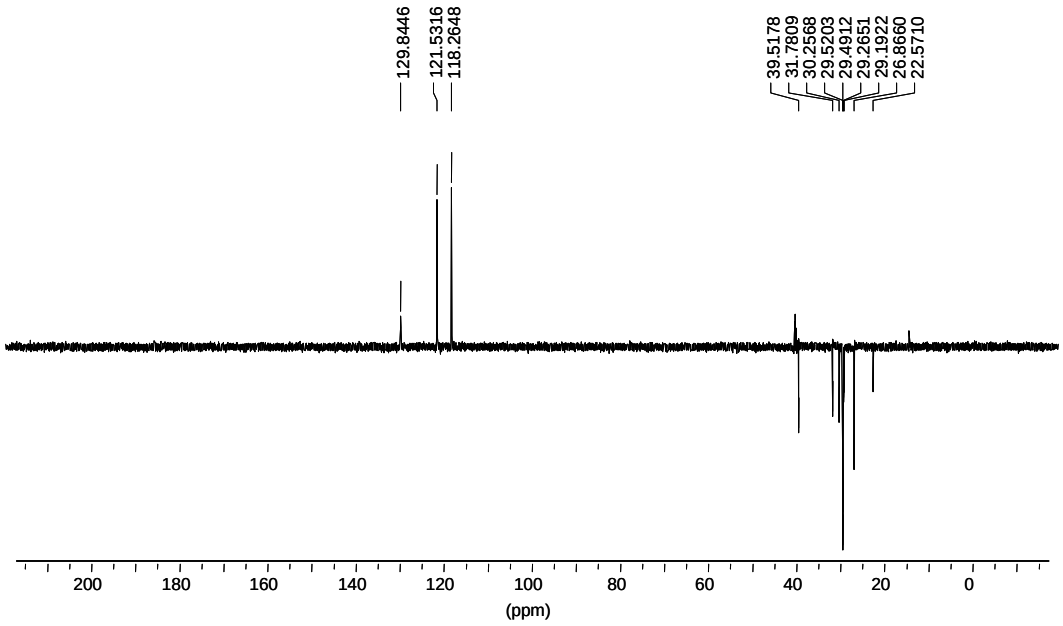
A)



B)


164.4310
155.5566
137.1733
135.8826
132.7105
129.6989
121.3786
118.1045
31.6133
30.0966
29.3601
29.3309
29.1048
29.0319
26.7058
22.4107
14.2655
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
(ppm)

C)


129.8446
121.5316
118.2648
39.5178
31.7809
30.2568
29.5203
29.4912
29.2651
29.1922
26.8660
22.5710
200 180 160 140 120 100 80 60 40 20 0
(ppm)

^{1}H NMR Titrations

^{1}H NMR titrations were carried out on a Bruker Spectrospin DPX-400 instrument at 25°C. Data analysis was conducted using Origin 7.5®, TopSpin, and Win-Eq NMR. The TBA salts of the anions used in the titrations were of spectroscopic grade and were purchased from Sigma Aldrich. All TBA salts were dried over P_2O_5 at 40°C under vacuum.

Preparation of Solutions for NMR Titrations with Anions

The concentrations of these solutions were prepared such that 2 µL would give *ca*. 0.1 molar equivalents of the anion. Host solutions of *ca.* 7.35×10^{-3} M were prepared by dissolving a known amount of host in 0.8 mL of solvent.

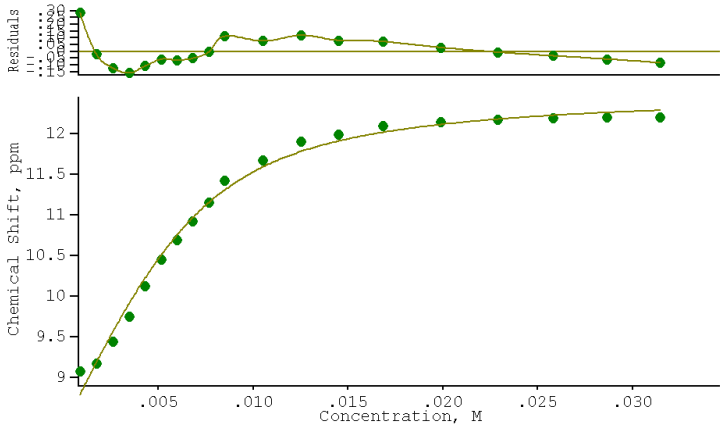


Figure S11: The experimental binding isotherms for ^{1}H NMR titration of **1** with AcO^- in DMSO-$_{d6}$ and the corresponding fit using Win-Eq NMR.

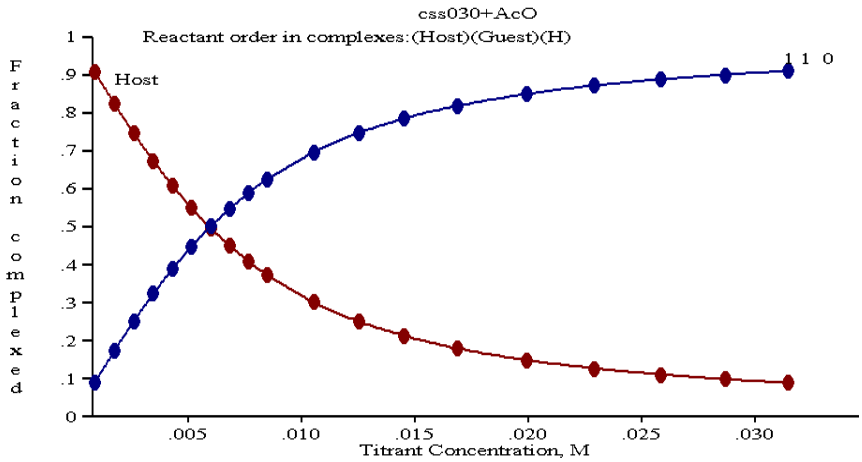


Figure S12: Speciation distribution diagram for the ^{1}H NMR titration of **1** with AcO^{-}

NO. A PARAMETER DELTA ERROR CONDITION DESCRIPTION

1 1 2.81838E+00 1.000E-02 7.195E-02 7.542E+00 K ass

2 1 8.37697E+00 1.000E-02 8.398E-02 1.987E+00 shift free

3 1 1.25157E+01 1.000E-02 8.622E-02 5.592E+00 shift compl

0RMS ERROR = 1.12E-01 MAX ERROR = 2.87E-01 AT OBS.NO. 1

RESIDUALS SQUARED = 2.02E-01

RFACTOR = 0.9248 PERCENT

0RMS ERROR = 1.22E-01 MAX ERROR = 3.15E-01 AT OBS.NO. 1

RESIDUALS SQUARED = 2.38E-01

RFACTOR = 0.9776 PERCENT

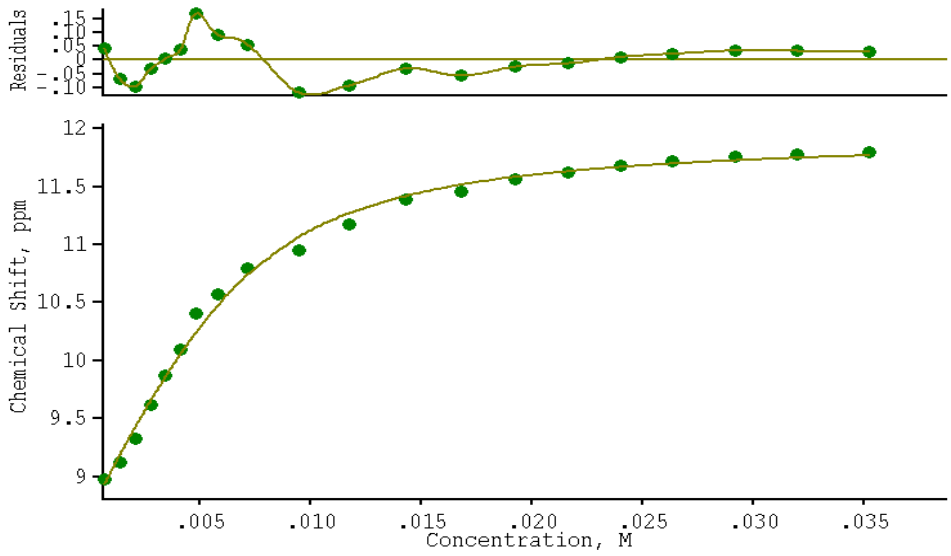


Figure S13: The experimental binding isotherms for ^{1}H NMR titration of **1** with SO_4^{2-} in DMSO-$_{d6}$ and the corresponding fit using Win-Eq NMR.

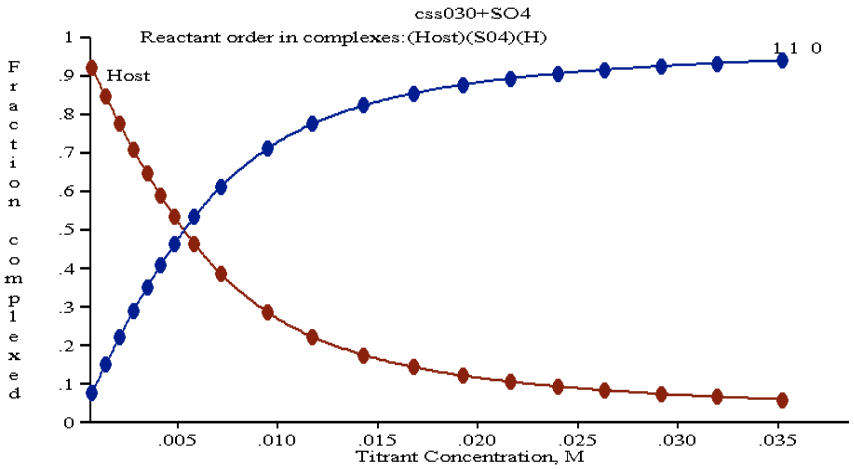


Figure S14: Speciation distribution diagram for the ^{1}H NMR titration of **1** with SO_4^{2-}

NO. A PARAMETER DELTA ERROR CONDITION DESCRIPTION

1 1 2.78136E+00 1.000E-02 5.917E-02 6.964E+00 K ass

2 1 8.67972E+00 1.000E-02 4.876E-02 1.900E+00 shift free

3 1 1.19408E+01 1.000E-02 5.209E-02 5.144E+00 shift compl

0RMS ERROR = 7.25E-02 MAX ERROR = 1.69E-01 AT OBS.NO. 7

RESIDUALS SQUARED = 8.95E-02

RFACTOR = 0.6178 PERCENT

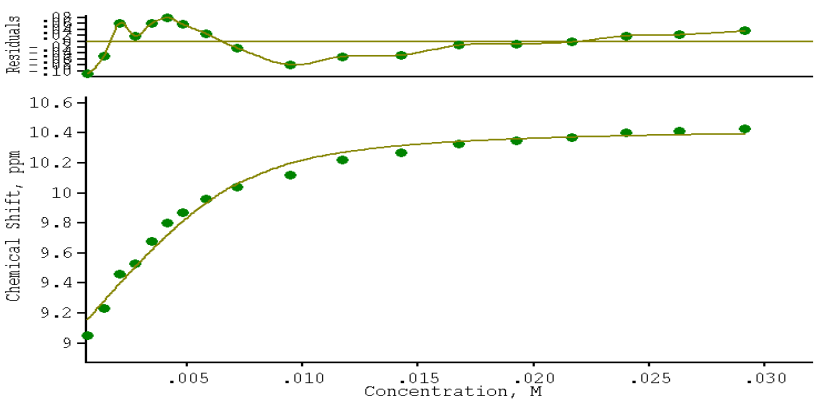


Figure S15: The experimental binding isotherms for ^{1}H NMR titration of **1** (Urea-NH) with $H_2PO_4^-$ in DMSO-$_{d6}$ and the corresponding fit using Win-Eq NMR.

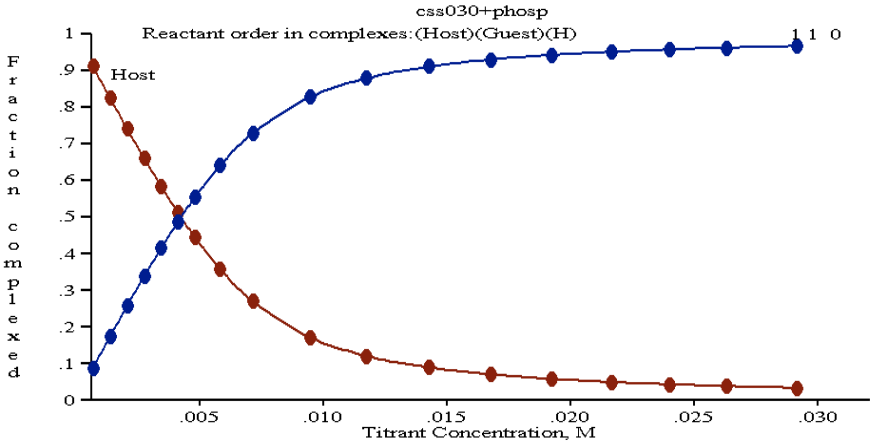


Figure S16: Speciation distribution diagram for the ^{1}H NMR titration of **1** (Urea-NH) with $H_2PO_4^-$.

NO. A PARAMETER DELTA ERROR CONDITION DESCRIPTION

1 1 3.09303E+00 1.000E-02 1.307E-01 5.284E+00 K ass

2 1 9.03393E+00 1.000E-02 3.660E-02 1.554E+00 shift free

3 1 1.04407E+01 1.000E-02 3.717E-02 4.289E+00 shift compl

0RMS ERROR = 5.55E-02 MAX ERROR = 1.09E-01 AT OBS.NO. 1

RESIDUALS SQUARED = 4.63E-02

RFACTOR = 0.5078 PERCENT

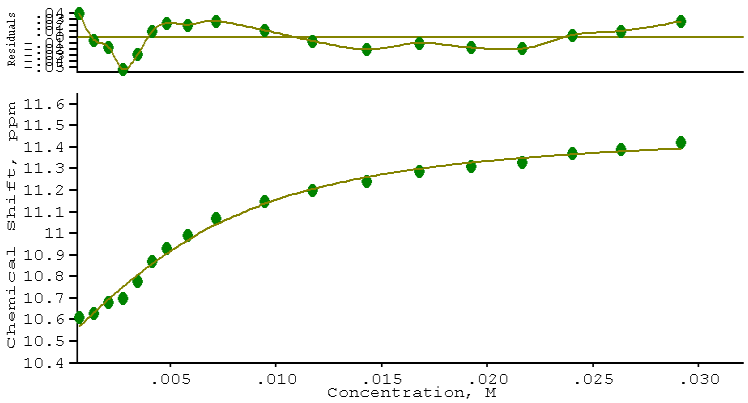


Figure S17: The experimental binding isotherms for ^{1}H NMR titration of **1** (Amido-NH) with $H_2PO_4^-$ in DMSO-$_{d6}$ and the corresponding fit using Win-Eq NMR.

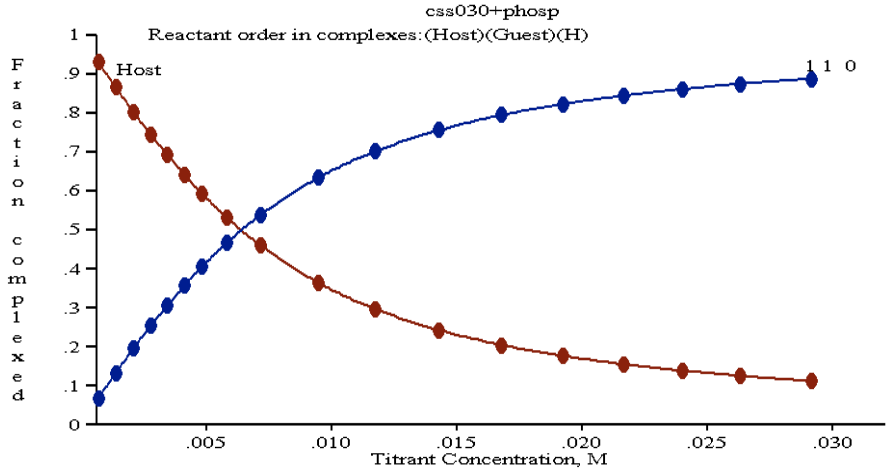


Figure S18: Speciation distribution diagram for the ^{1}H NMR titration of **1** (Amido-NH) with $H_2PO_4^-$.

NO. A PARAMETER DELTA ERROR CONDITION DESCRIPTION

1 1 2.52561E+00 1.000E-02 7.780E-02 1.394E+01 K ass

2 1 1.05003E+01 1.000E-02 1.777E-02 2.387E+00 shift free

3 1 1.15043E+01 1.000E-02 3.142E-02 1.020E+01 shift compl

0RMS ERROR = 2.57E-02 MAX ERROR = 5.44E-02 AT OBS.NO. 4

RESIDUALS SQUARED = 9.89E-03

RFACTOR = 0.2120 PERCENT

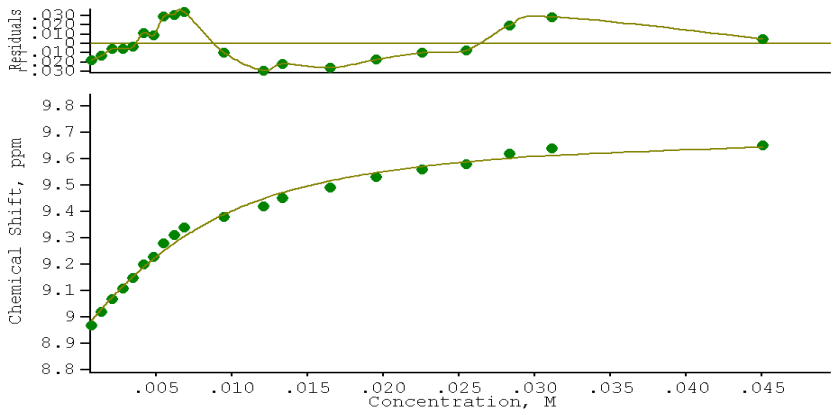


Figure S19: The experimental binding isotherms for ^{1}H NMR titration of **1** (Urea-NH) with Cl^- in DMSO-$_{d6}$ and the corresponding fit using Win-Eq NMR.

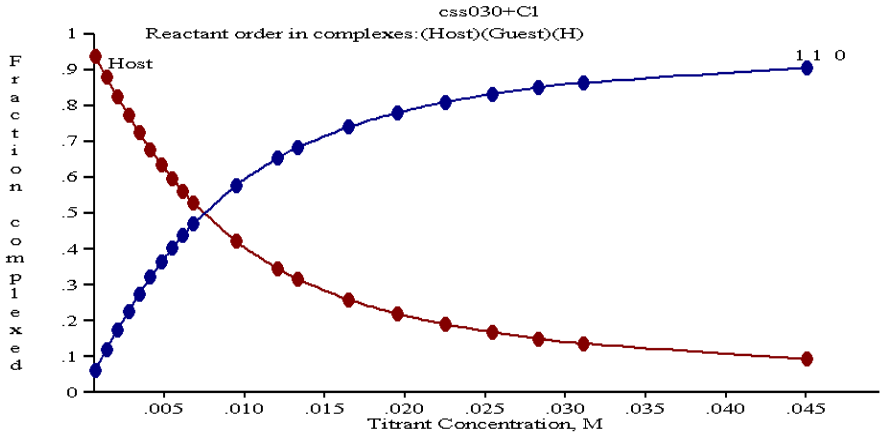


Figure S20: Speciation distribution diagram for the ^{1}H NMR titration of **1** (Urea-NH) with Cl^-.

NO. A PARAMETER DELTA ERROR CONDITION DESCRIPTION

1 1 2.39112E+00 1.000E-02 6.680E-02 1.233E+01 K ass

2 1 8.93975E+00 1.000E-02 1.393E-02 2.662E+00 shift free

3 1 9.71666E+00 1.000E-02 2.273E-02 8.334E+00 shift compl

0RMS ERROR = 2.08E-02 MAX ERROR = 3.37E-02 AT OBS.NO. 10

RESIDUALS SQUARED = 7.35E-03

RFACTOR = 0.2050 PERCENT

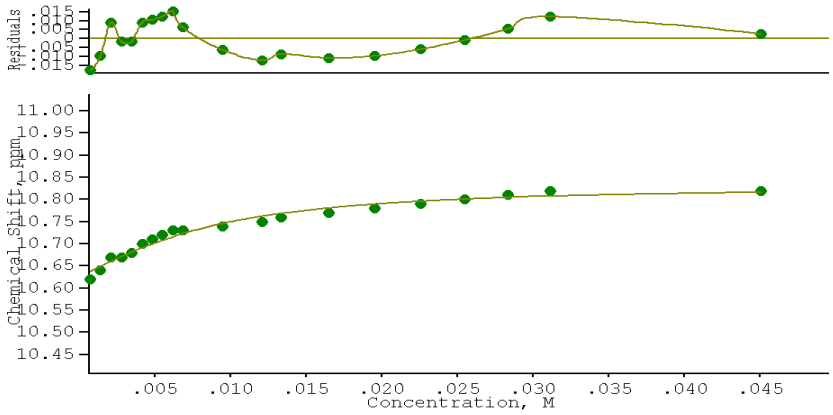


Figure S21: The experimental binding isotherms for ^{1}H NMR titration of **1** (Amido-NH) with Cl^- in DMSO-$_{d6}$ and the corresponding fit using Win-Eq NMR.

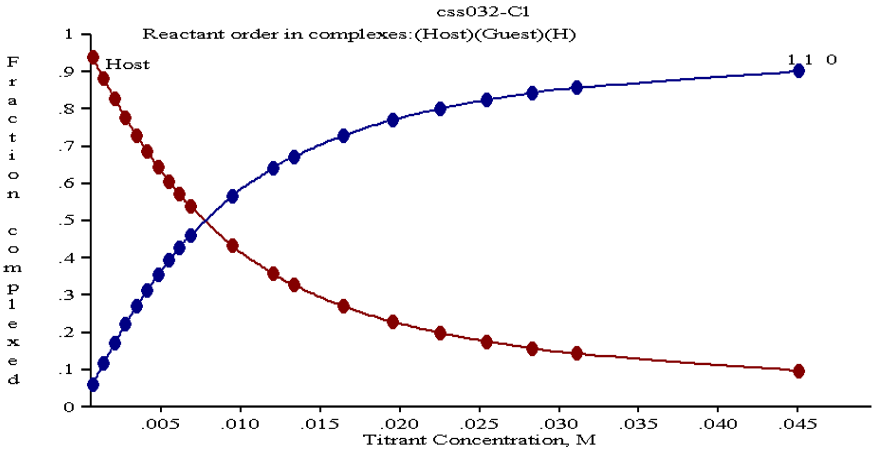


Figure S22: Speciation distribution diagram for the ^{1}H NMR titration of **1** (Amido-NH) with Cl^-.

NO. A PARAMETER DELTA ERROR CONDITION DESCRIPTION

1 1 2.36558E+00 1.000E-02 1.108E-01 1.124E+01 K ass

2 1 1.06250E+01 1.000E-02 6.610E-03 2.518E+00 shift free

3 1 1.08370E+01 1.000E-02 1.099E-02 7.736E+00 shift compl

0RMS ERROR = 1.03E-02 MAX ERROR = 1.75E-02 AT OBS.NO. 1

RESIDUALS SQUARED = 1.80E-03

RFACTOR = 0.0883 PERCENT

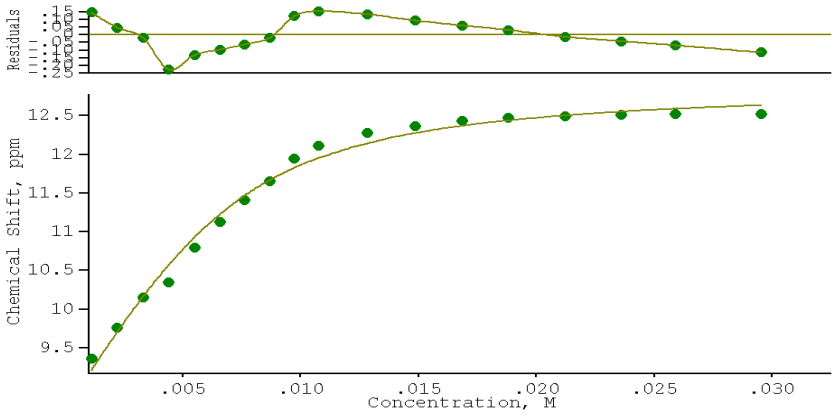


Figure S23: The experimental binding isotherms for ^{1}H NMR titration of **2** with AcO^{-} in DMSO-$_{d6}$ and the corresponding fit using Win-Eq NMR.

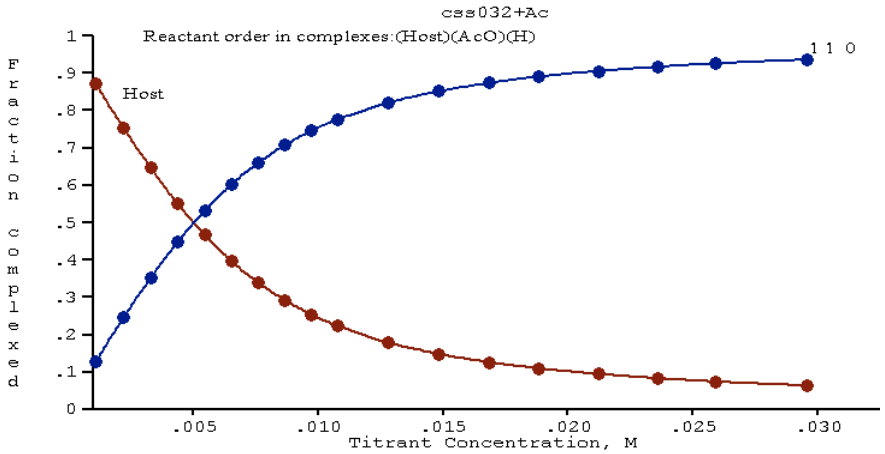


Figure S24: Speciation distribution diagram for the ^{1}H NMR titration of **2** with AcO^{-}.

NO. APARAMETER DELTA ERROR CONDITION DESCRIPTION

1 1 2.79637E+00 1.000E-02 7.709E-02 9.184E+00 K 1:1

2 1 8.67722E+00 1.000E-02 9.841E-02 2.100E+00 shift H

3 1 1.29000E+01 1.000E-02 9.679E-02 6.828E+00 shift HG

0RMS ERROR = 1.14E-01MAX ERROR = 2.27E-01 AT OBS.NO. 4

RESIDUALS SQUARED = 1.96E-01

RFACTOR =0.8988 PERCENT

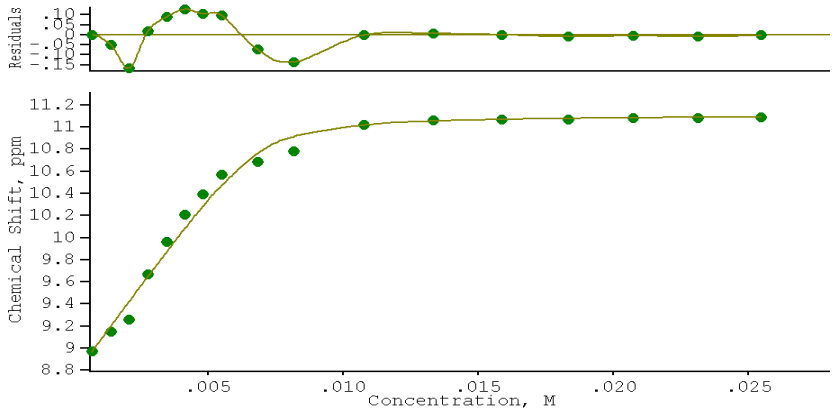


Figure S25: The experimental binding isotherms for ^{1}H NMR titration of **2** with SO_4^{2-} in DMSO-*d6* and the corresponding fit using Win-Eq NMR.

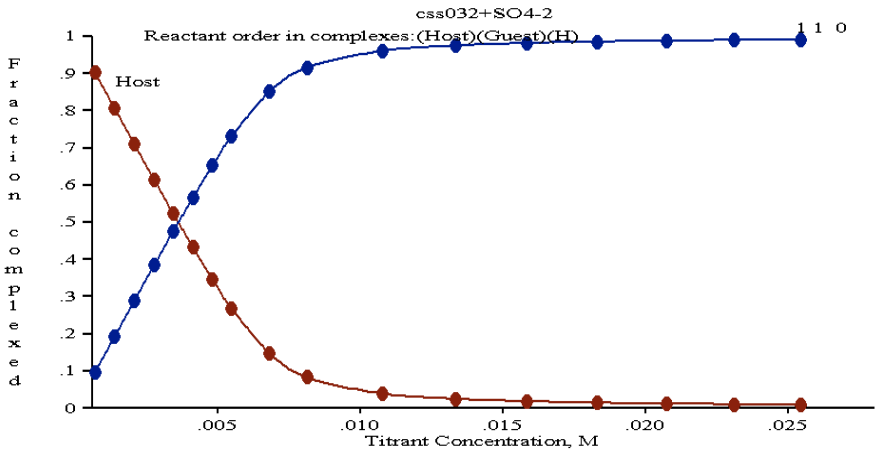


Figure S26: Speciation distribution diagram for the ^{1}H NMR titration of **2** with SO_4^{2-}.

NO. A PARAMETER DELTA ERROR CONDITION DESCRIPTION

1 1 3.75782E+00 1.000E-02 2.066E-01 3.018E+00 K ass

2 1 8.73768E+00 1.000E-02 5.279E-02 1.202E+00 shift free

3 1 1.11121E+01 1.000E-02 4.463E-02 2.862E+00 shift compl

0RMS ERROR = 8.39E-02 MAX ERROR = 1.65E-01 AT OBS.NO. 3

RESIDUALS SQUARED = 9.84E-02

RFACTOR = 0.7286 PERCENT

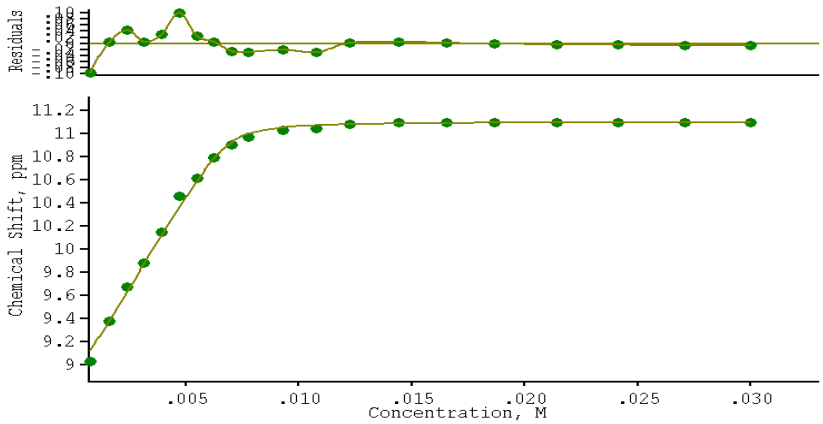


Figure S27: The experimental binding isotherms for ^{1}H NMR titration of **2** with $H_2PO_4^-$ in DMSO-*d6* and the corresponding fit using Win-Eq NMR.

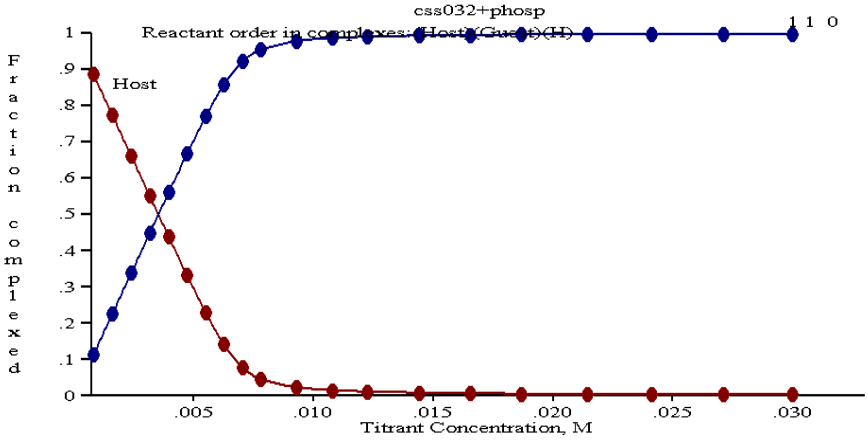


Figure S28: Speciation distribution diagram for the ^{1}H NMR titration of **2** with $H_2PO_4^-$.

NO. A PARAMETER DELTA ERROR CONDITION DESCRIPTION

1 1 4.19753E+00 1.000E-02 1.361E-01 2.229E+00 K ass

2 1 8.87262E+00 1.000E-02 2.569E-02 1.109E+00 Shift Free

3 1 1.11015E+01 1.000E-02 1.537E-02 2.218E+00 Shift Compl

0RMS ERROR = 3.87E-02 MAX ERROR = 1.01E-01 AT OBS.NO. 6

RESIDUALS SQUARED = 2.54E-02

RFACTOR = 0.3349 PERCENT

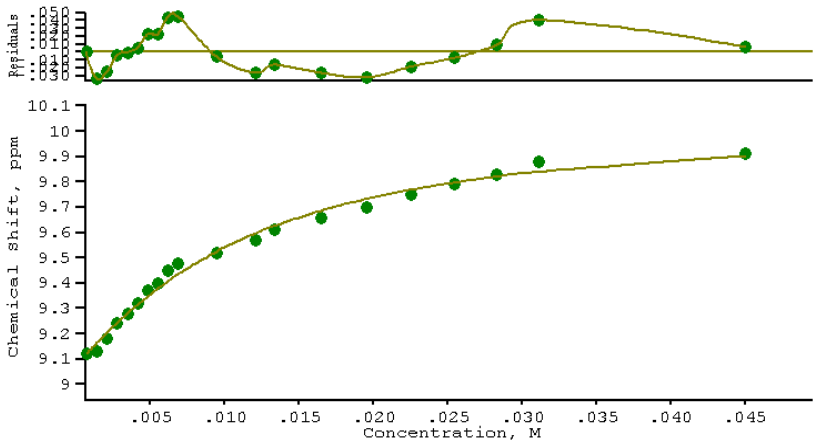


Figure S29: The experimental binding isotherms for ^{1}H NMR titration of **2** (Urea-NH) with Cl^- in DMSO-$_{d6}$ and the corresponding fit using Win-Eq NMR.

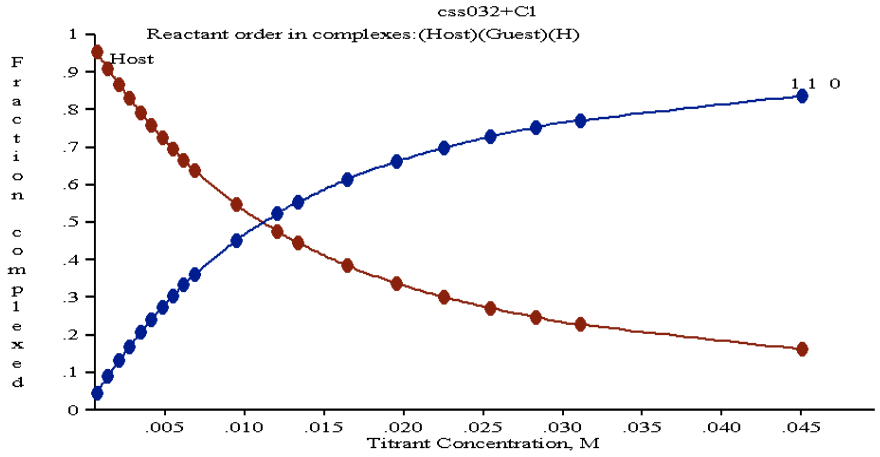


Figure S30: Speciation distribution diagram for the ^{1}H NMR titration of **2** (Urea-NH) with Cl^-.

NO. A PARAMETER DELTA ERROR CONDITION DESCRIPTION

1 1 2.12364E+00 1.000E-02 7.292E-02 1.912E+01 K ass

2 1 9.07395E+00 1.000E-02 1.701E-02 3.106E+00 shift free

3 1 1.00578E+01 1.000E-02 4.181E-02 1.307E+01 shift compl

0RMS ERROR = 2.63E-02 MAX ERROR = 4.56E-02 AT OBS.NO. 10

RESIDUALS SQUARED = 1.18E-02

RFACTOR = 0.2549 PERCENT

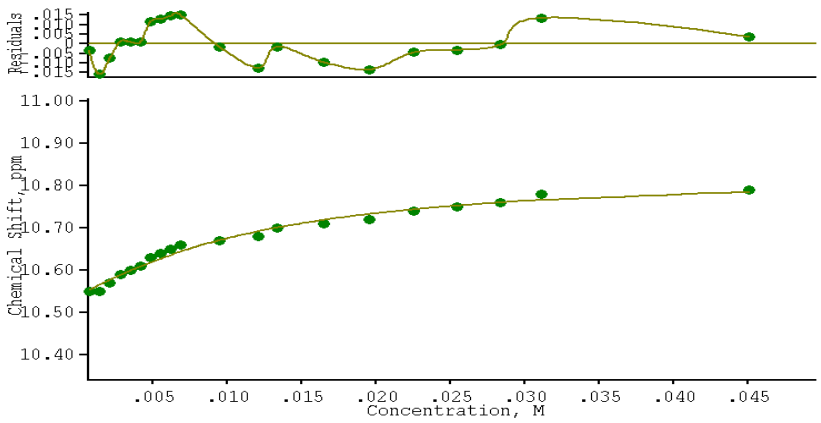


Figure S31: The experimental binding isotherms for ^{1}H NMR titration of **2** (Amido-NH) with Cl^- in DMSO-$_{d6}$ and the corresponding fit using Win-Eq NMR.

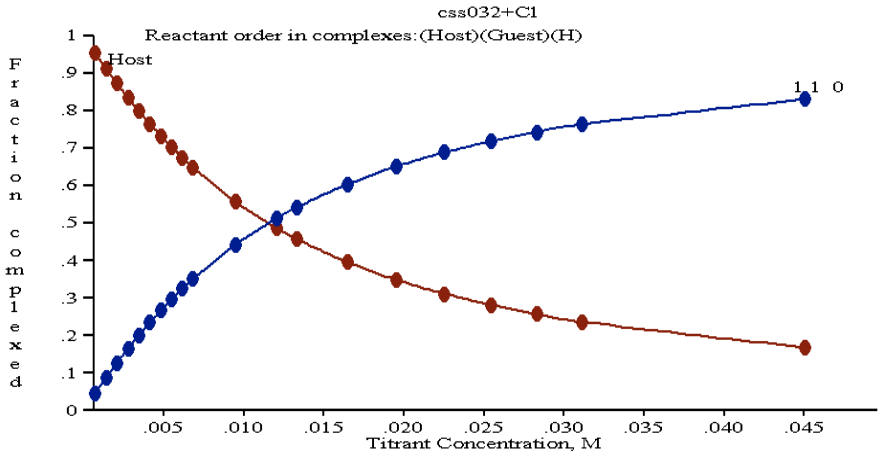


Figure S32: Speciation distribution diagram for the ^{1}H NMR titration of **2** (Amido-NH) with Cl^-.

NO. A PARAMETER DELTA ERROR CONDITION DESCRIPTION

1 1 2.08723E+00 1.000E-02 9.088E-02 1.963E+01 K ass

2 1 1.05405E+01 1.000E-02 6.257E-03 3.004E+00 shift free

3 1 1.08351E+01 1.000E-02 1.702E-02 1.374E+01 shift compl

0RMS ERROR = 1.01E-02 MAX ERROR = 1.59E-02 AT OBS.NO. 2

RESIDUALS SQUARED = 1.72E-03

RFACTOR = 0.0870 PERCENT

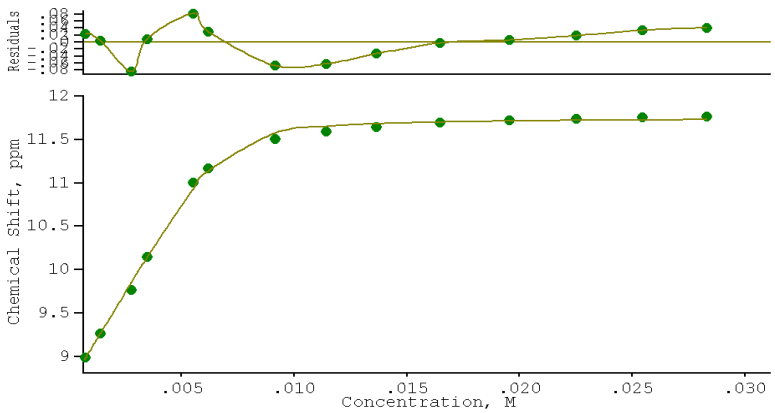


Figure S33: The experimental binding isotherms for ^{1}H NMR titration of **3** with AcO^{-} in DMSO-$_{d6}$ and the corresponding fit using Win-Eq NMR.

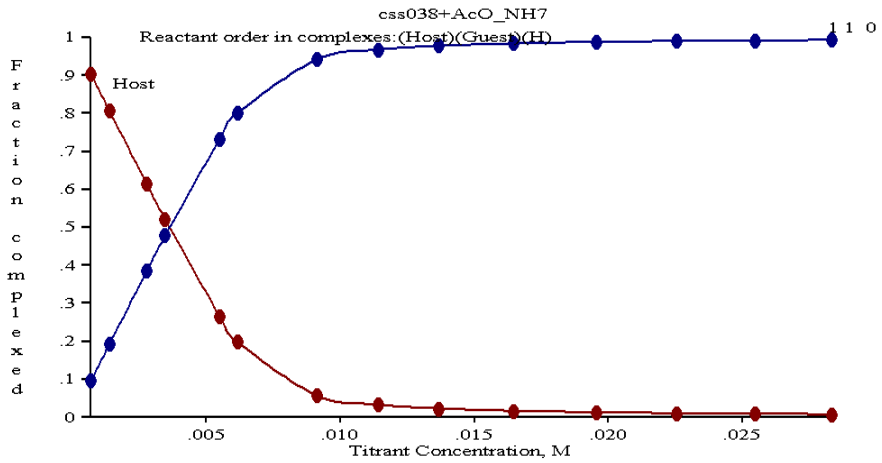


Figure S34: Speciation distribution diagram for the ^{1}H NMR titration of **3** with AcO^{-}.

NO. A PARAMETER DELTA ERROR CONDITION DESCRIPTION

1 1 3.77793E+00 1.000E-02 1.085E-01 2.789E+00 K ass

2 1 8.66651E+00 1.000E-02 3.606E-02 1.150E+00 shift free

3 1 1.17518E+01 1.000E-02 2.680E-02 2.627E+00 shift compl

0RMS ERROR = 5.03E-02 MAX ERROR = 8.38E-02 AT OBS.NO. 3

RESIDUALS SQUARED = 2.78E-02

RFACTOR = 0.4042 PERCENT

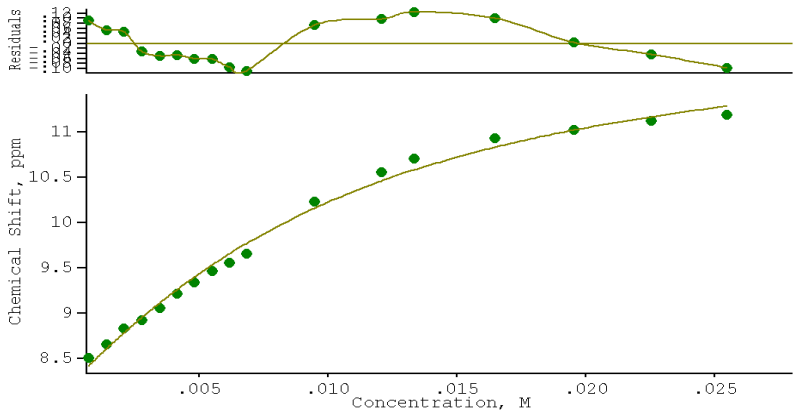


Figure S35: The experimental binding isotherms for ^{1}H NMR titration of **3** with SO_4^{2-} in DMSO-*d6* and the corresponding fit using Win-Eq NMR.

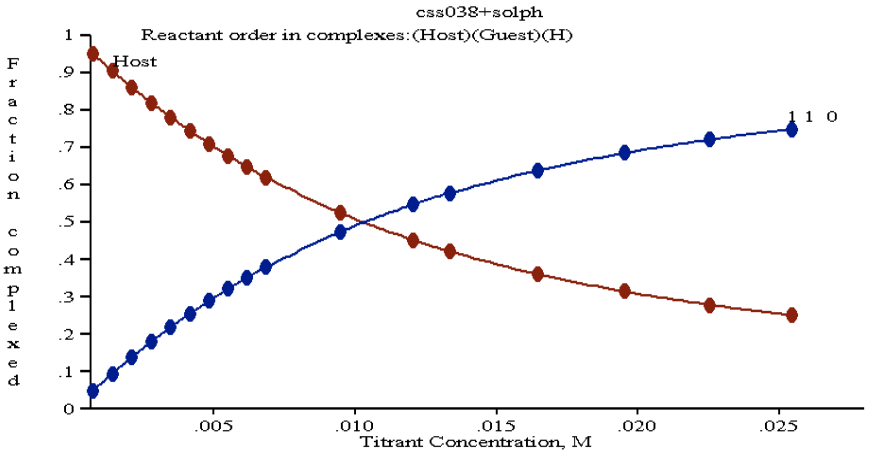


Figure S36: Speciation distribution diagram for the ^{1}H NMR titration of **3** with SO_4^{2-}.

NO. A PARAMETER DELTA ERROR CONDITION DESCRIPTION

1 1 2.15967E+00 1.000E-02 8.499E-02 3.659E+01 K ass

2 1 8.21441E+00 1.000E-02 5.963E-02 3.541E+00 shift free

3 1 1.23073E+01 1.000E-02 2.347E-01 2.677E+01 shift compl

0RMS ERROR = 8.44E-02 MAX ERROR = 1.25E-01 AT OBS.NO. 13

RESIDUALS SQUARED = 9.97E-02

RFACTOR = 0.7763 PERCENT

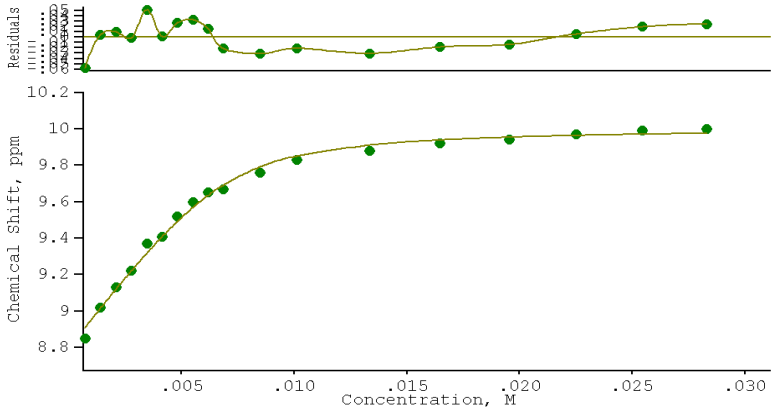


Figure S37: The experimental binding isotherms for ^{1}H NMR titration of **3** (Urea-NH) with $H_2PO_4^-$ in DMSO-*d6* and the corresponding fit using Win-Eq NMR.

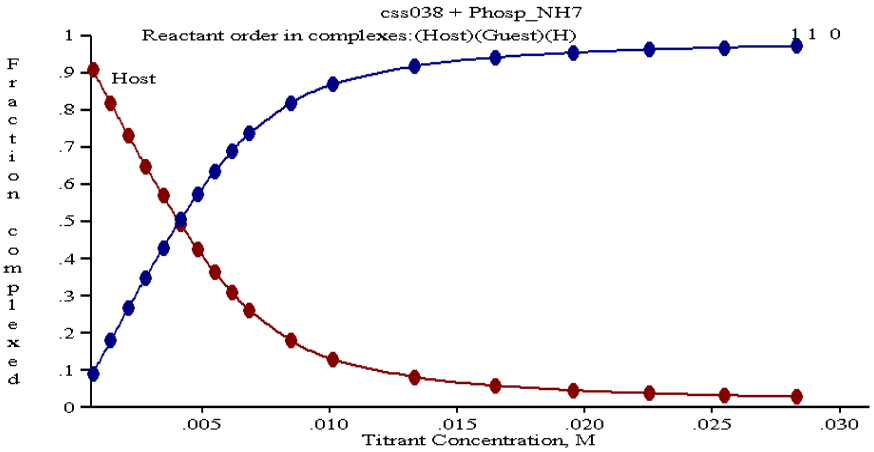


Figure S38: Speciation distribution diagram for the ^{1}H NMR titration of **3** (Urea-NH) with $H_2PO_4^-$.

NO. A PARAMETER DELTA ERROR CONDITION DESCRIPTION

1 1 3.19313E+00 1.000E-02 7.907E-02 4.932E+00 K ass

2 1 8.79803E+00 1.000E-02 1.881E-02 1.511E+00 shift free

3 1 1.00084E+01 1.000E-02 1.932E-02 4.138E+00 shift compl

0RMS ERROR = 2.89E-02 MAX ERROR = 5.77E-02 AT OBS.NO. 1

RESIDUALS SQUARED = 1.26E-02

RFACTOR = 0.2752 PERCENT

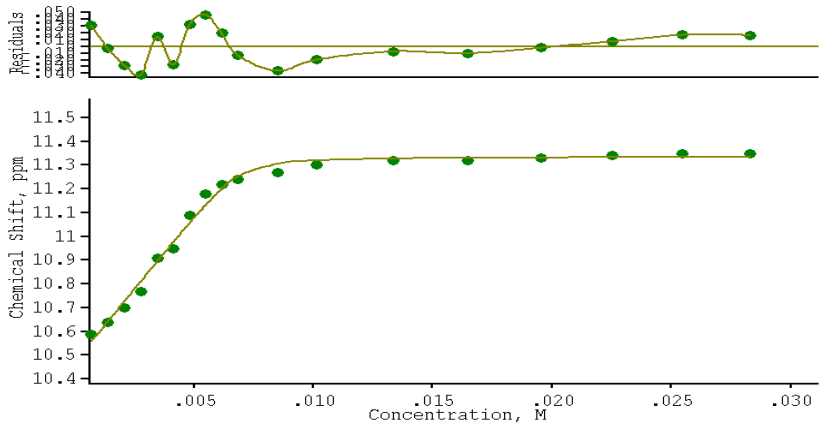


Figure S39: The experimental binding isotherms for ^{1}H NMR titration of **3** (Amido-NH) with $H_2PO_4^-$ in DMSO-$_{d6}$ and the corresponding fit using Win-Eq NMR.

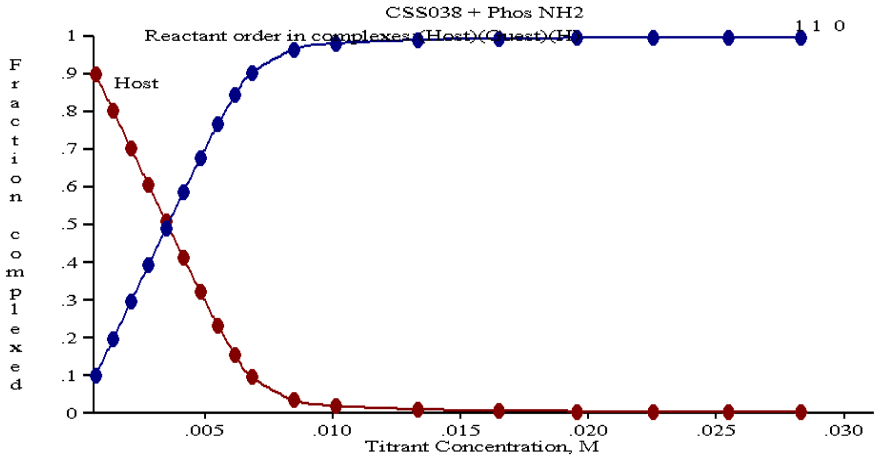


Figure S40: Speciation distribution diagram for the ^{1}H NMR titration of **3** (Amido-NH) with $H_2PO_4^-$.

NO. A PARAMETER DELTA ERROR CONDITION DESCRIPTION

1 1 4.15580E+00 1.000E-02 2.507E-01 2.473E+00 Kass

2 1 1.04730E+01 1.000E-02 1.666E-02 1.138E+00 Shift Free

3 1 1.13352E+01 1.000E-02 1.259E-02 2.481E+00 Shift Complex

0RMS ERROR = 2.68E-02 MAX ERROR = 4.70E-02 AT OBS.NO. 8

RESIDUALS SQUARED = 1.08E-02

RFACTOR = 0.2204 PERCENT

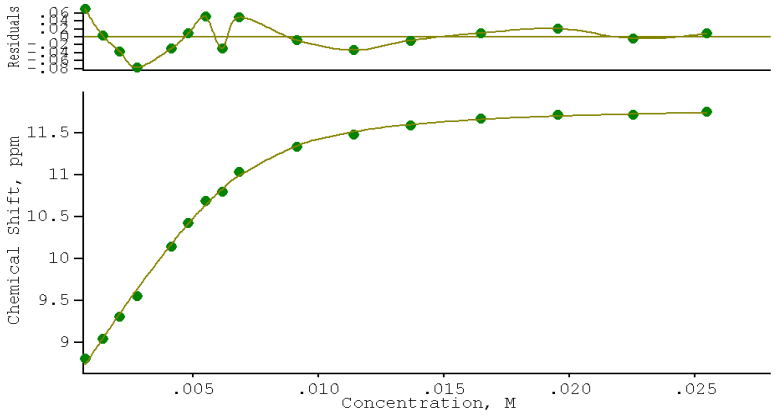


Figure S41: The experimental binding isotherms for ^{1}H NMR titration of **4** with AcO^{-} in DMSO-$_{d6}$ and the corresponding fit using Win-Eq NMR.

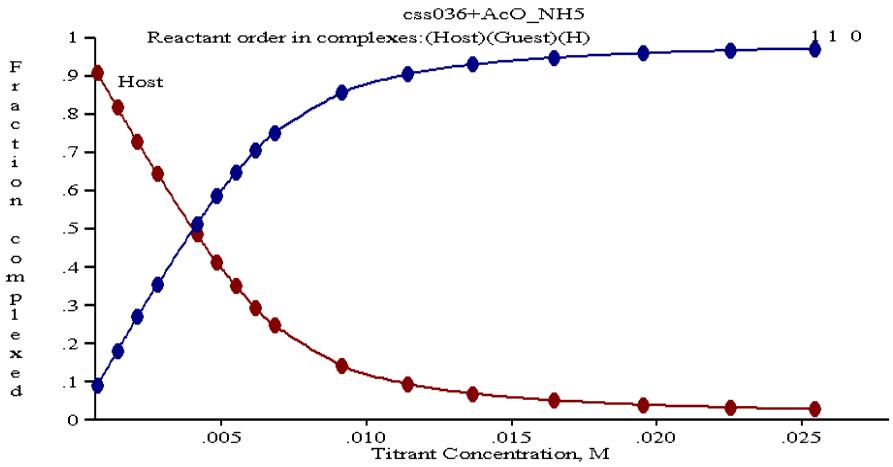


Figure S42: Speciation distribution diagram for the ^{1}H NMR titration of **4** with AcO^{-}.

NO. A PARAMETER DELTA ERROR CONDITION DESCRIPTION

1 1 3.25356E+00 1.000E-02 4.460E-02 5.100E+00 K ass

2 1 8.42501E+00 1.000E-02 2.695E-02 1.414E+00 shift free

3 1 1.18353E+01 1.000E-02 2.928E-02 4.455E+00 shift compl

0RMS ERROR = 4.03E-02 MAX ERROR = 7.73E-02 AT OBS.NO. 4

RESIDUALS SQUARED = 2.11E-02

RFACTOR = 0.3383 PERCENT

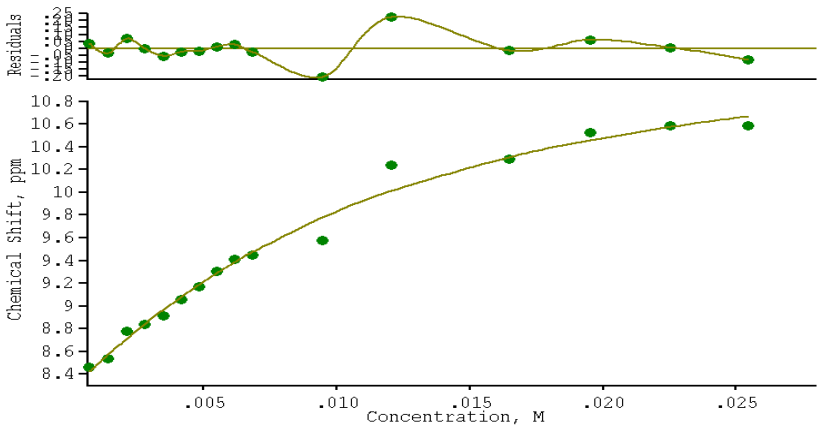


Figure S43: The experimental binding isotherms for ^{1}H NMR titration of **4** with SO_4^- in DMSO-*d6* and the corresponding fit using Win-Eq NMR.

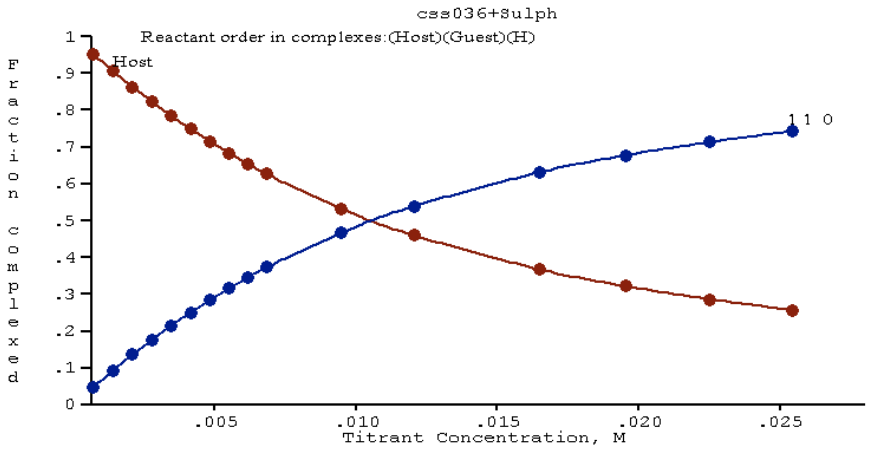


Figure S44: Speciation distribution diagram for the ^{1}H NMR titration of **4** with SO_4^-.

NO. A PARAMETER DELTA ERROR CONDITION DESCRIPTION

1 1 2.14337E+00 1.000E-02 1.258E-01 3.642E+01 K ass

2 1 8.27099E+00 1.000E-02 6.799E-02 3.655E+00 shift free

3 1 1.14983E+01 1.000E-02 2.781E-01 2.628E+01 shift compl

0RMS ERROR = 9.43E-02 MAX ERROR = 2.27E-01 AT OBS.NO. 12

RESIDUALS SQUARED = 1.16E-01

RFACTOR = 0.8937 PERCENT

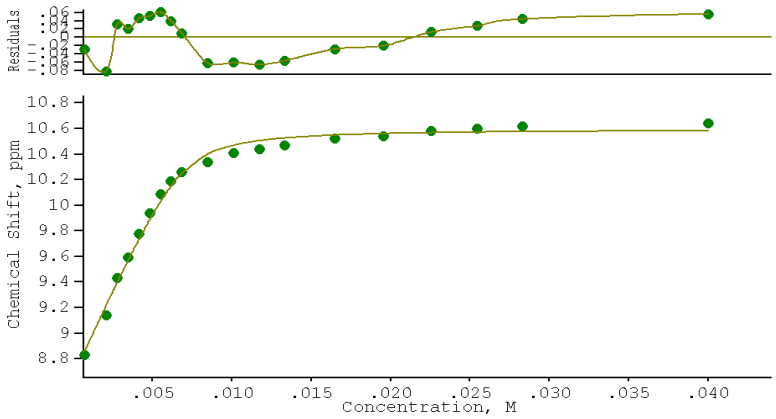


Figure S45: The experimental binding isotherms for ^{1}H NMR titration of **4** (Urea-NH) with $H_2PO_4^-$ in DMSO-$_{d6}$ and the corresponding fit using Win-Eq NMR.

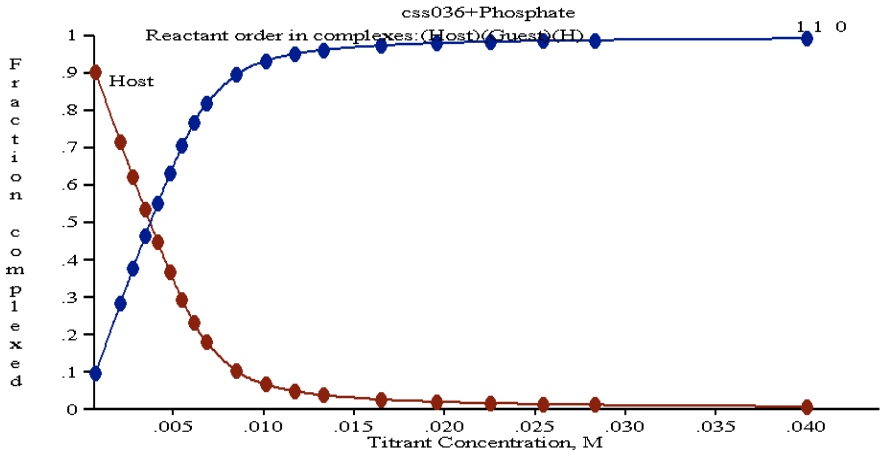


Figure S46: Speciation distribution diagram for the ^{1}H NMR titration of **4** (Urea-NH) with $H_2PO_4^-$.

NO. A PARAMETER DELTA ERROR CONDITION DESCRIPTION

1 1 3.56157E+00 1.000E-02 1.085E-01 3.449E+00 K ass

2 1 8.67462E+00 1.000E-02 3.668E-02 1.339E+00 shift free

3 1 1.05981E+01 1.000E-02 2.526E-02 3.030E+00 shift compl

0RMS ERROR = 5.06E-02 MAX ERROR = 8.11E-02 AT OBS.NO. 2

RESIDUALS SQUARED = 4.10E-02

RFACTOR = 0.4581 PERCENT

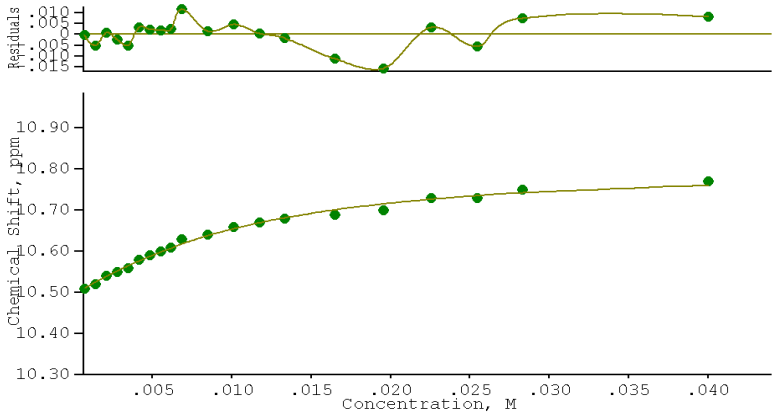


Figure S47: The experimental binding isotherms for ^{1}H NMR titration of **4** (Amido-NH) with $H_2PO_4^-$ in DMSO-$_{d6}$ and the corresponding fit using Win-Eq NMR.

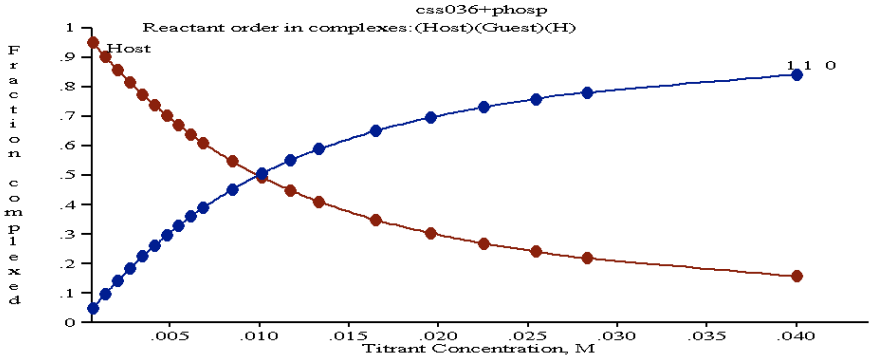


Figure S48: Speciation distribution diagram for the ^{1}H NMR titration of **4** (Amido-NH) with $H_2PO_4^-$.

NO. A PARAMETER DELTA ERROR CONDITION DESCRIPTION

1 1 2.18389E+00 1.000E-02 5.975E-02 2.090E+01 K ass

2 1 1.04945E+01 1.000E-02 4.398E-03 3.184E+00 shift free

3 1 1.08107E+01 1.000E-02 1.151E-02 1.443E+01 shift compl

0RMS ERROR = 6.74E-03 MAX ERROR = 1.55E-02 AT OBS.NO. 16

RESIDUALS SQUARED = 7.72E-04

RFACTOR = 0.0584 PERCENT

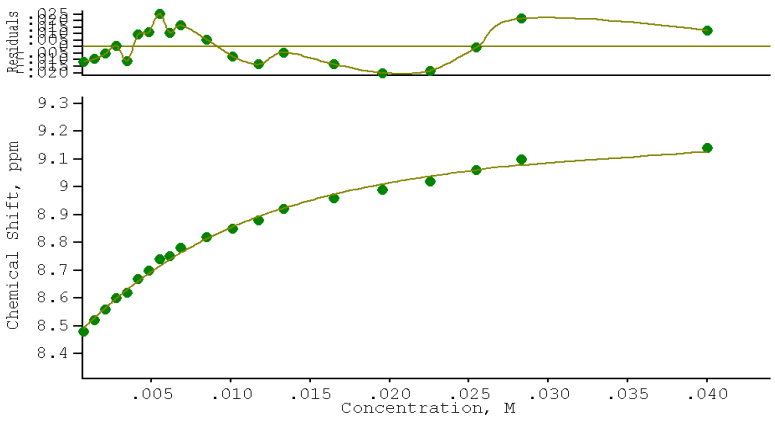


Figure S49: The experimental binding isotherms for ^{1}H NMR titration of **4** (Urea-NH) with Cl^- in DMSO-$_{d6}$ and the corresponding fit using Win-Eq NMR.

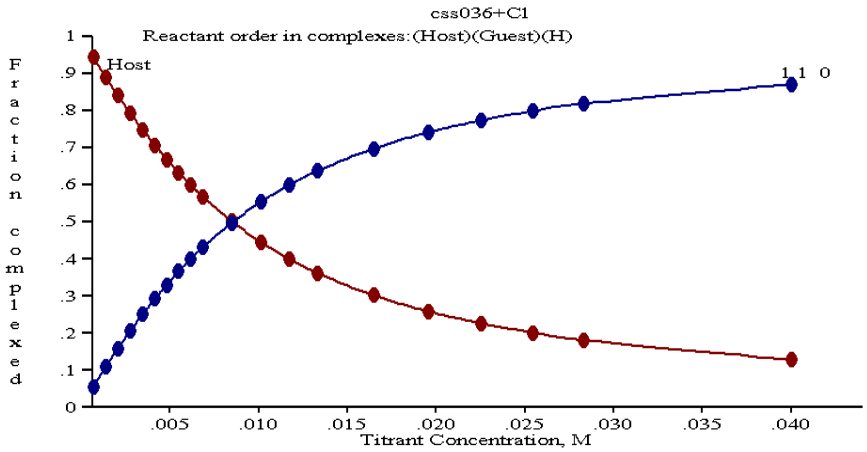


Figure S50: Speciation distribution diagram for the ^{1}H NMR titration of **4** (Urea-NH) with Cl^-.

NO. A PARAMETER DELTA ERROR CONDITION DESCRIPTION

1 1 2.18170E+00 1.000E-02 4.834E-02 1.922E+01 K ass

2 1 8.45122E+00 1.000E-02 9.241E-03 3.132E+00 shift free

3 1 9.25380E+00 1.000E-02 2.280E-02 1.317E+01 shift compl

0RMS ERROR = 1.42E-02 MAX ERROR = 2.52E-02 AT OBS.NO. 8

RESIDUALS SQUARED = 3.41E-03

RFACTOR = 0.1482 PERCENT

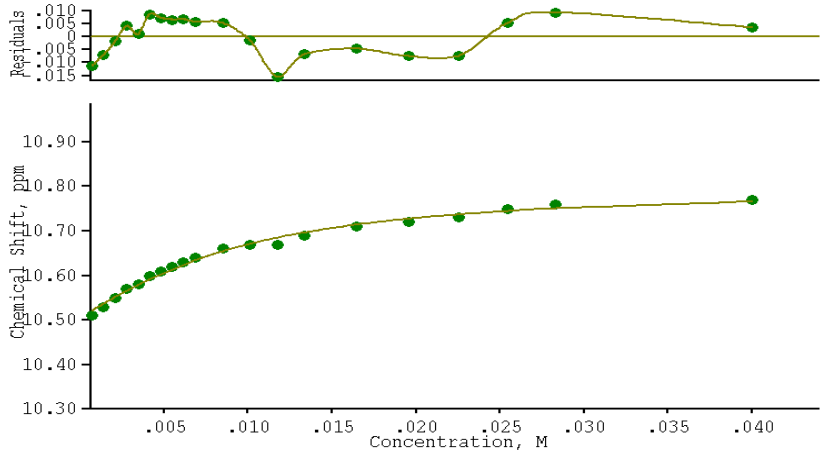


Figure S51: The experimental binding isotherms for ^{1}H NMR titration of **4** (Amido-NH) with Cl^- in DMSO-$_{d6}$ and the corresponding fit using Win-Eq NMR.

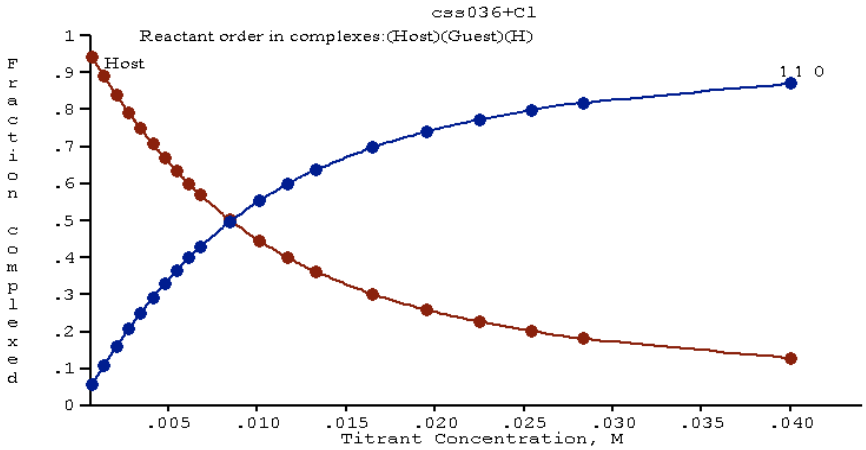


Figure S52: Speciation distribution diagram for the ^{1}H NMR titration of **4** (Amido-NH) with Cl^-.

NO. A PARAMETER DELTA ERROR CONDITION DESCRIPTION

1 1 2.28930E+00 1.000E-02 6.830E-02 1.586E+01 k ass

2 1 1.05046E+01 1.000E-02 5.036E-03 2.878E+00 shift free

3 1 1.08041E+01 1.000E-02 1.051E-02 1.091E+01 shift compl

0RMS ERROR = 7.68E-03 MAX ERROR = 1.53E-02 AT OBS.NO. 13

RESIDUALS SQUARED = 1.00E-03

RFACTOR = 0.0664 PERCENT

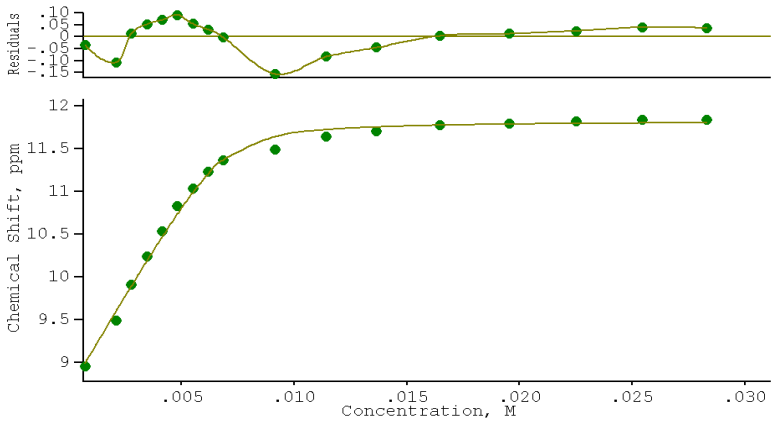


Figure S53: The experimental binding isotherms for ^{1}H NMR titration of **5** with AcO^{-} in DMSO-$_{d6}$ and the corresponding fit using Win-Eq NMR.

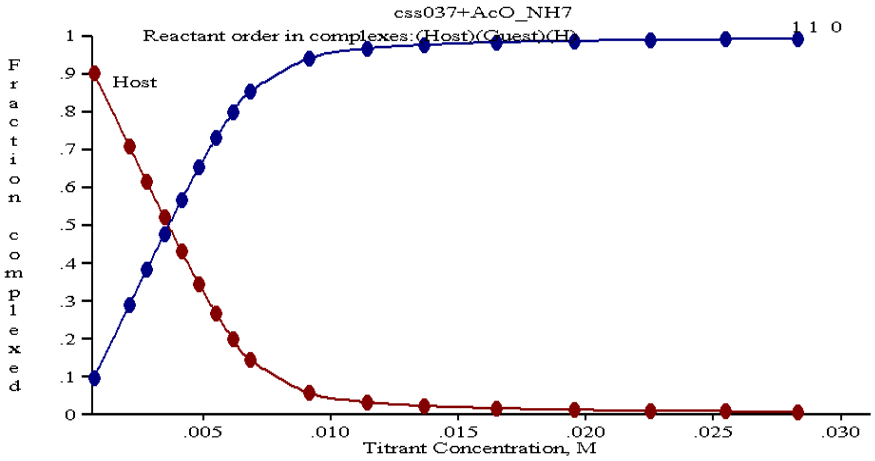


Figure S54: Speciation distribution diagram for the ^{1}H NMR titration of **5** with AcO^{-}.

NO. A PARAMETER DELTA ERROR CONDITION DESCRIPTION

1 1 3.77096E+00 1.000E-02 1.243E-01 3.048E+00 K ass

2 1 8.68813E+00 1.000E-02 5.106E-02 1.261E+00 shift free

3 1 1.18269E+01 1.000E-02 3.611E-02 2.808E+00 shift compl

0RMS ERROR = 7.07E-02 MAX ERROR = 1.56E-01 AT OBS.NO. 10

RESIDUALS SQUARED = 7.00E-02

RFACTOR = 0.5800 PERCENT

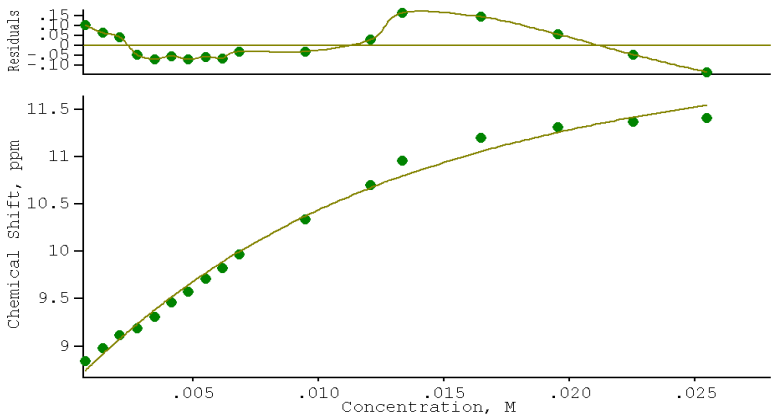


Figure S55: The experimental binding isotherms for ^{1}H NMR titration of **5** with SO_4^- in DMSO-*d6* and the corresponding fit using Win-Eq NMR.

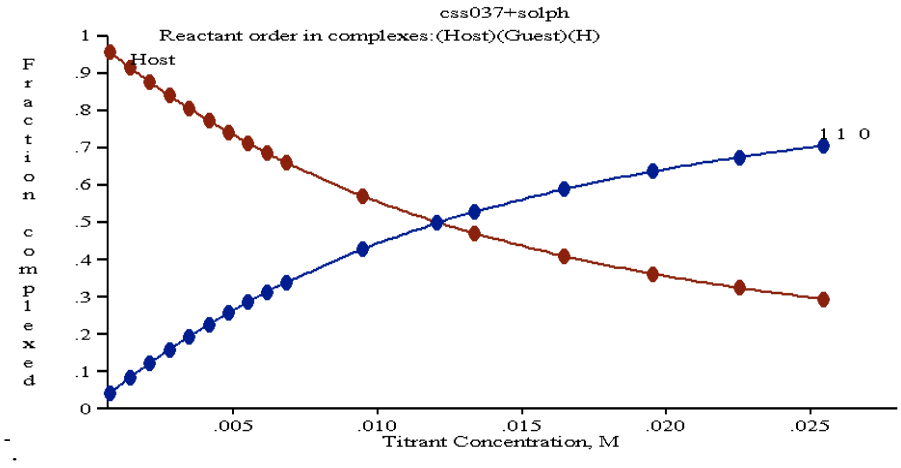


Figure S56: Speciation distribution diagram for the ^{1}H NMR titration of **5** with SO_4^-.

NO. A PARAMETER DELTA ERROR CONDITION DESCRIPTION

1 1 2.05787E+00 1.000E-02 9.663E-02 4.587E+01 K ass

2 1 8.55664E+00 1.000E-02 6.406E-02 3.821E+00 shift free

3 1 1.27964E+01 1.000E-02 3.102E-01 3.391E+01 shift compl

0RMS ERROR = 9.11E-02 MAX ERROR = 1.67E-01 AT OBS.NO. 13

RESIDUALS SQUARED = 1.16E-01

RFACTOR = 0.8173 PERCENT

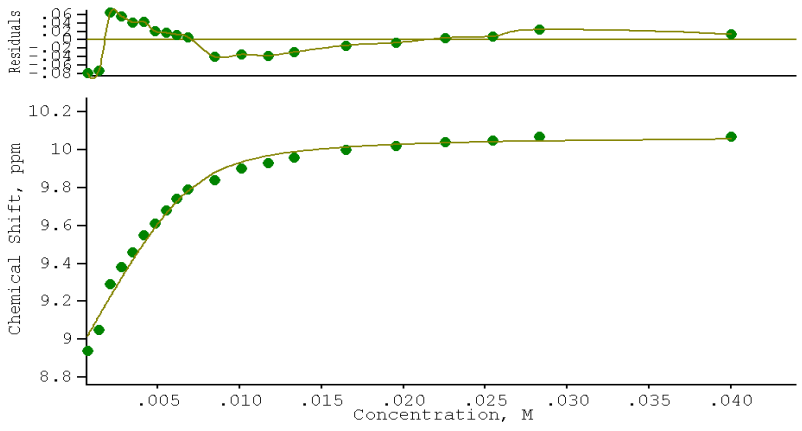


Figure S57: The experimental binding isotherms for ^{1}H NMR titration of **5** (Urea-NH) with $H_2PO_4^-$ in DMSO-*d6* and the corresponding fit using Win-Eq NMR.

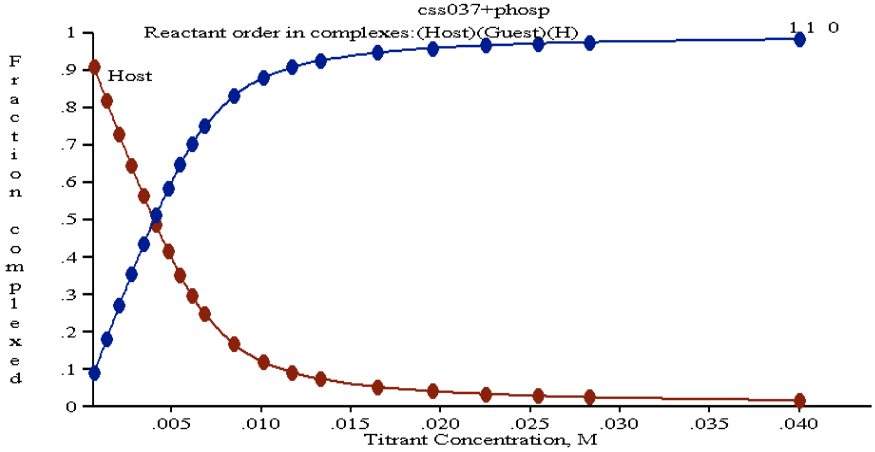


Figure S58: Speciation distribution diagram for the ^{1}H NMR titration of **5** (Urea-NH) with $H_2PO_4^-$.

NO. A PARAMETER DELTA ERROR CONDITION DESCRIPTION

1 1 3.24377E+00 1.000E-02 1.127E-01 4.249E+00 K ass

2 1 8.91235E+00 1.000E-02 2.679E-02 1.449E+00 shift free

3 1 1.00736E+01 1.000E-02 2.355E-02 3.588E+00 shift compl

0RMS ERROR = 4.17E-02 MAX ERROR = 7.87E-02 AT OBS.NO. 1

RESIDUALS SQUARED = 2.96E-02

RFACTOR = 0.3956 PERCENT

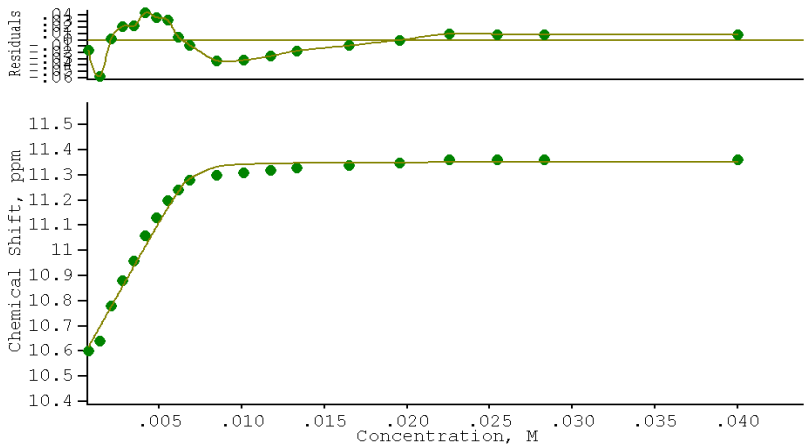


Figure S59: The experimental binding isotherms for ^{1}H NMR titration of **5** (Amido-NH) with $H_2PO_4^-$ in DMSO-*d6* and the corresponding fit using Win-Eq NMR.

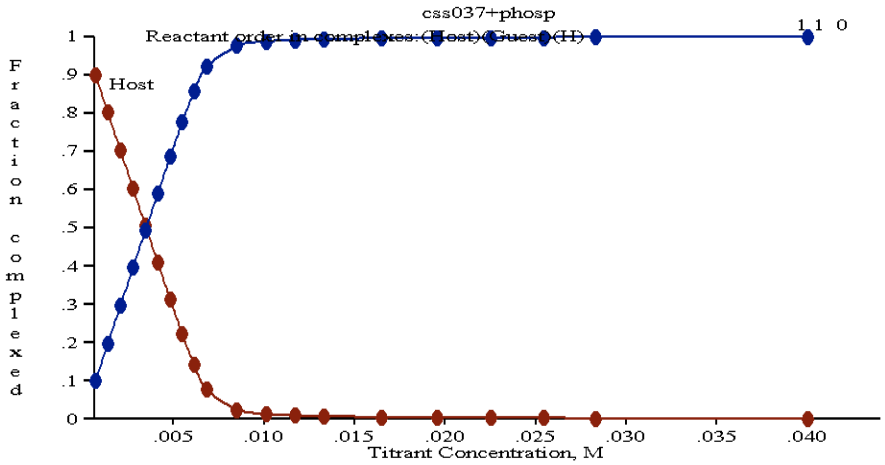


Figure S60: Speciation distribution diagram for the ^{1}H NMR titration of **5** (Amido-NH) with $H_2PO_4^-$.

NO. A PARAMETER DELTA ERROR CONDITION DESCRIPTION

1 1 4.33052E+00 1.000E-02 3.143E-01 2.043E+00 K ass

2 1 1.05358E+01 1.000E-02 1.664E-02 1.123E+00 shift free

3 1 1.13517E+01 1.000E-02 1.042E-02 2.019E+00 shift compl

0RMS ERROR = 2.68E-02 MAX ERROR = 5.72E-02 AT OBS.NO. 2

RESIDUALS SQUARED = 1.22E-02

RFACTOR = 0.2216 PERCENT

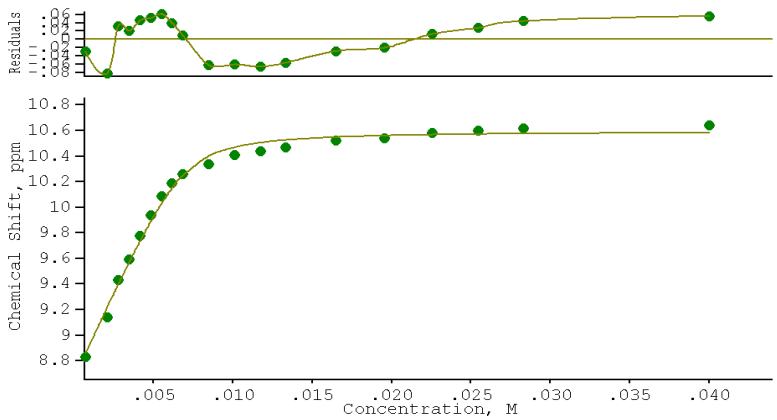


Figure S61: The experimental binding isotherms for ^{1}H NMR titration of **6** (Urea-NH) with $H_2PO_4^-$ in DMSO-*d6* and the corresponding fit using Win-Eq NMR.

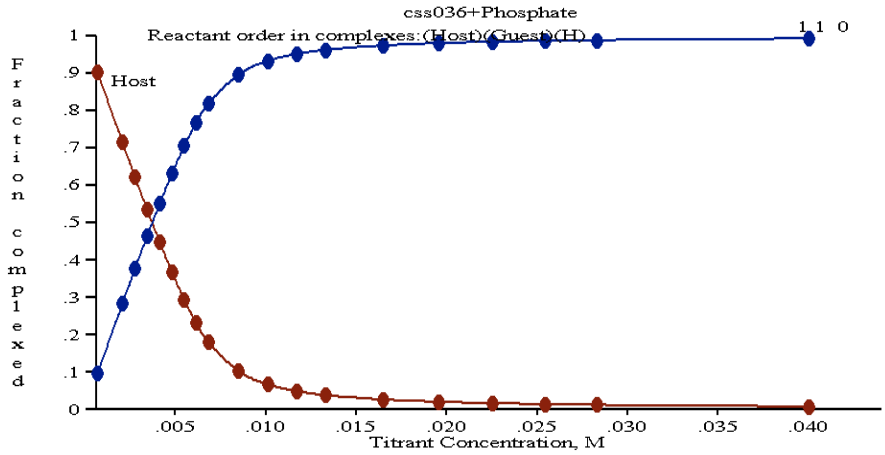


Figure S62: Speciation distribution diagram for the ^{1}H NMR titration of **6** (Urea-NH) with $H_2PO_4^-$.

NO. A PARAMETER DELTA ERROR CONDITION DESCRIPTION

1 1 3.56157E+00 1.000E-02 1.085E-01 3.449E+00 K ass

2 1 8.67462E+00 1.000E-02 3.668E-02 1.339E+00 shift free

3 1 1.05981E+01 1.000E-02 2.526E-02 3.030E+00 shift compl

0RMS ERROR = 5.06E-02 MAX ERROR = 8.11E-02 AT OBS.NO. 2

RESIDUALS SQUARED = 4.10E-02

RFACTOR = 0.4581 PERCENT

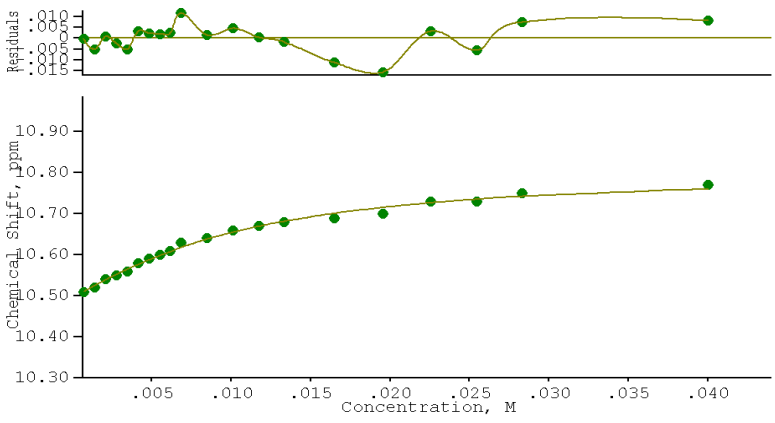


Figure S63: The experimental binding isotherms for ^{1}H NMR titration of **6** (Amido-NH) with $H_2PO_4^-$ in DMSO-*d6* and the corresponding fit using Win-Eq NMR.

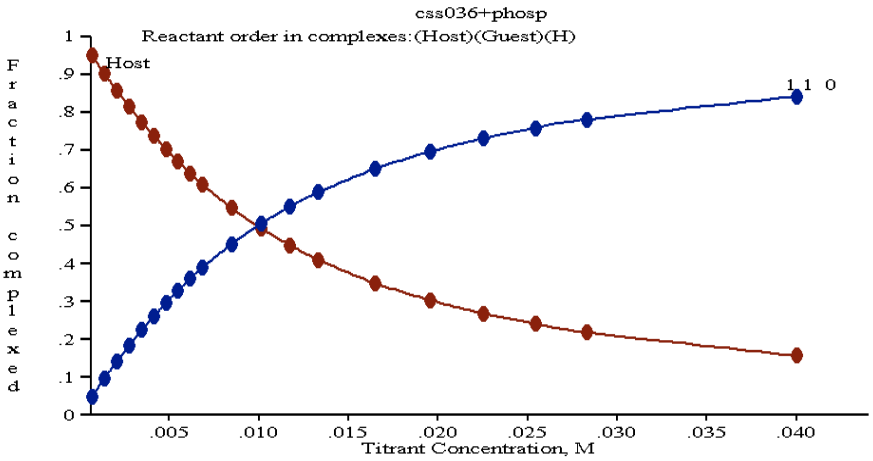


Figure S64: Speciation distribution diagram for the ^{1}H NMR titration of **6** (Amido-NH) with $H_2PO_4^-$.

NO. A PARAMETER DELTA ERROR CONDITION DESCRIPTION

1 1 2.18389E+00 1.000E-02 5.975E-02 2.090E+01 K ass

2 1 1.04945E+01 1.000E-02 4.398E-03 3.184E+00 shift free

3 1 1.08107E+01 1.000E-02 1.151E-02 1.443E+01 shift compl

0RMS ERROR = 6.74E-03 MAX ERROR = 1.55E-02 AT OBS.NO. 16

RESIDUALS SQUARED = 7.72E-04

RFACTOR = 0.0584 PERCENT

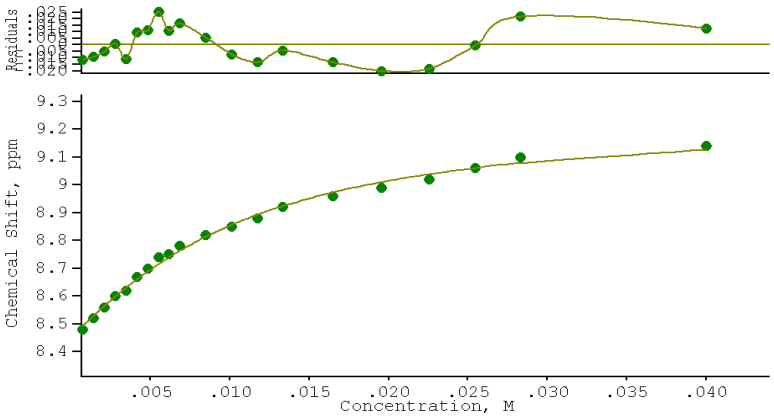


Figure S65: The experimental binding isotherms for ^{1}H NMR titration of **6** (Urea-NH) with Cl^- in DMSO-*d6* and the corresponding fit using Win-Eq NMR.

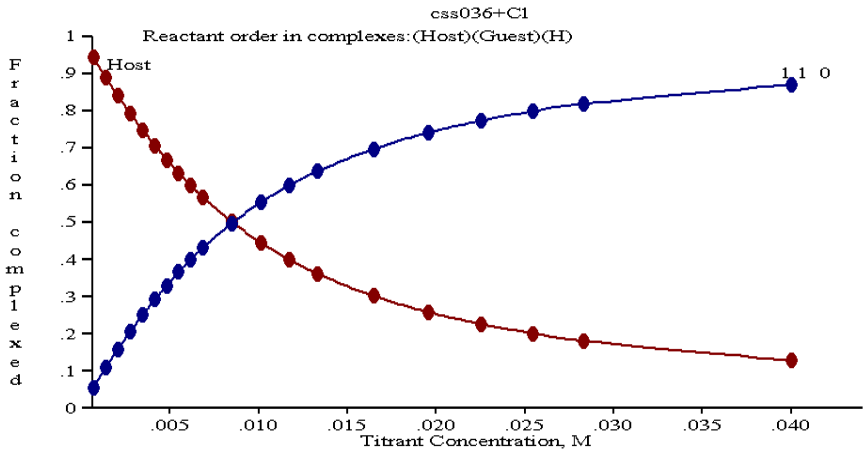


Figure S66: Speciation distribution diagram for the ^{1}H NMR titration of **6** (Urea-NH) with Cl^-.

NO. A PARAMETER DELTA ERROR CONDITION DESCRIPTION

1 1 2.18170E+00 1.000E-02 4.834E-02 1.922E+01 K ass

2 1 8.45122E+00 1.000E-02 9.241E-03 3.132E+00 shift free

3 1 9.25380E+00 1.000E-02 2.280E-02 1.317E+01 shift compl

0RMS ERROR = 1.42E-02 MAX ERROR = 2.52E-02 AT OBS.NO. 8

RESIDUALS SQUARED = 3.41E-03

RFACTOR = 0.1482 PERCENT

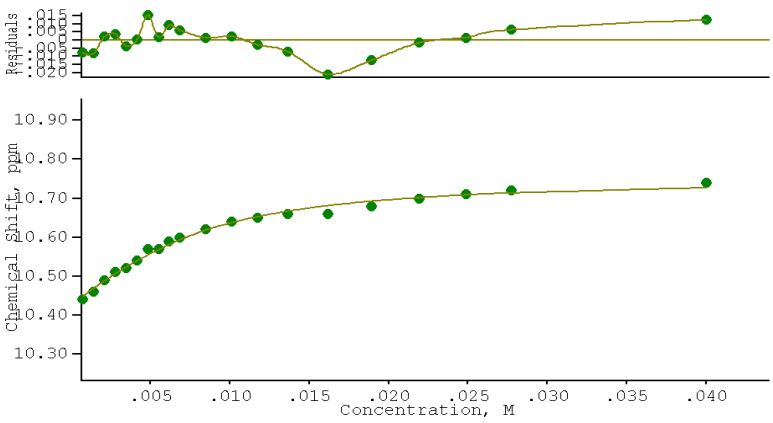


Figure S67: The experimental binding isotherms for ^{1}H NMR titration of **6** (Amido-NH) with Cl^- in DMSO-*d6* and the corresponding fit using Win-Eq NMR.

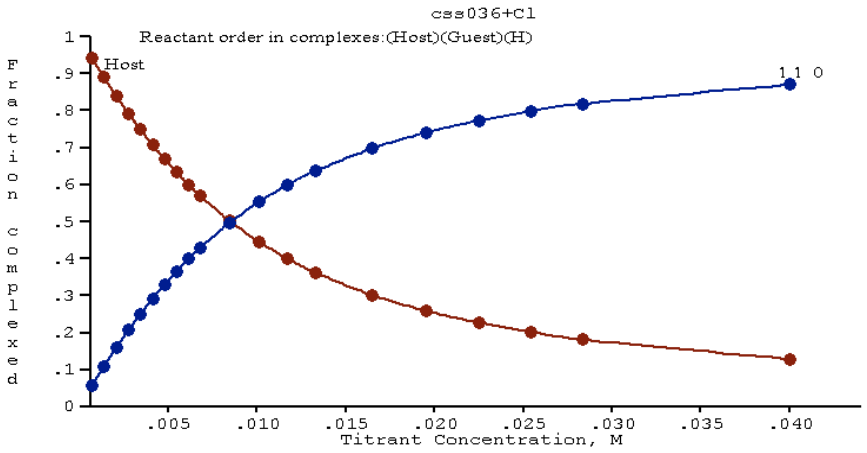


Figure S68: The calculated and observed isotopic distribution pattern (MALDI MS) for [**4** –H]$^-$ + AcO^- + K^+.

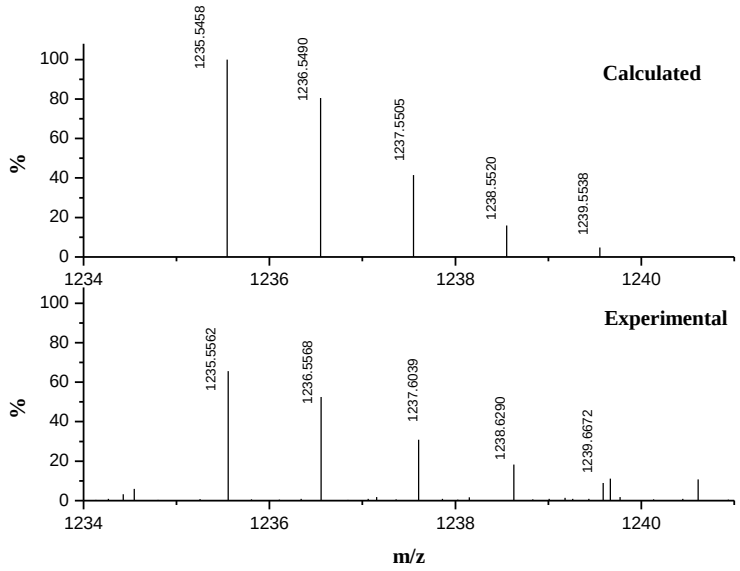


Figure S69: The calculated and observed isotopic distribution pattern (MALDI MS) for [**2** + H_2PO_4]$^-$.