Appendices and Supporting Information

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1.1 Appendix A – Fluorescence titration data

1.1.1 G1.5 PAMAM Dendron

Volume Cyt-C added (µL)	Volume Cyt-C added (L)	Moles Added	Vol. (L) in Cuvette	[Cyt-c] in Cuvette	Absorbance (run 1)	Absorbance (run 2)	Absorbance (run 3)
000	0.00000	0.00E+00	0.00300	0.00E+00	39501	33972	32573
010	0.00001	5.00E-08	0.00301	1.66E-05	25459	22877	22177
020	0.00002	1.00E-07	0.00302	3.31E-05	17082	15534	15136
030	0.00003	1.50E-07	0.00303	4.95E-05	11820	10525	10567
040	0.00004	2.00E-07	0.00304	6.58E-05	8392	7479	7646
050	0.00005	2.50E-07	0.00305	8.20E-05	5963	5420	5423
060	0.00006	3.00E-07	0.00306	9.80E-05	4454	4003	4059
070	0.00007	3.50E-07	0.00307	1.14E-04	3315	2891	3024
080	0.00008	4.00E-07	0.00308	1.30E-04	2523	2277	2400
090	0.00009	4.50E-07	0.00309	1.46E-04	1875	1796	1928
100	0.00010	5.00E-07	0.00310	1.61E-04	1399	1530	1569
110	0.00011	5.50E-07	0.00311	1.77E-04	1197	1317	1304
120	0.00012	6.00E-07	0.00312	1.92E-04	969	1111	1173
130	0.00013	6.50E-07	0.00313	2.08E-04	825	979	962
140	0.00014	7.00E-07	0.00314	2.23E-04	743	915	902
150	0.00015	7.50E-07	0.00315	2.38E-04	671	844	934
160	0.00016	8.00E-07	0.00316	2.53E-04	643	807	869
170	0.00017	8.50E-07	0.00317	2.68E-04	604	814	868
180	0.00018	9.00E-07	0.00318	2.83E-04	598	759	870
190	0.00019	9.50E-07	0.00319	2.98E-04	603	776	780
200	0.00020	1.00E-06	0.00320	3.13E-04	585	778	843

1.1.2 G2.5 PAMAM Dendron

Volume Cyt-C added (µL)	Volume Cyt-C added (L)	Moles Added	Vol. (L) in Cuvette	[Cyt-c] in Cuvette	Absorbance (run 1)	Absorbance (run 2)
0	0	0	0.003	0	22024	20147
10	0.00001	0.00000005	0.00301	1.66113E-05	12512	12824
20	0.00002	0.0000001	0.00302	3.31126E-05	8396	8469
30	0.00003	0.00000015	0.00303	4.9505E-05	4778.57143	5776
40	0.00004	0.0000002	0.00304	6.57895E-05	3272	3984
50	0.00005	0.00000025	0.00305	8.19672E-05	2304	2915
60	0.00006	0.0000003	0.00306	9.80392E-05	1554	2030
70	0.00007	0.00000035	0.00307	0.000114007	1048	1493
80	0.00008	0.0000004	0.00308	0.00012987	834	1249
90	0.00009	0.00000045	0.00309	0.000145631	645	996
100	0.0001	0.0000005	0.0031	0.00016129	626	816
150	0.00015	0.00000075	0.00315	0.000238095	414	556
200	0.0002	0.000001	0.0032	0.0003125	396	530

Volume Cyt-C added (µL)	Volume Cyt-C added (L)	Moles Added	Vol. (L) in Cuvette	[Cyt-c] in Cuvette	Absorbance (run 3)
0	0	0	0.003	0	17921
10	0.00001	0.00000005	0.00301	1.66113E-05	12164
20	0.00002	0.0000001	0.00302	3.31126E-05	8532
30	0.00003	0.00000015	0.00303	4.9505E-05	5855
40	0.00004	0.0000002	0.00304	6.57895E-05	4516
50	0.00005	0.00000025	0.00305	8.19672E-05	3079
60	0.00006	0.0000003	0.00306	9.80392E-05	2434
70	0.00007	0.00000035	0.00307	0.000114007	1845
80	0.00008	0.0000004	0.00308	0.00012987	1512
90	0.00009	0.00000045	0.00309	0.000145631	1290
100	0.0001	0.0000005	0.0031	0.00016129	1056
110	0.00011	0.00000055	0.00311	0.000176849	926
120	0.00012	0.0000006	0.00312	0.000192308	852
130	0.00013	0.00000065	0.00313	0.000207668	799
140	0.00014	0.0000007	0.00314	0.00022293	759
150	0.00015	0.00000075	0.00315	0.000238095	746
200	0.0002	0.000001	0.0032	0.0003125	687

1.2 Appendix B – X-ray Crystallography data

X-ray crystallography data was collected and analysed by Harry Adams from the University of Sheffield.

1.2.1 Compound 8

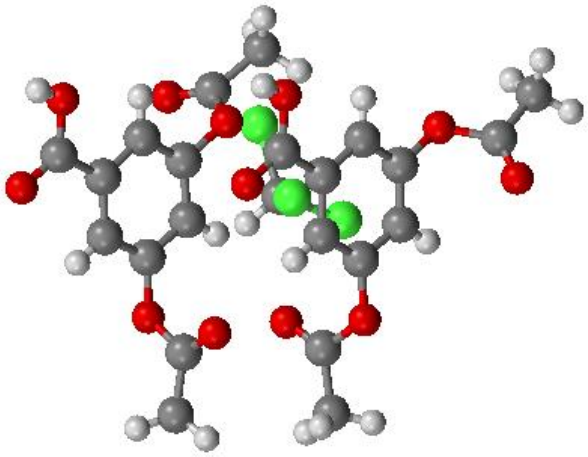


Table 1. Crystal data and structure refinement

Identification code	ilt1redo	
Empirical formula	C23 H19 Cl3 O12	
Formula weight	593.73	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 9.363(4) Å	α = 99.12(4)°.
	b = 9.477(4) Å	β = 95.23(4)°.
	c = 15.960(9) Å	γ = 110.10(3)°.
Volume	1296.9(11) $Å^3$	
Z	2	
Density (calculated)	1.520 Mg/m^3	
Absorption coefficient	0.416 mm^{-1}	
F(000)	608	
Crystal size	0.24 x 0.23 x 0.04 mm^3	
Theta range for data collection	1.31 to 27.78°.	
Index ranges	-12<=h<=11, -12<=k<=11, -20<=l<=20	
Reflections collected	14175	
Independent reflections	5855 [R(int) = 0.0885]	
Completeness to theta = 27.78°	95.5 %	

Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9835 and 0.9067
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5855 / 0 / 347
Goodness-of-fit on F^2	0.983
Final R indices [I>2sigma(I)]	R1 = 0.0647, wR2 = 0.1413
R indices (all data)	R1 = 0.1401, wR2 = 0.1740
Largest diff. peak and hole	0.508 and -0.552 e.$Å^{-3}$

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for ilt1redo. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	9742(3)	6316(3)	9512(2)	31(1)
O(2)	11777(3)	7010(3)	8835(2)	35(1)
O(3)	10808(3)	2492(3)	6447(2)	29(1)
O(4)	6577(3)	934(3)	8006(2)	27(1)
O(5)	10988(3)	449(3)	6945(2)	32(1)
O(6)	4991(3)	1931(3)	7380(2)	32(1)
C(1)	9825(4)	4556(4)	8303(2)	22(1)
C(2)	10620(4)	4220(4)	7654(2)	26(1)
C(3)	9986(4)	2798(4)	7109(2)	26(1)
C(4)	8625(4)	1711(4)	7193(2)	28(1)
C(5)	7864(4)	2074(4)	7848(2)	24(1)
C(6)	8453(4)	3494(4)	8410(2)	24(1)
C(7)	5159(4)	992(4)	7773(2)	24(1)
C(8)	3950(4)	-234(4)	8064(2)	31(1)
C(9)	11275(4)	1256(4)	6435(2)	26(1)
C(10)	12158(5)	1129(5)	5717(3)	37(1)
C(11)	10464(4)	6050(4)	8931(2)	26(1)
O(1A)	7282(3)	10410(3)	10021(2)	34(1)
O(2A)	9426(3)	11081(3)	9433(2)	29(1)
O(3A)	4311(3)	4944(3)	8426(2)	26(1)
O(4A)	8893(3)	6632(3)	7138(2)	27(1)
O(5A)	5548(3)	3950(3)	9316(2)	28(1)
O(6A)	7881(3)	7614(3)	6147(2)	35(1)
C(1A)	7543(4)	8617(4)	8869(2)	23(1)

C(2A)	6172(4)	7480(4)	8936(2)	23(1)
C(3A)	5719(4)	6071(4)	8385(2)	24(1)
C(4A)	6576(4)	5774(4)	7764(2)	28(1)
C(5A)	7921(4)	6934(4)	7711(2)	24(1)
C(6A)	8436(4)	8364(4)	8255(2)	25(1)
C(7A)	8800(4)	7069(4)	6368(2)	27(1)
C(8A)	9993(5)	6762(5)	5885(2)	35(1)
C(9A)	4370(5)	3936(4)	8953(2)	25(1)
C(10A)	2787(4)	2915(4)	9001(2)	30(1)
C(11A)	8079(4)	10117(4)	9490(2)	26(1)
C(1S)	5505(5)	3004(4)	4606(2)	34(1)
Cl(1)	5217(1)	1171(1)	4047(1)	50(1)
Cl(2)	6540(1)	3292(1)	5643(1)	53(1)
Cl(3)	6502(1)	4435(1)	4068(1)	51(1)

Table 3. Bond lengths [Å] and angles [°] for ilt1redo.

O(1)-C(11)	1.240(4)
O(2)-C(11)	1.293(4)
O(3)-C(9)	1.382(4)
O(3)-C(3)	1.413(4)
O(4)-C(7)	1.368(4)
O(4)-C(5)	1.390(4)
O(5)-C(9)	1.191(4)
O(6)-C(7)	1.211(4)
C(1)-C(6)	1.378(5)
C(1)-C(2)	1.389(5)
C(1)-C(11)	1.491(5)
C(2)-C(3)	1.382(5)
C(2)-H(2)	0.9500
C(3)-C(4)	1.370(5)
C(4)-C(5)	1.381(5)
C(4)-H(4)	0.9500
C(5)-C(6)	1.392(5)
C(6)-H(6)	0.9500
C(7)-C(8)	1.486(5)
C(8)-H(8A)	0.9800

C(8)-H(8B)	0.9800
C(8)-H(8C)	0.9800
C(9)-C(10)	1.486(5)
C(10)-H(10A)	0.9800
C(10)-H(10B)	0.9800
C(10)-H(10C)	0.9800
O(1A)-C(11A)	1.240(4)
O(2A)-C(11A)	1.300(4)
O(3A)-C(9A)	1.379(4)
O(3A)-C(3A)	1.398(4)
O(4A)-C(7A)	1.363(4)
O(4A)-C(5A)	1.412(4)
O(5A)-C(9A)	1.193(4)
O(6A)-C(7A)	1.200(4)
C(1A)-C(6A)	1.388(5)
C(1A)-C(2A)	1.391(5)
C(1A)-C(11A)	1.492(5)
C(2A)-C(3A)	1.380(5)
C(2A)-H(2A)	0.9500
C(3A)-C(4A)	1.386(5)
C(4A)-C(5A)	1.377(5)
C(4A)-H(4A)	0.9500
C(5A)-C(6A)	1.387(5)
C(6A)-H(6A)	0.9500
C(7A)-C(8A)	1.495(5)
C(8A)-H(8A1)	0.9800
C(8A)-H(8A2)	0.9800
C(8A)-H(8A3)	0.9800
C(9A)-C(10A)	1.482(5)
C(10A)-H(10D)	0.9800
C(10A)-H(10E)	0.9800
C(10A)-H(10F)	0.9800
C(1S)-Cl(1)	1.740(4)
C(1S)-Cl(3)	1.759(4)
C(1S)-Cl(2)	1.771(4)
C(1S)-H(1S)	1.0000

C(9)-O(3)-C(3)	117.4(3)

C(7)-O(4)-C(5)	118.3(3)
C(6)-C(1)-C(2)	121.0(3)
C(6)-C(1)-C(11)	117.9(3)
C(2)-C(1)-C(11)	121.0(3)
C(3)-C(2)-C(1)	118.1(4)
C(3)-C(2)-H(2)	120.9
C(1)-C(2)-H(2)	120.9
C(4)-C(3)-C(2)	122.7(4)
C(4)-C(3)-O(3)	120.3(3)
C(2)-C(3)-O(3)	117.0(3)
C(3)-C(4)-C(5)	117.9(3)
C(3)-C(4)-H(4)	121.1
C(5)-C(4)-H(4)	121.1
C(4)-C(5)-O(4)	118.8(3)
C(4)-C(5)-C(6)	121.6(3)
O(4)-C(5)-C(6)	119.2(3)
C(1)-C(6)-C(5)	118.7(4)
C(1)-C(6)-H(6)	120.7
C(5)-C(6)-H(6)	120.7
O(6)-C(7)-O(4)	122.0(3)
O(6)-C(7)-C(8)	127.8(3)
O(4)-C(7)-C(8)	110.2(3)
C(7)-C(8)-H(8A)	109.5
C(7)-C(8)-H(8B)	109.5
H(8A)-C(8)-H(8B)	109.5
C(7)-C(8)-H(8C)	109.5
H(8A)-C(8)-H(8C)	109.5
H(8B)-C(8)-H(8C)	109.5
O(5)-C(9)-O(3)	122.5(4)
O(5)-C(9)-C(10)	127.2(4)
O(3)-C(9)-C(10)	110.3(3)
C(9)-C(10)-H(10A)	109.5
C(9)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	109.5
C(9)-C(10)-H(10C)	109.5
H(10A)-C(10)-H(10C)	109.5
H(10B)-C(10)-H(10C)	109.5
O(1)-C(11)-O(2)	123.2(3)

O(1)-C(11)-C(1)	119.9(3)
O(2)-C(11)-C(1)	116.9(3)
C(9A)-O(3A)-C(3A)	115.9(3)
C(7A)-O(4A)-C(5A)	117.5(3)
C(6A)-C(1A)-C(2A)	121.3(3)
C(6A)-C(1A)-C(11A)	119.9(3)
C(2A)-C(1A)-C(11A)	118.8(3)
C(3A)-C(2A)-C(1A)	118.5(4)
C(3A)-C(2A)-H(2A)	120.7
C(1A)-C(2A)-H(2A)	120.7
C(2A)-C(3A)-C(4A)	121.9(3)
C(2A)-C(3A)-O(3A)	118.8(3)
C(4A)-C(3A)-O(3A)	119.2(3)
C(5A)-C(4A)-C(3A)	117.8(3)
C(5A)-C(4A)-H(4A)	121.1
C(3A)-C(4A)-H(4A)	121.1
C(4A)-C(5A)-C(6A)	122.5(4)
C(4A)-C(5A)-O(4A)	119.4(3)
C(6A)-C(5A)-O(4A)	117.8(3)
C(5A)-C(6A)-C(1A)	117.9(3)
C(5A)-C(6A)-H(6A)	121.1
C(1A)-C(6A)-H(6A)	121.1
O(6A)-C(7A)-O(4A)	122.8(4)
O(6A)-C(7A)-C(8A)	127.9(4)
O(4A)-C(7A)-C(8A)	109.3(3)
C(7A)-C(8A)-H(8A1)	109.5
C(7A)-C(8A)-H(8A2)	109.5
H(8A1)-C(8A)-H(8A2)	109.5
C(7A)-C(8A)-H(8A3)	109.5
H(8A1)-C(8A)-H(8A3)	109.5
H(8A2)-C(8A)-H(8A3)	109.5
O(5A)-C(9A)-O(3A)	123.0(3)
O(5A)-C(9A)-C(10A)	127.2(3)
O(3A)-C(9A)-C(10A)	109.8(3)
C(9A)-C(10A)-H(10D)	109.5
C(9A)-C(10A)-H(10E)	109.5
H(10D)-C(10A)-H(10E)	109.5
C(9A)-C(10A)-H(10F)	109.5

H(10D)-C(10A)-H(10F)	109.5
H(10E)-C(10A)-H(10F)	109.5
O(1A)-C(11A)-O(2A)	122.8(3)
O(1A)-C(11A)-C(1A)	121.7(3)
O(2A)-C(11A)-C(1A)	115.5(3)
Cl(1)-C(1S)-Cl(3)	112.1(2)
Cl(1)-C(1S)-Cl(2)	108.8(2)
Cl(3)-C(1S)-Cl(2)	110.1(2)
Cl(1)-C(1S)-H(1S)	108.6
Cl(3)-C(1S)-H(1S)	108.6
Cl(2)-C(1S)-H(1S)	108.6

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for ilt1redo. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	33(2)	29(2)	33(2)	4(1)	10(1)	11(1)
O(2)	30(2)	26(2)	40(2)	0(1)	11(1)	0(1)
O(3)	33(2)	28(2)	29(2)	8(1)	14(1)	12(1)
O(4)	23(2)	23(1)	37(2)	11(1)	10(1)	7(1)
O(5)	33(2)	29(2)	38(2)	12(1)	10(1)	12(1)
O(6)	30(2)	26(2)	38(2)	10(1)	1(1)	8(1)
C(1)	24(2)	17(2)	24(2)	4(1)	4(2)	7(2)
C(2)	21(2)	27(2)	29(2)	8(2)	4(2)	8(2)
C(3)	26(2)	28(2)	26(2)	6(2)	7(2)	12(2)
C(4)	29(2)	22(2)	30(2)	4(2)	4(2)	8(2)
C(5)	19(2)	25(2)	28(2)	7(2)	6(2)	6(2)
C(6)	28(2)	25(2)	24(2)	4(2)	6(2)	15(2)
C(7)	22(2)	24(2)	23(2)	-2(2)	6(2)	7(2)
C(8)	26(2)	28(2)	38(2)	8(2)	11(2)	8(2)
C(9)	21(2)	22(2)	30(2)	3(2)	2(2)	4(2)
C(10)	40(3)	40(3)	35(2)	6(2)	14(2)	19(2)
C(11)	28(2)	24(2)	28(2)	9(2)	5(2)	11(2)
O(1A)	36(2)	29(2)	33(2)	2(1)	15(1)	8(1)
O(2A)	25(2)	24(1)	34(2)	6(1)	10(1)	4(1)

O(3A)	25(1)	22(1)	28(1)	7(1)	0(1)	4(1)
O(4A)	30(2)	30(2)	24(1)	6(1)	8(1)	13(1)
O(5A)	26(2)	31(2)	29(2)	8(1)	4(1)	11(1)
O(6A)	35(2)	51(2)	26(2)	13(1)	7(1)	22(2)
C(1A)	27(2)	19(2)	22(2)	5(1)	3(2)	8(2)
C(2A)	25(2)	25(2)	21(2)	7(2)	8(2)	9(2)
C(3A)	24(2)	24(2)	25(2)	8(2)	4(2)	6(2)
C(4A)	34(2)	23(2)	22(2)	3(2)	-1(2)	8(2)
C(5A)	35(2)	25(2)	16(2)	3(1)	4(2)	15(2)
C(6A)	28(2)	22(2)	26(2)	6(2)	3(2)	10(2)
C(7A)	28(2)	24(2)	25(2)	0(2)	7(2)	4(2)
C(8A)	35(2)	37(2)	35(2)	5(2)	12(2)	14(2)
C(9A)	32(2)	22(2)	22(2)	3(2)	11(2)	10(2)
C(10A)	30(2)	25(2)	33(2)	8(2)	5(2)	6(2)
C(11A)	30(2)	22(2)	24(2)	6(2)	6(2)	8(2)
C(1S)	31(2)	33(2)	34(2)	-1(2)	9(2)	8(2)
Cl(1)	56(1)	39(1)	46(1)	-11(1)	-3(1)	18(1)
Cl(2)	59(1)	49(1)	33(1)	2(1)	0(1)	2(1)
Cl(3)	49(1)	51(1)	57(1)	23(1)	12(1)	17(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for ilt1redo.

	x	y	z	U(eq)
H(2)	11574	4948	7586	31
H(4)	8217	738	6813	33
H(6)	7919	3726	8859	29
H(8A)	4051	8	8692	46
H(8B)	4069	-1219	7883	46
H(8C)	2931	-298	7809	46
H(10A)	13255	1720	5920	55
H(10B)	11795	1535	5247	55
H(10C)	12006	50	5511	55
H(2A)	5560	7667	9352	28
H(4A)	6248	4802	7386	33
H(6A)	9370	9145	8209	30

H(8A1)	9824	6920	5298	52
H(8A2)	9917	5700	5868	52
H(8A3)	11019	7464	6174	52
H(10D)	2833	2064	9266	45
H(10E)	2195	2508	8420	45
H(10F)	2287	3499	9348	45
H(1S)	4478	3076	4669	41

1.2.2 Compound 11

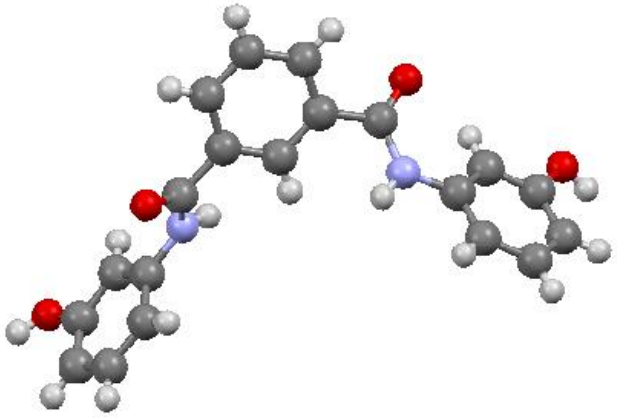


Table 1. Crystal data and structure refinement.

Identification code	iltgm1	
Empirical formula	C20 H16 N2 O4	
Formula weight	348.35	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 9.0833(8) Å	α = 103.777(3)°.
	b = 9.5341(8) Å	β = 90.893(3)°.
	c = 11.0670(9) Å	γ = 118.352(2)°.
Volume	809.85(12) $Å^3$	
Z	2	
Density (calculated)	1.429 Mg/m^3	
Absorption coefficient	0.101 mm^{-1}	
F(000)	364	
Crystal size	0.18 x 0.10 x 0.10 mm^3	
Theta range for data collection	2.53 to 27.52°.	
Index ranges	-11<=h<=11, -12<=k<=12, -14<=l<=13	
Reflections collected	10600	
Independent reflections	3561 [R(int) = 0.0416]	
Completeness to theta = 25.00°	99.3 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9900 and 0.9820	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3561 / 0 / 237	
Goodness-of-fit on F^2	1.045	

Final R indices [I>2sigma(I)]	R1 = 0.0449, wR2 = 0.0984
R indices (all data)	R1 = 0.0712, wR2 = 0.1108
Largest diff. peak and hole	0.383 and -0.427 e.Å^{-3}

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for iltgm1. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	6445(2)	4986(2)	-3733(1)	29(1)
O(2)	8055(2)	10167(2)	-700(1)	19(1)
O(3)	4738(2)	11650(2)	4891(1)	16(1)
O(4)	-2832(2)	8256(2)	3164(1)	20(1)
N(1)	2975(2)	9785(2)	3080(1)	15(1)
N(2)	7165(2)	8316(2)	474(1)	16(1)
C(1)	-1494(2)	7519(2)	4607(2)	16(1)
C(2)	-1443(2)	8230(2)	3641(2)	14(1)
C(3)	22(2)	8955(2)	3124(2)	15(1)
C(4)	1465(2)	8995(2)	3609(2)	14(1)
C(5)	4477(2)	11023(2)	3731(2)	13(1)
C(6)	5862(2)	11605(2)	2953(2)	14(1)
C(7)	6034(2)	10456(2)	2005(2)	14(1)
C(8)	7366(2)	10988(2)	1310(2)	15(1)
C(9)	7561(2)	9791(2)	265(2)	14(1)
C(10)	7137(2)	6927(2)	-378(2)	16(1)
C(11)	6863(2)	6644(2)	-1677(2)	19(1)
C(12)	6757(2)	5217(2)	-2466(2)	19(1)
C(13)	6965(2)	4102(2)	-1976(2)	20(1)
C(14)	7227(2)	4392(2)	-686(2)	21(1)
C(15)	7310(2)	5796(2)	123(2)	19(1)
C(16)	7030(2)	13293(2)	3199(2)	17(1)
C(17)	8336(2)	13823(2)	2494(2)	18(1)
C(18)	8508(2)	12680(2)	1546(2)	16(1)
C(19)	-43(2)	7548(2)	5064(2)	16(1)
C(20)	1448(2)	8282(2)	4569(2)	16(1)

Table 3. Bond lengths [Å] and angles [°] for iltgm1.

O(1)-C(12)	1.370(2)
O(1)-H(1)	0.8200
O(2)-C(9)	1.230(2)
O(3)-C(5)	1.246(2)
O(4)-C(2)	1.374(2)
O(4)-H(4)	0.8200
N(1)-C(5)	1.344(2)
N(1)-C(4)	1.430(2)
N(1)-H(1A)	0.8600
N(2)-C(9)	1.356(2)
N(2)-C(10)	1.420(2)
N(2)-H(2)	0.8600
C(1)-C(2)	1.385(3)
C(1)-C(19)	1.390(3)
C(1)-H(1B)	0.9300
C(2)-C(3)	1.384(2)
C(3)-C(4)	1.389(3)
C(3)-H(3)	0.9300
C(4)-C(20)	1.388(3)
C(5)-C(6)	1.493(2)
C(6)-C(7)	1.395(2)
C(6)-C(16)	1.397(2)
C(7)-C(8)	1.394(2)
C(7)-H(7)	0.9300
C(8)-C(18)	1.395(2)
C(8)-C(9)	1.496(2)
C(10)-C(15)	1.391(3)
C(10)-C(11)	1.393(3)
C(11)-C(12)	1.389(3)
C(11)-H(11)	0.9300
C(12)-C(13)	1.386(3)
C(13)-C(14)	1.382(3)
C(13)-H(13)	0.9300
C(14)-C(15)	1.389(3)
C(14)-H(14)	0.9300
C(15)-H(15)	0.9300
C(16)-C(17)	1.385(3)

C(16)-H(16)	0.9300
C(17)-C(18)	1.392(2)
C(17)-H(17)	0.9300
C(18)-H(18)	0.9300
C(19)-C(20)	1.389(3)
C(19)-H(19)	0.9300
C(20)-H(20)	0.9300

C(12)-O(1)-H(1)	109.5
C(2)-O(4)-H(4)	109.5
C(5)-N(1)-C(4)	125.41(15)
C(5)-N(1)-H(1A)	117.3
C(4)-N(1)-H(1A)	117.3
C(9)-N(2)-C(10)	127.13(15)
C(9)-N(2)-H(2)	116.4
C(10)-N(2)-H(2)	116.4
C(2)-C(1)-C(19)	119.18(17)
C(2)-C(1)-H(1B)	120.4
C(19)-C(1)-H(1B)	120.4
O(4)-C(2)-C(3)	117.27(16)
O(4)-C(2)-C(1)	121.64(16)
C(3)-C(2)-C(1)	121.09(17)
C(2)-C(3)-C(4)	118.81(17)
C(2)-C(3)-H(3)	120.6
C(4)-C(3)-H(3)	120.6
C(20)-C(4)-C(3)	121.36(17)
C(20)-C(4)-N(1)	120.75(16)
C(3)-C(4)-N(1)	117.89(16)
O(3)-C(5)-N(1)	124.15(16)
O(3)-C(5)-C(6)	121.20(15)
N(1)-C(5)-C(6)	114.65(15)
C(7)-C(6)-C(16)	119.53(16)
C(7)-C(6)-C(5)	120.05(15)
C(16)-C(6)-C(5)	120.38(15)
C(6)-C(7)-C(8)	120.28(16)
C(6)-C(7)-H(7)	119.9
C(8)-C(7)-H(7)	119.9
C(7)-C(8)-C(18)	119.78(16)

C(7)-C(8)-C(9)	121.57(16)
C(18)-C(8)-C(9)	118.58(16)
O(2)-C(9)-N(2)	124.15(16)
O(2)-C(9)-C(8)	120.62(16)
N(2)-C(9)-C(8)	115.23(15)
C(15)-C(10)-C(11)	120.32(17)
C(15)-C(10)-N(2)	117.82(16)
C(11)-C(10)-N(2)	121.78(17)
C(12)-C(11)-C(10)	119.29(18)
C(12)-C(11)-H(11)	120.4
C(10)-C(11)-H(11)	120.4
O(1)-C(12)-C(13)	122.60(16)
O(1)-C(12)-C(11)	116.61(17)
C(13)-C(12)-C(11)	120.78(17)
C(14)-C(13)-C(12)	119.37(17)
C(14)-C(13)-H(13)	120.3
C(12)-C(13)-H(13)	120.3
C(13)-C(14)-C(15)	120.88(18)
C(13)-C(14)-H(14)	119.6
C(15)-C(14)-H(14)	119.6
C(14)-C(15)-C(10)	119.33(18)
C(14)-C(15)-H(15)	120.3
C(10)-C(15)-H(15)	120.3
C(17)-C(16)-C(6)	120.18(16)
C(17)-C(16)-H(16)	119.9
C(6)-C(16)-H(16)	119.9
C(16)-C(17)-C(18)	120.38(16)
C(16)-C(17)-H(17)	119.8
C(18)-C(17)-H(17)	119.8
C(17)-C(18)-C(8)	119.83(17)
C(17)-C(18)-H(18)	120.1
C(8)-C(18)-H(18)	120.1
C(20)-C(19)-C(1)	120.86(18)
C(20)-C(19)-H(19)	119.6
C(1)-C(19)-H(19)	119.6
C(4)-C(20)-C(19)	118.68(17)
C(4)-C(20)-H(20)	120.7
C(19)-C(20)-H(20)	120.7

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for iltgm1. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	48(1)	17(1)	14(1)	3(1)	6(1)	11(1)
O(2)	22(1)	20(1)	14(1)	6(1)	6(1)	9(1)
O(3)	15(1)	18(1)	14(1)	3(1)	3(1)	8(1)
O(4)	15(1)	29(1)	17(1)	8(1)	5(1)	12(1)
N(1)	14(1)	18(1)	12(1)	4(1)	5(1)	8(1)
N(2)	21(1)	20(1)	10(1)	5(1)	5(1)	11(1)
C(1)	16(1)	16(1)	14(1)	4(1)	7(1)	8(1)
C(2)	14(1)	15(1)	14(1)	1(1)	1(1)	8(1)
C(3)	18(1)	16(1)	12(1)	5(1)	3(1)	9(1)
C(4)	14(1)	14(1)	13(1)	1(1)	4(1)	6(1)
C(5)	15(1)	14(1)	15(1)	6(1)	4(1)	10(1)
C(6)	14(1)	18(1)	12(1)	6(1)	2(1)	9(1)
C(7)	15(1)	14(1)	15(1)	4(1)	1(1)	8(1)
C(8)	14(1)	18(1)	14(1)	4(1)	2(1)	9(1)
C(9)	12(1)	18(1)	14(1)	5(1)	2(1)	7(1)
C(10)	13(1)	16(1)	17(1)	4(1)	4(1)	6(1)
C(11)	22(1)	18(1)	18(1)	7(1)	4(1)	9(1)
C(12)	19(1)	18(1)	14(1)	3(1)	6(1)	5(1)
C(13)	20(1)	16(1)	23(1)	3(1)	6(1)	9(1)
C(14)	24(1)	18(1)	23(1)	6(1)	1(1)	11(1)
C(15)	19(1)	20(1)	16(1)	5(1)	1(1)	9(1)
C(16)	19(1)	16(1)	16(1)	2(1)	3(1)	10(1)
C(17)	16(1)	16(1)	19(1)	5(1)	3(1)	4(1)
C(18)	15(1)	20(1)	15(1)	7(1)	4(1)	8(1)
C(19)	21(1)	14(1)	14(1)	5(1)	4(1)	9(1)
C(20)	16(1)	17(1)	17(1)	3(1)	2(1)	9(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2 x\ 10^3$)

for iltgm1.

	x	y	z	U(eq)
H(1)	6118	4013	-4108	43
H(4)	-3406	8301	3721	29
H(1A)	2918	9439	2280	18
H(2)	6901	8210	1203	19
H(1B)	-2487	7029	4944	19
H(3)	40	9408	2464	18
H(7)	5257	9331	1835	17
H(11)	6753	7402	-2012	23
H(13)	6928	3167	-2510	24
H(14)	7350	3638	-354	25
H(15)	7479	5979	990	23
H(16)	6931	14063	3838	21
H(17)	9102	14950	2655	22
H(18)	9382	13042	1071	19
H(19)	-71	7070	5710	20
H(20)	2415	8295	4875	20

1.2.3 Compound 12

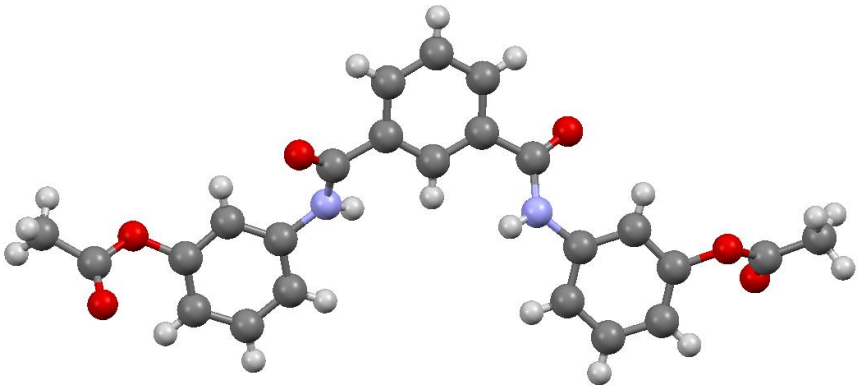


Table 1. Crystal data and structure refinement

Identification code	oltgmann1_0m	
Empirical formula	C24 H20 N2 O6	
Formula weight	432.42	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C2/c	
Unit cell dimensions	a = 29.4335(18) Å	α = 90°.
	b = 8.5428(5) Å	β = 103.117(3)°.
	c = 8.3216(5) Å	γ = 90°.
Volume	2037.8(2) $Å^3$	
Z	4	
Density (calculated)	1.409 Mg/m^3	
Absorption coefficient	0.103 mm^{-1}	
F(000)	904	
Crystal size	0.43 x 0.21 x 0.10 mm^3	
Theta range for data collection	1.42 to 27.51°.	
Index ranges	-38<=h<=37, -11<=k<=11, -10<=l<=10	
Reflections collected	14356	
Independent reflections	2336 [R(int) = 0.0655]	
Completeness to theta = 27.51°	99.2 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9898 and 0.9572	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2336 / 0 / 147	
Goodness-of-fit on F^2	0.908	

Final R indices [I>2sigma(I)]	R1 = 0.0430, wR2 = 0.1213
R indices (all data)	R1 = 0.0530, wR2 = 0.1311
Largest diff. peak and hole	0.377 and -0.208 e.Å^{-3}

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for oltgmann1_0m. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	3164(1)	7209(1)	3690(1)	32(1)
O(2)	2998(1)	8679(1)	1381(1)	27(1)
O(3)	4354(1)	11680(1)	634(1)	19(1)
N(1)	4262(1)	9715(1)	-1274(1)	17(1)
C(1)	2920(1)	8141(2)	2834(2)	23(1)
C(2)	3368(1)	8068(2)	752(2)	21(1)
C(3)	3641(1)	9181(2)	206(2)	19(1)
C(4)	3978(1)	8661(2)	-613(2)	17(1)
C(5)	4429(1)	11110(2)	-647(2)	15(1)
C(6)	4726(1)	11950(2)	-1612(2)	16(1)
C(7)	5000	11138(2)	-2500	15(1)
C(8)	2495(1)	8890(2)	3180(2)	31(1)
C(9)	4737(1)	13582(2)	-1579(2)	21(1)
C(10)	5000	14392(2)	-2500	24(1)
C(11)	4027(1)	7075(2)	-899(2)	22(1)
C(12)	3753(1)	5992(2)	-305(2)	27(1)
C(13)	3421(1)	6480(2)	535(2)	26(1)

Table 3. Bond lengths [Å] and angles [°] for oltgmann1_0m.

O(1)-C(1)	1.195(2)
O(2)-C(1)	1.3610(18)
O(2)-C(2)	1.4105(17)
O(3)-C(5)	1.2355(16)
N(1)-C(5)	1.3482(18)
N(1)-C(4)	1.4214(17)
N(1)-H(1)	0.8600

C(1)-C(8)	1.491(2)
C(2)-C(13)	1.382(2)
C(2)-C(3)	1.3867(19)
C(3)-C(4)	1.3967(18)
C(3)-H(3)	0.9300
C(4)-C(11)	1.389(2)
C(5)-C(6)	1.4989(17)
C(6)-C(9)	1.395(2)
C(6)-C(7)	1.3953(15)
C(7)-C(6)#1	1.3953(15)
C(7)-H(7)	0.9300
C(8)-H(8A)	0.9600
C(8)-H(8B)	0.9600
C(8)-H(8C)	0.9600
C(9)-C(10)	1.3903(17)
C(9)-H(9)	0.9300
C(10)-C(9)#1	1.3903(17)
C(10)-H(10)	0.9300
C(11)-C(12)	1.388(2)
C(11)-H(11)	0.9300
C(12)-C(13)	1.388(2)
C(12)-H(12)	0.9300
C(13)-H(13)	0.9300

C(1)-O(2)-C(2)	120.34(12)
C(5)-N(1)-C(4)	127.22(11)
C(5)-N(1)-H(1)	116.4
C(4)-N(1)-H(1)	116.4
O(1)-C(1)-O(2)	123.68(14)
O(1)-C(1)-C(8)	126.09(14)
O(2)-C(1)-C(8)	110.22(13)
C(13)-C(2)-C(3)	122.58(13)
C(13)-C(2)-O(2)	122.17(13)
C(3)-C(2)-O(2)	114.91(13)
C(2)-C(3)-C(4)	118.04(13)
C(2)-C(3)-H(3)	121.0
C(4)-C(3)-H(3)	121.0
C(11)-C(4)-C(3)	120.44(13)

C(11)-C(4)-N(1)	117.31(12)
C(3)-C(4)-N(1)	122.14(12)
O(3)-C(5)-N(1)	124.17(12)
O(3)-C(5)-C(6)	120.90(12)
N(1)-C(5)-C(6)	114.93(11)
C(9)-C(6)-C(7)	119.58(13)
C(9)-C(6)-C(5)	118.80(12)
C(7)-C(6)-C(5)	121.60(12)
C(6)#1-C(7)-C(6)	120.38(17)
C(6)#1-C(7)-H(7)	119.8
C(6)-C(7)-H(7)	119.8
C(1)-C(8)-H(8A)	109.5
C(1)-C(8)-H(8B)	109.5
H(8A)-C(8)-H(8B)	109.5
C(1)-C(8)-H(8C)	109.5
H(8A)-C(8)-H(8C)	109.5
H(8B)-C(8)-H(8C)	109.5
C(10)-C(9)-C(6)	119.98(13)
C(10)-C(9)-H(9)	120.0
C(6)-C(9)-H(9)	120.0
C(9)-C(10)-C(9)#1	120.34(18)
C(9)-C(10)-H(10)	119.8
C(9)#1-C(10)-H(10)	119.8
C(12)-C(11)-C(4)	119.86(13)
C(12)-C(11)-H(11)	120.1
C(4)-C(11)-H(11)	120.1
C(13)-C(12)-C(11)	120.68(14)
C(13)-C(12)-H(12)	119.7
C(11)-C(12)-H(12)	119.7
C(2)-C(13)-C(12)	118.33(14)
C(2)-C(13)-H(13)	120.8
C(12)-C(13)-H(13)	120.8

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,y,-z-1/2

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for oltgmann1_0m. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	41(1)	29(1)	29(1)	5(1)	14(1)	10(1)
O(2)	25(1)	29(1)	31(1)	7(1)	17(1)	5(1)
O(3)	26(1)	17(1)	19(1)	-1(1)	13(1)	0(1)
N(1)	22(1)	17(1)	16(1)	0(1)	12(1)	-1(1)
C(1)	25(1)	20(1)	25(1)	-2(1)	10(1)	-3(1)
C(2)	19(1)	25(1)	22(1)	0(1)	10(1)	0(1)
C(3)	21(1)	17(1)	20(1)	0(1)	8(1)	1(1)
C(4)	20(1)	17(1)	17(1)	0(1)	7(1)	-3(1)
C(5)	16(1)	15(1)	16(1)	3(1)	7(1)	3(1)
C(6)	19(1)	15(1)	15(1)	1(1)	7(1)	1(1)
C(7)	18(1)	12(1)	16(1)	0	5(1)	0
C(8)	27(1)	39(1)	31(1)	3(1)	15(1)	4(1)
C(9)	29(1)	16(1)	23(1)	-1(1)	14(1)	3(1)
C(10)	36(1)	10(1)	29(1)	0	17(1)	0
C(11)	25(1)	18(1)	29(1)	-2(1)	15(1)	-1(1)
C(12)	31(1)	17(1)	37(1)	-4(1)	17(1)	-6(1)
C(13)	27(1)	23(1)	32(1)	0(1)	15(1)	-7(1)

Table 5. Hydrogen coordinates ($x\ 10^4$) and isotropic displacement parameters ($Å^2 x\ 10^3$) for oltgmann1_0m.

	x	y	z	U(eq)
H(1)	4335	9432	-2174	21
H(3)	3601	10242	382	23
H(7)	5000	10050	-2500	18
H(8A)	2251	8123	3081	46
H(8B)	2393	9719	2403	46
H(8C)	2566	9309	4279	46
H(9)	4569	14129	-940	25
H(10)	5000	15480	-2500	28

H(11)	4242	6739	-1486	27
H(12)	3793	4929	-472	32
H(13)	3240	5756	941	31

1.3 Appendix C – ^{1}HNMR Titration data

1.3.1 Tetrabutylammonium fluoride

Core

Run 1		
[H] mmol	**[G] mmol**	**δ NH**
1	0	0
0.972	0.278	1.75
0.946	0.541	3.18
0.933	0.667	3.43
0.921	0.789	3.58
0.909	0.909	3.7
0.897	1.026	3.77
0.886	1.139	3.84

Run 2		
[H] mmol	**[G] mmol**	**δ NH**
1	0	0
0.986	0.141	0.85
0.972	0.278	1.7
0.959	0.411	2.59
0.946	0.541	3.12
0.933	0.667	3.39
0.921	0.789	3.54
0.909	0.909	3.64
0.897	1.026	3.71
0.886	1.139	3.76

1:1 HBP (Mn – 1600)

Run 1		
[H] mmol	**[G] mmol**	**δ NH**
5	0	0
4.795	1.027	1.27
4.605	1.974	2.57
4.516	2.419	2.89
4.43	2.848	3.09
4.348	3.261	3.22
4.268	3.659	3.3
4.192	4.042	3.34
4.118	4.412	3.4
4.046	4.769	3.45
3.977	5.114	3.49
3.911	5.447	3.52

Run 2		
[H] mmol	**[G] mmol**	**δ NH**
5	0	0
4.795	1.027	1.21
4.605	1.974	2.49
4.516	2.419	2.8
4.43	2.848	3
4.348	3.261	3.15
4.268	3.659	3.24
4.192	4.042	3.3
4.118	4.412	3.34
4.046	4.769	3.38
3.977	5.114	3.42
3.911	5.447	3.45

1:5 HBP (Mn – 4000)

Run 1		
[H] mmol	**[G] mmol**	**δ NH**
5	0	0
4.93	0.704	1.1
4.861	1.389	1.73
4.795	2.055	2.26
4.73	2.703	2.55
4.667	3.333	2.73
4.605	3.947	2.89
4.545	4.545	3.01
4.487	5.128	3.1
4.43	5.696	3.17
4.375	6.25	3.21

Run 2		
[H] mmol	**[G] mmol**	**δ NH**
5	0	0
4.93	0.704	1.1
4.861	1.389	1.83
4.795	2.055	2.37
4.73	2.703	2.67
4.667	3.333	2.88
4.605	3.947	3.05
4.545	4.545	3.16
4.487	5.128	3.24
4.43	5.696	3.3
4.375	6.25	3.36

1:20 HBP (Mn – 10343)

Run 1		
[H] mmol	**[G] mmol**	**δ NH**
5	0	0
4.93	0.704	0.64
4.861	1.389	1.02
4.795	2.055	1.38
4.73	2.703	1.71
4.667	3.333	2
4.605	3.947	2.21
4.545	4.545	2.38
4.487	5.128	2.53
4.43	5.696	2.63
4.375	6.25	2.7
4.321	6.79	2.75
4.242	7.576	2.84
4.167	8.333	2.89
4.07	9.302	2.96
3.977	10.227	3.04
3.889	11.111	3.11

Run 2		
[H] mmol	**[G] mmol**	**δ NH**
5	0	0
4.861	1.389	1.06
4.73	2.703	1.73
4.667	3.333	2.01
4.605	3.947	2.23
4.545	4.545	2.38
4.487	5.128	2.52
4.43	5.696	2.6
4.375	6.25	2.66
4.321	6.79	2.72
4.242	7.576	2.8
4.167	8.333	2.85
4.07	9.302	2.93
3.977	10.227	3.01
3.889	11.111	3.05

1.3.2 Tetrabutylammonium chloride

Core

Run 1		
[H] mmol	**[G] mmol**	**δ NH**
1	0	0
0.972	0.278	0.83
0.946	0.541	1.81
0.933	0.667	2.17
0.921	0.789	2.42
0.909	0.909	2.57
0.897	1.026	2.66
0.886	1.139	2.72
0.875	1.25	2.75

Run 2		
[H] mmol	**[G] mmol**	**δ NH**
1	0	0
0.972	0.278	0.76
0.946	0.541	1.69
0.933	0.667	2.07
0.921	0.789	2.34
0.909	0.909	2.51
0.897	1.026	2.62
0.886	1.139	2.69
0.875	1.25	2.73

1:1 HBP (Mn – 1600)

Run 1		
[H] mmol	**[G] mmol**	**δ NH**
5	0	0
4.895	0.524	0.41
4.795	1.027	0.85
4.698	1.51	1.28
4.605	1.974	1.64
4.516	2.419	1.96
4.43	2.848	2.2
4.348	3.261	2.35
4.268	3.659	2.43
4.217	3.916	2.47
4.167	4.167	2.5
4.118	4.412	2.52
4.07	4.651	2.54
3.977	5.114	2.56

Run 2		
[H] mmol	**[G] mmol**	**δ NH**
5	0	0
4.895	0.524	0.34
4.795	1.027	0.79
4.698	1.51	1.24
4.605	1.974	1.64
4.516	2.419	1.94
4.43	2.848	2.19
4.348	3.261	2.34
4.217	3.916	2.46
4.118	4.412	2.51
3.977	5.114	2.55

1:5 HBP (Mn – 4000)

Run 1		
[H] mmol	**[G] mmol**	**δ NH**
5	0	0
4.92957746	0.70422535	1.04
4.86111111	1.38888889	1.84
4.79452055	2.05479452	2.18
4.72972973	2.7027027	2.36
4.66666667	3.33333333	2.45
4.60526316	3.94736842	2.51
4.54545455	4.54545455	2.54
4.48717949	5.12820513	2.56
4.43037975	5.69620253	2.58
4.375	6.25	2.59

Run 2		
[H] mmol	**[G] mmol**	**δ NH**
5	0	0
4.92957746	0.70422535	1.25
4.86111111	1.38888889	2.01
4.79452055	2.05479452	2.33
4.72972973	2.7027027	2.45
4.66666667	3.33333333	2.51
4.60526316	3.94736842	2.55
4.54545455	4.54545455	2.57
4.48717949	5.12820513	2.59
4.43037975	5.69620253	2.6
4.375	6.25	2.61

1:20 HBP (Mn – 10343)

TBAC		
Run 1		
[H] mmol	**[G] mmol**	**δ NH**
5	0	0
4.92957746	0.70422535	0.77
4.86111111	1.38888889	1.38
4.79452055	2.05479452	1.8
4.72972973	2.7027027	2.03
4.66666667	3.33333333	2.19
4.60526316	3.94736842	2.31
4.54545455	4.54545455	2.39
4.48717949	5.12820513	2.44
4.43037975	5.69620253	2.48

Run 2		
[H] mmol	**[G] mmol**	**δ NH**
5	0	0
4.92957746	0.70422535	0.75
4.86111111	1.38888889	1.35
4.79452055	2.05479452	1.77
4.72972973	2.7027027	2.01
4.66666667	3.33333333	2.17
4.60526316	3.94736842	2.28
4.54545455	4.54545455	2.36
4.48717949	5.12820513	2.42
4.43037975	5.69620253	2.46

1.3.3 Tetrabutylammonium bromide

Core

Run 1		
[H] mmol	**[G] mmol**	**δ NH**
5	0	0
4.8951049	0.52447552	0.27
4.79452055	1.02739726	0.54
4.69798658	1.51006711	0.8
4.60526316	1.97368421	1.06
4.51612903	2.41935484	1.31
4.43037975	2.84810127	1.53
4.34782609	3.26086957	1.74
4.26829268	3.65853659	1.9
4.19161677	4.04191617	2.03
4.11764706	4.41176471	2.13
4.04624277	4.76878613	2.21
3.97727273	5.11363636	2.26
3.91061453	5.44692737	2.3
3.84615385	5.76923077	2.38
3.78378378	6.08108108	2.36
3.72340426	6.38297872	2.38
3.60824742	6.95876289	2.41
3.5	7.5	2.44
3.33333333	8.33333333	2.46
3.18181818	9.09090909	2.48

Run 2		
[H] mmol	**[G] mmol**	**δ NH**
5	0	0
4.79452055	1.02739726	0.58
4.60526316	1.97368421	1.11
4.43037975	2.84810127	1.58
4.26829268	3.65853659	1.94
4.19161677	4.04191617	2.07
4.11764706	4.41176471	2.16
4.04624277	4.76878613	2.24
3.97727273	5.11363636	2.29
3.91061453	5.44692737	2.33
3.84615385	5.76923077	2.36
3.78378378	6.08108108	2.38
3.72340426	6.38297872	2.4
3.60824742	6.95876289	2.43
3.5	7.5	2.45
3.33333333	8.33333333	2.47
3.18181818	9.09090909	2.49

1:1 HBP (Mn – 1600)

Run 1		
[H] mmol	**[G] mmol**	**δ NH**
5	0	0
4.79452055	1.02739726	0.6
4.60526316	1.97368421	1.22
4.43037975	2.84810127	1.63
4.34782609	3.26086957	1.76
4.26829268	3.65853659	1.86
4.19161677	4.04191617	1.93
4.11764706	4.41176471	1.98
4.04624277	4.76878613	2.02
3.97727273	5.11363636	2.05
3.91061453	5.44692737	2.07
3.84615385	5.76923077	2.1
3.72340426	6.38297872	2.13
3.60824742	6.95876289	2.15

Run 2		
[H] mmol	**[G] mmol**	**δ NH**
5	0	0
4.79452055	1.02739726	0.59
4.60526316	1.97368421	1.23
4.43037975	2.84810127	1.63
4.26829268	3.65853659	1.86
4.11764706	4.41176471	1.99
4.04624277	4.76878613	2.04
3.97727273	5.11363636	2.07
3.91061453	5.44692737	2.09
3.84615385	5.76923077	2.11
3.78378378	6.08108108	2.13
3.72340426	6.38297872	2.15
3.60824742	6.95876289	2.16

1:5 HBP (Mn – 4000)

Run 1		
[H] mmol	**[G] mmol**	**δ NH**
5	0	0
4.92957746	0.70422535	0.89
4.86111111	1.38888889	1.48
4.79452055	2.05479452	1.78
4.72972973	2.7027027	1.94
4.66666667	3.33333333	2.02
4.60526316	3.94736842	2.08
4.54545455	4.54545455	2.13
4.48717949	5.12820513	2.15
4.43037975	5.69620253	2.18
4.375	6.25	2.19
4.24242424	7.57575758	2.22
4.11764706	8.82352941	2.24

Run 2		
[H] mmol	**[G] mmol**	**δ NH**
5	0	0
4.92957746	0.70422535	0.89
4.86111111	1.38888889	1.48
4.79452055	2.05479452	1.74
4.72972973	2.7027027	1.9
4.66666667	3.33333333	1.98
4.60526316	3.94736842	2.04
4.54545455	4.54545455	2.09
4.48717949	5.12820513	2.11
4.43037975	5.69620253	2.14
4.375	6.25	2.15
4.24242424	7.57575758	2.19
4.11764706	8.82352941	2.21

1:20 HBP (Mn – 10343)

Run 1		
[H] mmol	**[G] mmol**	**δ NH**
5	0	0
4.8951049	1.04895105	0.88
4.79452055	2.05479452	1.38
4.69798658	3.02013423	1.68
4.60526316	3.94736842	1.86
4.51612903	4.83870968	1.97
4.43037975	5.69620253	2.03
4.34782609	6.52173913	2.08
4.26829268	7.31707317	2.11
4.19161677	8.08383234	2.15
4.11764706	8.82352941	2.17
4	10	2.19

Run 2		
[H] mmol	**[G] mmol**	**δ NH**
5	0	0
4.8951049	1.04895105	0.9
4.79452055	2.05479452	1.45
4.69798658	3.02013423	1.72
4.60526316	3.94736842	1.86
4.51612903	4.83870968	1.96
4.43037975	5.69620253	2.02
4.34782609	6.52173913	2.07
4.26829268	7.31707317	2.1
4.19161677	8.08383234	2.13

1.3.4 Tetrabutylammonium iodide

Core

Run 1		
[H] mmol	**[G] mmol**	**δ NH**
5	0	0
4.79452055	1.02739726	0.44
4.60526316	1.97368421	0.77
4.43037975	2.84810127	1.03
4.26829268	3.65853659	1.23
4.19161677	4.04191617	1.31
4.11764706	4.41176471	1.38
4.04624277	4.76878613	1.45
3.97727273	5.11363636	1.5
3.91061453	5.44692737	1.54
3.84615385	5.76923077	1.6
3.78378378	6.08108108	1.63
3.72340426	6.38297872	1.66
3.60824742	6.95876289	1.69
3.5	7.5	1.74
3.33333333	8.33333333	1.8
3.04347826	9.7826087	1.9
2.8	11	1.97

Run 2		
[H] mmol	**[G] mmol**	**δ NH**
5	0	0
4.79452055	1.02739726	0.37
4.60526316	1.97368421	0.7
4.43037975	2.84810127	0.96
4.26829268	3.65853659	1.17
4.19161677	4.04191617	1.26
4.11764706	4.41176471	1.33
4.04624277	4.76878613	1.4
3.97727273	5.11363636	1.46
3.91061453	5.44692737	1.51
3.84615385	5.76923077	1.56
3.78378378	6.08108108	1.6
3.72340426	6.38297872	1.63
3.60824742	6.95876289	1.69
3.5	7.5	1.74
3.33333333	8.33333333	1.81
3.04347826	9.7826087	1.91
2.8	11	1.97

1:1 HBP (Mn – 1600)

Run 1		
[H] mmol	**[G] mmol**	**δ NH**
5	0	0
4.79452055	1.02739726	0.35
4.60526316	1.97368421	0.68
4.43037975	2.84810127	1
4.26829268	3.65853659	1.19
4.11764706	4.41176471	1.32
4.04624277	4.76878613	1.37
3.97727273	5.11363636	1.42
3.91061453	5.44692737	1.46
3.84615385	5.76923077	1.5
3.78378378	6.08108108	1.53
3.72340426	6.38297872	1.56
3.60824742	6.95876289	1.61
3.5	7.5	1.65
3.33333333	8.33333333	1.71
3.18181818	9.09090909	1.76

Run 2		
[H] mmol	**[G] mmol**	**δ NH**
5	0	0
4.79452055	1.02739726	0.36
4.60526316	1.97368421	0.67
4.43037975	2.84810127	0.95
4.26829268	3.65853659	1.13
4.11764706	4.41176471	1.25
4.04624277	4.76878613	1.31
3.97727273	5.11363636	1.36
3.91061453	5.44692737	1.4
3.84615385	5.76923077	1.44
3.78378378	6.08108108	1.47
3.72340426	6.38297872	1.5
3.60824742	6.95876289	1.55
3.5	7.5	1.59
3.33333333	8.33333333	1.65
3.18181818	9.09090909	1.7

1:5 HBP (Mn – 4000)

Run 1		
[H] mmol	**[G] mmol**	**δ NH**
5	0	0
4.8951049	1.04895105	0.58
4.79452055	2.05479452	0.91
4.69798658	3.02013423	1.12
4.60526316	3.94736842	1.29
4.51612903	4.83870968	1.37
4.43037975	5.69620253	1.45
4.34782609	6.52173913	1.51
4.26829268	7.31707317	1.55
4.19161677	8.08383234	1.59
4.11764706	8.82352941	1.62

Run 2		
[H] mmol	**[G] mmol**	**δ NH**
5	0	0
4.8951049	1.04895105	0.5
4.79452055	2.05479452	0.86
4.69798658	3.02013423	1.1
4.60526316	3.94736842	1.27
4.51612903	4.83870968	1.37
4.43037975	5.69620253	1.44
4.34782609	6.52173913	1.51
4.26829268	7.31707317	1.55
4.19161677	8.08383234	1.59
4.11764706	8.82352941	1.61

1:20 HBP (Mn – 10343)

Run 1		
[H] mmol	**[G] mmol**	**δ NH**
5	0	0
4.79452055	1.02739726	0.35
4.60526316	1.97368421	0.68
4.43037975	2.84810127	1
4.26829268	3.65853659	1.19
4.11764706	4.41176471	1.32
4.04624277	4.76878613	1.37
3.97727273	5.11363636	1.42
3.91061453	5.44692737	1.46
3.84615385	5.76923077	1.5
3.78378378	6.08108108	1.53
3.72340426	6.38297872	1.56
3.60824742	6.95876289	1.61
3.5	7.5	1.65
3.33333333	8.33333333	1.71

Run 2		
[H] mmol	**[G] mmol**	**δ NH**
5	0	0
4.8951049	1.04895105	0.39
4.79452055	2.05479452	0.7
4.69798658	3.02013423	0.89
4.60526316	3.94736842	1.05
4.51612903	4.83870968	1.16
4.43037975	5.69620253	1.24
4.34782609	6.52173913	1.32
4.26829268	7.31707317	1.37
4.19161677	8.08383234	1.42
4.11764706	8.82352941	1.45
4.04624277	9.53757225	1.48
3.97727273	10.2272727	1.51
3.88888889	11.1111111	1.53

Run 3		
[H] mmol	**[G] mmol**	**δ NH**
5	0	0
4.79452055	1.02739726	0.36
4.60526316	1.97368421	0.67
4.43037975	2.84810127	0.95
4.26829268	3.65853659	1.13
4.11764706	4.41176471	1.25
4.04624277	4.76878613	1.31
3.97727273	5.11363636	1.36
3.91061453	5.44692737	1.4
3.84615385	5.76923077	1.44
3.78378378	6.08108108	1.47
3.72340426	6.38297872	1.5
3.60824742	6.95876289	1.55
3.5	7.5	1.59

1.3.5 Tetrabutylammonium benzoate

Core

Run 1		
[H] mmol	**[G] mmol**	**δ NH**
1	0	0
0.972222222	0.27777778	0.66
0.95890411	0.4109589	1.07
0.945945946	0.54054054	1.48
0.933333333	0.66666667	1.87
0.921052632	0.78947368	2.21
0.909090909	0.90909091	2.49
0.897435897	1.02564103	2.68
0.886075949	1.13924051	2.83
0.875	1.25	2.94
0.864197531	1.35802469	3.03
0.853658537	1.46341463	3.11
0.843373494	1.56626506	3.16
0.833333333	1.66666667	3.21
0.823529412	1.76470588	3.25

Run 2		
[H] mmol	**[G] mmol**	**δ NH**
1	0	0
0.933333333	0.66666667	1.9
0.921052632	0.78947368	2.32
0.909090909	0.90909091	2.61
0.897435897	1.02564103	2.81
0.886075949	1.13924051	2.94
0.875	1.25	3.04
0.864197531	1.35802469	3.11
0.853658537	1.46341463	3.18
0.843373494	1.56626506	3.23
0.833333333	1.66666667	3.27
0.823529412	1.76470588	3.3

1:1 HBP (Mn – 1600)

Run 1		
[H] mmol	**[G] mmol**	**δ NH**
5	0	0
4.794520548	1.02739726	0.87
4.605263158	1.97368421	1.77
4.430379747	2.84810127	2.46
4.347826087	3.26086957	2.69
4.268292683	3.65853659	2.86
4.191616766	4.04191617	2.98
4.117647059	4.41176471	3.07
4.046242775	4.76878613	3.14
3.977272727	5.11363636	3.19
3.910614525	5.44692737	3.23
3.846153846	5.76923077	3.27

Run 2		
[H] mmol	**[G] mmol**	**δ NH**
5	0	0
4.794520548	1.02739726	0.85
4.605263158	1.97368421	1.8
4.430379747	2.84810127	2.49
4.347826087	3.26086957	2.72
4.268292683	3.65853659	2.89
4.191616766	4.04191617	3.01
4.117647059	4.41176471	3.09
4.046242775	4.76878613	3.16
3.977272727	5.11363636	3.21
3.910614525	5.44692737	3.25
3.846153846	5.76923077	3.28

1:5 HBP (Mn – 4000)

Run 1		
[H] mmol	**[G] mmol**	**δ NH**
10	0	0
9.79020979	2.0979021	1.14
9.589041096	4.10958904	2.09
9.395973154	6.04026846	2.66
9.210526316	7.89473684	3.01
9.032258065	9.67741935	3.23
8.860759494	11.3924051	3.35
8.588957055	14.1104294	3.44
8.484848485	15.1515152	3.46
8.235294118	17.6470588	3.5
7.777777778	22.2222222	3.55

Run 2		
[H] mmol	**[G] mmol**	**δ NH**
5	0	0
4.895104895	1.04895105	1.14
4.794520548	2.05479452	2.01
4.72972973	2.7027027	2.43
4.666666667	3.33333333	2.74
4.605263158	3.94736842	2.94
4.545454545	4.54545455	3.07
4.487179487	5.12820513	3.15
4.430379747	5.69620253	3.24
4.375	6.25	3.3
4.242424242	7.57575758	3.37

1:20 HBP (Mn – 10343)

Run 1		
[H] mmol	**[G] mmol**	**δ NH**
5	0	0
4.794520548	2.05479452	1.04
4.605263158	3.94736842	1.88
4.430379747	5.69620253	2.53
4.347826087	6.52173913	2.76
4.268292683	7.31707317	2.95
4.191616766	8.08383234	3.07
4.117647059	8.82352941	3.16
4.046242775	9.53757225	3.23
3.977272727	10.2272727	3.28
3.910614525	10.8938547	3.32
3.846153846	11.5384615	3.36
3.76344086	12.3655914	3.4

Run 2		
[H] mmol	**[G] mmol**	**δ NH**
5	0	0
4.794520548	2.05479452	0.9
4.605263158	3.94736842	1.82
4.430379747	5.69620253	2.47
4.347826087	6.52173913	2.73
4.268292683	7.31707317	2.93
4.191616766	8.08383234	3.06
4.117647059	8.82352941	3.14
4.046242775	9.53757225	3.23
3.977272727	10.2272727	3.28
3.910614525	10.8938547	3.32
3.846153846	11.5384615	3.36
3.76344086	12.3655914	3.4

1.3.6 Tetrabutylammonium acetate

Core

Run 1		
[H] mmol	**[G] mmol**	**δ NH**
1	0	0
0.95890411	0.4109589	1.01
0.921052632	0.78947368	2.08
0.903225806	0.96774194	2.43
0.886075949	1.13924051	2.67
0.875	1.25	2.79
0.864197531	1.35802469	2.9
0.853658537	1.46341463	3.02
0.843373494	1.56626506	3.08
0.833333333	1.66666667	3.13
0.823529412	1.76470588	3.17
0.813953488	1.86046512	3.21
0.804597701	1.95402299	3.23
0.795454545	2.04545455	3.26
0.777777778	2.22222222	3.3
0.736842105	2.63157895	3.38

Run 2		
[H] mmol	**[G] mmol**	**δ NH**
1	0	0
0.979020979	0.20979021	0.43
0.95890411	0.4109589	1.05
0.939597315	0.60402685	1.62
0.921052632	0.78947368	2.1
0.903225806	0.96774194	2.45
0.886075949	1.13924051	2.7
0.875	1.25	2.82
0.864197531	1.35802469	2.92
0.853658537	1.46341463	3
0.843373494	1.56626506	3.06
0.833333333	1.66666667	3.11
0.823529412	1.76470588	3.16
0.813953488	1.86046512	3.19
0.804597701	1.95402299	3.22
0.795454545	2.04545455	3.25
0.777777778	2.22222222	3.3
0.736842105	2.63157895	3.38

1:1 HBP (Mn – 1600)

Run 1		
[H] mmol	**[G] mmol**	**δ NH**
5	0	0
4.795	1.027	0.74
4.605	1.974	1.53
4.43	2.848	2.07
4.268	3.659	2.52
4.118	4.412	2.85
4.046	4.769	2.94
3.977	5.114	3.01
3.911	5.447	3.06
3.846	5.769	3.1
3.784	6.081	3.14
3.723	6.383	3.17
3.608	6.959	3.21
3.5	7.5	3.25
3.333	8.333	3.29

Run 2		
[H] mmol	**[G] mmol**	**δ NH**
5	0	0
4.794520548	1.02739726	0.73
4.605263158	1.97368421	1.49
4.430379747	2.84810127	2.15
4.268292683	3.65853659	2.58
4.117647059	4.41176471	2.83
4.046242775	4.76878613	2.92
3.977272727	5.11363636	2.99
3.910614525	5.44692737	3.04
3.846153846	5.76923077	3.07
3.783783784	6.08108108	3.11
3.723404255	6.38297872	3.15
3.608247423	6.95876289	3.21
3.5	7.5	3.24
3.333333333	8.33333333	3.28

1:5 HBP (Mn – 4000)

Run 1		
[H] mmol	**[G] mmol**	**δ NH**
5	0	0
4.895104895	1.04895105	1.13
4.794520548	2.05479452	1.86
4.697986577	3.02013423	2.38
4.605263158	3.94736842	2.7
4.516129032	4.83870968	2.91
4.430379747	5.69620253	3.04
4.347826087	6.52173913	3.13
4.268292683	7.31707317	3.2
4.117647059	8.82352941	3.27

Run 2		
[H] mmol	**[G] mmol**	**δ NH**
5	0	0
4.895104895	1.04895105	1.12
4.794520548	2.05479452	1.82
4.697986577	3.02013423	2.35
4.605263158	3.94736842	2.7
4.516129032	4.83870968	2.9
4.430379747	5.69620253	3.04
4.347826087	6.52173913	3.14
4.268292683	7.31707317	3.2
4.117647059	8.82352941	3.28

1:20 HBP (Mn – 10343)

Run 1		
[H] mmol	**[G] mmol**	**δ NH**
5	0	0
4.895104895	1.04895105	0.44
4.794520548	2.05479452	0.82
4.697986577	3.02013423	1.11
4.605263158	3.94736842	1.42
4.516129032	4.83870968	1.73
4.430379747	5.69620253	2.02
4.347826087	6.52173913	2.27
4.268292683	7.31707317	2.48
4.191616766	8.08383234	2.64
4.117647059	8.82352941	2.78
4.046242775	9.53757225	2.89
3.977272727	10.2272727	2.96
3.910614525	10.8938547	3.03
3.846153846	11.5384615	3.1
3.76344086	12.3655914	3.17
3.684210526	13.1578947	3.21
3.58974359	14.1025641	3.26
3.5	15	3.29

Run 2		
[H] mmol	**[G] mmol**	**δ NH**
5	0	0
4.794520548	2.05479452	0.88
4.605263158	3.94736842	1.51
4.430379747	5.69620253	1.97
4.347826087	6.52173913	2.23
4.268292683	7.31707317	2.47
4.191616766	8.08383234	2.63
4.117647059	8.82352941	2.79
4.046242775	9.53757225	2.91
3.977272727	10.2272727	2.97
3.910614525	10.8938547	3.04
3.846153846	11.5384615	3.1
3.76344086	12.3655914	3.17
3.684210526	13.1578947	3.21
3.58974359	14.1025641	3.26
3.5	15	3.29

1.3.7 Tetrabutylammonium dihydrogen phosphate

Core

1:1 HBP (Mn – 1600)

Run 1		
[H] mmol	**[G] mmol**	**δ NH**
5	0	0
4.794520548	1.02739726	0.49
4.605263158	1.97368421	1.09
4.430379747	2.84810127	1.67
4.268292683	3.65853659	2.17
4.191616766	4.04191617	2.37
4.117647059	4.41176471	2.55
4.046242775	4.76878613	2.7
3.977272727	5.11363636	2.83
3.910614525	5.44692737	2.93
3.846153846	5.76923077	3.01
3.783783784	6.08108108	3.08
3.723404255	6.38297872	3.14
3.608247423	6.95876289	3.23
3.5	7.5	3.29
3.333333333	8.33333333	3.36
3.181818182	9.09090909	3.42

Run 2		
[H] mmol	**[G] mmol**	**δ NH**
5	0	0
4.794520548	1.02739726	0.49
4.605263158	1.97368421	1.09
4.430379747	2.84810127	1.66
4.268292683	3.65853659	2.15
4.191616766	4.04191617	2.35
4.117647059	4.41176471	2.53
4.046242775	4.76878613	2.69
3.977272727	5.11363636	2.82
3.910614525	5.44692737	2.93
3.846153846	5.76923077	3.02
3.783783784	6.08108108	3.08
3.723404255	6.38297872	3.14
3.608247423	6.95876289	3.23
3.5	7.5	3.3
3.333333333	8.33333333	3.37
3.181818182	9.09090909	3.43

Run 1		
[H] mmol	**[G] mmol**	**δ NH**
5	0	0
4.794520548	1.02739726	0.45
4.605263158	1.97368421	0.87
4.430379747	2.84810127	1.37
4.268292683	3.65853659	1.81
4.117647059	4.41176471	2.16
4.046242775	4.76878613	2.28
3.977272727	5.11363636	2.4
3.910614525	5.44692737	2.5
3.846153846	5.76923077	2.59
3.783783784	6.08108108	2.66
3.723404255	6.38297872	2.71
3.608247423	6.95876289	2.81
3.5	7.5	2.89
3.333333333	8.33333333	2.99
3.181818182	9.09090909	3.06

Run 2		
[H] mmol	**[G] mmol**	**δ NH**
5	0	0
4.794520548	1.02739726	0.51
4.605263158	1.97368421	0.9
4.430379747	2.84810127	1.38
4.268292683	3.65853659	1.81
4.117647059	4.41176471	2.15
4.046242775	4.76878613	2.29
3.977272727	5.11363636	2.41
3.910614525	5.44692737	2.49
3.846153846	5.76923077	2.58
3.783783784	6.08108108	2.66
3.723404255	6.38297872	2.71
3.608247423	6.95876289	2.81
3.5	7.5	2.88
3.333333333	8.33333333	2.99
3.181818182	9.09090909	3.06

1:5 HBP (Mn – 4000)

Run 1		
[H] mmol	**[G] mmol**	**δ NH**
10	0	0
9.79020979	8.39160839	2.28
9.589041096	16.4383562	3.02
9.395973154	24.1610738	3.25
9.210526316	31.5789474	3.36
9.032258065	38.7096774	3.44
8.860759494	45.5696203	3.46
8.588957055	56.4417178	3.52
8.484848485	60.6060606	3.53
8.235294118	70.5882353	3.6

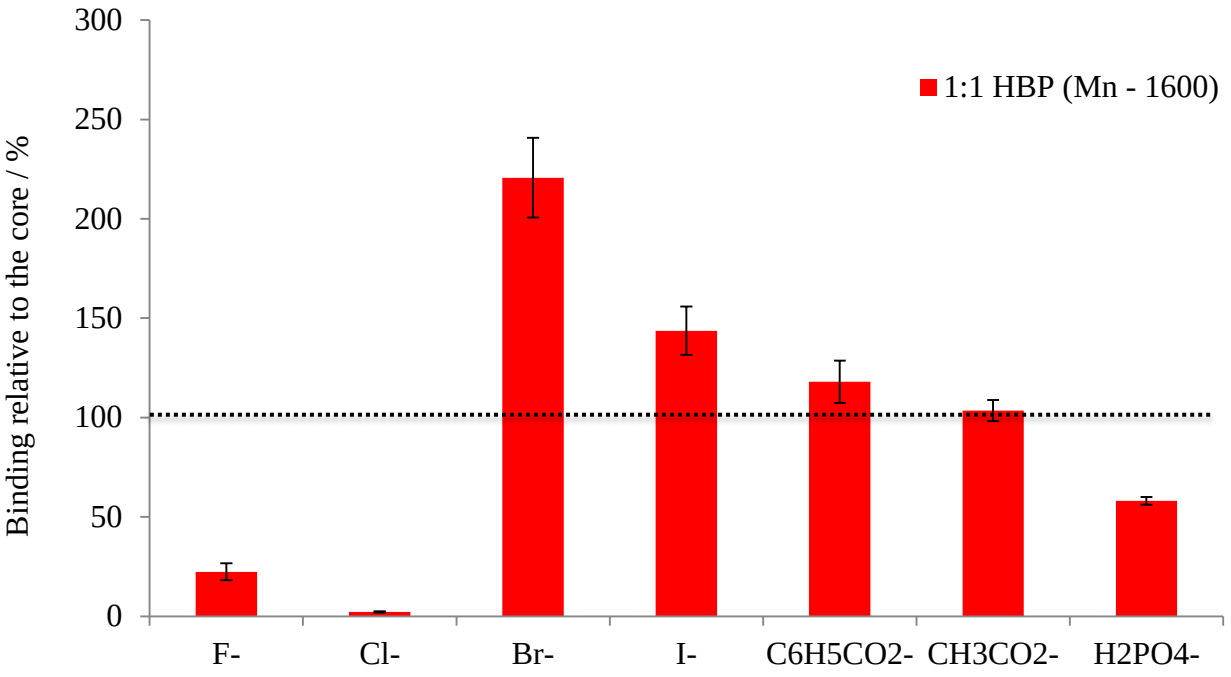
Run 2		
[H] mmol	**[G] mmol**	**δ NH**
10	0	0
9.79020979	8.39160839	2.2
9.589041096	16.4383562	2.99
9.395973154	24.1610738	3.24
9.210526316	31.5789474	3.34
9.032258065	38.7096774	3.41
8.860759494	45.5696203	3.44
8.588957055	56.4417178	3.48
8.484848485	60.6060606	3.52
8.235294118	70.5882353	3.59

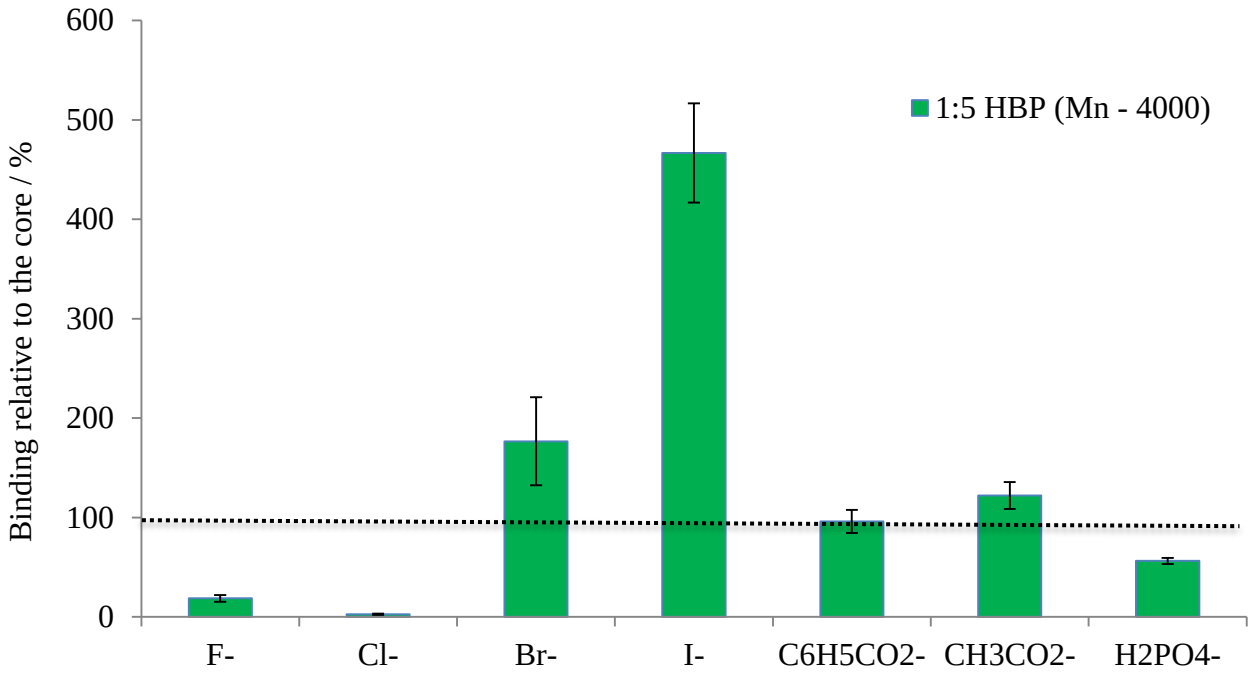
1:20 HBP (Mn – 10343)

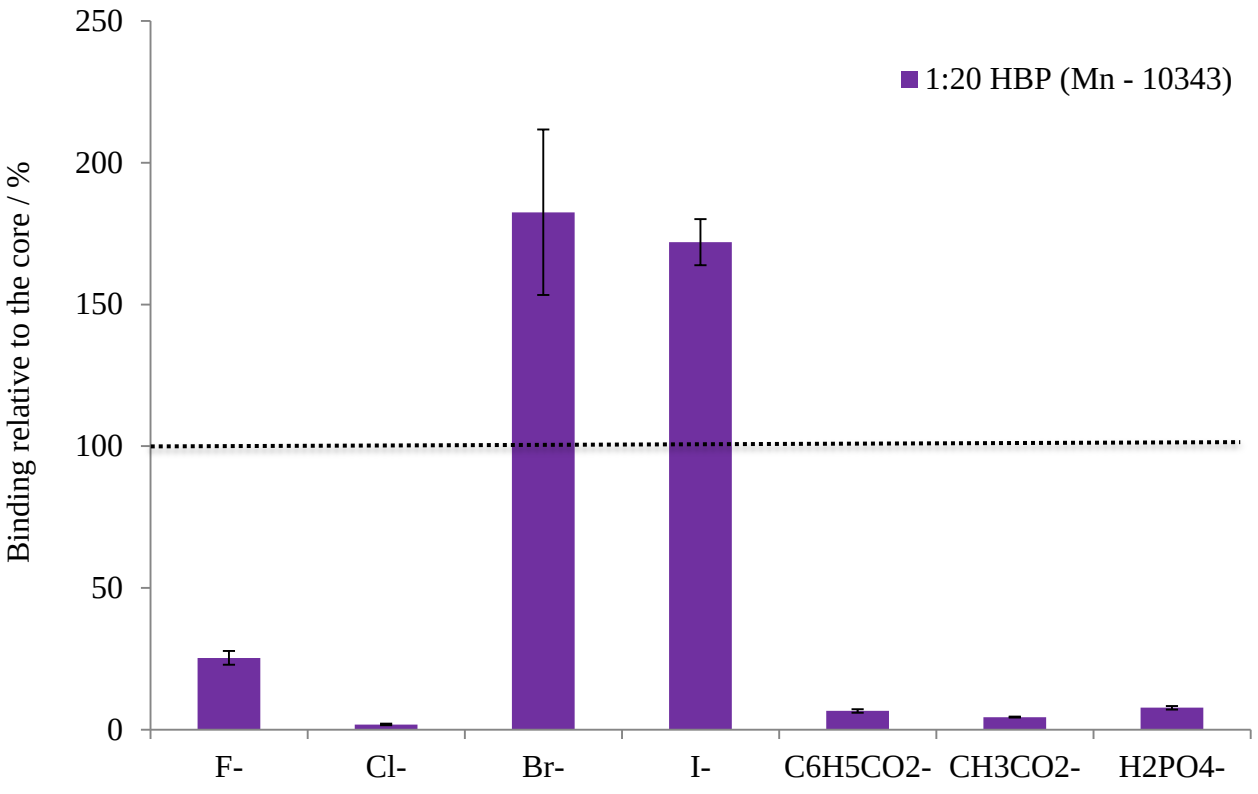
Run 1		
[H] mmol	**[G] mmol**	**δ NH**
10	0	0
9.79020979	8.39160839	0.89
9.589041096	16.4383562	1.96
9.395973154	24.1610738	2.7
9.210526316	31.5789474	3.01
9.032258065	38.7096774	3.15
8.860759494	45.5696203	3.26
8.695652174	52.173913	3.31
8.536585366	58.5365854	3.36
8.383233533	64.6706587	3.38

Run 2		
[H] mmol	**[G] mmol**	**δ NH**
10	0	0
9.79020979	8.39160839	0.92
9.589041096	16.4383562	1.99
9.395973154	24.1610738	2.68
9.210526316	31.5789474	3
9.032258065	38.7096774	3.15
8.860759494	45.5696203	3.26
8.695652174	52.173913	3.32
8.536585366	58.5365854	3.35
8.383233533	64.6706587	3.39

1.4 Appendix D – Anion binding data for hyperbranched polymer systems of different molecular weights.






250
200
150
100
50
0
Binding relative to the core / %
1:20 HBP (Mn - 10343)
F-
Cl-
Br-
I-
C6H5CO2-
CH3CO2-
H2PO4-