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Supplementary Information: Influence of Solution Chemistry on the Solubility, Crystallisability and Nucleation Behaviour of Eicosane in Toluene/Acetone Mixed-Solvents

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Abstract

This document contains supplementary information relating to the research article - Influence of Solution Chemistry on the Solubility and Crystallisability of Eicosane in Toluene/Acetone Mixed Solvent Solutions. Average crystallisation and dissolution temperatures from 5 repeats of measurements are presented in section S1, over the full mixed solvent compositional range studied, as a function of heating cycle rate and solution concentration. The full range of data collected for the solubility and crystallisability of the solutions, calculated solution thermodynamic parameters and determined nucleation mechanisms are provided in section S2, S3 and S4, respectively. Atomic partial charges of eicosane, toluene and acetone used in grid-based molecular modelling studies are presented in section S5. Predicted solvation sites of a single eicosane molecule solvated with single toluene and acetone molecules, at different energy cut-offs, are provided in section S6, alongside a description of the effect of calculating the intermolecular interactions of toluene with eicosane prior to acetone interactions with eicosane on the obtained results.

S1. Crystallisation and Dissolution Temperatures

Average crystallisation (Tc) and dissolution (Tdiss) temperatures for eicosane in toluene/acetone mixed solvent solutions at each cooling/heating rate (q) and each solution concentration, as a function of mol fraction of acetone (y), are shown in Table S1. The full compositional range from pure toluene to pure acetone are studied, with 11 compositions studied in total. The standard deviation (std) of the data is also displayed from 5 repeats of each crystallisation and dissolution experiment. The data provided for each solvent used highlights the influence that the solute composition, solute concentration and cooling rate has upon the crystallisation behaviour of eicosane in toluene/acetone mixed solvent solution.

Table S1. Average crystallisation (Tc) and dissolution (Tdiss) temperatures at different heating cycle rates (q) as a function of solvent composition and solution concentration. The standard deviations (SD) from 5 repeats of Tc and Tdiss are presented.

q (°C min^{-1})	Tc (°C)	SD	Tdiss (°C)	SD	Tc (°C)	SD	Tdiss (°C)	SD	Tc (°C)	SD	Tdiss (°C)	SD	Tc (°C)	SD	Tdiss (°C)	SD
y = 0																
	250 g L^{-1}				**300 g L^{-1}**				**350 g L^{-1}**				**450 g L^{-1}**			
0.25	9.74	0.25	11.96	0.11	11.36	0.09	13.27	0.19	12.58	0.12	14.62	0.15	14.75	0.09	16.40	0.37
1	9.22	0.20	13.01	0.54	10.74	0.30	15.05	0.38	12.03	0.09	15.48	0.65	14.19	0.18	18.06	0.18
2	8.27	0.26	15.08	0.49	9.75	0.19	16.83	0.30	11.22	0.22	18.51	0.53	13.28	0.16	20.44	0.27
3.2	7.57	0.27	17.26	0.53	8.97	0.16	19.52	0.25	10.34	0.12	20.44	0.62	12.68	0.11		
	550 g L^{-1}				**650 g L^{-1}**				**750 g L^{-1}**				**850 g L^{-1}**			
0.25	16.45	0.16	18.13	0.34	17.52	0.11	18.90	0.29	18.48	0.16	20.54	0.11	19.54	0.19	21.18	0.28
1	15.66	0.23	20.52	0.38	16.81	0.19	22.55	0.15	17.77	0.18	22.26	0.23	18.77	0.18	23.92	0.32
2	15.08	0.16	23.39	0.57	15.90	0.30	24.91	0.15	16.85	0.17	25.73	0.08	18.22	0.12	26.74	0.15
3.2	14.04	0.24	25.96	0.05	15.70	0.17	26.80	0.28	16.14	0.16	29.34	0.15	17.12	0.18	30.47	0.08
y = 0.14																
	200 g L^{-1}				**300 g L^{-1}**				**400 g L^{-1}**				**500 g L^{-1}**			
0.25	10.38	0.15	12.42	0.09	13.50	0.09	14.78	0.17	15.49	0.05	16.90	0.25	16.28	0.26	18.25	0.24
1	9.66	0.06	12.92	0.43	12.64	0.24	16.38	0.38	14.60	0.15	18.61	0.23	16.20	0.13	20.37	0.49
2	8.68	0.16	14.24	0.20	12.02	0.10	18.14	0.49	14.24	0.17	20.13	0.28	15.70	0.13	21.73	0.25
3.2	8.37	0.15	16.17	0.28	11.51	0.12	20.13	0.57	13.52	0.08	22.72	0.56	14.84	0.16	24.91	0.20
	700 g L^{-1}				**800 g L^{-1}**											
0.25	18.85	0.13	20.74	0.44	20.08	0.12	21.59	0.18								
1	18.53	0.21	23.01	0.30	19.37	0.21	24.13	0.46								
2	17.89	0.21	26.29	0.08	18.53	0.11	28.01	0.33								
3.2	16.73	0.28	30.33	0.21	17.32	0.22	31.59	0.15								
y = 0.26																
	200 g L^{-1}				**300 g L^{-1}**				**400 g L^{-1}**				**500 g L^{-1}**			
0.25	12.69	0.24	14.70	0.08	15.35	0.14	16.99	0.28	17.17	0.13	18.46	0.16	18.62	0.11	19.75	0.20
1	11.98	0.21	16.31	0.38	14.72	0.12	18.75	0.54	16.28	0.15	21.11	0.48	17.85	0.18	21.84	0.40
2	11.21	0.13	18.02	0.38	13.97	0.19	20.30	0.48	15.80	0.17	22.33	0.17	17.18	0.15	24.28	0.59

3.2	10.42	0.20	18.39	0.14	13.32	0.09	22.10	0.56	15.04	0.16	25.41	0.35	16.40	0.15	27.29	0.21
y = 0.38																
	200 g L^{-1}				**300 g L^{-1}**				**400 g L^{-1}**				**500 g L^{-1}**			
0.25	15.07	0.07	16.96	0.05	17.50	0.05	18.92	0.19	18.75	0.16	20.29	0.22	20.14	0.09	21.47	0.28
1	14.19	0.27	18.22	0.57	16.85	0.21	20.43	0.15	18.24	0.28	22.33	0.27	19.37	0.19	23.99	0.44
2	13.54	0.10	19.84	0.54	16.11	0.15	22.55	0.13	17.55	0.08	25.00	0.47	18.78	0.11	26.66	0.43
3.2	12.99	0.09	21.97	0.48	15.39	0.07	25.12	0.34	16.93	0.14	27.81	0.11	18.04	0.08	29.94	0.23
y = 0.49																
	150 g L^{-1}				**250 g L^{-1}**				**350 g L^{-1}**				**450 g L^{-1}**			
0.25	15.24	0.13	17.77	0.07	18.69	0.09	20.14	0.23	20.20	0.08	21.49	0.15	21.30	0.13	22.84	0.25
1	14.89	0.10	17.93	0.00	17.93	0.10	21.16	0.28	19.56	0.15	23.80	0.00	20.40	0.11	25.66	0.55
2	13.46	0.17	20.61	0.25	17.05	0.25	24.69	0.36	18.90	0.14	26.02	0.40	19.74	0.19	28.12	0.31
3.2	13.18	0.20	21.79	0.11	16.68	0.11	25.26	0.17	18.33	0.13	28.14	0.13	19.07	0.22	30.52	0.23
y = 0.59																
	150 g L^{-1}				**250 g L^{-1}**				**350 g L^{-1}**				**450 g L^{-1}**			
0.25	18.40	0.11	20.24	0.09	20.78	0.08	22.26	0.18	22.05	0.05	23.61	0.31	22.96	0.13	24.85	0.15
1	17.38	0.23	21.37	0.42	19.65	0.18	24.68	0.23	21.04	0.11	26.38	0.41	22.15	0.18	27.26	0.29
2	16.77	0.19	22.92	0.38	19.27	0.22	25.65	0.30	20.79	0.24	27.73	0.49	21.73	0.15	29.22	0.35
3.2	16.03	0.22	24.63	0.33	18.74	0.05	27.40	0.11	20.23	0.05	29.84	0.19	21.01	0.09	31.79	0.13
y = 0.68																
	150 g L^{-1}				**250 g L^{-1}**				**350 g L^{-1}**				**450 g L^{-1}**			
0.25	20.72	0.11	22.72	0.09	22.55	0.05	24.35	0.32	23.81	0.09	25.85	0.08	24.54	0.13	26.68	0.11
1	20.00	0.18	23.99	0.20	21.96	0.26	26.42	0.43	22.98	0.26	28.36	0.05	23.82	0.08	29.53	0.15
2	19.27	0.14	25.53	0.12	21.57	0.11	27.91	0.09	22.59	0.13	30.25	0.20	22.88	0.11	32.18	0.08
3.2	18.59	0.20	27.13	0.13	20.83	0.13	30.06	0.13	21.88	0.15	32.36	0.25	22.43	0.14	34.87	0.13
y = 0.77																
	100 g L^{-1}				**200 g L^{-1}**				**300 g L^{-1}**				**400 g L^{-1}**			
0.25	21.35	0.19	23.53	0.08	24.11	0.13	26.22	0.09	25.23	0.16	27.41	0.10	25.72	0.28	28.34	0.09
1	20.88	0.27	24.78	0.20	23.60	0.12	28.04	0.15	24.68	0.14	29.63	0.18	25.42	0.19	31.14	0.30
2	20.15	0.08	25.49	0.09	23.01	0.14	29.26	0.19	24.17	0.07	31.15	0.19	24.83	0.08	33.31	0.33
3.2	19.18	0.21	27.61	0.15	22.11	0.08	32.00	0.08	23.05	0.15	34.60	0.25	23.72	0.21	35.66	0.09
y = 0.85																

	75 g L^{-1}				175 g L^{-1}				275 g L^{-1}				375 g L^{-1}			
0.25	23.07	0.12	25.08	0.04	26.24	0.19	28.18	0.12	27.36	0.11	29.25	0.12	27.86	0.09	30.02	0.10
1	22.49	0.15	26.30	0.18	25.66	0.20	29.77	0.10	26.38	0.13	32.17	0.25	27.14	0.18	33.00	0.14
2	21.77	0.13	26.80	0.08	24.97	0.21	31.09	0.15	26.14	0.13	33.06	0.19				
3.2	21.14	0.14	28.18	0.16	24.59	0.13	32.22	0.18	25.41	0.16	35.48	0.07	26.00	0.17	37.14	0.20
y = 0.93																
	20 g L^{-1}				**60 g L^{-1}**				**100 g L^{-1}**				**140 g L^{-1}**			
0.25	18.71	0.43	20.74	0.14	25.00	0.15	26.89	0.09	27.36	0.11	28.92	0.11	28.24	0.18	30.13	0.08
1	17.57	0.30	21.59	0.15	24.33	0.21	28.08	0.11	26.60	0.15	30.41	0.13	27.81	0.23	31.98	0.18
2	17.16	0.21	21.63	0.18	24.03	0.15	28.42	0.15	26.06	0.11	31.19	0.15	27.07	0.16	33.10	0.18
3.2	15.82	0.30	23.03	0.11	23.13	0.16	29.70	0.13	25.76	0.13	32.12	0.09	26.58	0.08	34.35	0.16
y = 1																
	5 g L^{-1}				**15 g L^{-1}**				**25 g L^{-1}**				**35 g L^{-1}**			
0.25	12.34	0.73	13.71	0.26	20.47	0.15	21.97	0.25	23.55	0.07	25.43	0.24	25.95	0.04	27.05	0.37
1	11.08	0.10	14.81	0.30	19.49	0.20	22.86	0.30	23.09	0.08	26.13	0.19	25.13	0.05	28.44	0.11
2	10.14	0.33	15.19	0.40	18.59	0.16	23.37	0.13	22.66	0.19	26.72	0.14	24.57	0.13	28.87	0.13
3.2	10.75	0.28	18.53	0.22	18.63	0.24	25.71	0.04	22.64	0.32	29.61	0.08	24.46	0.14	31.91	0.19

S2. Solubility and Supersolubility Data

Table S2. Solubility (T_e) and supersolubility ($T_{c,l}$) data of eicosane in toluene:acetone solvent mixture solutions, together with the calculated steady-state MSZW over a range of concentrations. Standard error (SE) values are also presented.

Conc. (g L^{-1})	$T_{c,l}$ (°C)	SE	T_e (°C)	SE	MSZW (°C)	SE	Conc. (g L^{-1})	$T_{c,l}$ (°C)	SE	T_e (°C)	SE	MSZW (°C)	SE
y = 0							**y = 0.14**						
250	9.92	0.10	11.37	0.15	1.46	0.18	**200**	10.39	0.26	11.85	0.27	1.46	0.37
300	11.54	0.10	12.81	0.14	1.27	0.17	**300**	13.47	0.20	14.46	0.14	0.98	0.24
350	12.78	0.02	13.90	0.44	1.13	0.44	**400**	15.47	0.19	16.48	0.19	1.01	0.27
450	14.88	0.12	15.79	0.06	0.91	0.14	**500**	16.57	0.17	17.82	0.38	1.26	0.42
550	16.58	0.11	17.72	0.33	1.14	0.34	**700**	19.16	0.16	19.83	0.09	0.67	0.19
650	17.49	0.28	18.47	0.91	0.97	0.95	**800**	20.32	0.05	20.80	0.26	0.47	0.26
750	18.60	0.13	19.56	0.26	0.97	0.29							
850	19.69	0.11	20.57	0.19	0.88	0.22							
y = 0.26							**y = 0.38**						
200	12.81	0.08	14.30	0.16	1.49	0.18	**200**	15.05	0.20	16.51	0.05	1.47	0.21
300	15.45	0.09	16.80	0.24	1.35	0.26	**300**	17.61	0.08	18.36	0.04	0.75	0.09
400	17.18	0.17	18.24	0.51	1.06	0.53	**400**	18.87	0.06	19.74	0.13	0.88	0.14
500	18.70	0.11	19.20	0.08	0.50	0.14	**500**	20.20	0.12	20.94	0.18	0.74	0.22
y = 0.49							**y = 0.59**						
150	15.42	0.33	17.09	0.56	1.67	0.65	**150**	18.39	0.21	19.88	0.04	1.49	0.22
250	18.69	0.24	19.76	0.86	1.07	0.89	**250**	20.64	0.31	22.37	0.54	1.73	0.63
350	20.26	0.11	21.28	0.37	1.02	0.39	**350**	21.94	0.27	23.67	0.58	1.74	0.64
450	21.31	0.18	22.67	0.50	1.36	0.53	**450**	22.97	0.15	24.58	0.32	1.61	0.35
y = 0.68							**y = 0.77**						
150	20.80	0.11	22.44	0.11	1.65	0.16	**100**	21.59	0.05	23.23	0.29	1.64	0.30
250	22.63	0.09	24.16	0.31	1.53	0.32	**200**	24.29	0.05	25.84	0.31	1.55	0.32
350	23.80	0.17	25.75	0.45	1.95	0.48	**300**	25.45	0.12	26.92	0.39	1.47	0.41
450	24.58	0.21	26.41	0.44	1.83	0.49	**400**	26.02	0.16	28.22	0.50	2.20	0.52
y = 0.85							**y = 0.93**						
75	23.17	0.09	25.00	0.25	1.82	0.26	**20**	18.80	0.25	20.60	0.32	1.81	0.40
175	26.27	0.16	28.16	0.33	1.89	0.37	**60**	25.09	0.14	26.85	0.28	1.77	0.31
275	27.29	0.24	29.34	0.67	2.05	0.71	**100**	27.29	0.22	29.00	0.35	1.71	0.41
375	27.90	0.17	29.98	0.82	2.09	0.84	**140**	28.36	0.06	30.18	0.49	1.83	0.49
y = 1													
5	11.92	0.69	13.08	0.71	1.16	0.99							
15	20.27	0.43	21.53	0.43	1.26	0.61							
25	23.48	0.19	24.76	0.60	1.28	0.63							
35	25.81	0.20	26.57	0.52	0.76	0.55							

S3. Solution Thermodynamics Data

Table S3. Thermodynamic parameters and activity coefficients (Υ) as a function of temperature calculated from van't Hoff analysis. SE is the calculated standard error in results. The linear correlation values (R^2) of the van't Hoff plots are also provided.

Acetone mol fraction (y)	Enthalpy of dissolution (kJ mol^{-1})	SE - Enthalpy of dissolution (kJ mol^{-1})	Entropy of dissolution (kJ mol^{-1} K^{-1})	SE - Entropy of dissolution (kJ mol^{-1} K^{-1})	R^2	Enthalpy of mixing (kJ mol^{-1})	SE - Enthalpy of mixing (kJ mol^{-1})	Entropy of mixing (kJ mol^{-1} K^{-1})	SE - Entropy of mixing (kJ mol^{-1} K^{-1})	Conc. Range (g L^{-1})	$ln\,\Upsilon = aT + c$
0	78.36	1.41	0.255	0.005	0.998	35.50	1.41	0.116	0.005	250 - 850	-0.05T + 1.60
0.14	93.99	0.98	0.307	0.003	1.000	51.13	0.98	0.169	0.003	200 - 800	-0.07T + 2.16
0.26	116.28	5.80	0.382	0.020	0.995	73.42	5.80	0.243	0.020	200 - 500	-0.11T + 3.01
0.38	132.89	4.05	0.436	0.014	0.998	90.02	4.05	0.297	0.014	200 - 500	-0.13T + 3.76
0.49	130.71	3.00	0.425	0.010	0.999	87.85	3.00	0.286	0.010	150 - 450	-0.12T + 4.12
0.59	155.35	7.04	0.504	0.024	0.996	112.48	7.04	0.365	0.024	150 - 450	-0.16T + 5.32
0.68	182.22	10.69	0.590	0.036	0.993	139.36	10.69	0.452	0.036	150 - 450	-0.19T + 6.64
0.77	198.03	10.30	0.638	0.034	0.995	155.17	10.30	0.500	0.034	100 - 400	-0.21T + 7.73
0.85	224.72	17.66	0.721	0.059	0.988	181.86	17.66	0.582	0.059	75 - 375	-0.24T + 9.38
0.93	144.45	10.02	0.448	0.033	0.990	101.58	10.02	0.309	0.033	20 - 140	-0.14T + 7.24
1	100.52	5.53	0.296	0.019	0.994	57.65	5.53	0.157	0.019	5 - 35	-0.08T + 6.41

S4. Nucleation Mechanism Data

Representative examples of the polythermal data analysis of $\ln u_c$ vs. $\ln q$ plots of y = 0.38 and 0.68 solutions are given in Figure S1, with the resultant nucleation mechanisms provided in Table S4. Example plots of u_c vs. $\ln q$ for y = 0.68, for effective interfacial tension calculation, are given in Figure S2.

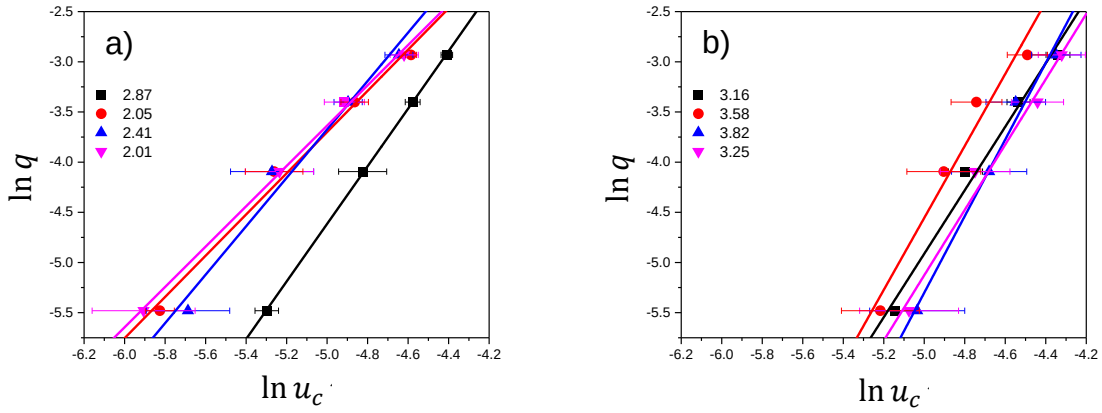

Figure S1. $\ln u_c$ vs. $\ln q$ plots for (a) y = 0.38 (showing IN) at concentrations of 200 (black square), 300 (red circle), 400 (blue upwards pointing triangle) and 500 g L^{-1} (pink downwards pointing triangle) and (b) y = 0.68 (showing PN) 150 (black square), 250 (red circle), 350 (blue upwards pointing triangle) and 450 g L^{-1} (pink downwards pointing triangle). Legend on graph gives values of slope for linear regressions fitted, for each concentration.

Table S4. Slopes of linear regressions of $\ln u_c$ vs. $\ln q$ plots for the range of solvent compositions studied, with the resultant nucleation mechanism determined from the "rule of three" KBHR analysis, alongside R^2 values of the fitted regressions and the standard errors (SE) of the slopes. The '*' denotes a low correlation fitting and as such the analysis has a lower confidence value and may be a potentially unreliable result.

Conc. (g L^{-1})	Slope of best-fit straight line of ln uc vs. ln q	SE	R^2, linear fitting	Nucleation mechanism	Conc. (g L^{-1})	Slope of best-fit straight line of ln uc vs. ln q	SE	R^2, linear fitting	Nucleation mechanism
y = 0					**y = 0.14**				
250	2.87	0.48	0.95	IN	**200**	2.80	0.27	0.98	IN
300	2.65	0.35	0.96	IN	**300**	2.26	0.04	0.99	IN
350	2.51	0.38	0.96	IN	**400**	2.37	0.18	0.99	IN

450	2.25	0.26	0.97	IN	**500**	3.15	1.32	0.74	PN*
550	2.45	0.25	0.98	IN	**700**	2.08	0.55	0.88	IN
650	2.24	0.21	0.98	IN	**800**	1.63	0.15	0.98	IN
750	2.18	0.18	0.98	IN					
850	2.16	0.23	0.98	IN					
y = 0.26					**y = 0.38**				
200	2.89	0.29	0.98	IN	**200**	2.87	0.02	0.99	IN
300	2.87	0.29	0.98	IN	**300**	2.05	0.14	0.99	IN
400	2.37	0.12	0.99	IN	**400**	2.41	0.27	0.97	IN
500	1.64	0.03	0.99	IN	**500**	2.01	0.07	0.99	IN
y = 0.49					**y = 0.59**				
150	2.82	0.75	0.88	IN	**150**	2.70	0.09	0.99	IN
250	2.32	0.14	0.99	IN	**250**	3.08	0.28	0.98	PN
350	2.53	0.15	0.99	IN	**350**	3.41	0.36	0.98	PN
450	2.67	0.06	0.99	IN	**450**	3.32	0.25	0.99	PN
y = 0.68					**y = 0.77**				
150	3.16	0.28	0.98	PN	**100**	3.18	0.67	0.92	PN
250	3.58	0.48	0.96	PN	**200**	3.27	0.61	0.93	PN
350	3.82	0.31	0.99	PN	**300**	3.04	0.63	0.92	PN
450	3.25	0.32	0.98	PN	**400**	3.91	1.30	0.82	PN
y = 0.85					**y = 0.93**				
75	3.61	0.45	0.97	PN	**20**	2.84	0.38	0.96	IN
175	4.00	0.38	0.98	PN	**60**	3.74	0.62	0.95	PN
275	3.84	0.41	0.97	PN	**100**	3.70	0.12	0.99	PN
375	4.04	0.41	0.99	PN	**140**	3.92	0.66	0.95	PN
y = 1									
5	1.68	0.49	0.85	IN					
15	2.28	0.33	0.96	IN					
25	4.16	0.48	0.97	PN					
35	1.95	0.24	0.97	IN					

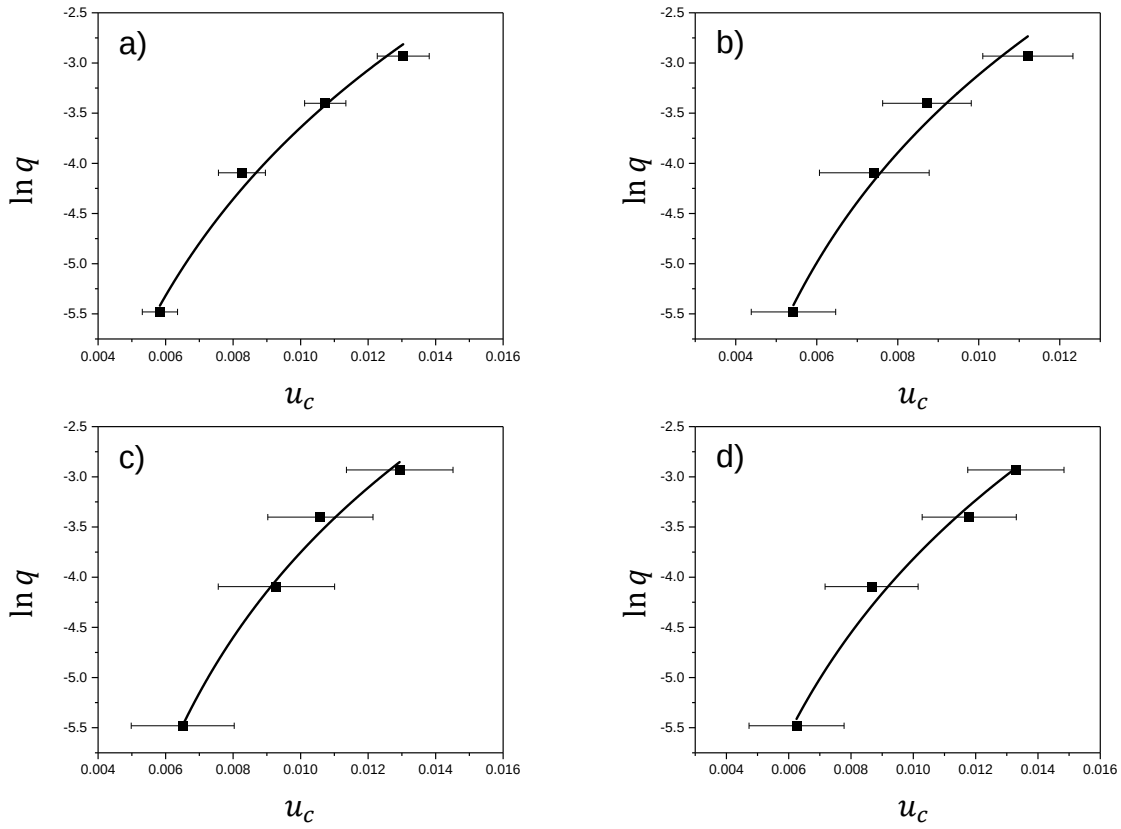

Figure S2. u_c vs. ln q plots for y = 0.68; (a) 150 g L^{-1}; (b) 250 g L^{-1}; (c) 350 g g L^{-1}; (d) 450 g L^{-1}. Data fitted with KBHR equation, $\ln q = \ln q_0 + a_1 \ln u_c - \frac{a_2}{(1-u_c)u_c^2}$, to determine nucleation kinetic parameters (black line on plots).

S5. Atomic Charges

The atomic partial charges calculated for eicosane, toluene and acetone are shown in Table S5, with the corresponding atomic labels represented in Figure S3.

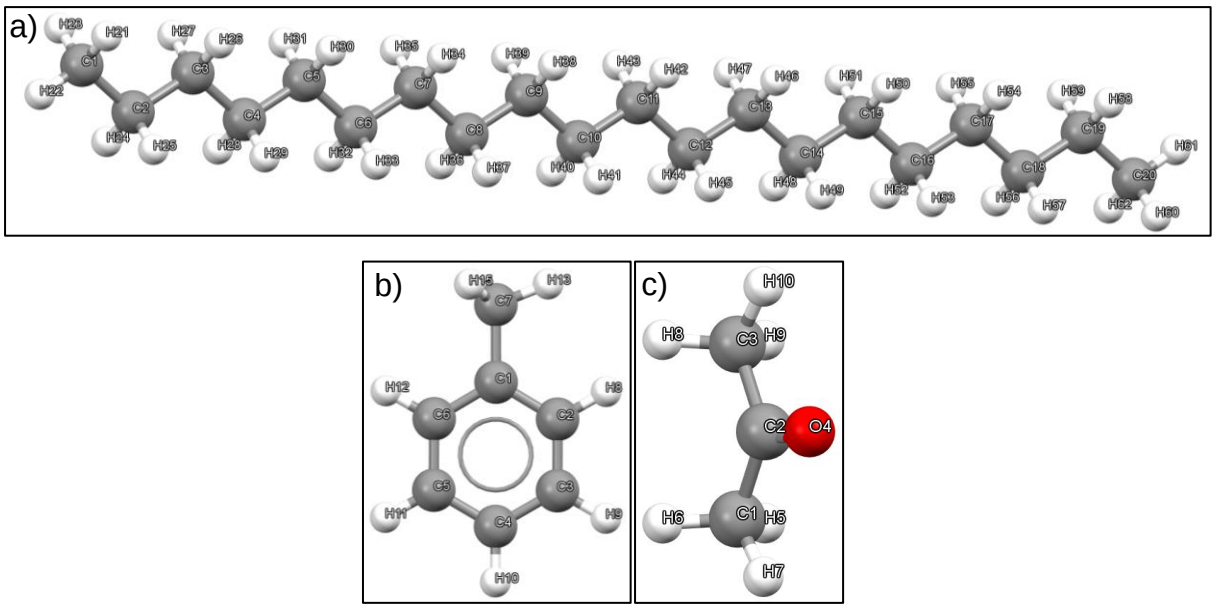

Figure S3. Atomic labels for a) eicosane, b) toluene and c) acetone. C represents carbon atoms, H represents hydrogen atoms and O represents and oxygen atom.

Table S5. Atomic partial charges and corresponding atomic labels calculated for eicosane, toluene and acetone molecules.

Eicosane Atomic Label	Eicosane Partial Charges	Toluene Atomic Label	Toluene Partial Charges	Acetone Atomic Label	Acetone Partial Charges
C1	-0.2170	C1	0.2056	C1	-0.3620
C2	0.1420	C2	-0.1970	C2	0.6768
C3	0.0171	C3	-0.0383	C3	-0.3623
C4	-0.0241	C4	-0.1522	O4	-0.5176
C5	0.0467	C5	-0.0248	H5	0.0889
C6	0.0096	C6	-0.2152	H6	0.0889
C7	0.0168	C7	-0.2530	H7	0.1046
C8	0.0396	H8	0.0992	H8	0.0891
C9	-0.0083	H9	0.0790	H9	0.0888
C10	0.0445	H10	0.0966	H10	0.1046
C11	0.0445	H11	0.0740		

C12	-0.0083	H12	0.1111
C13	0.0396	H13	0.0737
C14	0.0168	H14	0.0707
C15	0.0096	H15	0.0706
C16	0.0467		
C17	-0.0240		
C18	0.0171		
C19	0.1420		
C20	-0.2170		
H21	0.0463		
H22	0.0510		
H23	0.0463		
H24	-0.0270		
H25	-0.0269		
H26	-0.0078		
H27	-0.0076		
H28	-0.0037		
H29	-0.0039		
H30	-0.0136		
H31	-0.0137		
H32	-0.0068		
H33	-0.0067		
H34	-0.0102		
H35	-0.0103		
H36	-0.0136		
H37	-0.0138		
H38	-0.0053		
H39	-0.0051		
H40	-0.0172		
H41	-0.0170		
H42	-0.0170		
H43	-0.0172		
H44	-0.0051		
H45	-0.0053		
H46	-0.0138		
H47	-0.0136		
H48	-0.0103		
H49	-0.0102		
H50	-0.0067		
H51	-0.0068		
H52	-0.0137		
H53	-0.0136		
H54	-0.0039		
H55	-0.0037		
H56	-0.0076		
H57	-0.0078		
H58	-0.0269		
H59	-0.0270		

H60	0.0463		
H61	0.0510		
H62	0.0463		

S6. Grid-based Molecular Modelling

Figure S4 summarises the full results of the calculated solvation sites for a single eicosane molecule solvated with toluene and acetone, using different low-pass energy cut-off filters.

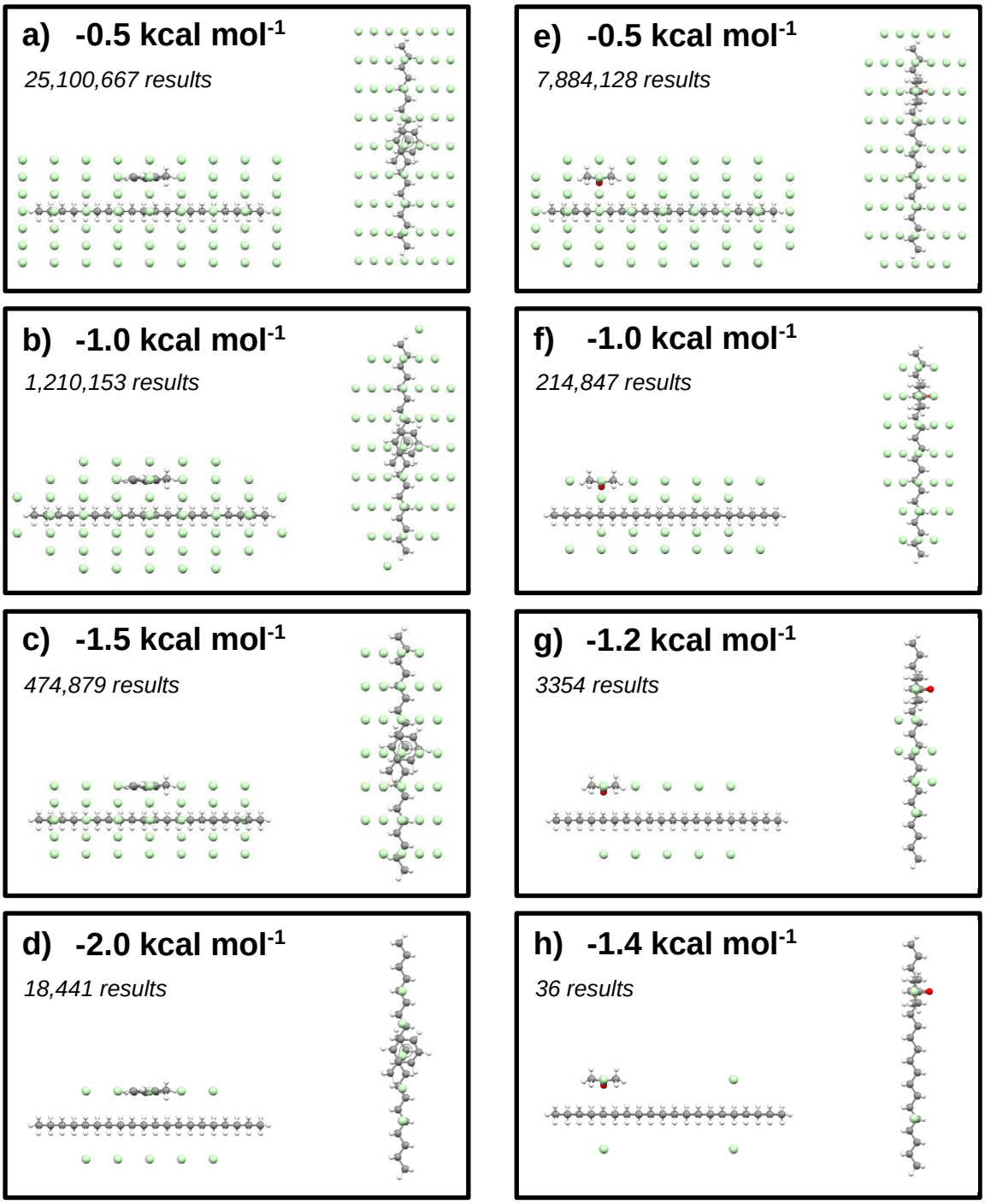

Figure S4. Interaction energy fields of toluene (a, b, c and d) and acetone (e, f, g and h) probe molecules, with a central eicosane molecule. Toluene and acetone molecules show most negative interaction energy site. The green dots represent interaction locations of the probes,

which passed the set energy filter cut-off, which is highlighted at the top left of images. A total of 331,986,600 points (location + rotation) were searched for each simulation, with the number of results found for each one shown below the high-energy cut-off values set. More negative energy filters highlight most favourable interaction sites with eicosane molecule.