Supplementary Materials

Transition state theory-inspired neural network for estimating the viscosity of deep eutectic solvents

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1 Comparison with traditional machine learning methods

In addition to the NN model in the main text, many other machine learning models can be used for quantitative structure-property relationship (QSPR), such as random forest, gradient boosting, and support vector machine. In this note, three tree models (random forest, gradient boosting, and LightGBM) have been applied to our dataset. We will discuss the hyperparameters settings and performance of these models, then compare these models with the TSTiNet model and the NN model.

1.1 NN

Benefit from the good designability, the NN model is the most extensively studied model currently in machine learning. The overall architecture of NN is as same as the MLP in the TSTiNet as the main text shows. We tune the hyperparameters of these MLPs manually, and the search space of the hyperparameters are shown in Table S1.

Table S1. The search space and results of parameters in the NN model.

Hyperparameters	Search space	Result
activation function	ReLU, Tanh, GELU	GELU
number of hidden layers	1, 2, 3	2
number of hidden neurons	32, 48, 64, 128	32
loss function	MSE loss, MAE loss, Huber loss	Huber loss

1.2 Random forest

Random forest has been widely used in classification and regression tasks related to molecular as a QSPR model. It is based on the decision tree model and bagging algorithm, and its core idea is selecting features randomly to grow each tree (74). The randomness reduces the risk of overfitting, which is the key benefit of the random forest model. To prove the superiority of our proposed TSTiNet model, a random forest model is applied to our dataset as a comparison.

The random forest model is performed in Python 3 with the scikit-learn package (75). The RandomizedSearchCV in the package is used to optimize the hyperparameters in the random forest with default settings, except for the number of parameter settings that are sampled is set to 50. The training set and validation set are concatenated as new training set for cross-validation (cv), and the cv score is a negative mean square error. The hyperparameters selected for optimization are the number of trees in the forest (n_estimators), the maximum depth of the tree (max_depth), the minimum number of samples required to split an internal node (min_samples_split), the minimum number of samples required to be at a leaf node (min_samples_leaf), and the number of features to consider when looking for the best split (max_features). Since the increase of n_estimators will lead to expensive computation, the n_estimators is initially set to 100. The search space and results of the parameters in the random forest model are shown in Table S2.

Table S2. The search space and results of parameters in the random forest model.

Hyperparameters	Search space	Result
max_features	20, 30, 40, 50, 60	40
max_depth	50, 75, 100, 125, 150	100
min_samples_split	2, 5, 10, 15, 20	2
min_samples_leaf	1, 2, 5, 10, 15	1
n_estimators	100	100

As Table S2 shows, the best values of min_samples_split and min_samples_leaf are 2 and 1, respectively, which are the default values of the model. The values of max_depth and max_features are 100 and 40, respectively. After these parameters are determined, we try the difference values of the n_estimators and find a minimum value that makes the model have acceptable results. As shown in Fig. S1, when the n_estimators is less than 130, the mean cv score gets higher as the n_estimators increases; when the n_estimators is more than 130, the mean cv score fluctuates up and down without a significant improvement. Therefore, the value of n_estimators is finally set to 130.

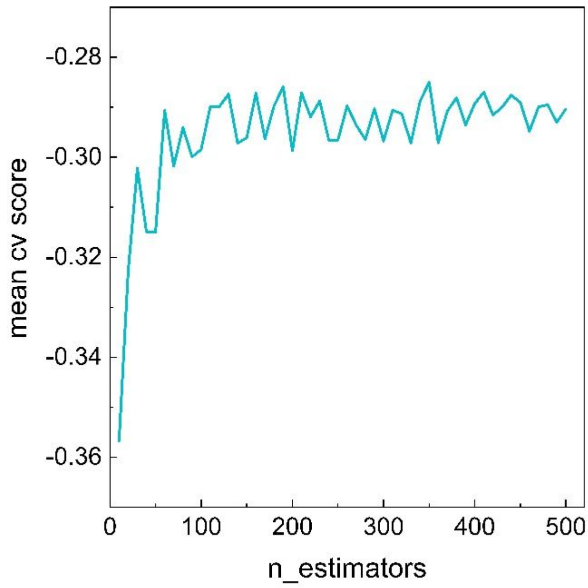


Fig. S1. Dependence of mean cv score on the n_estimators in the random forest model.

Under the above model settings, the performance of the model is evaluated on the test set and the new training set (see Fig. S2 and Fig. S3).

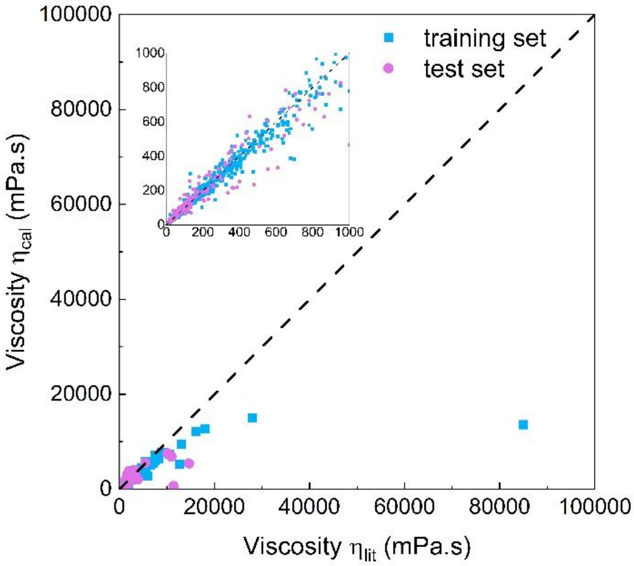


Fig. S2. Correlation between the predicted and reported viscosity values of datasets in the random forest model.

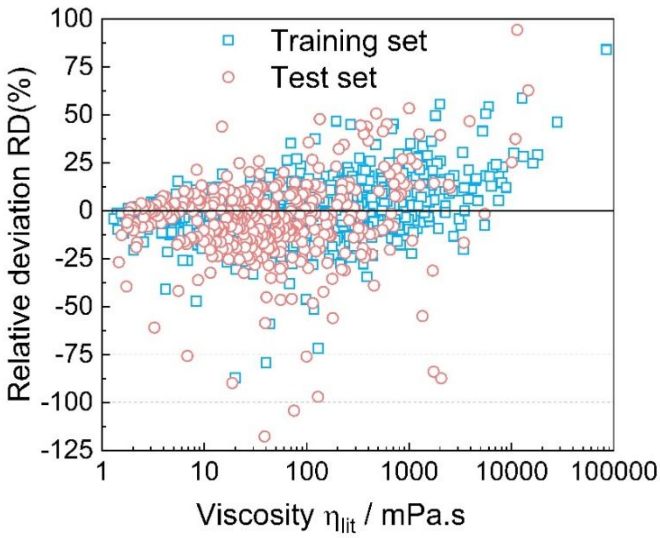


Fig. S3. Relative deviations between the literature and the predicted viscosities in both datasets in the random forest model.

As shown in Fig. S2, the calculated viscosities of DESs using the random forest model display a bad agreement with the corresponding experimental viscosity data. Even in the training set, the model performs very poorly, especially in the region of large viscosity (as already suggested by Fig. S3). Besides, there are also many points with huge RD, as seen in Fig. S3. Therefore, from the performance of the random forest model, the model is not suitable for the prediction of the viscosity of DESs.

1.3 Gradient boosting

Gradient boosting is a popular machine learning algorithm that has been proved successful across many domains. Unlike random forest that implements ensemble through deep independent trees, gradient boosting builds many weak estimators to fit the negative gradient of the loss function (76). Xu et al. (38) have applied the gradient boosting method to predict the thermophysical properties of DESs. And they get R^2=0.9773 on logarithm viscosity prediction, proving that the gradient boosting method may be a suitable method for viscosity prediction. Therefore, we implement a gradient boosting regressor to predict the viscosity of DESs as a comparison.

The gradient boosting model is performed in Python 3 with the scikit-learn package. The RandomizedSearchCV in the package is used to optimize the hyperparameters in the gradient boosting with default settings, except for the number of parameter settings that are sampled is set to 50. The training set and validation set are concatenated as new training set for cross-validation, and the cv score is a negative mean square error. The hyperparameters selected for optimization are the number of boosting stages to perform (n_estimators), the fraction of samples to be used for fitting the individual base learners (subsample), maximum depth of the individual regression estimators (max_depth), and learning rate. The search space and results of the parameters in the gradient boosting model are shown in Table S3.

Table S3. The search space and results of parameters in the gradient boosting model.

Hyperparameters	Search space	Result

subsample	0.25, 0.5, 0.75, 1	0.25
max_depth	4, 8, 10, 12, 14, 16	8
learning_rate	0.01, 0.03, 0.05, 0.07, 0.1	0.07
n_estimators	400, 800, 1200, 1600, 2000	1600

Under the above model settings, the performance of the model is evaluated on the test set and the new training set (see Fig. S4 and Fig. S5).

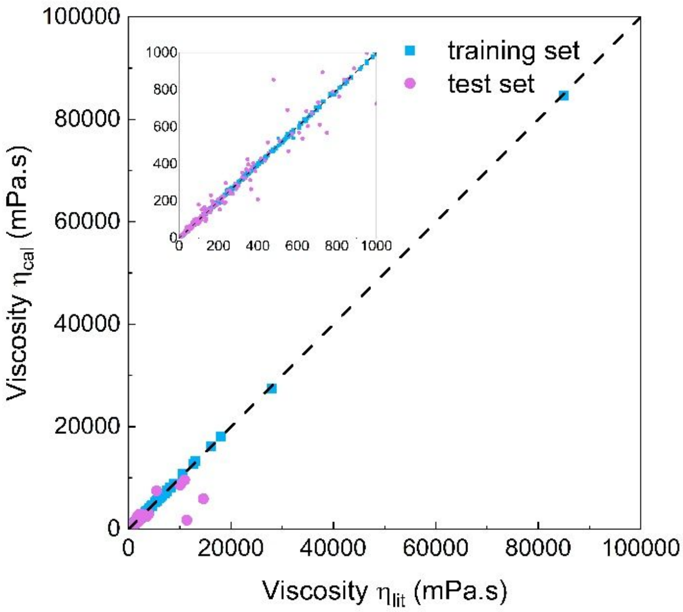


Fig. S4. Correlation between the predicted and reported viscosity values of datasets in the gradient boosting model.

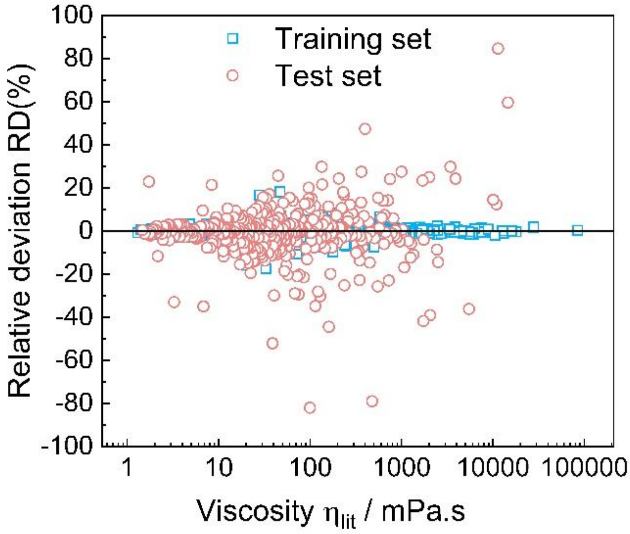


Fig. S5. Relative deviations between the literature and the predicted viscosities in both datasets in the gradient boosting model.

As shown in Fig. S4, the calculated viscosities of DESs using the gradient boosting model display a better agreement with the corresponding experimental viscosity data than the random forest model. Whereas the model gives excellent performance on the training set, some massive deviation points appear in the test set (as Fig. S5 shows). This result indicates that the model probably has an overfitting problem. Similar to the NN model, the gradient boosting model is not constrained by the equation, making it easily overfitting on the training set. Furthermore, the uneven distribution of the datasets makes it has some considerable deviation points in the region of high viscosity. Therefore, given the extensive viscosity range of DESs and the uneven distribution of viscosity data points, the gradient boosting model cannot provide a good solution.

1.4 LightGBM

With the popularity of the gradient boosting method, some new gradient boosting implementation models have been proposed (such as XGBoost, LightGBM (77)). These models improve the implementation algorithm of gradient boosting, which dramatically improves its accuracy and training speed. Among these models, whereas XGBoost has good performance on different tasks, it requires large memory and long calculation time. To address these drawbacks, LightGBM has been proposed. It has comparable performance, faster calculation, and minor memory usage than XGBoost. Furthermore, LightGBM has been widely used in many winning solutions of machine learning competitions. To explore the performance of the most advanced model on our dataset, we implement a LightGBM model to predict the viscosity of DESs as a comparison.

The LightGBM model is performed in Python 3 with the LightGBM package (https://github.com/microsoft/LightGBM). The package provides the interface in sckit-learn package, and we use this interface to implement the LightGBM model. The RandomizedSearchCV in the scikit-learn package is used to optimize the hyperparameters in the LightGBM model with default settings, except for the number of parameter settings that are sampled is set to 50. The training set and validation set are concatenated as new training set for cross-validation, and the cv score is a negative mean square error. The hyperparameters selected for optimization are subsample, max_depth, learning_rate, n_estimators, maximum tree leaves for base learners (num_leaves), frequency of subsample (subsample frequency), subsample ratio of columns when constructing each tree (colsample_bytree). The search space and results of the parameters in the LightGBM model are shown in Table S4.

Table S4. The search space and results of parameters in the LightGBM model.

Hyperparameters	Search space	Result
subsample	0.75, 0.78, 0.8, 0.82, 0.85	0.82
subsample_freq	2, 4, 6	6
colsample_bytree	0.25, 0.30, 0.35, 0.40, 0.45	0.35
max_depth	8, 10, 12, 14	10
learning_rate	0.1, 0.05, 0.01	0.1
n_estimators	1000, 2000, 3000, 4000	4000
num_leaves	5, 10, 15, 20, 25	10

There is a trade-off between learning_rate and n_estimators. To get better performance, different setups of the values of these two parameters are examined. And we find that when n_estimators = 40000 and learning_rate = 0.01, the model gets the best performance. Under the above model settings, the performance of the model is evaluated on the test set and the new training set (see Fig. S6 and Fig. S7).

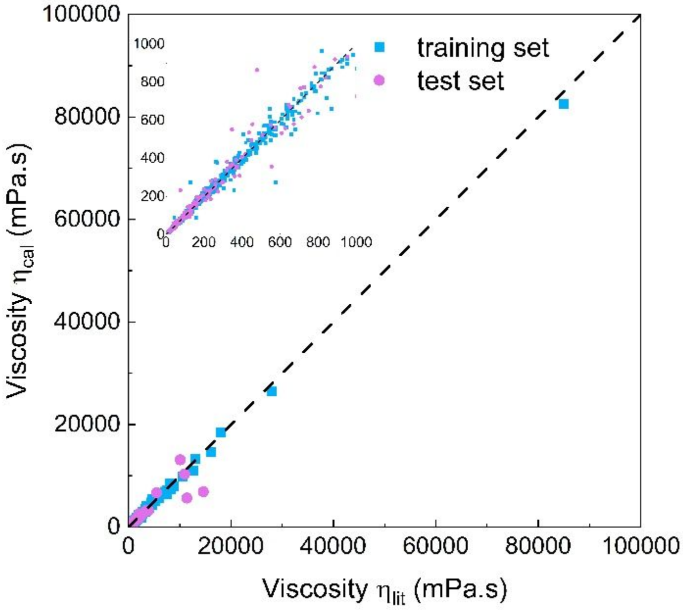


Fig. S6. Correlation between the predicted and reported viscosity values of datasets in the LightGBM model.

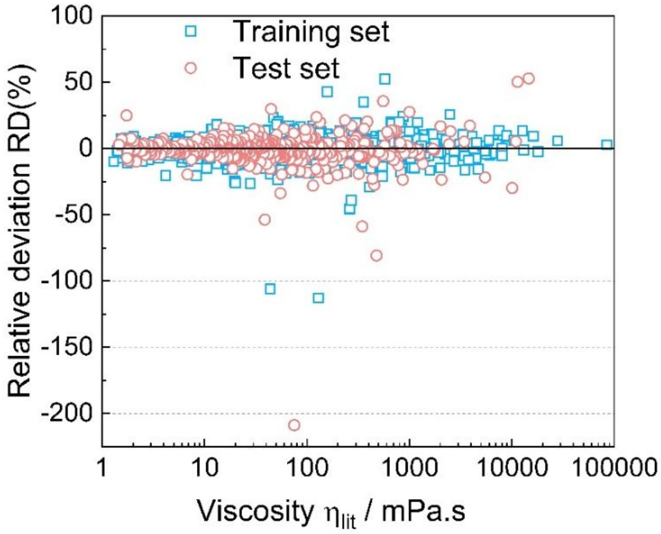


Fig. S7. Relative deviations between the literature and the predicted viscosities in both datasets in the LightGBM model.

As shown in Fig. S6, the calculated viscosities of DESs using the LightGBM model display a good agreement with the corresponding experimental viscosity data overall. However, as shown in the partial enlargement, the performance of LightGBM is highly variable and there are some big deviation points in the datasets. Fig. S7 also supports this result, and there are even some data points with the absolute value of RD greater than 100%. Although the number of big deviation points of the LightGBM model are significantly less than the gradient boosting model, the MRD of the LightGBM model is enormous (more than 200%). Therefore, the reliability of the LightGBM model is greatly reduced. And it cannot provide better performance than the TSTiNet model.

1.5 Summary

In addition to the NN model, we implement three decision tree models as comparisons with the TSTiNet model. These three decision tree models (random forest, gradient boosting and LightGBM) are very popular as machine learning methods. The performances of these three models are shown in Table S5. And the metrics we selected are AARD, MRD and R^2.

Table S5. The performance of different machine learning methods.

Model	AARD (%)	MRD (%)	R^2
Random forest	16.02	117.69	0.6308
Gradient boosting	8.30	84.66	0.7161
LightGBM	7.29	208.85	0.8353
Plain NN	5.23	82.15	0.7464
TSTiNet	6.85	49.28	0.9805

Table S5 shows that the LightGBM model has the best predictive effect among the decision tree models. Whereas the LightGBM model has a comparable AARD with the TSTiNet model, its MRD and R^2 are unacceptable. All these three models have larger AARD and MRD and lower R^2 than the TSTiNet model. And on the whole, the performances of the decision tree models are not as good as the NN model. Meanwhile, due to the poor designability of the decision tree model, it is difficult for them to combine with the equation. Therefore, the decision tree models are not as good and flexible as the neural network in predicting complex thermophysical properties.

2 Further validation of the TSTiNet model

From an industrial and application standpoint, the solvents' viscosity is one of the most critical parameters for solvent selection. The viscosity of mixtures is usually governed by the strength of intermolecular interactions between the constituents. Generally, polar solvents tend to be more viscous than similar non-polar solvents (78) (e.g., nonanoic acid>nonane). Since DESs are formed based on hydrogen bond molecular interactions, it is expected that high viscosities of these solvents would be observed as the hydrogen bonds formed between the molecules, which limit their mobility within the mixture. For instance, glycerol-based DESs such as potassium carbonate: glycerol are reported to have high viscosities in the range of 5500-28104 mPa·s at 298.15 K (79). The viscosities of DESs are relatively high compared to those of common organic solvents. Organic solvents typically have room temperature viscosities ranging from 0.2 to 10 mPa·s (80), whereas DESs display a broad range of room temperature viscosities, from 1.3 to greater than 85000 mPa·s (Supplementary data). This is of great significance as it enables an objective-oriented solvent design process.

2.1 Relationship between viscosity and temperature

The viscosity of the DESs is reported to be very sensitive to temperature (81, 82). A significant decrease in the viscosity of the DESs is observed when increasing the temperature. For the sake of a better overview, the temperature trends of the TSTiNet model to estimate the viscosities of some typical DESs are shown in Fig. S8 and Fig. S9. Because of the wide viscosity range of the investigated DESs, two figures were separately for the high and low viscosity ranges. Fig. S8 shows the viscosity-temperature behaviors of the TSTiNet model for five highly viscous DESs, while Fig. S9 focuses on four low viscosity DESs. The logarithmic decreasing trend of viscosity concerning the increasing temperature is successfully followed by the proposed model at both low and high viscosities of DESs.

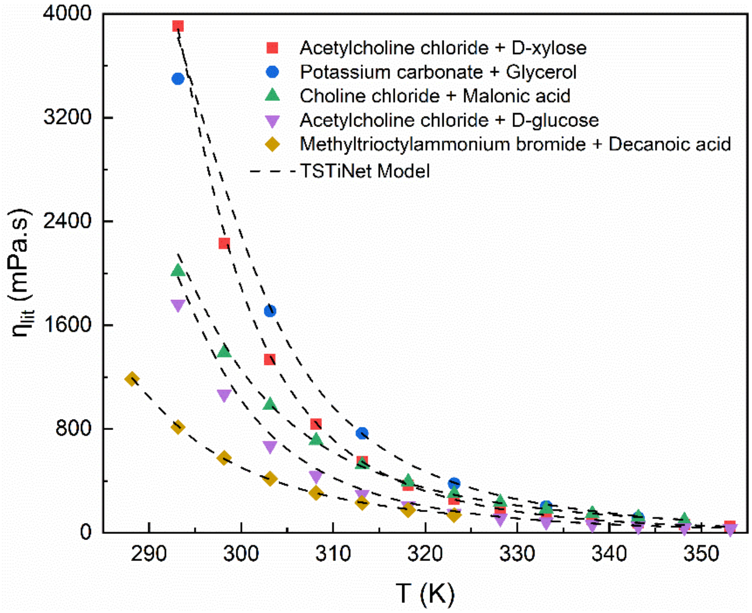


Fig. S8. Comparison between the trends of the experimental data and the proposed TSTiNet model for five randomly selected DESs in the high viscosity range. ■, Acetylcholine chloride: D-xylose (1:1); ●, Potassium carbonate: Glycerol (1:7); ▲, Choline chloride: Malonic acid (1:1); ▼, Acetylcholine chloride: D-xylose (1:1) and ◆, Methyltrioctylammonium bromide: Decanoic acid (1:2).

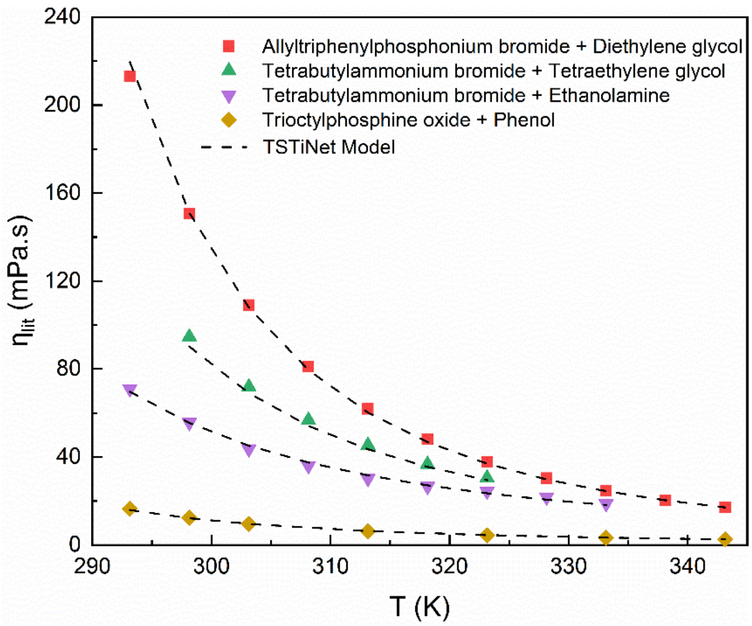


Fig. S9. Comparison between the trends of experimental data and the proposed TSTiNet model for five randomly chosen DESs in the low viscosity range. ■ , Allyltriphenylphosphonium bromide: Diethylene glycol (1:4); ▲ , Tetrabutylammonium bromide: Tetraethylene glycol (1:4); ▼, Tetrabutylammonium bromide: Ethanolamine (1:6) and ◆, Trioctylphosphine oxide: Phenol (1:2)

2.2 Relationship between viscosity and molar fraction

The effect of the molar fraction on viscosity is highly dependent on the intermolecular interactions among DES components. Fig. S10 shows the impact of changing the molar ratio of DES components on its viscosity. Five different molar ratios (1: 2, 1: 3, 1: 4, 1: 5, 1: 6) of DES composed of choline chloride and ethylene glycol are discussed. As shown in Fig. S10, the viscosity decreases along with increasing the ethylene glycol molar fraction. Increasing the number and strength of hydrogen bonds in the associative mixture will increase viscosity. Therefore, stronger bonds in the mixture lead to the more significant bonded molecules' resistance to moving next to each other. Fig. S10 demonstrates that in the studied DES, choline chloride: ethylene glycol with a ratio of 1:2 may have the most considerable hydrogen bond association strength. As the proportion of ethylene glycol increases, the change in viscosity behavior to temperature tends to be flat. Still, it can be seen that the proposed TSTiNet model can reasonably estimate all the discussed trends and changes in viscosity behavior.

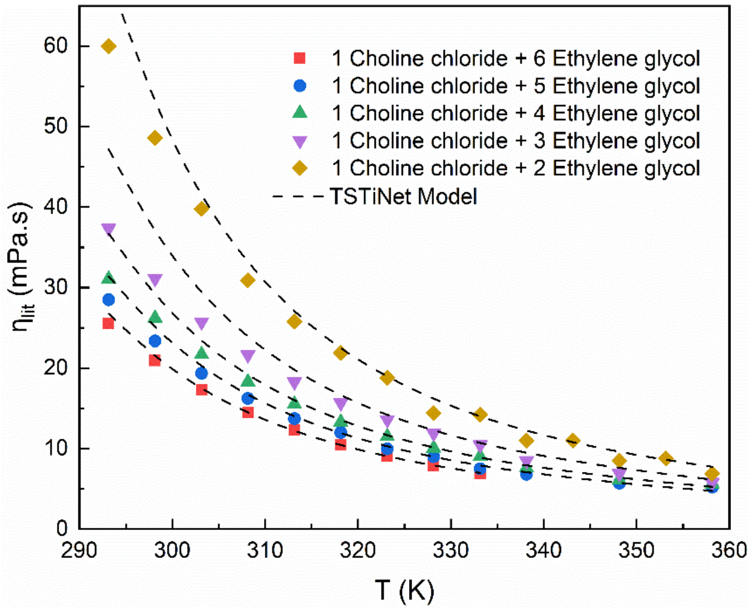


Fig. S10. Comparison of the viscosity behavior of choline chloride (HBA) with different ethylene glycol (HBD) ratios. ■, Choline chloride: Ethylene glycol (1:6); ●, Choline chloride: Ethylene glycol (1:5); ▲, Choline chloride: Ethylene glycol (1:4); ▼, Choline chloride: Ethylene glycol (1:3) and ◆, Choline chloride: Ethylene glycol (1:2).

2.3 Relationship between viscosity and types of HBA and HBD

It is known that the viscosity of DESs varies widely depending on the type of HBA and HBD. To study the proposed model's predictive ability more comprehensively, the influence of the component types of DESs on the viscosity is studied in Fig. S11 and Fig. S12. It can be seen that the model gives a reliable consistency between the experimental value and the estimated viscosity of DESs. Fig. S11 shows the effect of changing the HBD molecular type of a fixed HBA on the viscosity of DESs. In this figure, the choline chloride's viscosity-temperature behavior as HBA is compared, and four different HBDs, i.e., ethylene glycol, phenol, levulinic acid and urea, are compared. The molar ratio of HBA and HBD is 1: 2. As we know, the intermolecular interaction is the dominant force in the viscosity of a mixture. Therefore, the size of HBD, the number of hydrogen bonds between HBD and HBA, and the strength of hydrogen bonds are significant factors that should be considered when studying the viscosity behavior. It can be seen that the changing trend of viscosity is urea>levulinic acid>phenol>ethylene glycol. Fig. S12 shows the effect of changing the HBA molecule type of the fixed HBD on the viscosity of DESs. In this figure, the viscosity-temperature behavior of decanoic acid as HBD is compared, and three different HBAs, i.e., lidocaine, tetraoctylammonium chloride, and tetraoctylammonium bromide, are compared. The molar ratio of HBA to HBD is 1:2. It can be seen that the changing trend of viscosity is tetraoctylammonium bromide> tetraoctylammonium chloride> lidocaine. For the same cation and HBD, it is observed that the viscosity of bromide anion is higher than that of chloride anion (e.g., tetraoctylammonium bromide> tetraoctylammonium chloride). These trends are also consistent with the trends observed in the viscosity of ILs (82).

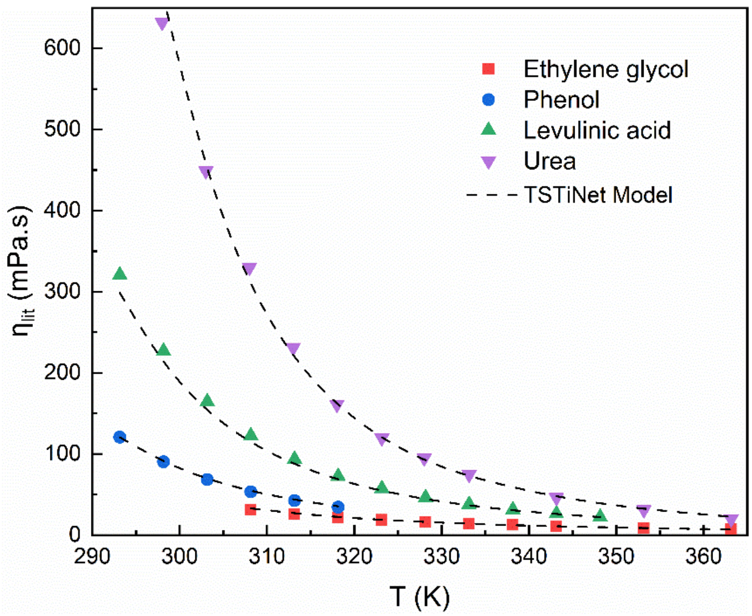


Fig. S11. Comparison of the viscosity behavior of choline chloride(HBA) with the different HBDs. ■, Choline chloride: Ethylene glycol (1:2); ●, Choline chloride: Phenol (1:2); ▲, Choline chloride: Levulinic acid (1:2) and ▼, Choline chloride: Urea (1:2).

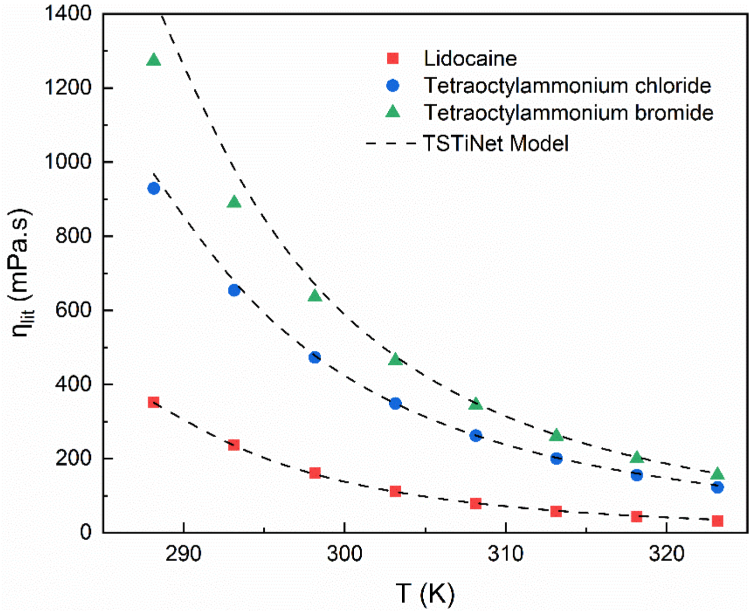


Fig. S12. Comparison of the viscosity behavior of decanoic acid (HBD) with the different HBAs. ■, Lidocaine: Decanoic acid(1:2); ●, Tetraoctylammonium chloride: Decanoic acid (1:2) and ▲, Tetraoctylammonium bromide: Decanoic acid (1:2).

3 Comparison with models reported by different research groups

Since the model proposed by Bakhtyari et al. is a global viscosity model covering extensive database, a detailed deviation comparison has been conducted.

Table S6. Comparison of the individual RD% values for DES by the TSTiNet model and the Bakhtyari et al. model.

HBA	HBD	HBA:HBD mole ratio	T	η_m^{lit}/ mPa·s	ARD%[a]	RD%[b]
Acetylcholine chloride	1,2,4-triazole	1:1	303.15	304.69	6.83	η_{ref}
			313.15	153.71	5.05	4.55
			323.15	83.06	9.56	11.54
			333.15	46.48	7.66	23.26
			343.15	27.73	4.10	35.19
			363.15	14.51	15.77	26.21
			373.15	8.37	5.99	61.10
Acetylcholine chloride/1,2,4-triazole				AARD%	7.85	26.98
Acetylcholine chloride	Imidazole	1:1.5	303.15	233.69	0.41	η_{ref}
			313.15	120.91	8.16	7.09
			323.15	59.05	1.22	31.42
			333.15	35.29	0.51	40.32
			343.15	18.67	21.60	78.11
			353.15	16.53	6.66	40.93
			363.15	11.69	5.88	44.64
Acetylcholine chloride	Imidazole	1:2	303.15	103.33	4.30	η_{ref}
			313.15	52.18	1.52	16.52
			323.15	31.63	11.98	20.89
			333.15	21.49	22.69	18.12
			343.15	11.37	6.02	54.94
			353.15	6.84	6.62	85.53
			363.15	4.17	25.21	126.23
Acetylcholine chloride	Imidazole	1:3	303.15	335.98	16.36	η_{ref}
			313.15	189.19	2.77	5.01
			323.15	98.80	0.26	5.91
			333.15	57.92	0.54	12.50
			343.15	35.77	3.82	19.82

			353.15	25.74	2.27	14.57
			363.15	17.68	1.18	19.18
Acetylcholine chloride/Imidazole				AARD%	7.14	35.65
Betaine	DL-Lactic acid	1:2	298.15	1266.00	3.75	η_{ref}
			303.15	818.60	5.04	1.79
			308.15	544.60	4.77	4.38
			313.15	374.60	4.03	6.78
			318.15	260.50	1.13	10.99
			323.15	190.20	0.17	12.52
			328.15	141.60	1.34	14.23
			333.15	107.50	3.13	15.86
			338.15	83.70	4.33	16.50
			343.15	65.90	6.18	17.60
Betaine	DL-Lactic acid	1:5	293.15	386.60	3.44	7.73
			298.15	245.30	1.12	η_{ref}
			303.15	167.70	1.64	3.67
			308.15	120.40	3.17	5.07
			313.15	86.10	1.10	9.40
			318.15	65.50	2.30	9.30
			323.15	50.60	2.60	9.50
			328.15	39.60	2.07	10.07
			333.15	31.10	0.01	11.89
			338.15	25.10	1.01	12.15
			343.15	20.60	1.85	11.89
Betaine/DL-Lactic acid				AARD%	2.58	10.07
Choline chloride	1,2-Butanediol	1:19	295.15	55.00	2.59	16.66
			297.15	48.00	1.59	13.75
			299.15	41.00	8.71	8.55
			301.15	34.00	10.33	0.14
			303.15	31.00	9.25	η_{ref}
			305.15	26.00	0.18	8.82
			307.15	22.00	9.96	17.66
			309.15	19.00	18.59	24.93
			311.15	17.00	23.80	28.31
Choline chloride	1,2-Butanediol	1:4	295.15	70.00	9.43	12.63
			297.15	62.00	8.01	11.12
			299.15	55.00	6.27	9.46
			301.15	48.00	2.51	5.99

			303.15	41.00	4.04	η_{ref}
			305.15	36.00	8.41	3.75
			307.15	31.00	3.30	10.02
			309.15	29.00	4.38	7.65
			311.15	26.00	1.04	10.15
Choline chloride	1,2-Butanediol	1:5.67	295.15	60.00	9.87	10.96
			297.15	53.00	7.78	9.05
			299.15	48.00	7.56	9.14
			301.15	38.00	6.45	4.14
			303.15	36.00	2.84	η_{ref}
			305.15	29.00	17.27	13.21
			307.15	26.00	3.93	15.44
			309.15	22.00	5.44	25.01
			311.15	19.00	13.70	32.93
Choline chloride	1,2-Butanediol	1:9	295.15	53.00	13.10	13.74
			297.15	45.00	7.06	8.18
			299.15	41.00	6.98	8.67
			301.15	36.00	3.01	5.48
			303.15	31.00	3.51	η_{ref}
			305.15	26.00	13.82	8.89
			307.15	22.00	24.45	17.80
			309.15	19.00	1.76	25.15
			311.15	17.00	6.31	28.60
Choline chloride/1,2-Butanediol				AARD%	7.98	13.31

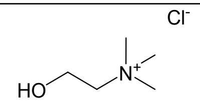
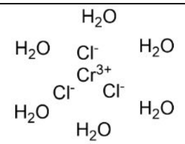
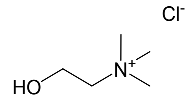
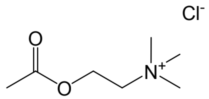
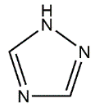
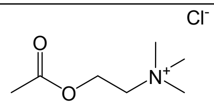
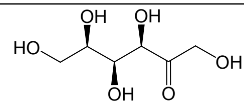
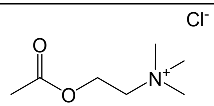
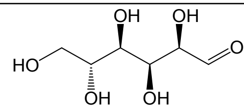
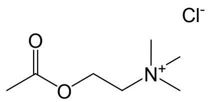
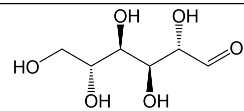
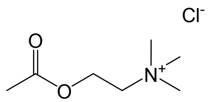
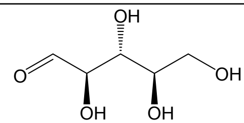
[a]the TSTiNet model; [b]the Bakhtyari et al. model.

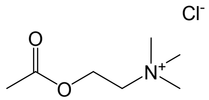
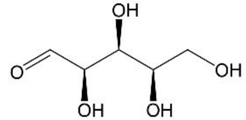
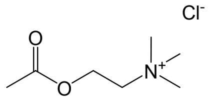
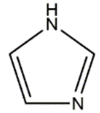
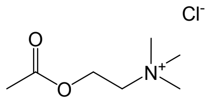
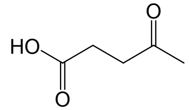
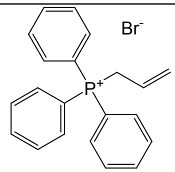
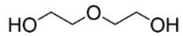
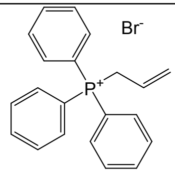
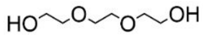
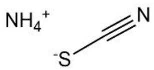
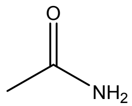
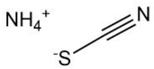
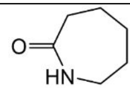
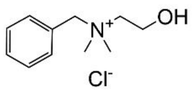
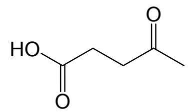
Table S7. Comparison of the individual AARD% values for DES by the TSTiNet model, the Bakhtyari et al. model, the Lewis and Squires model, the Haghbakhsh and Raeissi model, and the Dutt et al. model.

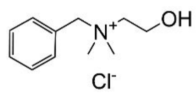
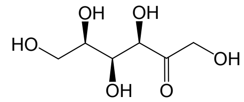
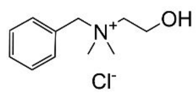
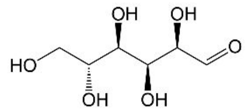
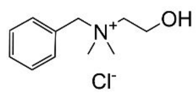
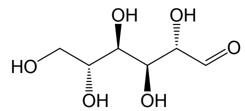
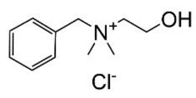
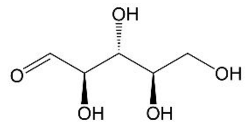
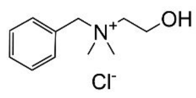
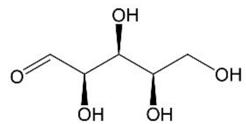
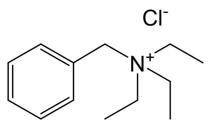
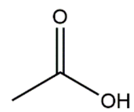
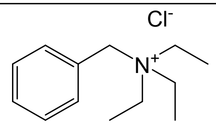
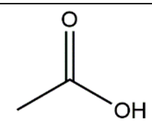
DES	AARD%				
	TSTiNet model	Bakhtyari et al. model	Lewis and Squires model	Haghbakhsh and Raeissi model	Dutt et al. model
Acetylcholine chloride/1,2,4-triazole	7.85	26.98	248.40	5.10	53.10

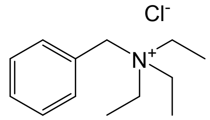
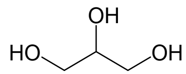
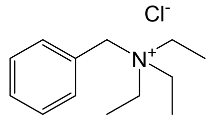
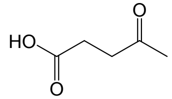
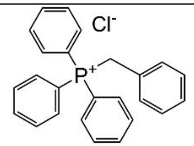
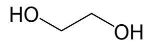
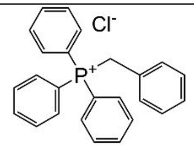
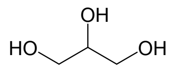
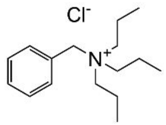
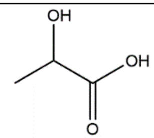
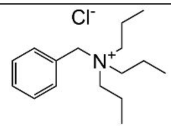
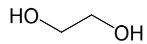
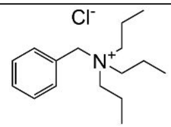
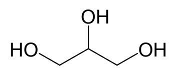
Acetylcholine chloride/Imidazole	7.14	35.65	235.73	12.40	40.77
Betaine/DL-Lactic acid	2.58	10.07	298.95	23.95	75.60
Choline chloride/1,2-Butanediol	7.98	13.31	32.05	11.68	12.40

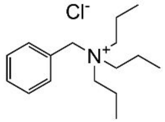
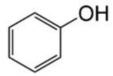
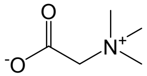
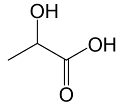
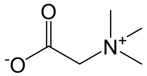
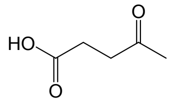
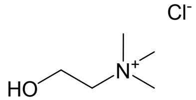
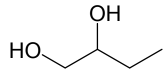
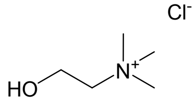
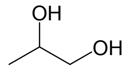
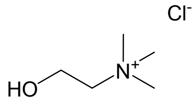
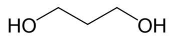
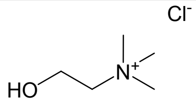
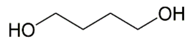
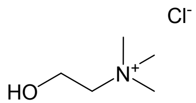
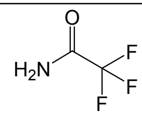
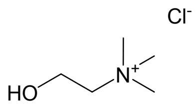
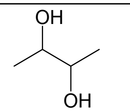
4 Chemical structure dataset for DESs

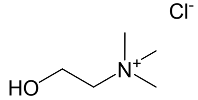
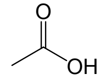
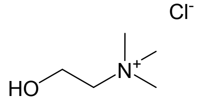
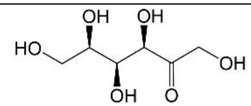
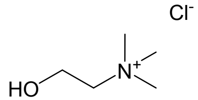
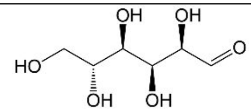
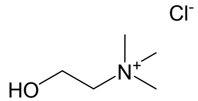
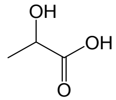
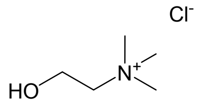
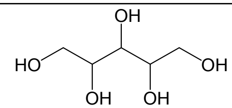
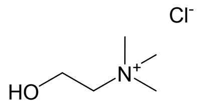
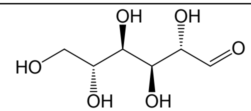
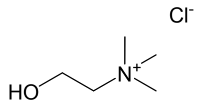
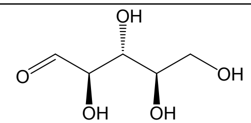
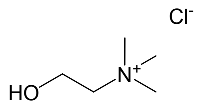
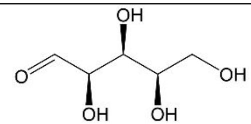
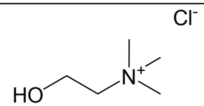
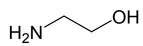
NO.	HBA	CAS register number	Molecular formula	Molecular Structure	Molecular Weight	HBD	CAS register number	Molecular formula	Molecular Structure	Molecular Weight
1	Zinc chloride	7646-85-7	$ZnCl_2$	Cl^- Zn^{2+} Cl^-	136.3	Choline chloride	67-48-1	$C_5H_{14}ClNO$		139.62
2	Chromic chloride hexahydrate	10060-12-5	$Cl_3CrH_{12}O_6$		266.45	Choline chloride	67-48-1	$C_5H_{14}ClNO$		139.62
3	Acetylcholine chloride	60-31-1	$C_7H_{16}ClNO_2$		181.66	1,2,4-Triazole	288-88-0	$C_2H_3N_3$		69.07
4	Acetylcholine chloride	60-31-1	$C_7H_{16}ClNO_2$		181.66	D-fructose	57-48-7	$C_6H_{12}O_6$		180.16
5	Acetylcholine chloride	60-31-1	$C_7H_{16}ClNO_2$		181.66	D-glucose	50-99-7	$C_6H_{12}O_6$		180.16
6	Acetylcholine chloride	60-31-1	$C_7H_{16}ClNO_2$		181.66	D-mannose	3458-28-4	$C_6H_{12}O_6$		180.16
7	Acetylcholine chloride	60-31-1	$C_7H_{16}ClNO_2$		181.66	D-ribose	50-69-1	$C_5H_{10}O_5$		150.13 (569)

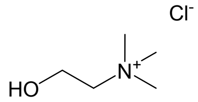
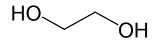
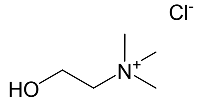
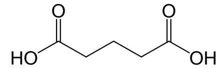
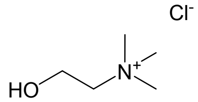
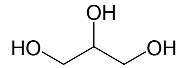
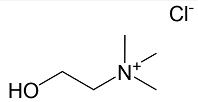
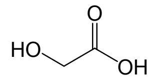
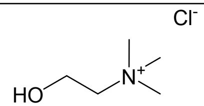
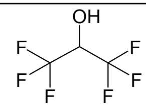
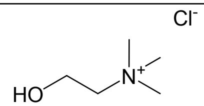
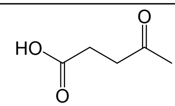
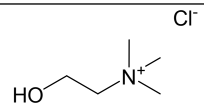
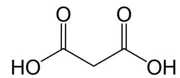
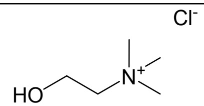
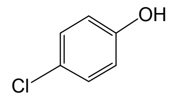
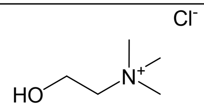
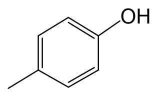
8	Acetylcholine chloride	60-31-1	$C_7H_{16}ClNO_2$		181.66	D-xylose	31178-70-8	$C_5H_{10}O_5$		150.13
9	Acetylcholine chloride	60-31-1	$C_7H_{16}ClNO_2$		181.66	Imidazole	288-32-4	$C_3H_4N_2$		68.08
10	Acetylcholine chloride	60-31-1	$C_7H_{16}ClNO_2$		181.66	Levulinic acid	123-76-2	$C_5H_8O_3$		116.11
11	Allyltriphenyl-phosphonium bromide	1560-54-9	$C_{21}H_{20}BrP$		383.26	Diethylene glycol	111-46-6	$C_4H_{10}O_3$		106.12
12	Allyltriphenylphos phonium bromide	1560-54-9	$C_{21}H_{20}BrP$		383.26	Triethylene glycol	112-27-6	$C_6H_{14}O_4$		150.17
13	Ammonium thiocyanate	1762-95-4	NH_4SCN		76.12	Acetamide	60-35-5	C_2H_5NO		59.07
14	Ammonium thiocyanate	1762-95-4	NH_4SCN		76.12	Caprolactam	105-60-2	$C_6H_{11}NO$		113.16
15	Benzyldimethyl(2-hydroxyethyl) ammonium chloride	7221-40-1	$C_{11}H_{18}ClNO$		215.72	Levulinic acid	123-76-2	$C_5H_8O_3$		116.11

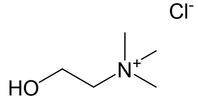
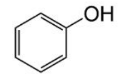
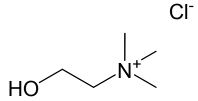
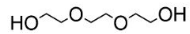
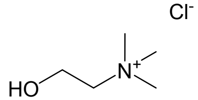
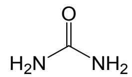
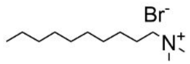
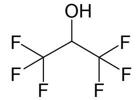
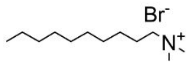
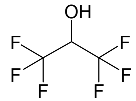
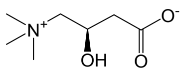
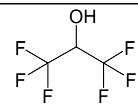
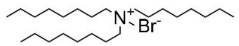
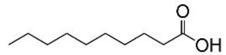
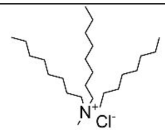
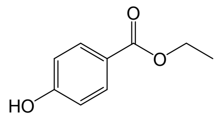
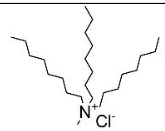
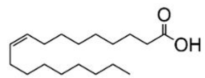
16	Benzyldimethyl(2-hydroxyethyl) ammonium chloride	7221-40-1	$C_{11}H_{18}ClNO$		215.72	D-fructose	57-48-7	$C_6H_{12}O_6$		180.16
17	Benzyldimethyl(2-hydroxyethyl) ammonium chloride	7221-40-1	$C_{11}H_{18}ClNO$		215.72	D-glucose	50-99-7	$C_6H_{12}O_6$		180.16
18	Benzyldimethyl(2-hydroxyethyl) ammonium chloride	7221-40-1	$C_{11}H_{18}ClNO$		215.72	D-mannose	3458-28-4	$C_6H_{12}O_6$		180.16
19	Benzyldimethyl(2-hydroxyethyl) ammonium chloride	7221-40-1	$C_{11}H_{18}ClNO$		215.72	D-ribose	50-69-1	$C_5H_{10}O_5$		150.13
20	Benzyldimethyl(2-hydroxyethyl) ammonium chloride	7221-40-1	$C_{11}H_{18}ClNO$		215.72	D-xylose	31178-70-8	$C_5H_{10}O_5$		150.13
21	Benzyltriethyl-ammonium chloride	56-37-1	$C_{13}H_{22}ClN$		227.77	Acetic acid	64-19-7	CH_3COOH		60.05
22	Benzyltrimethylammonium chloride	56-93-9,	$C_{10}H_{16}ClN$		185.69	Acetic acid	64-19-7	CH_3COOH		60.05

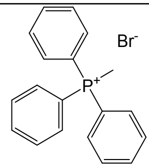
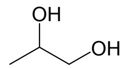
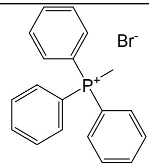
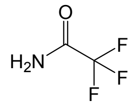
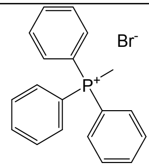
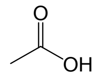
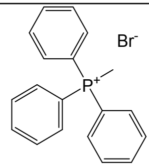
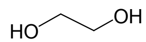
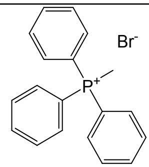
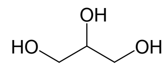
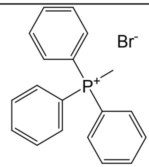
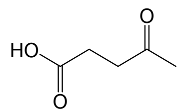
23	Benzyltrimethylammonium chloride	56-93-9,	$C_{10}H_{16}ClN$		185.69	Glycerol	56-81-5	$C_3H_8O_3$		92.09
24	Benzyltrimethylammonium chloride	56-93-9,	$C_{10}H_{16}ClN$		185.69	Levulinic acid	123-76-2	$C_5H_8O_3$		116.11
25	Benzyltriphenylphosphonium chloride	1100-88-5	$C_{25}H_{22}ClP$		388.87	Ethylene glycol	107-21-1	$C_2H_6O_2$		62.07
26	Benzyltriphenylphosphonium chloride	1100-88-5	$C_{25}H_{22}ClP$		388.87	Glycerol	56-81-5	$C_3H_8O_3$		92.09
27	Benzyltripropylammonium chloride	5197-87-5	$C_{16}H_{28}ClN$		269.85	DL-Lactic acid	598-82-3	$C_3H_6O_3$		90.08
28	Benzyltripropylammonium chloride	5197-87-5	$C_{16}H_{28}ClN$		269.85	Ethylene glycol	107-21-1	$C_2H_6O_2$		62.07
29	Benzyltripropylammonium chloride	5197-87-5	$C_{16}H_{28}ClN$		269.85	Glycerol	56-81-5	$C_3H_8O_3$		92.09

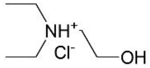
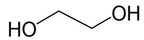
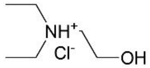
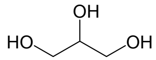
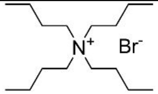
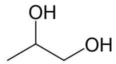
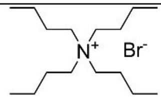
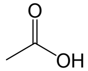
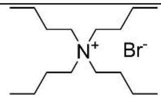
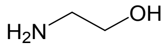
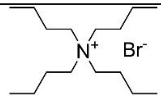
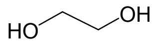
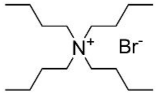
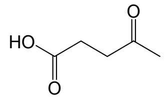
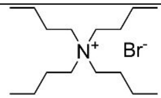
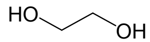
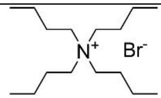
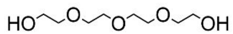
30	Benzyltripropylammonium chloride	5197-87-5	$C_{16}H_{28}ClN$		269.85	Phenol	108-95-2	C_6H_6O		94.11
31	Betaine	107-43-7	$C_5H_{11}NO_2$		117.15	DL-lactic acid	598-82-3	$C_3H_6O_3$		90.08
32	Betaine	107-43-7	$C_5H_{11}NO_2$		117.15	Levulinic acid	123-76-2	$C_5H_8O_3$		116.11
33	Choline chloride	. 67-48-1	$C_5H_{14}ClNO$		139.62	1,2-Butanediol	584-03-2	$C_4H_{10}O_2$		90.12
34	Choline chloride	. 67-48-1	$C_5H_{14}ClNO$		139.62	1,2-Propanediol	57-55-6	$C_3H_8O_2$		76.09
35	Choline chloride	. 67-48-1	$C_5H_{14}ClNO$		139.62	1,3-Propanediol	504-63-2	$C_3H_8O_2$		76.09
36	Choline chloride	. 67-48-1.	$C_5H_{14}ClNO$		139.62	1,4-Butanediol	110-63-4	$C_4H_{10}O_2$		90.12
37	Choline chloride	. 67-48-1	$C_5H_{14}ClNO$		139.62	2,2,2-Trifluoroacetamide	354-38-1	$C_2H_2F_3NO$		113.04
38	Choline chloride	. 67-48-1	$C_5H_{14}ClNO$		139.62	2,3-Butanediol	513-85-9	$C_4H_{10}O_2$		90.12

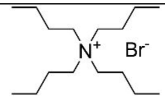
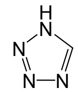
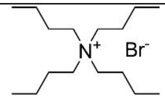
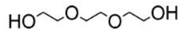
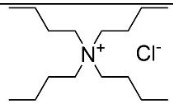
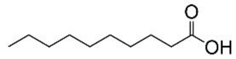
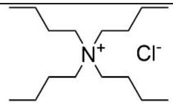
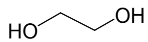
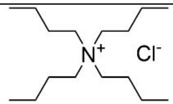
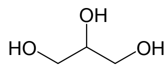
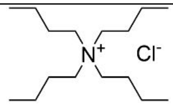
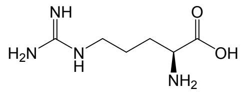
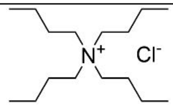
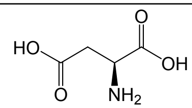
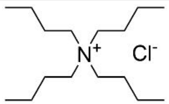
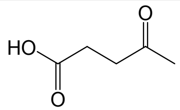
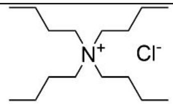
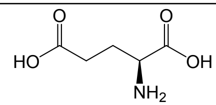
39	Choline chloride	. 67-48-1.	$C_5H_{14}ClNO$		139.62	Acetic acid	64-19-7	CH_3COOH		60.05
40	Choline chloride	. 67-48-1.	$C_5H_{14}ClNO$		139.62	D-fructose	57-48-7	$C_6H_{12}O_6$		180.16
41	Choline chloride	. 67-48-1	$C_5H_{14}ClNO$		139.62	D-glucose	50-99-7	$C_6H_{12}O_6$		180.16
42	Choline chloride	. 67-48-1.	$C_5H_{14}ClNO$		139.62	DL-lactic acid	598-82-3	$C_3H_6O_3$		90.08
43	Choline chloride	. 67-48-1	$C_5H_{14}ClNO$		139.62	DL-Xylitol	87-99-0	$C_5H_{12}O_5$		152.15
44	Choline chloride	. 67-48-1	$C_5H_{14}ClNO$		139.62	D-mannose	3458-28-4	$C_6H_{12}O_6$		180.16
45	Choline chloride	. 67-48-1	$C_5H_{14}ClNO$		139.62	D-ribose	50-69-1	$C_5H_{10}O_5$		150.13
46	Choline chloride	. 67-48-1	$C_5H_{14}ClNO$		139.62	D-xylose	31178-70-8	$C_5H_{10}O_5$		150.13
47	Choline chloride	. 67-48-1	$C_5H_{14}ClNO$		139.62	Ethanolamine	141-43-5	C_2H_7NO		61.08

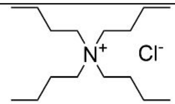
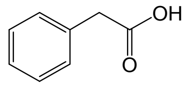
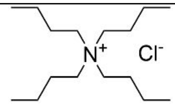
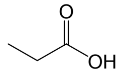
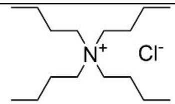
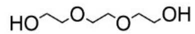
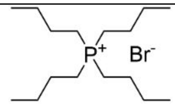
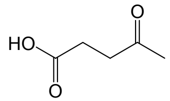
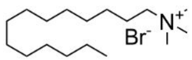
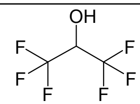
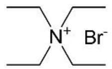
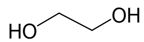
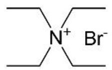
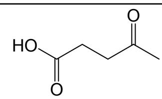
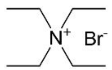
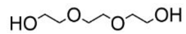
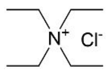
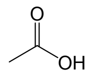
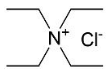
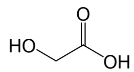
48	Choline chloride	. 67-48-1	$C_5H_{14}ClNO$		139.62	Ethylene glycol	107-21-1	$C_2H_6O_2$		62.07
49	Choline chloride	. 67-48-1	$C_5H_{14}ClNO$		139.62	Glutaric acid	110-94-1	$C_5H_8O_4$		132.11
50	Choline chloride	. 67-48-1.	$C_5H_{14}ClNO$		139.62	Glycerol	56-81-5	$C_3H_8O_3$		92.09
51	Choline chloride	. 67-48-1	$C_5H_{14}ClNO$		139.62	Glycolic acid	79-14-1	$C_2H_4O_3$		76.05
52	Choline chloride	. 67-48-1	$C_5H_{14}ClNO$		139.62	Hexafluoroisopropanol	920-66-1	$C_3H_2F_6O$		168.04
53	Choline chloride	. 67-48-1.	$C_5H_{14}ClNO$		139.62	Levulinic acid	123-76-2	$C_5H_8O_3$		116.11
54	Choline chloride	. 67-48-1	$C_5H_{14}ClNO$		139.62	Malonic acid	141-82-2	$C_3H_4O_4$		104.06
55	Choline chloride	. 67-48-1	$C_5H_{14}ClNO$		139.62	P-chlorophenol	106-48-9	C_6H_5ClO		128.56
56	Choline chloride	. 67-48-1	$C_5H_{14}ClNO$		139.62	P-cresol	106-44-5	C_7H_8O		108.14

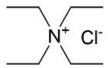
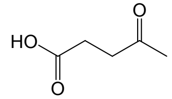
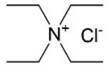
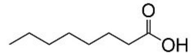
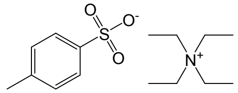
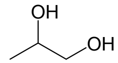
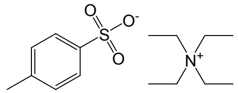
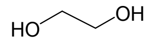
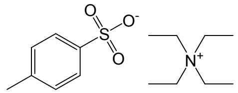
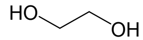
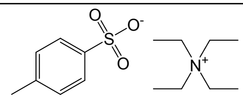
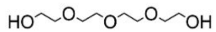
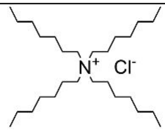
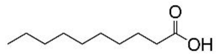
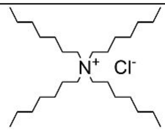
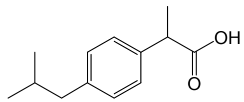
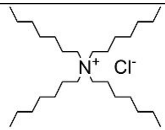
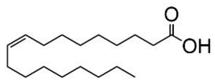
57	Choline chloride	. 67-48-1	$C_5H_{14}ClNO$		139.62	Phenol	108-95-2	C_6H_6O		94.11
58	Choline chloride	. 67-48-1	$C_5H_{14}ClNO$		139.62	Triethylene glycol	112-27-6	$C_6H_{14}O_4$		150.17
59	Choline chloride	. 67-48-1	$C_5H_{14}ClNO$		139.62	Urea	57-13-6	CH_4N_2O		60.06
60	Decyltrimethylammonium bromide	2082-84-0	$C_{13}H_{30}BrN$		280.29	Hexafluoroisopropanol	920-66-1	$C_3H_2F_6O$		168.04
61	Dodecyltrimethylammonium bromide	1119-94-4	$C_{15}H_{34}BrN$		308.34	Hexafluoroisopropanol	920-66-1	$C_3H_2F_6O$		168.04
62	L-carnitine	541-15-1	$C_7H_{15}NO_3$		161.20	Hexafluoroisopropanol	920-66-1	$C_3H_2F_6O$		168.04
63	Methyltrioctylammonium bromide	35675-80-0	$C_{25}H_{54}BrN$		448.61	Decanoic acid	334-48-5	$C_{10}H_{20}O_2$		172.26
64	Methyltrioctylammonium chloride	5137-55-3	$C_{25}H_{54}ClN$		404.16	Ethylparaben	120-47-8	$C_9H_{10}O_3$		166.17
65	Methyltrioctylammonium chloride	5137-55-3	$C_{25}H_{54}ClN$		404.16	Oleic acid	112-80-1	$C_{18}H_{34}O_2$		282.46

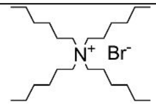
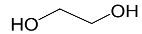
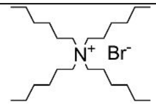
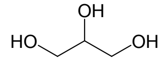
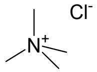
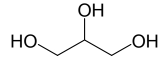
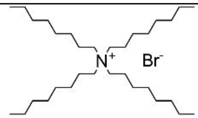
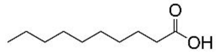
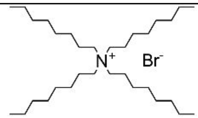
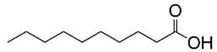
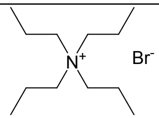
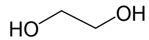
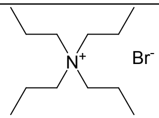
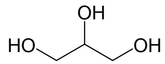
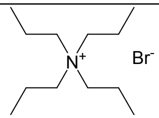
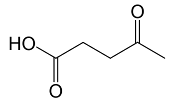
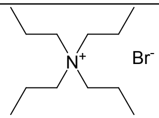
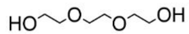
66	Methyltriphenylphosphonium bromide	1779-49-3	$C_{19}H_{18}BrP$		357.22	1,2-Propanediol	57-55-6	$C_3H_8O_2$		76.09
67	Methyltriphenylphosphonium bromide	1779-49-3	$C_{19}H_{18}BrP$		357.22	2,2,2-Trifluoroacetamide	354-38-1	C2H2F3NO		113.04
68	Methyltriphenylphosphonium bromide	1779-49-3	$C_{19}H_{18}BrP$		357.22	Acetic acid	64-19-7	CH_3COOH		60.05
69	Methyltriphenylphosphonium bromide	1779-49-3	$C_{19}H_{18}BrP$		357.22	Ethylene glycol	107-21-1	$C_2H_6O_2$		62.07
70	Methyltriphenylphosphonium bromide	1779-49-3	$C_{19}H_{18}BrP$		357.22	Glycerol	56-81-5	$C_3H_8O_3$		92.09
71	Methyltriphenylphosphonium bromide	1779-49-3	$C_{19}H_{18}BrP$		357.22	Levulinic acid	123-76-2	$C_5H_8O_3$		116.11

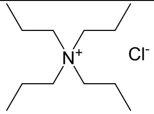
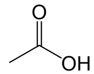
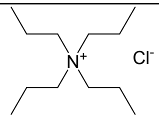
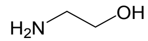
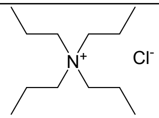
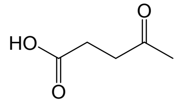
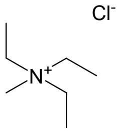
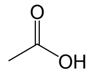
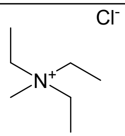
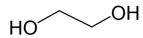
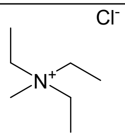
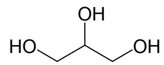
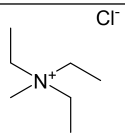
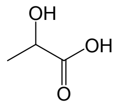
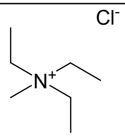
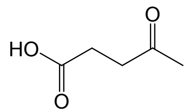
72	N,N-diethylethanol-ammonium chloride	13989-32-7	$C_6H_{16}ClNO$		153.65	Ethylene glycol	107-21-1	$C_2H_6O_2$		62.07
73	N,N-diethylethanol-ammonium chloride	13989-32-7	$C_6H_{16}ClNO$		153.65	Glycerol	56-81-5	$C_3H_8O_3$		92.09
74	Tetrabutyl-ammonium bromide	1643-19-2	$C_{16}H_{36}BrN$		322.37	1,2-Propanediol	57-55-6	$C_3H_8O_2$		76.09
75	Tetrabutyl-ammonium bromide	1643-19-2	$C_{16}H_{36}BrN$		322.37	Acetic acid	64-19-7	CH_3COOH		60.05
76	Tetrabutyl-ammonium bromide	1643-19-2	$C_{16}H_{36}BrN$		322.37	Ethanolamine	141-43-5	C_2H_7NO		61.08
77	Tetrabutyl-ammonium bromide	1643-19-2	$C_{16}H_{36}BrN$		322.37	Ethylene glycol	107-21-1	$C_2H_6O_2$		62.07
78	Tetrabutyl-ammonium bromide	1643-19-2	$C_{16}H_{36}BrN$		322.37	Levulinic acid	123-76-2	$C_5H_8O_3$		116.11
79	Tetrabutyl-ammonium bromide	1643-19-2	$C_{16}H_{36}BrN$		322.37	Polyethylene glycol	25322-68-3	$C_{2n}H_{4n+2}O_{n+1}$		697.61
80	Tetrabutyl-ammonium bromide	1643-19-2	$C_{16}H_{36}BrN$		322.37	Tetraethylene glycol	112-60-7	$C_8H_{18}O_5$		194.23

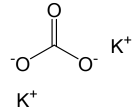
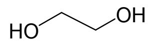
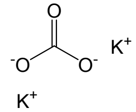
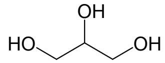
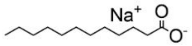
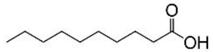
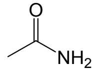
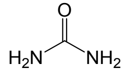
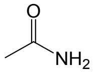
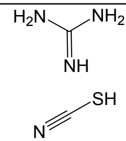
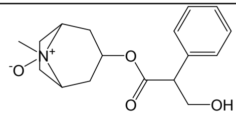
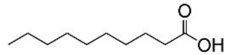
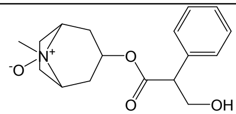
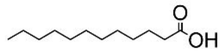
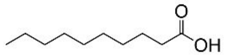
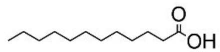
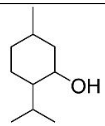
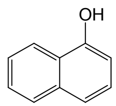
81	Tetrabutyl-ammonium bromide	1643-19-2	$C_{16}H_{36}BrN$		322.37	Tetrazole	288-94-8	CH_2N_4		70.05
82	Tetrabutyl-ammonium bromide	1643-19-2	$C_{16}H_{36}BrN$		322.37	Triethylene glycol	112-27-6	$C_6H_{14}O_4$		150.17
83	Tetrabutylammonium chloride	1112-67-0	$C_{16}H_{36}ClN$		277.92	Decanoic acid	334-48-5	$C_{10}H_{20}O_2$		172.26
84	Tetrabutyl-ammonium chloride	1112-67-0	$C_{16}H_{36}ClN$		277.92	Ethylene glycol	107-21-1	$C_2H_6O_2$		62.07
85	Tetrabutyl-ammonium chloride	1112-67-0	$C_{16}H_{36}ClN$		277.92	Glycerol	56-81-5	$C_3H_8O_3$		92.09
86	Tetrabutyl-ammonium chloride	1112-67-0	$C_{16}H_{36}ClN$		277.92	L-arginine	74-79-3	$C_6H_{14}N_4O_2$		174.20
87	Tetrabutyl-ammonium chloride	1112-67-0	$C_{16}H_{36}ClN$		277.92	L-aspartic acid	56-84-8	$C_4H_7NO_4$		133.10
88	Tetrabutyl-ammonium chloride	1112-67-0	$C_{16}H_{36}ClN$		277.92	Levulinic acid	123-76-2	$C_5H_8O_3$		116.11
89	Tetrabutyl-ammonium chloride	1112-67-0	$C_{16}H_{36}ClN$		277.92	L-glutamic acid	56-86-0	$C_5H_9NO_4$		147.13

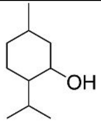
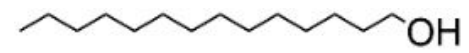
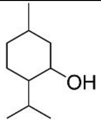
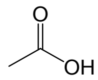
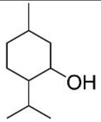
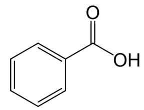
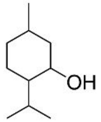
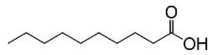
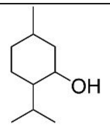
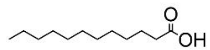
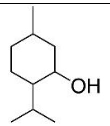
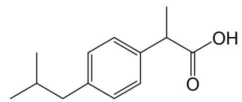
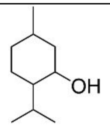
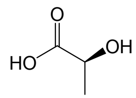
90	Tetrabutyl-ammonium chloride	1112-67-0	$C_{16}H_{36}ClN$		277.92	Phenylacetic acid	103-82-2	$C_8H_8O_2$		136.15
91	Tetrabutyl-ammonium chloride	1112-67-0	$C_{16}H_{36}ClN$		277.92	Propionic acid	79-09-4	$C_3H_6O_2$		74.08
92	Tetrabutyl-ammonium chloride	1112-67-0	$C_{16}H_{36}ClN$		277.92	Triethylene glycol	112-27-6	$C_6H_{14}O_4$		150.17
93	Tetrabutyl-phosphonium bromide	3115-68-2	$C_{16}H_{36}BrP$		339.33	Levulinic acid	123-76-2	$C_5H_8O_3$		116.11
94	Tetradecyl-trimethylammonium bromide	1119-97-7	$C_{17}H_{38}BrN$		336.39	Hexafluoroisopropanol	920-66-1	$C_3H_2F_6O$		168.04
95	Tetraethyl-ammonium bromide	71-91-0	$C_8H_{20}NBr$		210.16	Ethylene glycol	107-21-1	$C_2H_6O_2$		62.07
96	Tetraethyl-ammonium bromide	71-91-0	$C_8H_{20}NBr$		210.16	Levulinic acid	123-76-2	$C_5H_8O_3$		116.11
97	Tetraethyl-ammonium bromide	71-91-0	$C_8H_{20}NBr$		210.16	Triethylene glycol	112-27-6	$C_6H_{14}O_4$		150.17
98	Tetraethyl-ammonium chloride	56-34-8	$C_8H_{20}ClN$		165.7	Acetic acid	64-19-7	CH_3COOH		60.05
99	Tetraethyl-ammonium chloride	56-34-8	$C_8H_{20}ClN$		165.7	Glycolic acid	79-14-1	$C_2H_4O_3$		76.05

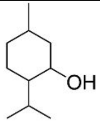
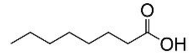
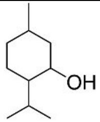
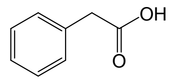
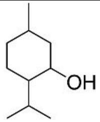
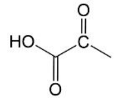
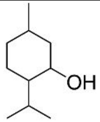
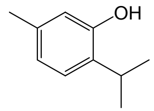
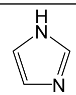
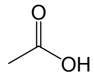
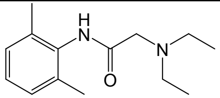
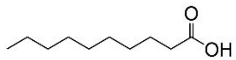
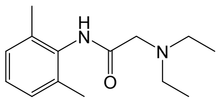
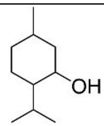
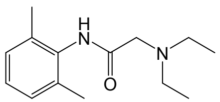
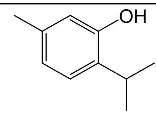
100	Tetraethyl-ammonium chloride	56-34-8	$C_8H_{20}ClN$		165.7	Levulinic acid	123-76-2	$C_5H_8O_3$		116.11
101	Tetraethyl-ammonium chloride	56-34-8	$C_8H_{20}ClN$		165.7	Octanoic acid	124-07-2	C8H16O2		144.21
102	Tetraethyl-ammonium p-toluenesulfonate	733-44-8	$C_{15}H_{27}NO_3S$		322.37	1,2-Propanediol	57-55-6	$C_3H_8O_2$		76.09
103	Tetraethyl-ammonium p-toluenesulfonate	733-44-8	$C_{15}H_{27}NO_3S$		322.37	Ethylene glycol	107-21-1	$C_2H_6O_2$		62.07
104	Tetraethyl-ammonium p-toluenesulfonate	733-44-8	$C_{15}H_{27}NO_3S$		322.37	Polyethylene glycol	25322-68-3	$C_{2n}H_{4n+2}O_{n+1}$		697.61
105	Tetraethyl-ammonium p-toluenesulfonate	733-44-8	$C_{15}H_{27}NO_3S$		322.37	Tetraethylene glycol	112-60-7	$C_8H_{18}O_5$		194.23
106	Tetraheptylammonium chloride	10247-90-2	$C_{28}H_{60}ClN$		446.24	Decanoic acid	334-48-5	$C_{10}H_{20}O_2$		172.26
107	Tetraheptyl-ammonium chloride	10247-90-2	$C_{28}H_{60}ClN$		446.24	Ibuprofen	15687-27-1	$C_{13}H_{18}O_2$		206.28
108	Tetraheptylammonium chloride	10247-90-2	$C_{28}H_{60}ClN$		446.24	Oleic acid	112-80-1	$C_{18}H_{34}O_2$		282.46

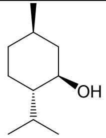
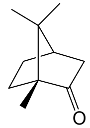
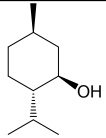
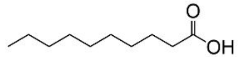
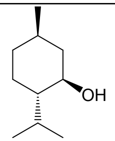
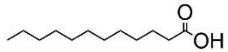
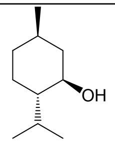
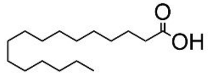
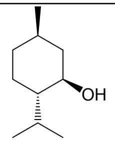
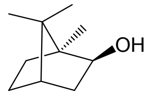
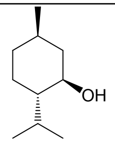
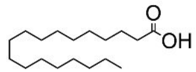
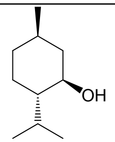
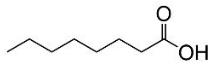
109	Tetrahexyl-ammonium bromide	4328-13-6.	$C_{24}H_{52}BrN$		434.58	Ethylene glycol	107-21-1	$C_2H_6O_2$		62.07
110	Tetrahexyl-ammonium bromide	4328-13-6.	$C_{24}H_{52}BrN$		434.58	Glycerol	56-81-5	$C_3H_8O_3$		92.09
111	Tetramethylammonium chloride	75-57-0	$C_4H_{12}NCl$		109.60	Glycerol	56-81-5	$C_3H_8O_3$		92.09
112	Tetraoctylammonium bromide	14866-33-2	$C_{32}H_{68}BrN$		546.79	Decanoic acid	334-48-5	$C_{10}H_{20}O_2$		172.26
113	Tetraoctylammonium chloride	3125-07-3	$C_{32}H_{68}ClN$		502.34	Decanoic acid	334-48-5	$C_{10}H_{20}O_2$		172.26
114	Tetrapropylammonium bromide	1941-30-6	$C_{12}H_{28}N.Br$		266.26	Ethylene glycol	107-21-1	$C_2H_6O_2$		62.07
115	Tetrapropylammonium bromide	1941-30-6	$C_{12}H_{28}N.Br$		266.26	Glycerol	56-81-5	$C_3H_8O_3$		92.09
116	Tetrapropylammonium bromide	1941-30-6	$C_{12}H_{28}N.Br$		266.26	Levulinic acid	123-76-2	$C_5H_8O_3$		116.11
117	Tetrapropylammonium bromide	1941-30-6	$C_{12}H_{28}N.Br$		266.26	Triethylene glycol	112-27-6	$C_6H_{14}O_4$		150.17

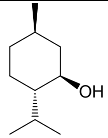
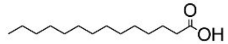
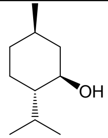
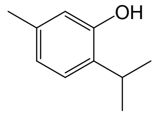
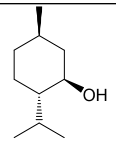
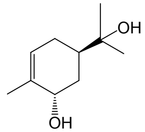
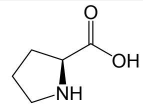
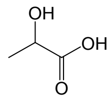
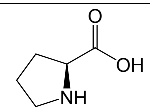
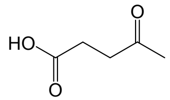
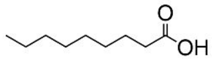
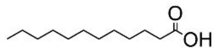
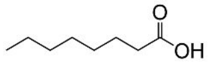
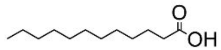
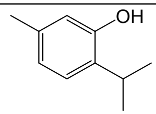
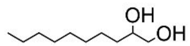
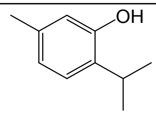
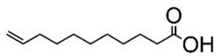
118	Tetrapropylammonium chloride	5810-42-4	$C_{12}H_{28}ClN$		221.81	Acetic acid	64-19-7	CH_3COOH		60.05
119	Tetrapropylammonium chloride	5810-42-4	$C_{12}H_{28}ClN$		221.81	Ethanolamine	141-43-5	C_2H_7NO		61.08
120	Tetrapropylammonium chloride	5810-42-4	$C_{12}H_{28}ClN$		221.81	Levulinic acid	123-76-2	$C_5H_8O_3$		116.11
121	Triethylmethylammonium chloride	10052-47-8	$C_7H_{18}ClN$		151.68	Acetic acid	64-19-7	CH_3COOH		60.05
122	Triethylmethylammonium chloride	10052-47-8	$C_7H_{18}ClN$		151.68	Ethylene glycol	107-21-1	$C_2H_6O_2$		62.07
123	Triethylmethylammonium chloride	10052-47-8	$C_7H_{18}ClN$		151.68	Glycerol	56-81-5	$C_3H_8O_3$		92.09
124	Triethylmethylammonium chloride	10052-47-8	$C_7H_{18}ClN$		151.68	DL-lactic acid	598-82-3	$C_3H_6O_3$		90.08
125	Triethylmethylammonium chloride	10052-47-8	$C_7H_{18}ClN$		151.68	Levulinic acid	123-76-2	$C_5H_8O_3$		116.11

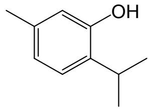
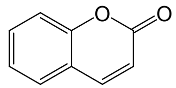
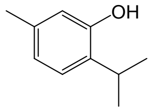
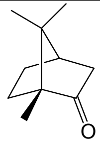
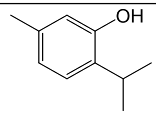
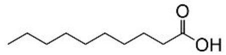
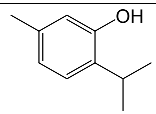
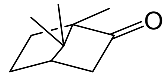
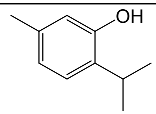
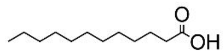
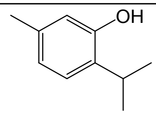
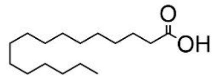
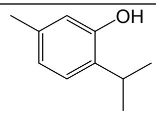
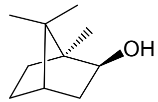
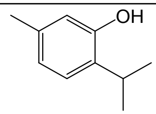
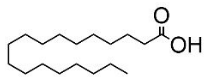
126	Potassium carbonate	584-08-7	K_2CO_3		138.21	Ethylene glycol	107-21-1	$C_2H_6O_2$		62.07
127	Potassium carbonate	584-08-7	K_2CO_3		138.21	Glycerol	56-81-5	$C_3H_8O_3$		92.09
128	Sodium dodecanoate	629-25-4	$C_{12}H_{23}O_2Na$		222.30	Decanoic acid	334-48-5	$C_{10}H_{20}O_2$		172.26
129	Zinc chloride	7646-85-7	$ZnCl_2$	Cl^- Zn^{2+} Cl^-	136.3	Acetamide	60-35-5	C_2H_5NO		59.07
130	Zinc chloride	7646-85-7	$ZnCl_2$	Cl^- Zn^{2+} Cl^-	136.3	Urea	57-13-6	CH_4N_2O		60.06
131	Acetamide	60-35-5	C_2H_5NO		59.07	Guanidine isothiocyanate	593-84-0	$C_2H_6N_4S$		118.16
132	Atropine	51-55-8	$C_{17}H_{23}NO_3$		289.37	Decanoic acid	334-48-5	$C_{10}H_{20}O_2$		172.26
133	Atropine	51-55-8	$C_{17}H_{23}NO_3$		289.37	Dodecanoic acid	143-07-7	$C_{12}H_{24}O_2$		200.32
134	Decanoic acid	334-48-5	$C_{10}H_{20}O_2$		172.26	Dodecanoic acid	143-07-7	$C_{12}H_{24}O_2$		200.32
135	DL-menthol	89-78-1	$C_{10}H_{20}O$		156.27	1-Naphthol	90-15-3	$C_{10}H_8O$		144.17

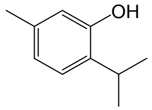
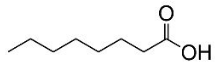
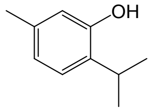
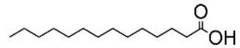
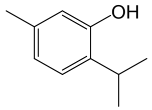
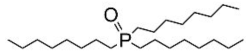
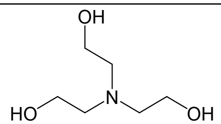
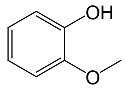
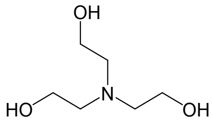
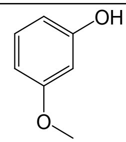
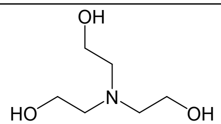
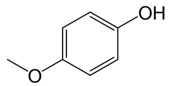
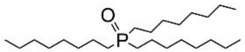
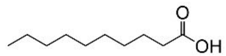
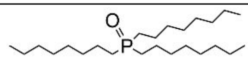
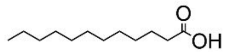
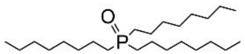
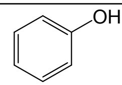
136	DL-menthol	89-78-1	$C_{10}H_{20}O$		156.27	1-Tetradecanol	112-72-1	$C_{14}H_{30}O$		214.39
137	DL-menthol	89-78-1	$C_{10}H_{20}O$		156.27	Acetic acid	64-19-7	CH_3COOH		60.05
138	DL-menthol	89-78-1	$C_{10}H_{20}O$		156.27	Benzoic acid	65-85-0	$C_7H_6O_2$		122.12
139	DL-menthol	89-78-1	$C_{10}H_{20}O$		156.27	Decanoic acid	334-48-5	$C_{10}H_{20}O_2$		172.26
140	DL-menthol	89-78-1	$C_{10}H_{20}O$		156.27	Dodecanoic acid	143-07-7	$C_{12}H_{24}O_2$		200.32
141	DL-menthol	89-78-1	$C_{10}H_{20}O$		156.27	Ibuprofen	15687-27-1	$C_{13}H_{18}O_2$		206.28
142	DL-menthol	89-78-1	$C_{10}H_{20}O$		156.27	L-lactic acid	79-33-4	$C_3H_6O_3$		90.08

143	DL-menthol	89-78-1	$C_{10}H_{20}O$		156.27	Octanoic acid	124-07-2	$C_8H_{16}O_2$		144.21
144	DL-menthol	89-78-1	$C_{10}H_{20}O$		156.27	Phenylacetic acid	103-82-2	$C_8H_8O_2$		136.15
145	DL-menthol	89-78-1	$C_{10}H_{20}O$		156.27	Pyruvic acid	127-17-3	$C_3H_4O_3$		88.06
146	DL-menthol	89-78-1	$C_{10}H_{20}O$		156.27	Thymol	89-83-8	$C_{10}H_{14}O$		150.22
147	Imidazole	288-32-4	$C_3H_4N_2$		68.08	Acetic acid	64-19-7	CH_3COOH		60.05
148	Lidocaine	137-58-6	$C_{14}H_{22}N_2O$		234.34	Decanoic acid	334-48-5	$C_{10}H_{20}O_2$		172.26
149	Lidocaine	137-58-6	$C_{14}H_{22}N_2O$		234.34	DL-menthol	89-78-1	$C_{10}H_{20}O$		156.27
150	Lidocaine	137-58-6	$C_{14}H_{22}N_2O$		234.34	Thymol	89-83-8	$C_{10}H_{14}O$		150.22

151	L-menthol	2216-51-5	$C_{10}H_{20}O$		156.27	D-camphor	464-49-3	$C_{10}H_{16}O$		152.23
152	L-menthol	2216-51-5	$C_{10}H_{20}O$		156.27	Decanoic acid	334-48-5	$C_{10}H_{20}O_2$		172.26
153	L-menthol	2216-51-5	$C_{10}H_{20}O$		156.27	Dodecanoic acid	143-07-7	$C_{12}H_{24}O_2$		200.32
154	L-menthol	2216-51-5	$C_{10}H_{20}O$		156.27	Hexadecanoic acid	57-10-3	$C_{16}H_{32}O_2$		256.43
155	L-menthol	2216-51-5	$C_{10}H_{20}O$		156.27	L-borneol	464-45-9	$C_{10}H_{18}O$		154.25
156	L-menthol	2216-51-5	$C_{10}H_{20}O$		156.27	Octadecanoic acid	57-11-4	$C_{18}H_{36}O_2$		284.48
157	L-menthol	2216-51-5	$C_{10}H_{20}O$		156.27	Octanoic acid	124-07-2	$C_8H_{16}O_2$		144.21

158	L-menthol	2216-51-5	$C_{10}H_{20}O$		156.27	Tetradecanoic acid	544-63-8	$C_{14}H_{28}O_2$		228.37
159	L-menthol	2216-51-5	$C_{10}H_{20}O$		156.27	Thymol	89-83-8	$C_{10}H_{14}O$		150.22
160	L-menthol	2216-51-5	$C_{10}H_{20}O$		156.27	Trans-sobrerol	42370-41-2	$C_{10}H_{18}O_2$		170.25
161	L-proline	147-85-3	$C_5H_9NO_2$		115.13	DL-lactic acid	598-82-3	$C_3H_6O_3$		90.08
162	L-proline	147-85-3	$C_5H_9NO_2$		115.13	Levulinic acid	123-76-2	$C_5H_8O_3$		116.11
163	Nonanoic acid	112-05-0	$C_9H_{18}O_2$		158.24	Dodecanoic acid	143-07-7	$C_{12}H_{24}O_2$		200.32
164	Octanoic acid	124-07-2	$C_8H_{16}O_2$		144.21	Dodecanoic acid	143-07-7	$C_{12}H_{24}O_2$		200.32
165	Thymol	89-83-8	$C_{10}H_{14}O$		150.22	1,2-Decanediol	1119-86-4	$C_{10}H_{22}O_2$		174.28
166	Thymol	89-83-8	$C_{10}H_{14}O$		150.22	10-Undecylenic acid	112-38-9	$C_{11}H_{20}O_2$		184.28

167	Thymol	89-83-8	$C_{10}H_{14}O$		150.22	Coumarin	91-64-5	$C_9H_6O_2$		146.14
168	Thymol	89-83-8	$C_{10}H_{14}O$		150.22	D-camphor	464-49-3	$C_{10}H_{16}O$		152.23
169	Thymol	89-83-8	$C_{10}H_{14}O$		150.22	Decanoic acid	334-48-5	$C_{10}H_{20}O_2$		172.26
170	Thymol	89-83-8	$C_{10}H_{14}O$		150.22	DL-camphor	21368-68-3	$C_{10}H_{16}O$		152.23
171	Thymol	89-83-8	$C_{10}H_{14}O$		150.22	Dodecanoic acid	143-07-7	$C_{12}H_{24}O_2$		200.32
172	Thymol	89-83-8	$C_{10}H_{14}O$		150.22	Hexadecanoic acid	57-10-3	$C_{16}H_{32}O_2$		256.43
173	Thymol	89-83-8	$C_{10}H_{14}O$		150.22	L-borneol	464-45-9	$C_{10}H_{18}O$		154.25
174	Thymol	89-83-8	$C_{10}H_{14}O$		150.22	Octadecanoic acid	57-11-4	$C_{18}H_{36}O_2$		284.48

175	Thymol	89-83-8	$C_{10}H_{14}O$		150.22	Octanoic acid	124-07-2	$C_8H_{16}O_2$		144.21
176	Thymol	89-83-8	$C_{10}H_{14}O$		150.22	Tetradecanoic acid	544-63-8	$C_{14}H_{28}O_2$		228.37
177	Thymol	89-83-8	$C_{10}H_{14}O$		150.22	Trioctyl-phosphine oxide	78-50-2	$C_{24}H_{51}OP$		386.63
178	Triethanolamine	102-71-6	$C_6H_{15}NO_3$		149.19	2-Methoxyphenol	90-05-1	$C_7H_8O_2$		124.14
179	Triethanolamine	102-71-6	$C_6H_{15}NO_3$		149.19	3-Methoxyphenol	150-19-6	$C_7H_8O_2$		124.14
180	Triethanolamine	102-71-6	$C_6H_{15}NO_3$		149.19	4-Methoxyphenol	150-76-5	$C_7H_8O_2$		124.14
181	Trioctylphosphine oxide	78-50-2	$C_{24}H_{51}OP$		386.63	Decanoic acid	334-48-5	$C_{10}H_{20}O_2$		172.26
182	Trioctylphosphine oxide	78-50-2	$C_{24}H_{51}OP$		386.63	Dodecanoic acid	143-07-7	$C_{12}H_{24}O_2$		200.32
183	Trioctylphosphine oxide	78-50-2	$C_{24}H_{51}OP$		386.63	Phenol	108-95-2	C_6H_6O		94.11

5 Measurement methods dataset for DESs

Ref. *	DES preparation method	Measurement apparatus	Uncertainty	Source	Purity	Purification method
1	Heating method	Brookfield DV-E viscometer	N/A	Sigma-Aldrich	N/A	N/A
2	Heating method	Brookfield R/S Plus Rheometer	The uncertainty in the viscosity and the temperature measurements are 3-5% of the measured value and ±0.01 K, respectively.	Merck Chemicals	Choline chloride, ethylene glycol, triethylene glycol, urea and malonic acid, >98 wt%.	The studied DES components were dried in a vacuum oven overnight.
3	Heating method	Pinkevitch method	Uncertainty of viscosity is ±0.2%.	Shanghai Aladdin Chemical Company	Acetylcholine chloride, 99.0 wt%; Imidazole, 99.0 wt%; 1,2,4-Triazole, 99.5 wt%.	The obtained DESs were further dried under vacuum at 353 K for 48 h before use.
4	Heating method	SVM 3000 Anton Paar rotational Stabinger viscometer-densimeter	The repeatability of the dynamic viscosity	Sigma Aldrich	Cholinium chloride, acetylcholinium chloride and benzyldimethyl(2-	Cholinium chloride, acetylcholinium chloride and

			measurements in this equipment is ±0.35%.		hydroxyethyl) ammonium chloride, >98wt%; D-(+)-Xylose, D-(+)-Mannose, D-(-)-Fructose, D-(+)-Glucose and D-(-)-Ribose, ≥99.0 wt%.	benzyldimethyl(2-hydroxyethyl) ammonium chloride were dried under vacuum prior to use.
5	Heating method	Pinkevitch method	The relative standard uncertainty of viscosity was 0.2%.	Aladdin Chemical Company	Choline chloride, >98.5 wt%; Levulinic acid, acetylcholine chloride, tetraethylammonium bromide, Tetrabutylammonium bromide, >99 wt%; Tetrabutylammonium chloride, >97 wt%; Tetraethylammonium chloride, trimethyl hydrochloride, >98 wt%.	without further purification
6	Heating method	digital rolling ball micro-viscometer(Anton Par, model Lovis-2000M/ME)	The viscosity meter has a measuring uncertainty of $\pm 5\times10^{-3}$ mPa.s and	R＆M Chemicals	Allyltriphenyl phosphonium bromide, diethylene glycol and triethylene glycol, >99	without further purification

			temperature of ±0.02 K.		wt%.	
7	Heating method	Pinkevitch method	Uncertainty of viscosity is ±0.2%.	N/A	KSCN, >99wt% ; NH4SCN, >98.5wt% ; Acetamide, >98.5wt% ; Caprolactam, >99wt%; Urea, >99wt%.	KSCN, NH4SCN and urea were fully dried under vacuum at 105 ºC to constant weight before use.
8	Grinding method	SM 3000 Anton Paar rotational Stabinger viscometer-densimeter	The highest relative standard uncertainty registered for the dynamic viscosity measurements was 2×10^{-5}Pa·s, respectively.	Sigma-Aldrich	Choline chloride,≥98 wt%; Benzylcholine chloride,≥97 wt%; Tetrabutylammonium chloride, ≥97 wt%; Levulinic acid, 98 wt%.	The DES were dried under vacuum(1 Pa) at room temperature for at least 3 days.
9	Heating method	Bohlin CVO 100 rheometer	N/A	Sigma-Aldrich, Shanghai Shenbo Chemical Company, VWR, Merck, Shanghai Lingfeng chemical reagent	N/A	All chemicals were analytical grade reagents and were used as received.

				company, Simopharm chemical reagent company and Aladdin company		
10	Heating method	Anton Paar Automated micro viscometer	The uncertainty in viscosity measurements was estimated to be less than ±1%.	Aladdin Chemicals Co., Ltd, Shanghai, China	Choline chloride, >98 wt%; Choline bromide, >98 wt%; Tetramethylammonium chloride, >98 wt%; Tetraethylammonium chloride, >98 wt%; Tetraethylammonium bromide, >98 wt%; Tetra-propylammonium chloride, >97 wt%; Tetrapropyl-ammonium bromide, >98 wt%; Tetrabutylammonium chloride, >97 wt%; Tetrabutylammonium bromide, >98 wt%; Benzyltrimethyl-	without further purification

					ammonium chloride, >98 wt%; Trioctylmethyl-ammonium chloride, >97 wt%; Triethylene glycol, >98 wt%; Tetraethylene glycol, >98 wt%; Phenylpropionic acid, >99 wt%; Malonic acid, >98 wt%; Glutaric acid, >98 wt%; Lactic acid, 98 wt%; sorbitol, >98 wt%; xylitol, >99 wt%.	
11	Heating method	Brookfield R/S plus Rheometer	(3-5)% of measured value	Merck Chemicals (Darmstadt, Germany)	All the chemicals used were of high purity(>99wt%).	N/A
12	Heating method	Anton Paar Lovis 2000 ME	Temperature is kept constant through a built-in Peltier device with an accuracy of 0.02 K.	Sigma-Aldrich and Merck	Benzyltripropylammonium Chloride, ≥97.0 wt%; Ethylene Glycol, ≥99.0 wt%; Lactic Acid, ≥90.0 wt%; Glycerol Anhydrous, ≥99.5 wt%; Phenol, ≥99.0 wt%.	All initial components except lactic acid were kept in vacuum and dried for 48 h prior to synthesis.

13	Heating method	A microviscosimeter Lovis 2000/ME connected to the Anton Paar DSA-5000M densimeter	N/A	Sigma-Aldrich, Labkem, Acros and Panreac	Levulinic acid, 99 wt%; DL-lactic acid, 90 wt%; Citric acid, 99 wt%; Betaine, 98 wt%; L-proline, 98 wt%.	without further purification
14	Heating method	Anton Paar Physica MCR 301 rheometer	N/A	Sigma-Aldrich	Imidazole, >99 wt%; Choline chloride, >99 wt%; Betaine, >99 wt%; Tetraethylammonium chloride, >96 wt%; Acetic acid, 99.7 wt%; Urea, >98 wt%; Levulinic acid, >97 wt%; Glycerol, 99 wt%; Ethylene glycol, >99 wt%; Decanoic acid, >98 wt%.	without further purification
15	Heating method	Anton Paar Lovis 2000ME microviscometer(Graz, Austria)	The uncertainty is nearer to 2%.	Acros Organics	Choline chloride, >99 wt%; Ethylene glycol, >99.8 wt%; 1,2-Propanediol, >99 wt%; 1,3-Propanediol, >98 wt%;	Choline chloride, which is a very hygroscopic compound, was dried in a Schlenk line under a high

					1,4-Butanediol, >99 wt%.	vacuum(10^{-4} mbar) for three days, while ethylene glycol, 1,2-propanediol, 1,3-propanediol, and 1,4-butanediol were placed in molecular sieves for at least one day.
16	Heating method	Anton Paar Lovis 2000ME	The accuracy of viscosity measurement was better than ±0.02 mPa s.	Shanghai Aladdin Industrial Co, Ltd.	1,4-butanediol, 99 wt%; 2,3-butanediol, 98 wt%; 1,3-propanediol, 98 wt%; choline chloride, 98 wt%.	The water in the DESs was swept away by flowing dried nitrogen at 353.15 K. Finally, the DESs were stored in closed bottles.
17	Heating method	Brookfield instrument	N/A	Merck(Germany)	All chemicals are high purity, ≥98 wt%.	N/A
18	Heating method	NDJ-8S rotational viscometer	N/A	Sinopharm Chemical Reagent Co, Ltd.	Choline chloride, 98.0-101.0 wt%); urea, ≥99.0	Choline chloride was chosen as

					wt%; ethylene glycol, ≥99.0 wt%; glycerol, ≥99.0 wt%; lactic acid, ≥99.0 wt%; acetic acid, ≥99.5 wt% and oxalic acid, ≥99.5 wt%.	HBA and dried under vacuum at 80 ºC for 48 h before use.
19	Heating method	a rotational viscometer(Anton Paar Rheolab QC)	(3-5)% of measured value	Merck Chemicals(Darmstadt, Germany)	Choline chloride ,D-fructose anhydrous , 98wt%.	Chemicals were dried in a vacuum oven prior to use to eliminate moisture contamination.
20	Heating method	Anton Paar Rheolab Qc.	(3-5)% of measured value	Merck Chemicals(Darmstadt, Germany)	Choline chloride (2-hydroxyethyl-trimethylammonium) and D-glucose anhydrous, >98 wt%.	without further purification
21	Heating method	MCR 301 rheometer from Anton Paar with a thermostated jacket	N/A	N/A	N/A	N/A
22	Heating method	automated rolling-ball viscometer (Anton Paar AMVn)	The expanded (k = 2) relative uncertainty of	Sigma-Aldrich	Choline chloride, ≥98 wt%; Ethylene glycol, ≥99.8 wt%.	Choline chloride was dried for 4 days at 313 K with a

			viscosity is 1.5%			high-vacuum line(pressure p<10-9 bar). Ethylene glycol(EG) was dried by 3A molecular sieve.
23	Heating method	N/A	N/A	Scionix Ltd	N/A	N/A
24	N/A	nonequilibrium periodic perturbation method	N/A	N/A	N/A	N/A
25	Heating method and Grinding method	automated SM 3000 Anton Paar rotational Stabinger viscometer densimeter	The temperature uncertainty is ±0.02 K. The precision of the viscosity measurements is ±0.5%.	Sigma-Aldrich	Choline chloride, ≥98 wt%; Oxalic, malonic, adipic, levulinic, glutaric, glycolic, succinic, malic, tartaric, fumaric, azelaic, and citric acids, all ≥99 wt%.	Cholinium chloride was first dried in a high vacuum pump at 40 °C for at least 2 days, while the hydrogen bond donors were used without any further purification.
26	Heating method	Brookfield DV-E viscometer	N/A	Sigma-Aldrich	Choline chloride, 99wt%; Ethylene glycol,1,4-butanediol, and	Choline chloride was recrystallized from absolute

					glycerol, >99wt%.	ethanol, filtered, and dried under vacuum. Others were used as received.
27	Heating method	Anton Paar SVM 3000/G2 Stabinger viscometer	The temperature uncertainty is 0.02 K and the relative uncertainty of the dynamic viscosity is 0.35%.	Sigma-Aldrich and Merck	Choline chloride, ≥98.0 wt%; Tetramethylammonium chloride, ≥98.0 wt%; Glycerol, ≥99.0 wt%.	The choline chloride was kept in a vacuum desiccator before it was used. All the chemicals were used without further purification.
28	Heating method	automated Anton Paar microviscometer (model AMVn)	The uncertainties associated with the viscosity measurements are ≤0.5%.	Sigma-Aldrich	Choline chloride, ≥98 wt%; Glycerol, ≥99.5 wt%.	N/A
29	Heating method	Brookfield DV-E viscometer	N/A	Sigma-Aldrich	N/A	Choline chloride(ChCl) was recrystallized from absolute ethanol,

						filtered, and dried under vacuum.
30	Heating method	Rheometer (DISCOVERY HR-2, USA)	N/A	Aladdin Chemistry Co. and Sinopharm Chemical Reagent Co.	N/A	N/A
31	Heating method	viscometer（Model DV2T，Brookfield）	The relative uncertainty is within 1.0%.	Aladdin Reagent Co. Ltd., Shanghai, China	Choline chloride, 98.0 wt%; Phenol, 99.0 wt%; P-cresol, 99.0 wt%); P-chlorophenol, 99.0 wt%.	Choline chloride was dried for 48 h at 313.2 K under vacuum condition beforeuse. Other reagents were used for the synthesis of DESs without additional purification.
32	Heating method	Ubbelohde viscometer	The uncertainty of the viscosity was less than ±3%.	Aladdin Chemical Co., Ltd. And Beijing Chemical Plant	Choline chloride, o-cresol, and 2,3-xylenol, >99 wt%; Phenol, 98 wt%.	without further purification
33	Heating method	automated Anton Paar microviscometer (model AMVn)	The deviation in viscosity was ≤0.5%.	Sigma-Aldrich	Choline chloride, ≥99 wt%; Urea, ≥99 wt%.	N/A

34	Heating method	Rheometer(DISCOVERY HR-2, USA)	N/A	Aladdin Chemistry Co., Sinopharm Chemical Reagent Co., Ltd.	All reagents used are of analytical grade.	N/A
35	Heating method	Anton Paar SVM 3000 Stabinger Viscometer	The temperature uncertainty is ±0.02 K and the relative uncertainty of the dynamic viscosity is ±0.35%.		Tetrabutylammonium chloride, ≥95 wt%; Tetraheptylammonium chloride, 95 wt%; Methyltrioctylammonium chloride, 97 wt%; Tetraoctylammonium chloride, 97 wt%; Methyltrioctylammonium bromide, 97 wt%; Tetraoctylammonium bromide, 98 wt%; Decanoic acid, >98 wt%.	N/A
36	Heating method	viscometer(DMA 5000M, Anton Paar GmbH)	N/A	Aladdin Reagent Co., Ltd.(Shanghai, China)	N/A	without further purification
37	Heating method	automated falling ball microviscometer(Anton Paar GmbH, model	The overall uncertainty was estimated to be	Merck	N,N-diethylethanolammonium chloride, >98 wt%;	The DES was vacuum dried at 343 K, and kept in a

		AMVn)	±1%.		Glycerol, >99.5wt%); Ethylene glycol, >99.9wt%.	dry box prior to use.
38	Heating method	Anton Paar Lovis 2000 ME micro viscometer	accuracy up to 0.5%	Acros Organics, Belgium Loba Chemie, India Sigma Aldrich, Switzerland Sigma Aldrich, USA Acros Organics, India WINLAB, UK Sigma Aldrich, USA WINLAB, Belgium AVONCHEM, UK Loba Chemie, India	Choline chloride, 99 wt%; Tetrabutylammonium bromide, 98 wt%; Tetraethylammonium chloride, 98 wt%; Tetraethylammonium p-toluene sulfonate, , 97 wt%; Methyl triphenyl phosphonium bromide, 98 wt%; Mono-ethylene glycol, 99 wt%; Tetra-ethylene glycol, 99 wt%; Poly-ethylene glycol, 99 wt%; Levulinic acid, 98 wt%; Ethanolamine, 99 wt%; Acetic acid, 99.7 wt%; 1,2-propanediol, 99 wt%.	without further purification
39	Heating	Brookfield DV-II+ Pro	N/A	J&K Chemical, Ltd.	All reagents were	The prepared DESs

	method	viscometer			obtained with purity more than 98 wt%.	were dried at 373.15 K under vacuum for 24 h to ensure that the water content in DESs was less than 0.2 wt%.
40	Heating method	Anton Paar Rheolab Qc.	5% of measured value	Merck Chemicals (Darmstadt, Germany)	Tetrabutylammonium chloride, glycerol, ethylene glycol, and triethylene glycol, >98 wt%.	Prior to being used, these chemicals were treated by drying in a vacuum oven to ensure a low moisture content of less than 200 ppm.
41	Heating method	Ostwald viscometer（Dalian Instruments an Meters Co.，P.R.China）	The uncertainties were estimated to be 1%.	Tianjin Kermel, Aladdin, Tianjin Kermel, and Tianjin Kcrmel	Tetrabutylammonium chloride, ≥98 wt%; Propionic acid, ≥99 wt %; Ethylene glycol, ≥98 wt %; Polyethylene glycol, ≥98 wt %; Phenylacetic acid, ≥99 wt %.	All the materials were purified before use according to crystallization, distillation, and vacuum drying.

42	Heating method	Anton Paar Rheolab Qc	5% of measured value	Sisco Research Lab(Mumbai, India)	Tetrabutylammonium chloride, N/A; Glutamic acid , aspartic acid , arginine, >99.0 wt%.	All chemicals were pretreated by drying for a minimum of 3 h in a vacuum oven.
43	Heating method	Cannon-Ubbelohde Size 400 viscometer	N/A	VWR	Tetraheptylammonium chloride, 95 wt%; DL-menthol; Decanoic, dodecanoic, and oleic acids, >98 wt%; Ibuprofen, 98 wt%.	without further purification
44	Heating method	Anton Paar SVM 3000/G2 Stabinger densimeter- viscosimeter	reproducibility: temperature 0.03K; viscosity 0.35%	Sigma-Aldrich, VWR, Acros Organics, Merck and Reidel-de Haen	Tetrahexylammonium bromide, ≥99.0 wt%; Ethylene glycol, ≥99.0 wt%; Glycerol, ≥99.0 wt%;	without further purification
45	Heating method	Anton Paar Rheolab Qc	(3-5)% of measured value	Merck Chemicals(Darmstadt, Germany)	Tetrapropylammonium bromide, ethylene glycol, triethylene glycol and glycerol, >98 wt%.	N/A
46	Heating method	Anton Paar Rheolab Qc	(3-5)% of measured value	Merck Chemicals(Darmstadt, Germany)	Potassium carbonate, ethylene glycol and glycerol, >98 wt%.	Prior to use, these chemicals were treated by drying in

						a vacuum oven to assure a low moisture content of below 200 ppm.
47	Heating method	Anton Paar(model SVM 3000) automated rotational Stabinger viscometer-densimeter	The temperature uncertainty is ± 0.01 ºC. The relative uncertainty of the dynamic viscosity is ±0.25%.	Sigma-Aldrich	Dodecanoate sodium salt, 99-100 wt%; Decanoic acid, >98 wt%.	without further purification
48	Heating method	Anton Paar AMVn falling ball automated microviscometer	The accuracy of viscosity measurement was better than ±0.02 mPa.s.	Shanghai Aladdin Chemical Company	Guanidine isothiocyanate(GI) and acetamide(AT) were AR grade with the mass purity higher than 0.99.	without further purification The DES was dried under vacuum at 353 K for 24 h prior to utilization, with the water content less than 2.0·10-3(mass fraction) in all cases.
49	Heating method	Anton Paar Lovis 2000 ME rolling ball	N/A	Sigma-Aldrich	1-Tetradecanol, ≥97.0 wt%; Thymol, ≥99.0 wt%;	N/A

		viscometer			Decanoic acid, ≥98.0 wt%; 1-Napthol, ≥99.0 wt%; Dodecanoic acid, ≥99.0 wt%; Menthol, ≥99.0 wt%; Coumarin, ≥99.0 wt%; 1,2-Decanediol, ≥98.0 wt%; Lidocaine, N/A; Atropine, ≥99.0 wt%.	
50	Heating method	Anton Paar(modelSVM 3000) automated rotational Stabinger viscometer-densimeter	The temperature uncertainty is±0.01 ºC. The relative uncertainty of the dynamic viscosity is ±0.25%.	Sigma-Aldrich	Octanoic acid,≥98 wt%; Decanoic acid,≥98 wt%; Nonanoic acid,≥98 wt%; Dodecanoic acid,≥98 wt%;	without further purification
51	Heating method	Anton Paar Lovis 2000 ME rolling ball viscometer	N/A	Sigma-Aldrich	1-Tetradecanol, ≥97 wt%; DL-menthol, ≥99 wt%.	N/A
52	Heating method	Anton Paar（model SVM 3000 ） automated rotational Stabinger viscometer-densimeter	The temperature uncertainty is ±0.02 K. The relative uncertainty of the	Sigma-Aldrich and Fluka	DL-Menthol, ≥95 wt%; Pyruvic acid, >98 wt%; Acetic acid, ≥99.7 wt%; Dodecanoic acid, >98	For the preparation of the dried samples, the DL-menthol-based

			dynamic viscosity is ±0.35%.		wt%; Caffeine, 99 wt%; Vanillic acid, ≥97 wt%; Tetracycline, >98 wt%; tryptophan, ≥98 wt%; L-Lactic acid solution (81 wt% in water).	eutectic mixtures were maintained for at least 4 days in a Schlenk under high vacuum(ca.10^{-1} Pa) at room temperature.
53	Heating method	Kinexus Prot Rheometer(Kinexus Prot, MAL1097376, Malvern)	N/A	Sigma	Menthol, 99wt%; Ibuprofen, >98wt%; Benzoic acid, >99.5wt%; Phenylacetic acid, 99wt%.	without further purification
54	Heating method	Anton Paar SVM 3000/G2 type Stabinger instrument	uncertainty of ±0.005 mPa s for the viscosity.	Sigma Aldrich	Tetraoctylammonium bromide, >96wt%; Menthol, ≈99wt%; Lidocaine, ≈99wt%; Thymol, ≈99wt%; Decanoic acid, >98wt%.	N/A
55	Heating method	Anton Paar Physica MCR 301 rheometer	Temperature accuracy is ±0.03 K, and the torque uncertainty is max 0.5%.	Sigma-Aldrich and TCI Chemicals	Lidocaine, >99 wt%; Decanoic acid, >98 wt%; Thymol, >99 wt%; Menthol, >99 wt%;	without further purification

56	Heating method	automated Anton Paar SVM 3000 Stabinger viscosimeter-densimeter	The relative uncertainty in the dynamic viscosity was ±0.35%.	Sigma-Aldrich	DL-Menthol, ≥95 wt%; Octanoic acid, ≥99 wt%.	All of the mixtures and pure compounds were carefully dried under vacuum at room temperature for a minimum of 2 h in order to remove traces of water and other volatile compounds.
57	Heating method	Anton Paar Physica MCR 301 rheometer	N/A	Sigma-Aldrich	Lidocaine, >99 wt%; Decanoic acid, >98 wt%.	N/A
58	Heating method	SVM 3001 Anton Paar viscometer	reproducibility: temperature 0.03K; viscosity 0.35%	N/A	L-menthol, ≥99.5 wt%; Thymol, >99 wt%; (+)-Camphor, 98 wt%; (-)-Borneol, ≥99 wt%; Trans-sobrerol, 99 wt%.	without further purification
59	Heating method	automated SVM 3000 Anton Paar rotational Stabinger viscometer-densimeter	temperature uncertainty:±0.02 K; dynamic viscosity relative	Acros, Sigma, Aldrich and Merck	L-Menthol, 99.7 wt%; Thymol, ≥99.5 wt%; Octanoic acid,≥99 wt%; Decanoic acid, 99-100	without further purification

			uncertainty:±0.35%.		wt%; Dodecanoic acid,≥99 wt%; Myristic acid, ≈95 wt%; Palmitic acid, ≥98 wt%; Stearic acid, ≥97 wt%.	
60	Heating method	a commercial rolling ball viscometer(Lovis 2000 M/ME, Anton Paar, Germany)	N/A	Sigma-Aldrich	N/A	without further purification
61	Heating method	BROOKFIELD LVDV-II+ viscometer(Labo-Plus, Poland)	N/A	Sigma-Aldrich and Merck.	Thymol, ≥99 wt%; ±Camphor, >95 wt%; Decanoic acid, >98 wt%; 10-Undecylenic acid, >97 wt%.	N/A
62	Heating method	SVM 3001 Anton Paar viscometer	reproducibility: temperature 0.03K; viscosity 0.35%	Merck and Acros Organic	Thymol, >99 wt%; Trioctylphosphine oxide, 99 wt%; Decanoic acid, 99 wt%; Hydrocinnamic acid, 99 wt%;	N/A
63	Heating method	Brookfield DVII+Pro rotary viscometer	with a precision of ±0.1 mPa.s.	Aladdin Chem. Co and Alfa Aesar	Monoethanolamine, 99 wt%; Diethanolamine, 99 wt%; Triethanolamine, 99	The as-prepared DESs were then dried under vacuum

					wt%; 2-methoxyphenol, 98 wt%; 3-methoxyphenol, 99 wt% and 4-methoxyphenol, 99 wt%.	to remove the traces of moisture.
64	Heating method	microviscosimeter Lovis 2000/ME connected to the Anton Paar DSA-5000M densimeter	The measurement uncertainty is ±0.03 mPa-s.	Scharlau, Sigma-Aldrich, Sigma and Acros Organics	Adipic acid, 99.5 wt%; Succinic acid, 99 wt%; Levulinic acid, 99 wt%; Decanoic acid,≥98 wt%; Dodecanoic acid, 99 wt%; Trioctylphosphine oxide, 99 wt%;	without further purification
65	Evaporating method	Bohlin Gemini cone and plate rheometer	N/A	Acros Organics	Trioctylphosphine oxide, >97 wt%; Phenol, 99.5 wt%.	Materials were stored under an inert atmosphere until used.
66	Heating method	interfacial rheometer(model: Physica MCR301, Anton-Paar Make)	The relative uncertainty of the dynamic viscosity is ±3.3%.	Merck	DL-Menthol, ≥95 wt%; Dodecanoic acid, ≥99 wt%; Ethanol, ≥99.9 wt%; 1-Propanol, ≥99 wt%; 1-Butanol, ≥99 wt%.	a vacuum at T=60 C for at least 48 h was applied to the DES samples

*: The references in this table is corresponding to the Sheet2 in Supplementary Data.