Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry

A Simple Ionic Triphenylene Receptor for Catecholamines, Serotonin and *D*-Glucosamine in Phosphate Buffered Water

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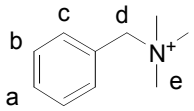
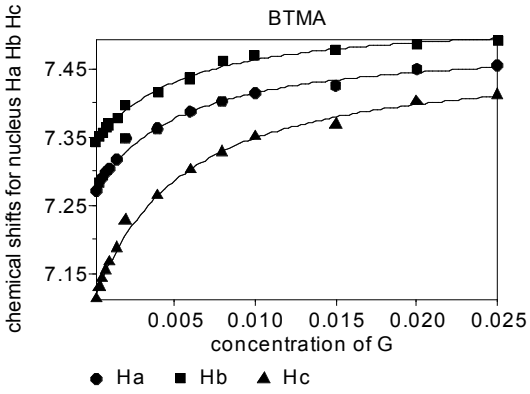
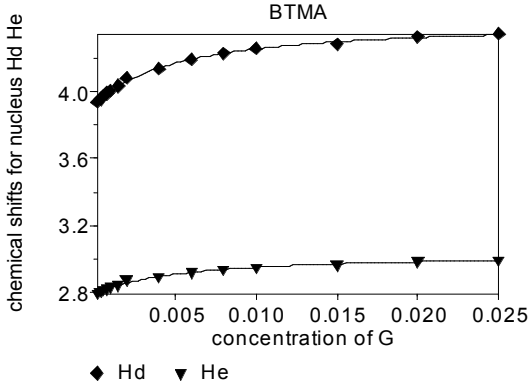


Experimental Data Table (300MHz, Buffered D_2O, δ in ppm)

Host (M)	Guest (M)	δ Ha	δ Hb	δ Hc	δ Hd	δ He
0.001	0.0002	7.2718	7.3433	7.1136	3.9364	2.7991
0.001	0.0004	7.2831	7.3521	7.1312	3.9577	2.8104
0.001	0.0006	7.2906	7.3571	7.1437	3.9753	2.8191
0.001	0.0008	7.2981	7.3634	7.155	3.9891	2.8254
0.001	0.001	7.3044	7.3684	7.1676	4.0054	2.833
0.001	0.0015	7.317	7.3785	7.1877	4.033	2.8455
0.001	0.002	7.3484	7.3974	7.2278	4.0807	2.8794
0.001	0.004	7.3622	7.4149	7.2642	4.1372	2.8945
0.001	0.006	7.3873	7.4362	7.3032	4.1912	2.9208
0.001	0.008	7.4023	7.4613	7.3283	4.2264	2.9384
0.001	0.01	7.4149	7.4688	7.3509	4.2552	2.9522
0.001	0.015	7.4263	7.4776	7.3684	4.2816	2.9648
0.001	0.02	7.4489	7.4866	7.4025	4.3282	2.989
0.001	0.025	7.4551	7.4915	7.4124	4.3431	2.9948
	$\Delta\delta_{max}$	**+0.18**	**+0.15**	**+0.30**	**+0.41**	**+0.20**

Fitting (1:1 Model, Protons H_a, H_b, H_c, H_d H_e, NH)

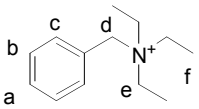




Results

```
 no. of spectra            14
 no. of resonance values   65
 no. of resonant nuclei     5

Chi-squared =  19.80
 Chi-squared should be less than 12.60 at the 95% confidence level

   sigma =   0.00433736002          RMS weighted residual =   0.00395335372
       stoich            value   relative    log    standard
       coeff                     std devn    beta   deviation

 Beta  1  1 refined  2.7729E+002  0.0446    2.4429   0.0194  (   2.44293224943464     )

 Individual chemical shifts
        +
                     G                          1,1
 ========================================================
        +        value    error         value    error
Ha      +       7.4873   0.0033         6.4824   0.0426
Hb      +       7.5244   0.0031         6.6725   0.0371
Hc      +       7.4675   0.0041         5.8159   0.0667
Hd      +       4.4162   0.0049         2.1622   0.0897
He      +       3.0296   0.0033         1.9494   0.0453
```

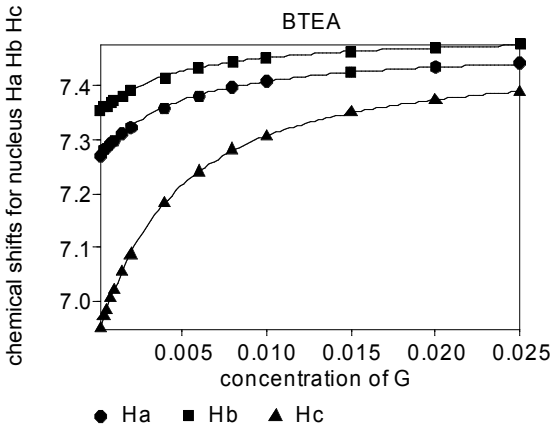
^{1}H NMR titrations between Host 1 and Benzyltriethylammonium 2b

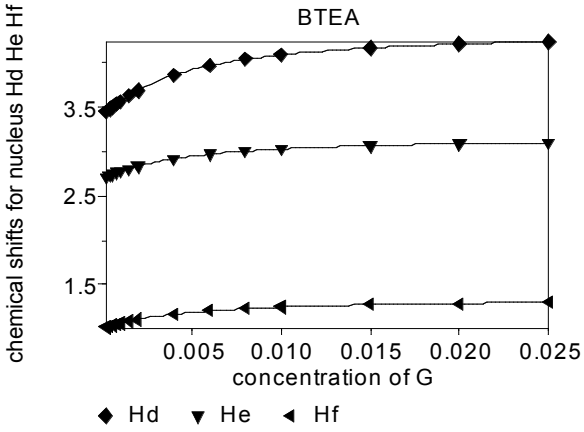


Experimental Data Table (300MHz, Buffered D_2O)

Host (M)	Guest (M)	δ Ha (ppm)	δ Hb (ppm)	δ Hc (ppm)	δ Hd (ppm)	δ He (ppm)	δ Hf (ppm)
0.001	0.0002	7.2705	7.3559	6.9492	3.4455	2.715	1.0165
0.001	0.0004	7.2806	7.3622	6.9705	3.4769	2.7325	1.0303
0.001	0.0006	7.2843	7.3634	6.9831	3.4983	2.7426	1.0378
0.001	0.0008	7.2919	7.3697	7.0044	3.5372	2.7614	1.0516
0.001	0.001	7.2981	7.3735	7.0195	3.5661	2.7752	1.0617
0.001	0.0015	7.3119	7.3822	7.0546	3.6301	2.8066	1.0843
0.001	0.002	7.3232	7.391	7.086	3.6878	2.8342	1.1031
0.001	0.004	7.3584	7.4161	7.1826	3.8636	2.9183	1.1646
0.001	0.006	7.381	7.4325	7.2404	3.969	2.9698	1.201
0.001	0.008	7.3986	7.445	7.2818	4.0443	3.0062	1.2274
0.001	0.01	7.4086	7.4525	7.3069	4.0908	3.0288	1.2437
0.001	0.015	7.4262	7.4651	7.3509	4.1686	3.0664	1.2713
0.001	0.02	7.4362	7.4726	7.3735	4.2113	3.0865	1.2851
0.001	0.025	7.4425	7.4776	7.3885	4.2364	3.0991	1.2952
	$\Delta\delta_{max}$	**+0.17**	**+0.12**	**+0.44**	**+0.79**	**+0.38**	**+0.28**

Fitting (1:1 Model, *Protons H_a, H_b, H_c, H_d, H_e, H_f)*

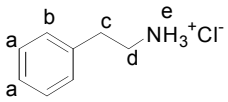




Results

```
no. of spectra            14
 no. of resonance values   84
 no. of resonant nuclei     6

 Chi-squared =  13.52
 Chi-squared should be less than 12.60 at the 95% confidence level

   sigma =   0.00228743803          RMS weighted residual =   0.00210299804
stoich            value   relative    log    standard
       coeff                      std devn    beta   deviation
Beta  1  1 refined  3.5196E+002  0.0130    2.5465   0.0056  (   2.54648955154416     )

 Individual chemical shifts
                  G                     1,1
 ============================================================
        +        value    error         value    error
Ha      +       7.4697   0.0014         6.6746   0.0107
Hb      +       7.4960   0.0014         6.9298   0.0090
Hc      +       7.4639   0.0017         5.4077   0.0224
Hd      +       4.3747   0.0024         0.6377   0.0394
He      +       3.1659   0.0017         1.3596   0.0199
Hf      +       1.3428   0.0015         0.0402   0.0151
```

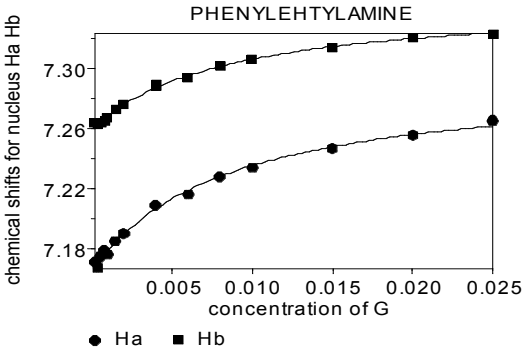
^{1}H NMR titrations between Host 1 and Phenylethylamine 2c

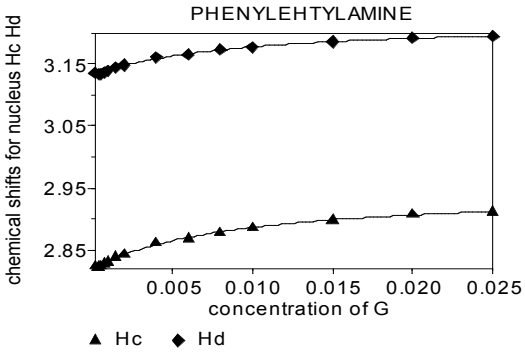


Experimental Data Table (300MHz, Buffered D_2O)

Host (mol.L^{-1})	Guest (mol.L^{-1})	δ Ha (ppm)	δ Hb (ppm)	δ Hc (ppm)	δ Hd (ppm)
0.001	0.0002	7.1713	7.2642	2.8229	3.1355
0.001	0.0004	7.1676	7.263	2.8217	3.1342
0.001	0.0006	7.1751	7.2642	2.8242	3.1342
0.001	0.0008	7.1789	7.2655	2.8279	3.1367
0.001	0.001	7.1764	7.268	2.8304	3.1387
0.001	0.0015	7.1852	7.273	2.838	3.1443
0.001	0.002	7.1902	7.2768	2.843	3.148
0.001	0.004	7.209	7.2893	2.8606	3.1606
0.001	0.006	7.2165	7.2944	2.8681	3.1656
0.001	0.008	7.2278	7.3019	2.8781	3.1731
0.001	0.01	7.2341	7.3069	2.8857	3.1769
0.001	0.015	7.2467	7.3145	2.8982	3.1857
0.001	0.02	7.2555	7.3207	2.907	3.192
0.001	0.025	7.2655	7.3232	2.9108	3.1945
	$\Delta\delta_{max}$	**+0.09**	**+0.06**	**+0.09**	**+0.06**

Fitting (1:1 Model, Protons H_a, H_b, H_c, H_d)





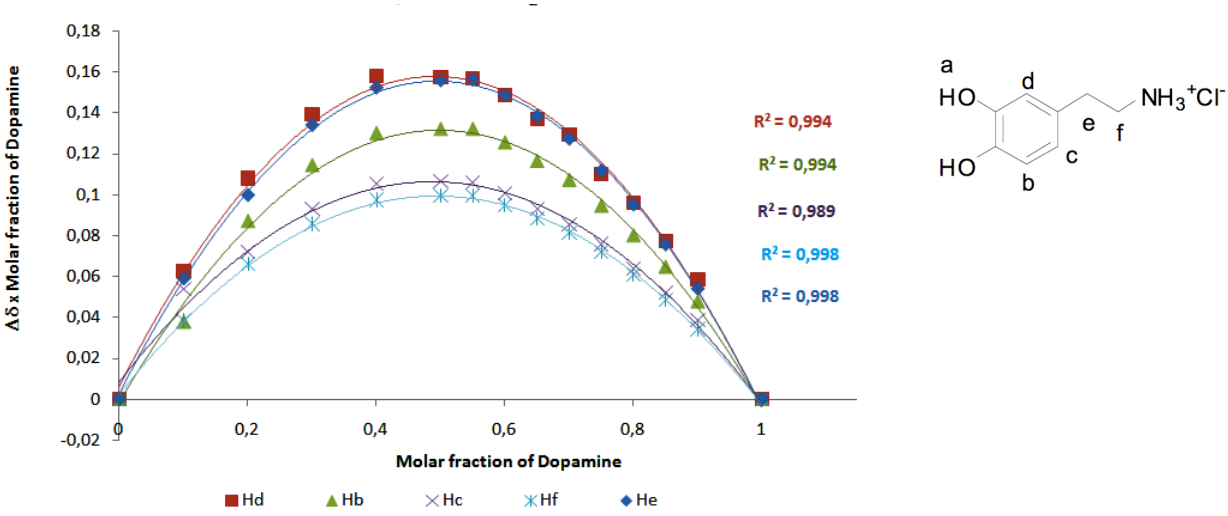
Results

```
no. of spectra            14
no. of resonance values   56
no. of resonant nuclei     4
Chi-squared =   8.86
Chi-squared should be less than 12.60 at the 95% confidence level

  sigma =   0.00170576933          RMS weighted residual =   0.00156269857

      stoich            value   relative    log    standard
      coeff                     std devn    beta   deviation

Beta  1   1 refined  1.4947E+002  0.0586    2.1746   0.0254  (   2.17456396608709     )

Individual chemical shifts
       +
                  G                        1,1
 ========================================================
       +        value    error         value    error
Ha     +       7.2924   0.0024         6.3200   0.0617
Hb     +       7.3443   0.0019         6.6967   0.0421
Hc     +       2.9411   0.0024         1.9964   0.0600
Hd     +       3.2155   0.0019         2.5663   0.0422
```

^{1}H NMR titrations between Host 1 and Dopamine 3a

Job plot for (Host 1:Dopamine 3a) Complex using NMR monitoring

Stock solutions of guest (2.5 mM) and host **4** (2.5 mM) were independently prepared in buffered D_2O (pH 7.1, Na_2HPO_4 100 mM). Fourteen NMR tubes were fulfilled with increasing aliquots of guest stock solution (from 0 to 500 µL) and the total volume (500 µL) was adjusted with host stock solution. Guest Protons were monitored by ^{1}H NMR.

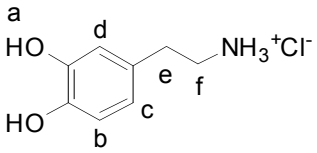


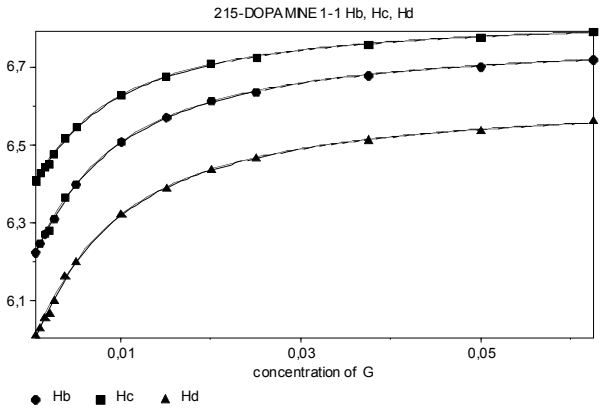
Titration

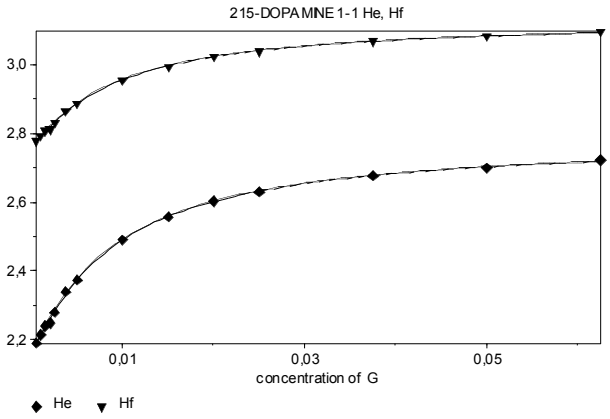
Experimental Data (300MHz, buffered D_2O, pH 7.2)

Host (mol.L^{-1})	Guest (mol.L^{-1})	δ Hb (ppm)	δ Hc (ppm)	δ Hd (ppm)	δ He (ppm)	δ Hf (ppm)
0.001	0.0005	6.4094	6.0127	6.2261	2.1927	2.779
0.001	0.001	6.4282	6.0328	6.2487	2.2166	2.794
0.001	0.0015	6.4458	6.0579	6.2738	2.2417	2.8078
0.001	0.002	6.4533	6.0679	6.2826	2.2505	2.8129
0.001	0.0025	6.4772	6.1018	6.3115	2.2819	2.8317
0.001	0.00375	6.5198	6.1646	6.3667	2.3409	2.8656
0.001	0.005	6.5462	6.2022	6.4006	2.376	2.8869
0.001	0.01	6.629	6.3228	6.5098	2.4928	2.9547
0.001	0.015	6.6768	6.3905	6.5713	2.5593	2.9949
0.001	0.02	6.7081	6.4382	6.614	2.6045	3.0238
0.001	0.025	6.7257	6.4659	6.6366	2.6308	3.0388
0.001	0.0375	6.7583	6.5136	6.6793	2.6773	3.0677
0.001	0.05	6.7747	6.5374	6.7019	2.7011	3.0828
0.001	0.0625	6.7910	6.5625	6.7194	2.7237	3.0966
	$\Delta\delta_{max}$	**+0.38**	**+0.55**	**+0.49**	**+0.53**	**+0.32**

Fitting (1:1 Model, Protons H_b, H_c, H_d, H_e, H_f)



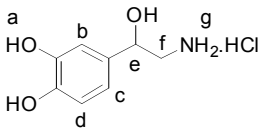




Results

```
no. of spectra            14
 no. of resonance values   72
 no. of resonant nuclei     5

  Chi-squared =   4.80
 Chi-squared should be less than 12.60 at the 95% confidence level

   sigma =   0.00240618884          RMS weighted residual =   0.00217446351

       stoich            value   relative    log    standard
       coeff                     std devn    beta   deviation

 Beta  1   1 refined  1.9367E+002  0.0156    2.2871   0.0068  (   2.28706671797779     )

 Individual chemical shifts
+
                    G                      1,1
 ============================================================
        +        value    error         value    error
Hb      +       6.7848   0.0018         4.9958   0.0207
Hc      +       6.8400   0.0016         5.4648   0.0163
Hd      +       6.6308   0.0019         4.6351   0.0229
He      +       2.7898   0.0018         0.8715   0.0221
Hf      +       3.1343   0.0015         1.9910   0.0139
```

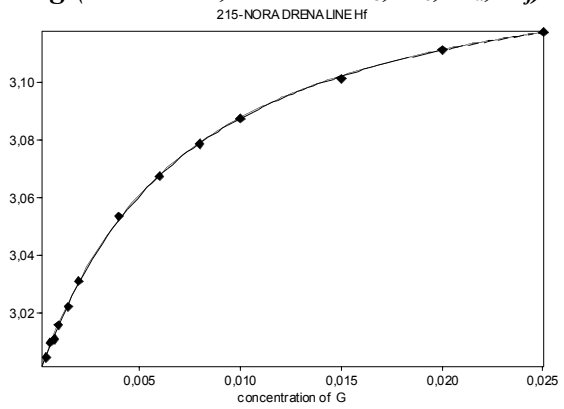
^{1}H NMR titrations between Host 1 and *L*-Noradrenaline (Norepinephrine) **3b**

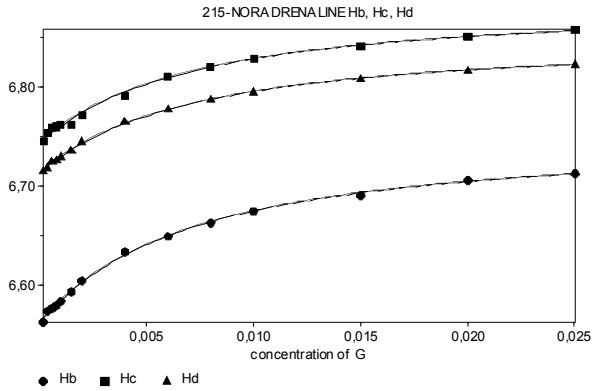


Experimental Data Table (300 MHz, Buffered D_2O)

Host (mol.L^{-1})	Guest (mol.L^{-1})	δ Hb (ppm)	δ Hc (ppm)	δ Hd (ppm)	δ Hf (ppm)
0.001	0.0002	6.5638	6.7458	6.7157	3.0049
0.001	0.0004	6.5751	6.7546	6.7194	3.01
0.001	0.0006	6.5776	6.7596	6.7257	3.0112
0.001	0.0008	6.5801	6.7609	6.727	3.0162
0.001	0.001	6.5851	6.7634	6.7307	3.0225
0.001	0.0015	6.5939	6.7636	6.737	3.0313
0.001	0.002	6.6052	6.7722	6.7458	3.0539
0.001	0.004	6.6341	6.7922	6.7659	3.0677
0.001	0.006	6.6504	6.8111	6.7784	3.079
0.001	0.008	6.6642	6.8211	6.7885	3.0878
0.001	0.01	6.6755	6.8299	6.796	3.1016
0.001	0.015	6.6918	6.8425	6.8086	3.1116
0.001	0.02	6.7069	6.8525	6.8173	3.1179
0.001	0.025	6.7132	6.8588	6.8236	3.1249
	$\Delta\delta_{max}$	**+0.15**	**+0.11**	**+0.11**	**+0.12**

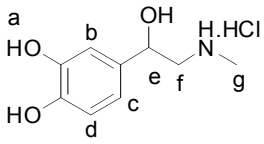
Fitting (1:1 Model, Protons H_b, H_c, H_d, H_f)





Results

```
 no. of spectra            14
 no. of resonance values   55
 no. of resonant nuclei     4

 Chi-squared =  12.35
 Chi-squared should be less than 12.60 at the 95% confidence level

   sigma =   0.00190632424          RMS weighted residual =   0.00174338916

       stoich            value   relative    log    standard
       coeff                     std devn    beta   deviation

 Beta  1   1 refined  1.8603E+002  0.0436    2.2696   0.0189  (   2.26957529634707     )

 Individual chemical shifts
        +
                    G                      1,1
 ========================================================
        +        value    error         value    error
Hb      +       6.7528   0.0024         5.5400   0.0536
Hc      +       6.8871   0.0020         5.9786   0.0408
Hd      +       6.8524   0.0020         5.9699   0.0397
Hf      +       3.1492   0.0021         2.1835   0.0427
```

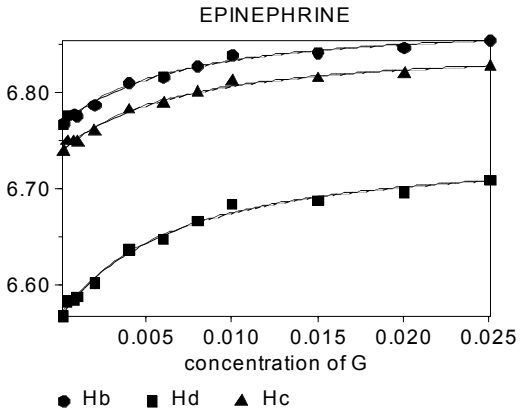


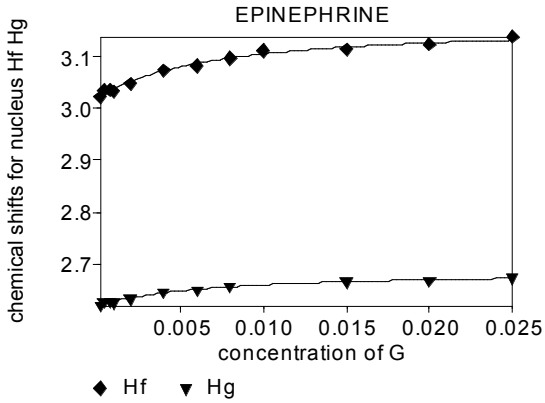
^{1}H NMR titrations between Host 1 and *L*-Adrenaline (epinephrine) **3c**

Experimental Data Table (300MHz, Buffered D_2O)

Host (mol.L^{-1})	Guest (M)	δ Hb (ppm)	δ Hc (ppm)	δ Hd (ppm)	δ Hf (ppm)	δ Hg (ppm)
0.001	0.0002	6.7671	6.7395	6.5688	3.0225	2.6208
0.001	0.0004	6.7759	6.7496	6.5839	3.0351	2.6271
0.001	0.0008	6.7772	6.7496	6.5851	3.0351	2.6271
0.001	0.001	6.7759	6.7483	6.5889	3.0325	2.6258
0.001	0.002	6.7872	6.7596	6.6027	3.0476	2.6334
0.001	0.004	6.8098	6.7822	6.6378	3.074	2.6459
0.001	0.006	6.8161	6.7885	6.6479	3.0815	2.6497
0.001	0.008	6.8274	6.801	6.6667	3.0966	2.6572
0.001	0.01	6.8387	6.8123	6.6843	3.1116	
0.001	0.015	6.8412	6.8148	6.688	3.1141	2.666
0.001	0.02	6.8462	6.8199	6.6968	3.1229	2.6685
0.001	0.025	6.8538	6.8274	6.7094	3.138	2.6735
	$\Delta\delta_{max}$	**+0.09**	**+0.09**	**+0.14**	**+0.12**	**+0.05**

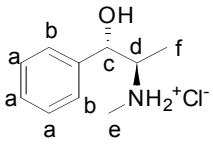
Fitting (1:1 Model, Protons, H_b, H_c, H_d, H_f, H_g)





Results

```
no. of spectra            12
 no. of resonance values   59
 no. of resonant nuclei     5

 Chi-squared =  10.29
 Chi-squared should be less than 12.60 at the 95% confidence level

   sigma =   0.00395633718          RMS weighted residual =   0.00356851815

       stoich            value   relative    log    standard
       coeff                     std devn    beta   deviation

 Beta  1  1 refined  2.0384E+002  0.1013    2.3093   0.0440  (   2.30928086348477     )


 Individual chemical shifts
        +
                    G                        1,1
 ============================================================
        +        value    error          value    error
Hb      +       6.8751   0.0037         6.2282   0.0667
Hd      +       6.7426   0.0049         5.7105   0.1029
Hc      +       6.8489   0.0037         6.1937   0.0675
Hf      +       3.1592   0.0042         2.3351   0.0832
Hg      +       2.6850   0.0032         2.3012   0.0434
```

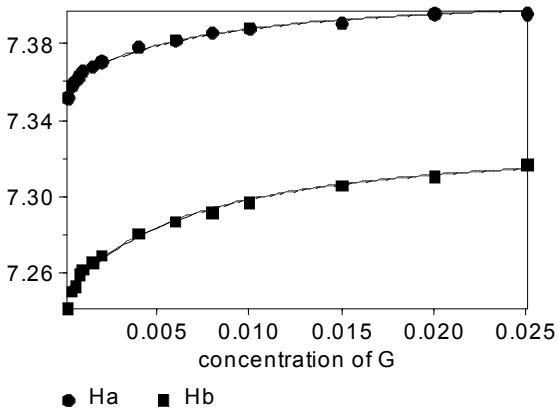


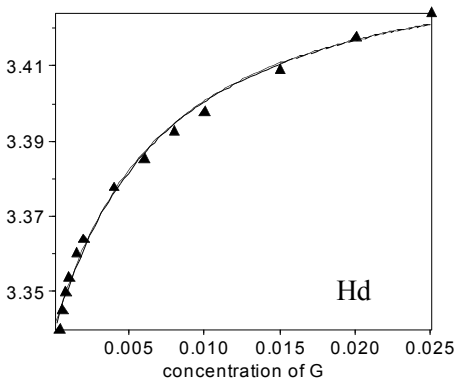
^{1}H NMR titrations between Host 1 and (–)-Ephedrine 3d

Experimental Data Table (300MHz, Buffered D_2O)

Host (mol.L^{-1})	Guest (mol.L^{-1})	δ Ha (ppm)	δ Hb (ppm)	δ Hd (ppm)
0.001	0.0002	7.3521	7.2416	
0.001	0.0004	7.3584	7.2504	3.3401
0.001	0.0006	7.3609	7.2529	3.3451
0.001	0.0008	7.3634	7.2592	3.3501
0.001	0.001	7.3659	7.2617	3.3539
0.001	0.0015	7.3684	7.2655	3.3602
0.001	0.002	7.3709	7.2693	3.364
0.001	0.004	7.3785	7.2806	3.3778
0.001	0.006	7.3822	7.2868	3.3853
0.001	0.008	7.386	7.2919	3.3928
0.001	0.01	7.3885	7.2969	3.3978
0.001	0.015	7.391	7.3057	3.4091
0.001	0.02	7.3961	7.3107	3.4179
0.001	0.025	7.3961	7.317	3.4242
	$\Delta\delta_{max}$	**+0.04**	**+0.07**	**+0.08**

Fitting (1:1 Model, Protons H_a, H_b, H_d)

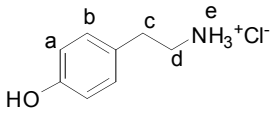




Results

```
no. of spectra            14
 no. of resonance values   52
 no. of resonant nuclei     5

Chi-squared =  10.77
 Chi-squared should be less than 12.60 at the 95% confidence level

   sigma =   0.00201646588          RMS weighted residual =   0.00183367952

       stoich            value   relative    log    standard
       coeff                     std devn    beta   deviation

 Beta  1   1 refined  1.8321E+002  0.0993    2.2630   0.0431  (   2.26295959280669     )

Individual chemical shifts
                 G                      1,1
 ============================================================
        +        value    error         value    error
Ha      +       7.4080   0.0019         7.0911   0.0333
Hb      +       7.3320   0.0024         6.8001   0.0533
Hd      +       3.4431   0.0029         2.7730   0.0664
```

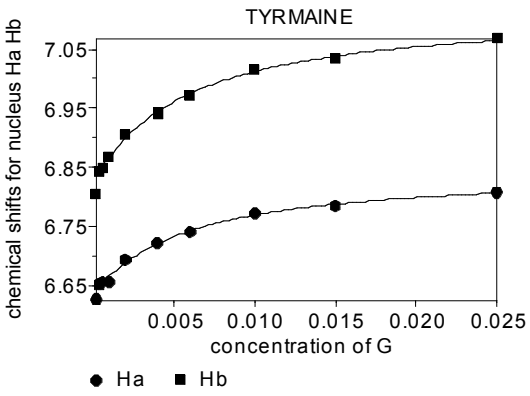
^{1}H NMR titrations between Host 1 and Tyramine 3e

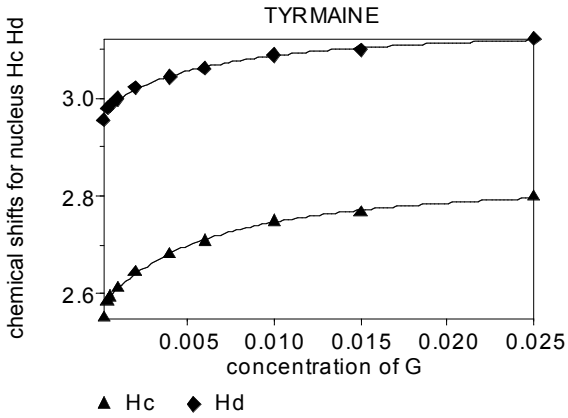


Experimental Data Table (300MHz, Buffered D_2O)

Host (mol.L^{-1})	Guest (mol.L^{-1})	δ Ha (ppm)	δ Hb (ppm)	δ Hc (ppm)	δ Hd (ppm)
0.001	0.0002	6.6253	6.8048	2.5505	2.956
0.001	0.0004	6.6504	6.8412	2.5844	2.9798
0.001	0.0006	6.6554	6.8487	2.5932	2.9861
0.001	0.001	6.6554	6.8688	2.612	2.9987
0.001	0.002	6.6931	6.904	2.6447	3.0212
0.001	0.004	6.7207	6.9416	2.6811	3.0438
0.001	0.006	6.7395	6.9705	2.7074	3.0614
0.001	0.01	6.7709	7.0144	2.7476	3.0878
0.001	0.015	6.7835	7.0333	2.7652	3.0991
0.001	0.025	6.8073	7.0684	2.7991	3.1217
	$\Delta\delta_{max}$	**+0.18**	**+0.26**	**+0.25**	**+0.17**

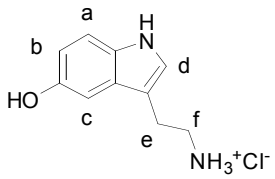
Fitting (1:1 Model, Protons H_a, H_b, H_c, H_d)





Results

```
no. of spectra            10
 no. of resonance values   36
 no. of resonant nuclei     4
 Chi-squared =  10.22
 Chi-squared should be less than 12.60 at the 95% confidence level

   sigma =   0.00408860231          RMS weighted residual =   0.00354083347

       stoich            value   relative    log    standard
       coeff                     std devn    beta   deviation

 Beta  1   1 refined  2.3740E+002  0.0716    2.3755   0.0311  (   2.37547875922881     )

 Individual chemical shifts
        +
                    G                        1,1
 ============================================================
        +        value    error          value    error
Ha      +       6.8426   0.0045          5.7658   0.0737
Hb      +       7.1160   0.0054          5.6050   0.1009
Hc      +       2.8435   0.0052          1.4263   0.0950
Hd      +       3.1509   0.0042          2.2187   0.0649
```

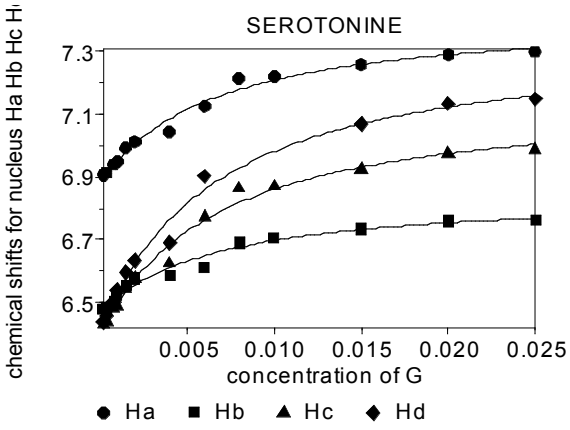


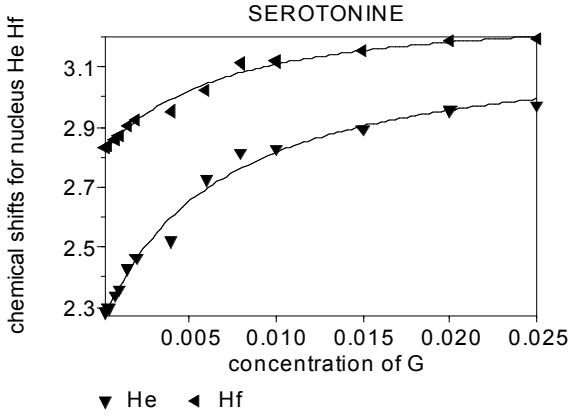
^{1}H NMR titrations between Host 1 and Serotonin 3f

Experimental Data Table (300MHz, Buffered D_2O)

Host (M)	Guest (M)	δ Ha (ppm)	δ Hb (ppm)	δ Hc (ppm)	δ Hd (ppm)	δ He (ppm)	δ Hf (ppm)
0.001	0.0002	6.9065	6.4772	6.4307	6.4382	2.2844	2.8317
0.001	0.0004	6.914	6.4822	6.4395	6.4596	2.2968	2.8367
0.001	0.0006	6.9394	6.5023	6.4809	6.5023	2.3384	2.8593
0.001	0.0008	6.9492	6.5223	6.4885	6.5387	2.3572	2.8694
0.001	0.001	6.9906	6.555	6.5462	6.5952	2.4275	2.9045
0.001	0.0015	7.0107	6.5763	6.5763	6.6328	2.4639	2.9233
0.001	0.002	7.0446	6.5864	6.6228	6.6893	2.5191	2.9522
0.001	0.004	7.1248	6.6139	6.7733	6.9014	2.7249	3.0212
0.001	0.008	7.214	6.69	6.8625		2.8154	3.1116
0.001	0.01	7.2203	6.7081	6.8713		2.8267	3.1179
0.001	0.015	7.2567	6.7345	6.9241	7.0684	2.892	3.1531
0.001	0.02	7.2906	6.7596	6.9743	7.1324	2.9547	3.1882
0.001	0.025	7.2981	6.7646	6.9868	7.1488	2.971	3.1957
	$\Delta\delta_{max}$	**+0.39**	**+0.29**	**+0.56**	**+0.71**	**+0.69**	**+0.36**

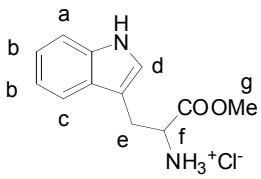
Fitting (1:1 Model, Protons H_a, H_b, H_c, H_d H_e, H_f)





Results

```
no. of spectra            13
 no. of resonance values   76
 no. of resonant nuclei     6
Chi-squared =  27.58
 Chi-squared should be less than 12.60 at the 95% confidence level

   sigma =   0.02371121755          RMS weighted residual =   0.02158824479

      stoich            value   relative    log    standard
      coeff                     std devn    beta   deviation

 Beta  1  1 refined  2.0124E+002  0.1013    2.3037   0.0440  (   2.30370528462867     )

 Individual chemical shifts
                  G                      1,1
 ============================================================
        +        value    error         value    error
Ha      +       7.4136   0.0204         4.2677   0.3329
Hb      +       6.8419   0.0184         4.6240   0.2521
Hc      +       7.1516   0.0239         2.6797   0.4547
Hd      +       7.3424   0.0269         1.7945   0.5490
He      +       3.1757   0.0270        -2.3544   0.5543
Hf      +       3.2982   0.0199         0.3802   0.3126
```

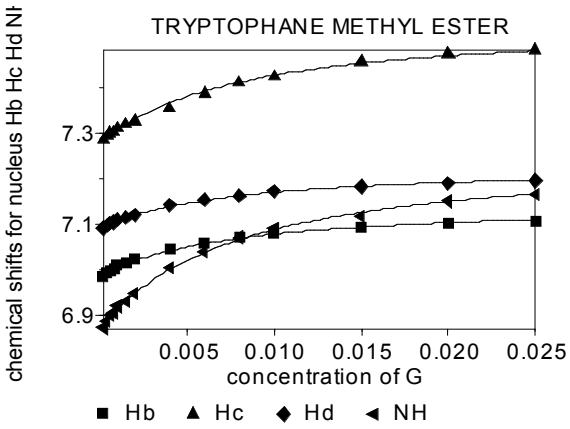


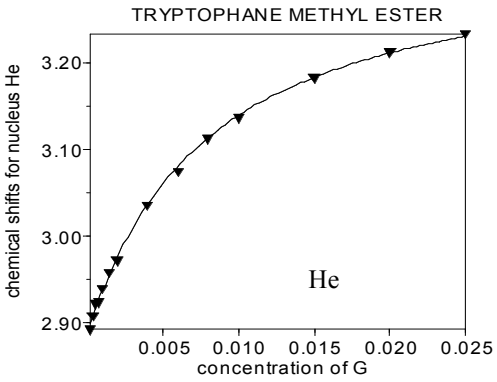
^{1}H NMR titrations between Host 1 and Tryptophane methyl ester 4e

Experimental Data Table (300MHz, Buffered D_2O)

Host (M)	Guest (M)	δ Ha (ppm)	δ Hb (ppm)	δ Hc (ppm)	δ Hd (ppm)	δ He (ppm)	δ NH
0.001	0.0002	7.2329	6.9818	7.2831	7.0898	2.8932	6.8701
0.001	0.0004	7.2504	6.9918	7.2931	7.096	2.9083	6.8851
0.001	0.0006	7.263	6.9969	7.2994	7.1011	2.9221	6.8977
0.001	0.0008	7.2693	7.0019	7.3019	7.1023	2.9246	6.904
0.001	0.001	7.2818	7.0092	7.3107	7.1086	2.9397	6.9178
0.001	0.0015	7.2931	7.0132	7.3182	7.1136	2.9585	6.9291
0.001	0.002	7.3069	7.0207	7.3245	7.1186	2.9723	6.9454
0.001	0.004	7.3534	7.0433	7.3534	7.14	3.0363	7.0031
0.001	0.006	7.3684	7.0571	7.3861	7.1513	3.0752	7.0358
0.001	0.008	7.3849	7.0697	7.4111	7.1613	3.1129	7.0697
0.001	0.01	7.3935	7.0772	7.4237	7.1713	3.1367	7.0885
0.001	0.015	7.4124	7.091	7.4563	7.1814	3.1832	7.1149
0.001	0.02	7.4212	7.0998	7.4726	7.1877	3.2121	7.1488
0.001	0.025	7.4287	7.1061	7.4827	7.1939	3.2334	7.1651
	$\Delta\delta_{max}$	**+0.20**	**+0.12**	**+0.20**	**+0.10**	**+0.34**	**+0.30**

Fitting (1:1 Model, Protons H_b, H_c, H_d H_e, NH)

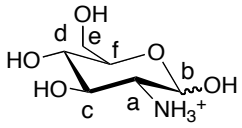




Results

```
no. of spectra            14
 no. of resonance values   70
no. of resonant nuclei     6

 Chi-squared =  10.91
 Chi-squared should be less than 12.60 at the 95% confidence level
sigma =   0.00394367168          RMS weighted residual =   0.00362057658
stoich            value   relative    log    standard
       coeff                       std devn    beta   deviation

 Beta  1   1 refined  1.5976E+002  0.0420    2.2035    0.0183  (   2.20346830171945     )

 Individual chemical shifts
                   G                        1,1
 ========================================================
        +        value    error         value    error
Hb      +       7.1454   0.0034         5.9959   0.0568
Hc      +       7.5410   0.0041         5.6274   0.0878
Hd      +       7.2276   0.0033         6.2385   0.0508
He      +       3.3333   0.0058         0.0956   0.1440
NH      +       7.2535   0.0052         4.4705   0.1245
```

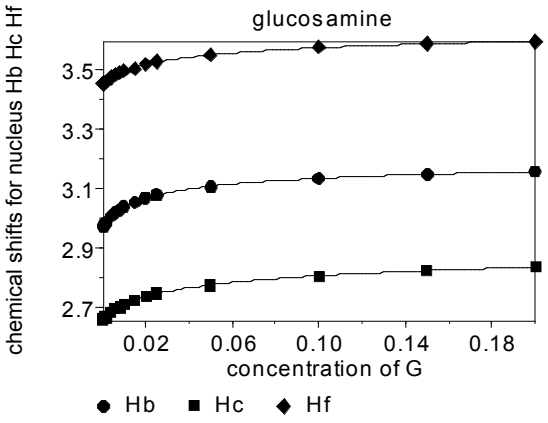
^{1}H NMR titrations between Host 1 and Glucosamine 5a

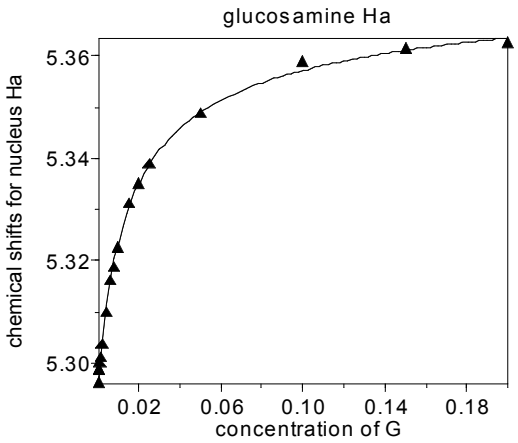


Experimental Data Table (300MHz, Buffered D_2O)

Host (mol.L^{-1})	Guest (mol.L^{-1})	δ Ha (ppm)	δ Hb (ppm)	δ Hc (ppm)	δ Hf (ppm)
0.001	0.0004	5.2959	2.971	2.6585	3.4531
0.001	0.0006	5.2984	2.9773	2.6622	3.4556
0.001	0.0008	5.2984		2.6622	3.4568
0.001	0.001	5.2997	2.9798	2.6647	3.4581
0.001	0.0015	5.3009	2.9836	2.6672	3.4585
0.001	0.002	5.3034	2.9899	2.671	3.4631
0.001	0.004	5.3097	3.0062	2.6836	3.4744
0.001	0.006	5.316	3.02	2.6949	3.4832
0.001	0.008	5.3185	3.0275	2.7011	3.4895
0.001	0.01	5.3223	3.0388	2.7099	3.497
0.001	0.015	5.331	3.0564	2.7262	3.5048
0.001	0.02	5.3348	3.0702	2.7375	3.5209
0.001	0.025	5.3386	3.079	2.7476	3.5284
	$\Delta\delta_{max}$	**+0.04**	**+0.11**	**+0.09**	**+0.08**

Fitting (1:1 Model, Protons, H_a, H_b, H_c, H_f)





Results

```
no. of spectra            17
 no. of resonance values   67
 no. of resonant nuclei     4

 Chi-squared =  14.07
 Chi-squared should be less than 12.60 at the 95% confidence level

   sigma =   0.00134892447          RMS weighted residual =   0.00119974284

       stoich            value   relative    log    standard
       coeff                     std devn    beta   deviation

 Beta  1   1 refined  8.7386E+001  0.0037    1.9414   0.0016  (   1.94144218843385     )

Individual chemical shifts
                  G                      1,1
 ========================================================
        +        value    error         value    error
Hb      +       3.1021   0.0001         1.4428   0.0000
Hc      +       2.7454   0.0001         1.6316   0.0000
Ha      +       5.3533   0.0003         4.6224   0.0000
Hf      +       3.5307   0.0001         2.5271   0.0000
```

Molecular Mechanics Calculations

To evaluate π-stacking, aromatic moieties were defined as centroids ($Ar_{centroid}$) using mercury software (version 2.3, CCDC Cambridge) and the distance inter-centroids was measured, in complement with the distance between aromatic planes. Distance between the triphenylene aromatic carbons (C_{Ar}) and CH groups of the guests were also measured to estimate CH-π interactions.

Measured distances (Å) for host :guest interactions and aromatics proximity in the minimized complexes

Host / Guest Atoms	(**1** : **2a**)	(**1** : **3a**)	(**1** : **5a**)
2 $COO^- \cdots H–N^+$	2.18 and 2.56	2.20 and 2.63	2.67 and 2.82
$Ar_{centroid} \cdots Ar_{centroid}$ distance between aromatic planes	3.80 (centroid off-set : 2.0) 3.48-3.50	3.96 and 4.30 (centroid off-set: 2.3) 3.50-3.70	-
$COO^- \cdots H–O$	-	2.47 and 2.96	2.39 & 2.87 (H1, 2 pts binding) and 2.35 (H4)
$C_{Ar} \cdots H–C$	2.59, 2.78 (CH_2) and 3.01 (CH_2)	2.72, 3.08 (CH_2)	2.67 (H3 & H5), 2.82 (H5), 2.94 (H3), 2.99 (CH_2)