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.

| 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).
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 |
|-----------------|--------------|--------|

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| Parameter       | Settings                                      | Value |
|-----------------|----------------------------------------------|-------|
| 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.](image)

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 scikit-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.
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 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).
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.
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   | $\eta_t^{\text{ref}}$ | ARD%a | RD%b   |
|----------------------|-------------------|--------------------|-----|-----------------------|-------|--------|
| Acetylcholine chloride | 1,2,4-triazole    | 1:1                | 303.15 | 304.69              | 6.83  | $\eta_{\text{ref}}$ |
|                      |                   |                    | 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  | $\eta_{\text{ref}}$ |
|                      |                   |                    | 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  | $\eta_{\text{ref}}$ |
|                      |                   |                    | 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 | $\eta_{\text{ref}}$ |
|                      |                   |                    | 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  |
| Temperature  | Acetylcholine chloride/Imidazole | Betaine/DL-Lactic acid | Choline chloride 1,2-Butanediol | Choline chloride 1,2-Butanediol |
|--------------|---------------------------------|------------------------|-------------------------------|-------------------------------|
| 353.15       | 25.74                           | 2.27                   | 14.57                         | 14.57                         |
| 363.15       | 17.68                           | 1.18                   | 19.18                         | 19.18                         |
|              | Acetylcholine chloride/Imidazole|                        |                               |                               |
|              | AARD%                           | 7.14                   |                               |                               |
|              | AARD%                           | 35.65                  |                               |                               |
|              |                                  |                        |                               |                               |
| Betaine      |                                 |                        |                               |                               |
| DL-Lactic acid 1:2 |                       |                        |                               |                               |
| 298.15       | 1266.00                         | 3.75                   | η<sub>ref</sub>              |                               |
| 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<sub>ref</sub>              |                               |
| 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 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<sub>ref</sub>              |                               |
| 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                        |                               |
| Betaine      |                                 |                        |                               |                               |
| DL-Lactic acid 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                         |                               |
| Choline chloride/1,2-Butanediol | AARD% | 7.98 | 13.31 |

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.
|                             | 7.14 | 35.65 | 235.73 | 12.40 | 40.77 |
|-----------------------------|------|-------|--------|-------|-------|
| Acetylcholine chloride/Imidazole |      |       |        |       |       |
| Betaine/DL-Lactic acid      | 2.58 | 10.07 | 298.95 | 23.95 | 75.60 |
| Choline chloride/1,2-      | 7.98 | 13.31 | 32.05  | 11.68 | 12.40 |
| Butanediol                  |      |       |        |       |       |
## 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           | ZnCl₂             | Cl⁻ Cl²⁺ Cl⁻       | 136.3            | Choline chloride| 67-48-1           | C₅H₁₅ClNO        | HO⁻ N⁺ Cl⁻         | 139.62           |
| 2   | Chom chloride hexahydrate | 10060-12-5 | Cl₃CrH₂O₆         | 266.45             | Choline chloride| 67-48-1           | C₅H₁₅ClNO        | Ho⁻ N⁺ Cl⁻         | 139.62           |
| 3   | Acetylcholine chloride | 60-31-1 | C₇H₁₄ClNO₂        | 181.66             | 1,2,4-Triazole   | 288-88-0           | C₃H₇N₃           | 181.66             | 69.07             |
| 4   | Acetylcholine chloride | 60-31-1 | C₇H₁₄ClNO₂        | 181.66             | D-fructose       | 57-48-7           | C₆H₁₂O₃           | 181.66             | 180.16            |
| 5   | Acetylcholine chloride | 60-31-1 | C₇H₁₄ClNO₂        | 181.66             | D-glucose        | 50-99-7           | C₆H₁₂O₃           | 181.66             | 180.16            |
| 6   | Acetylcholine chloride | 60-31-1 | C₇H₁₄ClNO₂        | 181.66             | D-mannose        | 3458-28-4         | C₆H₁₂O₃           | 181.66             | 180.16            |
| 7   | Acetylcholine chloride | 60-31-1 | C₇H₁₄ClNO₂        | 181.66             | D-ribose         | 50-69-1           | C₆H₁₄O₃           | 181.66             | 150.13 (569)      |
|   | Compound                                      | CAS   | Molecular Formula | Molecular Weight | 1st Name     | CAS       | Molecular Formula | Molecular Weight |
|---|----------------------------------------------|-------|-------------------|------------------|--------------|-----------|-------------------|------------------|
| 8 | Acetylcholine chloride                       | 60-31-1 | C<sub>7</sub>H<sub>16</sub>ClNO<sub>2</sub> | 181.66           | D-xylose     | 31178-70-8 | C<sub>5</sub>H<sub>10</sub>O | 150.13           |
| 9 | Acetylcholine chloride                       | 60-31-1 | C<sub>7</sub>H<sub>16</sub>ClNO<sub>2</sub> | 181.66           | Imidazole    | 288-32-4  | C<sub>3</sub>H<sub>4</sub>N<sub>2</sub> | 68.08            |
|10 | Acetylcholine chloride                       | 60-31-1 | C<sub>7</sub>H<sub>16</sub>ClNO<sub>2</sub> | 181.66           | Levulinic acid | 123-76-2 | C<sub>5</sub>H<sub>8</sub>O<sub>3</sub> | 116.11           |
|11 | Allytriphenylphosphonium bromide             | 1560-54-9 | C<sub>23</sub>H<sub>22</sub>BrP | 383.26           | Diethylene glycol | 111-46-6 | C<sub>4</sub>H<sub>10</sub>O<sub>3</sub> | 106.12           |
|12 | Allytriphenylphosphonium bromide             | 1560-54-9 | C<sub>23</sub>H<sub>22</sub>BrP | 383.26           | Triethylene glycol | 112-27-6 | C<sub>6</sub>H<sub>14</sub>O<sub>4</sub> | 150.17           |
|13 | Ammonium thiocyanate                        | 1762-95-4 | NH<sub>4</sub>SCN | 76.12            | Acetamide    | 60-35-5  | C<sub>2</sub>H<sub>4</sub>NO | 59.07            |
|14 | Ammonium thiocyanate                        | 1762-95-4 | NH<sub>4</sub>SCN | 76.12            | Caprolactam  | 105-60-2 | C<sub>6</sub>H<sub>11</sub>NO | 113.16           |
|15 | Benzylidimethyl(2-hydroxyethyl) ammonium chloride | 7221-40-1 | C<sub>11</sub>H<sub>12</sub>ClNO | 215.72           | Levulinic acid | 123-76-2 | C<sub>5</sub>H<sub>8</sub>O<sub>3</sub> | 116.11           |
|   | Chemical Name                                   | CAS Number | Chemical Structure | Molecular formula | Molecular Weight | Additional Information |
|---|------------------------------------------------|------------|--------------------|-------------------|------------------|------------------------|
| 16| Benzyldimethyl(2-hydroxyethyl) ammonium chloride | 7221-40-1  | ![Structure1](image) | C<sub>11</sub>H<sub>18</sub>ClNO | 215.72           | D-fructose 57-48-7     |
| 17| Benzyldimethyl(2-hydroxyethyl) ammonium chloride | 7221-40-1  | ![Structure2](image) | C<sub>11</sub>H<sub>18</sub>ClNO | 215.72           | D-glucose 50-99-7      |
| 18| Benzyldimethyl(2-hydroxyethyl) ammonium chloride | 7221-40-1  | ![Structure3](image) | C<sub>11</sub>H<sub>18</sub>ClNO | 215.72           | D-mannose 3458-28-4    |
| 19| Benzyldimethyl(2-hydroxyethyl) ammonium chloride | 7221-40-1  | ![Structure4](image) | C<sub>11</sub>H<sub>18</sub>ClNO | 215.72           | D-ribose 50-69-1       |
| 20| Benzyldimethyl(2-hydroxyethyl) ammonium chloride | 7221-40-1  | ![Structure5](image) | C<sub>11</sub>H<sub>18</sub>ClNO | 215.72           | D-xylose 31178-70-8    |
| 21| Benzytrimethylammonium chloride                | 56-37-1    | ![Structure6](image) | C<sub>13</sub>H<sub>22</sub>CIN | 227.77           | Acetic acid 64-19-7    |
| 22| Benzytrimethylnitromethane amylmonium chloride  | 56-93-9    | ![Structure7](image) | C<sub>10</sub>H<sub>16</sub>CIN | 185.69           | Acetic acid 64-19-7    |
|   | Name                                                                 | CAS    | Molecular Formula | Molecular Weight | Reactant          | CAS    | Molecular Formula    |
|---|----------------------------------------------------------------------|--------|-------------------|------------------|-------------------|--------|---------------------|
| 23| Benzyltrimethylammonium chloride                                       | 56-93-9| C_{10}H_{16}ClN   | 185.69           | Glycerol          | 56-81-5| C_{3}H_{8}O_{3}      | 92.09 |
| 24| Benzyltrimethylammonium chloride                                       | 56-93-9| C_{10}H_{16}ClN   | 185.69           | Levulinic acid    | 123-76-2| C_{3}H_{6}O_{2}     | 116.11|
| 25| Benzyltriphenylphosphonium chloride                                     | 1100-88-5| C_{25}H_{22}ClP | 388.87           | Ethylene glycol   | 107-21-1| C_{2}H_{6}O_{2}     | 62.07 |
| 26| Benzyltriphenylphosphonium chloride                                     | 1100-88-5| C_{25}H_{22}ClP | 388.87           | Glycerol          | 56-81-5| C_{3}H_{8}O_{3}      | 92.09 |
| 27| Benzyltripropylammonium chloride                                        | 5197-87-5| C_{16}H_{28}ClN | 269.85           | DL-Lactic acid    | 598-82-3| C_{3}H_{6}O_{3}     | 90.08 |
| 28| Benzyltripropylammonium chloride                                        | 5197-87-5| C_{16}H_{28}ClN | 269.85           | Ethylene glycol   | 107-21-1| C_{2}H_{6}O_{2}     | 62.07 |
| 29| Benzyltripropylammonium chloride                                        | 5197-87-5| C_{16}H_{28}ClN | 269.85           | Glycerol          | 56-81-5| C_{3}H_{8}O_{3}      | 92.09 |
| No. | Compound                        | CAS Registry Number | Molecular Formula | Molecular Weight | Chemical Name | CAS Registry Number | Molecular Structure |
|-----|--------------------------------|---------------------|-------------------|------------------|---------------|---------------------|---------------------|
| 30  | Benzyltripropylammonium chloride | 5197-87-5           | C_{18}H_{28}ClN   | 269.85           | Phenol        | 108-95-2            | ![Molecular Structure](image1.png) |
| 31  | Betaine                         | 107-43-7            | C_{6}H_{11}NO_{2}  | 117.15           | DL-lactic acid| 598-82-3            | ![Molecular Structure](image2.png) |
| 32  | Betaine                         | 107-43-7            | C_{6}H_{11}NO_{2}  | 117.15           | Levulinic acid | 123-76-2            | ![Molecular Structure](image3.png) |
| 33  | Choline chloride                | 67-48-1             | C_{5}H_{11}ClN    | 139.62           | 1,2-Butanediol| 584-03-2            | ![Molecular Structure](image4.png) |
| 34  | Choline chloride                | 67-48-1             | C_{5}H_{11}ClN    | 139.62           | 1,2-Propanediol| 57-55-6             | ![Molecular Structure](image5.png) |
| 35  | Choline chloride                | 67-48-1             | C_{5}H_{11}ClN    | 139.62           | 1,3-Propanediol| 504-63-2            | ![Molecular Structure](image6.png) |
| 36  | Choline chloride                | 67-48-1             | C_{5}H_{11}ClN    | 139.62           | 1,4-Propanediol| 110-63-4            | ![Molecular Structure](image7.png) |
| 37  | Choline chloride                | 67-48-1             | C_{5}H_{11}ClN    | 139.62           | 2,2,2-Trifluoroacetamide| 354-38-1          | ![Molecular Structure](image8.png) |
| 38  | Choline chloride                | 67-48-1             | C_{5}H_{11}ClN    | 139.62           | 2,3-Propanediol| 513-85-9            | ![Molecular Structure](image9.png) |
| No. | Compound         | CAS Number | Molecular Formula | MW  | Chemical Formula | Molecular Weight |
|-----|------------------|------------|-------------------|-----|------------------|------------------|
| 39  | Choline chloride | 67-48-1    | C₅H₁₄ClNO        | 139.62 | Acetic acid (CH₃COOH) | 60.05 |
| 40  | Choline chloride | 67-48-1    | C₅H₁₄ClNO        | 139.62 | D-fructose (C₆H₁₂O₅) | 180.16 |
| 41  | Choline chloride | 67-48-1    | C₅H₁₄ClNO        | 139.62 | D-glucose (C₆H₁₂O₅) | 180.16 |
| 42  | Choline chloride | 67-48-1    | C₅H₁₄ClNO        | 139.62 | DL-lactic acid (C₃H₆O₃) | 90.08 |
| 43  | Choline chloride | 67-48-1    | C₅H₁₄ClNO        | 139.62 | DL-Xylitol (C₅H₁₀O₅) | 152.15 |
| 44  | Choline chloride | 67-48-1    | C₅H₁₄ClNO        | 139.62 | D-mannose (C₆H₁₂O₅) | 180.16 |
| 45  | Choline chloride | 67-48-1    | C₅H₁₄ClNO        | 139.62 | D-ribose (C₆H₁₀O₅) | 150.13 |
| 46  | Choline chloride | 67-48-1    | C₅H₁₄ClNO        | 139.62 | D-xylose (C₅H₁₀O₅) | 150.13 |
| 47  | Choline chloride | 67-48-1    | C₅H₁₄ClNO        | 139.62 | Ethanolamine (C₂H₇NO) | 61.08 |
|   |   |   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|---|---|
| 48 | Choline chloride | . 67-48-1 | C₅H₁₄ClNO | Cl⁻ | 139.62 | Ethylene glycol | 107-21-1 | C₂H₅O₂ | HO—OH | 62.07 |
| 49 | Choline chloride | . 67-48-1 | C₅H₁₄ClNO | Cl⁻ | 139.62 | Glutaric acid | 110-94-1 | C₃H₆O₄ | O—O—O—OH | 132.11 |
| 50 | Choline chloride | . 67-48-1 | C₅H₁₄ClNO | Cl⁻ | 139.62 | Glycerol | 56-81-5 | C₃H₈O₃ | HO—OH—OH | 92.09 |
| 51 | Choline chloride | . 67-48-1 | C₅H₁₄ClNO | Cl⁻ | 139.62 | Glycolic acid | 79-14-1 | C₂H₄O₃ | O—O—OH | 76.05 |
| 52 | Choline chloride | . 67-48-1 | C₅H₁₄ClNO | Cl⁻ | 139.62 | Hexafluoroisopropyl alcohol | 92-66-1 | C₃H₆F₆O | O—F—F—F—F—F | 168.04 |
| 53 | Choline chloride | . 67-48-1 | C₅H₁₄ClNO | Cl⁻ | 139.62 | Levulinic acid | 123-76-2 | C₅H₈O₃ | HO—O—CO—CO—OH | 116.11 |
| 54 | Choline chloride | . 67-48-1 | C₅H₁₄ClNO | Cl⁻ | 139.62 | Malonic acid | 141-82-2 | C₃H₄O₄ | O—O—CO—OH | 104.06 |
| 55 | Choline chloride | . 67-48-1 | C₅H₁₄ClNO | Cl⁻ | 139.62 | P-chlorophenol | 106-48-9 | C₆H₅ClO | O—Cl—C₆H₄—OH | 128.56 |
| 56 | Choline chloride | . 67-48-1 | C₅H₁₄ClNO | Cl⁻ | 139.62 | P-cresol | 106-44-5 | C₆H₅O | O—OH | 108.14 |
|   | Name                                      | CAS Number | Molecular Formula   | Molecular Weight | Function                                   | CAS Number | Formula       | Molecular Weight |
|---|-------------------------------------------|------------|---------------------|------------------|-------------------------------------------|------------|---------------|------------------|
| 57| Choline chloride                           | .67-48-1   | C₅H₁₄ClNO          | 139.62           | Phenol                                    | 108-95-2   | C₅H₈O         | 94.11            |
| 58| Choline chloride                           | .67-48-1   | C₅H₁₄ClNO          | 139.62           | Triethylene glycol                        | 112-27-6   | C₆H₁₂O₄       | 150.17           |
| 59| Choline chloride                           | .67-48-1   | C₅H₁₄ClNO          | 139.62           | Urea                                      | 57-13-6    | CH₅N₂O        | 60.06            |
| 60| Decyltrimethylammonium bromide             | 2082-84-0  | C₁₃H₂₆BrN          | 280.29           | Hexafluoroisopropyl alcohol               | 920-66-1   | C₂₀H₂₆F₆      | 268.04           |
| 61| Dodecyltrimethylammonium bromide           | 1119-94-4  | C₁₅H₃₀BrN          | 308.34           | Hexafluoroisopropyl glyceride              | 920-66-1   | C₂₀H₂₆F₆      | 268.04           |
| 62| L-carnitine                                | 541-15-1   | C₇H₁₅NO₃           | 161.20           | Hexafluoroisopropyl glyceride              | 920-66-1   | C₂₀H₂₆F₆      | 268.04           |
| 63| Methyltrioctylammonium bromide             | 35675-80-0 | C₂₅H₅₄BrN          | 448.61           | Decanoic acid                             | 334-48-5   | C₁₈H₃₂O₂      | 172.26           |
| 64| Methyltrioctylammonium chloride            | 5137-55-3  | C₂₅H₅₄ClN          | 404.16           | Ethylparaben                              | 120-47-8   | C₁₀H₁₂O₃      | 166.17           |
| 65| Methyltrioctylammonium chloride            | 5137-55-3  | C₂₅H₅₄ClN          | 404.16           | Oleic acid                                | 112-80-1   | C₁₈H₃₂O₂      | 282.46           |
|   | Name                                      | CAS Number | Molecular Formula | Molecular Weight | Basic Solution | Molar Mass | Density | Boiling Point | Formula |   |
|---|-------------------------------------------|------------|-------------------|------------------|---------------|------------|--------|---------------|---------|---|
|66 | Methyltriphenylphosphonium bromide        | 1779-49-3  | C19H18BrP         | 357.22           | 1,2-Propanediol | 57-55-6    |        |               | C2H5O2  | 76.09 |
|67 | Methyltriphenylphosphonium bromide        | 1779-49-3  | C19H18BrP         | 357.22           | 2,2,2-Trifluoroacetamide | 354-38-1 |        |               | C2H2F3N | 113.04 |
|68 | Methyltriphenylphosphonium bromide        | 1779-49-3  | C19H18BrP         | 357.22           | Acetic acid    | 64-19-7    |        |               | CH3COOH | 60.05 |
|69 | Methyltriphenylphosphonium bromide        | 1779-49-3  | C19H18BrP         | 357.22           | Ethylene glycol | 107-21-1  |        |               | C2H4O2  | 62.07 |
|70 | Methyltriphenylphosphonium bromide        | 1779-49-3  | C19H18BrP         | 357.22           | Glycerol       | 56-81-5    |        |               | C3H8O3  | 92.09 |
|71 | Methyltriphenylphosphonium bromide        | 1779-49-3  | C19H18BrP         | 357.22           | Levulinic acid | 123-76-2   |        |               | C4H6O3  | 116.11 |
| ID | Name                                         | CAS Number | Molecular Formula | Molecular Weight | Purity | CAS Number | Formula   | Purity | CAS Number | Formula   |
|----|----------------------------------------------|------------|-------------------|------------------|--------|------------|-----------|--------|------------|-----------|
| 72 | N,N-diethylethanolammonium chloride          | 13989-32-7 | C₆H₁₆ClNO         | 153.65           | Ethylene glycol | 107-21-1 | C₆H₂O₂   | 153.65 | Ethylene glycol | 62.07     |
| 73 | N,N-diethylethanolammonium chloride          | 13989-32-7 | C₆H₁₆ClNO         | 153.65           | Glycerol      | 56-81-5  | C₆H₂O₂   | 153.65 | Glycerol      | 92.09     |
| 74 | Tetrabutylammonium bromide                  | 1643-19-2  | C₁₆H₃₆BrN         | 322.37           | 1,2-Propanediol| 57-55-6  | C₆H₂O₂   | 322.37 | 1,2-Propanediol| 76.09     |
| 75 | Tetrabutylammonium bromide                  | 1643-19-2  | C₁₆H₃₆BrN         | 322.37           | Acetic acid   | 64-19-7  | CH₃COOH  | 322.37 | Acetic acid   | 60.05     |
| 76 | Tetrabutylammonium bromide                  | 1643-19-2  | C₁₆H₃₆BrN         | 322.37           | Ethanolamine  | 141-43-5 | C₇H₁₄NO | 322.37 | Ethanolamine  | 61.08     |
| 77 | Tetrabutylammonium bromide                  | 1643-19-2  | C₁₆H₃₆BrN         | 322.37           | Ethylene glycol| 107-21-1 | C₆H₂O₂   | 322.37 | Ethylene glycol| 62.07     |
| 78 | Tetrabutylammonium bromide                  | 1643-19-2  | C₁₆H₃₆BrN         | 322.37           | Levulinic acid| 123-76-2 | C₇H₁₄O₂  | 322.37 | Levulinic acid| 116.11    |
| 79 | Tetrabutylammonium bromide                  | 1643-19-2  | C₁₆H₃₆BrN         | 322.37           | Polyethylene glycol| 25322-68-3 | C₉H₁₄O₂₃ | 322.37 | Polyethylene glycol| 697.61 |
| 80 | Tetrabutylammonium bromide                  | 1643-19-2  | C₁₆H₃₆BrN         | 322.37           | Tetraethylene glycol| 112-60-7  | C₈H₁₈O₃ | 322.37 | Tetraethylene glycol| 194.23 |
|   | Compound                        | CAS Number | Formula   | Molecular Weight | Molecular Structure | 81      | 82      | 83      | 84      | 85      | 86      | 87      | 88      | 89      |
|---|---------------------------------|------------|-----------|------------------|---------------------|---------|---------|---------|---------|---------|---------|---------|---------|---------|
| 81| Tetrabutylammonium bromide      | 1643-19-2  | C_{16}H_{36}BrN | 322.37          | Tetrazole           |         |         | 288-94-8| CH_{3}N_{4} | N | N | N | N | 70.05    |
| 82| Tetrabutylammonium bromide      | 1643-19-2  | C_{16}H_{36}BrN | 322.37          | Triethylene glycol  |         |         |         | C_{6}H_{12}O_{4} | O | O | O | O | 150.17   |
| 83| Tetrabutylammonium chloride     | 1112-67-0  | C_{16}H_{36}ClN | 277.92          | Decanoic acid       |         |         |         | C_{10}H_{20}O_{2} | O | O | HO | HO | 172.26   |
| 84| Tetrabutylammonium chloride     | 1112-67-0  | C_{16}H_{36}ClN | 277.92          | Ethylene glycol     |         |         |         | C_{2}H_{6}O_{2} | HO | HO | HO | HO | 62.07    |
| 85| Tetrabutylammonium chloride     | 1112-67-0  | C_{16}H_{36}ClN | 277.92          | Glycerol            |         |         |         | C_{3}H_{8}O_{3} | HO | OH | HO | HO | 92.09    |
| 86| Tetrabutylammonium chloride     | 1112-67-0  | C_{16}H_{36}ClN | 277.92          | L-arginine          |         |         |         | C_{6}H_{14}N_{4}O_{2} | N | NH | NH | NH | 174.20   |
| 87| Tetrabutylammonium chloride     | 1112-67-0  | C_{16}H_{36}ClN | 277.92          | L-aspartic acid     |         |         |         | C_{4}H_{7}NO_{4} | O | O | HO | O | 133.10   |
| 88| Tetrabutylammonium chloride     | 1112-67-0  | C_{16}H_{36}ClN | 277.92          | Levulinic acid      |         |         |         | C_{5}H_{8}O_{3} | HO | O | HO | O | 116.11   |
| 89| Tetrabutylammonium chloride     | 1112-67-0  | C_{16}H_{36}ClN | 277.92          | L-glutamic acid     |         |         |         | C_{5}H_{9}NO_{4} | O | O | O | O | 147.13   |
|   | Name                          | CAS Number | Structure       | Molecular Weight | Formula | Function          | CAS Number | Molecular Weight |
|---|-------------------------------|------------|----------------|------------------|--------|-------------------|------------|------------------|
| 90 | Tetrabutylammonium chloride   | 1112-67-0  | N⁺Cl⁻          | 277.92           | C₁₆H₃₆ClN | Phenylacetic acid | 103-82-2  | C₉H₁₀O₂         | 136.15 |
| 91 | Tetrabutylammonium chloride   | 1112-67-0  | N⁺Cl⁻          | 277.92           | C₁₆H₃₆ClN | Propionic acid    | 79-09-4   | C₅H₁₀O₂         | 74.08  |
| 92 | Tetrabutylammonium chloride   | 1112-67-0  | N⁺Cl⁻          | 277.92           | C₁₆H₃₆ClN | Triethylene glycol | 112-27-6  | C₆H₁₂O₄       | 150.17 |
| 93 | Tetrabutylphosphonium bromide | 3115-68-2  | P⁺Br⁻          | 339.33           | C₁₆H₃₆BrP | Levulinic acid    | 123-76-2  | C₅H₈O₃         | 116.11 |
| 94 | Tetradecyltrimethylammonium bromide | 1119-97-7 | C₁₇H₃₈BrN⁺     | 336.39           | C₁₇H₃₈BrN⁺ | Hexafluoroisopropanol | 920-66-1 | C₃H₂F₆O | 168.04 |
| 95 | Tetrathyldiammonium bromide   | 71-91-0    | N⁺Br⁻          | 210.16           | C₈H₁₆BrN⁺ | Ethylene glycol   | 107-21-1  | C₂H₄O₂         | 62.07  |
| 96 | Tetrathyldiammonium bromide   | 71-91-0    | N⁺Br⁻          | 210.16           | C₈H₁₆BrN⁺ | Levulinic acid    | 123-76-2  | C₇H₁₄O₃       | 116.11 |
| 97 | Tetrathyldiammonium bromide   | 71-91-0    | N⁺Br⁻          | 210.16           | C₈H₁₆BrN⁺ | Triethylene glycol | 112-27-6  | C₆H₁₂O₄       | 150.17 |
| 98 | Tetrathyldiammonium chloride  | 56-34-8    | N⁺Cl⁻          | 165.7            | C₈H₁₆ClN | Acetic acid       | 64-19-7   | CH₃COOH        | 60.05  |
| 99 | Tetrathyldiammonium chloride  | 56-34-8    | N⁺Cl⁻          | 165.7            | C₈H₁₆ClN | Glycolic acid     | 79-14-1   | C₂H₂O₂         | 76.05  |
| No. | Compound Description                                      | CAS Number | Molecular Formula    | Molecular Weight | Companion Description             | CAS Number | Molecular Formula    | Molecular Weight |
|-----|----------------------------------------------------------|------------|---------------------|------------------|-----------------------------------|------------|---------------------|------------------|
| 100 | Tetraethylammonium chloride                              | 56-34-8    | C<sub>8</sub>H<sub>20</sub>ClN | 165.7            | Levulinic acid                    | 123-76-2   | C<sub>5</sub>H<sub>8</sub>O<sub>3</sub> | 116.11           |
| 101 | Tetraethylammonium chloride                              | 56-34-8    | C<sub>8</sub>H<sub>20</sub>ClN | 165.7            | Octanoic acid                     | 124-07-2   | C<sub>8</sub>H<sub>16</sub>O<sub>2</sub> | 144.21           |
| 102 | Tetraethylammonium p-toluenesulfonate                    | 733-44-8   | C<sub>15</sub>H<sub>27</sub>NO<sub>3</sub>S | 322.37           | 1,2-Propanediol                   | 57-55-6    | C<sub>2</sub>H<sub>6</sub>O<sub>2</sub> | 76.09            |
| 103 | Tetraethylammonium p-toluenesulfonate                    | 733-44-8   | C<sub>15</sub>H<sub>27</sub>NO<sub>3</sub>S | 322.37           | Ethylene glycol                   | 107-21-1   | C<sub>2</sub>H<sub>6</sub>O<sub>2</sub> | 62.07            |
| 104 | Tetraethylammonium p-toluenesulfonate                    | 733-44-8   | C<sub>15</sub>H<sub>27</sub>NO<sub>3</sub>S | 322.37           | Polyethylene glycol               | 25322-68-3 | C<sub>2n</sub>H<sub>4n+2</sub>O<sub>n+1</sub> | 697.61           |
| 105 | Tetraethylammonium p-toluenesulfonate                    | 733-44-8   | C<sub>15</sub>H<sub>27</sub>NO<sub>3</sub>S | 322.37           | Tetraethylene glycol              | 112-60-7   | C<sub>10</sub>H<sub>16</sub>O<sub>3</sub> | 194.23           |
| 106 | Tetraheptylammonium chloride                             | 10247-90-2 | C<sub>28</sub>H<sub>60</sub>ClN | 446.24           | Decanoic acid                     | 334-48-5   | C<sub>10</sub>H<sub>20</sub> | 172.26           |
| 107 | Tetraheptylammonium chloride                             | 10247-90-2 | C<sub>28</sub>H<sub>60</sub>ClN | 446.24           | Ibuprofen                        | 15687-27-1 | C<sub>13</sub>H<sub>18</sub>O<sub>2</sub> | 206.28           |
| 108 | Tetraheptylammonium chloride                             | 10247-90-2 | C<sub>28</sub>H<sub>60</sub>ClN | 446.24           | Oleic acid                       | 112-80-1   | C<sub>18</sub>H<sub>34</sub>O<sub>2</sub> | 282.46           |
|   | Compound                        | CAS Registry Number | Molecular Formula | MW (g/mol) | Co-solvent          | Chemical Formula | Boiling Point (°C) | Density (g/cm³) |
|---|---------------------------------|---------------------|-------------------|------------|---------------------|------------------|-------------------|------------------|
| 109 | Tetrahexylammonium bromide     | 4328-13-6           | C_{24}H_{52}BrN   | 434.58     | Ethylene glycol     | C_{2}H_{6}O_{2}  | 107-21-1          | 62.07            |
| 110 | Tetrahexylammonium bromide     | 4328-13-6           | C_{24}H_{52}BrN   | 434.58     | Glycerol            | C_{3}H_{8}O_{3}  | 56-81-5           | 92.09            |
| 111 | Tetramethylammonium chloride   | 75-57-0             | C_{6}H_{12}NCl    | 109.60     | Glycerol            | C_{3}H_{8}O_{3}  | 56-81-5           | 92.09            |
| 112 | Tetraoctylammonium bromide     | 14866-33-2          | C_{32}H_{68}BrN   | 546.79     | Decanoic acid       | C_{10}H_{20}O_{2} | 334-48-5         | 172.26           |
| 113 | Tetraoctylammonium chloride    | 3125-07-3           | C_{32}H_{68}ClN   | 502.34     | Decanoic acid       | C_{10}H_{20}O_{2} | 334-48-5         | 172.26           |
| 114 | Tetrapropylammonium bromide    | 1941-30-6           | C_{12}H_{28}N.Br  | 266.26     | Ethylene glycol     | C_{2}H_{6}O_{2}  | 107-21-1          | 62.07            |
| 115 | Tetrapropylammonium bromide    | 1941-30-6           | C_{12}H_{28}N.Br  | 266.26     | Glycerol            | C_{3}H_{8}O_{3}  | 56-81-5           | 92.09            |
| 116 | Tetrapropylammonium bromide    | 1941-30-6           | C_{12}H_{28}N.Br  | 266.26     | Levulinic acid      | C_{5}H_{8}O_{3}  | 123-76-2          | 116.11           |
| 117 | Tetrapropylammonium bromide    | 1941-30-6           | C_{12}H_{28}N.Br  | 266.26     | Triethylene glycol  | C_{6}H_{12}O_{4} | 112-27-6          | 150.17           |
| No. | Name                  | CAS No. | Molecular Formula | Molecular Weight | Formula | Melting Point | Solvent | Density |
|-----|-----------------------|---------|-------------------|------------------|--------|--------------|---------|---------|
| 118 | Tetrapropylammonium chloride | 5810-42-4 | C_{12}H_{25}ClN | 221.81          | CH₃COOH | 64-19-7      | 60.05   |
| 119 | Tetrapropylammonium chloride | 5810-42-4 | C_{12}H_{25}ClN | 221.81          | C₂H₅NO  | 141-43-5     | 61.08   |
| 120 | Tetrapropylammonium chloride | 5810-42-4 | C_{12}H_{25}ClN | 221.81          | Leuvinic acid | 123-76-2 | 116.11   |
| 121 | Triethylmethylammonium chloride | 10052-47-8 | C₇H₁₈ClN | 151.68          | Acetic acid | 64-19-7 | 60.05   |
| 122 | Triethylmethylammonium chloride | 10052-47-8 | C₇H₁₈ClN | 151.68          | Ethylene glycol | 107-21-1 | 62.07   |
| 123 | Triethylmethylammonium chloride | 10052-47-8 | C₇H₁₈ClN | 151.68          | Glycerol | 56-81-5 | 92.09   |
| 124 | Triethylmethylammonium chloride | 10052-47-8 | C₇H₁₈ClN | 151.68          | DL-lactic acid | 598-82-3 | 90.08   |
| 125 | Triethylmethylammonium chloride | 10052-47-8 | C₇H₁₈ClN | 151.68          | Leuvinic acid | 123-76-2 | 116.11   |
| No. | Compound                           | CAS No.  | Molecular Structure | Molecular Formula | Molecular Weight |
|-----|------------------------------------|----------|---------------------|-------------------|------------------|
| 126 | Potassium carbonate               | 584-08-7 | ![Structure](image)  | K₂CO₃             | 138.21           |
|     |                                    |          |                     |                   |                  |
| 127 | Potassium carbonate               | 584-08-7 | ![Structure](image)  | K₂CO₃             | 138.21           |
|     |                                    |          |                     |                   |                  |
| 128 | Sodium dodecanoate                | 629-25-4 | ![Structure](image)  | C₁₂H₂₃O₂Na        | 222.30           |
|     |                                    |          |                     |                   |                  |
| 129 | Zinc chloride                     | 7646-85-7| ![Structure](image)  | ZnCl₂             | 136.3            |
|     |                                    |          |                     |                   |                  |
| 130 | Zinc chloride                     | 7646-85-7| ![Structure](image)  | ZnCl₂             | 136.3            |
|     |                                    |          |                     |                   |                  |
| 131 | Acetamide                          | 60-35-5  | ![Structure](image)  | C₂H₅NO            | 59.07            |
|     |                                    |          |                     |                   |                  |
| 132 | Atropine                           | 51-55-8  | ![Structure](image)  | C₁₇H₂₃NO₃        | 289.37           |
|     |                                    |          |                     |                   |                  |
| 133 | Atropine                           | 51-55-8  | ![Structure](image)  | C₁₇H₂₃NO₃        | 289.37           |
|     |                                    |          |                     |                   |                  |
| 134 | Decanoic acid                      | 334-48-5 | ![Structure](image)  | C₁₀H₂₀O₂          | 172.26           |
|     |                                    |          |                     |                   |                  |
| 135 | DL-menthol                         | 89-78-1  | ![Structure](image)  | C₁₀H₁₆O           | 156.27           |
|     |                                    |          |                     |                   |                  |
| 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_{7}H_{6}O_2 | 122.2 |
| 139 | DL-menthol | 89-78-1 | C_{10}H_{20}O | 156.27 | Decanoic acid | 334-48-5 | C_{10}H_{20}O_2 | 172.2 |
| 140 | DL-menthol | 89-78-1 | C_{10}H_{20}O | 156.27 | Dodecanoic acid | 143-07-7 | C_{12}H_{20}O_2 | 200.3 |
| 141 | DL-menthol | 89-78-1 | C_{10}H_{20}O | 156.27 | Ibuprofen | 15687-27-1 | C_{13}H_{18}O_2 | 206.2 |
| 142 | DL-menthol | 89-78-1 | C_{10}H_{20}O | 156.27 | L-lactic acid | 79-33-4 | C_{3}H_{6}O_3 | 90.08 |
|    |     |          |     |        |      |       |          |     |          |      |
|----|-----|----------|-----|--------|------|-------|----------|-----|----------|------|
| 143| DL-menthol | 89-78-1 | C\textsubscript{10}H\textsubscript{20}O | 156.27 | Octanoic acid | 124-07-2 | C\textsubscript{6}H\textsubscript{12}O\textsubscript{2} | 144.21 |
| 144| DL-menthol | 89-78-1 | C\textsubscript{10}H\textsubscript{20}O | 156.27 | Phenylacetic acid | 103-82-2 | C\textsubscript{6}H\textsubscript{6}O\textsubscript{2} | 136.15 |
| 145| DL-menthol | 89-78-1 | C\textsubscript{10}H\textsubscript{20}O | 156.27 | Pyruvic acid | 127-17-3 | C\textsubscript{4}H\textsubscript{4}O\textsubscript{3} | 88.06  |
| 146| DL-menthol | 89-78-1 | C\textsubscript{10}H\textsubscript{20}O | 156.27 | Thymol | 89-83-8 | C\textsubscript{10}H\textsubscript{14}O | 150.22 |
| 147| Imidazole  | 288-32-4 | C\textsubscript{3}H\textsubscript{4}N\textsubscript{2} | 68.08 | Acetic acid | 64-19-7 | CH\textsubscript{3}COOH | 60.05  |
| 148| Lidocaine  | 137-58-6 | C\textsubscript{14}H\textsubscript{22}N\textsubscript{2}O | 234.34 | Decanoic acid | 334-48-5 | C\textsubscript{10}H\textsubscript{20}O\textsubscript{2} | 172.26 |
| 149| Lidocaine  | 137-58-6 | C\textsubscript{14}H\textsubscript{22}N\textsubscript{2}O | 234.34 | DL-menthol | 89-78-1 | C\textsubscript{10}H\textsubscript{20}O | 156.27 |
| 150| Lidocaine  | 137-58-6 | C\textsubscript{14}H\textsubscript{22}N\textsubscript{2}O | 234.34 | Thymol | 89-83-8 | C\textsubscript{10}H\textsubscript{20}O | 150.22 |
| No. | Compound   | CAS Number | Molecular Formula | Molecular Weight | Other Compound | CAS Number | Molecular Formula | Molecular Weight |
|-----|------------|------------|-------------------|------------------|---------------|------------|-------------------|------------------|
| 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_{18}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_{22}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_{8}H_{16}O_{2}  | 144.21           |
| No. | Name                  | CAS No.  | molecular formula | molecular weight | common name                  | CAS No. | molecular formula | molecular weight |
|-----|-----------------------|----------|-------------------|------------------|-----------------------------|---------|-------------------|------------------|
| 158 | L-menthol             | 2216-51-5| C₁₀H₂₀O           | 156.27           | Tetradecanoic acid          | 544-63-8| C₁₄H₂₉O₂          | 228.37           |
| 159 | L-menthol             | 2216-51-5| C₁₀H₂₀O           | 156.27           | Thymol                      | 89-83-8 | C₁₀H₁₄O           | 150.22           |
| 160 | L-menthol             | 2216-51-5| C₁₀H₂₀O           | 156.27           | Trans-sobrerol              | 42370-41-2| C₁₀H₂₀O           | 170.25           |
| 161 | L-proline             | 147-85-3 | C₅H₉NO₂           | 115.13           | DL-lactic acid              | 598-82-3| C₅H₉O₂            | 90.08            |
| 162 | L-proline             | 147-85-3 | C₅H₉NO₂           | 115.13           | Levulinic acid              | 123-76-2| C₅H₉O₂            | 116.11           |
| 163 | Hexanoic acid         | 112-05-0 | C₆H₁₄O₂           | 158.24           | Dodecanoic acid             | 143-07-7| C₁₀H₂₀O₂          | 200.32           |
| 164 | Octanoic acid         | 124-07-2 | C₈H₁₆O₂           | 144.21           | Dodecanoic acid             | 143-07-7| C₁₀H₂₀O₂          | 200.32           |
| 165 | Thymol                | 89-83-8  | C₁₀H₁₄O           | 150.22           | 1,2-Decanediol              | 1119-86-4| C₁₀H₂₀O₂          | 174.28           |
| 166 | Thymol                | 89-83-8  | C₁₀H₁₄O           | 150.22           | 10-Undecylenic acid         | 112-38-9| C₁₁H₂₂O₂          | 184.28           |
| No. | Compound   | CAS     | Molecular Formula | Molecular Weight | CAS     | Molecular Formula | Molecular Weight |
|-----|------------|---------|-------------------|------------------|---------|-------------------|------------------|
| 167 | Thymol     | 89-83-8 | C₆H₁₂O            | 150.22           | Coumarin | 91-64-5 | C₈H₈O₂ | 146.14 |
| 168 | Thymol     | 89-83-8 | C₆H₁₂O            | 150.22           | D-camphor | 464-49-3 | C₁₀H₁₆O | 152.23 |
| 169 | Thymol     | 89-83-8 | C₆H₁₂O            | 150.22           | Decanoic acid | 334-48-5 | C₁₀H₂₀O₂ | 172.26 |
| 170 | Thymol     | 89-83-8 | C₆H₁₂O            | 150.22           | DL-camphor | 21368-68-3 | C₁₀H₁₆O | 152.23 |
| 171 | Thymol     | 89-83-8 | C₆H₁₂O            | 150.22           | Dodecanoic acid | 143-07-7 | C₁₂H₂₆O₂ | 200.32 |
| 172 | Thymol     | 89-83-8 | C₆H₁₂O            | 150.22           | Hexadecanoic acid | 57-10-3 | C₁₆H₃₂O₂ | 256.43 |
| 173 | Thymol     | 89-83-8 | C₆H₁₂O            | 150.22           | L-borneol | 464-45-9 | C₁₀H₁₆O | 154.25 |
| 174 | Thymol     | 89-83-8 | C₆H₁₂O            | 150.22           | Octadecanoic acid | 57-11-4 | C₁₈H₃₆O₂ | 284.48 |
|   |     |     |     |     |     |     |     |     |     |     |     |     |
|---|----|----|----|----|----|----|----|----|----|----|----|----|
| 175 | Thymol | 89-83-8 | C₁₀H₁₄O | 150.22 | Octanoic acid | 124-07-2 | C₇H₁₄O₂ | 144.21 |
| 176 | Thymol | 89-83-8 | C₁₀H₁₄O | 150.22 | Tetradecanoic acid | 544-63-8 | C₁₄H₂₀O₂ | 228.37 |
| 177 | Thymol | 89-83-8 | C₁₀H₁₄O | 150.22 | Triocetylphosphine oxide | 78-50-2 | C₂₄H₅₁O₅P | 386.63 |
| 178 | Triethanolamine | 102-71-6 | C₆H₁₅NO₃ | 149.19 | 2-Methoxyphenol | 90-05-1 | C₇H₈O₂ | 124.14 |
| 179 | Triethanolamine | 102-71-6 | C₆H₁₅NO₃ | 149.19 | 3-Methoxyphenol | 150-19-6 | C₇H₈O₂ | 124.14 |
| 180 | Triethanolamine | 102-71-6 | C₆H₁₅NO₃ | 149.19 | 4-Methoxyphenol | 150-76-5 | C₇H₈O₂ | 124.14 |
| 181 | Triocetylphosphine oxide | 78-50-2 | C₃₀H₅₁O₅P | 386.63 | Decanoic acid | 334-48-5 | C₁₀H₁₈O₂ | 172.26 |
| 182 | Triocetylphosphine oxide | 78-50-2 | C₃₀H₅₁O₅P | 386.63 | Dodecanoic acid | 143-07-7 | C₁₂H₂₄O₂ | 200.32 |
| 183 | Triocetylphosphine oxide | 78-50-2 | C₃₀H₅₁O₅P | 386.63 | Phenol | 108-95-2 | C₆H₅O | 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, acetylocholinium chloride and benzylidimethyl(2- |
|      |                        |                        |             |        |        | Cholinium chloride, acetylocholinium chloride and |
| No. | Heating method | Method | 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 microviscometer(Anton Par, model Lovis-2000M/ME) | The viscosity meter has a measuring uncertainty of ±5×10⁻³ mPa.s and | R&M Chemicals | Allyltriphenyl phosphonium bromide, diethylene glycol and triethylene glycol, >99 | Without further purification |
| Location | Heating method | Method | Uncertainty of viscosity | N/A | Chemicals |
|----------|----------------|--------|--------------------------|-----|-----------|
| 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%. |
| 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. |
| 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%; Tetrapropylammonium chloride, >97 wt%; Tetrapropyl-ammonium bromide, >98 wt%; Tetrabutylammonium chloride, >97 wt%; Tetrabutylammonium bromide, >98 wt%; Benzyltrimethyl- without further purification |
|    | Heating method | Instrument | Heating method details | Chemicals Used | Purity Remarks |
|----|----------------|------------|------------------------|----------------|---------------|
| 11 | Heating method | Brookfield R/S plus Rheometer | (3-5)% of measured value | ammonium chloride, >98 wt%; Trioctylmethylammonium 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%. | All the chemicals used were of high purity(>99wt%). |
| 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. | 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. |
|   | Heating method | Equipment | Supplier | Chemicals | Remarks |
|---|----------------|-----------|----------|-----------|---------|
| 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 |
| No. | Heating Method | Instrument/Company | Accuracy | Chemicals | Notes |
|-----|---------------|--------------------|----------|-----------|-------|
| 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%. 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. |
| 17  | Heating method | Brookfield instrument | N/A | Merck(Germany) | All chemicals are high purity, ≥98 wt%. |
| 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 |
| 19 | Heating method | a rotational viscometer (Anton Paar Rheolab QC) | (3-5)% of measured value | Merck Chemicals (Darmstadt, Germany) | Choline chloride (D-fructose anhydrous), 98 wt%. | HBA and dried under vacuum at 80 °C for 48 h before use. |
| 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%. | Chemicals were dried in a vacuum oven prior to use to eliminate moisture contamination. |
| 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% solution in high-vacuum line (pressure \( p < 10^{-9} \) bar). Ethylene glycol (EG) was dried by 3A molecular sieve.

|   | Heating method | Heating method | Grinding method | Scionix Ltd | N/A |
|---|----------------|----------------|-----------------|-------------|-----|
| 23 | N/A            | Automated SM 3000 Anton Paar rotational Stabinger viscometer densimeter | Sigma-Aldrich | N/A | Choline chloride, \( \geq 98 \) wt%; Oxalic, malonic, adipic, levulinic, glutaric, glycolic, succinic, malic, tartaric, fumaric, azelaic, and citric acids, all \( \geq 99 \) 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.

|   | N/A            | Nonequilibrium periodic perturbation method | N/A | N/A |
|---|----------------|--------------------------------------------|-----|-----|
| 24 | Heating method | Automated SM 3000 Anton Paar rotational Stabinger viscometer densimeter | Sigma-Aldrich | N/A | Choline chloride, 99wt%; Ethylene glycol, 1,4-butanediol, and citric acid.

Choline chloride was recrystallized from absolute
| Method   | Instrument                  | Uncertainty of Temperature | Supplier 1 | Supplier 2 | Notes                                                                 |
|----------|-----------------------------|-----------------------------|------------|------------|----------------------------------------------------------------------|
| 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, |
| 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 before use. 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 |
|   | Heating method | Instrument | Supplier | Comments |
|---|----------------|------------|----------|----------|
| 34 | Heating method | Rheometer(DISCOVER Y HR-2, USA) | N/A | Aladdin Chemistry Co., Sinopharm Chemical Reagent Co., Ltd. | All reagents used are of analytical grade. |
| 35 | Heating method | Anton Paar SVM 3000 Stabinger Viscometer | N/A | 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%. |
| 36 | Heating method | viscometer(DMA 5000M, Anton Paar GmbH) | N/A | N/A | without further purification |
| 37 | Heating method | automated falling ball microviscometer(Anton Paar GmbH, model) | N/A | Merck | N,N-diethylethanalammonium chloride, >98 wt%; The DES was vacuum dried at 343 K, and kept in a |
| Page | Heating method | Antisolvent | Rotor | VG | Reagents |
|------|----------------|-------------|-------|----|----------|
| 38   | Heating method | Anton Paar Lovis 2000 ME micro viscometer | ±1% | accuracy up to 0.5% | Glycerol, >99.5wt%; Ethylene glycol, >99.9wt%.
|      |                |             |       |     | dry box prior to use. |
| 39   | Heating        | Brookfield DV-II+ Pro | N/A | J&K Chemical, Ltd. | All reagents were without further purification. | The prepared DESs.
|   | Heating method | Viscometer | Uncertainties | Chemicals | Prior treatment |
|---|----------------|------------|---------------|-----------|----------------|
| 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) | Tetraethylammonium 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 |
| #  | Heating method | Heating method | Sigma-Aldrich | Sigma-Aldrich | N/A |
|----|----------------|----------------|---------------|---------------|-----|
| 47 | Anton Paar (model SVM 3000) automated rotational Stabinger viscometer-densimeter | Dodecanoate sodium salt, 99-100 wt%; Decanoic acid, >98 wt% | a vacuum oven to assure a low moisture content of below 200 ppm. | without further purification |
| 48 | Anton Paar AMVn falling ball automated microviscometer | Guanidine isothiocyanate (GI) and acetamide (AT) were AR grade with the mass purity higher than 0.99. 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. | Shanghai Aladdin Chemical Company | without further purification |
| 49 | Anton Paar Lovis 2000 ME rolling ball | 1-Tetradecanol, ≥97.0 wt%; Thymol, ≥99.0 wt% | Sigma-Aldrich | N/A |
| 50 | Heating method | Anton Paar (model SVM 3000) automated rotational Stabinger viscometer-densimeter | 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%. |
| 51 | Heating method | Anton Paar Lovis 2000 ME rolling ball viscometer | Sigma-Aldrich | Octanoic acid, ≥98 wt%; Decanoic acid, ≥98 wt%; Nonanoic acid, ≥98 wt%; Dodecanoic acid, ≥98 wt%; |
| 52 | Heating method | Anton Paar (model SVM 3000) automated rotational Stabinger viscometer-densimeter | Sigma-Aldrich and Fluka | 1-Tetradecanol, ≥97 wt%; DL-menthol, ≥99 wt%; |

Sigma-Aldrich and Fluka

50 Heating method
Anton Paar (model SVM 3000) automated rotational Stabinger viscometer-densimeter
The temperature uncertainty is ±0.01 °C. 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

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
| Heating method | Instrument         | Dynamic viscosity/Composition | Uncertainty/Additional Information |
|----------------|--------------------|-------------------------------|------------------------------------|
| 53             | Kinexus Prot Rheometer (Kinexus Prot, MAL1097376, Malvern) | 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. |
| 54             | Anton Paar SVM 3000/G2 type Stabinger instrument | Uncertainty of ±0.005 mPa s for the viscosity. | Sigma Aldrich Tetraoctylammonium bromide, >96 wt%; Menthol, ≥99 wt%; Lidocaine, ≥99 wt%; Thymol, ≥99 wt%; Decanoic acid, >98 wt%. | N/A |
| 55             | 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 |
| Page | Heating method | Equipment | Relative uncertainty | Supplier | Compounds |
|------|----------------|-----------|----------------------|----------|-----------|
| 56   | Automated      | Anton Paar SVM 3000 Stabinger viscosimeter-densimeter | Dynamic viscosity ±0.35% | Sigma-Aldrich | Sigma-Aldrich DL-Menthol, ≥95 wt%; Octanoic acid, ≥99 wt%.
|      | method         |           |                      |          | 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        | Anton Paar Physica MCR 301 rheometer | N/A | Sigma-Aldrich | Sigma-Aldrich Lidocaine, >99 wt%; Decanoic acid, >98 wt%.
| method|               |           |                      |          | N/A |
| 58   | Heating        | 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%.
| method|               |           |                      |          | without further purification |
| 59   | Heating        | 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 |
| method|               |           |                      |          | without further purification |
| Table 2 | Heating method | Measurement method | Reproducibility | Supplier | N/A | N/A | Notes |
|---------|----------------|--------------------|-----------------|----------|-----|-----|-------|
| 60      | Heating method | a commercial rolling ball viscometer (Lovis 2000 M/ME, Anton Paar, Germany) | N/A | Sigma-Aldrich | N/A | 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%; Trioclylphosphine 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 wt% | The as-prepared DESs were then dried under vacuum | |
| Method          | Equipment                                    | Uncertainty          | Contact          | Notes                                                                 |
|-----------------|----------------------------------------------|----------------------|------------------|----------------------------------------------------------------------|
| Heating method  | microviscosimeter Lovis 2000/ME connected to the Anton Paar DSA-5000M densimeter | ±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 |
| 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. |
| Heating method  | interfacial rheometer(model: Physica MCR301, Anton-Paar Make) | ±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.