CHEMPHYSCHEM

Supporting Information

Controlling the Formation of Ionic-Liquid-based Aqueous Biphasic Systems by Changing the Hydrogen-Bonding Ability of Polyethylene Glycol End Groups

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Supplementary Information

Experimental Section

Materials

The cholinium-chloride was acquired from Sigma Aldrich (St. Louis, MO) and the cholinium acetate, [Ch][OAc], was synthesized by our group according to standard protocols.[1] Both compounds were dried under constant agitation and vacuum, at a moderate temperature (50 ºC), for a minimum of 48 h, to reduce the volatile compounds and water contents to negligible values. ^{1}H and ^{13}C NMR were employed to evaluate the purity of each sample. Both salts showed a purity level higher than 98 wt%.

All the poly(ethylene glycol) methyl ether (OH-PEG-OMe) of average molecular weights 350 g mol^{-1}, 550 g mol^{-1} and 750 g mol^{-1} (abbreviated as OH-PEG-350-OMe, OH-PEG-550-OMe and OH-PEG-750-OMe, respectively) were supplied by Sigma Aldrich (St. Louis, MO), and used as received. Poly(ethylene glycol) dimethyl ether with an average molecular weight of 500 g mol^{-1} (MeO-PEG-500-OMe) was purchased from Sigma Aldrich (St. Louis, MO). Poly(ethylene glycol) methyl amine with an average molecular weight of 350 g mol^{-1} (MeO-PEG-350-NH_2) and poly(ethylene glycol) diamine with an average molecular weight of 600 g mol^{-1} (NH_2-PEG-600-NH_2) were synthesized according to the procedure described by Parker *et al.*[2] The composition of both PEG-amine-based polymers was then confirmed by ^{1}H and ^{13}C NMR:

- **MeO-PEG-350-NH_2** - ^{1}H NMR (500 MHz, DMSO-d6) δ ppm: 3.52 (m, 22H), 3.44 (t, 4H), 3.37 (t, 2H), 3.25 (s, 3H), 2.65 (t, 3H). ^{13}C NMR (125 MHz, DMSO-d6) δ ppm: 73.52 (s), 72.86 (s), 71.78 (s), 70.33 (s), 70.04 (s), 60.71 (s), 58.50 (s), 41.84 (s).
- **NH_2-PEG-600-NH_2** - ^{1}H NMR (500 MHz, loaded solventless in a flame-sealed capillary using $CDCl_3$ as external lock) δ ppm: 4.27 (s), 3.75 (m), 3.68 (t). ^{13}C NMR (500 MHz, loaded solventless in a flame-sealed capillary using $CDCl_3$ as external lock) δ ppm: 72.71 (s), 70.44 (s), 70.08 (s), 60.96 (s).

The water used was double distilled, passed across a reverse osmosis system and further treated with a Milli-Q plus 185 water purification apparatus.

Results

Tables S1 to S9 present the experimental weight fraction data corresponding to the solubility curves of each ABS.

Table S1. Experimental binodal weight fraction data for the systems composed of OH-PEG-350-OMe (1) + [Ch]Cl (2) + H_2O (3) at 25 ºC.

100 w_1	**100 w_2**	**100 w_1**	**100 w_2**	**100 w_1**	**100 w_2**
38.0515	39.3670	75.7079	11.8550	27.7214	48.4618
52.0244	28.9768	38.3497	39.6755	23.3240	53.1518
56.2501	26.1735	31.6189	45.3513	18.8495	56.7184
69.0070	16.0109				

Table S2. Experimental binodal weight fraction data for the systems composed of OH-PEG-550-OMe (1) + [Ch]Cl (2) + H_2O (3) at 25 ºC.

100 w_1	**100 w_2**	**100 w_1**	**100 w_2**	**100 w_1**	**100 w_2**
41.1973	29.1568	13.7647	51.2159	58.8054	18.7016
36.6949	32.7110	13.1248	51.5210	57.6695	19.3237
31.9424	36.3077	70.0878	11.7191	55.7938	20.4975
28.1844	38.9987	72.9982	10.4362	54.3964	21.4306
25.9002	40.0120	73.4944	9.9985	51.9932	22.7001
24.5702	41.3854	74.7257	9.3105	50.5166	23.3158
23.3732	42.1403	75.6485	8.8413	48.1196	24.7876
21.8046	43.5142	77.0804	8.2072	47.1204	25.3048
20.6313	44.6045	78.3146	7.5959	46.0338	25.8878
19.3523	45.7041	79.4987	6.7798	44.5938	27.0870
17.9480	46.7363	82.6132	5.4889	43.2503	28.0063
16.7177	48.0318	66.0381	13.8914	41.8569	28.7900
15.5532	49.3343	63.6821	15.8196	40.5668	29.6160
14.8936	50.0755	62.2716	16.6917	39.3813	30.3430
14.3937	50.5391	60.0724	18.0098		

Table S3. Experimental binodal weight fraction data for the systems composed of OH-PEG-750-OMe (1) + [Ch]Cl (2) + H_2O (3) at 25 ºC.

100 w_1	**100 w_2**	**100 w_1**	**100 w_2**	**100 w_1**	**100 w_2**
39.8948	27.0815	19.4658	43.5563	60.4409	13.8083
36.9018	29.7609	18.4312	44.1227	64.1528	11.9674
35.2655	30.9880	17.4021	45.2787	65.9568	10.9889
33.5283	32.0551	16.1991	46.7140	66.6279	10.4624
32.2713	33.3847	15.5114	47.3027	67.9468	9.7201
30.7813	34.1078	14.8661	47.6147	69.6545	8.9176
27.8918	36.8055	14.2031	48.5952	71.2269	8.2713
26.5098	38.0078	13.6921	49.1986	72.0495	7.8971
24.8277	39.3767	12.9236	49.6567	72.6251	7.5097
23.8039	40.2768	45.3468	22.7242	73.4027	7.2284
22.7793	40.9954	53.4746	18.0895	73.9917	6.9646
21.3129	41.6306	59.0077	15.1936	74.6564	6.6508

Table S4. Experimental binodal weight fraction data for the systems composed of OH-PEG-350-OMe (1) + [Ch][OAc] (2) + H_2O (3) at 25 ºC.

100 w_1	**100 w_2**	**100 w_1**	**100 w_2**	**100 w_1**	**100 w_2**
36.3725	32.4861	68.3853	12.9512	23.2090	44.0335
39.1554	30.4024	68.7030	12.4907	22.4734	44.8050
43.4976	28.1326	69.6703	11.9758	21.6990	45.4880
46.0815	26.6572	70.7773	11.4743	20.7096	46.3189
48.5818	25.2119	71.5313	11.0155	19.6265	47.4390
50.6435	23.9502	72.4912	10.4629	18.2624	48.2575
53.4724	22.5164	73.1659	10.0874	17.0239	49.1024
54.5295	21.3483	73.5689	9.7022	15.6618	51.2475
56.4632	20.2328	74.8920	9.1772	15.1410	52.2684
57.7072	19.4525	75.5379	8.8101	14.3993	52.7450
59.1940	18.3818	76.0420	8.5009	13.7675	53.5832
60.1545	17.7178	33.3450	34.7527	12.9561	54.7884
61.7749	16.5812	31.2841	36.9447	12.3260	55.7469
63.7993	15.6823	30.2993	37.3911	11.7335	56.4135
64.8692	15.0041	27.8717	40.0442	11.1503	57.3762
65.8952	14.3631	26.2010	41.2785	10.6608	58.1395
67.7100	13.4406	24.3434	43.0096		

Table S5. Experimental binodal weight fraction data for the systems composed of OH-PEG-550-OMe (1) + [Ch][OAc] (2) + H_2O (3) at 25 ºC.

100 w_1	**100 w_2**	**100 w_1**	**100 w_2**	**100 w_1**	**100 w_2**
19.3723	42.7978	7.5678	54.9289	36.5682	31.5295
18.6927	43.4757	7.2777	55.5395	35.1592	32.2066
17.6236	44.4425	7.0167	55.7612	34.1756	33.0711
16.3373	45.4723	6.7817	56.1164	32.9304	33.9847
15.5369	46.0987	6.4489	56.5309	32.0471	34.7362
14.6516	47.1253	6.1509	56.9589	31.1636	35.3065
14.0344	47.8281	5.8565	57.4114	30.1873	35.5433
13.4523	48.6715	5.6324	57.6814	28.9615	36.5727
12.8217	49.2791	5.3591	57.6968	28.3585	36.9778
12.1894	49.7568	5.0838	58.5386	27.3924	37.6441
11.7621	50.0351	55.2766	20.7707	26.9346	37.7750
11.2854	50.4783	52.4297	22.1461	26.3958	38.3577
10.7021	50.9569	50.0000	23.5951	25.6659	38.9482
10.1963	51.2907	48.7137	24.6308	25.1728	39.0670
9.6513	52.1375	46.7415	26.0594	24.4055	39.1894
9.2053	52.6776	44.4379	26.9963	23.8161	39.7638
8.8333	53.1880	43.0439	28.0230	23.2874	39.9170
8.5407	53.6270	41.1362	29.1619	22.3541	40.2257
8.2569	53.8716	39.4479	30.0217	21.3148	40.7158
7.8546	54.5017	37.7718	30.7877	20.7008	41.5281

Table S6. Experimental binodal weight fraction data for the systems composed of OH-PEG-750-OMe (1) + [Ch][OAc] (2) + H_2O (3) at 25 ºC.

100 w_1	100 w_2	100 w_1	100 w_2	100 w_1	100 w_2
40.6634	24.8909	22.1559	37.0393	50.9555	19.1458
39.6529	25.0347	21.7305	37.1200	51.3764	18.8777
38.4926	25.5004	21.3451	37.3371	52.0207	18.5113
37.2154	26.4124	21.0535	37.7599	52.4831	18.2367
35.9000	27.3260	20.5633	37.8522	53.1102	17.8979
34.9142	27.9885	20.0198	38.5930	53.4176	17.6983
34.1006	28.4415	19.6087	38.6658	53.9016	17.4101
33.2457	29.0251	19.0433	39.1583	54.3270	17.1677
32.4326	29.5326	18.6914	39.3383	54.8912	16.8677
31.7396	30.1337	18.1309	39.7357	55.0893	16.6979
30.7300	30.7507	17.5239	39.8686	55.5513	16.4349
29.9268	31.3114	16.8110	40.9370	55.9807	16.1582
29.6897	31.5471	42.1652	24.1884	56.4647	15.8874
29.1542	31.9284	43.1000	23.6581	56.9984	15.6291
28.4237	32.4972	44.0191	23.1506	57.3510	15.3439
27.6902	33.1036	44.7809	22.6935	57.8766	15.0785
27.0674	33.5485	45.3269	22.3514	58.4035	14.7412
26.2654	34.1079	46.2083	21.8858	58.8135	14.5386
25.8630	34.5230	46.6915	21.5840	59.0061	14.2134
25.3461	34.6870	47.6583	21.1064	60.1624	13.6082
24.8246	35.2688	48.1971	20.7747	60.6900	13.2623
24.2561	35.4515	48.8117	20.4164	61.0167	13.0421
23.8640	35.8573	49.0691	20.1835	62.0386	12.3808
22.9729	36.3945	49.6789	19.8460	63.9181	11.5930
22.5252	36.6296	50.1376	19.5532	64.6601	11.2123

Table S7. Experimental binodal weight fraction data for the systems composed of MeO-PEG-500-OMe (1) + [Ch][OAc] (2) + H_2O (3) at 25 ºC.

100 w_1	**100 w_2**	**100 w_1**	**100 w_2**	**100 w_1**	**100 w_2**
58.1324	9.4424	29.5389	26.2106	13.9821	40.1964
55.6560	11.2732	27.9201	27.7697	13.2779	41.4539
54.7901	11.6906	27.4117	28.5122	12.2631	42.2603
53.7432	12.8118	26.3815	29.3494	11.1427	42.9983
51.3384	14.0322	25.5816	29.8550	10.0282	45.3617
48.9791	15.2752	24.5192	30.6876	9.1826	45.3909
46.6331	16.3304	23.5374	31.8091	8.5462	46.7288
44.9261	16.7757	22.3675	32.4868	7.9131	47.9724
43.3210	17.4750	21.6686	33.2984	7.5115	48.6118
41.3865	18.3832	20.5546	34.3756	7.0036	48.5255
39.3212	19.6727	19.8436	34.8907	6.4349	50.0172
38.3422	20.4793	19.3414	35.6381	6.2020	50.7158
38.1184	20.4800	18.9000	36.0049	5.9530	51.1785
37.6297	20.7179	18.3154	36.6746	5.6461	51.0743
37.0006	21.2139	17.7620	37.0397	5.3623	51.7454
35.6396	21.8956	17.2572	37.8192	5.0798	52.0637
34.4805	22.9944	16.7747	37.9340	4.8564	52.4467
33.3313	23.7456	16.1900	38.8085	4.7208	52.8430
32.6831	24.1310	15.7707	39.2646	4.5376	53.1243
31.4912	24.7771	15.3331	39.9929	4.3816	53.0563
30.5275	25.4570	14.9770	40.4516	4.1883	53.6937

Table S8. Experimental binodal weight fraction data for the systems composed of NH_2-PEG-600-NH_2 (1) + [Ch][OAc] (2) + H_2O (3) at 25 ºC.

100 w_1	**100 w_2**	**100 w_1**	**100 w_2**	**100 w_1**	**100 w_2**
66.0411	6.3634	38.0105	19.8150	24.9342	28.4115
48.8498	14.2052	29.9142	23.7981	21.6766	30.9281

Table S9. Experimental binodal weight fraction data for the systems composed of MeO-PEG-350-NH_2 (1) + [Ch][OAc] (2) + H_2O (3) at 25 ºC.

100 w_1	**100 w_2**	**100 w_1**	**100 w_2**	**100 w_1**	**100 w_2**
44.0381	30.7329	54.9517	24.9643	26.6947	35.7744
33.2571	32.2984	53.0328	25.9976	25.1021	36.9705
71.7066	14.0852	50.8199	27.4807	23.5585	37.6985
12.2741	45.7539	48.4494	28.6238	21.8980	38.8119
10.1806	47.2173	46.9516	29.3243	20.6949	39.2765
8.8420	48.4999	45.4947	30.1140	19.1635	40.4545
7.5775	49.2930	44.3617	30.6283	17.7716	41.6189
6.1523	51.0827	41.6840	31.3950	16.7686	42.3300
4.8616	54.2121	38.1276	32.0675	16.1048	42.5789
69.5113	15.3149	35.5996	32.1834	15.3995	43.3769
63.3854	19.1870	33.1219	32.6087	14.6368	43.8398
59.4974	21.5722	31.5406	33.7409	13.7103	44.7815
56.9550	23.2010	29.1906	34.3587	13.7103	44.7815

Computational Detail

COSMO-RS

COSMO-RS is a well-known predictive method developed by Klamt and co-workers[3] able to provide the thermodynamic properties and equilibrium of pure fluids and mixtures. It uses a statistical thermodynamic approach based on the results of unimolecular quantum chemical calculations. The detailed theory regarding COSMO-RS, HB_bond3, HB_acc3 can be found in the original work of Klamt.[4] In a first step, the continuum solvation COSMO calculations of electronic density and molecular geometry of all compounds (PEG-400 and its derivatives) were performed with the TURBOMOLE 6.1 program package on the density functional theory (DFT) level, employing the BP functional B88-P86 with a triple-ζ valence polarized basis set (TZVP) and the resolution of identity standard (RI) approximation.[5] All the optimized structures were confirmed to be minima on potential energy surface via vibrational frequency analysis. The absence of imaginary or negative frequencies indicates that the structure is a global minimum.[6] The estimation of the activity coefficient at infinite dilution of PEG-400 molecules or its derivatives in water or [Ch][OAc] was performed with the COSMOtherm program using the parameter file BP_TZVP_C30_1301 (COSMOlogic GmbH & Co KG, Leverkusen, Germany).[7] The HB_don3 and HB_acc3 of all compounds were also estimated using the same parameterization *via* activating atomic sigma moment as the output during COSMO-RS calculations.

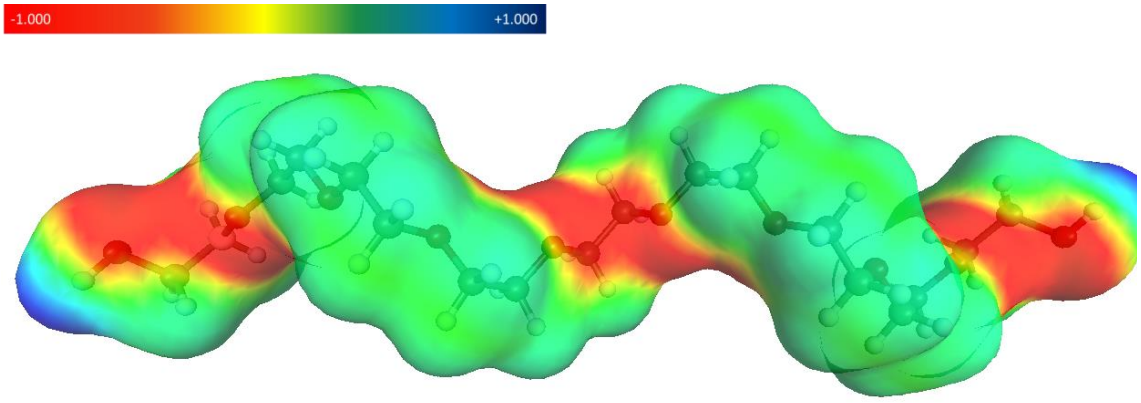
Partial Charges of the Atoms

The optimized geometries of PEG-400 molecules or its derivatives in the gas phase obtained with TURBOMOLE 6.1 were used as starting structures for the calculations in Gaussian 03 Revision D.02 software.[8] The partial charges of the atoms composing the PEG-400 or its derivatives were retrieved by electrostatic surface potential (ESP) fits, using the CHelpG algorithm[9] to the electron densities obtained at the BP_TZVP level of theory.

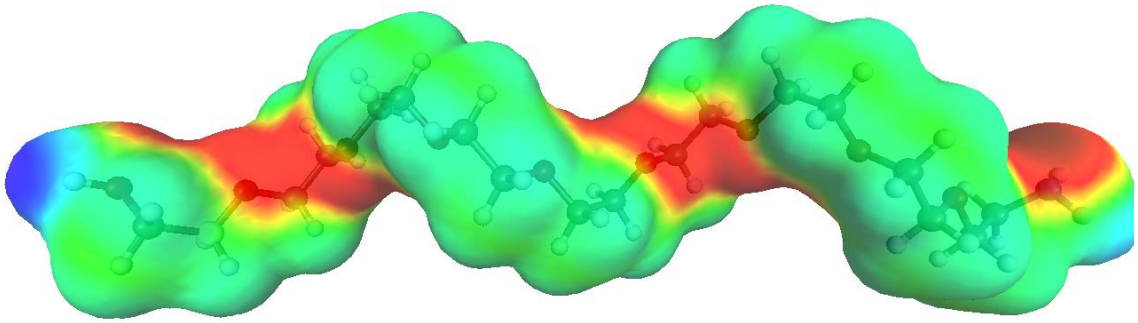
Results

Figure S1 presents the results according partial electrostatic potential-derived CHelpG charges for the various functionalized PEG-400 molecules retrieved at the BP_TZVP level of theory.

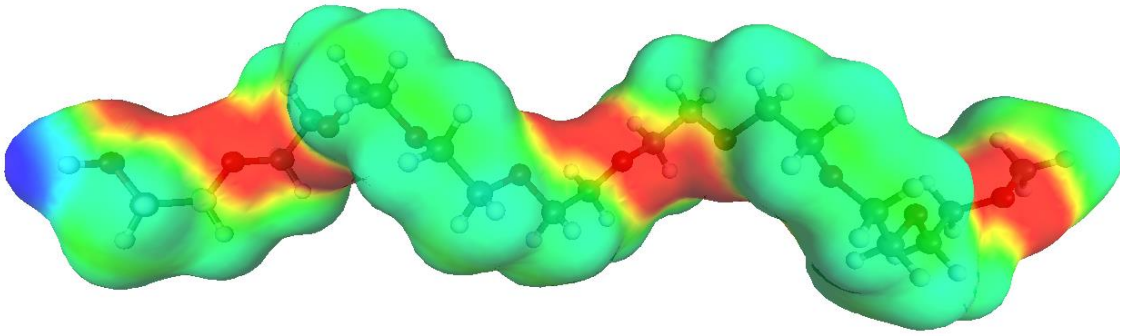
Tables S10 to S16 present the results corresponding to the computational approaches used in this work.



(a) PEG-400



(b) OH-PEG-400-NH_2



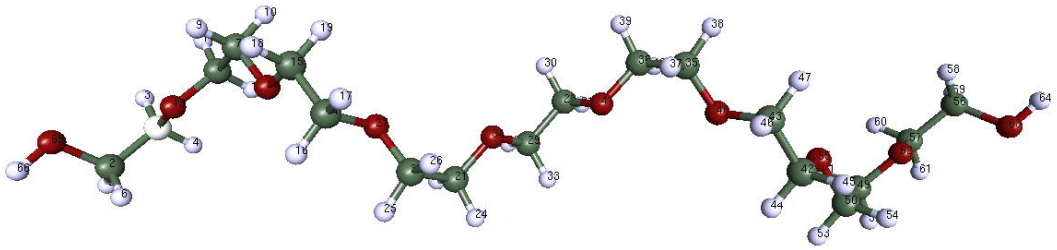
(c) OH-PEG-400-OMe

Figure S1. Partial electrostatic potential-derived CHelpG charges for the various functionalized PEG-400 molecules retrieved at the BP_TZVP level of theory.

Table S10. Atom coordinates, electrostatic potential-derived (CHelpG) charges, HB_don3, and HB_acc3 calculated at the BP-TZVP level of theory for water.

Centre Number	Atomic Number	Atom	Coordinate/Å			CHelpG	Hb_acc3	Hb_don3
			x	y	z			
1	1	H	0.6391	-0.0279	0.4947	0.3952	0	1.9255
2	8	O	0.1598	0.0324	-0.3698	-0.7904	5.6933	0
3	1	H	-0.7990	-0.0045	-0.1249	0.3952	0	1.9252

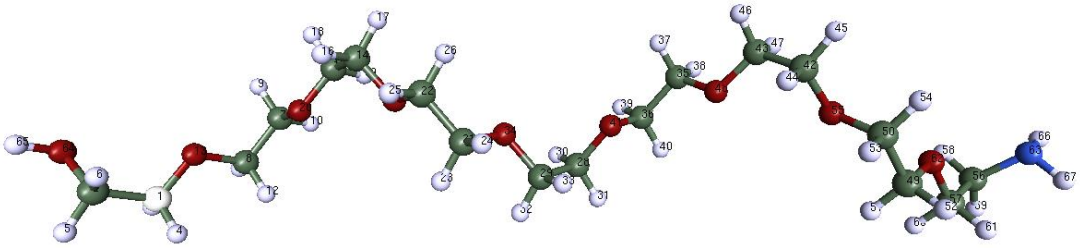
Table S11. Atom coordinates, electrostatic potential-derived (CHelpG) charges, HB_don3, and HB_acc3 calculated at the BP-TZVP level of theory for PEG-400.



Centre Number	Atomic Symbol	Atomic Number	Coordinates/Å			CHelpG	Hb_acc3	Hb_don3
			x	y	z			
1	C	6	9.63482	-1.61631	0.23367	0.1397	0	0
2	C	6	10.49817	-1.46018	-1.01250	0.2521	0.0004	0
3	H	1	10.31267	-1.74015	1.10953	0.0309	0	0
4	H	1	9.00851	-2.52778	0.09866	-0.0182	0	0
5	H	1	11.12627	-2.37178	-1.12699	-0.0334	0	0
6	H	1	9.83540	-1.34506	-1.89943	-0.0112	0	0
7	C	6	7.13973	0.62459	1.68478	0.1166	0	0
8	C	6	8.02310	-0.60867	1.53764	0.1474	0	0
9	H	1	7.80380	1.51458	1.77959	0.0326	0	0
10	H	1	6.53076	0.49757	2.60916	0.0087	0	0
11	H	1	8.65923	-0.68163	2.44945	-0.0052	0	0
12	H	1	7.35882	-1.50007	1.45845	0.0277	0	0
13	O	8	8.82272	-0.47128	0.38231	-0.3056	2.6094	0
14	C	6	4.58686	1.98830	-0.54564	0.1619	0	0
15	C	6	5.49106	1.88123	0.67655	0.1400	0	0
16	H	1	5.23586	2.07478	-1.44753	0.0199	0	0
17	H	1	3.96491	2.90531	-0.42864	-0.0070	0	0
18	H	1	6.11360	2.80423	0.72041	-0.0002	0	0
19	H	1	4.84196	1.81041	1.57975	0.0254	0	0
20	O	8	6.30655	0.73585	0.55070	-0.3422	2.4704	0
21	C	6	2.05084	-0.31136	-1.82294	0.1368	0	0
22	C	6	2.93731	0.92658	-1.75626	0.1318	0	0
23	H	1	2.71257	-1.20494	-1.89869	0.0287	0	0
24	H	1	1.41417	-0.22460	-2.73316	0.0013	0	0
25	H	1	3.54608	0.95913	-2.68884	0.0014	0	0
26	H	1	2.27527	1.82113	-1.69626	0.0276	0	0
27	O	8	3.77066	0.83898	-0.62023	-0.3294	2.4458	0
28	C	6	-0.43028	-1.57601	0.54260	0.1515	0	0
29	C	6	0.43551	-1.52264	-0.71051	0.1048	0	0
30	H	1	0.24673	-1.62242	1.42673	0.0251	0	0
31	H	1	-1.05414	-2.49738	0.48575	-0.0007	0	0

32	H	1	1.05803	-2.44643	-0.73278	0.0086	0	0
33	H	1	-0.24118	-1.49196	-1.59551	0.0348	0	0
34	O	8	1.25238	-0.37246	-0.66044	-0.3215	2.3773	0
35	C	6	-2.92698	0.77863	1.79693	0.1179	0	0
36	C	6	-2.03940	-0.45970	1.75851	0.1264	0	0
37	H	1	-2.26576	1.67577	1.80691	0.0326	0	0
38	H	1	-3.53140	0.73456	2.73185	0.0076	0	0
39	H	1	-1.39874	-0.44682	2.66998	0.0049	0	0
40	H	1	-2.70020	-1.35716	1.76404	0.0300	0	0
41	O	8	-1.24584	-0.42486	0.59158	-0.3288	2.4746	0
42	C	6	-5.49545	1.92380	-0.53607	0.1387	0	0
43	C	6	-4.58049	1.93546	0.68273	0.1314	0	0
44	H	1	-4.85447	1.92154	-1.44779	0.0283	0	0
45	H	1	-6.11637	2.84836	-0.50341	0.0017	0	0
46	H	1	-3.95756	2.85778	0.63127	0.0025	0	0
47	H	1	-5.22175	1.95337	1.59412	0.0276	0	0
48	O	8	-3.76584	0.78282	0.66158	-0.3171	2.5024	0
49	C	6	-8.04121	-0.48835	-1.56217	0.1426	0	0
50	C	6	-7.15668	0.75137	-1.62219	0.1212	0	0
51	H	1	-7.37809	-1.38411	-1.55894	0.0292	0	0
52	H	1	-8.68652	-0.48958	-2.47045	-0.0053	0	0
53	H	1	-6.55709	0.69554	-2.55963	0.0069	0	0
54	H	1	-7.81976	1.64694	-1.64114	0.0317	0	0
55	O	8	-6.31219	0.77329	-0.49124	-0.3400	2.457	0
56	C	6	-10.49217	-1.53175	0.93953	0.2368	0.0009	0
57	C	6	-9.64211	-1.59175	-0.32399	0.1479	0	0
58	H	1	-9.82000	-1.48693	1.82573	-0.0076	0	0
59	H	1	-11.12112	-2.44858	0.98938	-0.0291	0	0
60	H	1	-9.01651	-2.51188	-0.26681	-0.0201	0	0
61	H	1	-10.32922	-1.64610	-1.19969	0.0302	0	0
62	O	8	-8.82901	-0.43979	-0.39166	-0.3053	2.5388	0
63	O	8	-11.31203	-0.39682	0.90336	-0.5895	3.8833	0
64	H	1	-11.83748	-0.41085	1.74509	0.3793	0	2.0252
65	O	8	11.31926	-0.33336	-0.87968	-0.5919	3.8705	0
66	H	1	11.85357	-0.28314	-1.71442	0.3790	0	2.0085

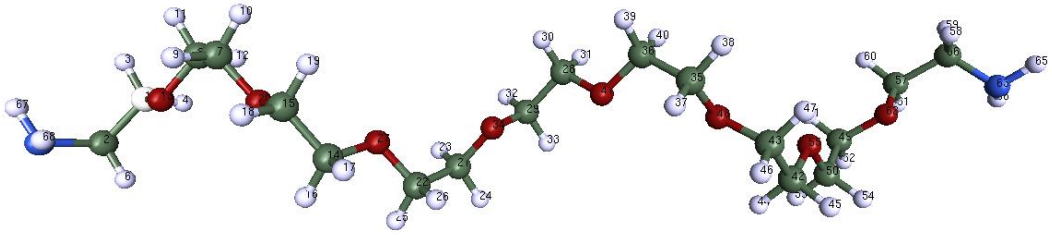
Table S12. Atom coordinates, electrostatic potential-derived (CHelpG) charges, HB_don3, and HB_acc3 calculated at the BP-TZVP level of theory for OH-PEG-400-NH_2.



Centre Number	Atomic Symbol	Atomic Number	Coordinates/Å			CHelpG	Hb_acc3	Hb_don3
			x	y	z			
1	C	6	9.63737	-1.61007	0.26495	0.1312	0	0
2	C	6	10.49959	-1.48155	-0.98514	0.2498	0.0003	0
3	H	1	10.31602	-1.71437	1.14274	0.0338	0	0
4	H	1	9.01103	-2.52435	0.15077	-0.0147	0	0
5	H	1	11.12768	-2.39541	-1.07994	-0.0331	0	0
6	H	1	9.83602	-1.38619	-1.87382	-0.0097	0	0
7	C	6	7.14334	0.66229	1.66821	0.1277	0	0
8	C	6	8.02670	-0.57386	1.54768	0.1469	0	0
9	H	1	7.80739	1.55422	1.74264	0.0286	0	0
10	H	1	6.53520	0.55576	2.59571	0.0049	0	0
11	H	1	8.66365	-0.62652	2.46033	-0.0056	0	0
12	H	1	7.36243	-1.46685	1.48888	0.0265	0	0
13	O	8	8.82527	-0.46208	0.38887	-0.3046	2.6128	0
14	C	6	4.58833	1.97594	-0.58966	0.1253	0	0
15	C	6	5.49363	1.89609	0.63380	0.1389	0	0
16	H	1	5.23652	2.04244	-1.49382	0.0299	0	0
17	H	1	3.96639	2.89527	-0.49248	0.0034	0	0
18	H	1	6.11612	2.81988	0.65661	0.0029	0	0
19	H	1	4.84535	1.84528	1.53892	0.0281	0	0
20	O	8	6.30914	0.74827	0.53268	-0.3412	2.528	0
21	C	6	2.05143	-0.35172	-1.81334	0.1420	0	0
22	C	6	2.93782	0.88748	-1.77493	0.1381	0	0
23	H	1	2.71318	-1.24670	-1.86984	0.0262	0	0
24	H	1	1.41392	-0.28523	-2.72469	-0.0008	0	0
25	H	1	3.54576	0.89938	-2.70856	-0.0009	0	0
26	H	1	2.27574	1.78308	-1.73421	0.0260	0	0
27	O	8	3.77219	0.82518	-0.63799	-0.3206	2.4459	0
28	C	6	-0.42744	-1.56381	0.58191	0.1440	0	0
29	C	6	0.43723	-1.53815	-0.67287	0.1180	0	0

30	H	1	0.25037	-1.59053	1.46622	0.0272	0	0
31	H	1	-1.05125	-2.48625	0.54606	0.0004	0	0
32	H	1	1.05982	-2.46216	-0.67521	0.0048	0	0
33	H	1	-0.24027	-1.52718	-1.55774	0.0321	0	0
34	O	8	1.25401	-0.38709	-0.64906	-0.3283	2.4402	0
35	C	6	-2.92317	0.81789	1.78599	0.1321	0	0
36	C	6	-2.03557	-0.42095	1.77422	0.1242	0	0
37	H	1	-2.26201	1.71505	1.77553	0.0295	0	0
38	H	1	-3.52680	0.79450	2.72218	0.0039	0	0
39	H	1	-1.39410	-0.38782	2.68457	0.0039	0	0
40	H	1	-2.69631	-1.31810	1.80020	0.0305	0	0
41	O	8	-1.24307	-0.41191	0.60605	-0.3267	2.4852	0
42	C	6	-5.49271	1.91162	-0.56998	0.1603	0	0
43	C	6	-4.57752	1.94981	0.64798	0.1420	0	0
44	H	1	-4.85199	1.89009	-1.48154	0.0231	0	0
45	H	1	-6.11450	2.83611	-0.55690	-0.0039	0	0
46	H	1	-3.95476	2.87082	0.57594	-0.0039	0	0
47	H	1	-5.21841	1.98754	1.55905	0.0246	0	0
48	O	8	-3.76293	0.79698	0.65158	-0.3281	2.5913	0
49	C	6	-8.03078	-0.52658	-1.54680	0.2038	0	0
50	C	6	-7.15244	0.71526	-1.63094	0.0801	0	0
51	H	1	-7.36419	-1.41959	-1.53105	0.0205	0	0
52	H	1	-8.68039	-0.54533	-2.45184	-0.0185	0	0
53	H	1	-6.55366	0.64410	-2.56771	0.0102	0	0
54	H	1	-7.81953	1.60738	-1.66531	0.0373	0	0
55	O	8	-6.30789	0.76161	-0.50070	-0.3347	2.5065	0
56	C	6	-10.48152	-1.52119	0.97771	0.3401	0.0015	0
57	C	6	-9.62277	-1.61198	-0.28216	0.0830	0	0
58	H	1	-9.81733	-1.46232	1.86769	0.0230	0	0
59	H	1	-11.10867	-2.43606	1.06578	-0.0771	0	0
60	H	1	-8.99441	-2.52828	-0.19978	-0.0174	0	0
61	H	1	-10.30220	-1.69353	-1.16172	0.0292	0	0
62	O	8	-8.81228	-0.46034	-0.37352	-0.3166	3.327	0
63	N	7	-11.33604	-0.33755	0.93552	-0.9139	5.2565	0
64	O	8	11.32068	-0.35200	-0.87810	-0.5910	3.8765	0
65	H	1	11.85424	-0.32028	-1.71423	0.3788	0	2.0086
66	H	1	-11.91073	-0.31043	1.80873	0.3358	0	0.0382
67	H	1	-11.99316	-0.41271	0.12513	0.3388	0	0.0258

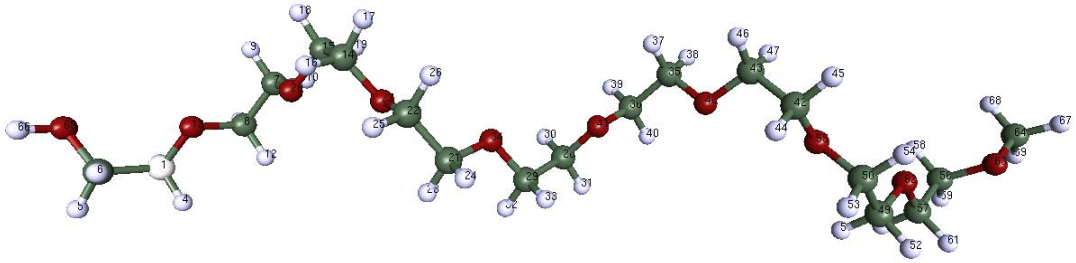
Table S13. Atom coordinates, electrostatic potential-derived (CHelpG) charges, HB_don3, and HB_acc3 calculated at the BP-TZVP level of theory for NH_2-PEG-400-NH_2.



Centre Number	Atomic Symbol	Atomic Number	Coordinates/Å			CHelpG	Hb_acc3	Hb_don3
			x	y	z			
1	C	6	9.62007	-1.63843	0.17760	-0.0100	0	0
2	C	6	10.49528	-1.45850	-1.06664	0.3968	0	0
3	H	1	10.28908	-1.78575	1.05645	0.0334	0	0
4	H	1	8.99419	-2.54606	0.01821	-0.0046	0	0
5	H	1	11.11298	-2.37107	-1.21135	-0.0266	0	0
6	H	1	9.84949	-1.33326	-1.96273	0.0019	0	0
7	C	6	7.13923	0.58351	1.67895	0.0728	0	0
8	C	6	8.01412	-0.65241	1.50783	0.1429	0	0
9	H	1	7.81030	1.46766	1.77938	0.0333	0	0
10	H	1	6.53598	0.44979	2.60611	0.0209	0	0
11	H	1	8.65785	-0.74057	2.41297	0.0010	0	0
12	H	1	7.34579	-1.54022	1.42212	0.0489	0	0
13	O	8	8.80213	-0.50063	0.34649	-0.3073	1.6562	0
14	C	6	4.59042	1.99312	-0.52630	0.1213	0	0
15	C	6	5.49348	1.86324	0.69439	0.1611	0	0
16	H	1	5.24027	2.09127	-1.42644	0.0296	0	0
17	H	1	3.97154	2.91027	-0.39539	0.0025	0	0
18	H	1	6.12217	2.78139	0.75130	-0.0035	0	0
19	H	1	4.84427	1.78334	1.59666	0.0248	0	0
20	O	8	6.29999	0.71384	0.55163	-0.3257	2.4677	0
21	C	6	2.05023	-0.28094	-1.83990	0.1173	0	0
22	C	6	2.93681	0.95557	-1.75255	0.1316	0	0
23	H	1	2.71173	-1.17297	-1.93393	0.0323	0	0
24	H	1	1.41104	-0.17742	-2.74660	0.0066	0	0
25	H	1	3.54417	1.00487	-2.68536	0.0046	0	0
26	H	1	2.27513	1.84898	-1.67515	0.0307	0	0
27	O	8	3.77119	0.84737	-0.61922	-0.3220	2.436	0
28	C	6	-0.42357	-1.58873	0.50966	0.1260	0	0
29	C	6	0.43795	-1.51235	-0.74519	0.1298	0	0
30	H	1	0.25636	-1.65230	1.39046	0.0301	0	0

31	H	1	-1.04842	-2.50835	0.43756	0.0045	0	0
32	H	1	1.06001	-2.43578	-0.78685	0.0035	0	0
33	H	1	-0.24170	-1.46480	-1.62716	0.0305	0	0
34	O	8	1.25523	-0.36351	-0.67639	-0.3223	2.4166	0
35	C	6	-2.91391	0.74412	1.81590	0.1368	0	0
36	C	6	-2.02802	-0.49430	1.75142	0.1179	0	0
37	H	1	-2.25168	1.64016	1.84187	0.0284	0	0
38	H	1	-3.51647	0.68254	2.75105	0.0028	0	0
39	H	1	-1.38489	-0.49975	2.66120	0.0056	0	0
40	H	1	-2.68995	-1.39091	1.74143	0.0321	0	0
41	O	8	-1.23777	-0.43795	0.58310	-0.3224	2.4583	0
42	C	6	-5.48621	1.93538	-0.48912	0.1620	0	0
43	C	6	-4.56970	1.92297	0.72840	0.0969	0	0
44	H	1	-4.84669	1.95291	-1.40169	0.0250	0	0
45	H	1	-6.10856	2.85806	-0.43642	-0.0012	0	0
46	H	1	-3.94741	2.84653	0.69521	0.0084	0	0
47	H	1	-5.20990	1.92159	1.64072	0.0370	0	0
48	O	8	-3.75472	0.77133	0.68243	-0.3152	2.5688	0
49	C	6	-8.02992	-0.45966	-1.55794	0.1921	0	0
50	C	6	-7.14938	0.78368	-1.59440	0.1107	0	0
51	H	1	-7.36468	-1.35364	-1.57782	0.0206	0	0
52	H	1	-8.67966	-0.44214	-2.46287	-0.0168	0	0
53	H	1	-6.55374	0.75082	-2.53544	0.0019	0	0
54	H	1	-7.81523	1.67740	-1.59022	0.0278	0	0
55	O	8	-6.30049	0.78260	-0.46670	-0.3396	2.5936	0
56	C	6	-10.48040	-1.55557	0.92669	0.3438	0.0015	0
57	C	6	-9.62316	-1.59327	-0.33688	0.0616	0	0
58	H	1	-9.81555	-1.53243	1.81771	0.0234	0	0
59	H	1	-11.10712	-2.47364	0.97781	-0.0776	0	0
60	H	1	-8.99519	-2.51224	-0.29070	-0.0113	0	0
61	H	1	-10.30342	-1.63881	-1.21842	0.0357	0	0
62	O	8	-8.81169	-0.43908	-0.38269	-0.3079	3.3319	0
63	N	7	-11.33698	-0.37335	0.93405	-0.9163	5.3463	0
64	N	7	11.38135	-0.30206	-0.94530	-0.9486	5.1958	0
65	H	1	-11.89453	-0.37383	1.81862	0.3360	0	0.0393
66	H	1	-12.00948	-0.43111	0.13487	0.3403	0	0.0275
67	H	1	11.99318	-0.41199	-0.10410	0.3437	0	0.0307
68	H	1	10.81721	0.57278	-0.84510	0.3498	0	0.001

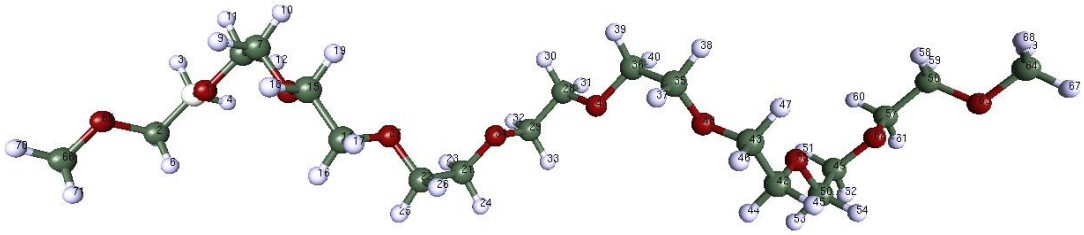
Table S14. Atom coordinates, electrostatic potential-derived (CHelpG) charges, HB_don3, and HB_acc3 calculated at the BP-TZVP level of theory for OH-PEG-400-OMe.



Centre Number	Atomic Symbol	Atomic Number	Coordinates/Å			CHelpG	Hb_acc3	Hb_don3
			x	y	z			
1	C	6	10.03114	-1.63827	-0.33868	0.1214	0	0
2	C	6	10.91218	-1.02061	-1.41800	0.2583	0.0004	0
3	H	1	10.69631	-2.09872	0.42779	0.0353	0	0
4	H	1	9.40167	-2.41974	-0.82277	-0.0122	0	0
5	H	1	11.53670	-1.82318	-1.87020	-0.0341	0	0
6	H	1	10.26216	-0.56408	-2.19789	-0.0119	0	0
7	C	6	7.52875	-0.10871	1.84111	0.1458	0	0
8	C	6	8.40728	-1.19775	1.23686	0.1342	0	0
9	H	1	8.19624	0.66813	2.28045	0.0255	0	0
10	H	1	6.90645	-0.57769	2.63751	0.0002	0	0
11	H	1	9.03039	-1.62490	2.05581	-0.0028	0	0
12	H	1	7.73923	-1.98188	0.81143	0.0302	0	0
13	O	8	9.22345	-0.63183	0.23355	-0.3019	2.6096	0
14	C	6	5.01415	2.03888	0.28665	0.1404	0	0
15	C	6	5.89964	1.45614	1.38168	0.1521	0	0
16	H	1	5.67681	2.46312	-0.50264	0.0262	0	0
17	H	1	4.39436	2.84409	0.74374	-0.0018	0	0
18	H	1	6.52536	2.28335	1.78862	-0.0026	0	0
19	H	1	5.23694	1.04589	2.17831	0.0226	0	0
20	O	8	6.71198	0.44199	0.83000	-0.3509	2.5089	0
21	C	6	2.48883	0.44134	-1.81620	0.1541	0	0
22	C	6	3.37735	1.54790	-1.26049	0.1050	0	0
23	H	1	3.14933	-0.35668	-2.22730	0.0244	0	0
24	H	1	1.86516	0.88184	-2.62762	-0.0016	0	0
25	H	1	3.99912	1.93747	-2.09897	0.0078	0	0
26	H	1	2.71686	2.35304	-0.86350	0.0343	0	0
27	O	8	4.19446	1.01696	-0.23915	-0.3160	2.4257	0
28	C	6	-0.02863	-1.62774	-0.16316	0.1367	0	0
29	C	6	0.85484	-1.09549	-1.28519	0.1406	0	0

30	H	1	0.63550	-2.02172	0.64048	0.0274	0	0
31	H	1	-0.65401	-2.44844	-0.58358	0.0004	0	0
32	H	1	1.47507	-1.94197	-1.65965	-0.0012	0	0
33	H	1	0.19068	-0.71578	-2.09562	0.0253	0	0
34	O	8	1.67406	-0.06304	-0.77965	-0.3346	2.3789	0
35	C	6	-2.53798	0.06810	1.88099	0.1377	0	0
36	C	6	-1.65588	-1.06455	1.36935	0.1330	0	0
37	H	1	-1.87295	0.88059	2.25472	0.0273	0	0
38	H	1	-3.15951	-0.33506	2.71322	0.0015	0	0
39	H	1	-1.03174	-1.42021	2.22102	0.0017	0	0
40	H	1	-2.32105	-1.88344	1.01009	0.0273	0	0
41	O	8	-0.84145	-0.58088	0.32272	-0.3270	2.4798	0
42	C	6	-5.05625	2.07320	0.15203	0.1610	0	0
43	C	6	-4.17080	1.58511	1.29243	0.1314	0	0
44	H	1	-4.39361	2.43249	-0.66887	0.0217	0	0
45	H	1	-5.67857	2.91184	0.54041	-0.0046	0	0
46	H	1	-3.54752	2.44467	1.63022	0.0002	0	0
47	H	1	-4.83348	1.24047	2.11956	0.0272	0	0
48	O	8	-3.35551	0.53076	0.82730	-0.3291	2.5543	0
49	C	6	-7.57282	0.30023	-1.81654	0.1742	0	0
50	C	6	-6.69156	1.45266	-1.34949	0.1138	0	0
51	H	1	-6.90684	-0.52366	-2.16267	0.0228	0	0
52	H	1	-8.19804	0.67121	-2.66086	-0.0071	0	0
53	H	1	-6.07122	1.77821	-2.21590	0.0043	0	0
54	H	1	-7.35707	2.28283	-1.01792	0.0290	0	0
55	O	8	-5.87262	1.00921	-0.28864	-0.3313	2.5056	0
56	C	6	-10.07504	-1.65299	-0.00575	0.2014	0	0
57	C	6	-9.19742	-1.20062	-1.16707	0.0667	0	0
58	H	1	-9.40610	-1.97803	0.82447	0.0218	0	0
59	H	1	-10.69268	-2.50978	-0.36088	-0.0095	0	0
60	H	1	-8.57068	-2.06840	-1.47633	0.0159	0	0
61	H	1	-9.86530	-0.88986	-2.00336	0.0370	0	0
62	O	8	-8.38608	-0.12562	-0.74411	-0.3295	2.4404	0
63	O	8	-10.89808	-0.58035	0.40028	-0.3331	2.5093	0
64	C	6	-11.70258	-0.99468	1.48044	0.0372	0	0
65	O	8	11.73762	-0.04179	-0.85050	-0.5901	3.8702	0
66	H	1	12.28351	0.32227	-1.59501	0.3770	0	2.0097
67	H	1	-12.34482	-0.14252	1.78365	0.0629	0	0
68	H	1	-11.08452	-1.26711	2.36476	0.0274	0	0
69	H	1	-12.38202	-1.82499	1.18508	0.0234	0	0

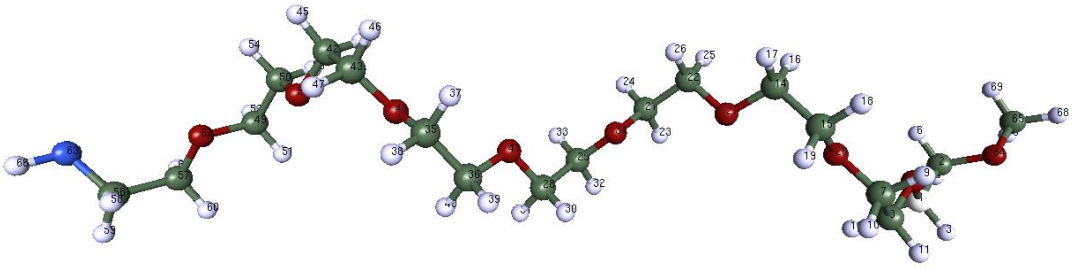
Table S15. Atom coordinates, electrostatic potential-derived (CHelpG) charges, HB_don3, and HB_acc3 calculated at the BP-TZVP level of theory for MeO-PEG-400-OMe.



Centre Number	Atomic Symbol	Atomic Number	Coordinates/Å			CHelpG	Hb_acc3	Hb_don3
			x	y	z			
1	C	6	9.58903	-0.75520	-1.55311	0.0981	0	0
2	C	6	10.49424	0.47119	-1.55976	0.1841	0	0
3	H	1	10.23679	-1.66195	-1.56831	0.0290	0	0
4	H	1	8.95874	-0.71626	-2.47111	0.0084	0	0
5	H	1	11.10696	0.43563	-2.48982	-0.0060	0	0
6	H	1	9.84538	1.37750	-1.56007	0.0240	0	0
7	C	6	7.06969	-1.82722	0.86684	0.1060	0	0
8	C	6	7.94536	-1.86681	-0.37994	0.1645	0	0
9	H	1	7.73875	-1.83125	1.75812	0.0314	0	0
10	H	1	6.42957	-2.73918	0.86095	0.0067	0	0
11	H	1	8.55073	-2.80134	-0.34042	-0.0030	0	0
12	H	1	7.27540	-1.87856	-1.27053	0.0244	0	0
13	O	8	8.78332	-0.73081	-0.39422	-0.3332	2.4793	0
14	C	6	4.60420	0.64221	1.95074	0.1085	0	0
15	C	6	5.46405	-0.61545	1.99259	0.1642	0	0
16	H	1	5.28494	1.52422	1.92461	0.0330	0	0
17	H	1	3.98443	0.66057	2.87648	0.0068	0	0
18	H	1	6.09079	-0.56793	2.91257	-0.0044	0	0
19	H	1	4.78310	-1.49670	2.03474	0.0226	0	0
20	O	8	6.27558	-0.66048	0.83843	-0.3254	2.4612	0
21	C	6	2.10235	1.71893	-0.48494	0.1079	0	0
22	C	6	2.98656	1.76840	0.75540	0.1488	0	0
23	H	1	2.76599	1.67126	-1.37904	0.0348	0	0
24	H	1	1.49369	2.65194	-0.50566	0.0072	0	0
25	H	1	3.62354	2.67963	0.68204	-0.0003	0	0
26	H	1	2.32343	1.83210	1.64885	0.0268	0	0
27	O	8	3.78426	0.60473	0.80228	-0.3271	2.4645	0
28	C	6	-0.44768	-0.70187	-1.47906	0.1188	0	0
29	C	6	0.45288	0.52465	-1.56509	0.1377	0	0
30	H	1	0.20411	-1.60424	-1.42426	0.0319	0	0
31	H	1	-1.07049	-0.73144	-2.40244	0.0064	0	0

32	H	1	1.07480	0.42528	-2.48421	0.0008	0	0
33	H	1	-0.19864	1.42609	-1.63567	0.0285	0	0
34	O	8	1.26899	0.58172	-0.41472	-0.3206	2.4129	0
35	C	6	-2.97764	-1.61247	0.99505	0.1420	0	0
36	C	6	-2.09206	-1.73722	-0.23901	0.1320	0	0
37	H	1	-2.31535	-1.54487	1.88884	0.0265	0	0
38	H	1	-3.61078	-2.52751	1.05242	0.0006	0	0
39	H	1	-1.47975	-2.66115	-0.12572	0.0014	0	0
40	H	1	-2.75476	-1.82054	-1.13121	0.0273	0	0
41	O	8	-1.26302	-0.59843	-0.33137	-0.3231	2.4216	0
42	C	6	-5.46903	0.91126	1.87538	0.1589	0	0
43	C	6	-4.59916	-0.33209	2.01736	0.1276	0	0
44	H	1	-4.79526	1.79447	1.78578	0.0230	0	0
45	H	1	-6.09443	0.99479	2.79370	-0.0052	0	0
46	H	1	-3.97828	-0.20935	2.93435	0.0015	0	0
47	H	1	-5.27306	-1.21347	2.12283	0.0286	0	0
48	O	8	-3.78043	-0.45765	0.87431	-0.3316	2.5529	0
49	C	6	-7.96383	1.77905	-0.64942	0.1518	0	0
50	C	6	-7.08676	1.93053	0.58776	0.1248	0	0
51	H	1	-7.29477	1.66624	-1.53360	0.0271	0	0
52	H	1	-8.57786	2.70373	-0.74593	-0.0003	0	0
53	H	1	-6.45506	2.83750	0.44691	0.0011	0	0
54	H	1	-7.75508	2.05912	1.47028	0.0277	0	0
55	O	8	-6.28198	0.77941	0.72889	-0.3274	2.5777	0
56	C	6	-10.49121	-0.73024	-1.46856	0.1854	0	0
57	C	6	-9.59831	0.49276	-1.64324	0.0802	0	0
58	H	1	-9.83327	-1.62051	-1.33831	0.0255	0	0
59	H	1	-11.10530	-0.83676	-2.39226	-0.0050	0	0
60	H	1	-8.96871	0.32639	-2.54736	0.0129	0	0
61	H	1	-10.25509	1.38127	-1.78890	0.0344	0	0
62	O	8	-8.79115	0.64562	-0.49524	-0.3287	2.4618	0
63	O	8	-11.31806	-0.54470	-0.33954	-0.3306	2.4473	0
64	C	6	-12.13660	-1.67931	-0.17128	0.0383	0	0
65	O	8	11.32217	0.44406	-0.41669	-0.3360	2.4388	0
66	C	6	12.15236	1.58267	-0.41684	0.0542	0	0
67	H	1	-12.78174	-1.51515	0.71609	0.0627	0	0
68	H	1	-11.53005	-2.58994	0.03138	0.0269	0	0
69	H	1	-12.81312	-1.82430	-1.04283	0.0229	0	0
70	H	1	12.79808	1.54330	0.48432	0.0586	0	0
71	H	1	11.55542	2.51928	-0.34875	0.0232	0	0
72	H	1	12.82808	1.59188	-1.30093	0.0195	0	0

Table S16. Atom coordinates, electrostatic potential-derived (CHelpG) charges, HB_don3, and HB_acc3 calculated at the BP-TZVP level of theory for MeO-PEG-400-NH_2.



Centre Number	Atomic Symbol	Atomic Number	Coordinates/Å			CHelpG	Hb_acc3	Hb_don3
			x	y	z			
1	C	6	-9.16945	-1.49898	-0.78741	0.0756	0	0
2	C	6	-10.06456	-1.58762	0.44322	0.1816	0	0
3	H	1	-9.82453	-1.45584	-1.68801	0.0351	0	0
4	H	1	-8.53650	-2.41554	-0.81490	0.0158	0	0
5	H	1	-10.67884	-2.51275	0.35258	-0.0037	0	0
6	H	1	-9.40685	-1.64803	1.34122	0.0258	0	0
7	C	6	-6.67223	1.00158	-1.71394	0.1306	0	0
8	C	6	-7.54640	-0.24079	-1.83584	0.1387	0	0
9	H	1	-7.34283	1.88877	-1.64147	0.0265	0	0
10	H	1	-6.04388	1.06669	-2.63171	0.0010	0	0
11	H	1	-8.16599	-0.13214	-2.75541	0.0028	0	0
12	H	1	-6.87561	-1.12641	-1.92470	0.0300	0	0
13	O	8	-8.36650	-0.34211	-0.69154	-0.3231	2.4998	0
14	C	6	-4.17954	1.89729	0.80238	0.1228	0	0
15	C	6	-5.05488	2.03615	-0.43739	0.1410	0	0
16	H	1	-4.84944	1.80124	1.68787	0.0317	0	0
17	H	1	-3.55921	2.81905	0.88597	0.0051	0	0
18	H	1	-5.68299	2.94754	-0.30996	-0.0003	0	0
19	H	1	-4.38512	2.14940	-1.32096	0.0281	0	0
20	O	8	-5.86375	0.88624	-0.56269	-0.3226	2.4994	0
21	C	6	-1.67104	-0.61881	1.65300	0.1452	0	0
22	C	6	-2.55014	0.61588	1.81120	0.1366	0	0
23	H	1	-2.33861	-1.50467	1.54457	0.0253	0	0
24	H	1	-1.04950	-0.71424	2.57274	-0.0018	0	0
25	H	1	-3.17622	0.47254	2.72165	-0.0002	0	0
26	H	1	-1.88347	1.50010	1.93638	0.0271	0	0
27	O	8	-3.36104	0.75566	0.66440	-0.3305	2.4304	0
28	C	6	0.83594	-1.42599	-0.87890	0.1480	0	0
29	C	6	-0.04492	-1.60672	0.35145	0.1318	0	0
30	H	1	0.16951	-1.29792	-1.76302	0.0242	0	0

31	H	1	1.45499	-2.34533	-0.99233	-0.0018	0	0
32	H	1	-0.67296	-2.51266	0.18935	0.0005	0	0
33	H	1	0.62044	-1.75112	1.23375	0.0269	0	0
34	O	8	-0.85373	-0.46127	0.51305	-0.3281	2.4207	0
35	C	6	3.35398	1.11206	-1.63162	0.1456	0	0
36	C	6	2.46377	-0.10712	-1.84070	0.1178	0	0
37	H	1	2.69451	1.99741	-1.47858	0.0269	0	0
38	H	1	3.97053	1.24447	-2.55013	0.0012	0	0
39	H	1	1.83424	0.08211	-2.74030	0.0048	0	0
40	H	1	3.12269	-0.98996	-2.00954	0.0317	0	0
41	O	8	1.65668	-0.29200	-0.69753	-0.3281	2.4596	0
42	C	6	5.89089	1.78011	0.91148	0.1891	0	0
43	C	6	4.99489	2.02769	-0.29622	0.0941	0	0
44	H	1	5.23577	1.60919	1.79676	0.0190	0	0
45	H	1	6.51538	2.69018	1.06370	-0.0096	0	0
46	H	1	4.37356	2.92686	-0.07988	0.0072	0	0
47	H	1	5.64997	2.21443	-1.17832	0.0368	0	0
48	O	8	4.17753	0.89607	-0.50573	-0.3222	2.5671	0
49	C	6	8.40885	-0.80147	1.49952	0.1911	0	0
50	C	6	7.52997	0.41160	1.78019	0.0913	0	0
51	H	1	7.74109	-1.67501	1.31721	0.0242	0	0
52	H	1	9.03987	-0.97975	2.40027	-0.0160	0	0
53	H	1	6.91515	0.18416	2.68114	0.0073	0	0
54	H	1	8.19712	1.28211	1.97806	0.0335	0	0
55	O	8	6.70415	0.65379	0.66130	-0.3407	2.5839	0
56	C	6	10.89573	-1.37196	-1.12169	0.3541	0.0014	0
57	C	6	10.02026	-1.66481	0.09518	0.0690	0	0
58	H	1	10.24373	-1.15533	-1.99604	0.0201	0	0
59	H	1	11.51576	-2.26556	-1.35679	-0.0815	0	0
60	H	1	9.38772	-2.54823	-0.15078	-0.0149	0	0
61	H	1	10.68683	-1.89978	0.95680	0.0331	0	0
62	O	8	9.21516	-0.53848	0.37098	-0.3108	3.3334	0
63	N	7	11.76198	-0.22397	-0.87039	-0.9142	5.3427	0
64	O	8	-10.89176	-0.44496	0.49832	-0.3277	2.4449	0
65	C	6	-11.69576	-0.50727	1.65383	0.0276	0	0
66	H	1	12.33153	-0.04489	-1.72881	0.3344	0	0.0396
67	H	1	12.42321	-0.45605	-0.09373	0.3385	0	0.0278
68	H	1	-12.34418	0.39258	1.67583	0.0650	0	0
69	H	1	-11.07767	-0.48540	2.57890	0.0307	0	0
70	H	1	-12.36911	-1.39290	1.63250	0.0258	0	0

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