Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information

Amphiphilic Nanostructure in Choline Carboxylate and Amino Acid Ionic Liquids and Solutions

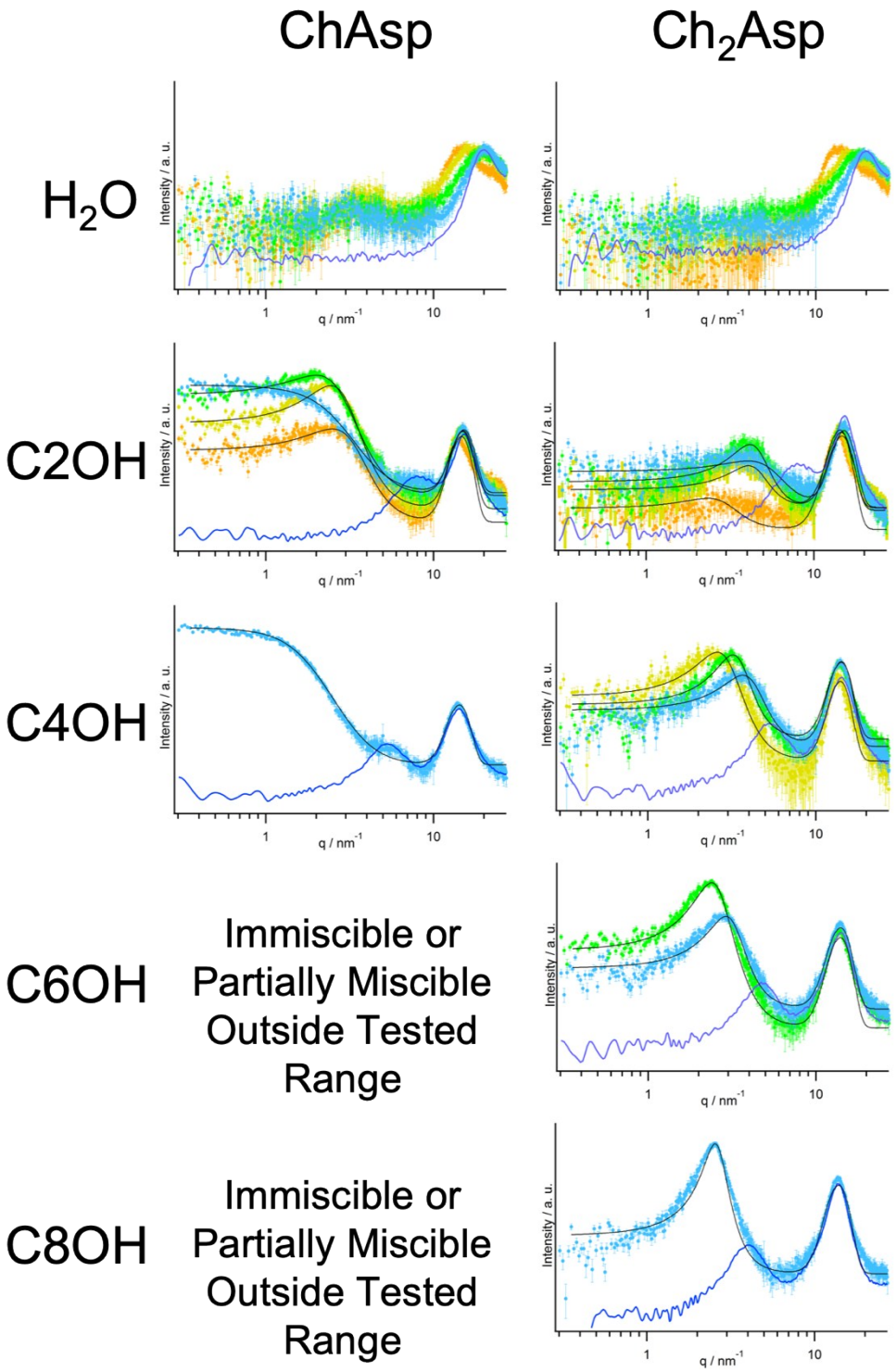
Shurui Miao,[1] Rob Atkin,[2] and Gregory G. Warr[11]

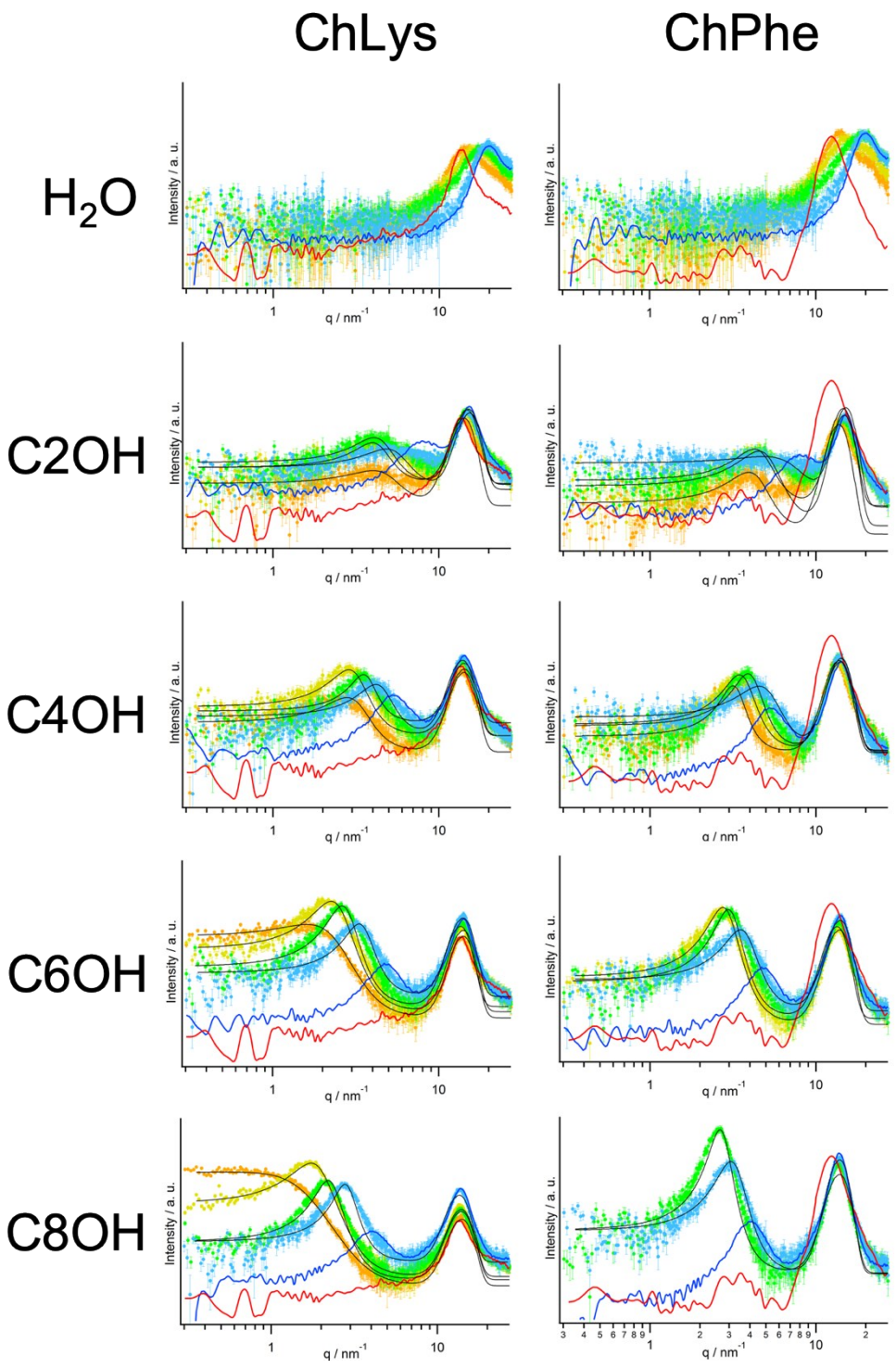
1. School of Chemistry and University of Sydney Nano Institute, The University of Sydney, NSW 2006, Australia

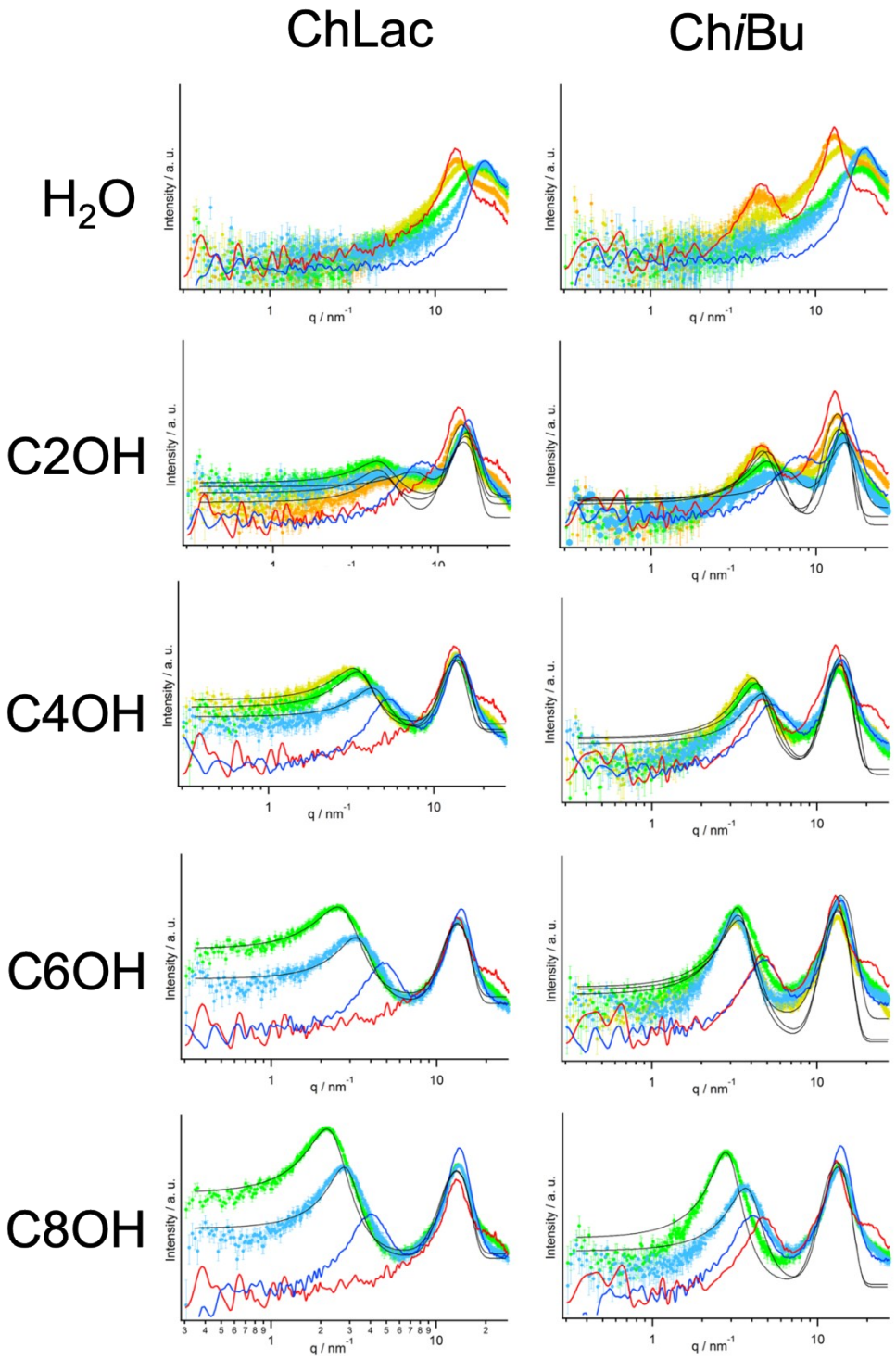
2. School of Molecular Sciences, The University of Western Australia, WA 6009, Australia

[1] Corresponding Author: Tel.: +16 02 9351 2106. E-mail: gregory.warr@sydney.edu.au

Figure S1. SAXS/WAXS patterns of bio-ILs and their mixtures. Each plot shows pure bio-IL (red), pure alkanol or water (blue) and four mixtures at 20, 40, 60 and 80 wt% ILs. Fits of the Teubner-Strey model are shown in black lines.*




ChLys
ChPhe
H2O
C2OH
C4OH
C6OH
C8OH
Intensity / a. u.
q / nm-1
1
10



*Due to the low scattering intensity of IL + water samples, upon background subtraction, most water-containing scattering patterns have no obvious prepeak features (e.g. ChLys + water) and hence are not fitted using the Teubner-Strey model. For those with a noticeable prepeak (e.g. Ch*i*Bu + water), its proximity to the nearest neighbour peak makes it difficult to determine an unambiguous best fit; various combinations of background, periodicity and correlation lengths can describe the observed features. Similar effects are present in all Ch*i*Bu patterns and some IL + ethanol systems, but diminish as the prepeak becomes more pronounced, enabling a unique set of periodicity and correlation lengths at a fixed background to be determined.

Table S1. Teubner-Strey best-fit parameters of all SAXS/WAXS patterns

Sample	bkg	TS scale	SLD a	SLD b	d (nm)	δ_d (nm)	ξ (nm)	δ_ξ (nm)	Gaus. peak	Gaus. sigma
ChLac + 20 wt% C_2H_5OH	0.0012	7.0	0.3	6.3	1.381	0.002	0.700	0.004	13.9	2.1
ChLac + 40 wt% C_2H_5OH	0.0016	5.4	0.3	6.3	1.392	0.010	0.813	0.034	14.3	2.3
ChLac + 60 wt% C_2H_5OH	0.0019	8.0	0.3	6.3	1.401	0.010	0.700	0.015	14.7	2.1
ChLac + 80 wt% C_2H_5OH	0.0018	19.1	0.3	6.3	0.858	0.009	0.430	0.018	15.0	2.4
ChLac + 40 wt% C_4H_9OH	0.0020	6.9	0.3	6.3	1.837	0.008	0.942	0.017	13.8	2.0
ChLac + 60 wt% C_4H_9OH	0.0017	7.6	0.3	6.3	1.665	0.006	0.940	0.017	14.0	2.1
ChLac + 80 wt% C_4H_9OH	0.0017	8.1	0.3	6.3	1.427	0.006	0.813	0.020	14.1	2.2
ChLac + 60 wt% $C_6H_{13}OH$	0.0019	8.1	0.3	6.3	2.268	0.006	1.098	0.012	13.8	2.2
ChLac + 80 wt% $C_6H_{13}OH$	0.0018	7.2	0.3	6.3	1.807	0.006	1.066	0.017	13.9	2.2
ChLac + 60 wt% $C_8H_{17}OH$	0.0017	7.5	0.3	6.3	2.682	0.004	1.595	0.012	13.8	2.3
ChLac + 80 wt% $C_8H_{17}OH$	0.0016	5.7	0.3	6.3	2.135	0.005	1.529	0.018	13.8	2.2
Ch*i*Bu + 20 wt% C_2H_5OH	0.0008	17.7	0.3	6.3	1.199	0.001	0.731	0.010	13.5	2.0
Ch*i*Bu + 40 wt% C_2H_5OH	0.0012	10.0	0.3	6.3	1.309	0.010	0.900	0.006	13.8	2.0
Ch*i*Bu + 60 wt% C_2H_5OH	0.0012	16.0	0.3	6.3	1.211	0.008	0.700	0.005	14.5	2.0
Ch*i*Bu + 80 wt% C_2H_5OH	0.0015	16.1	0.3	6.3	0.925	0.006	0.622	0.018	15.0	2.8
Ch*i*Bu + 40 wt% C_4H_9OH	0.0010	11.0	0.3	6.3	1.502	0.004	1.033	0.013	13.6	2.0
Ch*i*Bu + 60 wt% C_4H_9OH	0.0010	12.0	0.3	6.3	1.420	0.003	0.940	0.012	13.8	2.0
Ch*i*Bu + 80 wt% C_4H_9OH	0.0010	15.0	0.3	6.3	1.301	0.004	0.800	0.007	14.1	2.0
Ch*i*Bu + 40 wt% $C_6H_{13}OH$	0.0010	10.5	0.3	6.3	1.781	0.004	1.100	0.012	13.5	2.0
Ch*i*Bu + 60 wt% $C_6H_{13}OH$	0.0010	10.0	0.3	6.3	1.850	0.003	1.300	0.012	13.7	2.0
Ch*i*Bu + 80 wt% $C_6H_{13}OH$	0.0010	5.3	0.3	6.3	1.895	0.005	1.656	0.027	13.8	2.3
Ch*i*Bu + 60 wt% $C_8H_{17}OH$	0.0010	6.6	0.3	6.3	2.136	0.003	1.689	0.016	13.6	2.1
Ch*i*Bu + 80 wt% $C_8H_{17}OH$	0.0010	9.7	0.3	6.3	1.608	0.004	1.081	0.014	13.8	2.1
Ch_2Asp + 20 wt% C_2H_5OH	0.0010	1.0	0.3	6.3	2.337	0.030	0.752	0.041	14.3	2.2
Ch_2Asp + 40 wt% C_2H_5OH	0.0014	4.3	0.3	6.3	1.540	0.016	0.944	0.042	14.7	2.1
Ch_2Asp + 60 wt% C_2H_5OH	0.0012	9.3	0.3	6.3	1.402	0.016	0.718	0.002	14.9	2.3
Ch_2Asp + 80 wt% C_2H_5OH	0.0010	11.1	0.3	6.3	1.291	0.024	0.373	0.018	15.2	2.1

Ch_2Asp + 40 wt% C_4H_9OH	0.0005	3.1	0.3	6.3	2.274	0.015	1.041	0.022	14.0	1.9
Ch_2Asp + 60 wt% C_4H_9OH	0.0016	8.6	0.3	6.3	1.881	0.006	1.102	0.021	14.2	2.0
Ch_2Asp + 80 wt% C_4H_9OH	0.0010	7.8	0.3	6.3	1.605	0.010	0.755	0.019	14.2	2.0
Ch_2Asp + 60 wt% $C_6H_{13}OH$	0.0007	6.7	0.3	6.3	2.539	0.006	1.541	0.014	14.0	2.0
Ch_2Asp + 80 wt% $C_6H_{13}OH$	0.0012	6.6	0.3	6.3	2.082	0.007	1.232	0.019	14.0	2.0
Ch_2Asp + 80 wt% $C_8H_{17}OH$	0.0010	5.1	0.3	6.3	2.426	0.004	2.334	0.026	13.9	2.0
ChAsp + 20 wt% C_2H_5OH	0.0010	7.7	0.3	6.3	2.202	0.014	0.720	0.012	14.7	2.0
ChAsp + 40 wt% C_2H_5OH	0.0012	11.0	0.3	6.3	2.366	0.008	0.952	0.009	14.9	2.0
ChAsp + 60 wt% C_2H_5OH	0.0011	9.1	0.3	6.3	2.673	0.010	0.806	0.009	15.0	2.1
ChAsp + 80 wt% C_2H_5OH	0.0012	7.6	0.3	6.3	3.513	0.034	0.490	0.013	15.2	2.1
ChAsp + 80 wt% C_4H_9OH	0.0012	6.8	0.3	6.3	5.374	0.027	0.764	0.009	14.3	1.9
ChLys + 20 wt% C_2H_5OH	0.0008	6.0	0.3	6.3	1.414	0.003	0.500	0.040	14.2	2.2
ChLys + 40 wt% C_2H_5OH	0.0008	4.0	0.3	6.3	1.507	0.016	0.800	0.015	14.8	2.2
ChLys + 60 wt% C_2H_5OH	0.0008	6.0	0.3	6.3	1.458	0.011	0.700	0.013	15.1	2.2
ChLys + 80 wt% C_2H_5OH	0.0008	10.0	0.3	6.3	1.201	0.011	0.500	0.011	15.3	2.2
ChLys + 20 wt% C_4H_9OH	0.0011	3.5	0.3	6.3	2.092	0.020	0.905	0.025	14.2	2.2
ChLys + 40 wt% C_4H_9OH	0.0011	3.9	0.3	6.3	2.093	0.011	1.126	0.023	14.2	2.2
ChLys + 60 wt% C_4H_9OH	0.0011	2.9	0.3	6.3	1.747	0.010	1.300	0.059	14.2	2.2
ChLys + 80 wt% C_4H_9OH	0.0011	8.0	0.3	6.3	1.411	0.009	0.800	0.030	14.2	2.2
ChLys + 20 wt% $C_6H_{13}OH$	0.0009	4.1	0.3	6.3	3.165	0.017	0.863	0.014	14.0	2.1
ChLys + 40 wt% $C_6H_{13}OH$	0.0008	4.8	0.3	6.3	2.656	0.008	1.391	0.015	14.1	2.1
ChLys + 60 wt% $C_6H_{13}OH$	0.0008	4.7	0.3	6.3	2.249	0.006	1.567	0.020	14.0	2.1
ChLys + 80 wt% $C_6H_{13}OH$	0.0010	5.3	0.3	6.3	1.845	0.007	1.300	0.026	14.0	2.1
ChLys + 20 wt% $C_8H_{17}OH$	0.0009	4.5	0.3	6.3	5.277	0.020	0.931	0.010	14.0	2.1
ChLys + 40 wt% $C_8H_{17}OH$	0.0007	4.3	0.3	6.3	3.431	0.007	1.760	0.012	13.9	2.1
ChLys + 60 wt% $C_8H_{17}OH$	0.0009	4.3	0.3	6.3	2.796	0.006	2.297	0.023	14.0	2.1
ChLys + 80 wt% $C_8H_{17}OH$	0.0007	3.3	0.3	6.3	2.174	0.006	2.060	0.033	13.9	2.0
ChPhe + 20 wt% C_2H_5OH	0.0007	6.0	0.3	6.3	1.489	0.003	0.700	0.003	13.8	2.1
ChPhe + 40 wt% C_2H_5OH	0.0007	6.0	0.3	6.3	1.412	0.011	0.700	0.013	14.6	2.1
ChPhe + 60 wt% C_2H_5OH	0.0006	11.0	0.3	6.3	1.306	0.005	0.600	0.005	14.8	2.1
ChPhe + 80 wt% C_2H_5OH	0.0007	28.0	0.3	6.3	1.037	0.105	0.250	0.007	15.2	2.1
ChPhe + 20 wt% C_4H_9OH	0.0009	2.2	0.3	6.3	1.941	0.013	1.500	0.049	13.8	2.2

ChPhe + 40 wt% C_4H_9OH	0.0012	5.9	0.3	6.3	1.757	0.008	1.117	0.025	14.1	2.2
ChPhe + 60 wt% C_4H_9OH	0.0009	6.0	0.3	6.3	1.567	0.007	1.056	0.030	14.1	2.2
ChPhe + 80 wt% C_4H_9OH	0.0009	12.5	0.3	6.3	1.290	0.011	0.577	0.015	14.2	2.2
ChPhe + 40 wt% $C_6H_{13}OH$	0.0009	5.6	0.3	6.3	2.221	0.006	1.520	0.019	13.9	2.2
ChPhe + 60 wt% $C_6H_{13}OH$	0.0009	5.8	0.3	6.3	2.000	0.006	1.529	0.021	13.9	2.2
ChPhe + 80 wt% $C_6H_{13}OH$	0.0009	6.1	0.3	6.3	1.727	0.009	1.072	0.021	14.0	2.2
ChPhe + 60 wt% $C_8H_{17}OH$	0.0008	4.3	0.3	6.3	2.342	0.004	2.193	0.025	13.9	2.2
ChPhe + 80 wt% $C_8H_{17}OH$	0.0008	5.4	0.3	6.3	1.988	0.007	1.359	0.021	13.9	2.0