

Extraction of Phenolic Compound from Model Pyrolysis Oil Using Deep Eutectic Solvents: Computational Screening and Experimental Validation

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Table S1: Standard deviation (STDEV) for the ternary system MTPPBr/EG (1:3) (1) / phenol (2) / toluene (3) for mole fractions x: Top layer.

feed% phenol	Mole fraction			Average mole fraction			STDEV mole fraction		
	X ₁	X ₂	X ₃	X ₁	X ₂	X ₃	X ₁	X ₂	X ₃
5	0	0.00036	0.99964	0	0.00036	0.99964	0	0.00001	0.00001
	0	0.00037	0.99963						
	0	0.00036	0.99964						
10	0	0.00082	0.99918	0	0.00081	0.99919	0	0.00001	0.00001
	0	0.00080	0.99920						
	0	0.00081	0.99919						
15	0	0.00119	0.99881	0	0.00116	0.99884	0	0.00002	0.00002
	0	0.00115	0.99885						
	0	0.00114	0.99886						
20	0	0.00169	0.99831	0	0.00169	0.99831	0	0.00002	0.00002
	0	0.00171	0.99829						
	0	0.00167	0.99833						
25	0	0.00218	0.99782	0	0.00218	0.99782	0	0.00001	0.00001
	0	0.00218	0.99782						
	0	0.00219	0.99781						

Table S2: Standard deviation (STDEV) for the ternary system MTPPBr/EG (1:3) (1) / phenol (2) / toluene (3) for mole fractions x: bottom layer.

feed% phenol	Mole fraction			Average mole fraction			STDEV mole fraction		
	X ₁	X ₂	X ₃	X ₁	X ₂	X ₃	X ₁	X ₂	X ₃
5	0.59857	0.15582	0.24561	0.59622	0.15519	0.24860	0.00213	0.00057	0.00270
	0.59442	0.15470	0.25089						
	0.59567	0.15505	0.24929						
10	0.46513	0.27500	0.25987	0.46327	0.27393	0.26280	0.00193	0.00112	0.00305
	0.46340	0.27403	0.26257						
	0.46129	0.27276	0.26595						
15	0.37544	0.31675	0.30781	0.37434	0.31587	0.30979	0.00111	0.00090	0.00201
	0.37436	0.31590	0.30975						
	0.37322	0.31496	0.31182						
20	0.31407	0.36010	0.32584	0.31314	0.35904	0.32781	0.00083	0.00094	0.00176
	0.31289	0.35874	0.32838						
	0.31247	0.35830	0.32923						
25	0.26587	0.38354	0.35060	0.26463	0.38176	0.35362	0.00109	0.00157	0.00266
	0.26420	0.38115	0.35465						
	0.26381	0.38058	0.35561						

Table S3: Standard deviation (STDEV) for the ternary system MTPPBr/EG (1:3) (1) / phenol (2) / heptane (3) for mole fractions x: Top layer.

feed% phenol	Mole fraction			Average mole fraction			STDEV mole fraction		
	x ₁	x ₂	x ₃	x ₁	x ₂	x ₃	x ₁	x ₂	x ₃
5	0	0.00011	0.99989	0	0.00011	0.99989	0	0.00000	0.00000
	0	0.00011	0.99989						
	0	0.00011	0.99989						
10	0	0.00012	0.99988	0	0.00012	0.99988	0	0.00001	0.00001
	0	0.00011	0.99989						
	0	0.00012	0.99988						
15	0	0.00016	0.99984	0	0.00015	0.99985	0	0.00001	0.00001
	0	0.00014	0.99986						
	0	0.00014	0.99986						
18	0	0.00022	0.99978	0	0.00021	0.99979	0	0.00000	0.00000
	0	0.00021	0.99979						
	0	0.00021	0.99979						
20	0	0.00022	0.99978	0	0.00022	0.99978	0	0.00001	0.00001
	0	0.00022	0.99978						
	0	0.00024	0.99976						

Table S4: Standard deviation (STDEV) for the ternary system MTPPBr/EG (1:3) (1) / phenol (2) / heptane (3) for mole fractions x: bottom layer.

feed% phenol	Mole fraction			Average mole fraction			STDEV mole fraction		
	X ₁	X ₂	X ₃	X ₁	X ₂	X ₃	X ₁	X ₂	X ₃
5	0.77030	0.22486	0.00484	0.77010	0.22481	0.00510	0.00017	0.00005	0.00022
	0.77000	0.22478	0.00522						
	0.77000	0.22477	0.00523						
10	0.62698	0.36458	0.00845	0.62697	0.36459	0.00844	0.00001	0.00002	0.00001
	0.62696	0.36461	0.00843						
	0.62696	0.36458	0.00845						
15	0.53089	0.46133	0.00777	0.53090	0.46136	0.00774	0.00003	0.00004	0.00006
	0.53087	0.46135	0.00778						
	0.53093	0.46140	0.00767						
18	0.48335	0.50704	0.00961	0.48336	0.50705	0.00959	0.00001	0.00002	0.00002
	0.48336	0.50705	0.00958						
	0.48337	0.50707	0.00956						
20	0.46122	0.53017	0.00861	0.46121	0.53014	0.00864	0.00000	0.00002	0.00003
	0.46121	0.53014	0.00865						
	0.46121	0.53012	0.00867						

Table S5: Standard deviation (STDEV) for the ternary system ChCl/EtA (1:5) (1) / phenol (2) / toluene (3) for mole fractions x: Top layer.

feed% phenol	Mole fraction			Average mole fraction			STDEV mole fraction		
	x ₁	x ₂	x ₃	x ₁	x ₂	x ₃	x ₁	x ₂	x ₃
5	0	0.00043	0.99957	0	0.00043	0.99957	0	0.00001	0.00002
	0	0.00042	0.99958						
	0	0.00044	0.99956						
10	0	0.00088	0.99912	0	0.00091	0.99909	0	0.00004	0.00004
	0	0.00089	0.99911						
	0	0.00095	0.99905						
15	0	0.00194	0.99806	0	0.00193	0.99807	0	0.00004	0.00004
	0	0.00198	0.99802						
	0	0.00189	0.99811						
20	0	0.00308	0.99692	0	0.00321	0.99679	0	0.00030	0.00030
	0	0.00300	0.99700						
	0	0.00356	0.99644						
25	0	0.00488	0.99512	0	0.00506	0.99494	0	0.00017	0.00017
	0	0.00523	0.99477						
	0	0.00508	0.99492						

Table S6: Standard deviation (STDEV) for the ternary system ChCl/EtA (1:5) (1) / phenol (2) / toluene (3) for mole fractions x: bottom layer.

feed% phenol	Mole fraction			Average mole fraction			STDEV mole fraction		
	X ₁	X ₂	X ₃	X ₁	X ₂	X ₃	X ₁	X ₂	X ₃
5	0.71703	0.16361	0.11936	0.71833	0.16391	0.11776	0.00112	0.00026	0.00138
	0.71889	0.16408	0.11702						
	0.71905	0.16404	0.11691						
10	0.60074	0.27901	0.12025	0.60050	0.27883	0.12067	0.00023	0.00019	0.00042
	0.60047	0.27886	0.12067						
	0.60028	0.27863	0.12109						
15	0.51441	0.35722	0.12837	0.51371	0.35674	0.12954	0.00071	0.00045	0.00116
	0.51375	0.35668	0.12957						
	0.51299	0.35632	0.13069						
20	0.44812	0.42465	0.12723	0.44712	0.42349	0.12938	0.00102	0.00139	0.00240
	0.44717	0.42388	0.12895						
	0.44608	0.42195	0.13197						
25	0.40548	0.46217	0.13235	0.40488	0.46125	0.13387	0.00057	0.00081	0.00137
	0.40481	0.46095	0.13424						
	0.40435	0.46063	0.13502						

Table S7: Standard deviation (STDEV) for the ternary system ChCl/EtA (1:5) (1) / phenol (2) / heptane (3) for mole fractions x: Top layer.

feed% phenol	Mole fraction			Average mole fraction			STDEV mole fraction		
	X ₁	X ₂	X ₃	X ₁	X ₂	X ₃	X ₁	X ₂	X ₃
5	0	0.00109	0.99891	0	0.00106	0.99894	0	0.00003	0.00003
	0	0.00106	0.99894						
	0	0.00102	0.99898						
10	0	0.00099	0.99901	0	0.00102	0.99898	0	0.00005	0.00005
	0	0.00100	0.99900						
	0	0.00107	0.99893						
15	0	0.00144	0.99856	0	0.00140	0.99860	0	0.00004	0.00004
	0	0.00139	0.99861						
	0	0.00138	0.99862						
18	0	0.00152	0.99848	0	0.00153	0.99847	0	0.00003	0.00003
	0	0.00157	0.99843						
	0	0.00151	0.99849						
20	0	0.00187	0.99813	0	0.00179	0.99821	0	0.00015	0.00015
	0	0.00187	0.99813						
	0	0.00162	0.99838						

Table S8: Standard deviation (STDEV) for the ternary system ChCl/EtA (1:5) (1) / phenol (2) / heptane (3) for mole fractions x: Bottom layer.

feed% phenol	Mole fraction			Average mole fraction			STDEV mole fraction		
	X ₁	X ₂	X ₃	X ₁	X ₂	X ₃	X ₁	X ₂	X ₃
5	0.84220	0.15751	0.00030	0.84209	0.15759	0.00032	0.00012	0.00010	0.00002
	0.84210	0.15757	0.00033						
	0.84197	0.15770	0.00033						
10	0.81105	0.18837	0.00058	0.81113	0.18828	0.00059	0.00013	0.00012	0.00001
	0.81106	0.18834	0.00060						
	0.81129	0.18814	0.00058						
15	0.72534	0.27379	0.00088	0.72526	0.27388	0.00086	0.00007	0.00008	0.00002
	0.72524	0.27392	0.00084						
	0.72521	0.27394	0.00085						
18	0.68556	0.31332	0.00112	0.68559	0.31330	0.00112	0.00005	0.00006	0.00001
	0.68565	0.31323	0.00112						
	0.68555	0.31334	0.00111						
20	0.59166	0.40727	0.00107	0.59153	0.40739	0.00108	0.00019	0.00021	0.00002
	0.59163	0.40727	0.00110						
	0.59131	0.40763	0.00106						

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Figure S2. GC calibration curve of toluene/phenol.

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Figure S4. ^1H NMR spectra of ChCl/EtA pure DES (1:5, molar ratio) in DMSO-d_6

Figure S5. ^1H NMR spectra of MTPPBr/EG DES (1:3, molar ratio) in DMSO-d_6 : (a) pure DES; and (b) heptane rich phase (Top Layer).

Figure S6. ^1H NMR spectra of ChCl/EtA DES (1:5, molar ratio) in DMSO-d_6 : (a) pure DES; and (b) heptane rich phase (Top Layer).

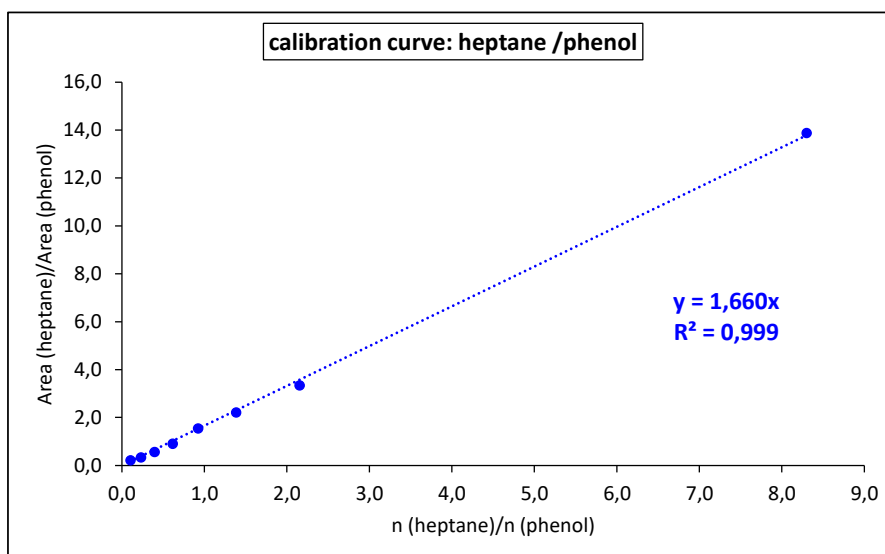


Figure S1. GC calibration curve of heptane/phenol.

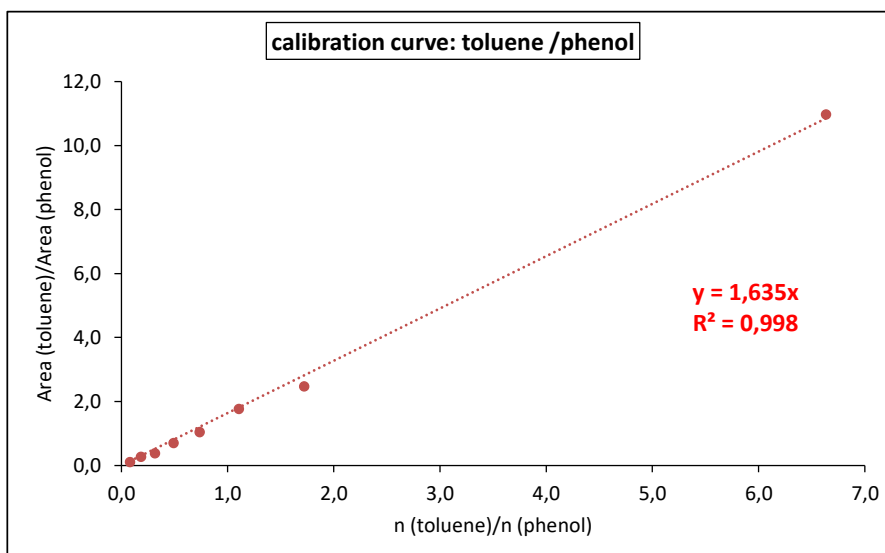


Figure S2. GC calibration curve of toluene/phenol.

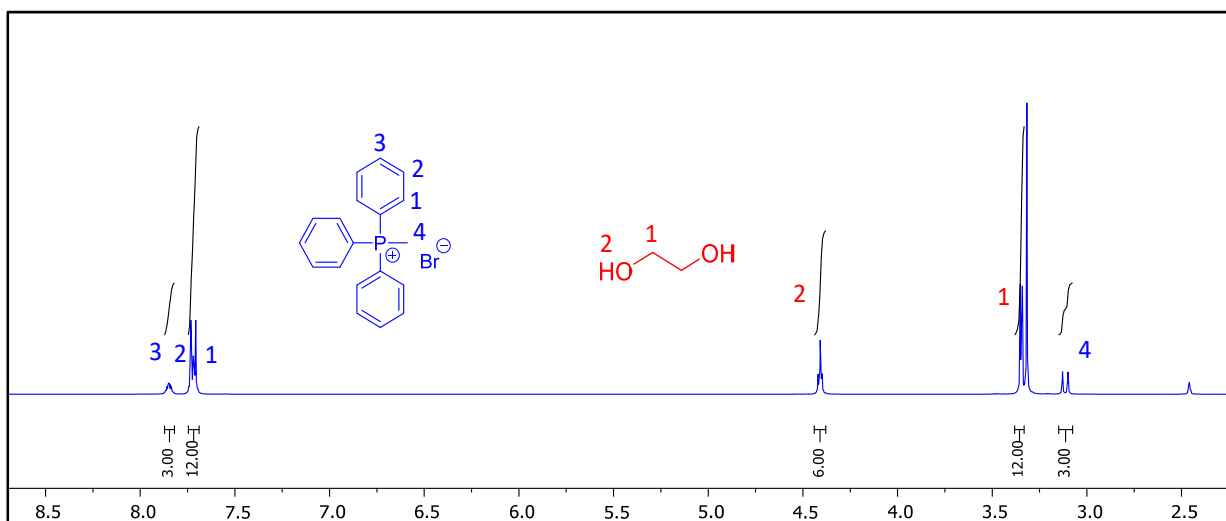


Figure S3. ^1H NMR spectra of MTPPBr/EG pure DES (1:3, molar ratio) in DMSO-d_6

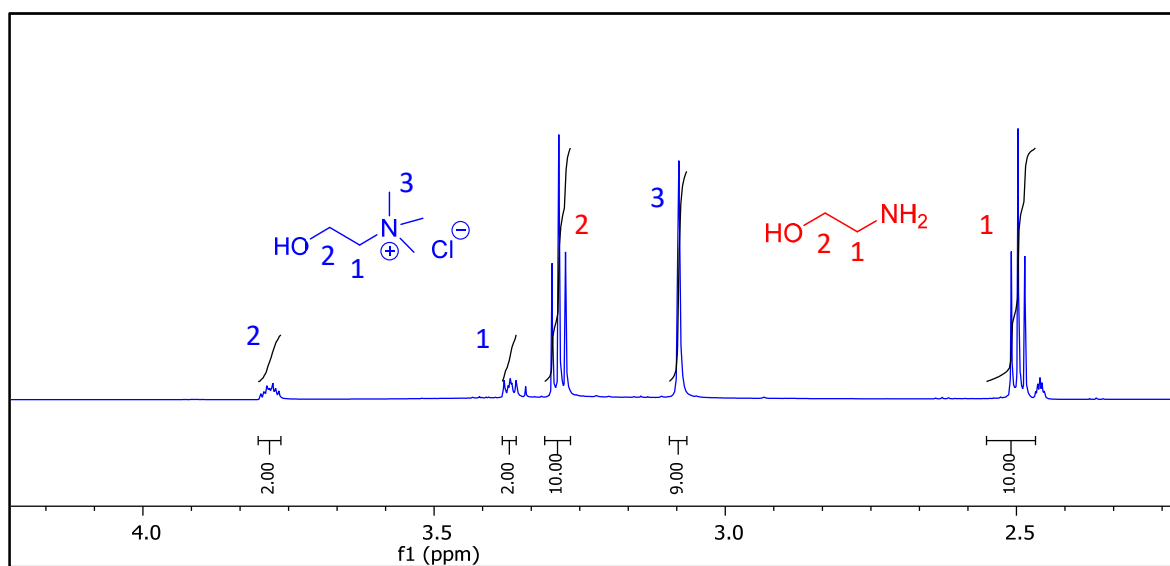


Figure S4. ^1H NMR spectra of ChCl/EtA pure DES (1:5, molar ratio) in DMSO-d_6

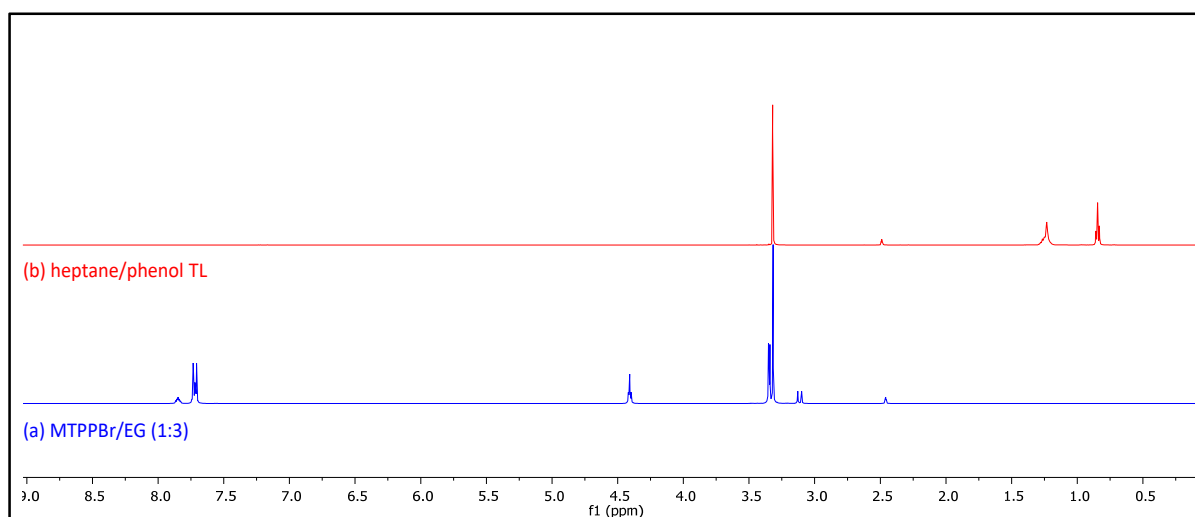


Figure S5. ^1H NMR spectra of MTPPBr/EG DES (1:3, molar ratio) in DMSO-d_6 : (a) pure DES; and (b) heptane rich phase (Top Layer).

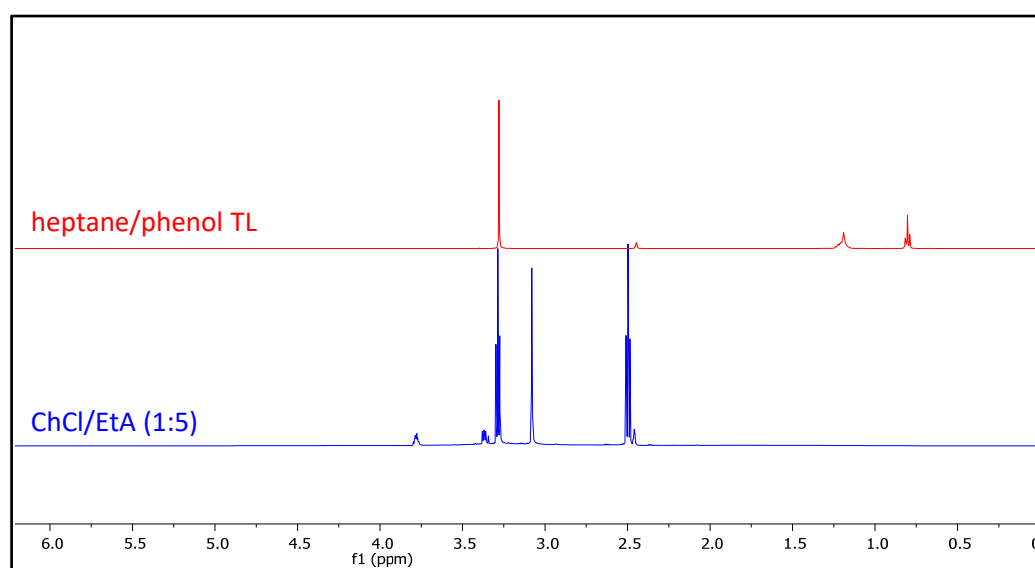


Figure S6. ^1H NMR spectra of ChCl/EtA DES (1:5, molar ratio) in DMSO-d_6 : (a) pure DES; and (b) heptane rich phase (Top Layer).