**SUPPLEMENTARY MATERIAL**

**QSAR Study of octanol/water partition coefficient of organophosphorous compounds: Hybrid (GA/ MLR) Approach and Hybrid (GA/ ANN) Approach.**

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The comparative results of MLR and ANN model are showed in TABLE S-I. The results demonstrated that ANN was more powerful than MLR, because the ANN model presented a high statistical quality and low prediction error.

TABLE S-I. Comparative results of MLR and ANN.

|  |  |  |  |
| --- | --- | --- | --- |
| Méthodes | | | |
| Training set= 28 |  | MLR | SVM |
| R2 | 94.09% | 97.24% |
| Q2ext | 92.43% | 92.17% |
| SDEC | 0.471 | 0.332 |
| SDEPext | 0.533 | 0.466 |
| Validation set=15 | R2test | 89.35% | 92.53% |
| Q2ext | 89.73% | 92.17% |
| (r2-r20)/ r2<0.1 | -0.1188 | -0.075 |
| (r2-r’20)/ r2<0.1 | -0.118 | -0.0797 |
| 0.85 < k< 1.15 | 0.9917 | 0.9701 |
| 0.85< k’< 1.15 | 0.9851 | 1.0138 | |

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