

Electronic supplementary information (ESI)

Selective binding and dynamics of imidazole alkyl sulfate ionic liquids with human serum albumin and collagen –A detailed NMR investigation

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Fig. S1 ^1H NMR (A) and ^{13}C NMR (B) spectra of IL4.

Fig. S2 FT-IR spectra of lyophilized collagen in the presence of ILs at higher concentration (5mM). Concentration of collagen was 5 μM .

Fig. S3A ^1H NMR spectra of IL2 at various concentrations of HSA, showing (a) 0 μM , (b) 1 μM , (c) 5 μM , (d) 10 μM , (e) 20 μM , (f) 30 μM (g) 40 μM and (h) 50 μM . Concentration of IL was 5 mM.

Fig. S3B ^1H NMR spectra of IL3 at various concentrations of HSA, showing (a) 0 μM , (b) 1 μM , (c) 5 μM , (d) 10 μM , (e) 20 μM , (f) 30 μM (g) 40 μM and (h) 50 μM . Concentration of IL was 5 mM. The expanded regions of broadened signals (anionic part) are marked up.

Fig. S3C ^1H NMR spectra of IL4 at various concentrations of HSA, showing (a) 0 μM , (b) 1 μM , (c) 5 μM , (d) 10 μM , (e) 20 μM , (f) 30 μM (g) 40 μM and (h) 50 μM . Concentration of IL was 5 mM.

Fig. S4A ^1H NMR spectra of IL1 (5 mM) at various concentrations of collagen, showing (a) 0 μM , (b) 0.2 μM (c) 0.6 μM , (d) 1 μM , (e) 1.5 μM , (f) 2.2 μM and (g) 3.6 μM .

Fig. S4B ^1H NMR spectra of IL2 (5 mM) at various concentrations of collagen, showing (a) 0 μM , (b) 0.6 μM (c) 1 μM , (d) 1.8 μM , (e) 2.2 μM , (f) 3.6 μM and (g) 5 μM .

Fig. S4C ^1H NMR spectra of IL3 (5 mM) at various concentrations of collagen, showing (a) 0 μM , (b) 0.4 μM (c) 0.6 μM , (d) 0.8 μM , (e) 1 μM , (f) 1.8 μM , (g) 2.2 μM of collagen and (h) 3.6 μM .

Fig. S4D ^1H NMR spectra of IL4 (5 mM) at various concentrations of collagen, showing (a) 0 nM, (b) 20 nM (c) 40 nM, (d) 60 nM, (e) 80 nM, and (f) 100 nM.

Fig. S5 ^1H NMR spectrum of 1-Butyl 3-Methylimidazolium chloride (5 mM) in the presence of HSA (50 μM) and the corresponding STD NMR spectrum.

Fig. S6 STD NMR (A) IL3 Control (B) IL3 in the presence of HSA at different on-resonance irradiation positions (0.5, 0, -0.5 and -1 ppm).

Fig. S7 ^1H NMR spectrum (blue) of IL1 (A), IL2 (B) and IL4 (C) in the presence of collagen (5 μM), whereas for IL4 collagen concentration was 0.1 μM and the corresponding STD NMR spectrum (red) for each IL is shown in the top. Concentration of ILs was 5 mM.

Fig. S8 STD NMR profiles for IL4 (5 mM) in the presence of HSA (A) and collagen (B). The solid lines represent the best fit of experimental data to eqn (1) for various protons of IL3. The concentrations of HSA and collagen were (50 μM and 0.1 μM), respectively.

Fig. S9 Selective and nonselective relaxation rates (R_{ISEL} and R_{INS}) for IL1 (A), IL2 (B) and IL4 (C) as a function of HSA.

Fig. S10 Selective and nonselective relaxation rates (R_{ISEL} and R_{INS}) for IL1 (A), IL2 (B) and IL4 (C) as a function of collagen.

Fig. S11 Selective and non-selective relaxation rates for IL3 (5 mM) in the presence of HSA (50 μM) as a function of temperature.

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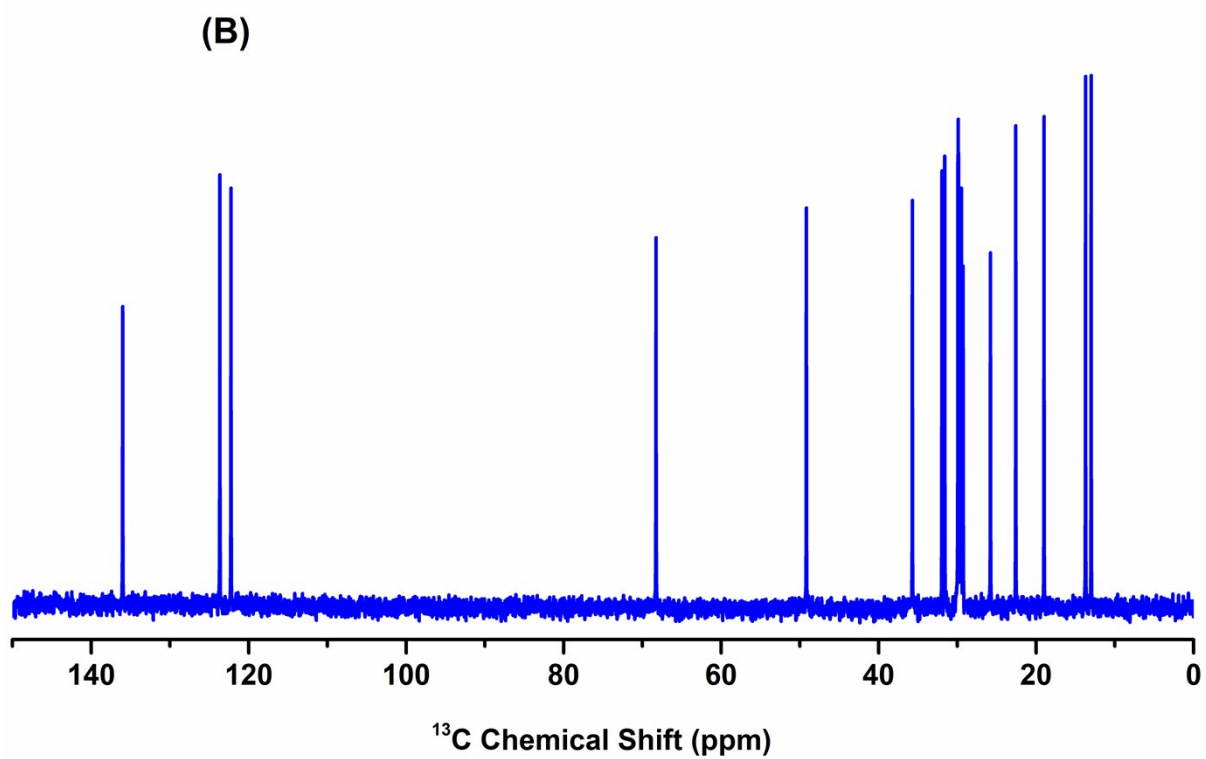
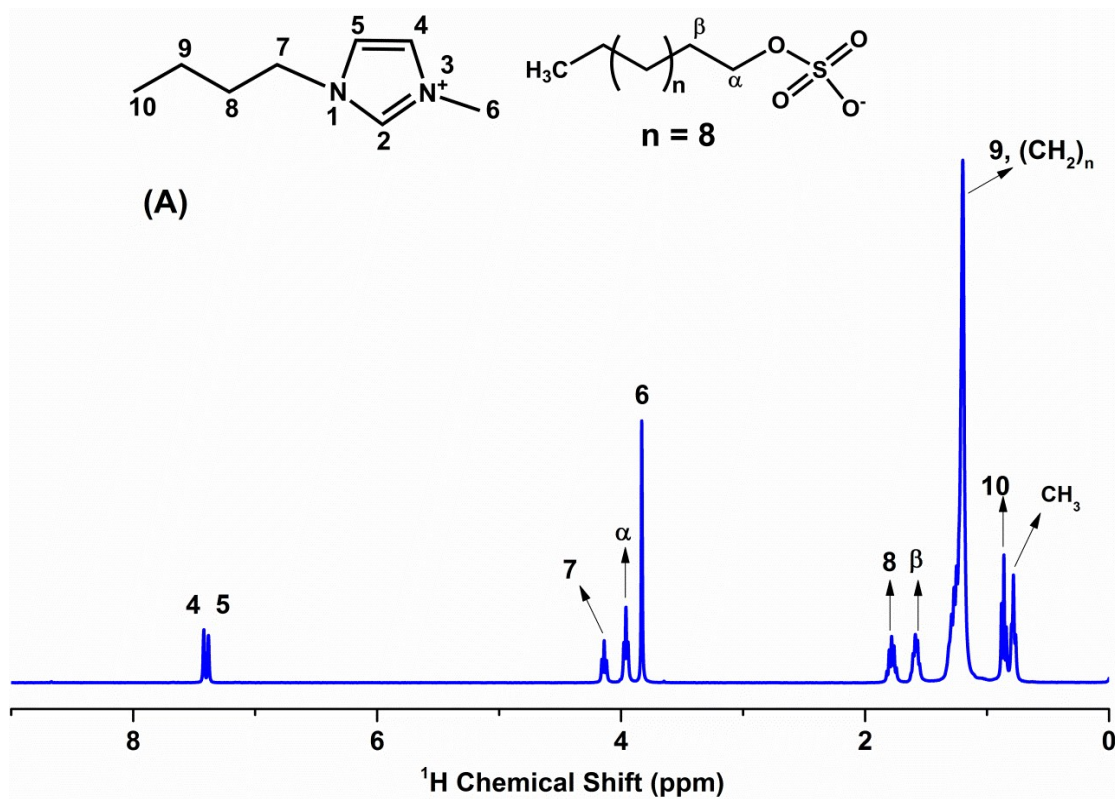


Fig. S1

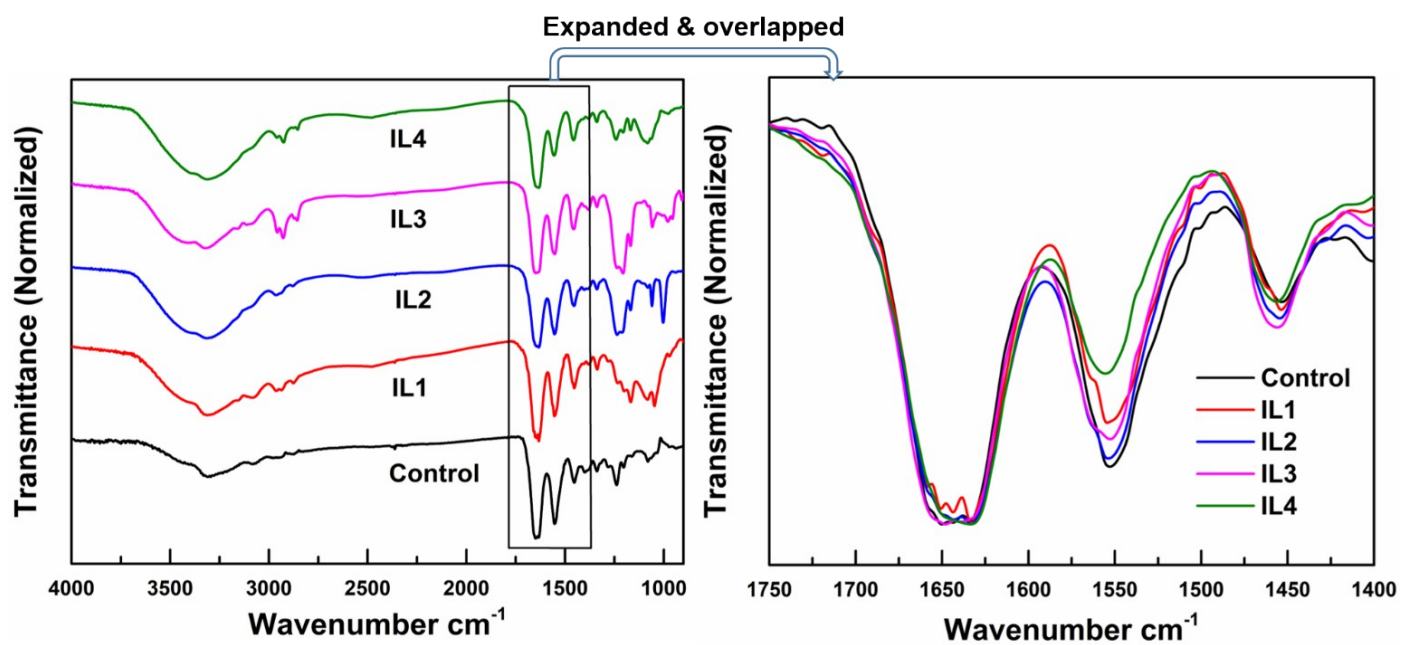


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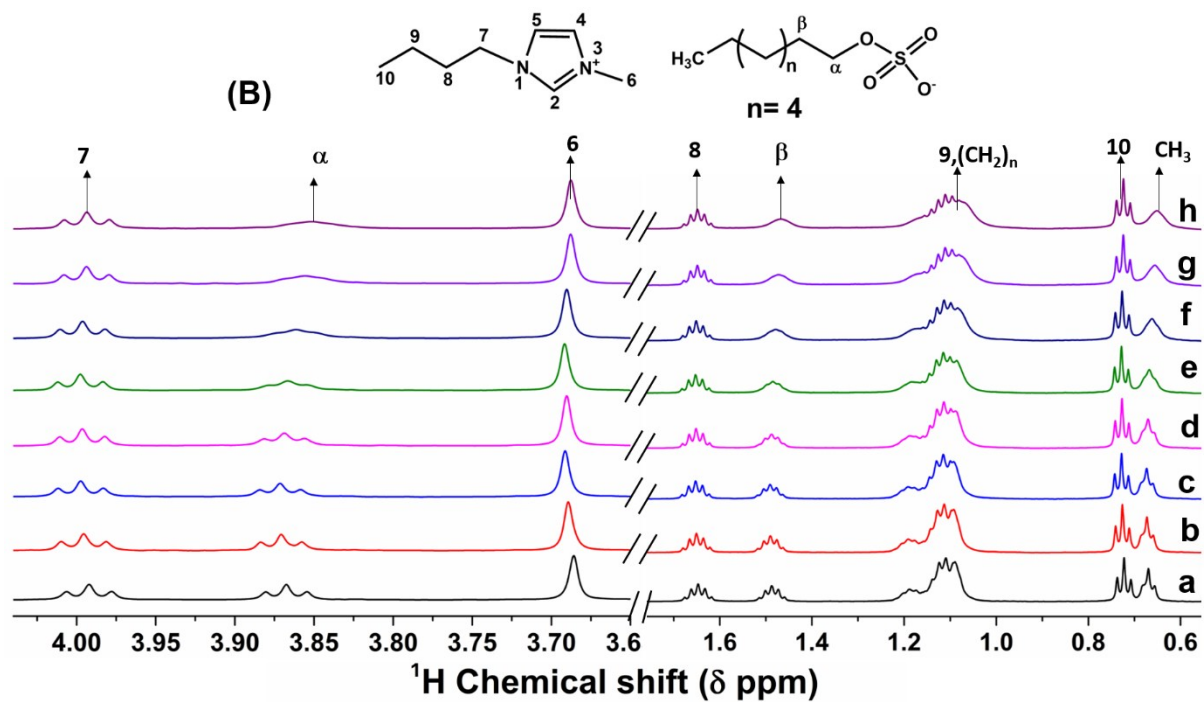
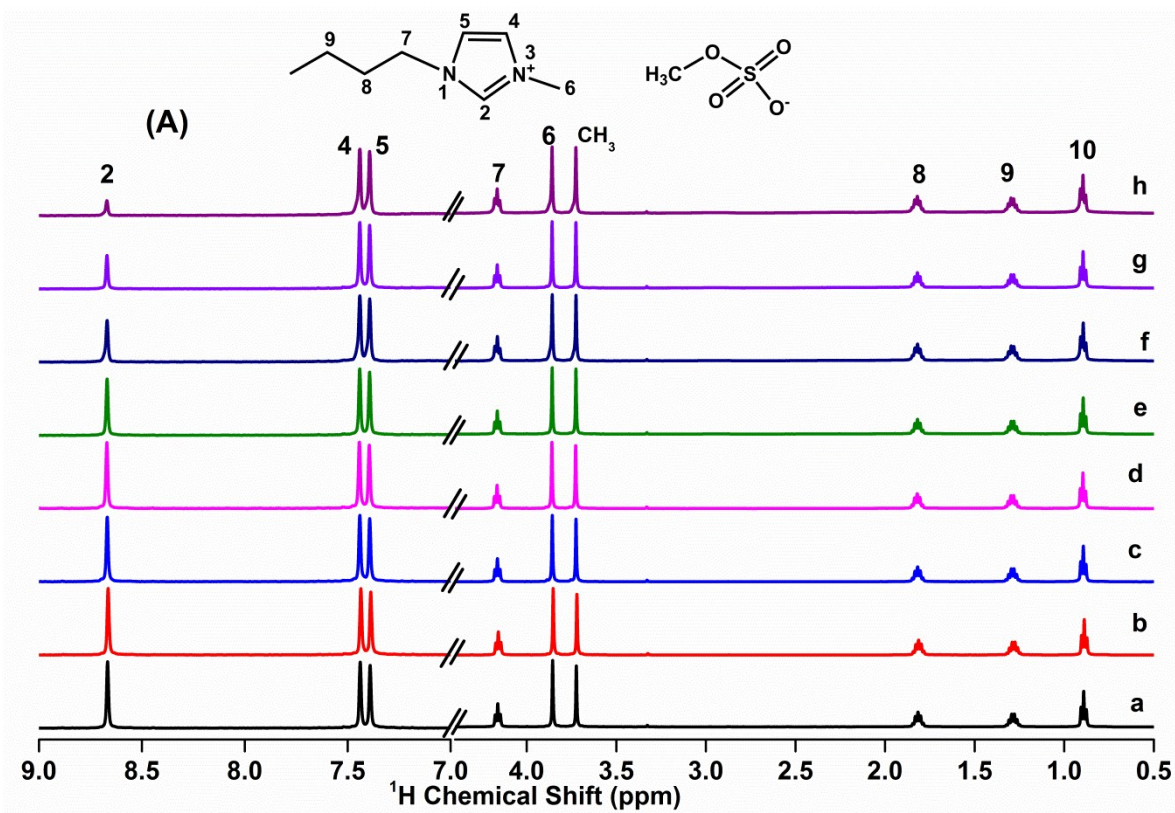


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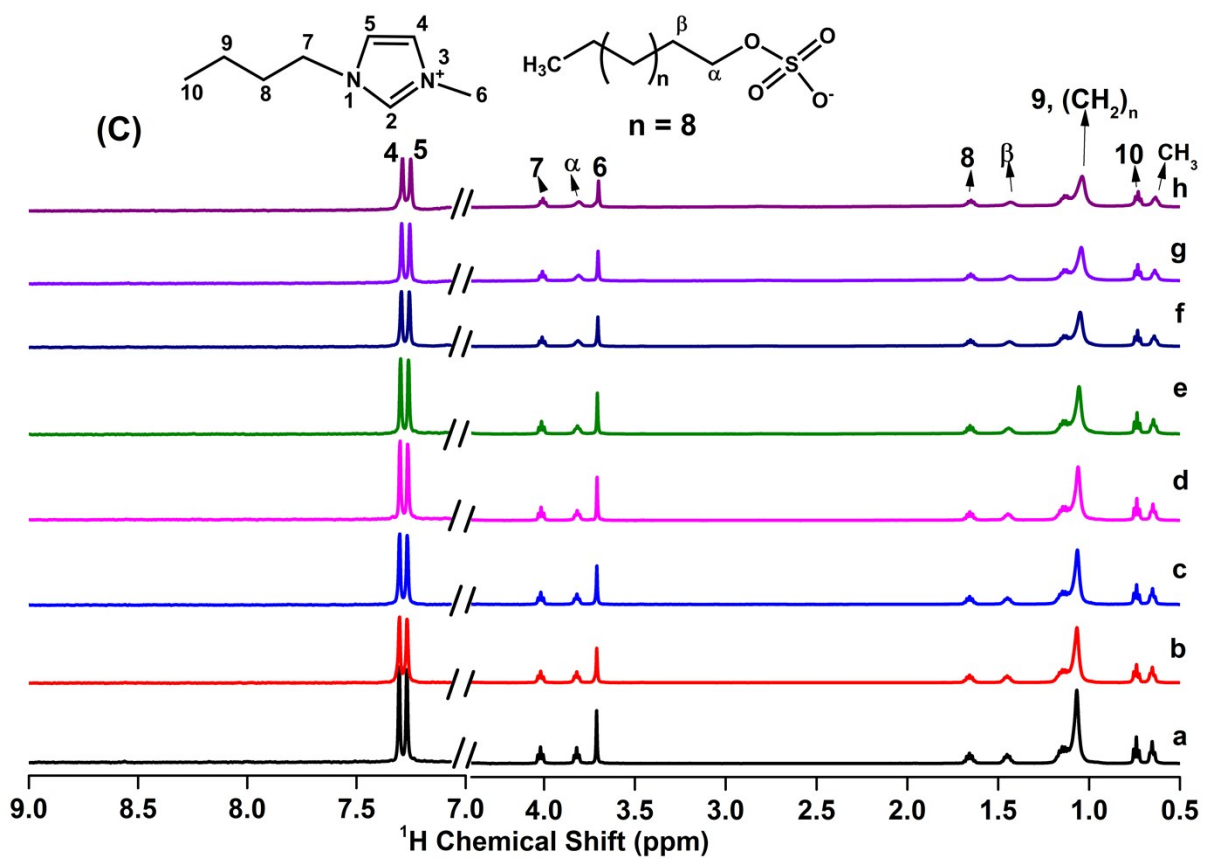


Fig. S3

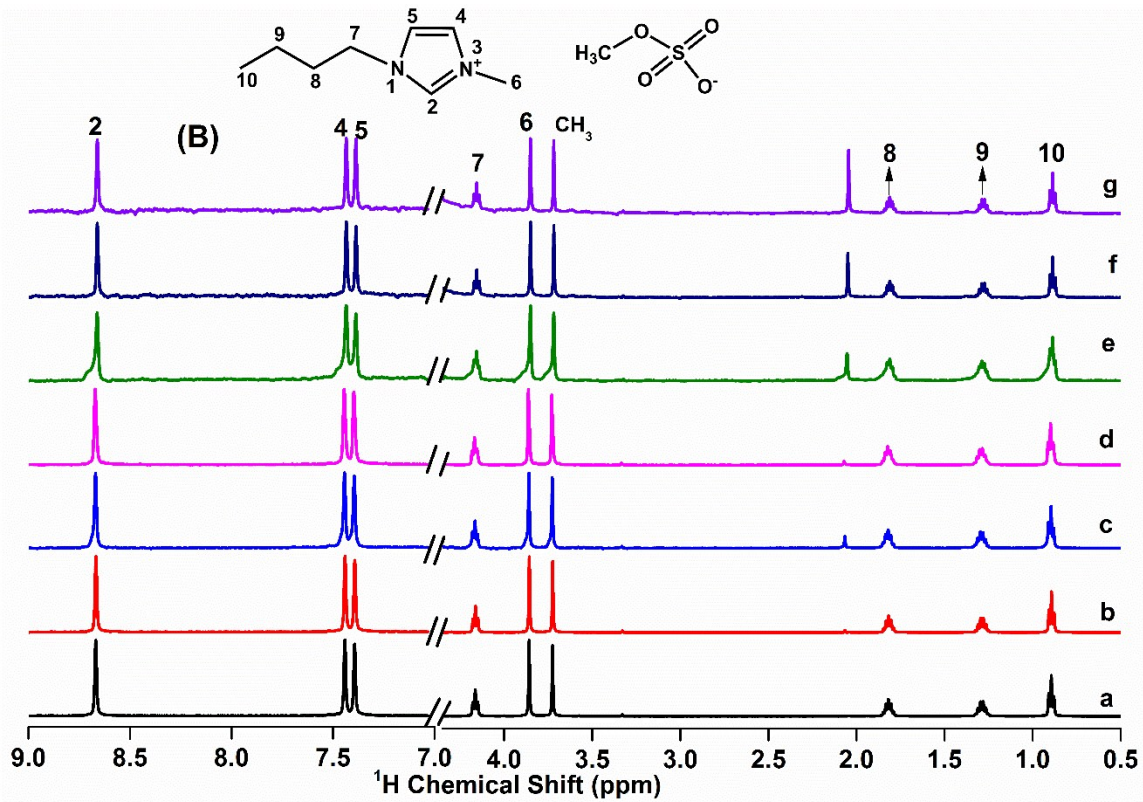
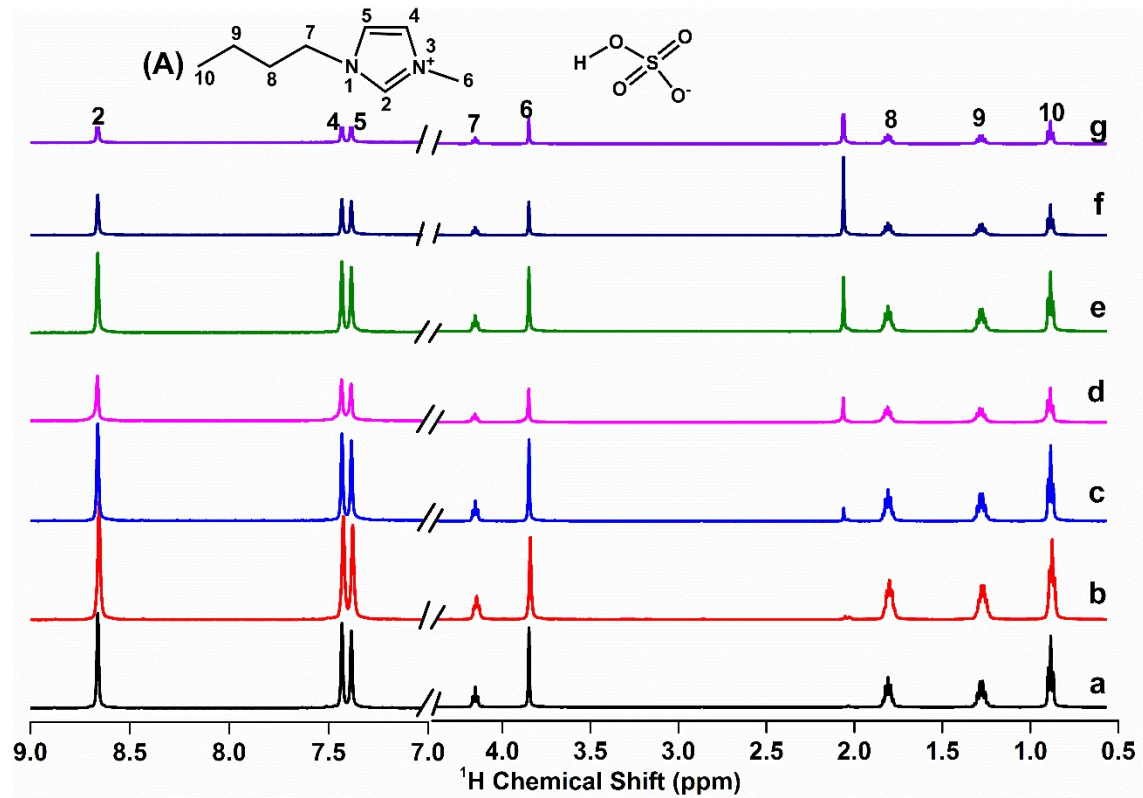


Fig. S4

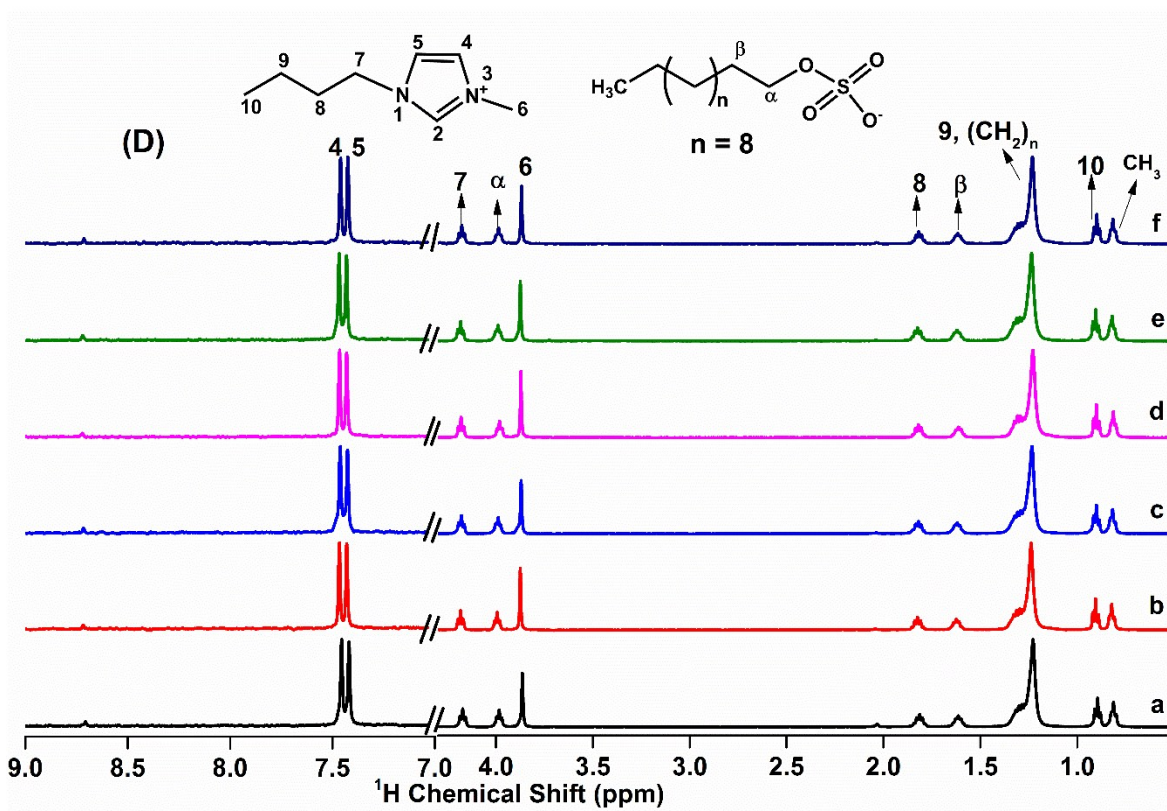
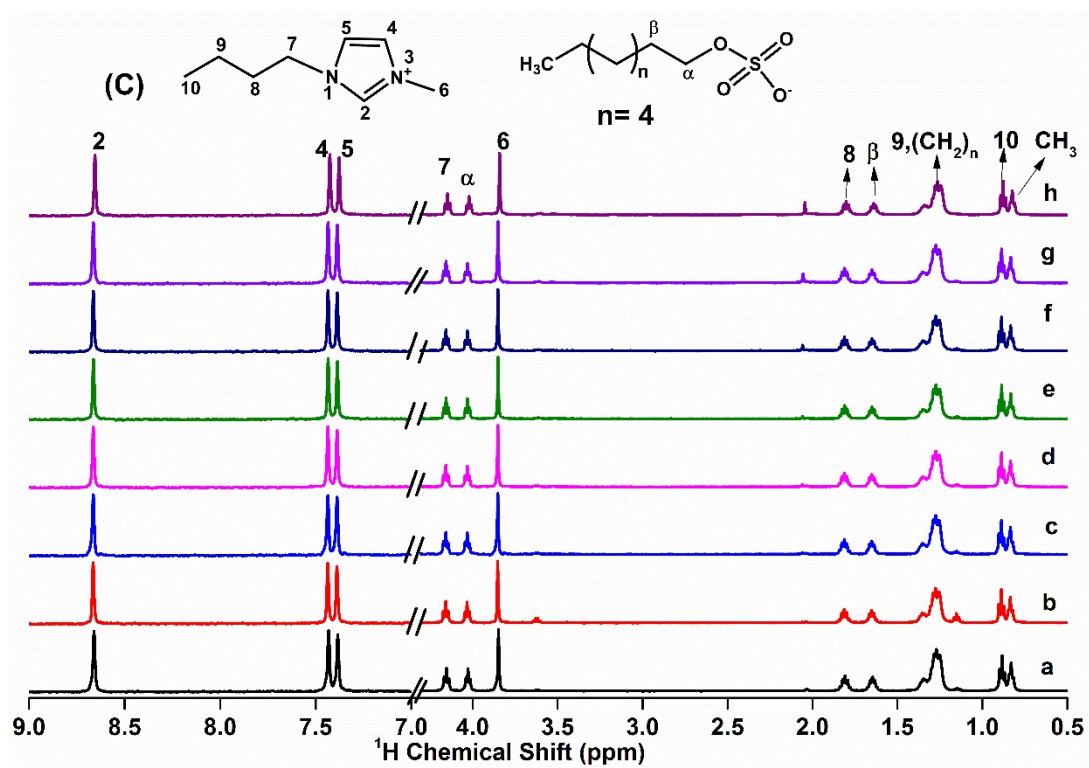


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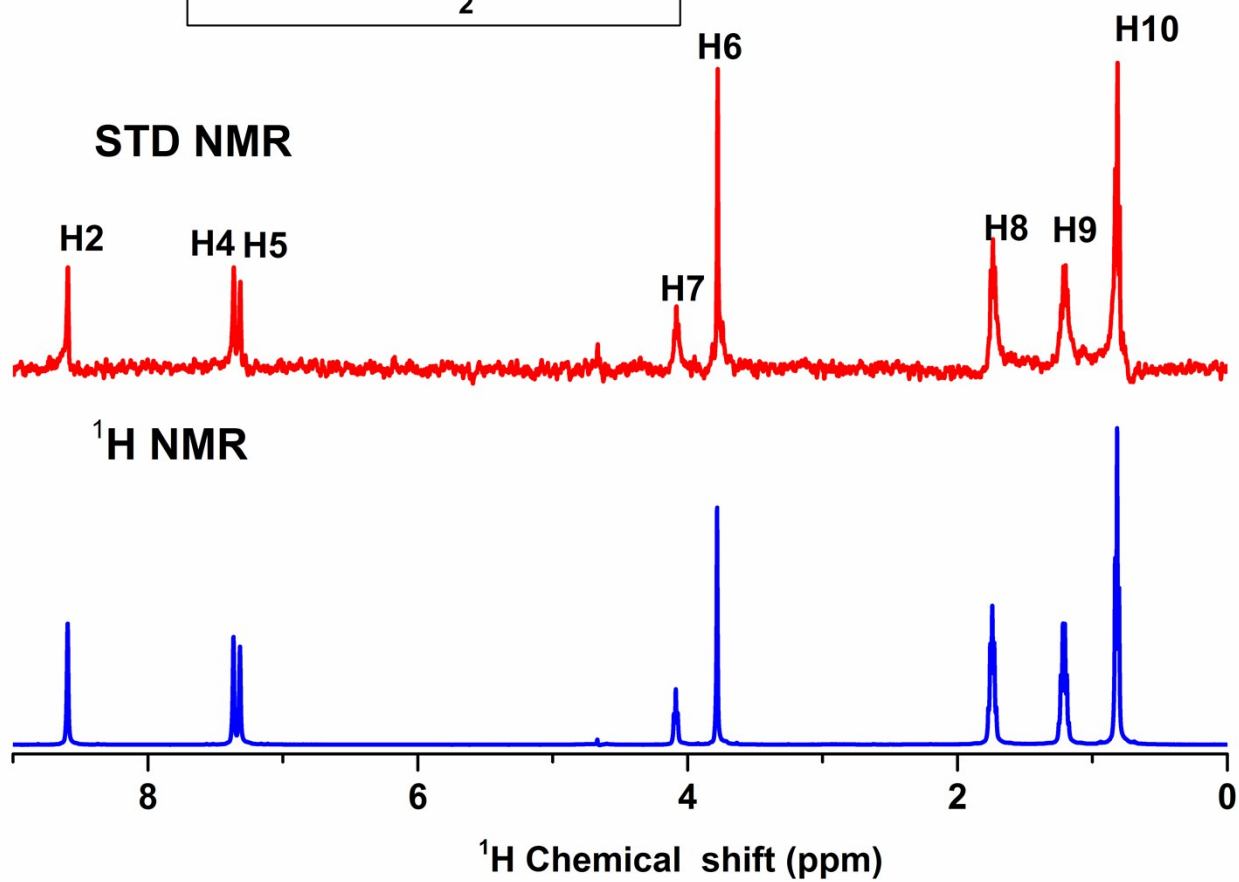
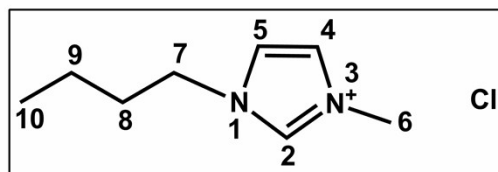


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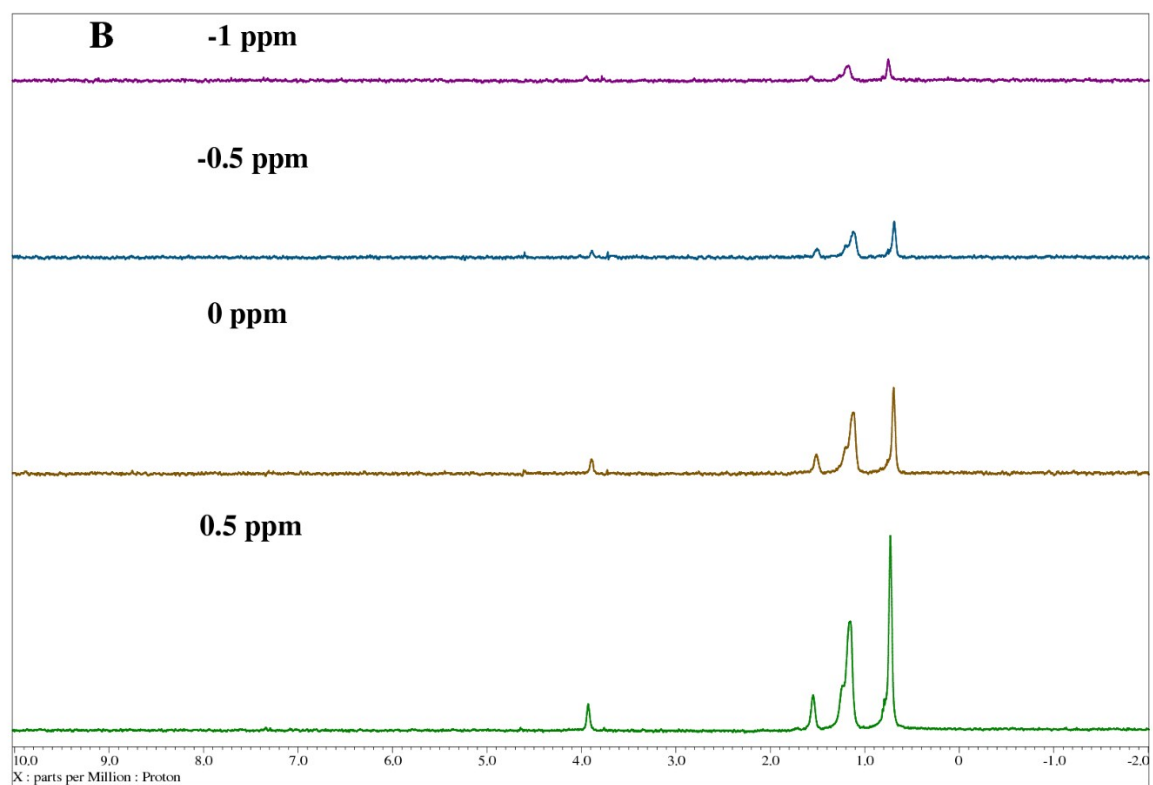
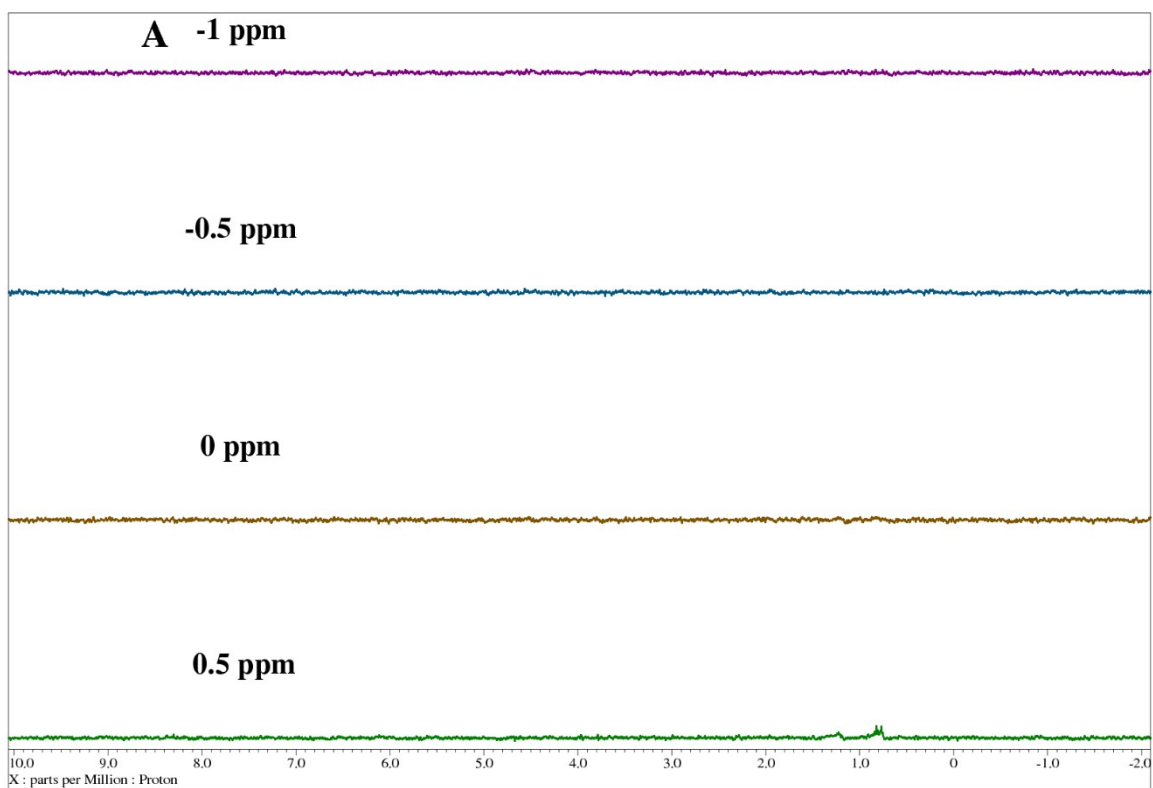


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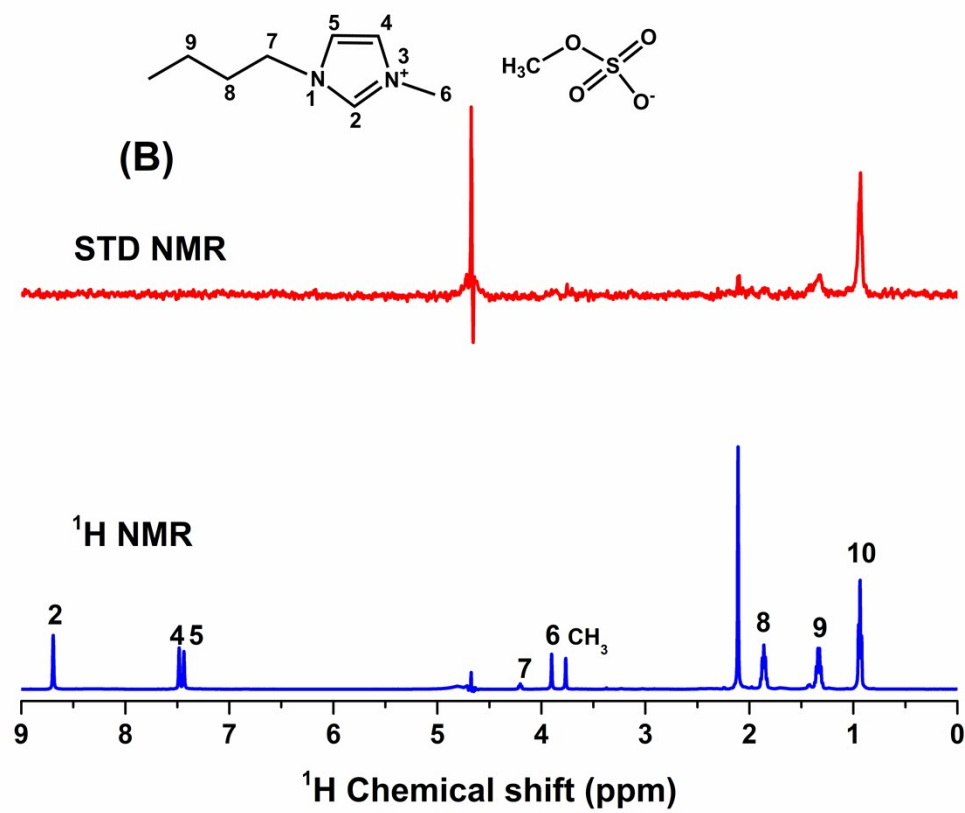
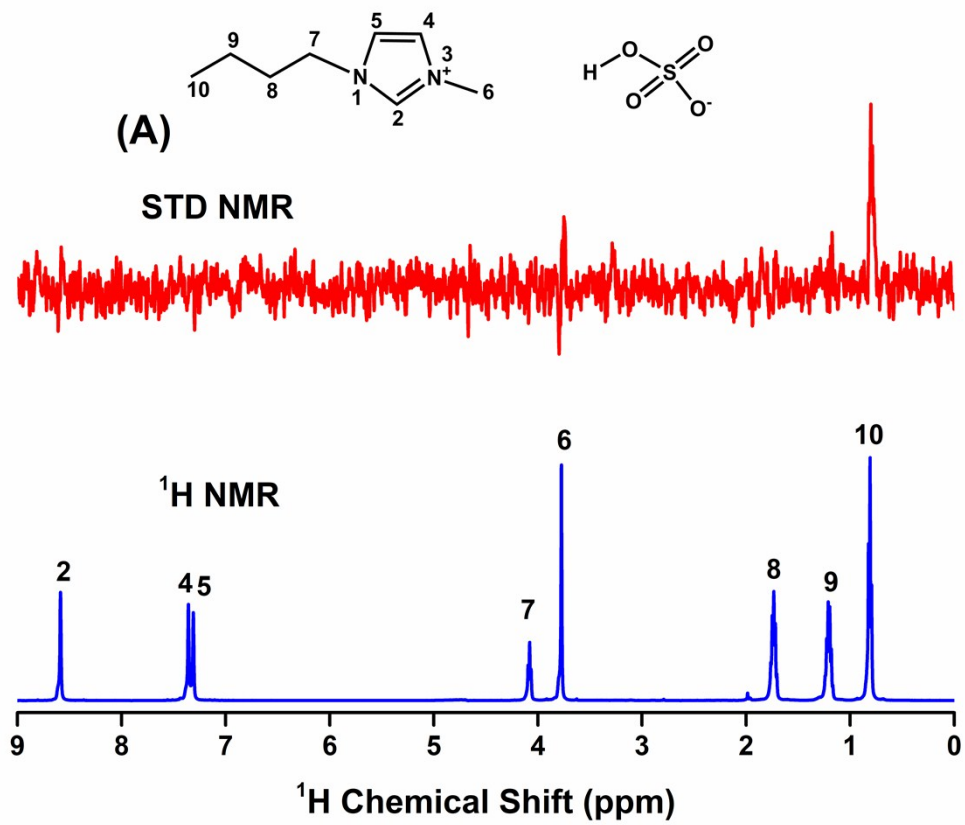


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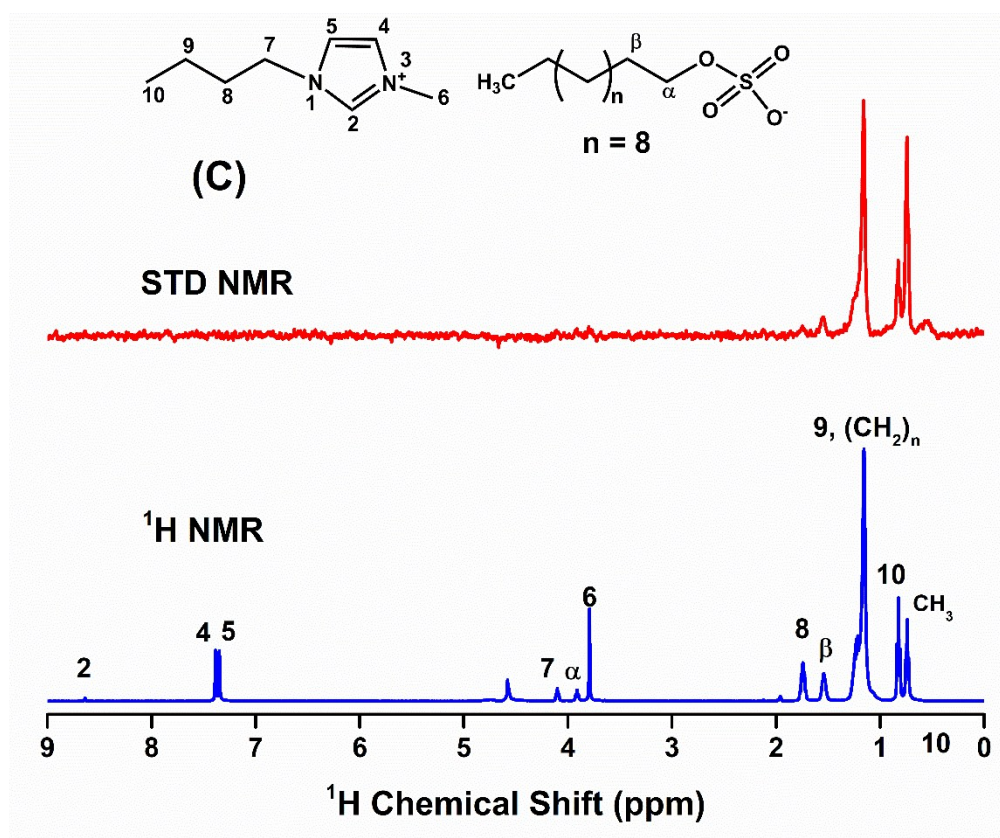


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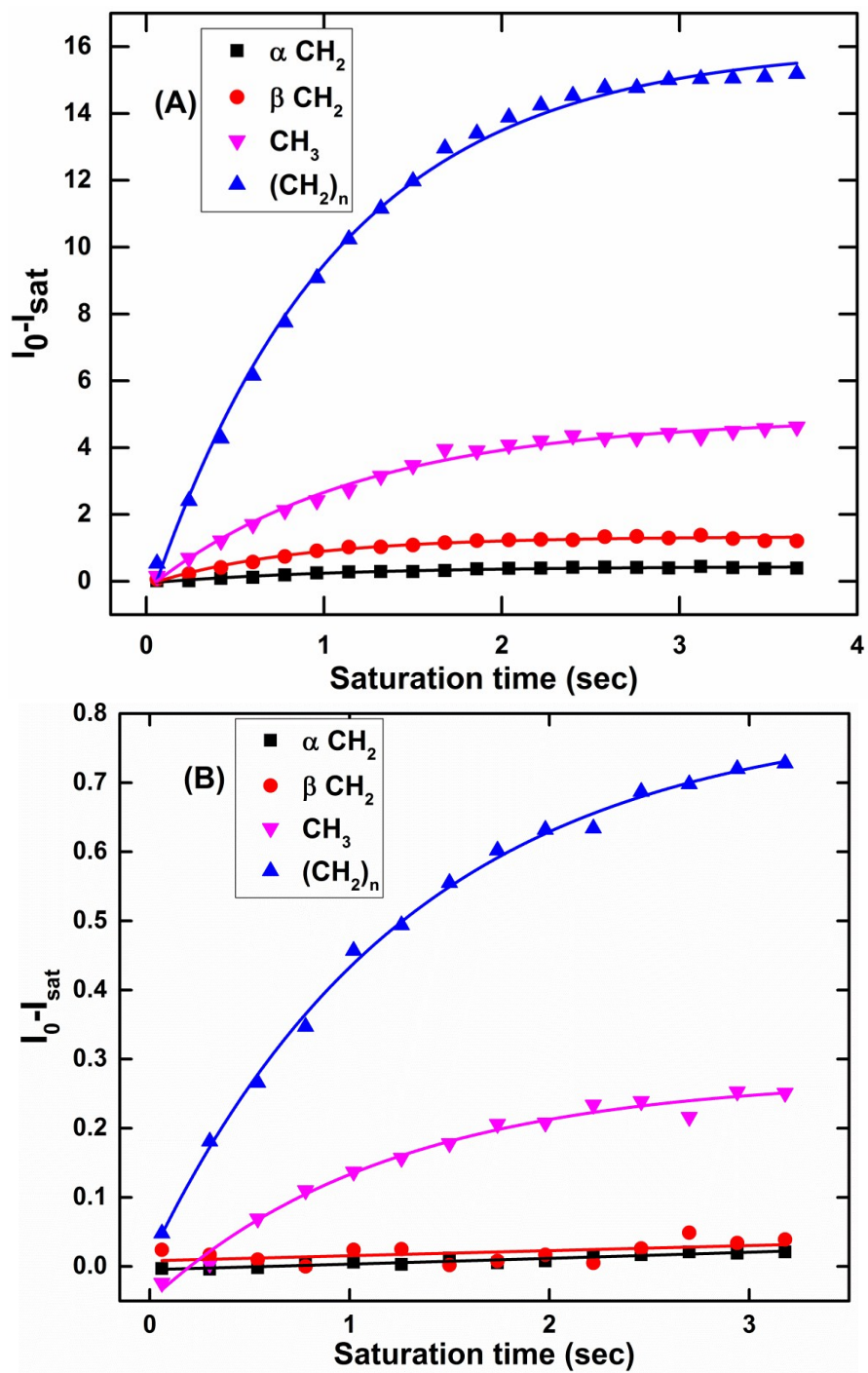


Fig. S8

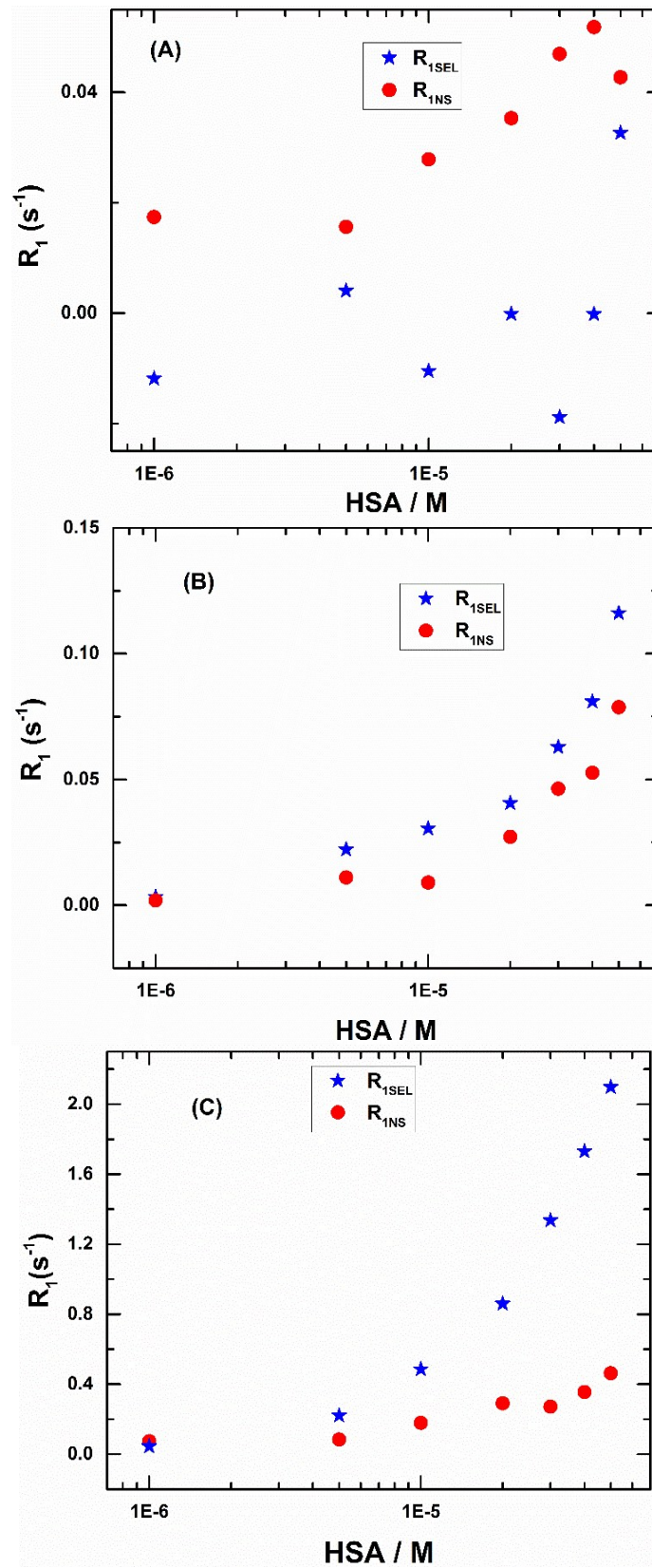


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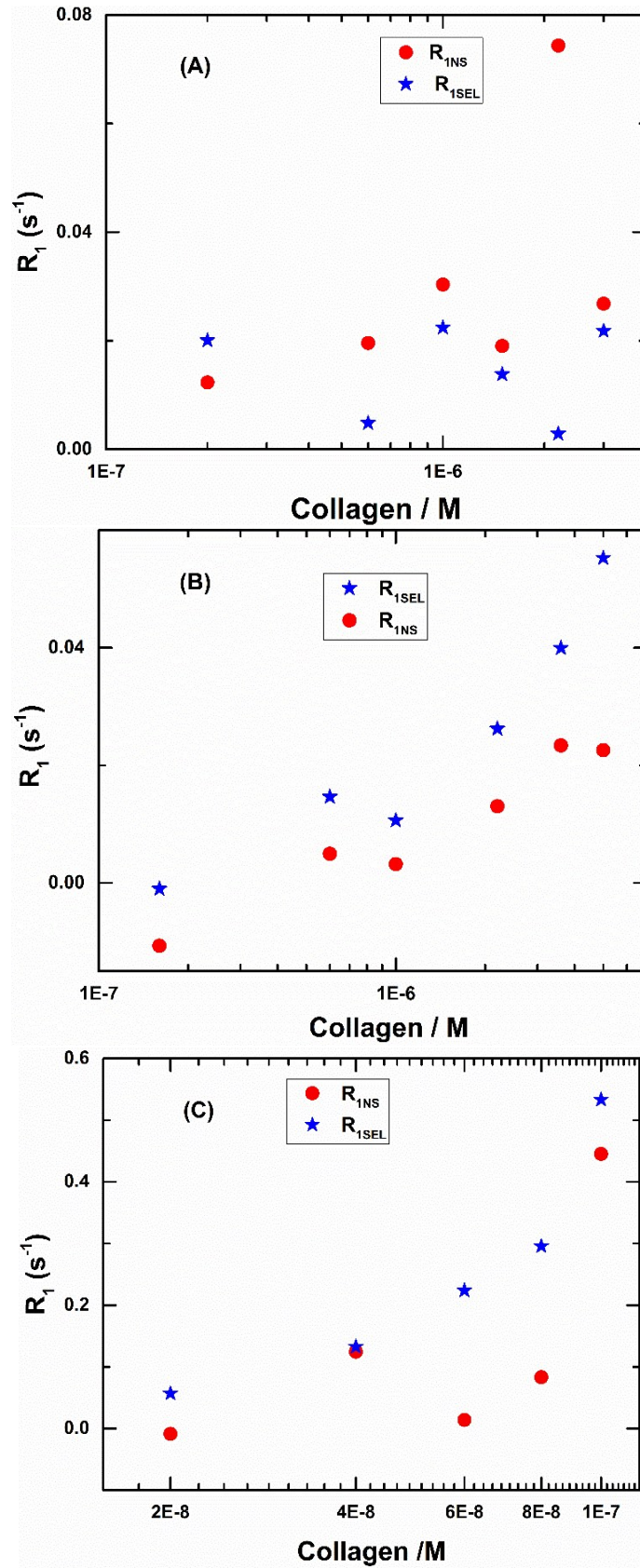


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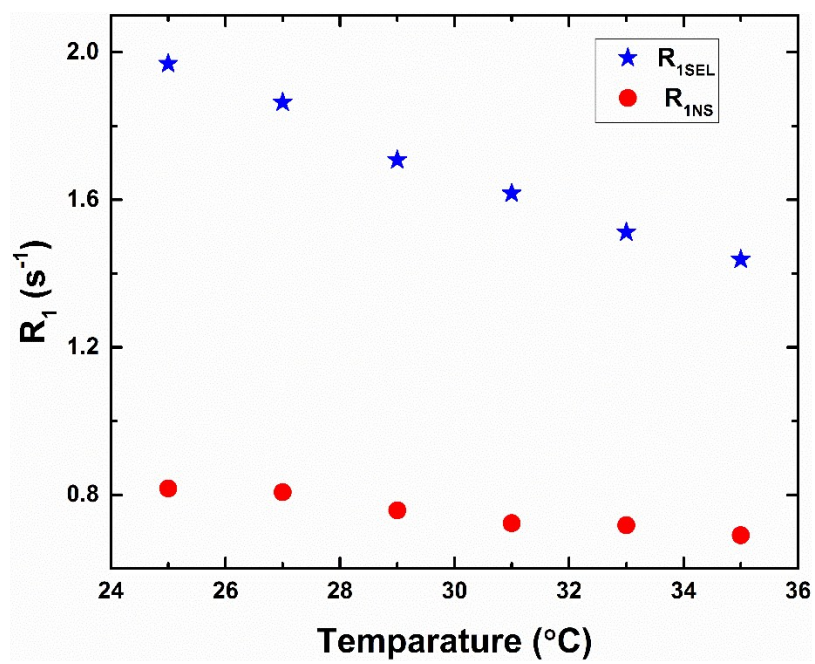


Fig. S11

Table S1 T₁ and T₂ values of IL1 as a function of HSA.

Conc (μ M)	CH ₃ C		γ -CH ₂ C		β -CH ₂ C		N-CH ₃ C		α -CH ₂ C	
	T ₁	T ₂	T ₁	T ₂	T ₁	T ₂	T ₁	T ₂	T ₁	T ₂
0	3.598	2.242	2.952	1.941	2.523	1.950	3.877	2.438	2.642	1.440
	(0.014)	(0.040)	(0.012)	(0.03)	(0.007)	(0.064)	(0.028)	(0.053)	(0.008)	(0.047)
1	3.306	2.30	2.787	2.134	2.405	1.90	3.569	2.390	2.476	1.292
	(0.014)	(0.028)	(0.014)	(0.02)	(0.01)	(0.06)	(0.025)	(0.04)	(0.005)	(0.063)
5	3.326	2.151	2.804	1.554	2.423	2.019	3.598	2.1867	2.518	1.241
	(0.017)	(0.030)	(0.016)	(0.031)	(0.010)	(0.097)	(0.024)	(0.034)	(0.008)	(0.051)
10	3.196	2.254	2.518	1.833	2.336	1.733	3.524	2.315	2.412	1.125
	(0.017)	(0.025)	(0.025)	(0.030)	(0.008)	(0.057)	(0.022)	(0.030)	(0.006)	(0.063)
20	3.121	2.323	2.673	1.86	2.294	1.678	3.498	2.290	2.374	1.248
	(0.023)	(0.033)	(0.019)	(0.030)	(0.011)	(0.1321)	(0.020)	(0.029)	(0.008)	(0.085)
30	3.012	2.410	2.590	2.104	2.175	1.738	3.480	2.471	2.370	1.210
	(0.040)	(0.037)	(0.028)	(0.030)	(0.020)	(0.07)	(0.036)	(0.045)	(0.010)	(0.055)
40	2.968	2.4041	2.55	1.982	2.183	1.532	3.427	2.347	2.302	1.237
	(0.030)	(0.023)	(0.023)	(0.030)	(0.013)	(0.162)	(0.025)	(0.018)	(0.007)	(0.091)
50	3.051	2.192	2.63	1.986	2.252	1.702	3.675	2.274	2.414	1.413
	(0.044)	(0.033)	(0.029)	(0.05)	(0.018)	(0.082)	(0.025)	(0.026)	(0.006)	(0.071)

Table S2 T₁ and T₂ values of IL2 as a function of HSA.

Conc (μ M)	CH ₃ C		γ -CH ₂ C		β -CH ₂ C		CH ₃ A		N-CH ₃ C		α -CH ₂ C	
	T ₁	T ₂	T ₁	T ₂	T ₁	T ₂	T ₁	T ₂	T ₁	T ₂	T ₁	T ₂
0	3.316	2.77	2.827	2.326	2.347	2.320	8.535	6.740	3.798	3.355	2.475	1.585
	(0.01)	(0.013)	(0.012)	(0.032)	(0.015)	(0.026)	(0.037)	(0.052)	(0.0367)	(0.024)	(0.015)	(0.034)
1	3.266	2.726	2.745	2.337	2.356	1.983	8.40	5.371	3.662	3.090	2.425	1.467
	(0.023)	(0.02)	(0.015)	(0.032)	(0.008)	(0.049)	(0.077)	(0.098)	(0.060)	(0.016)	(0.008)	(0.052)
5	3.308	2.610	2.795	2.030	2.40	1.639	7.797	3.851	3.735	2.905	2.466	1.384
	(0.006)	(0.025)	(0.007)	(0.037)	(0.007)	(0.090)	(0.012)	(0.062)	(0.040)	(0.021)	(0.008)	(0.062)
10	3.471	2.656	2.878	2.376	2.44	2.133	7.924	3.568	3.891	3.078	2.552	1.519
	(0.023)	(0.02)	(0.007)	(0.030)	(0.010)	0.0364)	(0.155)	(0.054)	(0.030)	(0.016)	(0.018)	(0.037)
20	3.463	2.606	2.833	2.157	2.435	1.910	6.926	2.615	3.972	2.991	2.596	1.218
	(0.050)	(0.018)	(0.026)	(0.035)	(0.016)	(0.06)	(0.033)	(0.015)	(0.087)	(0.011)	(0.019)	(0.050)
30	3.232	2.40	2.7094	2.075	2.339	1.878	6.116	1.974	3.757	2.779	2.447	1.130
	(0.012)	(0.013)	(0.014)	(0.030)	(0.007)	(0.048)	(0.068)	(0.005)	(0.045)	(0.016)	(0.006)	(0.042)
40	3.323	2.55	2.742	2.049	2.321	1.972	5.888	1.860	3.892	3.037	2.535	1.317
	(0.011)	(0.02)	(0.013)	(0.04)	(0.008)	(0.052)	(0.098)	(0.007)	(0.045)	(0.013)	(0.006)	(0.042)
50	3.160	2.485	2.645	1.935	2.308	1.904	5.104	1.407	3.770	2.907	2.470	1.215
	(0.017)	(0.018)	(0.017)	(0.045)	(0.008)	(0.048)	(0.092)	(0.004)	(0.040)	(0.017)	(0.006)	(0.040)

Table S3 T₁ and T₂ values of IL3 as a function of HSA.

Conc (μ M)	CH ₃ A		CH ₃ C		β -CH ₂ A		β -CH ₂ C		N-CH ₃ C		α -CH ₂ A		α -CH ₂ C	
	T ₁	T ₂	T ₁	T ₂	T ₁	T ₂	T ₁	T ₂	T ₁	T ₂	T ₁	T ₂	T ₁	T ₂
	2.887	1.958	3.172	2.305	1.418	1.211	2.357	1.823	3.557	2.689	1.795	0.485	2.48	1.258
0	(0.013)	(0.128)	(0.013)	(0.296)	(0.004)	(0.070)	(0.001)	(0.105)	(0.025)	(0.465)	(0.004)	(0.067)	(0.008)	(0.128)
1	2.73	1.221	3.183	2.131	1.392	0.848	2.356	1.992	3.598	2.359	1.80	0.708	2.530	1.371
	(0.006)	(0.012)	(0.006)	(0.02)	(0.003)	(0.020)	(0.007)	(0.048)	(0.014)	(0.030)	(0.004)	(0.024)	(0.006)	(0.042)
5	2.406	0.580	3.056	2.068	1.337	0.387	2.281	1.896	3.456	2.514	1.640	0.431	2.408	1.100
	(0.018)	(0.005)	(0.007)	(0.02)	(0.003)	(0.013)	(0.008)	(0.063)	(0.021)	(0.046)	(0.006)	(0.017)	(0.004)	(0.087)
10	2.176	0.332	3.210	2.068	1.303	0.2169	2.312	1.709	3.718	2.333	1.574	0.267	2.488	1.213
	(0.03)	(0.004)	(0.01)	(0.02)	(0.003)	(0.009)	(0.007)	(0.077)	(0.020)	(0.044)	(0.009)	(0.016)	(0.011)	(0.056)
20	1.892	0.189	2.943	1.938	1.276	0.1242	2.361	1.596	3.413	2.180	1.503	0.168	2.3351	1.095
	(0.06)	(0.002)	(0.04)	(0.06)	(0.02)	(0.004)	(0.105)	(0.076)	(0.063)	(0.073)	(0.054)	(0.009)	(0.025)	(0.056)
30	1.553	0.119	2.682	1.96	1.152	0.083	2.060	1.547	3.130	2.185	1.286	0.1182	2.175	1.012
	(0.02)	(0.002)	(0.03)	(0.06)	(0.005)	(0.003)	(0.014)	(0.065)	(0.065)	(0.087)	(0.011)	(0.008)	(0.014)	(0.051)
40	1.490	0.097	2.478	1.911	1.143	0.065	2.135	1.486	3.364	2.01	1.265	0.091	2.280	1.036
	(0.02)	(0.002)	(0.03)	(0.02)	(0.006)	(0.002)	(0.012)	(0.068)	(0.026)	(0.020)	(0.010)	(0.006)	(0.009)	(0.054)
50	1.392	0.077	2.79	1.764	1.105	0.052	2.083	1.450	3.34	1.925	1.191	0.074	2.233	0.999
	(0.02)	(0.001)	(0.001)	(0.02)	(0.005)	(0.001)	(0.012)	(0.069)	(0.019)	(0.035)	(0.012)	(0.005)	(0.005)	(0.051)

Table S4 T₁ and T₂ values of IL4 as a function of HSA.

Conc (μ M)	CH ₃ A		CH ₃ C		β -CH ₂ A		β -CH ₂ C		N-CH ₃ C		α -CH ₂ A		α -CH ₂ C	
	T ₁	T ₂	T ₁	T ₂	T ₁	T ₂	T ₁	T ₂	T ₁	T ₂	T ₁	T ₂	T ₁	T ₂
0	1.86 (0.009)	0.988 (0.006)	2.374 (0.02)	1.28 (0.008)	0.924 (0.003)	0.328 (0.026)	1.684 (0.006)	0.813 (0.063)	2.752 (0.035)	1.533 (0.013)	1.201 (0.006)	0.278 (0.027)	1.804 (0.011)	0.657 (0.055)
1	1.711 (0.002)	0.737 (0.006)	2.176 (0.00)	1.007 (0.012)	0.885 (0.004)	0.250 (0.014)	1.582 (0.006)	0.795 (0.037)	2.474 (0.025)	1.396 (0.021)	1.103 (0.003)	0.206 (0.023)	1.681 (0.002)	0.584 (0.051)
5	1.637 (0.010)	0.470 (0.004)	2.250 (0.006)	0.944 (0.013)	0.897 (0.004)	0.185 (0.006)	1.625 (0.005)	0.834 (0.015)	2.628 (0.022)	1.349 (0.011)	1.090 (0.004)	0.185 (0.017)	1.746 (0.007)	0.598 (0.033)
10	1.452 (0.02)	0.314 (0.004)	2.064 (0.008)	1.115 (0.010)	0.843 (0.004)	0.088 (0.006)	1.540 (0.007)	0.594 (0.07)	2.421 (0.020)	1.274 (0.016)	0.988 (0.008)	0.104 (0.017)	1.618 (0.009)	0.460 (0.061)
20	1.251 (0.013)	0.178 (0.004)	1.956 (0.007)	0.890 (0.008)	0.794 (0.005)	0.056 (0.004)	1.480 (0.006)	0.482 (0.058)	2.368 (0.019)	0.961 (0.014)	0.890 (0.010)	0.064 (0.015)	1.555 (0.010)	0.338 (0.058)
30	1.216 (0.016)	0.124 (0.004)	1.985 (0.011)	0.872 (0.011)	0.822 (0.007)	0.043 (0.005)	1.50 (0.006)	0.420 (0.052)	2.382 (0.016)	0.897 (0.016)	0.905 (0.006)	0.046 (0.017)	1.591 (0.004)	0.284 (0.064)
40	1.111 (0.015)	0.091 (0.003)	1.860 (0.014)	0.7325 (0.011)	0.796 (0.009)	0.033 (0.004)	1.420 (0.007)	0.398 (0.046)	2.243 (0.014)	0.72 (0.013)	0.842 (0.010)	0.037 (0.013)	1.490 (0.009)	0.260 (0.052)
50	1.03 (0.010)	0.076 (0.004)	1.798 (0.015)	0.656 (0.014)	0.761 (0.010)	0.028 (0.006)	1.394 (0.008)	0.296 (0.043)	2.276 (0.016)	0.56 (0.018)	0.77 (0.020)	0.028 (0.026)	1.442 (0.016)	0.166 (0.066)

Table S5 T₁ and T₂ values of IL1 as a function of collagen.

Conc (μ M)	CH ₃ C T ₁	γ -CH ₂ C T ₁	β -CH ₂ C T ₁	N CH ₃ C T ₁	α -CH ₂ C T ₁
0	3.405 (0.025)	2.872 (0.03)	2.44 (0.025)	3.692 (0.03)	2.653 (0.05)
0.2	3.268 (0.009)	2.778 (0.01)	2.402 (0.008)	3.5038 (0.01)	2.433 (0.027)
0.6	3.192 (0.015)	2.617 (0.021)	2.213 (0.033)	3.519 (0.02)	2.535 (0.066)
1	3.086 (0.03)	2.520 (0.048)	2.212 (0.032)	3.437 0.034)	2.616 (0.072)
1.5	3.120 (0.028)	2.721 (0.052)	2.350 (0.046)	3.504 (0.037)	2.635 (0.118)
2.2	3.285 (0.037)	2.852 (0.061)	2.587 (0.070)	3.900 (0.112)	3.47 (0.100)
3.6	3.120 (0.05)	2.834 (0.123)	2.46 (0.082)	3.455 (0.08)	2.451 (0.080)

Table S6 T₁ and T₂ values of IL2 as a function of collagen.

Conc (μ M)	CH ₃ C		γ -CH ₂ C		β -CH ₂ C		CH ₃ A		N CH ₃ C		α -CH ₂ C	
	T ₁	T ₂	T ₁	T ₂	T ₁	T ₂	T ₁	T ₂	T ₁	T ₂	T ₁	T ₂
0	3.245 (0.044)	2.625 (0.013)	2.70 (0.030)	2.086 (0.037)	2.305 (0.027)	2.044 (0.051)	8.386 (0.149)	6.293 (0.104)	3.886 (0.061)	3.121 (0.015)	2.325 (0.033)	1.395 (0.036)
0.2	3.355 (0.005)	2.956 (0.060)	2.767 (0.011)	2.286 (0.042)	2.373 (0.027)	2.248 (0.05)	8.750 (0.031)	7.236 (0.230)	3.891 (0.044)	3.616 (0.065)	2.483 (0.008)	1.417 (0.038)
0.4	3.407 (0.018)	2.854 (0.056)	2.823 (0.027)	2.012 (0.023)	2.408 (0.012)	2.224 (0.032)	8.775 (0.102)	6.501 (0.026)	3.811 (0.076)	3.214 (0.065)	2.445 (0.030)	1.203 (0.040)
0.6	3.36 (0.046)	2.620 (0.170)	2.761 (0.019)	1.724 (0.118)	2.367 (0.023)	1.443 (0.129)	7.821 (0.188)	4.926 (0.353)	3.792 (0.054)	2.750 (0.188)	2.39 (0.033)	0.798 (0.06)
0.8	3.380 (0.023)	2.2905 (0.015)	2.8240 (0.022)	2.1291 (0.020)	2.3703 (0.028)	2.0941 (0.010)	8.4491 (0.116)	3.6103 (0.036)	3.7758 (0.053)	2.6669 (0.023)	2.488 (0.065)	1.315 (0.018)
1	3.238 (0.006)	2.606 (0.022)	2.680 (0.011)	2.0193 (0.026)	2.250 (0.015)	1.185 (0.033)	7.898 (0.03)	4.153 (0.047)	3.677 (0.036)	2.692 (0.014)	2.381 (0.017)	0.907 (0.065)
1.4	3.148 (0.005)	2.386 (0.018)	2.616 (0.013)	1.806 (0.035)	2.263 (0.014)	1.698 (0.043)	7.455 (0.023)	3.640 (0.037)	3.559 (0.033)	2.5665 (0.018)	2.331 (0.015)	0.868 (0.038)
1.8	3.115 (0.007)	2.516 (0.012)	2.571 (0.012)	1.788 (0.031)	2.240 (0.014)	1.520 (0.086)	7.238 (0.035)	3.585 (0.021)	3.520 (0.037)	2.6075 (0.026)	2.315 (0.012)	0.771 (0.054)
2.2	3.114 (0.005)	2.383 (0.007)	2.555 (0.013)	1.671 (0.03)	2.202 (0.018)	1.537 (0.072)	7.396 (0.04)	3.313 (0.022)	3.554 (0.041)	2.440 (0.023)	2.241 (0.018)	0.671 (0.053)
3.6	3.141 (0.030)	2.185 (0.007)	2.587 (0.06)	1.410 (0.023)	2.182 (0.078)	1.322 (0.08)	7.122 (0.25)	2.391 (0.01)	3.563 (0.08)	2.112 (0.022)	2.268 (0.26)	0.550 (0.06)

Table S7 T₁ and T₂ values of IL3 as a function of collagen.

Conc (μ M)	CH ₃ A		CH ₃ C		β -CH ₂ A		β -CH ₂ C		N-CH ₃ C		α -CH ₂ A		α -CH ₂ C	
	T ₁	T ₂	T ₁	T ₂	T ₁	T ₂	T ₁	T ₂	T ₁	T ₂	T ₁	T ₂	T ₁	T ₂
0	2.63	1.703	3.208	2.050	1.43	0.800	2.355	1.19	3.47	1.598	1.741	0.370	2.490	0.405
	(0.008)	(0.02)	(0.008)	(0.018)	(0.008)	(0.027)	(0.014)	(0.016)	(0.02)	(0.036)	(0.015)	(0.078)	(0.025)	(0.07)
0.2	2.632	1.138	3.026	1.867	1.35	0.583	2.223	1.114	3.31	1.67	1.741	0.335	2.360	0.498
	(0.008)	(0.022)	(0.008)	(0.026)	(0.007)	(0.048)	(0.010)	(0.055)	(0.017)	(0.025)	(0.010)	(0.078)	(0.013)	(0.093)
0.4	2.466	0.943	2.903	1.397	1.321	0.540	2.15	1.343	3.20	1.785	1.644	0.375	2.221	0.598
	(0.01)	(0.025)	(0.012)	(0.024)	(0.006)	(0.040)	(0.010)	(0.05)	(0.024)	(0.055)	(0.009)	(0.073)	(0.015)	(0.08)
0.6	2.479	0.756	3.018	1.853	1.373	0.438	2.223	1.203	3.32	1.663	1.73	0.305	2.350	0.541
	(0.015)	(0.02)	(0.009)	(0.025)	(0.009)	(0.038)	(0.010)	(0.05)	(0.020)	(0.025)	(0.015)	(0.07)	(0.01)	(0.09)
0.8	2.261	0.640	2.850	2.084	1.255	0.326	2.063	1.102	3.14	1.828	1.547	0.275	2.15	0.37
	(0.02)	(0.017)	(0.024)	(0.043)	(0.01)	(0.038)	(0.014)	(0.08)	(0.036)	(0.040)	(0.008)	(0.069)	(0.017)	(0.115)
1	2.590	0.527	3.710	1.926	1.542	0.32	2.560	1.261	4.102	1.755	2.044	0.271	2.782	0.571
	(0.018)	(0.02)	(0.051)	(0.013)	(0.023)	(0.043)	(0.023)	(0.035)	(0.063)	(0.02)	(0.021)	(0.068)	(0.04)	(0.091)
1.8	2.142	0.34	3.030	1.852	1.360	0.218	2.209	0.98	3.382	1.440	1.594	0.217	2.325	0.468
	(0.02)	(0.02)	(0.007)	(0.012)	(0.016)	(0.03)	(0.010)	(0.06)	(0.012)	(0.02)	(0.017)	(0.077)	(0.007)	(0.10)
2.2	2.125	0.305	3.064	1.867	1.423	0.190	2.241	1.171	3.356	1.80	1.738	0.190	2.455	0.6383
	(0.022)	(0.02)	(0.057)	(0.042)	(0.021)	(0.025)	(0.021)	(0.060)	(0.065)	(0.03)	(0.02)	(0.05)	(0.034)	(0.07)

Table S8 T₁ and T₂ values of IL4 as a function of collagen.

Conc (nM)	CH ₃ A		CH ₃ C		β-CH ₃ A		β-CH ₃ C		N CH ₃ C		α-CH ₃ A		α-CH ₃ C	
	T ₁	T ₂	T ₁	T ₂	T ₁	T ₂	T ₁	T ₂	T ₁	T ₂	T ₁	T ₂	T ₁	T ₂
0	1.607	0.754	2.024	0.963	0.744	0.276	1.466	0.611	2.110	0.968	0.834	0.200	1.503	0.334
	(0.004)	(0.008)	(0.004)	(0.007)	(0.012)	(0.020)	(0.012)	(0.025)	(0.013)	(0.012)	(0.006)	(0.041)	(0.007)	(0.06)
20	1.560	0.660	2.01	0.970	0.728	0.233	1.452	0.494	2.090	0.946	0.840	0.211	1.610	0.354
	(0.004)	(0.022)	(0.007)	(0.021)	(0.009)	(0.046)	(0.013)	(0.06)	(0.015)	(0.041)	(0.006)	(0.068)	(0.013)	(0.111)
40	1.395	0.566	1.796	0.902	0.722	0.217	1.358	0.494	1.806	0.941	0.755	0.203	1.381	0.350
	(0.005)	(0.015)	(0.004)	(0.014)	(0.004)	(0.029)	(0.007)	(0.052)	(0.006)	(0.032)	(0.009)	(0.056)	(0.011)	(0.090)
60	1.424	0.445	1.905	0.746	0.747	0.234	1.383	0.542	2.153	0.980	0.824	0.250	1.351	0.450
	(0.015)	(0.003)	(0.019)	(0.005)	(0.017)	(0.008)	(0.025)	(0.011)	(0.018)	(0.010)	(0.027)	(0.02)	(0.050)	(0.033)
80	1.494	0.758	1.915	1.032	0.726	0.314	1.407	0.783	1.922	1.062	0.780	0.312	1.404	0.490
	(0.005)	(0.007)	(0.004)	(0.009)	(0.009)	(0.009)	(0.008)	(0.015)	(0.015)	(0.015)	(0.006)	(0.034)	(0.007)	(0.04)
100	1.435	0.416	1.845	0.756	0.648	0.161	1.290	0.413	1.724	0.720	0.608	0.140	1.224	0.270
	(0.007)	(0.014)	(0.004)	(0.014)	(0.010)	(0.028)	(0.010)	(0.045)	(0.015)	(0.032)	(0.010)	(0.063)	(0.009)	(0.08)

Table S9 T_{1NS} and T_{1SEL} values of IL1 against HSA.

Conc (μ M)	CH ₃ C T_{1NS}	CH ₃ C T_{1SEL}	α -CH ₂ C T_{1NS}	α -CH ₂ C T_{1SEL}
0	3.598 (0.014)	3.508 (0.012)	2.642 (0.008)	2.775 (0.053)
1	3.306 (0.015)	3.660 (0.076)	2.476 (0.005)	2.761 (0.009)
5	3.326 (0.016)	3.460 (0.05)	2.518 (0.008)	2.612 (0.012)
10	3.196 (0.016)	3.642 (0.027)	2.411 (0.006)	2.76 (0.006)
20	3.122 (0.023)	3.510 (0.037)	2.373 (0.008)	2.708 (0.010)
30	3.012 (0.04)	3.756 (0.307)	2.370 (0.01)	2.728 (0.035)
40	2.968 (0.030)	3.510 (0.137)	2.302 (0.008)	2.70 (0.104)
50	3.051 (0.044)	3.147 (0.127)	2.413 (0.006)	2.535 (0.053)

Table S10 T_{INS} and T_{ISEL} values of IL2 against HSA .

Conc (μ M)	CH ₃ A		α -CH ₂ C	
	T _{INS}	T _{ISEL}	T _{INS}	T _{ISEL}
0	8.535	9.224	2.475	3.52
	(0.037)	(0.070)	(0.015)	(0.031)
1	8.396	8.952	2.425	3.401
	(0.07)	(0.147)	(0.008)	(0.026)
5	7.80	7.659	2.466	3.624
	(0.012)	(0.064)	(0.008)	(0.050)
10	7.924	7.196	2.552	3.483
	(0.155)	(0.05)	(0.018)	(0.041)
20	6.926	6.710	2.596	3.553
	(0.03)	(0.04)	(0.02)	(0.06)
30	6.116	5.84	2.450	3.495
	(0.068)	(0.05)	(0.006)	(0.051)
40	5.888	5.28	2.535	3.412
	(0.098)	(0.04)	(0.006)	(0.054)
50	5.104	4.453	2.470	3.40
	(0.092)	(0.02)	(0.006)	(0.053)

Table S11 T_{INS} and T_{ISEL} values of IL3 against HSA.

Conc (μ M)	CH ₃ A		α - CH ₂ A	
	T _{INS}	T _{ISEL}	T _{INS}	T _{ISEL}
0	2.887 (0.01)	3.026 (0.027)	1.795 (0.004)	1.964 (0.005)
1	2.73 (0.006)	2.634 (0.013)	1.80 (0.004)	1.953 (0.030)
5	2.406 (0.018)	2.052 (0.011)	1.640 (0.006)	1.513 (0.003)
10	2.176 (0.032)	1.547 (0.013)	1.574 (0.009)	1.226 (0.003)
20	1.892 (0.058)	1.097 (0.008)	1.503 (0.05)	0.923 (0.011)
30	1.553 (0.026)	0.804 (0.009)	1.286 (0.01)	0.705 (0.003)
40	1.490 (0.023)	0.702 (0.008)	1.265 (0.01)	0.616 (0.004)
50	1.392 (0.019)	0.588 (0.01)	1.191 (0.01)	0.54 (0.028)

Table S12 T_{INS} and T_{ISEL} values of IL4 against HSA.

Conc (μ M)	CH ₃ A		α -CH ₂ A	
	T _{INS}	T _{ISEL}	T _{INS}	T _{ISEL}
0	1.860	1.812	1.201	1.101
	(0.009)	(0.007)	(0.006)	(0.003)
1	1.711	1.723	1.102	1.050
	(0.002)	(0.01)	(0.003)	(0.002)
5	1.640	1.45	1.090	0.885
	(0.01)	(0.02)	(0.004)	(0.001)
10	1.452	1.161	0.98	0.717
	(0.018)	(0.015)	(0.008)	(0.001)
20	1.25	0.830	0.88	0.565
	(0.01)	(0.006)	(0.01)	(0.002)
30	1.215	0.680	0.906	0.445
	(0.01)	(0.008)	(0.006)	(0.002)
40	1.11	0.536	0.842	0.378
	(0.01)	(0.005)	(0.01)	(0.003)
50	1.030	0.453	0.772	0.333
	(0.01)	(0.002)	(0.020)	(0.004)

Table S13 T_{INS} and T_{ISEL} values of IL1 against collagen.

Conc (μ M)	CH ₃ C T _{INS}	CH ₃ C T _{ISEL}
0	3.405 (0.025)	3.550 (0.04)
0.2	3.268 (0.009)	3.314 (0.02)
0.6	3.192 (0.015)	3.49 (0.02)
1	3.086 (0.029)	3.288 (0.05)
1.4	3.120 (0.028)	3.384 (0.05)
2.2	2.717 (0.114)	3.514 (0.07)
3.6	3.120 (0.05)	3.295 (0.05)

Table S14 T_{INS} and T_{ISEL} values of IL2 against collagen.

Conc (μ M)	T _{INS}	CH ₃ A	T _{ISEL}
	8.385		8.890
0	(0.145)		(0.12)
0.2	8.750 (0.03)		8.847 (0.16)
0.6	7.821 (0.188)		8.344 (0.14)
0.8	8.45 (0.12)		8.055 (0.044)
1	7.898 (0.03)		8.156 (0.16)
1.4	7.455 (0.02)		7.482 (0.050)
1.8	7.238 (0.03)		7.293 (0.102)
2.2	7.396 (0.04)		7.174 (0.08)
3.6	7.122 (0.24)		6.622 (0.08)

Table S15 T_{INS} and T_{ISEL} values of IL3 against collagen.

Conc (μ M)	CH ₃ A		α -CH ₂ A	
	T _{INS}	T _{ISEL}	T _{INS}	T _{ISEL}
0	2.632	3.340	1.741	2.034
	(0.008)	(0.02)	(0.01)	(0.018)
0.2	2.466	2.596	1.644	1.756
	(0.01)	(0.06)	(0.009)	(0.026)
0.4	2.48	2.244	1.723	1.452
	(0.01)	(0.02)	(0.01)	(0.01)
0.6	2.261	2.015	1.547	1.360
	(0.02)	(0.02)	(0.008)	(0.018)
0.8	2.5903	1.74	2.044	1.156
	(0.018)	(0.01)	(0.02)	(0.015)
1.0	2.23	1.628	1.583	1.078
	(0.02)	(0.01)	(0.01)	(0.007)
1.4	2.141	1.396	1.502	0.934
	(0.02)	(0.02)	(0.01)	(0.013)
1.8	2.125	1.130	1.593	0.794
	(0.02)	(0.01)	(0.01)	(0.007)
2.2	2.632	1.020	1.737	0.755
	(0.008)	(0.02)	(0.02)	(0.009)

Table S16 T_{INS} and T_{ISEL} values of IL4 against collagen.

Conc (nM)	CH ₃ A		α -CH ₂ A	
	T _{INS}	T _{ISEL}	T _{INS}	T _{ISEL}
0	1.607	1.703	0.833	0.868
	(0.004)	(0.013)	(0.006)	(0.007)
20	1.560	1.605	0.840	0.827
	(0.004)	(0.010)	(0.006)	(0.015)
40	1.395	1.510	0.755	0.778
	(0.005)	(0.010)	(0.009)	(0.005)
60	1.424	1.425	0.824	0.727
	(0.015)	(0.009)	(0.027)	(0.012)
80	1.494	1.405	0.778	0.690
	(0.005)	(0.006)	(0.006)	(0.005)
100	1.435	1.306	0.608	0.593
	(0.007)	(0.004)	(0.010)	(0.006)