

Supporting information

**The solvation properties and effect of D-fructose on taste behavior of
Citrus aurantium active components in aqueous solutions**

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Table S1. Provenance and purity of the samples.

Chemical Name	Source	Mass Fraction Purity	Purification Method
Hydrochloric acid solution	Sigma-Aldrich, Darmstadt, Germany	-	none
(±)-synephrine	Sigma-Aldrich, Darmstadt, Germany	≥ 0.98	none
(±)-synephrine hydrochloride	synthesis	-	none
(±)-octopamine hydrochloride	Sigma-Aldrich, Darmstadt, Germany	≥ 0.98	none
D-(-)-fructose	TCI, Eschborn, Germany	≥ 0.99	none

Table S2. Molality, (m), Density, (d), and apparent molar volume, (V_ϕ) of synephrine-HCl and octopamine-HCl in aqueous solutions with a different molality of D-fructose in the temperature range from (293.15 to 313.15) K at $p=1\cdot 10^5$ Pa.

$m /$ (mol·kg ⁻¹)		$d /$ (g·cm ⁻³)					$V_\phi /$ (cm ³ ·mol ⁻¹)				
$T /$ K	293.15	298.15	303.15	308.15	313.15	293.15	298.15	303.15	308.15	313.15	
Synephrine-HCl + water											
0.0203	0.99920	0.99803	0.99661	0.99498	0.99314	155.09	155.62	156.74	158.16	159.17	
0.0304	0.99969	0.99851	0.99708	0.99544	0.99360	154.95	155.67	156.81	158.15	159.06	
0.0503	1.00065	0.99946	0.99802	0.99636	0.99449	155.01	155.69	156.64	157.92	159.16	
0.0607	1.00115	0.99995	0.99851	0.99684	0.99496	154.96	155.72	156.53	157.80	159.02	
0.0812	1.00212	1.00092	0.99947	0.99778	0.99587	155.08	155.68	156.45	157.69	159.03	
0.0984	1.00294	1.00173	1.00027	0.99857	0.99664	155.07	155.69	156.45	157.61	158.96	
0.1493	1.00536	1.00411	1.00264	1.00091	0.99889	154.85	155.58	156.20	157.23	158.82	
0.2018	1.00785	1.00658	1.00506	1.00331	1.00122	154.60	155.27	156.03	156.94	158.53	
0.2959	1.01225	1.01092	1.00934	1.00755	1.00540	154.25	154.96	155.74	156.56	157.92	
0.4011	1.01713	1.01575	1.01415	1.01232	1.01004	153.77	154.46	155.13	155.89	157.30	
0.4732	1.02045	1.01901	1.01746	1.01561	1.01324	153.45	154.18	154.68	155.38	156.83	
Synephrine-HCl + water + 0.1 mol·kg ⁻¹ D-fructose											
0.0000	1.00580	1.00460	1.00314	1.00142	0.99944						
0.1002	1.00971	1.00845	1.00696	1.00520	1.00319	156.75	157.38	157.94	158.63	159.55	
0.2015	1.01418	1.01286	1.01132	1.00952	1.00746	156.82	157.50	158.11	158.76	159.58	
0.2975	1.01828	1.01691	1.01532	1.01348	1.01139	156.87	157.55	158.19	158.83	159.57	
0.4308	1.02377	1.02233	1.02068	1.01879	1.01670	156.92	157.60	158.27	158.87	159.48	
0.6024	1.03059	1.02899	1.02726	1.02532	1.02326	156.84	157.66	158.33	158.93	159.36	

Synephrine-HCl + water + 0.3 mol·kg ⁻¹ D-fructose										
0.0000	1.01838	1.01705	1.01548	1.01365	1.01163					
0.0989	1.02298	1.02159	1.01997	1.01807	1.01594	158.36	159.00	159.48	160.48	161.54
0.2081	1.02744	1.02600	1.02433	1.02240	1.02022	158.47	159.09	159.66	160.44	161.31
0.3073	1.03136	1.02987	1.02817	1.02620	1.02399	158.52	159.16	159.70	160.43	161.19
0.4522	1.03690	1.03534	1.03359	1.03152	1.02925	158.49	159.14	159.68	160.48	161.22
0.6056	1.04245	1.04084	1.03904	1.03699	1.03473	158.58	159.19	159.73	160.36	160.97
Synephrine-HCl + water + 0.5 mol·kg ⁻¹ D-fructose										
0.0000	1.03167	1.03023	1.02858	1.02665	1.02453					
0.1028	1.03566	1.03419	1.03248	1.03053	1.02836	160.14	160.49	160.97	161.39	161.92
0.1958	1.03920	1.03769	1.03596	1.03398	1.03178	160.02	160.49	160.93	161.41	161.96
0.3025	1.04315	1.04160	1.03981	1.03782	1.03559	159.92	160.42	160.97	161.39	161.96
0.4491	1.04834	1.04673	1.04489	1.04284	1.04056	159.92	160.44	161.00	161.49	162.09
0.6054	1.05370	1.05200	1.05012	1.04802	1.04573	159.78	160.37	160.91	161.42	161.96
Synephrine-HCl + water + 1.0 mol·kg ⁻¹ D-fructose										
0.0000	1.06096	1.05929	1.05739	1.05526	1.05294					
0.0998	1.06488	1.06292	1.06097	1.05882	1.05651	162.29	162.71	163.13	163.41	163.60
0.2035	1.06814	1.06617	1.06421	1.06205	1.05972	162.38	162.75	163.13	163.45	163.77
0.3007	1.07110	1.06913	1.06714	1.06496	1.06262	162.40	162.73	163.16	163.52	163.87
0.4472	1.07537	1.07340	1.07144	1.06919	1.06684	162.44	162.75	163.07	163.54	163.89
0.6037	1.07975	1.07780	1.07579	1.07352	1.07110	162.42	162.67	163.06	163.51	163.96
Octopamine-HCl + water										
0.1013	1.00342	1.00222	1.00077	0.99910	0.99719	137.66	138.14	138.75	139.55	140.62

0.1322	1.00498	1.00377	1.00231	1.00061	0.99868	137.65	138.12	138.70	139.57	140.59
0.1476	1.00576	1.00454	1.00307	1.00137	0.99942	137.62	138.12	138.71	139.51	140.58
0.1697	1.00687	1.00564	1.00416	1.00244	1.00048	137.57	138.07	138.67	139.50	140.51
0.1989	1.00833	1.00708	1.00559	1.00385	1.00188	137.52	138.07	138.65	139.48	140.42
0.2557	1.01115	1.00987	1.00834	1.00657	1.00458	137.42	137.99	138.63	139.43	140.28
0.3056	1.01361	1.01228	1.01073	1.00894	1.00692	137.30	137.96	138.58	139.35	140.19
0.3062	1.01364	1.01231	1.01076	1.00897	1.00694	137.29	137.95	138.57	139.34	140.21
0.3391	1.01523	1.01389	1.01232	1.01052	1.00850	137.27	137.91	138.55	139.28	140.06
0.3947	1.01792	1.01653	1.01495	1.01312	1.01108	137.15	137.85	138.44	139.17	139.91
0.4051	1.01842	1.01703	1.01544	1.01361	1.01156	137.14	137.82	138.42	139.14	139.89
Octopamine-HCl + water + 0.1 mol·kg ⁻¹ D-fructose										
0.0000	1.00580	1.00460	1.00314	1.00142	0.99944					
0.0487	1.00827	1.00705	1.00557	1.00382	1.00179	138.16	138.56	139.11	139.91	141.09
0.0969	1.01066	1.00943	1.00792	1.00614	1.00406	138.32	138.74	139.31	140.12	141.34
0.2066	1.01594	1.01467	1.01311	1.01126	1.00906	138.60	139.07	139.67	140.51	141.74
0.3085	1.02068	1.01936	1.01776	1.01582	1.01353	138.81	139.31	139.92	140.79	142.03
0.4098	1.02523	1.02386	1.02221	1.02019	1.01779	138.98	139.52	140.14	141.04	142.31
Octopamine-HCl + water + 0.3 mol·kg ⁻¹ D-fructose										
0.0000	1.01838	1.01705	1.01548	1.01365	1.01163					
0.0573	1.02118	1.01984	1.01826	1.01638	1.01431	138.69	138.98	139.45	140.30	141.42
0.1148	1.02391	1.02256	1.02096	1.01905	1.01693	139.02	139.31	139.79	140.55	141.68
0.2171	1.02859	1.02723	1.02559	1.02364	1.02142	139.48	139.74	140.24	140.95	142.05
0.3208	1.03312	1.03174	1.03007	1.02809	1.02580	139.89	140.17	140.65	141.29	142.32
0.4350	1.03786	1.03650	1.03479	1.03277	1.03042	140.36	140.55	141.04	141.65	142.61

Octopamine-HCl + water + 0.5 mol·kg ⁻¹ D-fructose										
0.0000	1.03167	1.03023	1.02858	1.02665	1.02453					
0.0549	1.03424	1.03277	1.03110	1.02914	1.02699	139.52	140.16	140.66	141.36	142.07
0.1107	1.03671	1.03523	1.03355	1.03154	1.02936	140.36	140.84	141.25	142.12	142.84
0.2120	1.04089	1.03934	1.03765	1.03557	1.03338	141.68	142.32	142.66	143.53	144.10
0.3286	1.04849	1.04671	1.04499	1.04280	1.04064	144.52	145.45	145.78	146.58	146.91
0.4278	1.04521	1.04358	1.04182	1.03967	1.03751	143.23	143.93	144.43	145.28	145.64
Octopamine-HCl + water + 1.0 mol·kg ⁻¹ D-fructose										
0.0000	1.06096	1.05929	1.05739	1.05526	1.05294					
0.0596	1.06341	1.06173	1.05981	1.05766	1.05530	141.92	142.24	142.72	143.24	144.08
0.1204	1.06577	1.06406	1.06213	1.05998	1.05759	142.61	143.07	143.49	143.85	144.61
0.2404	1.07009	1.06836	1.06636	1.06423	1.06177	143.76	144.16	144.74	144.96	145.73
0.3575	1.07392	1.07217	1.07010	1.06795	1.06543	144.77	145.15	145.82	146.06	146.83
0.4782	1.07755	1.07581	1.07365	1.07143	1.06895	145.65	145.96	146.70	147.08	147.65

Standard uncertainties are: $u(d) = 8.2 \cdot 10^{-4} \text{ g} \cdot \text{cm}^{-3}$, $u(m) = 3.5 \cdot 10^{-4} \text{ mol} \cdot \text{kg}^{-1}$, $u(T) = 0.015 \text{ K}$, $u(V_{\phi}) = 9.1 \cdot 10^{-3} \text{ cm}^3 \cdot \text{mol}^{-1}$

Relative standard uncertainty: $u_r(p)=0.015$

Table S3. Fitting parameters, obtained using equation (7), for synephrine-HCl and octopamine-HCl in aqueous solutions with a different molality of D-fructose in the temperature range from (293.15 to 313.15) K with the deviations of their fit (σ) and regression coefficient (R^2).

$T / (\text{K})$	$V_{\phi}^o / (\text{cm}^3 \cdot \text{mol}^{-1})$	$S_v' / (\text{cm}^{3/2} \cdot \text{mol}^{-1/2})^2$	$b / (\text{cm}^3 \cdot \text{mol}^{-1})^2$	σ	R^2
Synephrine-HCl + water					
293.15	154.96	1.78	-5.99	0.087	0.9956
298.15	155.60	1.87	-5.92	0.077	0.9964
303.15	156.55	1.96	-7.06	0.084	0.9970
308.15	157.90	2.05	-8.88	0.116	0.9964
313.15	159.06	2.14	-8.15	0.079	0.9979
Synephrine-HCl + water + 0.1 mol·kg ⁻¹ D-fructose					
293.15	156.33	1.78	-1.44	0.026	0.9961
298.15	156.90	1.87	-1.16	0.016	0.9977
303.15	157.44	1.96	-1.00	0.008	0.9991
308.15	158.11	2.05	-1.29	0.012	0.9990
313.15	159.13	2.14	-2.49	0.027	0.9999
Synephrine-HCl + water + 0.3 mol·kg ⁻¹ D-fructose					
293.15	157.92	1.78	-1.27	0.034	0.9912
298.15	158.55	1.87	-1.39	0.024	0.9962
303.15	159.03	1.96	-1.38	0.032	0.9934
308.15	160.00	2.05	-2.14	0.058	0.9908
313.15	161.07	2.14	-3.15	0.116	0.9834
Synephrine-HCl + water + 0.5 mol·kg ⁻¹ D-fructose					
293.15	159.74	1.78	-2.44	0.073	0.9887
298.15	160.07	1.87	-2.04	0.050	0.9925
303.15	160.50	1.96	-1.93	0.047	0.9925
308.15	160.88	2.05	-1.81	0.051	0.9899
313.15	161.41	2.14	-1.87	0.057	0.9880
Synephrine-HCl + water + 1.0 mol·kg ⁻¹ D-fructose					
293.15	161.88	1.78	-1.45	0.013	0.9988
298.15	162.31	1.87	-1.92	0.023	0.9980
303.15	162.71	1.96	-2.13	0.034	0.9963
308.15	162.93	2.05	-1.75	0.025	0.9969
313.15	163.09	2.14	-1.30	0.024	0.9953
Octopamine-HCl + water					
293.15	137.48	1.78	-3.84	0.020	0.9988
298.15	137.84	1.87	-3.07	0.013	0.9992

303.15	138.41	1.96	-3.10	0.022	0.9977
308.15	139.28	2.05	-3.60	0.019	0.9987
313.15	140.45	2.14	-4.93	0.021	0.9991
Octopamine-HCl + water + 0.1 mol·kg ⁻¹ D-fructose					
293.15	137.75	1.78	3.99	0.004	0.9976
298.15	138.11	1.87	3.82	0.005	0.9989
303.15	138.64	1.96	2.97	0.006	0.9987
308.15	139.42	2.05	2.74	0.007	0.9990
313.15	140.58	2.14	2.99	0.007	0.9992
Octopamine-HCl + water + 0.3 mol·kg ⁻¹ D-fructose					
293.15	138.12	1.78	2.77	0.017	0.9993
298.15	138.41	1.87	2.44	0.016	0.9991
303.15	138.88	1.96	2.38	0.010	0.9996
308.15	139.71	2.05	1.61	0.018	0.9976
313.15	140.87	2.14	1.01	0.012	0.9970
Octopamine-HCl + water + 0.5 mol·kg ⁻¹ D-fructose					
293.15	138.43	1.78	13.03	0.045	0.9997
298.15	138.89	1.87	13.94	0.134	0.9981
303.15	139.34	1.96	13.60	0.162	0.9971
308.15	140.11	2.05	13.70	0.090	0.9991
313.15	140.91	2.14	12.27	0.081	0.9991
Octopamine-HCl + water + 1.0 mol·kg ⁻¹ D-fructose					
293.15	141.45	1.78	10.58	0.058	0.9992
298.15	141.86	1.87	10.46	0.116	0.9965
303.15	142.25	1.96	11.33	0.091	0.9982
308.15	142.67	2.05	11.00	0.042	0.9996
313.15	143.54	2.14	10.43	0.071	0.9985

Table S4. Fitting coefficients obtained using equation (9), a_1 and a_2 of synephrine-HCl and octopamine-HCl in aqueous solutions with a different molality of D-fructose in the temperature range from (293.15 to 313.15) K.

$m / \text{mol} \cdot \text{kg}^{-1}$	$a_1 / (\text{cm}^3 \cdot \text{mol}^{-1})$	$a_2 / (\text{cm}^3 \cdot \text{mol}^{-1})$	R^2
Synephrine-HCl			
0	-2.28	0.0041	0.9946
0.1	-1.65	0.0029	0.9939
0.3	-2.22	0.0039	0.9930
0.5	-0.52	0.0010	0.9978
1	1.31	-0.0021	0.9976
Octopamine-HCl			
0	-3.18	0.0055	0.9997
0.1	-3.06	0.0053	0.9983
0.3	-3.50	0.0060	0.9988
0.5	-1.61	0.0029	0.9971
1	-1.55	0.0027	0.9938

Table S5. Values of the limiting apparent molar expansibilities and Hepler's coefficients of synephrine-HCl and octopamine-HCl in aqueous solutions with a different molality of D-fructose in the temperature range from (293.15 to 313.15) K.

$T / (\text{K})$	293.15	298.15	303.15	308.15	313.15	$\left(\frac{\partial E_\phi^\circ}{\partial T} \right)_p / (\text{cm}^3 \cdot \text{mol}^{-1} \cdot \text{K}^{-2})$
$m / (\text{mol} \cdot \text{kg}^{-1})$	$E_\phi^\circ / (\text{cm}^3 \cdot \text{mol}^{-1} \cdot \text{K}^{-1})$ of synephrine-HCl					
0	0.1238	0.1648	0.2058	0.2468	0.2878	0.0082
0.1	0.0503	0.0793	0.1083	0.1373	0.1663	0.0058
0.3	0.0742	0.1133	0.1524	0.1915	0.2306	0.0078

0.5	0.0642	0.0743	0.0843	0.0943	0.1043	0.0020
1	0.1003	0.0797	0.0591	0.0385	0.0179	-0.0041
$m / (\text{mol} \cdot \text{kg}^{-1})$	$E_{\phi}^{\circ} / (\text{cm}^3 \cdot \text{mol}^{-1} \cdot \text{K}^{-1})$ of octopamine-HCl					$\left(\frac{\partial E_{\phi}^{\circ}}{\partial T} \right)_p / (\text{cm}^3 \cdot \text{mol}^{-1} \cdot \text{K}^{-2})$
0	0.0404	0.0953	0.1502	0.2051	0.2600	0.0110
0.1	0.0362	0.0891	0.1420	0.1949	0.2478	0.0106
0.3	0.0178	0.0778	0.1378	0.1978	0.2578	0.0120
0.5	0.0903	0.1193	0.1483	0.1773	0.2063	0.0058
1	0.0330	0.0600	0.0870	0.1140	0.1410	0.0054

Table S6. The viscosity of synephrine-HCl and octopamine-HCl in aqueous solutions (η) as a function of synephrine-HCl and octopamine-HCl molality (m) in the temperature range from (293.15 to 313.15) K at $p = 0.1$ MPa.

$m /$ ($\text{mol} \cdot \text{kg}^{-1}$)	$T / (\text{K})$				
	293.15	298.15	303.15	308.15	313.15
$\eta / (\text{mPa} \cdot \text{s})$ synephrine-HCl					
0.0811	1.055	0.936	0.838	0.755	0.685
0.0984	1.064	0.944	0.845	0.761	0.690
0.1502	1.093	0.969	0.866	0.780	0.707
0.2022	1.117	0.989	0.885	0.796	0.721
0.2544	1.142	1.011	0.903	0.812	0.735
0.3001	1.164	1.029	0.919	0.826	0.747
$\eta / (\text{mPa} \cdot \text{s})$ of octopamine-HCl					
0.0494	1.027	0.913	0.819	0.740	0.672
0.0749	1.037	0.923	0.827	0.748	0.680
0.0989	1.047	0.931	0.835	0.755	0.687
0.2045	1.086	0.968	0.868	0.785	0.714
0.3000	1.124	1.000	0.899	0.813	0.739
0.3911	1.164	1.037	0.931	0.840	0.764

Relative standard uncertainties: $u_r(\eta) = 0.01$, $u_r(p) = 0.015$;
Standard uncertainties: $u(T) = 0.015$ K, $u(m) = 3.5 \cdot 10^{-4} \text{mol} \cdot \text{kg}^{-1}$

Table S7. Extended Jones–Dole’s equation (14) fitting parameters for the viscosity of synephrine-HCl and octopamine-HCl in aqueous solutions in the temperature range from (293.15 to 313.15) K with the deviations of their fit (σ) and regression coefficient (R^2).

$T / (\text{K})$	$A / (\text{dm}^{3/2}\cdot\text{mol}^{-1/2})$	$B / (\text{dm}^3\cdot\text{mol}^{-1})$	$D / (\text{dm}^3\cdot\text{mol}^{-1})^2$	σ	R^2
Synephrine-HCl					
293.15	0.093	0.401	0.206	0.001	0.9996
298.15	0.097	0.382	0.195	0.002	0.9994
303.15	0.101	0.359	0.182	0.002	0.9993
308.15	0.105	0.331	0.147	0.001	0.9999
313.15	0.109	0.312	0.123	0.001	0.9999
Octopamine-HCl					
293.15	0.068	0.347	0.322	0.005	0.9980
298.15	0.077	0.323	0.317	0.006	0.9988
303.15	0.079	0.295	0.306	0.005	0.9997
308.15	0.079	0.282	0.238	0.004	0.9992
313.15	0.081	0.266	0.196	0.003	0.9995

Table S8. Values of hydration numbers of synephrine-HCl and octopamine-HCl calculated with equation (16) in the temperature range from (293.15 to 313.15) K and hydration number calculated with equation (18).

$T / (\text{K})$	$h_n^{(16)}$	$h_n^{(18)}$
	Synephrine-HCl	
293.15	12.26	-
298.15	11.99	10.12
303.15	11.66	-
308.15	11.14	-
313.15	10.57	-
$T / (\text{K})$	Octopamine-HCl	
293.15	7.91	-
298.15	7.08	6.60
303.15	6.54	-
308.15	5.83	-
313.15	4.93	-

Table S9. Contribution of methyl group to transfer volumes $\Delta_{\text{tr}}V_{\phi}^{\circ}$ with molality of D-fructose at different temperatures.

$T / (\text{K})$	293.15	298.15	303.15	308.15	313.15
$m / (\text{mol} \cdot \text{kg}^{-1})$	$\Delta_{\text{tr}}V_{\phi}^{\circ} (\text{CH}_3) / (\text{cm}^3 \cdot \text{mol}^{-1})$				
0	/	/	/	/	/
0.1	1.10	1.04	0.66	0.07	-0.06
0.3	2.32	2.38	2.02	1.67	1.59
0.5	3.83	3.42	3.02	2.16	1.90
1	2.95	2.70	2.32	1.64	0.94

Table S10. Apparent specific volume at infinite dilution, v_{ϕ}° of synephrine-HCl and octopamine-HCl in aqueous solutions in the temperature range from (293.15 to 313.15) K, and v_{ϕ}° of epinephrine-HCl, norepinephrine-HCl and tyramine-HCl in aqueous solutions calculated from literature V_{ϕ}° values at $T=298.15$ K [29].

Compound	$T / (\text{K})$				
	293.15	298.15	303.15	308.15	313.15
	$v_{\phi}^{\circ} / (\text{cm}^3 \cdot \text{mol}^{-1})$				
Synephrine-HCl	0.76	0.76	0.77	0.78	0.78
Octopamine-HCl	0.72	0.73	0.73	0.73	0.74
Epinephrine-HCl	-	0.71	-	-	-
Norepinephrine-HCl	-	0.67	-	-	-
Tyramine-HCl	-	0.78	-	-	-

Table S11. Apparent specific volume at infinite dilution, v_{ϕ}° of synephrine-HCl and octopamine-HCl in aqueous solutions with a different molality of D-fructose in the temperature range from (293.15 to 313.15) K.

$m /$ ($\text{mol} \cdot \text{kg}^{-1}$)	$T / (\text{K})$				
	293.15	298.15	303.15	308.15	313.15
	$v_{\phi}^{\circ} / (\text{cm}^3 \cdot \text{mol}^{-1})$				
Synephrine-HCl					
0.0	0.76	0.76	0.77	0.78	0.78
0.1	0.77	0.77	0.77	0.78	0.78
0.3	0.78	0.78	0.78	0.79	0.79
0.5	0.78	0.79	0.79	0.79	0.79
1.0	0.79	0.80	0.80	0.80	0.80
Octopamine-HCl					
0.0	0.72	0.73	0.73	0.73	0.74
0.1	0.73	0.73	0.73	0.74	0.74
0.3	0.73	0.73	0.73	0.74	0.74
0.5	0.73	0.73	0.73	0.74	0.74
1.0	0.75	0.75	0.75	0.75	0.76

Table S12. The docking parameters for investigated ligands.

Ligand	Binding free energy / kJ·mol ⁻¹	Docking score
Synephrine-HCl	-24.98	-7.332
Octopamine-HCl	-22.36	-6.928
Fructose	-18.64	-5.023

Table S13. List and type of interactions obtained from molecular docking simulations.

Interactions	Type of interactions
Synephrine-HCl	
Met 100	Hydrophobic
Met 111	Hydrophobic
Asn 183	H-bond
Ser 194	Hydrophobic
Arg 197	Van der Waals
Cys 198	Hydrophobic
Tyr 199	H-bond
Trp 201	Van der Waals
Arg 206	Van der Waals
Phe 264	H-bond
Ser 266	Hydrophobic
Val 267	H-bond
Ile 271	Hydrophobic
Cys 282	Hydrophobic
Octopamine-HCl	
Met 100	Hydrophobic
Asn 183	H-bond
Ser 189	Hydrophobic
Ser 194	Hydrophobic
Arg 197	Van der Waals
Cys 198	Hydrophobic
Tyr 199	H-bond
Ala 262	Van der Waals
Phe 264	H-bond
Val 267	H-bond
Cys 282	Hydrophobic
Fructose	
Asn 189	H-bond
Trp 201	Van der Waals
Ile 271	Hydrophobic
Asn 292	H-bond
Asp 328	H-bond
Cys 365	Hydrophobic
Asn 371	H-bond

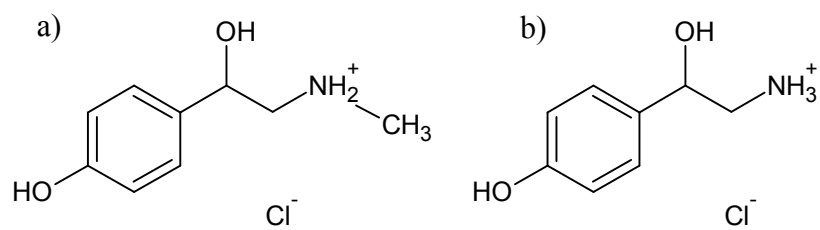


Fig. S1. Structure of a) synephrine-HCl and b) octopamine-HCl

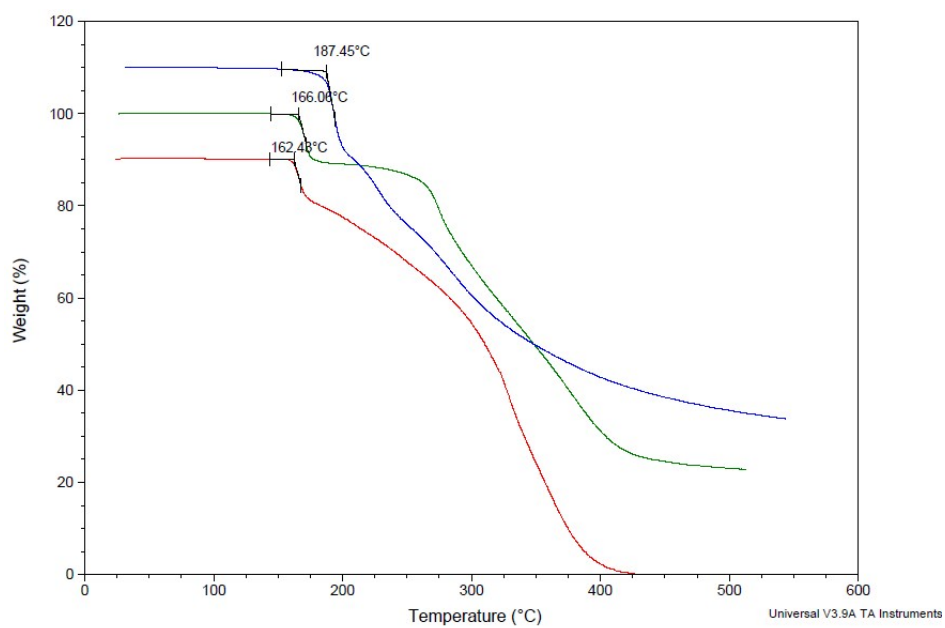


Fig. S2. TG curves for (red line) synephrine-HCl, (green line) octopamine-HCl and (blue line) synephrine.

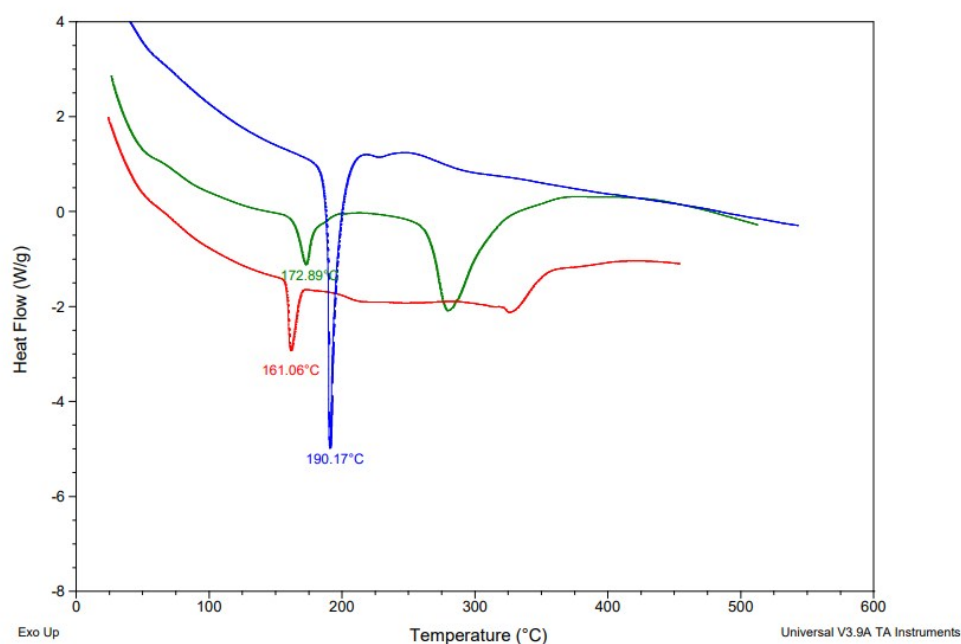


Fig. S3. DSC curves for (red line) synephrine-HCl, (green line) octopamine-HCl and (blue line) synephrine.

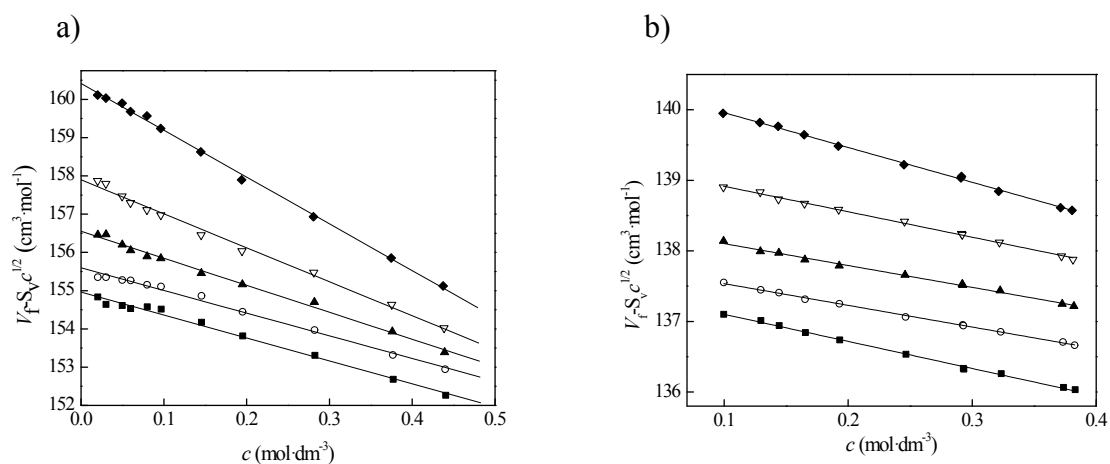


Fig. S4. Variation of $V_\phi - S_v c^{1/2}$ with a) synephrine-HCl and b) octopamine-HCl concentration at different temperatures: (●), 293.15; (○), 298.15; (▲), 303.15; (▽), 308.15 and (◆) 313.15 K.

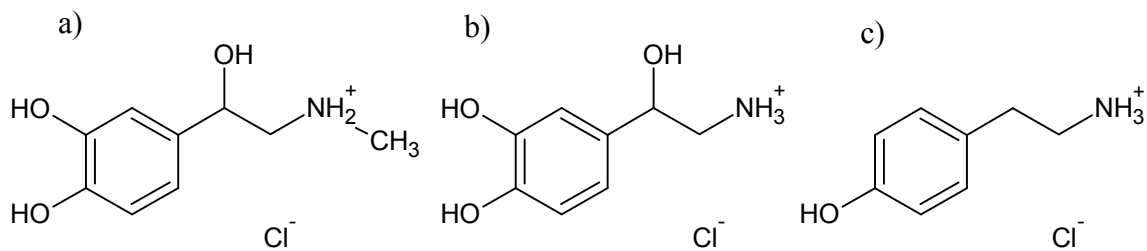


Fig. S5. Structure of a) epinephrine-HCl b) norepinephrine-HCl and c) tyramine-HCl

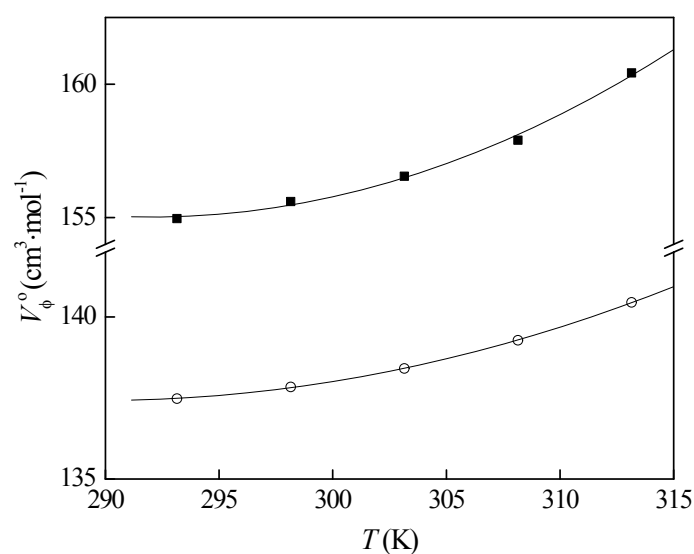


Fig. S6. Variation of the apparent molar volume at infinite dilution (V_{ϕ}^0) with a temperature of synephrine-HCl (O) and octopamine-HCl (■).

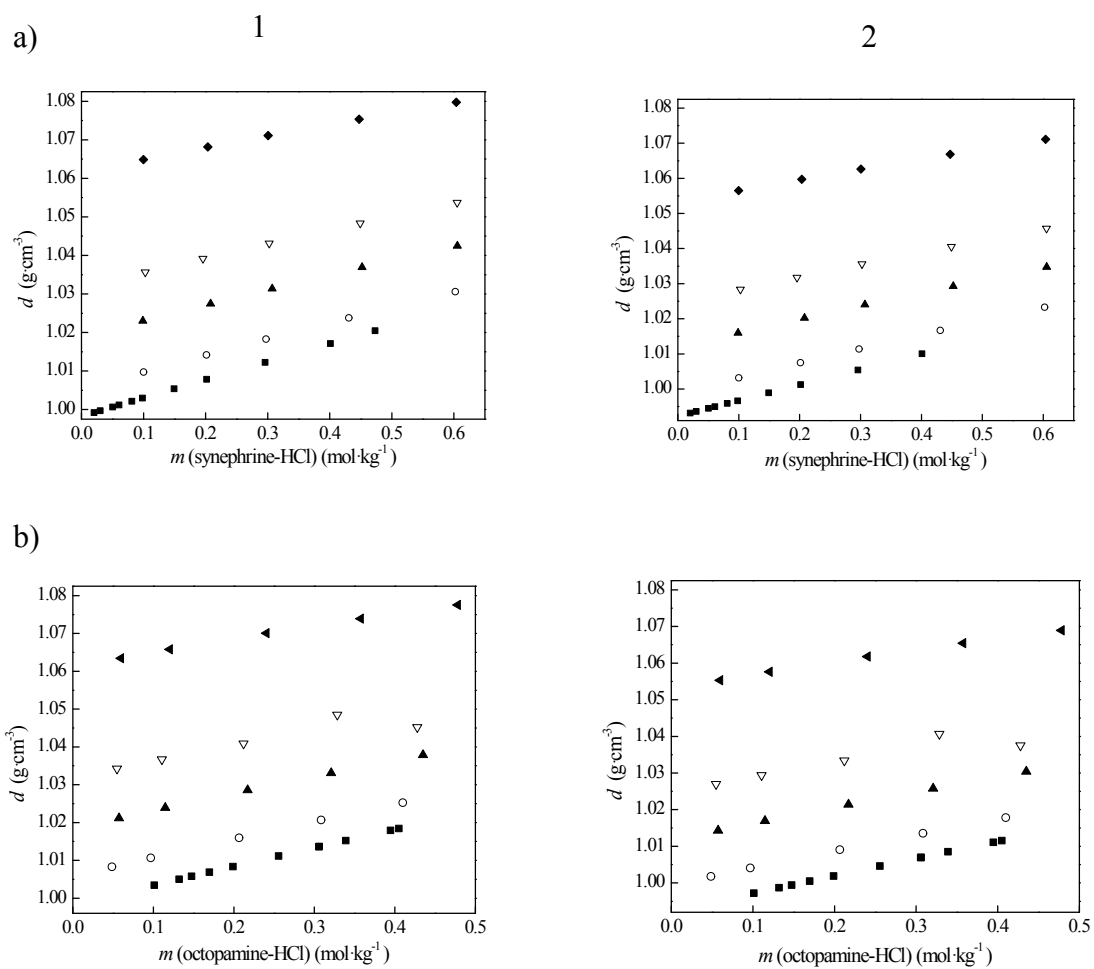


Fig. S7. Density for a) synephrine-HCl and b) octopamine-HCl versus molality of synephrine/octopamine-HCl at (1) $T=293.15$ K and (2) $T=313.15$ K in aqueous solutions with different molality of D-fructose: (●), 0.0; (⊗), 0.1; (▲), 0.3; (▽), 0.5 and (◆) $1.0 \text{ mol}\cdot\text{kg}^{-1}$.

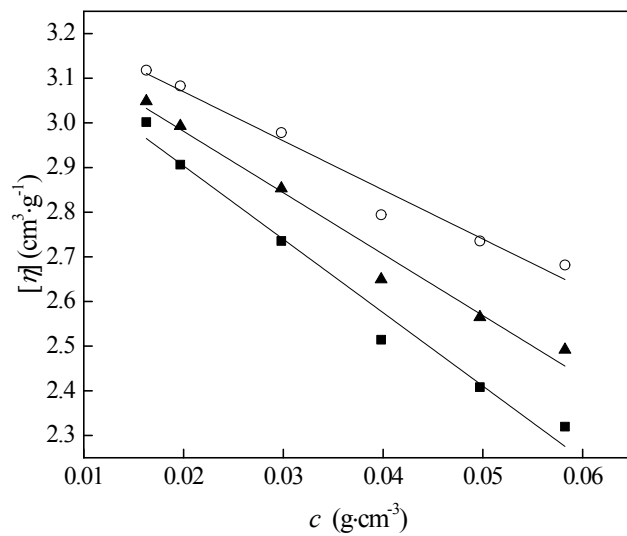


Fig. S8. Determination of intrinsic viscosity, $[\eta]$, of synephrine-HCl by extrapolation of: (○) η_{sp}/c ; (◻) $(\ln \eta/\eta_0)/c$ and (▲) η_{diff}/c .