Supplementary Material

Predicting retention times of polycyclic aromatic hydrocarbons in reversed-phase liquid chromatography: A quantitative structure retention relationship (QSRR) approach

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**Table. SI**. Experimental (Exp.), Predicted (Pred.) and Residual (Res.) values of log I for PAHs.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Name |   | polymeric |   |   | Monomeric |   |
| Exp. | Pred. | Res. | Exp.  | Pred. | Res. |
| Naphthalene | 2 | 2.0532 | 0.0532 | 2 | 2.0802 | 0.0802 |
| Fluorene | 2.7 | 2.7374 | 0.0374 | 2.75 | 2.7566 | 0.0066 |
| Anthracene | 3.16 | 3.132 | -0.028 | 3.11 | 3.1157 | 0.0057 |
| Fluoranthene | 3.39 | 3.5593 | 0.1693 | 3.43 | 3.3816 | -0.0484 |
| Aceanthrylene | 3.39 | 3.5146 | 0.1246 | 3.39 | 3.4995 | 0.1095 |
| pyrene | 3.55 | 3.6231 | 0.0731 | 3.63 | 3.4899 | -0.1401 |
| 11H-Benzo[a]fluorene | 3.81 | 3.749 | -0.061 | 3.75 | 3.7988 | 0.0488 |
| 11H-Benzo[b]fluorene | 3.82 | 3.7031 | -0.1169 | 3.78 | 3.828 | 0.048 |
| Cyclopenta[cd]pyrene | 3.94 | 3.8861 | -0.0539 | 3.95 | 4.0903 | 0.1403 |
| Benzo[ghi]fluoranthene | 3.95 | 3.8594 | -0.0906 | 4.07 | 4.0969 | 0.0269 |
| Triphenylene | 3.75 | 3.6021 | -0.1479 | 3.82 | 3.6972 | -0.1228 |
| Benzo[c]phenanthrene | 3.69 | 3.7788 | 0.0888 | 3.91 | 3.7039 | -0.2061 |
| Benz[a]anthracene | 4 | 3.995 | -0.005 | 4 | 3.9853 | -0.0147 |
| Chrysene | 4.06 | 4.1373 | 0.0773 | 3.97 | 3.9523 | -0.0177 |
| Benz[e]aceanthrylene | 4.25 | 4.2389 | -0.0111 | 4.34 | 4.5578 | 0.2178 |
| Benz[l]aceanthrylene | 4.26 | 4.2413 | -0.0187 | 4.38 | 4.4269 | 0.0469 |
| Benz[k]acephenanthrylene | 4.39 | 4.3584 | -0.0316 | 4.43 | 4.5273 | 0.0973 |
| Benz[a]aceanthrylene | 4.24 | 4.0922 | -0.1478 | 4.45 | 4.4899 | 0.0399 |
| Benzo[j]fluoranthene | 4.26 | 4.3209 | 0.0609 | 4.37 | 4.4568 | 0.0868 |
| Benzo[k]fluoranthene | 4.38 | 4.4403 | 0.0603 | 4.5 | 4.5022 | 0.0022 |
| Benzo[e]pyrene | 4.29 | 4.2252 | -0.0648 | 4.51 | 4.4802 | -0.0298 |
| Perylene | 4.33 | 4.3808 | 0.0508 | 4.52 | 4.497 | -0.023 |
| Benzo[a]pyrene | 4.51 | 4.5548 | 0.0448 | 4.68 | 4.6848 | 0.0048 |
| 13H-Dibenzo[a,g]fluorene | 4.53 | 4.5413 | 0.0113 | 4.62 | 4.6876 | 0.0676 |
| 11H-Indeno[2,1-a]phenanthrene | 4.91 | 4.8396 | -0.0704 | 4.74 | 4.8004 | 0.0604 |
| 13H-Dibenzo[a,h]fluorene | 4.96 | 4.8445 | -0.1155 | 4.77 | 4.8101 | 0.0401 |
| Indeno[1,2,3-cd]pyrene | 4.84 | 4.7669 | -0.0731 | 5.23 | 5.2265 | -0.0035 |
| Indeno[1,2,3-cd]fluoranthene | 4.93 | 4.9587 | 0.0287 | 5.05 | 5.1578 | 0.1078 |
| Benzo[ghi]perylene | 4.76 | 4.7061 | -0.0539 | 5.36 | 5.3214 | -0.0386 |
| Dibenzo[def,mno]chrysene | 5.08 | 4.9348 | -0.1452 | 5.61 | 5.6305 | 0.0205 |
| Dibenzo[c,g]phenanthrene | 4.07 | 4.0412 | -0.0288 | 4.51 | 4.2953 | -0.2147 |
| Benzo[b]triphenylene | 4.4 | 4.4598 | 0.0598 | 4.73 | 4.7379 | 0.0079 |
| Benzo[g]chrysene | 4.27 | 4.3909 | 0.1209 | 4.71 | 4.7247 | 0.0147 |
| Benzo[c]chrysene | 4.45 | 4.7367 | 0.2867 | 4.85 | 4.7213 | -0.1287 |
| Dibenz[a,j]anthracene | 4.56 | 4.5969 | 0.0369 | 4.84 | 4.653 | -0.187 |
| Pentaphene | 4.67 | 4.8886 | 0.2186 | 4.96 | 4.9748 | 0.0148 |
| Benzo[a]naphthacene | 4.99 | 5.0465 | 0.0565 | 4.5 | 4.964 | 0.464 |
| Benzo[b]chrysene | 5 | 5.1483 | 0.1483 | 5 | 4.9949 | -0.0051 |
| Picene | 5.18 | 5.1848 | 0.0048 | 5.02 | 4.9239 | -0.0961 |
| Dibenz[a,e]acephenanthrylene | 4.8 | 4.5894 | -0.2106 | 5.48 | 5.2584 | -0.2216 |
| Dibenzo[j,l]fluoranthene | 4.79 | 4.7415 | -0.0485 | 5.35 | 5.4208 | 0.0708 |
| Naphth[2,3-a]aceanthrylene | 4.91 | 4.7772 | -0.1328 | 5.51 | 5.4563 | -0.0537 |
| Naphth[2,3-e]acephenanthrylene | 5.27 | 5.257 | -0.013 | 5.64 | 5.5046 | -0.1354 |
| Naphtho[2,3-j]fluoranthene | 4.98 | 5.1963 | 0.2163 | 5.4 | 5.4736 | 0.0736 |
| Dibenz[e,k]acephenanthrylene | 5.28 | 5.2857 | 0.0057 | 5.59 | 5.5167 | -0.0733 |

**Table. SI**. Continued

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Name |   | Polymeric |   |   | Monomeric |   |
| Exp. | Pred. | Res. | Exp.  | Pred. | Res. |
| 7H-Benzo[c]fluorene | 3.49 | 3.4851 | -0.0049 | 3.64 | 3.6692 | 0.0292 |
| Benz[j]aceanthrylene | 4.26 | 4.3223 | 0.0623 | 4.29 | 4.4481 | 0.1581 |
| Benz[e]acephenanthrylene | 4.29 | 4.2918 | 0.0018 | 4.44 | 4.4668 | 0.0268 |
| Dibenzo[b,g]phenanthrene | 4.33 | 4.4514 | 0.1214 | 4.8 | 4.6493 | -0.1507 |
| Dibenz[a,h]anthracene | 4.73 | 4.9839 | 0.2539 | 4.86 | 4.8862 | 0.0262 |
| Dibenz[a,e]aceanthrylene | 4.9 | 4.5897 | -0.3103 | 5.5 | 5.3982 | -0.1018 |
| Indeno[1,2,3-fg]naphthacene | 5.07 | 4.7944 | -0.2756 | 5.71 | 5.628 | -0.082 |
| Benzo[rst]pentaphene | 5.74 | 5.4542 | -0.2858 | 5.93 | 5.8178 | -0.1122 |
| Anthracene, 1-methyl | 3.43 | 3.2975 | -0.1325 | 3.57 | 3.5323 | -0.0377 |
| Phenanthrene, 2-methyl | 3.68 | 3.476 | -0.204 | 3.71 | 3.6171 | -0.0929 |
| Phenanthrene, 3-methyl | 3.34 | 3.2989 | -0.0411 | 3.47 | 3.362 | -0.108 |
| Phenanthrene, 4-methyl | 3.26 | 3.3252 | 0.0652 | 3.4 | 3.3892 | -0.0108 |
| Phenanthrene, 9-methyl | 3.38 | 3.3532 | -0.0268 | 3.51 | 3.4003 | -0.1097 |
| Fluoranthene, 3-methyl | 3.86 | 3.8745 | 0.0145 | 3.91 | 3.9518 | 0.0418 |
| Pyrene, 1-methyl | 3.98 | 3.9024 | -0.0776 | 4.15 | 3.9512 | -0.1988 |
| Benz[a]anthracene, 1-methyl | 4.18 | 4.1046 | -0.0754 | 4.39 | 4.4171 | 0.0271 |
| Benz[a]anthracene, 2-methyl | 4.14 | 4.0963 | -0.0437 | 4.43 | 4.3685 | -0.0615 |
| Benz[a]anthracene, 4-methyl | 4.33 | 4.3361 | 0.0061 | 4.44 | 4.4917 | 0.0517 |
| Benz[a]anthracene, 6-methyl | 4.15 | 4.0944 | -0.0556 | 4.41 | 4.4644 | 0.0544 |
| Benz[a]anthracene, 8-methyl | 4.21 | 4.2051 | -0.0049 | 4.4 | 4.4258 | 0.0258 |
| Benz[a]anthracene, 10-methyl | 4.18 | 4.2514 | 0.0714 | 4.42 | 4.4419 | 0.0219 |
| Benz[a]anthracene, 12-methyl | 4.14 | 4.2485 | 0.1085 | 4.37 | 4.5758 | 0.2058 |
| Benzo[c]phenanthrene, 3-methyl | 4.09 | 4.0318 | -0.0582 | 4.41 | 4.357 | -0.053 |
| Benzo[c]phenanthrene, 5-methyl | 4.04 | 4.0741 | 0.0341 | 4.37 | 4.3441 | -0.0259 |
| Benzo[c]phenanthrene, 6-methyl | 4.17 | 3.8761 | -0.2939 | 4.37 | 4.2106 | -0.1594 |
| Chyrsene, 3-methyl | 4.28 | 4.3594 | 0.0794 | 4.41 | 4.4067 | -0.0033 |
| Chyrsene, 4-methyl | 4.2 | 4.2145 | 0.0145 | 4.36 | 4.3813 | 0.0213 |
| Chyrsene, 6-methyl | 4.17 | 4.2617 | 0.0917 | 4.35 | 4.3736 | 0.0236 |
| Benzo[a]pyrene, 1-methyl | 4.83 | 4.7796 | -0.0504 | 5.24 | 5.0683 | -0.1717 |
| Benzo[a]pyrene, 4-methyl | 4.84 | 4.7412 | -0.0988 | 5.26 | 5.1368 | -0.1232 |
| Benzo[a]pyrene, 5-methyl | 4.64 | 4.6567 | 0.0167 | 5.15 | 5.1626 | 0.0126 |
| Benzo[a]pyrene, 11-methyl | 4.66 | 4.6984 | 0.0384 | 5.14 | 5.2735 | 0.1335 |
| Benzo[a]pyrene, 1,2-dimethyl | 5.21 | 5.2264 | 0.0164 | 5.73 | 5.7094 | -0.0206 |
| Benzo[a]pyrene, 1,3-dimethyl | 5.26 | 5.0922 | -0.1678 | 5.75 | 5.512 | -0.238 |
| Benzo[a]pyrene, 1,4-dimethyl | 5.08 | 4.8818 | -0.1982 | 5.77 | 5.4979 | -0.2721 |
| Benzo[a]pyrene, 1,6-dimethyl | 5.1 | 4.9867 | -0.1133 | 5.65 | 5.4879 | -0.1621 |
| Benzo[a]pyrene, 3,12-dimethyl | 4.94 | 4.9331 | -0.0069 | 5.62 | 5.5425 | -0.0775 |
| Perylene, 3-methyl | 4.69 | 4.7255 | 0.0355 | 4.57 | 5.0275 | 0.4575 |
| Naphtho[1,2-k]fluoranthene | 5 | 5.2213 | 0.2213 | 5.34 | 5.3113 | -0.0287 |
| Naphtho[2,3-k]fluoranthene | 5.92 | 5.5952 | -0.3248 | 5.79 | 5.5242 | -0.2658 |
| Dibenzo[def,p]chrysene | 4.65 | 4.7862 | 0.1362 | 5.57 | 5.5884 | 0.0184 |
| Benzo[a]perylene | 4.93 | 5.2096 | 0.2796 | 5.54 | 5.6166 | 0.0766 |
| Naphtho[1,2,3,4-def]chrysene | 4.97 | 4.9702 | 0.0002 | 5.56 | 5.5666 | 0.0066 |

**Table. SI**. Continued

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Name |   | Polymeric |   |   | Monomeric |   |
| Exp. | Pred. | Res. | Exp.  | Pred. | Res. |
| Dibenzo[de,qr]naphthacene | 4.91 | 5.143 | 0.233 | 5.53 | 5.625 | 0.095 |
| Dibenzo[fg,op]naphthacene | 5.04 | 5.0321 | -0.0079 | 5.52 | 5.699 | 0.179 |
| Benzo[b]perylene | 5.04 | 4.8086 | -0.2314 | 5.56 | 5.5531 | -0.0069 |
| Naphtho[2,1,8-qra]naphthacene | 5.86 | 5.5916 | -0.2684 | 5.92 | 5.7437 | -0.1763 |
| Dibenzo[b,def]chrysene | 6 | 5.7094 | -0.2906 | 6 | 5.8644 | -0.1356 |
| Phenanthro[3,4-c]phenanthrene | 4.21 | 4.1858 | -0.0242 | 4.77 | 4.8017 | 0.0317 |
| Dibenzo[g,p]chrysene | 4.45 | 4.5961 | 0.1461 | 5.53 | 5.6454 | 0.1154 |
| Anthracene, 2-methyl | 3.69 | 3.4408 | -0.2492 | 3.69 | 3.723 | 0.033 |
| Anthracene, 9-methyl | 3.41 | 3.4833 | 0.0733 | 3.52 | 3.5974 | 0.0774 |
| Phenanthrene, 1-methyl | 3.4 | 3.4359 | 0.0359 | 3.5 | 3.4035 | -0.0965 |
| Fluoranthene, 1-methyl | 3.73 | 3.6879 | -0.0421 | 3.87 | 3.9504 | 0.0804 |
| Fluoranthene, 7-methyl | 3.8 | 3.7781 | -0.0219 | 3.91 | 3.9149 | 0.0049 |
| Fluoranthene, 8-methyl | 3.85 | 3.8324 | -0.0176 | 3.95 | 3.9809 | 0.0309 |
| Pyrene, 2-methyl | 4.04 | 3.9772 | -0.0628 | 4.21 | 4.3139 | 0.1039 |
| Pyrene, 4-methyl | 3.98 | 3.8308 | -0.1492 | 4.13 | 4.0205 | -0.1095 |
| Benz[a]anthracene, 3-methyl | 4.39 | 4.365 | -0.025 | 4.51 | 4.6163 | 0.1063 |
| Benz[a]anthracene, 5-methyl | 4.28 | 4.2072 | -0.0728 | 4.48 | 4.4358 | -0.0442 |
| Benz[a]anthracene, 7-methyl | 4.17 | 4.2448 | 0.0748 | 4.36 | 4.4645 | 0.1045 |
| Benz[a]anthracene, 9-methyl | 4.37 | 4.3714 | 0.0014 | 4.52 | 4.5525 | 0.0325 |
| Benz[a]anthracene, 11-methyl | 4.17 | 4.0218 | -0.1482 | 4.36 | 4.2997 | -0.0603 |
| Benzo[c]phenanthrene, 1-methyl | 3.73 | 3.787 | 0.057 | 4.1 | 4.1087 | 0.0087 |
| Benzo[c]phenanthrene, 2-methyl | 3.94 | 3.8032 | -0.1368 | 4.29 | 4.0115 | -0.2785 |
| Benzo[c]phenanthrene, 4-methyl | 4.04 | 4.0541 | 0.0141 | 4.37 | 4.2163 | -0.1537 |
| Chyrsene, 1-methyl | 4.39 | 4.3954 | 0.0054 | 4.46 | 4.3979 | -0.0621 |
| Chyrsene, 2-methyl | 4.49 | 4.5481 | 0.0581 | 4.54 | 4.5851 | 0.0451 |
| Chyrsene, 5-methyl | 4.17 | 4.2363 | 0.0663 | 4.36 | 4.5387 | 0.1787 |
| Triphenylene, 1-methyl | 3.88 | 3.8721 | -0.0079 | 4.19 | 4.2392 | 0.0492 |
| Benzo[a]pyrene, 2-methyl | 4.94 | 4.9836 | 0.0436 | 5.33 | 5.4154 | 0.0854 |
| Benzo[a]pyrene, 3-methyl | 4.9 | 4.8976 | -0.0024 | 5.25 | 5.1346 | -0.1154 |
| Benzo[a]pyrene, 6-methyl | 4.73 | 4.8103 | 0.0803 | 5.11 | 5.1064 | -0.0036 |
| Benzo[a]pyrene, 7-methyl | 4.74 | 4.7999 | 0.0599 | 5.13 | 5.1202 | -0.0098 |
| Benzo[a]pyrene, 8-methyl | 4.96 | 4.9365 | -0.0235 | 5.33 | 5.2481 | -0.0819 |
| Benzo[a]pyrene, 9-methyl | 4.78 | 4.8255 | 0.0455 | 5.18 | 5.1402 | -0.0398 |
| Benzo[a]pyrene, 10-methyl | 4.73 | 4.6615 | -0.0685 | 5.16 | 5.1126 | -0.0474 |
| Benzo[a]pyrene, 12-methyl | 4.61 | 4.6717 | 0.0617 | 5.14 | 5.1044 | -0.0356 |
| Benzo[a]pyrene, 2,3-dimethyl | 5.37 | 5.3198 | -0.0502 | 5.74 | 5.7253 | -0.0147 |
| Benzo[a]pyrene, 3,6-dimethyl | 5.09 | 5.0559 | -0.0341 | 5.63 | 5.5467 | -0.0833 |
| Benzo[a]pyrene, 3,11-dimethyl | 5.01 | 4.9604 | -0.0496 | 5.68 | 5.7123 | 0.0323 |
| Benzo[a]pyrene, 4,5-dimethyl | 4.9 | 4.9148 | 0.0148 | 5.54 | 5.5869 | 0.0469 |
| Benzo[a]pyrene, 7,10-dimethyl | 4.82 | 4.8266 | 0.0066 | 5.51 | 5.53 | 0.02 |
| Perylene, 1-methyl | 4.28 | 4.4591 | 0.1791 | 4.85 | 4.9304 | 0.0804 |
| Perylene, 2-methyl | 4.5 | 4.5484 | 0.0484 | 5.03 | 5.093 | 0.063 |
| Phenanthrene | 3 | 3.1353 | 0.1353 | 3 | 2.8838 | -0.1162 |
| Acephenanthrene | 3.37 | 3.4751 | 0.1051 | 3.38 | 3.4265 | 0.0465 |

**Table. SII**. Training and prediction sets for both columns by using Kennard and Stone algorithm.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| ID | Name | Status | ID | Name | Status |
| 1 | Naphthalene | Training | 44 | Naphtho[2,3-j]fluoranthene | Training |
| 2 | Fluorene | Training | 45 | Dibenz[e,k]acephenanthrylene | Training |
| 3 | Anthracene | Training | 46 | Naphtho[1,2-k]fluoranthene | Training |
| 4 | Fluoranthene | Training | 47 | Naphtho[2,3-k]fluoranthene | Training |
| 5 | Aceanthrylene | Training | 48 | Dibenzo[def,p]chrysene | Training |
| 6 | pyrene | Training | 49 | Benzo[a]perylene | Training |
| 7 | 11H-Benzo[a]fluorene | Training | 50 | Naphtho[1,2,3,4-def]chrysene | Training |
| 8 | 11H-Benzo[b]fluorene | Training | 51 | Dibenzo[de,qr]naphthacene | Training |
| 9 | Cyclopenta[cd]pyrene | Training | 52 | Dibenzo[fg,op]naphthacene | Training |
| 10 | Benzo[ghi]fluoranthene | Training | 53 | Benzo[b]perylene | Training |
| 11 | Triphenylene | Training | 54 | Naphtho[2,1,8-qra]naphthacene | Training |
| 12 | Benzo[c]phenanthrene | Training | 55 | Dibenzo[b,def]chrysene | Training |
| 13 | Benz[a]anthracene | Training | 56 | Phenanthro[3,4-c]phenanthrene | Training |
| 14 | Chrysene | Training | 57 | Dibenzo[g,p]chrysene | Training |
| 15 | Benz[e]aceanthrylene | Training | 58 | Anthracene, 2-methyl | Training |
| 16 | Benz[l]aceanthrylene | Training | 59 | Anthracene, 9-methyl | Training |
| 17 | Benz[k]acephenanthrylene | Training | 60 | Phenanthrene, 1-methyl | Training |
| 18 | Benz[a]aceanthrylene | Training | 61 | Fluoranthene, 1-methyl | Training |
| 19 | Benzo[j]fluoranthene | Training | 62 | Fluoranthene, 7-methyl | Training |
| 20 | Benzo[k]fluoranthene | Training | 63 | Fluoranthene, 8-methyl | Training |
| 21 | Benzo[e]pyrene | Training | 64 | Pyrene, 2-methyl | Training |
| 22 | Perylene | Training | 65 | Pyrene, 4-methyl | Training |
| 23 | Benzo[a]pyrene | Training | 66 | Benz[a]anthracene, 3-methyl | Training |
| 24 | 13H-Dibenzo[a,g]fluorene | Training | 67 | Benz[a]anthracene, 5-methyl | Training |
| 25 | 11H-Indeno[2,1-a]phenanthrene | Training | 68 | Benz[a]anthracene, 7-methyl | Training |
| 26 | 13H-Dibenzo[a,h]fluorene | Training | 69 | Benz[a]anthracene, 9-methyl | Training |
| 27 | Indeno[1,2,3-cd]pyrene | Training | 70 | Benz[a]anthracene, 11-methyl | Training |
| 28 | Indeno[1,2,3-cd]fluoranthene | Training | 71 | Benzo[c]phenanthrene, 1-methyl | Training |
| 29 | Benzo[ghi]perylene | Training | 72 | Benzo[c]phenanthrene, 2-methyl | Training |
| 30 | Dibenzo[def,mno]chrysene | Training | 73 | Benzo[c]phenanthrene, 4-methyl | Training |
| 31 | Dibenzo[c,g]phenanthrene | Training | 74 | Chyrsene, 1-methyl | Training |
| 32 | Benzo[b]triphenylene | Training | 75 | Chyrsene, 2-methyl | Training |
| 33 | Benzo[g]chrysene | Training | 76 | Chyrsene, 5-methyl | Training |
| 34 | Benzo[c]chrysene | Training | 77 | Triphenylene, 1-methyl | Training |
| 35 | Dibenz[a,j]anthracene | Training | 78 | Benzo[a]pyrene, 2-methyl | Training |
| 36 | Pentaphene | Training | 79 | Benzo[a]pyrene, 3-methyl | Training |
| 37 | Benzo[a]naphthacene | Training | 80 | Benzo[a]pyrene, 6-methyl | Training |
| 38 | Benzo[b]chrysene | Training | 81 | Benzo[a]pyrene, 7-methyl | Training |
| 39 | Picene | Training | 82 | Benzo[a]pyrene, 8-methyl | Training |
| 40 | Dibenz[a,e]acephenanthrylene | Training | 83 | Benzo[a]pyrene, 9-methyl | Training |
| 41 | Dibenzo[j,l]fluoranthene | Training | 84 | Benzo[a]pyrene, 10-methyl | Training |
| 42 | Naphth[2,3-a]aceanthrylene | Training | 85 | Benzo[a]pyrene, 12-methyl | Training |
| 43 | Naphth[2,3-e]acephenanthrylene | Training | 86 | Benzo[a]pyrene, 2,3-dimethyl | Training |

**Table S2.** Continued

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| ID | Name | Status | ID | Name | Status |
| 87 | Benzo[a]pyrene, 3,6-dimethyl | Training | 110 | Benz[a]anthracene, 1-methyl | Prediction |
| 88 | Benzo[a]pyrene, 3,11-dimethyl | Training | 111 | Benz[a]anthracene, 2-methyl | Prediction |
| 89 | Benzo[a]pyrene, 4,5-dimethyl | Training | 112 | Benz[a]anthracene, 4-methyl | Prediction |
| 90 | Benzo[a]pyrene, 7,10-dimethyl | Training | 113 | Benz[a]anthracene, 6-methyl | Prediction |
| 91 | Perylene, 1-methyl | Training | 114 | Benz[a]anthracene, 8-methyl | Prediction |
| 92 | Perylene, 2-methyl | Training | 115 | Benz[a]anthracene, 10-methyl | Prediction |
| 93 | Phenanthrene | Prediction | 116 | Benz[a]anthracene, 12-methyl | Prediction |
| 94 | Acephenanthrene | Prediction | 117 | Benzo[c]phenanthrene, 3-methyl | Prediction |
| 95 | 7H-Benzo[c]fluorene | Prediction | 118 | Benzo[c]phenanthrene, 5-methyl | Prediction |
| 96 | Benz[j]aceanthrylene | Prediction | 119 | Benzo[c]phenanthrene, 6-methyl | Prediction |
| 97 | Benz[e]acephenanthrylene | Prediction | 120 | Chyrsene, 3-methyl | Prediction |
| 98 | Dibenzo[b,g]phenanthrene | Prediction | 121 | Chyrsene, 4-methyl | Prediction |
| 99 | Dibenz[a,h]anthracene | Prediction | 122 | Chyrsene, 6-methyl | Prediction |
| 100 | Dibenz[a,e]aceanthrylene | Prediction | 123 | Benzo[a]pyrene, 1-methyl | Prediction |
| 101 | Indeno[1,2,3-fg]naphthacene | Prediction | 124 | Benzo[a]pyrene, 4-methyl | Prediction |
| 102 | Benzo[rst]pentaphene | Prediction | 125 | Benzo[a]pyrene, 5-methyl | Prediction |
| 103 | Anthracene, 1-methyl | Prediction | 126 | Benzo[a]pyrene, 11-methyl | Prediction |
| 104 | Phenanthrene, 2-methyl | Prediction | 127 | Benzo[a]pyrene, 1,2-dimethyl | Prediction |
| 105 | Phenanthrene, 3-methyl | Prediction | 128 | Benzo[a]pyrene, 1,3-dimethyl | Prediction |
| 106 | Phenanthrene, 4-methyl | Prediction | 129 | Benzo[a]pyrene, 1,4-dimethyl | Prediction |
| 107 | Phenanthrene, 9-methyl | Prediction | 130 | Benzo[a]pyrene, 1,6-dimethyl | Prediction |
| 108 | Fluoranthene, 3-methyl | Prediction | 131 | Benzo[a]pyrene, 3,12-dimethyl | Prediction |
| 109 | Pyrene, 1-methyl | Prediction | 132 | Perylene, 3-methyl | Prediction |

**Table. SIII.** Evaluation metrics formulas and their accepted thresholds.

|  |  |
| --- | --- |
| Metric | Threshold |
|  | R²ext >0.7 |
|  | Q²F1> 0.6 |
|  | Q²F2> 0.6 |
|  | Q²F3> 0.6 |
|  | CCC> 0.85 |

Where  is the predicted value calculated using the regression of the predicted and experimental data of the prediction set, the mean experimental value in the training set and *next*the number of molecules in the validation set,  the mean experimental value in the prediction set,  is the mean predicted values

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