

## Supporting Information

### Deep insights into the viscosity of Deep Eutectic Solvents by XGBoost-based model plus SHapley Additive exPlanation

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**Table S1.** Summary of the reported laboratory-measured viscosity for diverse deep eutectic solvents in the literature

DES	Composition	Ratio	Temperature	Viscosity	Ref
DES 1	ChCl:Ethylene glycol	1:2	20-80	4.3-60.9	1
DES 2	ChCl:Glycerol	1:2	10-90	11.4031-1003.94	2, 3
DES 3	ChCl:1,2-Propanediol	1:2	25-65	22.37-122.3028	2
DES 4	ChCl:Malonic acid	1:1	20-75	10.14-2016	4
DES 5	ChCl:Glutaric acid	1:1	20-80	9.323-2968	2, 4
DES 6	ChCl:Urea	1:2	20-80	13.6-1685.8	1
DES 7	Tetramethylammonium chloride:Ethylene glycol	1:3	25-65	8.3058-26.12	2
DES 8	Tetraethylammonium chloride:Ethylene glycol	1:2	25-65	13.153-50.426	2
DES 9	Tetrabutylammonium chloride:Ethylene glycol	1:2	25-65	12.499-61.159	2
DES10	[BMIM][PF <sub>6</sub> ]:N-Methylacetamide	1:2	25-65	5.396-17.306	2
DES 11	[HMIM][PF <sub>6</sub> ]:N-Methylacetamide	1:2	25-65	6.4785-23.456	2

DES 12	[OMIM][PF <sub>6</sub> ]:N-Methylacetamide	1:2	25-65	8.2708-35.488	2
DES 13	Tetramethylammonium acetate:Ethylene glycol	1:2	25-65	11.43-42.437	2
DES 14	Tetraethylammonium bromide:Ethylene glycol	1:2	25-65	8.5566-28.84	2
DES 15	[BMIM][CF <sub>3</sub> SO <sub>3</sub> ]:N-Methylacetamide	1:2	25-65	5.1486-16.332	2
DES 16	[BMIM][Ac]:N-Methylacetamide	1:2	25-65	8.5325-36.361	2
DES 17	Phenyltrimethylammonium chloride:Ethylene glycol	1:2	25-65	12.151-53.292	2
DES 18	Benzyltrimethylammonium chloride:Ethylene glycol	1:2	25-65	19.568-106.31	2
DES 19	Allyltrimethylammonium chloride:Ethylene glycol	1:2	25-65	3.6863-11.319	2
DES 20	ZnCl <sub>2</sub> :Ethylene glycol	1:2	25-65	34.206-274.75	2
DES 21	ZnCl <sub>2</sub> :Acetamide	1:3	25-65	36.519-602.51	2
DES 22	FeCl <sub>3</sub> ·6H <sub>2</sub> O:Ethylene glycol	2:1	25-65	3.85743-28.07838	2
DES 23	Lithium bis(trifluoromethanesulphonyl)imide:N-Methylacetamide	1:4	25-65	17.687-80.548	H
DES 24	Lithium bis(trifluoromethanesulphonyl)imide:Ethylene glycol	1:2	25-65	53.258-372.35	2
DES 25	ChCl:Ethylene glycol	1:2.00	20-60	15.31-60.00	5
DES 26	ChCl:Ethylene glycol	1:2.99	20-60	10.47-37.35	5
DES 27	ChCl:Ethylene glycol	1:3.99	20-60	9.01-31.80	5
DES28	ChCl:Ethylene glycol	1:4.99	20-60	7.50-28.49	5
DES29	ChCl:Ethylene glycol	1:1.59	20-60	6.91-25.56	5
DES30	ChCl:1,2-Propanediol	1:2.99	20-60	17.11-94.05	5
DES31	ChCl:1,2-Propanediol	1:4.00	20-60	14.43-80.19	5
DES32	ChCl:1,2-Propanediol	1:4.97	20-60	13.04-73.34	5
DES33	ChCl:1,2-Propanediol	1:5.97	20-60	12.21-70.57	5
DES34	ChCl:1,3-Propanediol	1:3.01	20-60	16.88-69.74	5
DES35	ChCl:1,3-Propanediol	1:4.00	20-60	14.66-61.31	5
DES36	ChCl:1,3-Propanediol	1:4.97	20-60	13.25-57.14	5
DES37	ChCl:1,3-Propanediol	1:5.97	20-60	12.83-53.95	5
DES38	ChCl:1,4-Butanediol	1:3.03	20-60	23.6-112.88	5
DES39	ChCl:1,4-Butanediol	1:3	30-70	15.7-60.64	6
DES40	ChCl:1,4-Butanediol	1:3.99	20-60	20.75-99.69	5

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DES41	ChCl:1,4-Butanediol	1:5.00	20-60	19.64-93.69	5
DES42	ChCl:1,4-Butanediol	1:6.01	20-60	18.98-91.44	5
DES43	ChCl:1,4-Butanediol	1:4	30-70	14-54.75	7
DES44	ChCl:2,3-Butanediol	1:4	30-70	11.89-71.79	7
DES45	ChCl:2,3-Butanediol	1:3	30-70	14.34-84.88	7
DES46	ChCl:1,3-Propanediol	1:4	30-70	10.26-34.43	7
DES47	ChCl:1,3-Propanediol	1:3	30-70	11.85-40.05	7
DES48	ChCl:Phenol	1:2	20-45	34.34-120.77	8
DES49	ChCl:Phenol	1:3	20-45	19.14-57.84	8
DES50	ChCl:Phenol	1:4	20-45	14.00-40.23	8
DES51	ChCl:Phenol	1:5	20-45	11.26-31.96	8
DES52	ChCl:Phenol	1:6	20-45	9.46-27.03	8
DES53	ChCl:O-cresol	1:2	25	207.41	8
DES54	ChCl:O-cresol	1:3	25	77.65	8
DES55	ChCl:O-cresol	1:3.91	25	46.95	8
DES56	ChCl:O-cresol	1:5	25	34.90	8
DES57	ChCl:O-cresol	1:6	25	27.82	8
DES58	Betaine:Lactic acid	1:2	20.21-69.66	70-1210	6
DES59	Histidine:Lactic acid	1:9	20.21-69.66	90-2130	6
DES60	Betaine:DL-Malic Acid	2:1	20.21-69.66	680-27310	6
DES61	Ethylamine hydrochloride:Urea	1:0.5	40-80	34.8-97.8	9
DES62	Ethylamine hydrochloride:Urea	1:1	40-80	34.8-197.7	9
DES63	Ethylamine hydrochloride:Urea	1:2	40-80	28.7-105.5	9
DES64	Betaine:Levulinic acid	1:7	25	117.7	10
DES65	ChCl:Levulinic acid	1:2	25-75	7.212-320.6	4, 11
DES66	ChCl:Glucose	1:1	50-100	216.83-34400	12, 13
DES67	ChCl:Fructose	1:1	50-100	199.59-5586.90	12
DES68	ChCl:Xylose	1:1	45-100	146.28-5999.90	12
DES69	ChCl : Mannose	1:1	60-100	356.01-6619.40	12
DES70	Allyltriphenylphosphonium bromide:Diethylene glycol	1:4	20-70	17.139-213.18	14
DES71	Allyltriphenylphosphonium bromide:Diethylene glycol	1:10	20-70	8.9700-70.916	14
DES72	Allyltriphenylphosphonium bromide:Diethylene glycol	1:16	20-70	7.870-57.19	14
DES73	Allyltriphenylphosphonium bromide:Triethylene glycol	1:4	20-70	19.402-233.75	14
DES74	Allyltriphenylphosphonium bromide:Triethylene glycol	1:10	20-70	11.402-95.287	14

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DES75	Allyltriphenylphosphonium bromide:Triethylene glycol	1:16	20-70	9.8905-76.6310	14
DES76	ChCl:Triethylene glycol	1:3	25-85	9.0-68.0	15
DES77	ChCl:Triethylene glycol	1:4	25-85	8.1-61.9	15
DES78	ChCl:Triethylene glycol	1:5	25-85	7.5-53.0	15
DES79	ChCl:Triethylene glycol	1:6	25-85	6.5-44.9	15
DES80	N,N-diethylethanolammonium chloride:Glycerol	1:2	25-70	42.5755-513.0930	16
DES81	N,N-diethylethanolammonium chloride : Ethylene glycol	1:2	25-70	9.9868-50.4466	16
DES82	ChCl:Imidazole	3:7	20-130	6.2-810.0	17
DES83	Tetrabutylammonium bromide:Imidazole	3:7	60-130	4.0-22.5	17
DES84	ChCl:Xylitol	1:1	30-70	250-5230	13
DES85	ChCl:D-Sorbitol	1:1	30-70	480-12730	13
DES86	ChCl:Oxalic acid	1:1	20-75	10-8953	4
DES87	ChCl:Glycolic acid	1:1	20-80	7.845-779.4	4
DES88	ChCl:Levulinic acid	1:3	20-60	20.21-134.23	18
DES89	Acetylcholine chloride:Levulinic acid	1:3	20-60	21.47-164.52	18
DES90	Tetraethylammonium chloride:Levulinic acid	1:3	20-60	18.71-130.07	18
DES91	Tetraethylammonium bromide:Levulinic acid	1:3	20-60	19.74-148.95	18
DES92	Tetrabutylammonium chloride:Levulinic acid	1:3	20-60	17.47-121.68	18
DES93	Tetrabutylammonium bromide:Levulinic_acid	1:3	20-60	33.85-376.50	18
DES94	Trimethylamine hydrochloride:Levulinic acid	1:3	20-60	12.70-74.02	18
DES 95	Acetylcholine chloride:1,2,4-Triazole	1:1	30-90	8.37-304.69	19
DES 96	Acetylcholine chloride:Imidazole	1:1.5	30-90	11.69-233.69	19
DES 97	Acetylcholine chloride:Imidazole	1:2	30-90	4.17-103.33	19
DES 98	Acetylcholine chloride:Imidazole	1:3	30-90	17.68-335.98	19
DES 99	Benzyltripropylammonium Chloride:Phenol	1:3	20-70	20.4-638.4	20
DES 100	Benzyltripropylammonium Chloride:Ethylene glycol	1:3	20-70	22.2-327.9	20
DES 101	Benzyltripropylammonium Chloride:Lactic acid	1:3	30-70	81.3-2276.7	20
DES 102	Benzyltripropylammonium Chloride:Glycerol	1:3	30-70	97-1890.5	20
DES 103	Methyltriphenylphosphonium bromide : Glycerol	1:1.75	45-95	36.9-887.1	21
DES 104	Methyltriphenylphosphonium bromide:Ethylene glycol	1:4	5-75	1.8-345	21
DES10	Methyltriphenylphosphonium bromide:Ethylene glycol	1:8	5-85	0.9-657.7	21

5	m bromide:2,2,2-Trifluoroacetamide				
DES10	Methyltriphenylphosphoni	1:5	55-95	38.7-553.7	21
6	m bromide:Glycerol				
DES10	Methyltriphenylphosphoni	1:3	55-95	35.9-201.9	21
7	m bromide:Ethylene glycol				

**Table S2.** The MSE and R2 of different models in training set and test set

Model	Representation	Data set	MSE	R <sup>2</sup>
Support Vector Regression	BP	Training set	1.9014	0.2765
		Test set	2.6443	0.1328
	BP _ W <sub>H2O</sub>	Training set	1.8144	0.3093
		Test set	2.6169	0.1418
	BP _ MF	Training set	0.5222	0.8012
		Test set	0.6595	0.7837
	BP _ W <sub>H2O</sub> _ MF	Training set	0.0877	0.9666
		Test set	0.2121	0.9304
Random Forest	BP	Training set	1.6629	0.3670
		Test set	2.4072	0.2105
	BP _ W <sub>H2O</sub>	Training set	0.2712	0.8968
		Test set	0.6854	0.7752
	BP _ MF	Training set	0.4999	0.8097
		Test set	0.6885	0.7742
	BP _ W <sub>H2O</sub> _ MF	Training set	0.0191	0.9927
		Test set	0.1199	0.9607
Neural Network	BP	Training set	2.2736	0.1346
		Test set	2.9722	0.0253
	BP _ W <sub>H2O</sub>	Training set	1.1609	0.5581
		Test set	2.2798	0.2523
	BP _ MF	Training set	0.3426	0.8696
		Test set	0.6997	0.7705
	BP _ W <sub>H2O</sub> _ MF	Training set	0.0312	0.9881
		Test set	0.0658	0.9784
Extreme Gradient boosting	BP	Training set	1.6868	0.3579
		Test set	2.3750	0.2211
	BP _ W <sub>H2O</sub>	Training set	0.2566	0.9023
		Test set	0.5547	0.8181
	BP _ MF	Training set	0.3487	0.8673
		Test set	0.5666	0.8142
	BP _ W <sub>H2O</sub> _ MF	Training set	0.0002	0.9999
		Test set	0.0422	0.9861

**Table S3.** The ranges of the grid-search for each algorithm in training the models

Algorithm	Hyperparameter	Range
Support Vector Regression	C	0.1,0.2,0.3, 1,2,3,10,20
	gamma	1, 0.1, 0.01,0.001
Random Forest	n_estimators	5,10,20,50,70,100
	max_depth	3,5,7,9,10,20
	max_features	0.6,0.7,1
Extreme Gradient boosting	n_estimators	5, 10, 20, 50, 70, 100, 200
	max_depth	5, 6, 7, 8
	max_delta_step	1, 3, 5, 7

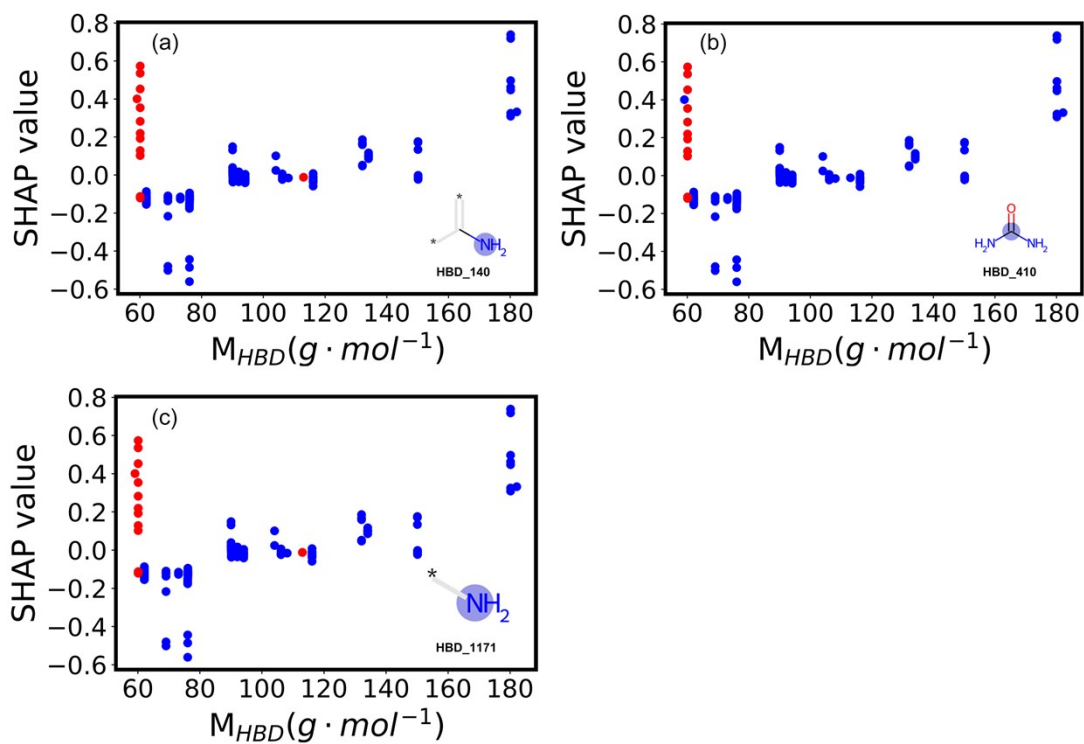


Fig. S1 The relationship between SHAP value and the NH<sub>2</sub> group related substructure for DESs. DESs with (a) HBD\_140, (b) HBD\_410, and (c) HBD\_1771 are highlighted in red.

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