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Catching chloride: searching for non-Hofmeister selectivity behavior in systematically varied polyamide macrocyclic receptors

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Contents

1. Binding data analysis

Table S1. Binding data for the studied receptors gathered from the literature [a]

Entry	Host	Ring-size	Linker	Titration method[b]	Solvent mixture			$K_{a.\ anion}$ (M^{-1})				K_{rel} = log ($K_{a.\ Cl^-}$ / K_{anion})			Ref.
					#1	#2	%#2 (v/v)	Cl^-	$H_2PO_4^-$	$MeCO_2^-$	$PhCO_2^-$	$H_2PO_4^-$	$MeCO_2^-$	$PhCO_2^-$	
1	Ac1	-	-	A	DMSO-d_6	-	0	12	-	45	-	n/a	-0.57	n/a	1
2	Ac2	-	-	A	DMSO-d_6	-	0	45	285	162	-	-0.80	-0.55	n/a	2
3	Ac3	-	-	A	DMSO-d_6	-	0	14	60	130	-	-0.63	-0.97	n/a	3
4	Ac4	-	-	A	DMSO-d_6	H_2O	5	5	150	-	13	-1.48	n/a	-0.41	4
5	Ac4	-	-	A	DMSO-d_6	MeOH	10	5	93	-	10	-1.27	n/a	-0.30	4
6	Ac5	-	-	B	MeCN	-	0	540000	31000	630000	-	1.24	-0.07	n/a	5
7	Ac5	-	-	B	DMSO	-	0	710	4200	2200	-	-0.77	-0.49	n/a	5
8	Ac6[c]	-	-	A	MeCN	-	0	1540	120	2410	-	1.11	-0.19	n/a	6
9	Ac7	-	-	A	Acetone	-	0	12000	-	4300	-	n/a	0.45	n/a	7
10	Ac8			B	MeCN	-	0	19000000	660000	-	-	1.46	n/a	n/a	8
11	M1	18	2	A	DMSO-d_6	-	0	65	1680	2640	-	-1.41	-1.61	n/a	1
12	M2	18	2	A	DMSO-d_6	-	0	390.5	2226	6331	-	-0.76	-1.21	n/a	9
13	M3	20	2	A	DMSO-d_6	-	0	204	617	-	260	-0.48	n/a	-0.11	10
14	M4	20	2	A	DMSO-d_6	-	0	29	327	-	-	-1.05	n/a	n/a	10
15	M5	18	2	A	DMSO-d_6	-	0	1100	3900	14000	-	-0.55	-1.10	n/a	11
16	M6	20	3	A	DMSO-d_6	-	0	1930	7410	3240	2283	-0.58	-0.22	-0.07	12
17	M6	20	3	A	DMSO-d_6	H_2O	5	373	575	-	292	-0.19	n/a	0.11	12
18	M7	20	3	A	DMSO-d_6	-	0	378	- [d]	3130		n/a	-0.92	n/a	13
19	M7	20	3	A	DMSO-d_6	H_2O	5	98	1320	-	169	-1.13	n/a	-0.24	13
20	M8	20	3	A	DMSO-d_6	MeOH	10	93	25000	-	13000	-2.43	n/a	-2.15	4
21	M9	20	3	A	DMSO-d_6	-	0	2148	8000	-	3612	-0.57	n/a	-0.23	14
22	M9	20	3	A	DMSO-d_6	H_2O	5	555	2680	-	666	-0.68	n/a	-0.08	14
23	M10	20	3	A	DMSO-d_6	H_2O	5	280	-	-	3700	n/a	n/a	-1.12	4
24	M10	20	3	A	DMSO-d_6	MeOH	10	270	4800	-	1700	-1.25	n/a	-0.80	4
25	M11	22	4	A	DMSO-d_6	-	0	296	573	552	302	-0.29	-0.27	-0.01	3
26	M12	24	5	A	DMSO-d_6	-	0	18	450	310	301	-1.40	-1.24	-1.22	12
27	M13	24	5	A	DMSO-d_6	-	0	48	- [d]	205	82	n/a	-0.63	-0.23	3
28	M14	24	2	A	DMSO-d_6	-	0	25	830	-	-	-1.52	n/a	n/a	15
29	M15	24	2	A	DMSO-d_6	-	0	490	11000	-	-	-1.35	n/a	n/a	15-16
30	M16	30	-	A	DMSO-d_6	-	0	28	1000	88	35	-1.55	-0.50	-0.10	17
31	M17	24	-	B	DMSO	-	0	4000	24000	3300	26300	-0.78	0.08	-0.82	18
32	M18	24	-	B	DMSO	-	0	19000	21000	43700	145000	-0.04	-0.36	-0.88	18
33	M19	22	-	B	MeCN	-	0	2000	342000	38000	64000	-2.23	-1.28	-1.51	19
34	M20	22	-	B	MeCN	-	0	116000	15500	67000	47000	0.87	0.24	0.39	20
35	M21 [e]	16	-	A	DMSO-d_6	-	0	100000	1400	140	-	1.85	2.85	n/a	21
36	M22 [e]	16	-	A	DMSO-d_6	-	0	270	15000	77000	-	-1.74	-2.46	n/a	21
37	M23	22	-	B	MeCN	-	0	11900000	4390000	15900000	-	0.43	-0.13	n/a	22
38	M23	22	-	B	MeCN	H_2O	5	995000	-	5430	-	n/a	2.26	n/a	22
39	M24	16	-	A	CD_2Cl_2	-	0	350	97	668	196	0.56	-0.28	0.25	23
40	M24 [e]	16	-	C	MeCN	-	0	140000	-	290000	115000	-	-0.31	0.09	24
41	M24 [e]	16	-	C	DMSO	-	0	1300	5100	6100	-	-0.59	-0.67	-	25
42	M25 [e]	16	-	C	MeCN	-	0	530000	-	1900000	1200000	-	-0.55	-0.35	25
43	M25 [e]	16	-	C	DMSO	-	0	1500	17000	48000	-	-1.05	-1.51	-	25
44	Uc1	22	2	A	DMSO-d_6	H_2O	0.5	96	- [d]	- [d]	95	n/a	n/a	0.00	26
45	Uc2	24	3	A	DMSO-d_6	H_2O	0.5	484	- [d]	490	269	n/a	-0.01	0.26	26
46	Uc3	24	3	A	DMSO-d_6	H_2O	0.5	778	1268	642	162	-0.21	0.08	0.68	26
47	Uc4	26	4	A	DMSO-d_6	H_2O	0.5	11	7286	191	128	-2.82	-1.24	-1.07	26
48	Uc5	26	4	A	DMSO-d_6	H_2O	0.5	9	1738	262	251	-2.29	-1.46	-1.45	27
49	Cr1	24	-	A	CD_2Cl_2	CD_3CN	75	40	25	770	-	0.20	-1.28	n/a	28
50	Cr2	24	2	A	DMSO-d_6	-	0	820	- [d]	46	-	n/a	1.25	n/a	29
51	Cr3	24	2	A	DMSO-d_6	-	0	2950	2040	2400	-	0.16	0.09	n/a	29, 30
52	Cr4	24	2	A	DMSO-d_6	-	0	35	2512	13000	-	-1.86	-2.57	n/a	30
53	Cr5	28	2	A	DMSO-d_6	-	0	180	170	130	-	0.02	0.14	n/a	31, 32

Table S1. Continuation.

Entry	Host	Ring-size	Linker	Titration method[b]	Solvent mixture			$K_{a.\ anion}$ (M^{-1})				K_{rel} = log ($K_{a.\ Cl^-}$ / K_{anion})			Ref.
					#1	#2	%#2 (v/v)	Cl^-	$H_2PO_4^-$	$MeCO_2^-$	$PhCO_2^-$	$H_2PO_4^-$	$MeCO_2^-$	$PhCO_2^-$	
55	Cr6	24.33	-	A	DMSO-d_6	-	0	350	- [d]	380	-	n/a	-0.04	n/a	31
56	Cr7	24.30	-	A	DMSO-d_6	-	0	10	740	100	-	-1.87	-1.00	n/a	32
57	Cr8	36	2	A	DMSO-d_6	-	0	850	760	1380	-	0.05	-0.21	n/a	33
58	Cr9 [e]	16.22	3	C	DMSO	H_2O	20	26000	10	10	-	3.41	3.41	n/a	34
59	Cr10 [e]	16.22	5	C	MeCN	-	0	2600000	2800	1600	6000	2.97	3.21	2.64	35
60	Cr11 [e]	16.22	3	C	MeCN	-	0	3500000	7700	-	2700	2.66	n/a	3.11	35
61	Cr12 [e]	16.23	4	C	MeCN	-	0	8700000	50000	-	55000	2.24	n/a	2.20	35
62	Cr13 [e]	16.24	5	C	MeCN	-	0	4000000	20000	280000	53000	2.30	1.15	1.88	35

[a] All titration experiments were conducted at 298K, if not otherwise stated; [b] A: ^{1}H NMR, B: UV-Vis, C: ITC; [c] temperature was not reported; [d] complex binding mode; [e] T = 303 K.

2. Crystal Data

2.1 Diffractometer and data collection

The x-ray measurements of **Uc1**·H_2O and **Uc1**·TBACl were performed at 100(2) K on a KM4CCD κ-axis diffractometer with graphite-monochromated MoK_α. The corresponding crystal was positioned at 62 mm from the CCD camera. 1200 (**Uc1**) or 750 (**Uc1**·TBACl) frames were measured at 1^o intervals with a counting time of 11 or 9 sec for **Uc1** and **Uc1**·TBACl, respectively. The data were corrected for Lorentz and polarization effects. Empirical correction for absorption was applied.[36] Data reduction and analysis were carried out with the Oxford Diffraction programs.[36-37]

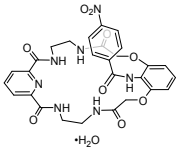
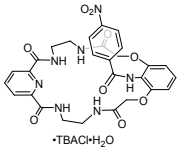
2.2 Structure refinement

The structure was solved by direct methods[38] and refined using WinGX[39] and SHELXL Software Package.[40]
The refinement was based on F^2 for all reflections except those with very negative F^2. Weighted R factors wR and all goodness-of-fit S values are based on F^2. Conventional R factors are based on F with F set to zero for negative F^2. The $F_o^2 > 2\sigma(F_o^2)$ criterion was used only for calculating R factors and is not relevant to the choice of reflections for the refinement. The R factors based on F^2 are about twice as large as those based on F. All hydrogen atoms were located geometrically and their position and temperature factors were not refined except those engaged in hydrogen bonds. Scattering factors were taken from Tables 6.1.1.4 and 4.2.4.2 in Ref. [41]. The H-bonds in crystal structure were determined according to IUPAC recommendation.[42]
The crystal structure of **Uc1** contains disordered *p*-nitrophenyl substituent and partially occupied solvent molecules such as disordered *n*-pentan, water, and methanol molecules. All of the oxygen-containing solvent molecules, except the water molecule located within macrocyclic cavity, were refinement without the hydrogen atoms. It is noteworthy that, the exact dimensions and cell volume should be probably doubled (i.e.: a = 8.214 Å, b = 19.363 Å, c = 23.930 Å, α = 109.07°, β = 97.28°, γ = 93.34°, V = 3547.71 Å^3) as compared to the data mentioned in the cif file. However, since the reflections proving this assumption were weak, the final structure was refinement as the average from two smaller elemental cells.
The crystal structure of **Uc1**·TBACl contains water molecule which is dislocated between two adjacent macrocycles. This results in incomplete hydrogen bond saturation of the water molecule which is engaged in just two, albeit strong, hydrogen bonds with the oxygen carbonyl atoms of the adjacent macrocyclic molecules.

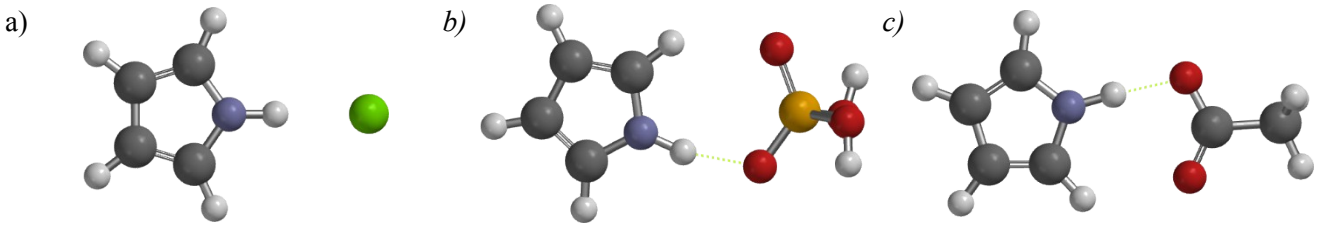
2.3 Crystallographic data

The structures discussed in this paper have been deposited with the Cambridge Crystallographic Data Centre. Copies of the data can be obtained, free of charge, on application to CCDC, 12 Union Road, Cambridge CB2 1EZ, UK [fax: +44(0)-1223-336033 or e-mail: deposit@ccdc.cam.ac.uk].

Tab. S2 Crystal data and structure refinement details for solvate (left) and TBACl complex (right) of **Uc1**.

Compound	**Uc1**·H_2O		**Uc1**·TBACl·H_2O	
Structure				
Empirical formula	$C_{30}H_{33.25}N_7O_{13.1}$		$C_{44}H_{65}ClN_8O_{10}$	
Moiety formula	$C_{28}H_{27}N_7O_8 \cdot H_2O$		$C_{28}H_{27}N_7O_8 \cdot C_{16}H_{36}NCl \cdot H_2O$	
Formula weight	701.49		901.49	
CCDC No.	1534255		1534256	
Temperature	100 K			
Wavelength	0.71073 Å (MoK_α)			
Crystal system	Triclinic		Monoclinic	
Space group	P-1		P21/c	
Unit cell dimensions	a = 8.2136(7) Å	α = 85.572(7) °	a = 9.9445(6) Å	α = 90.00 °
	b = 10.2940(9) Å	β = 88.689(9) °	b = 15.7022(8) Å	β = 98.244(5) °
	c = 22.413(2) Å	γ = 69.865(5) °	c = 30.3358(18) Å	γ = 90.00 °
Volume	V = 1773.9(3) Å^3		V = 4688.0(5) Å^3	
Z	2		4	
Density Calc.	1.313 g/cm^3		1.277 g/cm^3	
Absorption coefficient	0.105 mm^{-1}		0.146 mm^{-1}	
F(000)	734		1928	
Crystal	Prismatic, colorless		Prismatic, colorless	
Crystal size	0.71 × 0.53 × 0.24 mm		0.56× 0.35 × 0.21 mm	
θ range for data collection	2.76 – 28.62 °		2.68 – 28.66 °	
Index ranges	−11≤ h ≤11, −13≤ k ≤13, -30≤ l ≤29		−12≤ h ≤13, −21≤ k ≤21, -40≤ l ≤39	
Reflections collected (all/independent)	33596 / 7650 [R_{int} = 0.05]		11406 / 7415 [R_{int} = 0.033]	
Absorption correction	Multi-scan			
Refinement method	Full-matrix least-squares on F^2			
Data / restraints / parameters	8543/502/599		11406/0/838	
Goodness-of-fit on F^2	1.092		0.916	
Final R indices [$F^2 > 2\sigma(F^2)$]	R = 0.050, ωR = 0.163		R = 0.033, ωR = 0.073	
R indices (all data)	R = 0.068, ωR = 0.174		R = 0.062, ωR = 0.078	
Largest diff. peak and hole	0.579 and -0.498 e Å^{-3}		0.287 and -0.304 e Å^{-3}	

3. Visualization and Cartesian coordinates of calculated structures



Pyrrole@Cl^-
ΔE = -84.7 kJ/mol

Pyrrole@$H_2PO_4^-$
ΔE = -95.8 kJ/mol

Pyrrole@$MeCO_2^-$
ΔE = -120.4 kJ/mol

Fig. S21. Structures and relative energies of pyrrole with chloride (a), dihydrogenphosphate (b), and acetate (c) anions obtained at DFT/M06-2X/6-311G(d) level of theory; corresponding hydrogen bond interactions are $d_{N\cdots Cl^-}$ = 3.143, 2.756, and 2.737 Å, respectively.

Table S3. Cartesian coordinates of the structures of pyrrole, acetate, dihydrogenphosphate, and anion complexes with pyrrole calculated at DFT/M06-2X/6-311G(d) level of theory using program Spartan'16 Parallel Suite[43]

Pyrrole E = -210.122158 au E + ZPE = -670.337099 au				$MeCO_2^-$ E = -228.475980 au E + ZPE = -228.427217 au				$H_2PO_4^-$ E = -643.574252 au E + ZPE = -643.535888 au			
N	0.000000	0.000000	1.117622	C	0.220244	0.001583	0.000000	P	0.000000	0.000004	-0.174661
C	1.120010	0.000000	0.330394	O	0.689923	1.156582	0.000000	O	-0.883022	-0.990723	-0.848902
C	0.711051	0.000000	-0.979683	O	0.802227	-1.099097	0.000000	O	-0.964229	0.838773	0.883056
C	-0.711051	0.000000	-0.979683	C	-1.347137	-0.055435	0.000000	O	0.883018	0.990761	-0.848863
C	-1.120010	0.000000	0.330394	H	-1.715036	-1.083850	0.000000	O	0.964233	-0.838814	0.883014
H	2.106872	0.000000	0.765101	H	-1.730401	0.473540	-0.878782	H	1.746539	-0.302581	1.036738
H	1.358904	0.000000	-1.842493	H	-1.730401	0.473540	0.878782	H	-1.746541	0.302540	1.036747
H	-1.358904	0.000000	-1.842493								
H	-2.106872	0.000000	0.765101								
H	0.000000	0.000000	2.122901								

Pyrrole + Cl^- E = -670.420989 au E + ZPE = -670.337099 au				Pyrrole + $MeCO_2^-$ E = -438.645889 au E + ZPE = -438.511941 au				Pyrrole + $H_2PO_4^-$ E = -853.734493 au E + ZPE = -853.611268 au			
N	0.000000	0.000000	0.248273	N	1.028188	0.355076	0.000000	N	1.696177	-0.493211	0.025826
C	1.109423	0.000000	1.033500	C	2.121768	1.164623	0.000000	C	1.908739	0.845257	-0.100908
C	0.710715	0.000000	2.354524	C	3.254181	0.374394	0.000000	C	3.271124	1.064503	-0.094396
C	-0.710715	0.000000	2.354524	C	2.808171	-0.976209	0.000000	C	3.899187	-0.205107	0.040767
C	-1.109423	0.000000	1.033500	C	1.427387	-0.943293	0.000000	C	2.890297	-1.142783	0.110112
H	2.091853	0.000000	0.587072	H	2.012918	2.238884	-0.000000	H	1.056172	1.505946	-0.180646
H	1.362581	0.000000	3.216419	H	4.276710	0.726344	0.000000	H	3.759136	2.025117	-0.178286
H	-1.362581	0.000000	3.216419	H	3.423777	-1.864843	0.000000	H	4.960127	-0.408957	0.081286
H	-2.091853	0.000000	0.587072	H	0.672492	-1.714654	0.000000	H	2.930838	-2.216440	0.214316
H	0.000000	0.000000	-0.786973	H	0.024428	0.653610	0.000000	H	0.750371	-0.904841	0.045141
Cl	0.000000	0.000000	-2.894954	C	-2.228958	-0.039352	0.000000	P	-1.829538	0.030854	-0.009947
				O	-1.616009	1.062944	0.000000	O	-0.968782	-1.197469	0.009420
				O	-1.742851	-1.179803	0.000000	O	-2.924511	-0.201017	-1.214599
				C	-3.769078	0.086223	0.000000	O	-1.295923	1.414300	-0.118022
				H	-4.244680	-0.895172	0.000000	O	-2.777624	-0.029825	1.333821
				H	-4.086453	0.653426	-0.878934	H	-3.005976	0.870676	1.579962
				H	-4.086453	0.653426	0.878934	H	-2.962206	-1.140963	-1.411770

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