**Multilayered Variable Selection in QSPR: A Case Study of Modeling Melting Point of Bromide Ionic Liquids**

**Supplementary Materials**

*Table S1. The list of studied bromide ionic liquids (cationic part of* ***376*** *ILs shown) with their experimental and predicted (based on the consensus model) melting point* ***[****Log (Tm°C)]**values.*

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| N-alkyl-pyridinium based cation  R1-R5 can be a substituent or H | | | | | | | |
| **Compound Nos.** | **N- substituent** | **Other substituents** | | | **Exp. m.p. [Log (Tm°C)]** | **Predicted m.p. [Log (Tm°C)]** | |
| 1 | decyl | 3-pentyl | | | 1.477 | 1.670 | |
| 2\* | 11-propionylloxyundecyl |  | | | 1.544 | 1.740 | |
| 3 | benzyl | 4-dibenzyl; 3-ethoxycarbonyl | | | 1.544 | 1.901 | |
| 4 | octyl | 4-propyl | | | 1.568 | 1.712 | |
| 5 | tetradecyl | 4-hexyl | | | 1.568 | 1.640 | |
| 6 | tetradecyl | 3-pentyl | | | 1.591 | 1.650 | |
| 7 | decyl | 4-ethoxycarbonyl | | | 1.607 | 1.668 | |
| 8 | dodecyl | 4-propyl | | | 1.613 | 1.670 | |
| 9 | undecyl |  | | | 1.622 | 1.708 | |
| 10\* | octyl | 4-ethyl | | | 1.628 | 1.748 | |
| 11\* | dodecyl | 4-ethyl | | | 1.638 | 1.683 | |
| 12 | decyl |  | | | 1.648 | 1.719 | |
| 13 | dodecyl |  | | | 1.653 | 1.699 | |
| 14 | hexyl | 2-(2-methyloctyl) | | | 1.672 | 1.698 | |
| 15 | ethoxycarbonylmethyl | 5-butyl; 2-methyl | | | 1.708 | 1.861 | |
| 16 | 2,5- dimethoxyphenethyl |  | | | 1.731 | 2.037 | |
| 17 | tridecyl |  | | | 1.736 | 1.691 | |
| 18 | 4-fluoro-benzyl |  | | | 1.760 | 2.068 | |
| 19 | tetradecyl |  | | | 1.771 | 1.683 | |
| 20\* | butyl | 4-ethoxycarbonyl | | | 1.778 | 1.884 | |
| 21 | 2-methylpropyl |  | | | 1.806 | 1.959 | |
| 22 | methyl | 3-(3-hydroxypropyl) | | | 1.806 | 2.042 | |
| 23 | benzyl | 3-methyl | | | 1.810 | 2.049 | |
| 24 | butyl | 2-benzylsulfanyl | | | 1.813 | 1.869 | |
| 25 | 2-cyclohexyl-2-oxo-ethyl |  | | | 1.839 | 1.823 | |
| 26 | methylpropyl |  | | | 1.842 | 1.974 | |
| 27\* | 2-pyridinyl |  | | | 1.848 | 2.189 | |
| 28 | 2-(ethoxycarbonyl)ethyl |  | | | 1.851 | 1.956 | |
| 29 | 1-(ethjoxycarbonyl)propyl |  | | | 1.863 | 1.938 | |
| 31\* | ethyl | 3-diethylcarbamoyl | | | 1.878 | 1.949 | |
| 32 | 2-phenoxyethyl |  | | | 1.886 | 2.010 | |
| 33 | methyl | 2,4,6-tetramethyl | | | 1.892 | 1.993 | |
| 34 | methyl | 4-(3-hydroxypropyl) | | | 1.895 | 2.141 | |
| 35\* | ethyl | 2,6-dimethyl | | | 1.898 | 1.962 | |
| 36 | methyl | 3-pyridinyl | | | 1.903 | 2.033 | |
| 37 | isopropyloxycarbonylmethyl |  | | | 1.903 | 2.201 | |
| 38 | morpholinomethyl | 4-methyl | | | 1.903 | 2.026 | |
| 39 | methyl | 4-benzyl | | | 1.916 | 1.916 | |
| 40 | 2-fluroethyl | 3-ethoxycarbonyl | | | 1.932 | 2.081 | |
| 41 | phenethyl | 4-methyl | | | 1.940 | 2.027 | |
| 42\* | butyl | 3-carboxy | | | 1.954 | 2.010 | |
| 43 | allyl | 3-diethylcarbamoyl | | | 1.959 | 1.974 | |
| 44 | bis(ethoxycarbonyl)methyl |  | | | 1.964 | 2.040 | |
| 45 | 4-acetoxybutyl | 3-hydroxy | | | 1.971 | 1.987 | |
| 46\* | benzyloxy |  | | | 1.978 | 1.953 | |
| 47 | allyl |  | | | 1.978 | 2.008 | |
| 48 | methyl | 3-methoxycarbonyl | | | 1.980 | 2.067 | |
| 49 | 2-hydroxyethyl | 3-methyl | | | 1.982 | 2.070 | |
| 50\* | ethyl | 2-methyl | | | 1.987 | 1.987 | |
| 51 | isopropyl |  | | | 1.987 | 2.027 | |
| 52 | butyl |  | | | 1.987 | 2.042 | |
| 53 | ethyl | 4-(4-pyridyl) | | | 1.989 | 1.896 | |
| 54\* | allyl | 3-hydroxy | | | 1.991 | 2.114 | |
| 55 | benzyl |  | | | 1.991 | 2.096 | |
| 56 | methyl | 4-(2-ethoxycarbonylethyl) | | | 1.996 | 2.047 | |
| 57 | ethyl | 3-acetyl | | | 1.998 | 1.992 | |
| 58\* | allyl | 3-formyl | | | 2.000 | 2.061 | |
| 59 | acetonyl | 2,6-dimethyl | | | 2.000 | 2.096 | |
| 60 | ethyl | 3-hydroxy | | | 2.017 | 2.090 | |
| 61 | ethoxy | 4-methoxy | | | 2.025 | 2.057 | |
| 62 | propyloxycarbonylmethyl |  | | | 2.035 | 2.008 | |
| 63 | allyl | 2-hydroxymethyl | | | 2.041 | 1.949 | |
| 64 | 2-hydroxyethyl |  | | | 2.041 | 2.009 | |
| 65 | allyl | 4-hydroxymethyl | | | 2.041 | 1.979 | |
| 66 | 5-hexynyl |  | | | 2.045 | 2.009 | |
| 67 | 2-cyanoethyl | 3-methyl | | | 2.057 | 1.982 | |
| 68\* | pyridenyl |  | | | 2.064 | 2.094 | |
| 69 | isopropyl | 4-hydroxyethyl | | | 2.072 | 2.189 | |
| 70 | 3-cholropropyl |  | | | 2.076 | 1.995 | |
| 71 | ethyl |  | | | 2.079 | 2.075 | |
| 72\* | allyl | 4-cyan | | | 2.081 | 2.020 | |
| 73 | ethyl | 4-methyl | | | 2.083 | 2.152 | |
| 74 | isopropyl | 2-hydroxymethyl | | | 2.083 | 2.026 | |
| 75 | 2-hydroxyethyl | 3-hydroxy | | | 2.086 | 1.996 | |
| 76\* | 2-hydroxyethyl | 3,4-dimethyl | | | 2.088 | 2.015 | |
| 77 | 3,3-diethylallyl | 4-methyl | | | 2.102 | 1.992 | |
| 78 | 1-methyl-2-oxopropyl | 2-methyl | | | 2.106 | 2.017 | |
| 79 | 2-cyano-ethyl | 3,4-dimethyl | | | 2.124 | 2.099 | |
| 80\* | ethoxycarbonylmethyl |  | | | 2.124 | 2.095 | |
| 81 | 3-bromopropyl | 4-methyl | | | 2.137 | 1.999 | |
| 82 | (Z)-3-methylpent-2-en-4-inyl |  | | | 2.145 | 2.010 | |
| 83 | methyl | 3-methyoxycarbonyl | | | 2.145 | 2.126 | |
| 84\* | 2-cyanoethyl | 3-amino | | | 2.149 | 2.080 | |
| 85 | 1-metrhyl-2-oxopropyl |  | | | 2.152 | 2.158 | |
| 86 | cyanomethyl | 3,5-dimethyl | | | 2.158 | 2.097 | |
| 87 | methyl | 4-methyl-3-hydroxy | | | 2.158 | 2.148 | |
| 88\* | 2-cyanoethyl | 4-methyl | | | 2.164 | 2.176 | |
| 89 | 2-cyanoethyl |  | | | 2.167 | 2.094 | |
| 90 | methyl |  | | | 2.173 | 2.092 | |
| 91\* | methyl | 3-hydroxy | | | 2.176 | 2.154 | |
| 92 | vinyl |  | | | 2.186 | 2.184 | |
| 93 | phenyl |  | | | 2.189 | 2.147 | |
| 94 | (E)-3-hydroxyprop-1-en-1-yl |  | | | 2.190 | 2.101 | |
| 95 | 2-carboxyallyl |  | | | 2.195 | 2.026 | |
| 96\* | cyclohex-2-enyl |  | | | 2.195 | 2.126 | |
| 97 | 2-cyanoethyl | 3,5-dimethyl | | | 2.203 | 1.886 | |
| 98 | 3-carboxypropyl |  | | | 2.205 | 2.136 | |
| 99 | methyl | 4-methoxycarbonyl | | | 2.212 | 1.998 | |
| 100 | ethyl | 4-cyano | | | 2.215 | 2.080 | |
| 101 | cyanomethyl |  | | | 2.219 | 2.120 | |
| 102\* | methyl | 2-hydroxymethyl | | | 2.223 | 2.156 | |
| 103 | vinyl | 4-methyl | | | 2.224 | 2.078 | |
| 104 | isopropyl | 4-methoxy | | | 2.228 | 2.142 | |
| 105 | methyl | 4-methyl | | | 2.229 | 2.068 | |
| 106\* | methoxycarbonylmethyl |  | | | 2.238 | 2.148 | |
| 107 | propyl | 3-carbamoyl | | | 2.242 | 2.091 | |
| 108 | ethyl | 4-dimethylamino | | | 2.243 | 2.057 | |
| 109 | prop-2-ynyl | 4-methyl | | | 2.246 | 2.154 | |
| 110\* | cyanomethyl | 4-methyl | | | 2.250 | 2.099 | |
| 111 | 2-fluroethhyl |  | | | 2.253 | 2.152 | |
| 112 | methyl | 4-acetyl | | | 2.255 | 2.148 | |
| 113\* | allyl | 4-(hydroxyiminomethyl) | | | 2.264 | 2.169 | |
| 114 | hydrazinocarbonylmethyl |  | | | 2.267 | 2.251 | |
| 115 | 2-oxopropyl |  | | | 2.268 | 2.094 | |
| 116 | ethyl | 4-carbamoyl | | | 2.272 | 2.089 | |
| 117\* | (E)-2-carboxy-1-ethenyl | 3-methyl | | | 2.274 | 2.061 | |
| 118 | 2-propionamido |  | | | 2.275 | 2.152 | |
| 119 | (E)-2-carboxy-1-ethenyl | 3-methyl | | | 2.278 | 2.152 | |
| 120 | allyl | 2-(hydroxyiminomethyl) | | | 2.280 | 2.149 | |
| 121 | 2-oxopropyl | 2-methyl | | | 2.284 | 2.251 | |
| 122 | 2-hydroxyethyl | 2-(hydroxyiminomethyl) | | | 2.292 | 2.090 | |
| 123 | cyanomethyl | 2,4-dimethyl | | | 2.298 | 2.179 | |
| 124\* | carboxymethyl |  | | | 2.299 | 2.150 | |
| 125 | 2-carbamoylethyl |  | | | 2.299 | 2.108 | |
| 126 | carbamoylmethyl |  | | | 2.299 | 2.088 | |
| hydroxyalkylammonium cation | | | | | | | |
| **Compound Nos.** | **Cation name** | | | | **Exp. m.p. [Log (Tm°C)]** | **Predicted m.p. [Log (Tm°C)]** | |
| 127 | (2-hydroxyethyl)-dimethyl-pentyl-ammonium | | | | 1.699 | 2.180 | |
| 128\* | dibutyl-hexadecyl-(2-hydroxyethyl)-ammonium | | | | 1.740 | 1.862 | |
| 129 | tributyl-(2-hydroxyethyl)-ammonium | | | | 1.763 | 1.948 | |
| 130\* | ethyl-hexadecyl-(2-hydroxyethyl)-methyl-ammonium | | | | 1.806 | 1.927 | |
| 131 | didodecyl-(2-hydroxyethyl)-methyl-ammonium | | | | 1.813 | 1.889 | |
| 132 | diethyl-(2-hydroxyethyl)-tetradecyl-ammonium | | | | 1.813 | 1.955 | |
| 133\* | decyl-(3-hydroxypropyl)-dimethyl-ammonium | | | | 1.845 | 2.085 | |
| 134 | decyl-diethyl-(2-hydroxyethyl)-ammonium | | | | 1.886 | 2.098 | |
| 135 | hexadecyl-(3-hydroxypropyl)-dimethyl-ammonium | | | | 1.929 | 2.030 | |
| 136\* | (3-hydroxypropyl)-dimethyl-tetradecyl-ammonium | | | | 1.934 | 2.046 | |
| 137 | didodecyl-ethyl-(2-hydroxyethyl)-ammonium | | | | 2.000 | 1.897 | |
| 138 | (2-hydroxyethyl)-dimethyl-octyl-ammonium | | | | 2.061 | 2.116 | |
| 139 | (2-hydroxyethyl)-dimethyl-nonyl-ammonium | | | | 2.079 | 2.100 | |
| 140 | dodecyl-diethyl-(2-hydroxyethyl)-ammonium | | | | 2.079 | 2.062 | |
| 141 | diethyl-hexadecyl-(2-hydroxyethyl)-ammonium | | | | 2.114 | 1.944 | |
| 142 | (2-hydroxyethyl)-methyl-dioctadecyl-ammonium | | | | 2.114 | 1.911 | |
| 143\* | diethyl-(2-hydroxyethyl)-octadecyl-ammonium | | | | 2.134 | 1.934 | |
| 144 | dihexadecyl-(2-hydroxyethyl)-methyl-ammonium | | | | 2.176 | 1.871 | |
| 145 | decyl-(2-hydroxyethyl)-dimethyl-ammonium | | | | 2.190 | 2.087 | |
| 146 | (2-hydroxyethyl)-isopropyl-methyl-propyl-ammonium | | | | 2.190 | 2.214 | |
| 147 | diethyl-(3-hydroxypropyl)-methyl-ammonium | | | | 2.190 | 2.217 | |
| 148\* | triethyl-(3-hydroxypropyl)-ammonium | | | | 2.217 | 2.171 | |
| 149 | trimethyl-(3-hydroxypropyl)-ammonium | | | | 2.243 | 2.399 | |
| 150 | dodecyl-(2-hydroxyethyl)-dimethyl-ammonium | | | | 2.301 | 2.170 | |
| 151 | (2-hydroxyethyl)-dimethyl-tetradecyl-ammonium | | | | 2.301 | 2.045 | |
| 152 | (2-hydroxyethyl)-dimethyl-pentadecyl-ammonium | | | | 2.312 | 2.035 | |
| 153 | (2-hydroxyethyl)-dimethyl-octadecyl-ammonium | | | | 2.322 | 2.016 | |
| 154 | hexadecyl-(2-hydroxyethyl)-dimethyl-ammonium | | | | 2.352 | 2.028 | |
| 155 | (2-hydroxyethyl)-diisopropyl-methyl-ammonium | | | | 2.371 | 2.289 | |
| 156 | triethyl-(2-hydroxyethyl)-ammonium | | | | 2.407 | 2.394 | |
| 157\* | ethyl-(2-hydroxyethyl)-isopropyl-methyl-ammonium | | | | 2.415 | 2.266 | |
| 158 | (2-hydroxyethyl)-isopropyl-dimethyl-ammonium | | | | 2.439 | 2.307 | |
| 159 | ethyl-(2-hydroxyethyl)-dimethyl-ammonium | | | | 2.455 | 2.286 | |
| 160\* | (2-hydroxyethyl)-trimethyl-ammonium | | | | 2.477 | 2.394 | |
| tetraalkyl-ammonium based cation | | | | | | | |
| **Compound Nos.** | **Cation Name** | | | | **Exp. m.p. [Log (Tm°C)]** | **Predicted m.p. [Log (Tm°C)]** | |
| 161 | tributyl-(3-methylbutyl)-ammonium | | | | 1.230 | 1.963 | |
| 162 | butyl-dodecyl-dimethyl-ammonium | | | | 1.602 | 2.074 | |
| 163 | dimethyl-ditetradecyl-ammonium | | | | 1.699 | 2.009 | |
| 164 | dibutyl-hexadecyl-methyl-ammonium | | | | 1.708 | 1.969 | |
| 165\* | tributyl-hexyl-ammonium | | | | 1.716 | 1.937 | |
| 166 | dodecyl-tripropyl-ammonium | | | | 1.748 | 1.957 | |
| 167 | dimethyl-octadecyl-octyl-ammonium | | | | 1.756 | 2.017 | |
| 168\* | decyl-dimethyl-octadecyl-ammonium | | | | 1.778 | 2.009 | |
| 169 | dimethyl-octadecyl-tetradecyl-ammonium | | | | 1.792 | 1.995 | |
| 170 | dodecyl-dimethyl-octadecyl-ammonium | | | | 1.792 | 2.001 | |
| 171 | triheptyl-propyl-ammonium | | | | 1.813 | 1.965 | |
| 172 | dihexadecyl-dimethyl-ammonium | | | | 1.813 | 1.995 | |
| 173 | diethyl-hexadecyl-methyl-ammonium | | | | 1.851 | 2.031 | |
| 174\* | trioctyl-propyl-ammonium | | | | 1.851 | 1.955 | |
| 175 | tributyl-hexadecyl-ammonium | | | | 1.875 | 1.900 | |
| 176 | hexadecyl-dimethyl-pentyl-ammonium | | | | 1.881 | 2.041 | |
| 177\* | butyl-hexadecyl-dimethyl-ammonium | | | | 1.919 | 2.043 | |
| 178 | tetraheptyl-ammonium | | | | 1.954 | 1.947 | |
| 179\* | didocosyl-dimethyl-ammonium | | | | 1.954 | 2.024 | |
| 180 | tetradodecyl-ammonium | | | | 1.954 | 1.958 | |
| 181 | tetraoctyl-ammonium | | | | 1.978 | 1.978 | |
| 182\* | dodecyl-diethyl-propyl-ammonium | | | | 1.987 | 2.000 | |
| 183 | tetrahexyl-ammonium | | | | 2.000 | 1.916 | |
| 184 | tetrapentyl-ammonium | | | | 2.000 | 1.931 | |
| 185\* | triethyl-hexyl-ammonium | | | | 2.021 | 2.122 | |
| 186 | triethyl-octyl-ammonium | | | | 2.031 | 2.084 | |
| 187 | diethyl-methyl-(2,4,4-trimethylpentyl)-ammonium | | | | 2.041 | 2.221 | |
| 188 | tetrabutyl-ammonium | | | | 2.079 | 1.947 | |
| 189\* | triethyl-heptyl-ammonium | | | | 2.079 | 2.101 | |
| 190 | tributyl-methyl-ammonium | | | | 2.079 | 2.054 | |
| 191 | hexadecyl-tripropyl-ammonium | | | | 2.079 | 1.938 | |
| 192 | ethyl-methyl-bis(3-methylbutyl)-ammonium | | | | 2.104 | 2.125 | |
| 193\* | dodecyl-triethyl-ammonium | | | | 2.114 | 2.034 | |
| 194 | (2-methylbutyl)-triethyl-ammonium | | | | 2.134 | 2.137 | |
| 195 | diicosyl-dimethyl-ammonium | | | | 2.137 | 1.978 | |
| 196 | hexadecyl-dimethyl-octyl-ammonium | | | | 2.164 | 2.024 | |
| 197\* | triethyl-pentyl-ammonium | | | | 2.164 | 2.146 | |
| 198 | (2-isopropyl-5-methylhexyl)-trimethyl-ammonium | | | | 2.182 | 2.233 | |
| 199\* | hexadecyl-icosyl-dimethyl-ammonium | | | | 2.190 | 1.987 | |
| 200 | dibutyl-dimethyl-ammonium | | | | 2.220 | 2.195 | |
| 201\* | triethyl-hexadecyl-ammonium | | | | 2.243 | 2.000 | |
| 202 | triethyl-octadecyl-ammonium | | | | 2.255 | 1.986 | |
| 203 | trimethyl-pentyl-ammonium | | | | 2.255 | 2.361 | |
| 204\* | heptyl-trimethyl-ammonium | | | | 2.265 | 2.281 | |
| 205 | hexyl-trimethyl-ammonium | | | | 2.270 | 2.316 | |
| 206 | dodecyl-ethyl-dimethyl-ammonium | | | | 2.274 | 2.110 | |
| 207\* | ethyl-hexadecyl-dimethyl-ammonium | | | | 2.279 | 2.071 | |
| 208 | butyl-trimethyl-ammonium | | | | 2.290 | 2.406 | |
| 209 | (3-methylbutyl)-trimethyl-ammonium | | | | 2.301 | 2.354 | |
| 210\* | (1-isopropyl-3-methylbutyl)-trimethyl-ammonium | | | | 2.307 | 2.337 | |
| 211 | trimethyl-(4-methylpentyl)-ammonium | | | | 2.322 | 2.366 | |
| 212 | butyl-triethyl-ammonium | | | | 2.322 | 2.168 | |
| 213 | (1-methylheptyl)-trimethyl-ammonium | | | | 2.322 | 2.288 | |
| 214\* | trimethyl-octyl-ammonium | | | | 2.332 | 2.250 | |
| 215 | (2-methylbutyl)-trimethyl-ammonium | | | | 2.352 | 2.399 | |
| 216 | (2-ethyldecyl)-trimethyl-ammonium | | | | 2.354 | 2.156 | |
| 217 | trimethyl-nonyl-ammonium | | | | 2.362 | 2.225 | |
| 218 | trimethyl-propyl-ammonium | | | | 2.380 | 2.629 | |
| 219 | decyl-trimethyl-ammonium | | | | 2.380 | 2.204 | |
| 220\* | trimethyl-(1-butylpentyl)-ammonium | | | | 2.380 | 2.217 | |
| 221 | (1-ethylpropyl)-trimethyl-ammonium | | | | 2.389 | 2.554 | |
| 222 | trimethyl-octadecyl-ammonium | | | | 2.398 | 2.103 | |
| 223 | dodecyl-trimethyl-ammonium | | | | 2.398 | 2.170 | |
| 224\* | hexadecyl-trimethyl-ammonium | | | | 2.398 | 2.120 | |
| 225 | trimethyl-tetradecyl-ammonium | | | | 2.398 | 2.142 | |
| 226 | ethyl-diisopropyl-methyl-ammonium | | | | 2.398 | 2.417 | |
| 227 | triethyl-isopropyl-ammonium | | | | 2.422 | 2.364 | |
| 228 | tetraethyl-ammonium | | | | 2.431 | 2.384 | |
| 229\* | diethyl-isopropyl-methyl-ammonium | | | | 2.442 | 2.439 | |
| 230 | tetrapropyl-ammonium | | | | 2.447 | 2.061 | |
| 231 | (3,3-dimethylbutyl)-trimethyl-ammonium | | | | 2.458 | 2.341 | |
| 232 | triethyl-methyl-ammonium | | | | 2.477 | 2.477 | |
| 233 | diethyl-dimethyl-ammonium | | | | 2.505 | 2.589 | |
| 234 | isopropyl-trimethyl-ammonium | | | | 2.505 | 2.450 | |
| 235\* | ethyl-trimethyl-ammonium | | | | 2.519 | 2.435 | |
| Imidazolium cation | | | | | | |
| **Compound Nos.** | **1-substituent** | **3-substituent** | **other substituents** | **Exp. m.p. [Log (Tm°C)]** | **Predicted m.p. [Log (Tm°C)]** | |
| 236 | -CH3 | -CH2COPh |  | | 1.690 | 2.167 | |
| 237\* | -CH3 | -C2H5 |  | | 1.812 | 2.122 | |
| 238\* | -CH=CH2 | n-C4H9 |  | | 1.919 | 2.031 | |
| 239 | n-C10H21 | -CH3 | 2-CH3 | | 1.927 | 1.974 | |
| 240 | -CH3 | -CH2COC6H4(*m*-OC3H7) |  | | 1.929 | 2.111 | |
| 241 | -CH2CH=CH2 | -CH2CHCN |  | | 1.947 | 2.114 | |
| 242 | -CH3 | -CH2C6H4(*p*-COPh) |  | | 1.971 | 2.157 | |
| 243 | -CH3 | -CH2CH2OH |  | | 1.988 | 2.081 | |
| 244 | -CH=CH2 | -C2H5 |  | | 1.998 | 2.151 | |
| 245\* | -CH3 | -CH3 |  | | 2.039 | 2.258 | |
| 246\* | -CH3 | n-C4H9 | 5-CH3 | | 2.043 | 2.013 | |
| 247 | -CH3 | -CH2C6H4(*m*-CH3) |  | | 2.061 | 2.146 | |
| 248\* | -CH3 | -CH2C6H4(*o*-CH3) |  | | 2.061 | 2.146 | |
| 249 | -CH3 | -CH2COPh |  | | 2.068 | 2.167 | |
| 250 | -CH3 | -CH2Ph |  | | 2.100 | 2.145 | |
| 251 | -CH3 | -CH2COC6H4(*m*-OC2H5) |  | | 2.138 | 2.146 | |
| 252 | -CH3 | -C(CH3)2COPh |  | | 2.141 | 2.182 | |
| 253 | -CH3 | -CH2COC6H4(*p*-OC2H5) |  | | 2.160 | 2.105 | |
| 254 |  |  |  | | 2.167 | 2.166 | |
| 255 | -CH3 | -CH2COC6H4(*p*-Cl) |  | | 2.172 | 2.162 | |
| 256 | n-C3H7 | -CH2COPh |  | | 2.173 | 2.054 | |
| 257 | -CH3 | -CH2COC6H4(*o*-CH3) |  | | 2.185 | 2.208 | |
| 258 | -C2H5 | -C2H5 | 4-Ph,5-Ph | | 2.186 | 2.064 | |
| 259\* | -CH=CH2 | n-C3H7 |  | | 2.190 | 2.083 | |
| 260 | -CH3 | -CH2COC6H4 | (*p*-OMe) | | 2.197 | 2.177 | |
| 261 | n-C3H7 | n-C3H7 | 2-CH2CH(CH3)2 | | 2.211 | 2.006 | |
| 262 | -CH3 | -CH2COC6H3[3,4(-CH3)2] |  | | 2.215 | 2.234 | |
| 263 | -CH3 | -CH2COC6H4(*o*-OCH3) |  | | 2.220 | 2.177 | |
| 264 | -CH3 | -CH2COC6H4(*m*-Cl) |  | | 2.246 | 2.189 | |
| 265\* | -CH(CH3)2 | -CH2COC6H4(*m*-OCH3) |  | | 2.250 | 2.173 | |
| 266 | -CH3 | -CH2COC6H4(*o*-F) |  | | 2.253 | 2.185 | |
| 267\* | -CH3 | -CH2COC6H3[3,4-(Cl)2] |  | | 2.264 | 2.207 | |
| 268 | -CH3 | -CH2COPh | 2-CH(=CH2)Ph | | 2.267 | 2.366 | |
| 269 | -CH3 | -(CH2)2C6H4(*p*-NO2) |  | | 2.267 | 2.187 | |
| 270\* | -CH3 | -CH2Ph | 2-n-C7H15 | | 2.271 | 2.123 | |
| 271 | CH3 | -CH2COC6H4(*p*-NO2) |  | | 2.273 | 2.238 | |
| 272\* | -CH3 | -CH3 | 5-Cl | | 2.291 | 2.291 | |
| 273\* | -CH3 | -CH2COPh | 2-CH(=CH2)C(CH3)3 | | 2.301 | 2.253 | |
| 274 | -CH3 | -CH2COC6H4(*p*-Cl) | 2-CH3 | | 2.303 | 2.323 | |
| 275 | -CH3 | -CH2COC6H3[2,5-(OCH3)2] |  | | 2.319 | 2.225 | |
| 276 | -CH3 | -CH2COC6H4(*p*-CN) |  | | 2.326 | 2.298 | |
| 277 | -CH3 | -CH2COC6H3[2,3(-OCH3)2] |  | | 2.334 | 2.225 | |
| 278\* | -CH3 | -CH2COC6H4(*p*-Br) |  | | 2.339 | 2.190 | |
| 279 | -CH3 | -CH2COC6H2[2,4,6-(CH3)3] |  | | 2.347 | 2.290 | |
| 280 | -CH3 | -CH2C6H4[2-COOC6H4(*p*-NO2)] | 2-CH3 | | 2.349 | 2.346 | |
| 281 |  |  |  | | 2.363 | 2.347 | |
| 282 | -CH3 | -CH2COC6H3[3,4-(OCH3)2] |  | | 2.365 | 2.225 | |
| 283 |  |  |  | | 2.377 | 2.347 | |
| 284\* | -CH3 | -CH2COC6H3[3,5-(OCH3)2] |  | | 2.380 | 2.266 | |
| 285\* | -CH3 | -CH2COC6H4(*p*-Ph) |  | | 2.395 | 2.197 | |
| 286 | -CH3 | -CH3 | 2-Br,4-Br,5-Br | | 2.428 | 2.340 | |
| 287\* | -CH3 | -CH3 | 2-Ph | | 2.452 | 2.344 | |
| 288 | -OCH2C6H3[2,4(Cl)2] | -CH2COC6H4(*p*-Cl) |  | | 2.021 | 2.212 | |
| 289 | -OH | -CH2C6H3[2,4-(Cl)2] |  | | 2.061 | 2.176 | |
| 290\* | -OCH=CH2 | -CH2C6H3[2,4(Cl)2) |  | | 2.068 | 2.180 | |
| 291\* | -OC2H5 | -CH2C6H4(*p*-NO2) |  | | 2.079 | 2.166 | |
| 292 | -OC2H5 | -CH2COC6H4(*p*-Cl) |  | | 2.114 | 2.092 | |
| 293 | -OC2H5 | -CH2C6H3[2,4-(Cl)2] |  | | 2.127 | 2.092 | |
| 294 |  |  |  | | 2.137 | 2.155 | |
| 295\* | -OCH2CH2Ph | -CH2C6H3[2,5-(Cl)2] |  | | 2.140 | 2.160 | |
| 296 | -OCOC(CH3) | -CH2COC6H4(*p*-Cl) |  | | 2.146 | 2.134 | |
| 297 | -OPh | -CH2COC6H4(*p*-N(CH3)2) |  | | 2.149 | 2.245 | |
| 298\* | -OCH2Ph | -CH2C6H3[2,4-(Cl)2] |  | | 2.158 | 2.144 | |
| 299 | -OH | -OH | 2-Br,4-CH3,5-CH3 | | 2.182 | 2.226 | |
| 300 | -OH | -OH | 2-CH3,4-Br | | 2.188 | 2.368 | |
| 301 | -OCH2C6H3(2,6[Cl]2) | -OCH2C6H3(2,6[Cl2]) | 2-C2H5 | | 2.193 | 2.276 | |
| 302 | -OCH3 | -CH2COC6H4(*p*-Cl) |  | | 2.193 | 2.162 | |
| 303 | -OH | -OH | 2-Ph,4-Br | | 2.199 | 2.321 | |
| 304\* | -OCH2Ph | -CH2C6H2[3,4,5(-OCH3)3] | 2-C2H5 | | 2.201 | 2.283 | |
| 305 | -OCOCH(CH3)3 | -CH2COC6H4(*p*-Cl) |  | | 2.220 | 2.134 | |
| 306\* | -OCH2C6H4(p-NO2) | -OCH2C6H4(*p*-NO2) | 2-CH3 | | 2.225 | 2.380 | |
| 307 | -OCH2C6H4(p-Br) | -OCH2C6H4(*p*-Br) | 2-C2H5 | | 2.230 | 2.249 | |
| 308 | -OPh | -CH2COC6H4(*p*-Cl) | 2-C2H5 | | 2.233 | 2.292 | |
| 309 | -OCH2C6H4(p-Br) | -OCH2C6H4(*p*-Br) | 2-CH3 | | 2.241 | 2.282 | |
| 310 | -OCH2C6H3(2,4[Cl]2) | -OCH2C6H3(2,4-[Cl]2) | 2-C2H5 | | 2.246 | 2.276 | |
| 311 | -OH | -OH | 2-Br | | 2.258 | 2.249 | |
| 312 | -OCOC(CH3)3 | -CH2COC6H4(*p*-Cl) | 2-C2H5 | | 2.265 | 2.234 | |
| 313 | -OH | -CH2C6H2[3,4,5(-OCH3)3] |  | | 2.279 | 2.159 | |
| 314 | -OH | -CH2COC6H4(*p*-Cl) | 2-C2H5 | | 2.299 | 2.257 | |
| 315 | -OH | -CH2COC6H4(*p*-Cl) | 2-CH3 | | 2.301 | 2.306 | |
| 316 | -OH | -CH2COC6H4(*p*-Cl) |  | | 2.305 | 2.172 | |
| 317 | -CH2Ph | -CH2Ph |  | | 1.796 | 2.088 | |
| 318 | -CH2Ph | n-C10H21 | 2-CH3 | | 1.942 | 2.040 | |
| 319\* | -CH2Ph | n-C14H29 | 2-CH3 | | 2.013 | 1.984 | |
| 320 | -CH2Ph | n-C5H11 | 2-n-C11H23 | | 2.066 | 2.006 | |
| 321 | -CH2Ph | -CH2Ph | 4-C2H4OH | | 2.130 | 2.024 | |
| 322\* | -Ph | -CH2COC6H4(*m*-OCH3) |  | | 2.167 | 2.201 | |
| 323 | -CH2Ph | -CH3 | 2-n-C11H23 | | 2.271 | 2.052 | |
| 324 | -CH2CH2Ph | -CH2COC6H4(*p*-Br) | 2-CH3 | | 2.286 | 2.318 | |
| 325\* | -CH2Ph | -CH2COC6H4(*p*-OCH3) | 2-CH3 | | 2.305 | 2.292 | |
| 326 | -Ph | -CH2COC6H4(*p*-CH3) | 2-CH3 | | 2.313 | 2.329 | |
| 327\* | -C(Ph)3 | -CH2COPh | 4-CH3 | | 2.313 | 2.258 | |
| 328\* | -CH2Ph(p-OCH3) | -CH2COC6H4(*p*-CH3) | 2-CH3 | | 2.351 | 2.375 | |
| 329 | -CH2Ph | -CH2COC6H4(*p*-Cl) | 2-CH3 | | 2.359 | 2.300 | |
| 330 | -CH2Ph | -CH2COPh | 2-CH3 | | 2.378 | 2.283 | |
| 331 | -Ph | -Ph | 2-Ph,4-NH2 | | 2.428 | 2.340 | |
| 332 | -Ph | -CH3 | 2-Ph,4-NH2 | | 2.452 | 2.344 | |
| benzimidazolium cation | | | | | | | |
| **Compound Nos.** | **1-substituent** | **3-substituent** | **Other substituents** | | **Exp. m.p. [Log (Tm°C)]** | **Predicted m.p. [Log (Tm°C)]** | |
| 333\* | -(CH2)3CN | -(CH2)2CN |  | | 2.178 | 2.377 | |
| 334\* | -CH3 | -CH2CH=CH2 |  | | 2.212 | 2.315 | |
| 335 | -CH2COOH | -CH2COPh |  | | 2.244 | 2.239 | |
| 336 | -CH2OH | -CH2COPh |  | | 2.262 | 2.249 | |
| 337 | -CH3 | -CH2COPh | 5-OCH3 | | 2.292 | 2.274 | |
| 338\* | -C2H5 | -CH2COC6H4(*p*-Br) |  | | 2.297 | 2.220 | |
| 339 | -CH2COOCH3 | -CH2COPh | 2-CH3 | | 2.312 | 2.368 | |
| 340 | -C2H5 | -C2H5 |  | | 2.314 | 2.200 | |
| 341 | -CH(CH3)2 | -CH2COPh | 2-NH2 | | 2.318 | 2.342 | |
| 342\* | -CH2COOCH3 | -CH2COC6H4(*p*-Br) | 2-CH3 | | 2.324 | 2.384 | |
| 343 | -CH2COOCH3 | -CH2COC6H4(*p*-OCH3) | 2-CH3 | | 2.331 | 2.375 | |
| 344 | -CH2CH=CH2 | -CH2COC6H4(*p*-Br) |  | | 2.332 | 2.239 | |
| 345\* | -CH2COOC2H5 | -CH2COPh | 2-C2H5 | | 2.332 | 2.320 | |
| 346 | -CH3 | -CH2COOC2H5 | 2-CH3 | | 2.332 | 2.397 | |
| 347 | -CH2COOCH3 | -CH2COC6H4(p-CH3) | 2-CH3 | | 2.336 | 2.410 | |
| 348 | -CH3 | -CH2COPh | 5-NO2 | | 2.349 | 2.368 | |
| 349 | -Ph | -CH2COC6H4(*p*-NO2) | 2-CH3 | | 2.355 | 2.416 | |
| 350\* | -C4H9 | -CH2COOCH3 | 2-NH2 | | 2.357 | 2.228 | |
| 351\* | -(CH2)3COOC2H5 | -CH2Ph | 2-CH3 | | 2.364 | 2.248 | |
| 352 | -CH2COOCH3 | -CH2COCH3 | 2-CH3 | | 2.364 | 2.432 | |
| 353 | -C2H5 | -CH2COOC2H5 | 2-C2H5 | | 2.367 | 2.288 | |
| 354\* | -CH2COOCH3 | -CH3 | 2-CH3 | | 2.369 | 2.472 | |
| 355 | -CH2COOC2H5 | -CH2COPh | 2-C2H5 | | 2.370 | 2.320 | |
| 356\* | -(CH2)3COOH | -CH2Ph | 2-CH3 | | 2.371 | 2.307 | |
| 357 | -CH3 | -CH2COC6H4(*p*-NO2) | 5-NO2 | | 2.372 | 2.420 | |
| 358 | -C2H5 | -C2H5 | 2-CH3 | | 2.374 | 2.343 | |
| 359\* | n-C15H31 | n-C15H31 | 2-CH3 | | 2.377 | 2.060 | |
| 360 | -CH3 | -CH2COC6H4(*p*-NO2) | 5-OCH3 | | 2.378 | 2.331 | |
| 361 | -CH3 | -CH2COOCH3 | 2-NH2 | | 2.381 | 2.372 | |
| 362 | -CH3 | -CH2CN | 2-CH3 | | 2.384 | 2.504 | |
| 363 | n-C9H19 | n-C9H19 | 2-CH3 | | 2.391 | 2.142 | |
| 364 | -CH2Ph | -CH2COC6H4(*p*-NO2) | 2-CH3 | | 2.394 | 2.415 | |
| 365 | -CH2COOC2H5 | -CH2COOC2H5 | 2-CH3 | | 2.397 | 2.310 | |
| 366 | -CH3 | -CH2COOC2H5 | 2-NH2 | | 2.401 | 2.298 | |
| 367 | -C2H5 | -CH2COC6H4(*p*-NO2) | 5-CH3,6-CH3 | | 2.404 | 2.265 | |
| 368\* | -CH3 | -CH(CH3)COOCH3 | 2-CH3 | | 2.407 | 2.485 | |
| 369 | -NH2 | -CH2COPh | 2-NH2 | | 2.411 | 2.434 | |
| 370 | -C2H5 | -CH2CN | 2-CH3 | | 2.417 | 2.423 | |
| 371 | -CH3 | -CH2COPh | 2-CH3,5-NO2 | | 2.422 | 2.502 | |
| 372\* | -CH3 | -CH3 | 2-C2H5,5-NO2 | | 2.423 | 2.533 | |
| 373 | -CH3 | -CH3 | 5-Cl | | 2.439 | 2.406 | |
| 374\* | -NH2 | -CH2COC6H4(*p*-OCH3) | 2-NH2 | | 2.446 | 2.441 | |
| 375 |  | | | | 2.504 | 2.479 | |
| 376 | -CH2C6H4(p-NO2) | -CH2C6H4(*p*-NO2) | 2-NH2 | | 2.568 | 2.552 | |

\* indicates test set compounds

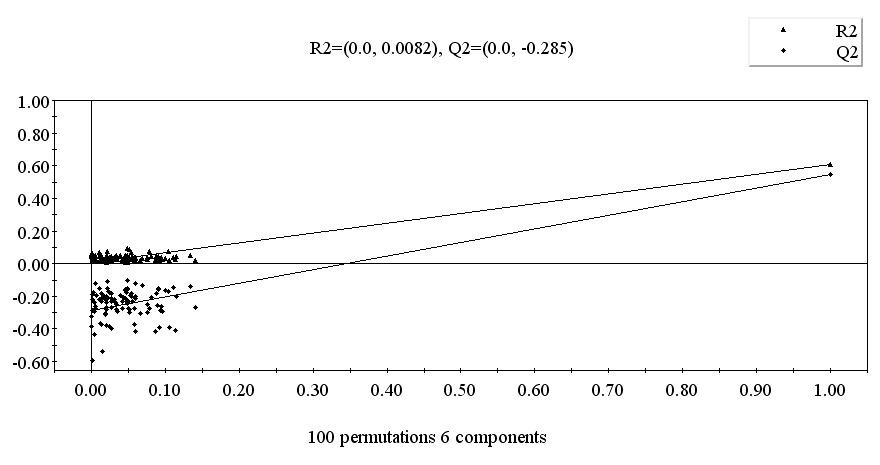
*Table S2. Relative importance of descriptors based on VIP plot.*

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Final PLS models** | | | | | |
| Model Nos. | Model-1 | Model-2 | Model-3 | Model-4 | Model-5 |
| Relative importance of Descriptors | F01[C-N] | F01[C-N] | <5-F01[C-N]> | F01[C-N] | <5-F01[C-N]> |
| ETA\_Shape\_P | ETA\_Shape\_P | ETA\_Shape\_P | ETA\_Shape\_P | ETA\_Shape\_P |
| ETA\_EtaP\_L | ETA\_EtaP\_L | ETA\_EtaP\_L | ETA\_EtaP\_L | ETA\_EtaP\_L |
| C-043 | C-043 | C-043 | C-043 | C-043 |
| <F07[C-N]-2> | <F07[C-N]-2> | <F07[C-N]-2> | <F07[C-N]-2> | <F07[C-N]-2> |
| NNRS | NNRS | NNRS | NNRS | NNRS |
| C-006 | C-006 | C-006 | C-006 | C-006 |
| <X4Av-0.111> | <X4Av-0.111> | <X4Av-0.111> | <X4Av-0.111> | <X4Av-0.111> |
| nArCOOR | nCH2RX | nCH2RX | nCH2RX | nCH2RX |
| nArCNO | nArCOOR | nArCOOR | nArCNO | nArCNO |

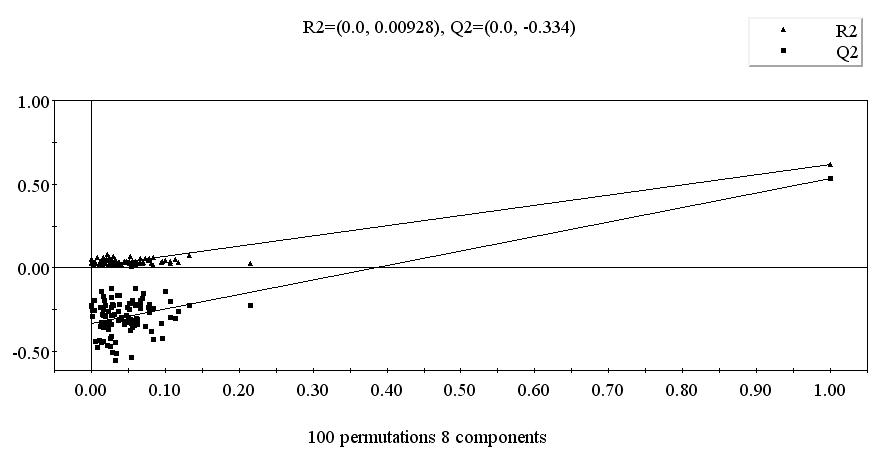
*Table S3. The quality of the consensus model obtained according to Golbraikh and Tropsha criteria.*

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | **Parameters** | **Consensus model** | **Remarks** | **Threshold value** |
| 1 | r^2 | 0.615 | Passed | r^2>0.6 |
| 2 | [(r^2-r0^2)/r^2] | 0.000113 | Passed | <0.1 |
| [(r^2-r0^'2)/r^2] | 0.411 | Failed |
| 3 | k | 1.0007 | Passed | 0.85<k or k'<1.15 |
|  | k' | 0.996 |

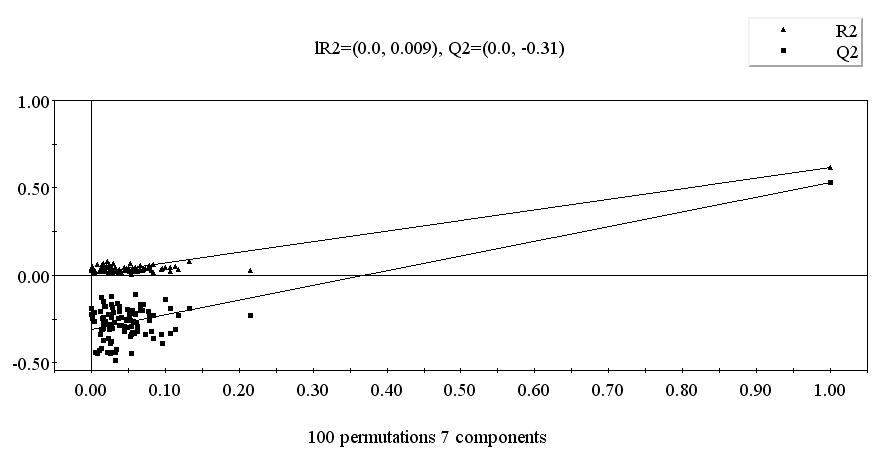
*Figure S1. Y-scrambling of the PLS model (model 1) based on 100 randomization cycles.*



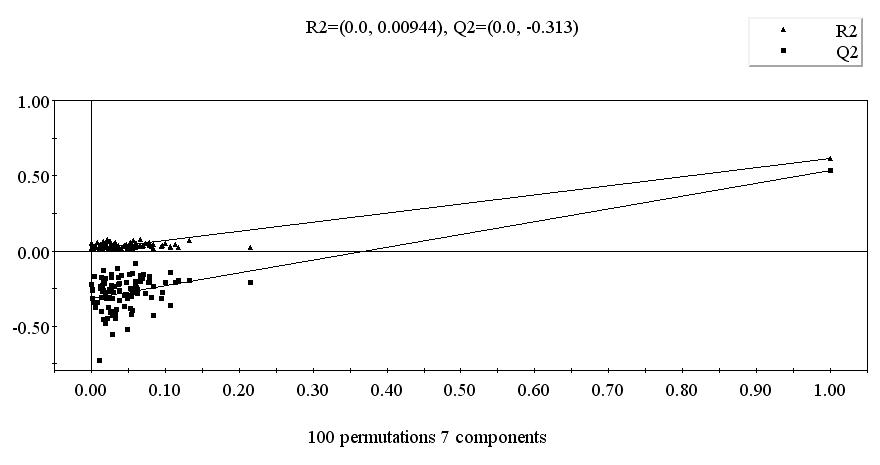
*Figure S2. Y-scrambling of the PLS model (model 2) based on 100 randomization cycles.*



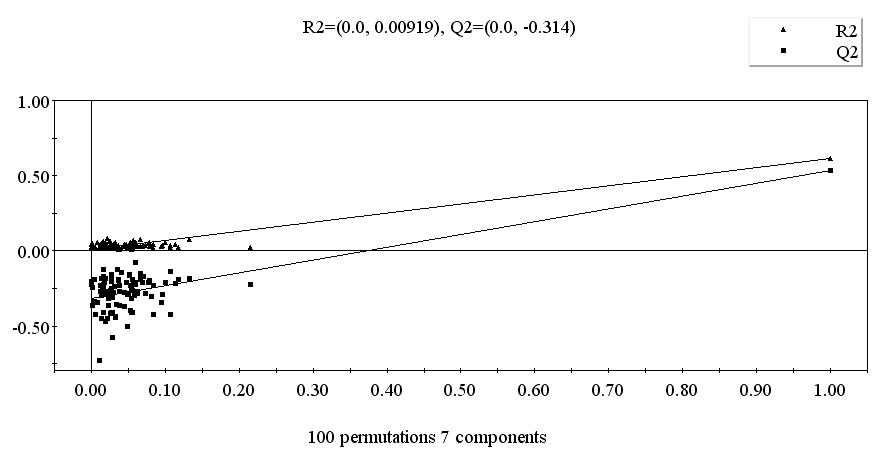
*Figure S3. Y-scrambling of the PLS model (model 3) based on 100 randomization cycles.*



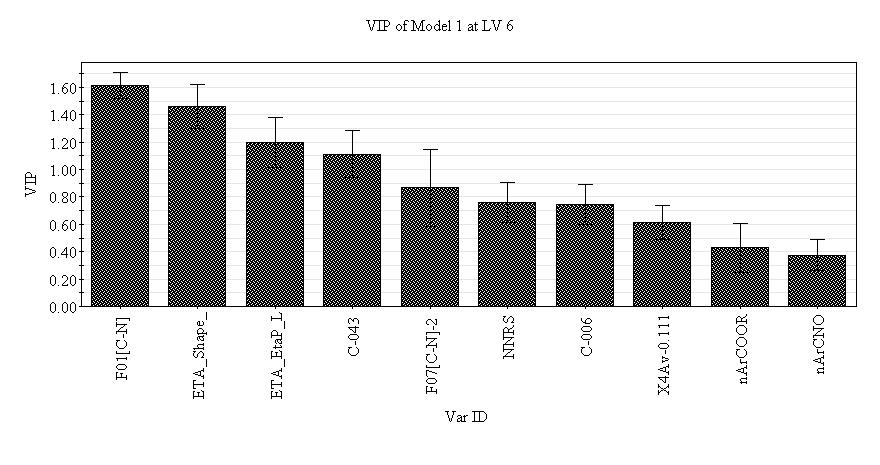
*Figure S4. Y-scrambling of the PLS model (model 4) based on 100 randomization cycles.*



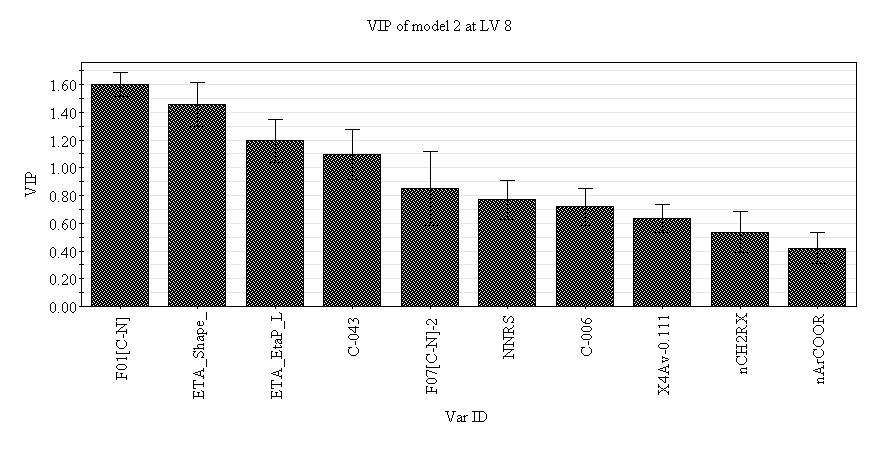
*Figure S5. Y-scrambling of the PLS model (model 5) based on 100 randomization cycles.*



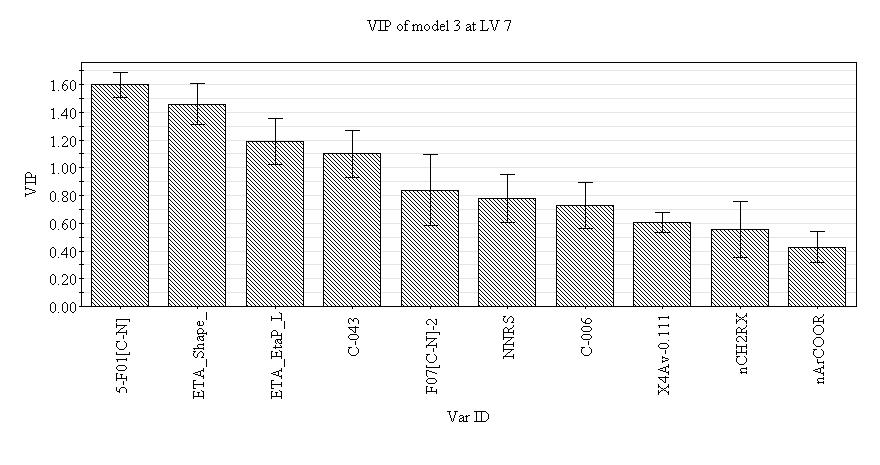
*Figure S6. Variable importance plot (VIP) of model 1.*



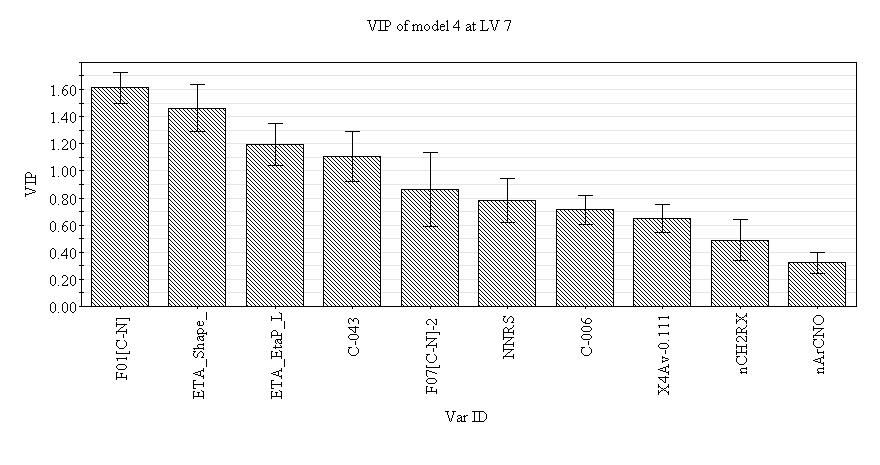
*Figure S7. Variable importance plot (VIP) of model 2.*



*Figure S8. Variable importance plot (VIP) of model 3.*



*Figure S9. Variable importance plot (VIP) of model 4.*



*Figure S10. Variable importance plot (VIP) of model 5.*

