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# Supporting Information

## Model Development and Design Criteria of Hypergolic Imidazolium Ionic Liquids from Ignition Delay Time and Viscosity Viewpoints

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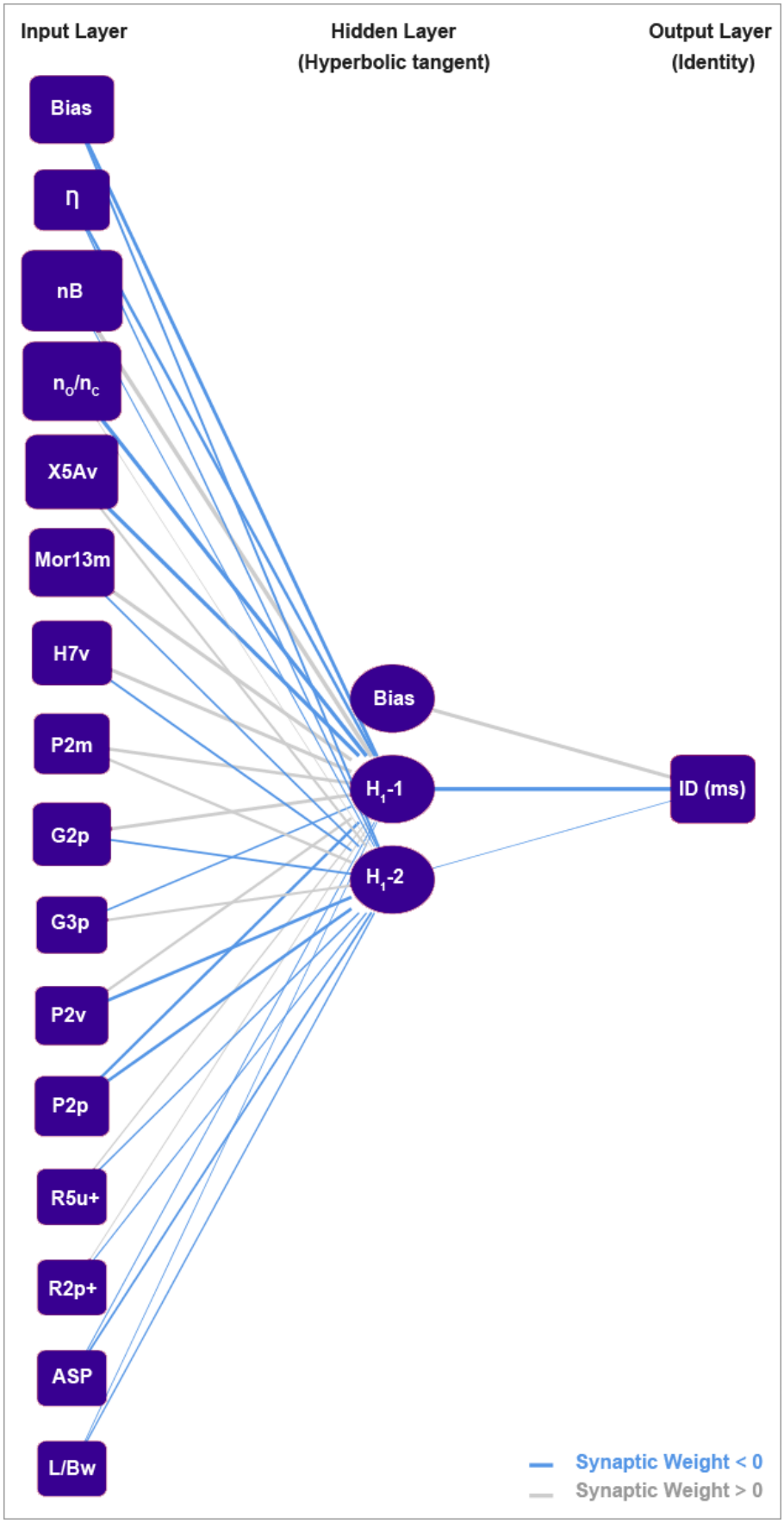


**Figure S1.** General structure of applied MLP-ANN networks for ID times of HEILs.

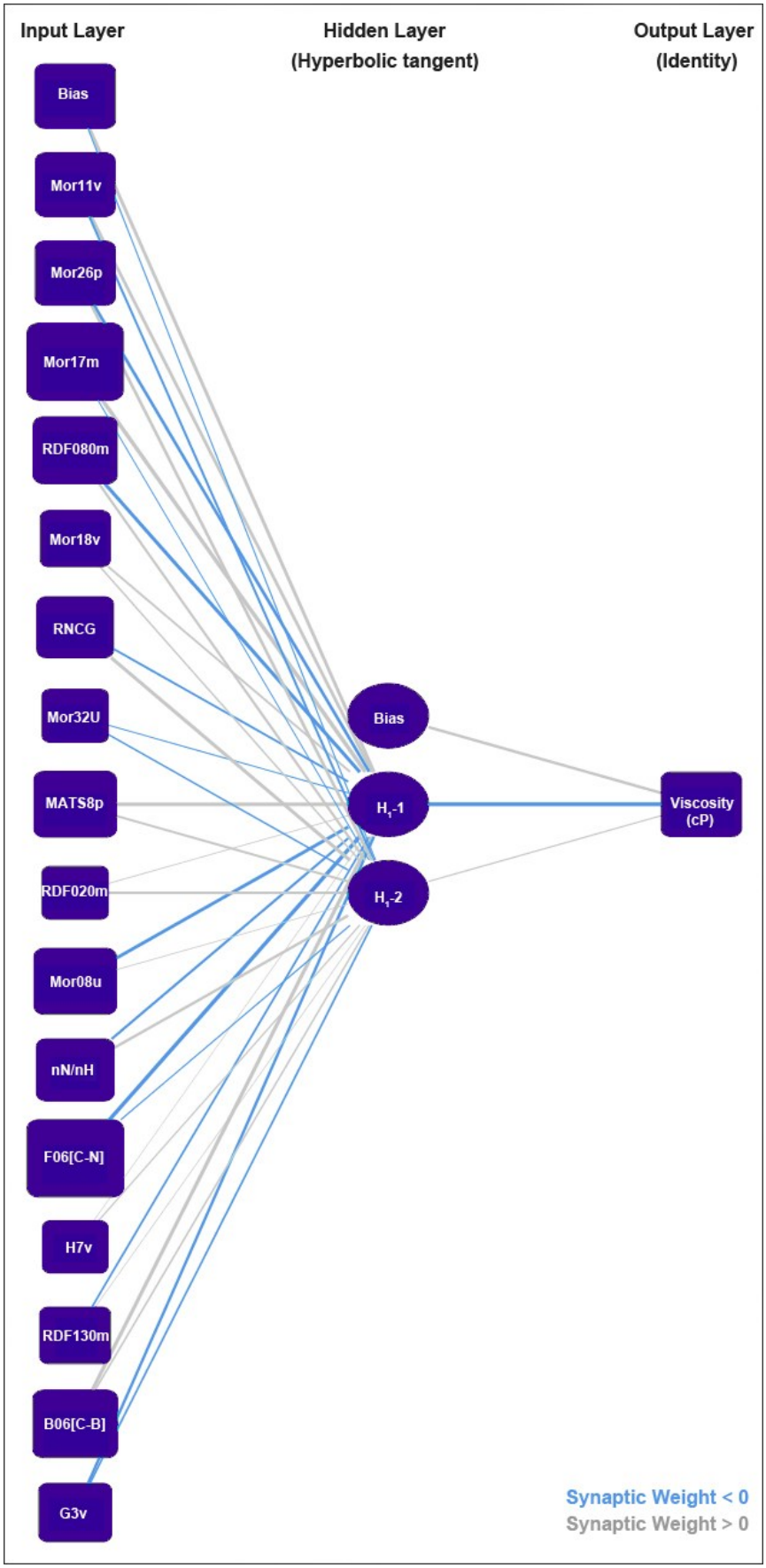


**Figure S2.** General structure of applied MLP-ANN networks for viscosity of HEILs.

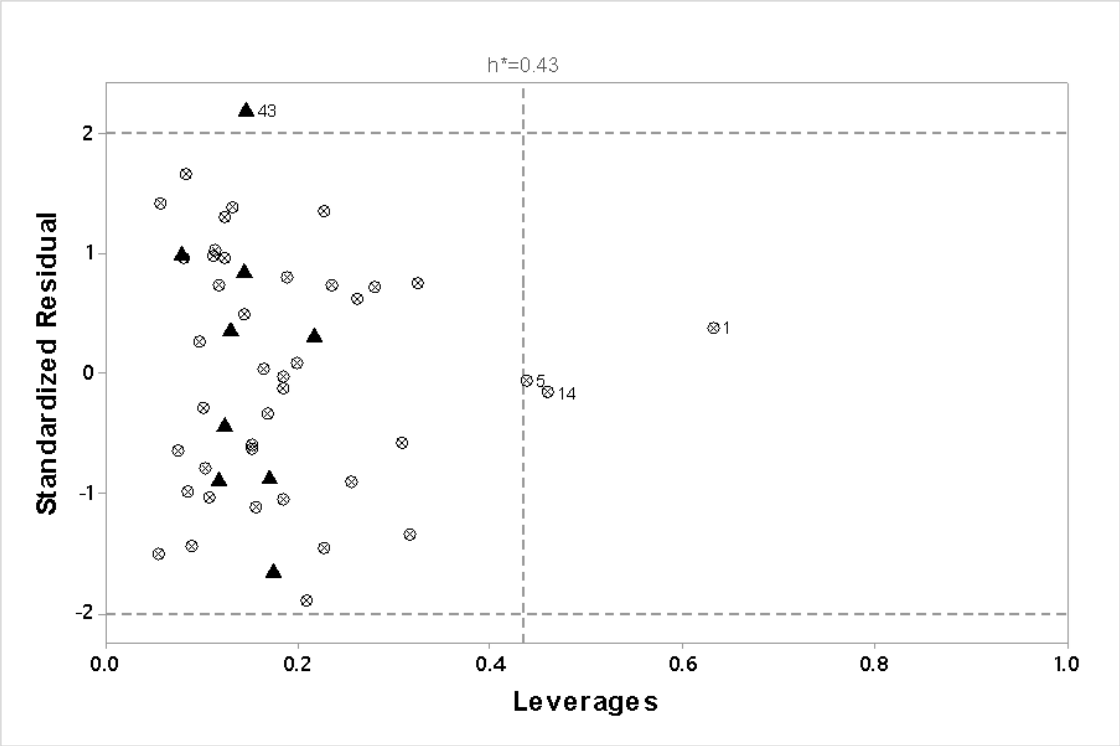


**Figure S3.** Leverage values versus residuals for ID times of ionic liquids.

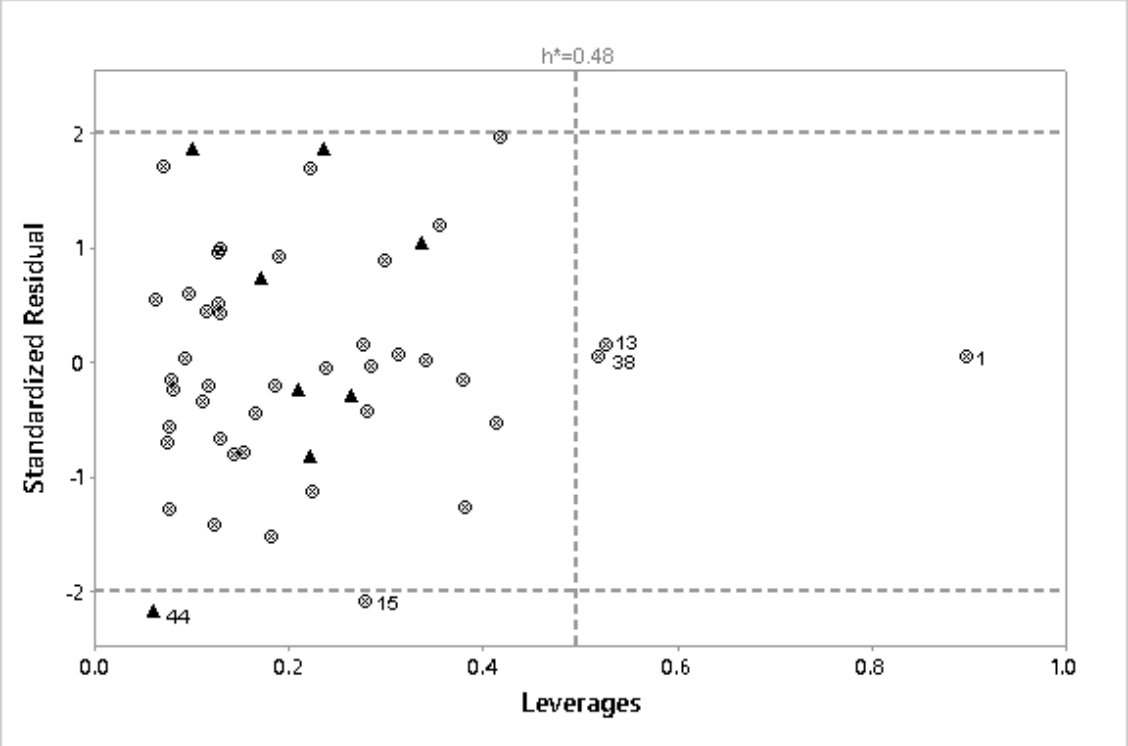


**Figure S4.** Leverage values versus residuals for viscosity of ionic liquids.

**Table S1.** Mean values of independent variable importance analysis (50 repetition) for ID times of HEILs.

| No. | Descriptor | Importance | Normalized importance |
|---|---|---|---|
| 1 | $\frac{n_o}{n_c}$ | 0.205 | 100.00% |
| 2 | $n_B$ | 0.188 | 91.70% |
| 3 | ***X5Av*** | 0.153 | 74.50% |
| 4 | η | 0.106 | 51.80% |
| 5 | ***H7v*** | 0.075 | 36.40% |
| 6 | ***Mor13m*** | 0.064 | 31.20% |
| 7 | ***G2p*** | 0.048 | 23.20% |
| 8 | ***G3p*** | 0.046 | 22.50% |
| 9 | ***R5u+*** | 0.040 | 19.40% |
| 10 | ***P2v*** | 0.031 | 15.30% |
| 11 | ***R2p+*** | 0.017 | 8.50% |
| 12 | ***P2m*** | 0.010 | 4.80% |
| 13 | ***P2p*** | 0.008 | 3.80% |
| 14 | ***ASP*** | 0.005 | 2.50% |
| 15 | ***L/Bw*** | 0.004 | 1.80% |

**Table S2.** The results of best subsets regression analysis on the selected molecular descriptors for ID times of HEILs.

| Variables | $R^2$ | $R^2$ (Adjusted) | PRESS | $R^2$ (predicted) | Mallows Cp | S | η (Cp) | nB | $n_o/n_c$ | X5Av | Mor13m | H7v | P2m | G2p | G3p | P2v | P2p | R5u+ | R2p+ | ASP | L/Bw |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 54.0 | 52.8 | 9337.2 | 48.9 | 171.7 | 14.869 | | | X | | | | | | | | | | | | |
| 1 | 45.4 | 44.0 | 11248.7 | 38.4 | 210.7 | 16.205 | | X | | | | | | | | | | | | | |
| 2 | 69.3 | 67.6 | 6413.9 | 64.9 | 104.9 | 12.323 | | X | X | | | | | | | | | | | | |
| 2 | 60.9 | 58.8 | 8694.6 | 52.4 | 142.4 | 13.888 | | | X | | | | | | | | | X | | | |
| 3 | 76.1 | 74.2 | 5150.1 | 71.8 | 75.8 | 11.005 | | X | X | X | | | | | | | | | | | |
| 3 | 72.3 | 70.0 | 6690.1 | 63.4 | 93.3 | 11.865 | X | X | X | | | | | | | | | | | | |
| 4 | 80.0 | 77.7 | 5045.7 | 72.4 | 60.6 | 10.229 | X | X | X | X | | | | | | | | | | | |
| 4 | 78.2 | 75.7 | 4973.1 | 72.8 | 68.4 | 10.664 | | X | X | X | | | | | | X | | | | | |
| 5 | 83.2 | 80.7 | 4160.6 | 77.2 | 47.9 | 9.5045 | X | X | X | X | | X | | | | | | | | | |
| 5 | 81.7 | 79.1 | 5113.8 | 72.0 | 54.5 | 9.9067 | X | X | X | X | X | | | | | | | | | | |
| 6 | 89.2 | 87.2 | 2736.4 | 85.0 | 23.0 | 7.7482 | X | X | X | X | X | X | | | | | | | | | |
| 6 | 86.4 | 83.9 | 3585.7 | 80.4 | 35.5 | 8.6816 | X | X | X | X | | X | | | | | X | | | | |
| 7 | 90.7 | 88.7 | 2467.0 | 86.5 | 17.9 | 7.2774 | X | X | X | X | X | X | X | | | | | | | | |
| 7 | 90.6 | 88.6 | 2486.9 | 86.4 | 18.3 | 7.3138 | X | X | X | X | X | X | | | | X | | | | | |
| 8 | 91.8 | 89.6 | 2187.7 | 88.0 | 15.2 | 6.9644 | X | X | X | X | X | X | X | X | | | | | | | |
| 8 | 91.6 | 89.4 | 2229.8 | 87.8 | 15.9 | 7.0313 | X | X | X | X | X | X | | X | | X | | | | | |
| 9 | 92.8 | 90.7 | 2186.0 | 88.0 | 12.4 | 6.6125 | X | X | X | X | X | X | X | X | | | | X | | | |
| 9 | 92.6 | 90.4 | 2214.6 | 87.9 | 13.2 | 6.6944 | X | X | X | X | X | X | | X | | X | | X | | | |
| 10 | 93.4 | 91.1 | 2138.9 | 88.3 | 12.0 | 6.4637 | X | X | X | X | X | X | X | X | | | | X | | X | |
| 10 | 93.3 | 91.0 | 2106.4 | 88.5 | 12.1 | 6.4838 | X | X | X | X | X | X | X | X | X | | | X | | | |
| 11 | 94.0 | 91.6 | 2187.2 | 88.0 | 11.1 | 6.2589 | X | X | X | X | X | X | X | X | X | | | X | | | X |
| 11 | 93.8 | 91.4 | 2048.0 | 88.8 | 11.8 | 6.3424 | X | X | X | X | X | X | X | X | X | | | X | | X | |
| 12 | 94.3 | 91.8 | 2149.0 | 88.2 | 11.7 | 6.2011 | X | X | X | X | X | X | X | X | X | | | X | X | | X |
| 12 | 94.3 | 91.8 | 2219.5 | 87.9 | 11.7 | 6.2090 | X | X | X | X | X | X | X | X | X | | X | X | | | X |
| 13 | 94.5 | 91.8 | 2230.5 | 87.8 | 12.8 | 6.2141 | X | X | X | X | X | X | X | X | X | | X | X | | X | X |
| 13 | 94.4 | 91.6 | 2451.4 | 86.6 | 13.2 | 6.2618 | X | X | X | X | X | X | | X | X | X | X | X | X | | X |
| 14 | 94.6 | 91.6 | 2548.8 | 86.1 | 14.3 | 6.2695 | X | X | X | X | X | X | X | X | X | X | X | X | | X | X |
| 14 | 94.5 | 91.5 | 2658.1 | 85.5 | 14.6 | 6.3148 | X | X | X | X | X | X | X | X | X | X | X | X | X | | X |
| 15 | 94.7 | 91.4 | 2826.9 | 84.5 | 16.0 | 6.3595 | X | X | X | X | X | X | X | X | X | X | X | X | X | X | X |

**Table S3.** The description of the selected molecular descriptors from Dragon software.

| Model | No. | Symbol | Descriptor Blocks | Description |
|---|---|---|---|---|
| ID Time | 1 | ***X5Av*** | Connectivity indices | Average valence connectivity index chi-5 |
| | 2 | ***Mor13m*** | 3D-MoRSE descriptors | 3D-MoRSE - signal 13 / weighted by atomic masses |
| | 3 | ***H7v*** | GETAWAY descriptors | H autocorrelation of lag 7 / weighted by van der Waals volume |
| Viscosity | 1 | ***F06[C-N]*** | 2D frequency fingerprints | Frequency of C-N at topological distance 06 |
| | 2 | ***Mor17m*** | 3D-MoRSE descriptors | 3D-MoRSE - signal 17 / weighted by atomic masses |
| | 3 | ***B06[C-B]*** | 2D binary fingerprints | Presence/absence of C-B at topological distance 06 |
| | 4 | ***RDF080m*** | RDF descriptors | Radial Distribution Function – 8.0 / weighted by atomic masses |
| | 5 | ***Mor08u*** | 3D-MoRSE descriptors | 3D-MoRSE - signal 08 / unweighted |
| | 6 | ***MATS8p*** | 2D autocorrelations | Moran autocorrelation – lag 8 / weighted by atomic polarizabilities |

**Table S4.** Mean values of independent variable importance analysis (50 repetition) for viscosity of HEILs.

| No. | Descriptor | Importance | Normalized importance |
|---|---|---|---|
| 1 | ***F06[C-N]*** | 0.146 | 100.00% |
| 2 | ***Mor17m*** | 0.144 | 98.30% |
| 3 | ***B06[C-B]*** | 0.091 | 62.10% |
| 4 | ***RDF080m*** | 0.088 | 60.10% |
| 5 | ***Mor08u*** | 0.082 | 55.80% |
| 6 | ***MATS8p*** | 0.081 | 55.50% |
| 7 | ***Mor26p*** | 0.072 | 49.10% |
| 8 | ***Mor11v*** | 0.068 | 46.60% |
| 9 | ***nN/nH*** | 0.059 | 40.20% |
| 10 | ***RNCG*** | 0.054 | 37.20% |
| 11 | ***G3v*** | 0.038 | 26.20% |
| 12 | ***RDF130m*** | 0.029 | 20.00% |
| 13 | ***Mor18v*** | 0.025 | 17.20% |
| 14 | ***Mor32u*** | 0.009 | 5.80% |
| 15 | ***RDF020m*** | 0.008 | 5.80% |
| 16 | ***H7v*** | 0.004 | 2.90% |

**Table S5.** The results of best subsets regression analysis on the selected molecular descriptors for viscosity of HEILs.

| Variables | $R^2$ | $R^2$ (Adjusted) | $R^2$ (predicted) | Mallows Cp | S | H7v | $n_N/n_H$ | Mor08u | MATS8p | RDF020m | RDF130m | RDF080m | Mor07v | Mor26p | Mor32u | Mor17m | Mor11v | Mor18v | G3v | RNCG | B06[C-B] | F06[C-N] |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 43.4 | 42.2 | 32.7 | 1674.6 | 141.30 | | | | | | | X | | | | | | | | | | |
| 1 | 39.3 | 38.0 | 27.3 | 1798.4 | 146.30 | | | | | | | | | | | | | | | | | X |
| 2 | 59.7 | 58.0 | 47.7 | 1181.0 | 120.49 | | | | | | | X | | | | | | | | | X | |
| 2 | 55.6 | 53.7 | 0.0 | 1305.4 | 126.46 | | | | | | X | | | | | | | | | | | X |
| 3 | 73.4 | 71.6 | 65.4 | 766.6 | 98.952 | | | X | | | | X | | | | | | | | | X | |
| 3 | 67.5 | 65.4 | 55.6 | 944.1 | 109.27 | | | | X | | | X | | | | | | | | | X | |
| 4 | 80.9 | 79.2 | 72.7 | 539.1 | 84.660 | | | X | | | | X | | | | | | | | | X | X |
| 4 | 80.7 | 78.9 | 74.6 | 547.5 | 85.275 | | | X | X | | | X | | | | | | | | | X | |
| 5 | 85.5 | 83.9 | 79.6 | 401.4 | 74.582 | | | X | | | X | X | | | | | | | | | X | X |
| 5 | 84.2 | 82.4 | 74.8 | 441.2 | 77.883 | | | X | | | | X | | | | | | | | X | X | X |
| 6 | 89.1 | 87.6 | 80.4 | 294.7 | 65.451 | | | X | | | X | X | | | | | | | | X | X | X |
| 6 | 88.8 | 87.2 | 83.6 | 304.9 | 66.447 | | | X | X | | | X | | | | X | | | | | X | X |
| 7 | 91.3 | 89.9 | 86.5 | 229.1 | 59.070 | | | X | X | | | X | | X | | X | | | | | X | X |
| 7 | 91.2 | 89.7 | 51.6 | 233.6 | 59.574 | | | X | | | X | X | | X | | | | | | X | X | X |
| 8 | 92.6 | 91.2 | 61.9 | 192.0 | 55.167 | | | X | | | X | X | | X | | | X | | | X | X | X |
| 8 | 92.5 | 91.1 | 88.7 | 195.0 | 55.537 | | | X | X | | | X | | X | | X | X | | | | X | X |
| 9 | 94.5 | 93.3 | 90.1 | 136.0 | 48.072 | | | X | X | | | X | | X | | X | X | | | X | X | X |
| 9 | 94.0 | 92.6 | 0.0 | 152.3 | 50.377 | X | | X | | | X | X | | X | | X | | | | X | X | X |
| 10 | 95.5 | 94.4 | 72.2 | 107.9 | 44.064 | X | | X | | X | X | X | | X | | X | | | X | | X | X |
| 10 | 95.2 | 94.0 | 56.0 | 117.3 | 45.551 | | | X | X | | X | X | | X | | X | X | | | X | X | X |
| 11 | 96.5 | 95.5 | 81.3 | 81.1 | 39.628 | X | | X | | X | X | X | | X | X | X | | | X | | X | X |
| 11 | 96.5 | 95.4 | 93.4 | 81.8 | 39.752 | X | | X | X | X | X | X | | X | | X | | | X | | X | X |
| 12 | 96.9 | 95.9 | 90.2 | 69.0 | 37.410 | X | | X | X | X | X | X | | X | | X | | X | X | | X | X |
| 12 | 96.9 | 95.9 | 81.9 | 71.0 | 37.814 | X | | X | X | X | X | X | X | X | | X | | | X | | X | X |
| 13 | 97.7 | 96.8 | 89.5 | 49.4 | 33.230 | X | | X | X | X | X | X | X | X | | X | | X | X | | X | X |
| 13 | 97.6 | 96.7 | 81.7 | 51.9 | 33.818 | X | | X | X | X | X | X | X | X | X | X | | | X | | X | X |
| 14 | 98.3 | 97.6 | 83.5 | 33.0 | 29.039 | X | X | X | X | X | X | X | X | X | | X | | X | X | | X | X |
| 14 | 98.2 | 97.5 | 96.3 | 34.9 | 29.552 | X | | X | X | X | X | X | X | X | | X | | X | X | X | X | X |
| 15 | 98.6 | 98.0 | 96.8 | 24.9 | 26.499 | X | | X | X | X | X | X | X | X | X | X | | X | X | X | X | X |
| 15 | 98.6 | 97.9 | 94.5 | 25.7 | 26.762 | X | X | X | X | X | X | X | X | X | | X | | X | X | X | X | X |
| 16 | 98.8 | 98.2 | 94.7 | 19.9 | 24.615 | X | X | X | X | X | X | X | X | X | X | X | | X | X | X | X | X |
| 16 | 98.8 | 98.2 | 97.3 | 21.1 | 25.027 | X | X | X | X | X | X | X | X | X | | X | X | X | X | X | X | X |
| 17 | 98.9 | 98.4 | 97.4 | 18.0 | 23.601 | X | X | X | X | X | X | X | X | X | X | X | X | X | X | X | X | X |

**Table S6.** The calculated values of the selected molecular descriptors from Dragon software.

| IL No. | X5Av | Mor13m | H7v | F06[C-N] | Mor17m | B06[C-B] | RDF080m | Mor08u | MATS8p |
|---|---|---|---|---|---|---|---|---|---|
| **1** | 0.040 | -0.460 | 0.079 | 4.000 | -0.240 | 1.000 | 4.457 | 1.122 | -0.028 |
| **2** | 0.054 | -0.396 | 0.014 | 1.000 | -0.297 | 0.000 | 0.170 | 0.928 | 0.000 |
| **3** | 0.040 | -0.354 | 0.002 | 0.000 | -0.263 | 0.000 | 0.013 | 1.040 | 0.000 |
| **4** | 0.040 | -0.465 | 0.018 | 4.000 | -0.255 | 1.000 | 2.120 | 0.905 | -0.028 |
| **5** | 0.050 | -0.290 | 0.015 | 0.000 | -0.255 | 0.000 | 0.000 | 0.690 | 0.000 |
| **6** | 0.054 | -0.319 | 0.006 | 1.000 | -0.361 | 0.000 | 0.055 | 1.136 | 0.000 |
| **7** | 0.046 | -0.156 | 0.008 | 2.000 | -0.501 | 0.000 | 0.109 | 1.069 | 0.045 |
| **8** | 0.045 | -0.469 | 0.023 | 1.000 | -0.26 | 0.000 | 0.688 | 1.527 | 0.200 |
| **9** | 0.036 | -0.218 | 0.008 | 0.000 | -0.245 | 0.000 | 0.001 | 0.352 | 0.000 |
| **10** | 0.040 | -0.278 | 0.014 | 4.000 | -0.326 | 1.000 | 2.029 | 0.560 | -0.028 |
| **11** | 0.046 | -0.143 | 0.01 | 2.000 | -0.546 | 0.000 | 0.203 | 1.285 | 0.045 |
| **12** | 0.050 | -0.303 | 0.014 | 0.000 | -0.258 | 0.000 | 0.000 | 0.571 | 0.000 |
| **13** | 0.055 | -0.600 | 0.056 | 1.000 | -0.351 | 0.000 | 1.178 | 1.620 | 0.222 |
| **14** | 0.069 | -0.473 | 0.018 | 2.000 | -0.562 | 0.000 | 0.148 | 1.436 | -0.222 |
| **15** | 0.035 | -0.434 | 0.005 | 0.000 | -0.223 | 0.000 | 0.005 | 0.659 | 0.222 |
| **16** | 0.040 | -0.408 | 0.013 | 0.000 | -0.254 | 0.000 | 0.001 | 0.629 | 0.000 |
| **17** | 0.039 | -0.413 | 0.013 | 0.000 | -0.223 | 0.000 | 0.088 | 1.332 | 0.000 |
| **18** | 0.045 | -0.454 | 0.019 | 1.000 | -0.420 | 0.000 | 1.157 | 1.354 | 0.200 |
| **19** | 0.058 | -0.655 | 0.02 | 2.000 | -0.588 | 0.000 | 0.785 | 1.932 | -0.143 |
| **20** | 0.038 | -0.481 | 0.008 | 4.000 | -0.503 | 0.000 | 1.026 | 0.804 | -0.073 |
| **21** | 0.054 | -0.457 | 0.024 | 1.000 | -0.423 | 0.000 | 0.013 | 0.924 | 0.000 |
| **22** | 0.040 | -0.406 | 0.016 | 0.000 | -0.226 | 0.000 | 0.994 | 1.421 | 0.222 |
| **23** | 0.043 | -0.473 | 0.021 | 1.000 | -0.281 | 0.000 | 0.026 | 1.262 | 0.000 |
| **24** | 0.054 | -0.400 | 0.009 | 1.000 | -0.254 | 0.000 | 0.310 | 0.647 | 0.000 |
| **25** | 0.054 | -0.373 | 0.003 | 1.000 | -0.368 | 0.000 | 0.039 | 0.741 | 0.000 |
| **26** | 0.040 | -0.402 | 0.006 | 0.000 | -0.222 | 0.000 | 0.004 | 0.567 | 0.000 |
| **27** | 0.049 | -0.269 | 0.000 | 0.000 | -0.243 | 0.000 | 0.000 | 0.721 | 0.000 |
| **28** | 0.054 | -0.395 | 0.007 | 1.000 | -0.286 | 0.000 | 0.172 | 0.959 | 0.000 |
| **29** | 0.040 | -0.373 | 0.009 | 0.000 | -0.192 | 0.000 | 0.011 | 0.764 | 0.000 |
| **30** | 0.035 | -0.553 | 0.003 | 0.000 | -0.100 | 0.000 | 0.064 | 1.020 | 0.222 |
| **31** | 0.050 | -0.287 | 0.008 | 0.000 | -0.29 | 0.000 | 0.000 | 0.641 | 0.000 |
| **32** | 0.040 | -0.363 | 0.009 | 0.000 | -0.212 | 0.000 | 0.010 | 0.851 | 0.000 |
| **33** | 0.035 | -0.469 | 0.037 | 0.000 | -0.149 | 0.000 | 0.273 | 0.921 | 0.222 |
| **34** | 0.050 | -0.325 | 0.016 | 0.000 | -0.252 | 0.000 | 0.000 | 0.717 | 0.000 |
| **35** | 0.054 | -0.343 | 0.017 | 1.000 | -0.308 | 0.000 | 0.160 | 1.100 | 0.000 |
| **36** | 0.054 | -0.372 | 0.013 | 1.000 | -0.328 | 0.000 | 0.104 | 1.418 | 0.000 |
| **37** | 0.040 | -0.406 | 0.004 | 0.000 | -0.226 | 0.000 | 0.004 | 0.769 | 0.000 |
| **38** | 0.046 | -0.234 | 0.029 | 4.000 | -0.606 | 0.000 | 2.027 | 0.919 | -0.073 |
| **39** | 0.040 | -0.401 | 0.013 | 4.000 | -0.550 | 1.000 | 4.207 | 1.476 | -0.028 |
| **40** | 0.050 | -0.315 | 0.013 | 0.000 | -0.245 | 0.000 | 0.000 | 0.786 | 0.000 |
| **41** | 0.040 | -0.428 | 0.012 | 0.000 | -0.143 | 0.000 | 0.027 | 1.004 | 0.000 |
| **42** | 0.040 | -0.309 | 0.029 | 4.000 | -0.565 | 1.000 | 2.749 | 0.915 | -0.028 |
| **43** | 0.050 | -0.318 | 0.011 | 0.000 | -0.288 | 0.000 | 0.000 | 0.839 | 0.000 |
| **44** | 0.054 | -0.291 | 0.026 | 1.000 | -0.328 | 0.000 | 0.654 | 1.238 | 0.000 |
| **45** | 0.050 | -0.295 | 0.015 | 0.000 | -0.266 | 0.000 | 0.000 | 0.722 | 0.000 |
| **46** | 0.036 | -0.484 | 0.007 | 0.000 | -0.244 | 0.000 | 0.006 | 0.552 | 0.000 |
| **47** | 0.035 | -0.461 | 0.026 | 0.000 | -0.168 | 0.000 | 0.123 | 0.785 | 0.222 |
| **48** | 0.040 | -0.428 | 0.021 | 0.000 | -0.165 | 0.000 | 0.020 | 1.009 | 0.000 |
| **49** | 0.040 | -0.434 | 0.026 | 0.000 | -0.126 | 0.000 | 0.000 | 0.826 | 0.000 |
| **50** | 0.040 | -0.421 | 0.002 | 4.000 | -0.357 | 1.000 | 2.420 | 0.932 | -0.028 |