Electronic Supplementary Material (ESI) for Molecular Systems Design & Engineering.

1. Solvent library

No.	CAS Number	Name	MW (g/mol)	B.P. (°C)	M.P. (°C)	Density (g/ml) @ 20 °C	Viscosity (cP) @ 20 °C	ICH Class
1	71-36-3	1-butanol	74	118	-89	0.810	3.006	3
2	71-41-0	1-pentanol	88	137	-78	0.815	3.512	3
3	71-23-8	1-propanol	60	97	-127	0.803	1.943	3
4	78-92-2	2-butanol	74	100	-115	0.808	2.998	3
5	78-93-3	2-butanone	72	80	-87	0.805	0.378	3
6	1634-04-4	2-methoxy-2-methylpropane	88	55	-109	0.760	0.340	3
7	78-83-1	2-methyl-1-propanol	74	108	-102	0.802	3.333	3
8	67-63-0	2-propanol	60	82	-88	0.785	2.430	3
9	123-51-3	3-methyl-1-butanol	88	131	-117	0.809	3.738	3
10	108-10-1	Methyl isobutyl ketone	100	117	-84	0.796	0.546	3
11	64-19-7	Acetic acid	60	118	17	1.049	1.130	3
12	67-64-1	Acetone	58	56	-95	0.791	0.303	3
13	100-66-3	Anisole	108	154	-38	0.994	0.789	3
14	123-86-4	Butyl acetate	116	126	-77	0.881	0.737	3
15	60-29-7	Diethylether	74	35	-116	0.713	0.242	3
16	67-68-5	Dimethylsulphoxide	78	189	19	1.101	1.991	3
17	64-17-5	Ethanol	46	78	-114	0.789	1.263	3
18	141-78-6	Ethyl acetate	88	77	-84	0.902	0.426	3
19	142-82-5	Heptane	100	98	-91	0.917	0.412	3
20	110-19-0	Isobutylacetate	116	118	-99	0.684	0.397	3
21	64-18-6	Methanoic acid	46	101	8	1.220	1.966	3
22	79-20-9	Methyl acetate	74	57	-98	0.934	0.364	3
23	7732-18-15	Water	18	100	0	1.000	1.000	3
24	109-94-4	Ethyl formate	74	54	-80	0.917	0.412	3
25	108-21-4	Isopropyl acetate	103	89	-73	0.870	0.520	3
26	109-66-0	Pentane	72	36	-131	0.626	0.225	3
27	109-60-4	Propyl acetate	102	102	-95	0.890	0.551	3
28	123-91-1	1,4-dioxane	88	102	12	1.033	1.087	2
29	110-71-4	1,2-dimethoxyethane	90	85	-58	0.868	0.455	2
30	110-80-5	2-ethoxyethanol	90	135	-70	0.931	1.850	2
31	109-86-4	2-methoxyethanol	76	124	-85	0.965	1.570	2
32	75-05-8	Acetonitrile	41	82	-45	0.786	0.358	2
33	67-66-3	Chloroform	119	61	-64	1.492	0.536	2
34	110-82-7	Cyclohexane	84	81	7	0.779	0.980	2
35	75-09-2	Dichloromethane	85	40	-95	1.325	0.404	2
36	75-12-7	Formamide	45	220	3	1.134	3.300	2
37	110-54-3	Hexane	86	69	-95	0.659	0.294	2
38	67-56-1	Methanol	32	65	-98	0.791	0.590	2
39	127-19-5	N, N-dimethylacetamide	87	165	-20	0.940	0.927	2
40	68-12-2	N, N-dimethylformamide	73	153	-61	0.944	0.802	2
41	75-52-5	Nitromethane	61	101	-29	1.130	0.647	2
42	872-50-4	N-methyl-2-pyrrolidone	99	202	-24	1.033	1.666	2
43	110-86-1	Pyridine	79	115	-42	0.978	0.880	2
44	109-99-9	Tetrahydrofuran	72	65	-108	0.889	0.460	2
45	108-88-3	Toluene	92	111	-95	0.867	0.553	2
46	79-01-6	Trichloroethylene	131	87	-73	1.460	0.592	2
47	106-42-3	o,m.p- xylene	106	138	-13	0.866	0.605	2
48	108-90-7	Chlorobenzene	113	131	-45	1.110	0.760	2

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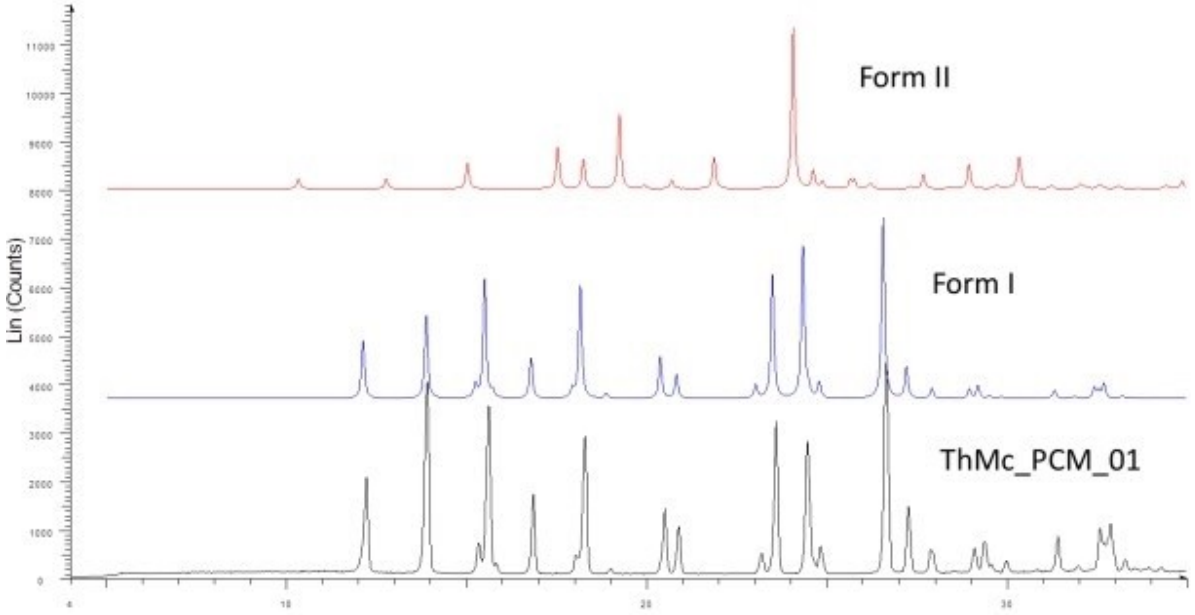
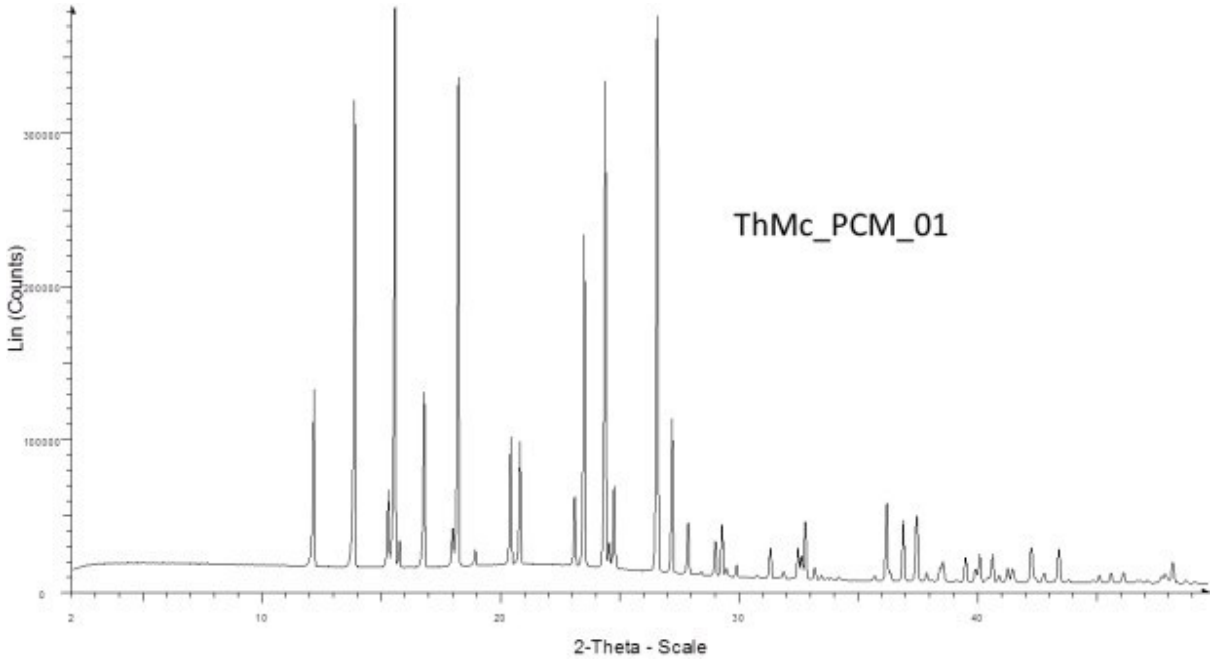
49	98-82-8	Cumene	120	152	-96	0.862	0.739	2
50	107-21-1	Ethylene glycol	62	197	-13	1.113	21.000	2
51	591-78-6	Methylbutyl ketone	100	128	-56	0.811	0.584	2
52	108-87-2	Methylcyclohexane	98	101	-126	0.770	0.670	2
53	126-33-0	Sulfolane	120	285	28	1.261	10.290	2
54	119-64-2	Tetralin	132	206	-36	0.970	2.140	2

Stage 1. Raw material characterisation

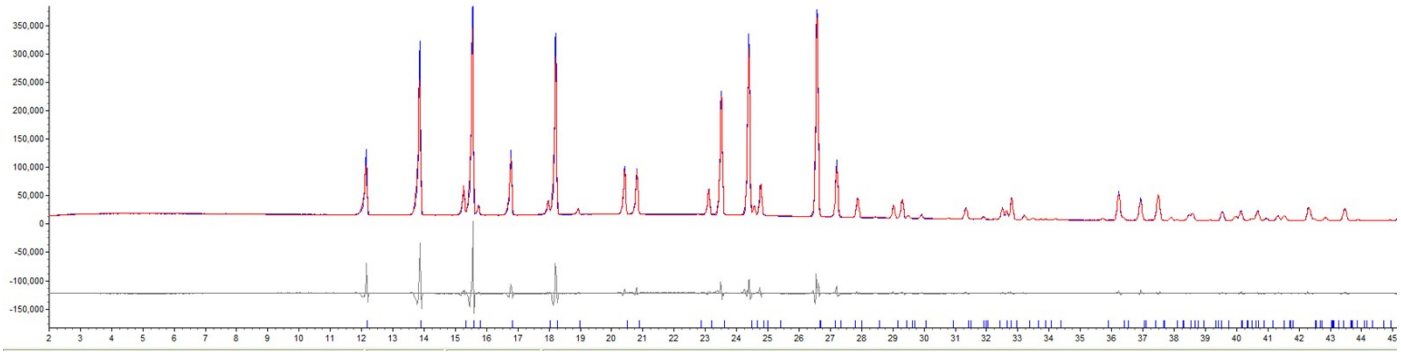
XRPD Plate



XRPD Capillary

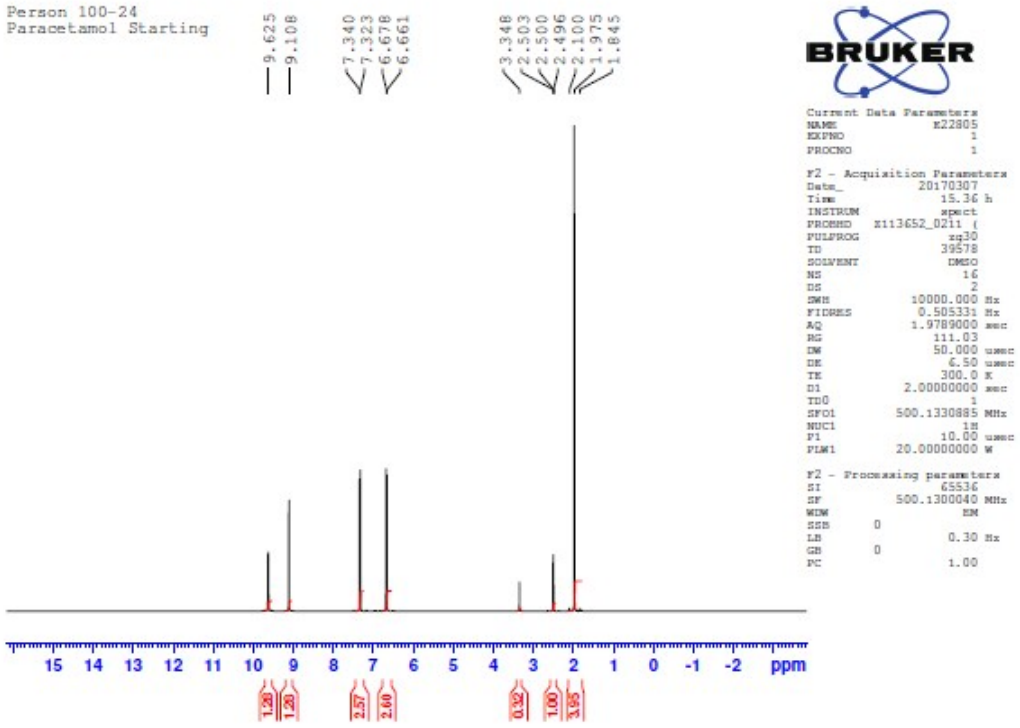


Pawley fitting

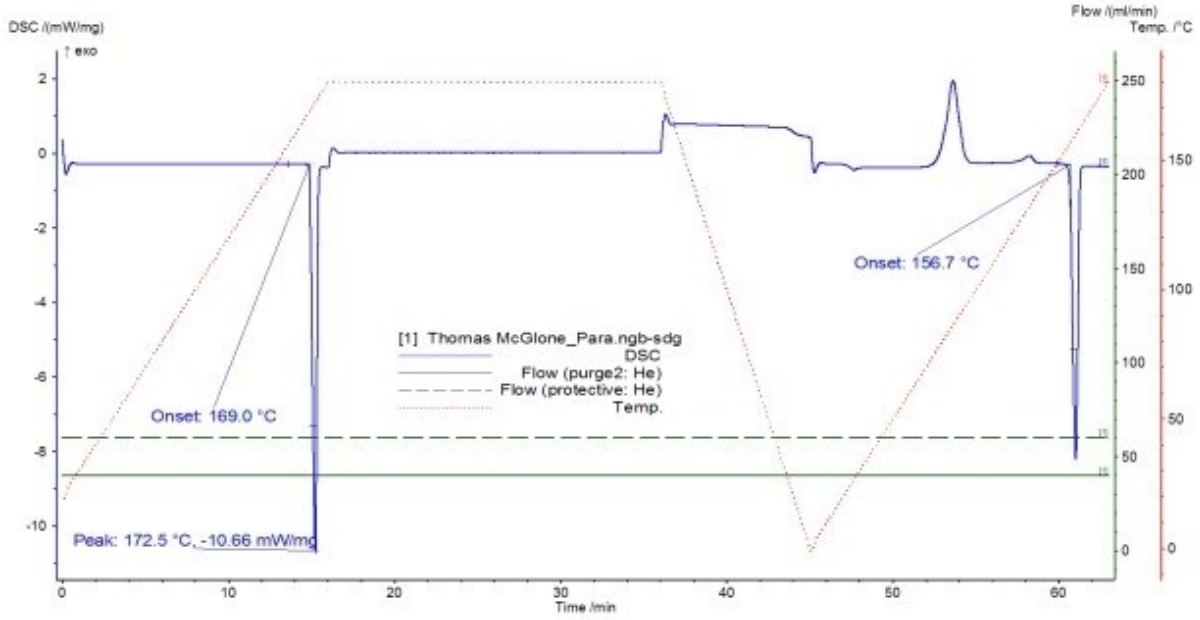


Parameter	Value
Rp	5.93%
Rwp	9.51%
a	7.0667883 Å
b	9.3380316 Å
c	11.6523207 Å
Beta	97.41708 °

NMR



DSC


DSC /(mW/mg)
↑ exo
Flow /(ml/min)
Temp. /°C
[1] Thomas McGlone_Para.ngb-sdg
DSC
Flow (purge2: He)
Flow (protective: He)
Temp.
Onset: 169.0 °C
Peak: 172.5 °C, -10.66 mW/mg
Onset: 156.7 °C
Time /min