

SUPPLEMENTARY MATERIAL

Title: Aggregation behaviour of betablockers drugs in aqueous media

Authors: Estefania Zuriaga, Laura Lomba, Félix M. Royo, Carlos Lafuente, Beatriz Giner

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Table 1. Densities, ρ , speeds of sound, u , isentropic compressibilities, κ_s , apparent molar volume, V_ϕ , and apparent molar isentropic compressions, $K_{S,\phi}$, of propranolol + water at $T = 298.15$ K

m (mol·kg ⁻¹)	ρ (kg·m ⁻³)	u (m·s ⁻¹)	κ_s (TPa ⁻¹)	$10^6 \cdot V_\phi$ (m ³ ·mol ⁻¹)	$K_{S,\phi}$ (TPa ⁻¹ ·m ³ ·mol ⁻¹)	m (mol·kg ⁻¹)	ρ (g·cm ⁻³)	u (m·s ⁻¹)	κ_s (TPa ⁻¹)	$10^6 \cdot V_\phi$ (m ³ ·mol ⁻¹)	$K_{S,\phi}$ (TPa ⁻¹ ·m ³ ·mol ⁻¹)
0.00093	997.241	1496.96	447.52	82.5030	-0.0331	0.03804	999.113	1503.43	446.43	241.4464	-0.0180
0.00104	997.251	1496.99	447.51	95.4793	-0.0415	0.04200	999.306	1504.4	445.99	241.9372	-0.0168
0.00116	997.261	1497.02	447.51	107.6164	-0.0468	0.04519	999.472	1504.62	441.95	242.0275	-0.0173
0.00123	997.267	1497.03	447.50	113.4662	-0.0458	0.04983	999.702	1505.30	441.45	242.3625	-0.0158
0.00135	997.274	1497.05	447.50	124.5309	-0.0435	0.05371	999.901	1506.04	440.93	242.4645	-0.0167
0.00149	997.281	1497.07	447.49	135.9744	-0.0392	0.05942	1000.181	1506.88	440.32	242.7989	-0.0152
0.00160	997.286	1497.09	447.49	143.8751	-0.0377	0.06250	1000.326	1507.67	439.79	243.0470	-0.0176
0.00175	997.292	1497.11	447.49	153.5180	-0.0330	0.06974	1000.693	1508.94	438.89	243.1490	-0.0178
0.00202	997.298	1497.13	447.46	169.6564	-0.0195	0.07675	1001.042	1509.79	438.24	243.2977	-0.0150
0.00239	997.324	1497.19	447.47	178.3654	-0.0208	0.08489	1001.442	1510.82	437.47	243.4852	-0.0126
0.00256	997.333	1497.25	447.46	182.6800	-0.0278	0.09470	1001.908	1512.28	436.42	243.8197	-0.0114
0.00303	997.351	1497.37	447.43	194.3733	-0.0320	0.10194	1002.216	1513.25	435.73	244.3724	-0.0098
0.00413	997.414	1497.53	447.40	206.2464	-0.0251	0.11123	1002.741	1514.57	434.74	243.7627	-0.0095
0.00726	997.555	1498.06	447.36	225.6291	-0.0184	0.11905	1003.197	1515.56	433.98	243.1867	-0.0088
0.01068	997.738	1498.67	447.31	231.0648	-0.0197	0.12626	1003.505	1516.38	433.38	243.6242	-0.0070
0.01273	997.848	1499.07	447.27	232.8872	-0.0218	0.13680	1003.845	1517.43	432.63	244.9983	-0.0034
0.01487	997.954	1499.44	447.23	234.8445	-0.0210	0.14472	1004.093	1518.22	432.07	245.9441	-0.0010
0.01789	998.112	1499.99	447.14	236.3249	-0.0215	0.15198	1004.303	1519.04	431.52	246.8367	0.0007
0.02066	998.246	1500.45	446.98	237.8260	-0.0200	0.16155	1004.513	1519.82	430.98	248.3127	0.0042

0.03019	998.731	1502.15	447.05	240.0362	-0.0202	0.16978	1004.741	1520.52	430.49	249.1533	0.0065
0.03432	998.928	1502.71	446.72	240.9812	-0.0169						

Table 2. Densities, ρ , speeds of sound, u , isentropic compressibilities, κ_s , apparent molar volume, V_ϕ , and apparent molar isentropic compressions, $K_{S,\phi}$, of atenolol + water at $T = 298.15$ K

m (mol·kg ⁻¹)	ρ (kg·m ⁻³)	u (m·s ⁻¹)	κ_s (TPa ⁻¹)	$10^6 \cdot V_\phi$ (m ³ ·mol ⁻¹)	$K_{S,\phi}$ (TPa ⁻¹ ·m ³ ·mol ⁻¹)	m (mol·kg ⁻¹)	ρ (g·cm ⁻³)	u (m·s ⁻¹)	κ_s (TPa ⁻¹)	$10^6 \cdot V_\phi$ (m ³ ·mol ⁻¹)	$K_{S,\phi}$ (TPa ⁻¹ ·m ³ ·mol ⁻¹)
0.00105	997.245	1496.91	447.52	73.5511	-0.0023	0.00583	997.438	1497.66	446.98	198.8555	-0.0094
0.00107	997.246	1496.91	447.51	76.2276	-0.0008	0.00533	997.419	1497.56	447.05	196.0527	-0.0071
0.00111	997.248	1496.92	447.51	81.2913	-0.0035	0.00862	997.559	1498.01	446.72	206.7664	-0.0047
0.00115	997.249	1496.93	447.50	86.8773	-0.0053	0.01126	997.654	1498.42	446.43	212.3744	-0.0051
0.00117	997.250	1496.93	447.50	89.0972	-0.0039	0.01469	997.851	1499.01	445.99	211.5882	-0.0122
0.00123	997.253	1496.94	447.49	95.3238	-0.0049	0.02060	998.030	1499.80	445.44	218.6761	-0.0053
0.00125	997.254	1496.94	447.49	97.2665	-0.0037	0.02555	998.196	1500.12	445.18	221.4384	0.0054
0.00129	997.255	1496.95	447.49	101.7508	-0.0052	0.03015	998.312	1500.91	444.66	224.4645	0.0035
0.00136	997.257	1496.99	447.46	108.7788	-0.0177	0.03577	998.594	1501.87	443.96	223.1248	-0.0016
0.00144	997.260	1496.97	447.47	115.4750	-0.0037	0.03981	998.813	1502.63	443.42	221.9704	-0.0057
0.00159	997.266	1496.98	447.46	125.9769	0.0008	0.04344	999.002	1503.31	442.93	221.2904	-0.0086
0.00170	997.270	1497.03	447.43	132.7369	-0.0113	0.04636	999.136	1503.92	442.51	221.2106	-0.0111
0.00199	997.284	1497.08	447.40	145.2297	-0.0136	0.05043	999.291	1504.42	442.15	221.7484	-0.0094
0.00248	997.303	1497.13	447.36	161.5862	-0.0063	0.05115	999.331	1504.52	442.07	221.5844	-0.0094
0.00283	997.318	1497.19	447.31	169.2927	-0.0083	0.05780	999.508	1505.29	441.54	223.6365	-0.0055
0.00316	997.331	1497.25	447.27	175.3585	-0.0100	0.06061	999.585	1505.51	441.38	224.3284	-0.0031
0.00358	997.349	1497.31	447.23	181.0516	-0.0094	0.06757	999.731	1506.17	440.93	226.4620	0.0016
0.00433	997.376	1497.44	447.14	189.6643	-0.0107	0.07283	999.815	1506.54	440.68	228.1681	0.0059

Table 3. Densities, ρ , speeds of sound, u , isentropic compressibilities, κ_s , apparent molar volume, V_ϕ , and apparent molar isentropic compressions, $K_{S,\phi}$, of nadolol + water at $T = 298.15$ K

m (mol·kg ⁻¹)	ρ (kg·m ⁻³)	u (m·s ⁻¹)	κ_s (TPa ⁻¹)	$10^6 \cdot V_\phi$ (m ³ ·mol ⁻¹)	$K_{S,\phi}$ (TPa ⁻¹ ·m ³ ·mol ⁻¹)	m (mol·kg ⁻¹)	ρ (g·cm ⁻³)	u (m·s ⁻¹)	κ_s (TPa ⁻¹)	$10^6 \cdot V_\phi$ (m ³ ·mol ⁻¹)	$K_{S,\phi}$ (TPa ⁻¹ ·m ³ ·mol ⁻¹)
0.00091	997.254	1496.95	447.49	77.0558	-0.0369	0.00477	997.452	1497.64	446.99	223.9721	-0.0189
0.00099	997.260	1496.96	447.48	89.8041	-0.0342	0.00519	997.475	1497.71	446.93	226.4880	-0.0182
0.00107	997.265	1496.97	447.47	101.5859	-0.0311	0.00617	997.522	1497.87	446.82	232.1112	-0.0157
0.00117	997.270	1496.98	447.46	115.1218	-0.0256	0.00732	997.581	1498.06	446.68	236.2563	-0.0142
0.00119	997.271	1496.98	447.46	117.5559	-0.0236	0.00895	997.652	1498.29	446.51	241.7211	-0.0090
0.00126	997.274	1496.99	447.45	125.8661	-0.0214	0.00990	997.697	1498.42	446.41	243.7047	-0.0068
0.00144	997.281	1497.01	447.44	144.0236	-0.0141	0.01222	997.827	1498.58	446.26	245.5863	0.0034
0.00162	997.292	1497.04	447.42	155.6620	-0.0143	0.01412	997.862	1498.79	446.12	251.7634	0.0104
0.00179	997.305	1497.09	447.38	163.0366	-0.0231	0.01597	998.003	1499.07	445.89	249.6075	0.0068
0.00205	997.318	1497.13	447.35	175.3260	-0.0200	0.01920	998.155	1499.57	445.52	251.7761	0.0061
0.00228	997.331	1497.18	447.31	183.1985	-0.0222	0.01955	998.168	1499.59	445.50	252.1465	0.0073
0.00264	997.351	1497.23	447.28	192.8983	-0.0184	0.02374	998.331	1500.16	445.09	255.4110	0.0098
0.00333	997.384	1497.36	447.18	207.2360	-0.0182	0.02614	998.395	1500.29	444.99	257.9391	0.0164
0.00346	997.391	1497.39	447.16	209.0691	-0.0193	0.03535	998.560	1500.87	444.57	266.7431	0.0340
0.00396	997.411	1497.49	447.09	216.7563	-0.0191	0.04579	998.699	1501.33	444.24	273.4834	0.0489
0.00420	997.423	1497.53	447.06	219.2204	-0.0183						

Table 4. Densities, ρ , speeds of sound, u , isentropic compressibilities, κ_s , apparent molar volume, V_ϕ , and apparent molar isentropic compressions, $K_{S,\phi}$, of metoprolol + water at $T = 298.15$ K

m (mol·kg ⁻¹)	ρ (kg·m ⁻³)	u (m·s ⁻¹)	κ_s (TPa ⁻¹)	$10^6 \cdot V_\phi$ (m ³ ·mol ⁻¹)	$K_{S,\phi}$ (TPa ⁻¹ ·m ³ ·mol ⁻¹)	m (mol·kg ⁻¹)	ρ (g·cm ⁻³)	u (m·s ⁻¹)	κ_s (TPa ⁻¹)	$10^6 \cdot V_\phi$ (m ³ ·mol ⁻¹)	$K_{S,\phi}$ (TPa ⁻¹ ·m ³ ·mol ⁻¹)
0.00108	997.258	1496.80	447.57	486.4794	0.2392	0.00803	998.319	1500.17	445.09	526.3194	-0.0729
0.00121	997.311	1497.00	447.43	463.9130	0.1079	0.01253	998.955	1502.00	443.73	532.3199	-0.0700
0.00141	997.376	1497.19	447.29	449.1178	0.0138	0.01255	998.958	1502.01	443.72	532.3225	-0.0701
0.00151	997.401	1497.32	447.20	448.1856	-0.0333	0.02187	1000.234	1505.77	440.94	538.3437	-0.0657
0.00176	997.445	1497.48	447.08	456.8909	-0.0619	0.03105	1001.372	1509.12	438.49	544.2295	-0.0541
0.00191	997.473	1497.58	447.01	460.1743	-0.0775	0.05086	1004.045	1517.09	432.74	544.5270	-0.0565
0.00201	997.489	1497.63	446.97	463.4250	-0.0805	0.07310	1006.839	1525.30	426.90	546.6657	-0.0499
0.00221	997.513	1497.72	446.91	472.6852	-0.0796	0.10173	1010.460	1535.32	419.84	546.8109	-0.0436
0.00244	997.535	1497.80	446.85	483.7651	-0.0709	0.11455	1012.078	1539.19	417.06	546.5666	-0.0390
0.00242	997.535	1497.80	446.85	482.0896	-0.0741	0.13774	1015.361	1547.25	411.39	543.0836	-0.0399
0.00300	997.618	1498.03	446.68	493.7510	-0.0713	0.14948	1016.985	1551.18	408.66	541.8027	-0.0395
0.00363	997.709	1498.35	446.45	501.9447	-0.0810	0.16722	1018.819	1556.31	405.24	543.9633	-0.0334
0.00467	997.853	1498.70	446.17	511.9472	-0.0674	0.19231	1021.055	1563.62	400.58	548.0398	-0.0254
0.00626	998.081	1499.39	445.66	519.5005	-0.0712	0.22831	1023.168	1570.50	396.26	557.1352	-0.0046

Table 5. Densities, ρ , speeds of sound, u , isentropic compressibilities, κ_s , apparent molar volume, V_ϕ , and apparent molar isentropic compressions, $K_{S,\phi}$, of timolol + water at $T = 298.15$ K

m (mol·kg ⁻¹)	ρ (kg·m ⁻³)	u (m·s ⁻¹)	κ_s (TPa ⁻¹)	$10^6 \cdot V_\phi$ (m ³ ·mol ⁻¹)	$K_{S,\phi}$ (TPa ⁻¹ ·m ³ ·mol ⁻¹)	m (mol·kg ⁻¹)	ρ (g·cm ⁻³)	u (m·s ⁻¹)	κ_s (TPa ⁻¹)	$10^6 \cdot V_\phi$ (m ³ ·mol ⁻¹)	$K_{S,\phi}$ (TPa ⁻¹ ·m ³ ·mol ⁻¹)
0.00098	997.304	1496.90	447.49	165.8307	0.0155	0.01047	998.346	1498.53	446.05	308.1898	-0.0059
0.00096	997.298	1496.89	447.50	166.5372	0.0237	0.01126	998.432	1498.69	445.92	309.2621	-0.0073
0.00112	997.324	1496.95	447.45	181.3483	-0.0050	0.01765	999.132	1499.71	445.00	314.0646	-0.0051
0.00130	997.339	1497.00	447.42	204.6771	-0.0109	0.01772	999.134	1499.73	444.99	314.4201	-0.0050
0.00165	997.378	1497.05	447.37	229.4692	-0.0069	0.02013	999.400	1500.12	444.64	315.2530	-0.0049
0.00221	997.438	1497.14	447.29	253.8873	-0.0048	0.02203	999.606	1500.49	444.33	315.9381	-0.0063
0.00314	997.536	1497.28	447.16	275.7073	-0.0008	0.02415	999.827	1500.81	444.04	316.9334	-0.0050
0.00323	997.551	1497.29	447.15	275.4325	-0.0014	0.03259	1000.742	1502.18	442.83	318.4260	-0.0044
0.00386	997.632	1497.37	447.07	280.1201	-0.0009	0.03683	1001.202	1502.84	442.23	318.8576	-0.0038
0.00408	997.646	1497.48	446.99	284.9383	-0.0096	0.04029	1001.560	1503.45	441.72	319.5568	-0.0041
0.00428	997.667	1497.50	446.97	286.9427	-0.0073	0.04634	1002.221	1504.39	440.88	319.7192	-0.0035
0.00463	997.683	1497.49	446.97	294.5436	0.0061	0.05025	1002.626	1505.03	440.32	320.2251	-0.0033
0.00545	997.800	1497.69	446.80	293.8354	-0.0070	0.06680	1004.366	1507.51	438.11	321.1470	-0.0010
0.00553	997.806	1497.71	446.78	294.7628	-0.0073	0.06743	1004.437	1507.62	438.02	321.0956	-0.0011
0.00640	997.907	1497.84	446.66	297.7228	-0.0063	0.08117	1005.856	1509.71	436.19	321.7194	0.0000
0.00782	998.052	1498.07	446.46	303.6808	-0.0043	0.09488	1007.290	1511.79	434.37	321.8340	0.0005
0.00881	998.161	1498.28	446.29	305.7847	-0.0075	0.10953	1008.784	1513.82	432.57	322.1579	0.0021

Table 6. Densities, ρ , speeds of sound, u , isentropic compressibilities, κ_s , apparent molar volume, V_ϕ , and apparent molar isentropic compressions, $K_{S,\phi}$, of acebutolol + water at $T = 298.15$ K

m (mol·kg ⁻¹)	ρ (kg·m ⁻³)	u (m·s ⁻¹)	κ_s (TPa ⁻¹)	$10^6 \cdot V_\phi$ (m ³ ·mol ⁻¹)	$K_{S,\phi}$ (TPa ⁻¹ ·m ³ ·mol ⁻¹)	m (mol·kg ⁻¹)	ρ (g·cm ⁻³)	u (m·s ⁻¹)	κ_s (TPa ⁻¹)	$10^6 \cdot V_\phi$ (m ³ ·mol ⁻¹)	$K_{S,\phi}$ (TPa ⁻¹ ·m ³ ·mol ⁻¹)
0.00097	997.259	1496.91	447.51	149.9602	0.0225	0.00752	997.701	1498.31	446.47	285.7875	-0.0160
0.00105	997.267	1496.93	447.49	159.3595	0.0153	0.00930	997.817	1498.67	446.21	290.0505	-0.0154
0.00110	997.274	1496.96	447.47	162.7107	0.0001	0.01322	998.071	1499.44	445.64	295.4684	-0.0136
0.00125	997.285	1497.00	447.44	179.2024	-0.0070	0.02065	998.564	1500.95	444.52	299.4454	-0.0141
0.00135	997.292	1497.02	447.43	188.4087	-0.0076	0.02788	999.041	1502.42	443.44	301.3021	-0.0143
0.00159	997.308	1497.06	447.40	206.2844	-0.0053	0.03418	999.450	1503.66	442.53	302.4262	-0.0136
0.00181	997.322	1497.13	447.35	218.8753	-0.0145	0.04114	999.905	1505.01	441.53	303.1451	-0.0129
0.00219	997.345	1497.21	447.29	235.2060	-0.0143	0.05168	1000.593	1507.05	440.03	303.8142	-0.0122
0.00250	997.365	1497.27	447.25	244.3519	-0.0134	0.05787	1001.001	1508.21	439.18	303.9882	-0.0116
0.00301	997.402	1497.37	447.17	253.9269	-0.0138	0.06527	1001.477	1509.57	438.18	304.3059	-0.0107
0.00375	997.450	1497.54	447.05	264.7098	-0.0168	0.08217	1002.581	1512.73	435.87	304.5073	-0.0098
0.00540	997.559	1497.83	446.82	277.7290	-0.0110	0.08749	1002.919	1513.70	435.17	304.6396	-0.0094
0.00613	997.608	1497.99	446.71	281.1194	-0.0126	0.10428	1003.605	1515.91	433.60	308.6639	-0.0003

Table 7. Conductivities, κ , of propanolol + water at $T = 298.15$ K

m (mol·kg ⁻¹)	κ (mS·cm ⁻¹)	m (mol·kg ⁻¹)	κ (mS·cm ⁻¹)
0.00075	0.168	0.02617	2.470
0.00095	0.205	0.03203	2.830
0.00117	0.240	0.04056	3.360
0.00147	0.288	0.04922	3.920
0.00239	0.425	0.05941	4.550
0.00387	0.613	0.07282	5.590
0.00590	0.827	0.08577	6.160
0.00835	1.066	0.10600	7.120
0.01287	1.456	0.13568	8.180
0.01853	1.930	0.16683	9.010
0.02056	2.070		

Table 8. Conductivities, κ , of metoprolol + water at $T = 298.15$ K

m (mol·kg ⁻¹)	κ (mS·cm ⁻¹)	m (mol·kg ⁻¹)	κ (mS·cm ⁻¹)
0.00064	0.163	0.03090	3.200
0.00083	0.210	0.04460	4.150
0.00105	0.250	0.06240	5.280
0.00149	0.325	0.07940	6.250
0.00243	0.483	0.09680	7.150
0.00317	0.603	0.11408	7.960
0.00524	0.891	0.12640	8.440
0.00763	1.154	0.13330	8.710
0.00998	1.421	0.14520	9.130
0.01520	1.940	0.17060	9.850
0.02000	2.360		

Table 9. Conductivities, κ , of timolol + water at $T = 298.15$ K

m (mol·kg ⁻¹)	κ (mS·cm ⁻¹)	m (mol·kg ⁻¹)	κ (mS·cm ⁻¹)
0.00098	0.103	0.01973	1.016
0.00111	0.119	0.02360	1.180
0.00133	0.149	0.02973	1.387
0.00172	0.162	0.03412	1.540
0.00253	0.230	0.03758	1.689
0.00348	0.275	0.04602	1.947
0.00532	0.392	0.05068	2.090
0.00737	0.492	0.05748	2.290
0.00955	0.600	0.06188	2.400
0.01122	0.680	0.07217	2.650
0.01356	0.770	0.07878	2.840
0.01657	0.908		

Table 10. Conductivities, κ , of acebutolol + water at $T = 298.15$ K

m (mol·kg ⁻¹)	κ (mS·cm ⁻¹)	m (mol·kg ⁻¹)	κ (mS·cm ⁻¹)
0.00061	0.175	0.02600	2.330
0.00086	0.212	0.02952	2.550
0.00095	0.222	0.03266	2.740
0.00132	0.289	0.03600	2.960
0.00177	0.370	0.03967	3.190
0.00285	0.508	0.04510	3.420
0.00471	0.748	0.05030	3.710
0.00774	1.016	0.05730	4.080
0.01177	1.336	0.06636	4.480
0.01584	1.621	0.08140	5.310
0.02039	1.957	0.10660	6.170