Electronic Supplementary Material (ESI) for RSC Advances.


# Supporting Information

# (Submitted to the RSC Advances)

## Role of Exchange and Correlation in the Real External Prediction of Mutagenicity: Performance of Hybrid and Meta-hybrid Exchange-correlation Functionals

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# Table of Contents

| | |
|---|---|
| **Table S2f.** | Same as **Table S2a** but for electrophilicity index descriptor ($\omega$). |
| **Table S3.** | Compounds in the training set (T), prediction set (P) and excluded set (E) in different types of splitting methods employed for TA100 mutagenicity. Excluded compounds are either response or structural outliers (determined from Williams plot). |
| **Table S4.** | Compounds in the training set (T), prediction set (P) and excluded set (E) in different types of splitting methods employed for TA98 mutagenicity. Excluded compounds are either response or structural outliers (determined from Williams plot). |
| **Table S5.** | Comparison of the key internal and external validation parameters for the models based on the total energy ($E$) and energy of HOMO ($E_{HOMO}$) computed with the Exchange (X) only, Exchange + Correlation (X+C) methods, and with the effect of electron-correlation (CORR) of the descriptors, for modeling TA98 mutagenicity of nitrated-PAHs. |
| **Table S6.** | Same as **Table S5** but for the models based on the total electronic energy ($E$) and energy of the LUMO ($E_{LUMO}$). |
| **Table S7.** | Same as **Table S5** but for the models based on the total electronic energy ($E$) and absolute electronegativity ($\chi$). |
| **Table S8.** | Same as **Table S5** but for the models based on the total energy ($E$) and chemical hardness ($\eta$). |
| **Table S9.** | Same as **Table S5** but for the models based on the total electronic energy ($E$) and electrophilicity index ($\omega$). |
| **Table S10.** | Comparison of the key internal and external validation parameters for the models developed with the total energy ($E$), energy of HOMO ($E_{HOMO}$), energy of LUMO ($E_{LUMO}$), absolute electronegativity ($\chi$), chemical hardness ($\eta$) and electrophilicity index ($\omega$) computed with the Exchange (X) only Hartree-Fock (HF) method, for modeling TA100 mutagenicity and TA98 mutagenicity of nitrated-PAHs. |
| **Table S11.** | Value of internal and external validation parameters of two-descriptor QSAR models, for mutagenicity (LogTA100), developed using exchange (X) only (B88, HFX and HF) based methods through activity sampling (ordered response) splitting method. |
| **Table S12.** | Value of internal and external validation parameters of two-descriptor QSAR models, for mutagenicity (LogTA100), developed using exchange (X) only (B88, HFX and HF) based methods through 30% (random) splitting method. |
| **Table S13.** | Value of internal and external validation parameters of two-descriptor QSAR models, for mutagenicity (LogTA98), developed using exchange (X) only (B88, HFX and HF) based methods through activity sampling (ordered response) splitting method. |
| **Table S14.** | Value of internal and external validation parameters of two-descriptor QSAR models, for mutagenicity (LogTA98), developed using exchange (X) only (B88, HFX and HF) based methods through 30% (random) splitting method. |
| **Table S15.** | Value of internal and external validation parameters of two-descriptor QSAR models, for mutagenicity (LogTA100), developed using exchange-correlation (HFX+LYP, BLYP and B3LYP) based methods through activity sampling (ordered response) splitting method. |
| **Table S16.** | Value of internal and external validation parameters of two-descriptor QSAR models, for mutagenicity (LogTA100), developed using exchange-correlation (HFX+LYP, BLYP and B3LYP) based methods through 30% (random) splitting method. |
| **Table S17.** | Value of internal and external validation parameters of two-descriptor QSAR models, for mutagenicity (LogTA100), developed using meta exchange-correlation functionals (M06, M06-L and M06-2X) based methods through activity sampling (ordered response) splitting method. |
| **Table S18.** | Value of internal and external validation parameters of two-descriptor QSAR models, for mutagenicity (LogTA100), developed using meta exchange-correlation functionals (M06, M06-L and M06-2X) based methods through 30% (random) splitting method. |

| | |
|---|---|
| **Table S19.** | Value of internal and external validation parameters of two-descriptor QSAR models, for mutagenicity (LogTA98), developed using exchange-correlation (HFX+LYP, BLYP and B3LYP) based methods through activity sampling (ordered response) splitting method. |
| **Table S20.** | Value of internal and external validation parameters of two-descriptor QSAR models, for mutagenicity (LogTA98), developed using exchange-correlation (HFX+LYP, BLYP and B3LYP) based methods through 30% (random) splitting method. |
| **Table S21.** | Value of internal and external validation parameters of two-descriptor QSAR models, for mutagenicity (LogTA98), developed using meta exchange-correlation functionals (M06, M06-L and M06-2X) based methods through activity sampling (ordered response) splitting method. |
| **Table S22.** | Value of internal and external validation parameters of two-descriptor QSAR models, for mutagenicity (LogTA98), developed using meta exchange-correlation functionals (M06, M06-L and M06-2X) based methods through 30% (random) splitting method. |
| **Table S23.** | Value of internal and external validation parameters of two-descriptor QSAR models, for mutagenicity (LogTA100), developed using electron-correlation (CORR(HFX+LYP), CORR(BLYP), CORR(B3LYP)) based methods through activity sampling (ordered response) splitting method. |
| **Table S24.** | Value of internal and external validation parameters of two-descriptor QSAR models, for mutagenicity (LogTA100), developed using electron-correlation (CORR(HFX+LYP), CORR(BLYP), CORR(B3LYP)) based methods through 30% (random) splitting method. |
| **Table S25.** | Value of internal and external validation parameters of two-descriptor QSAR models, for mutagenicity (LogTA98), developed using electron-correlation (CORR(HFX+LYP), CORR(BLYP), CORR(B3LYP)) based methods through activity sampling (ordered response) splitting method. |
| **Table S26.** | Value of internal and external validation parameters of two-descriptor QSAR models, for mutagenicity (LogTA98), developed using electron-correlation (CORR(HFX+LYP), CORR(BLYP), CORR(B3LYP)) based methods through 30% (random) splitting method. |
| **Table S27.** | Value of internal and external validation parameters of two-descriptor QSAR models, for mutagenicity (LogTA100), developed using electron-correlation (CORR(M06), CORR(M06-L), CORR(M06-2X)) based methods through activity sampling (ordered response) splitting method. |
| **Table S28.** | Value of internal and external validation parameters of two-descriptor QSAR models, for mutagenicity (LogTA100), developed using electron-correlation (CORR(M06) CORR(M06-L), CORR(M06-2X)) based methods through 30% (random) splitting method. |
| **Table S29.** | Value of internal and external validation parameters of two-descriptor QSAR models, for mutagenicity (LogTA98), developed using electron-correlation (CORR(M06), CORR(M06-L), CORR(M06-2X)) based methods through activity sampling (ordered response) splitting method. |
| **Table S30.** | Value of internal and external validation parameters of two-descriptor QSAR models, for mutagenicity (LogTA98), developed using electron-correlation (CORR(M06), CORR(M06-L), CORR(M06-2X)) based methods through activity sampling 30% (random) splitting method. |

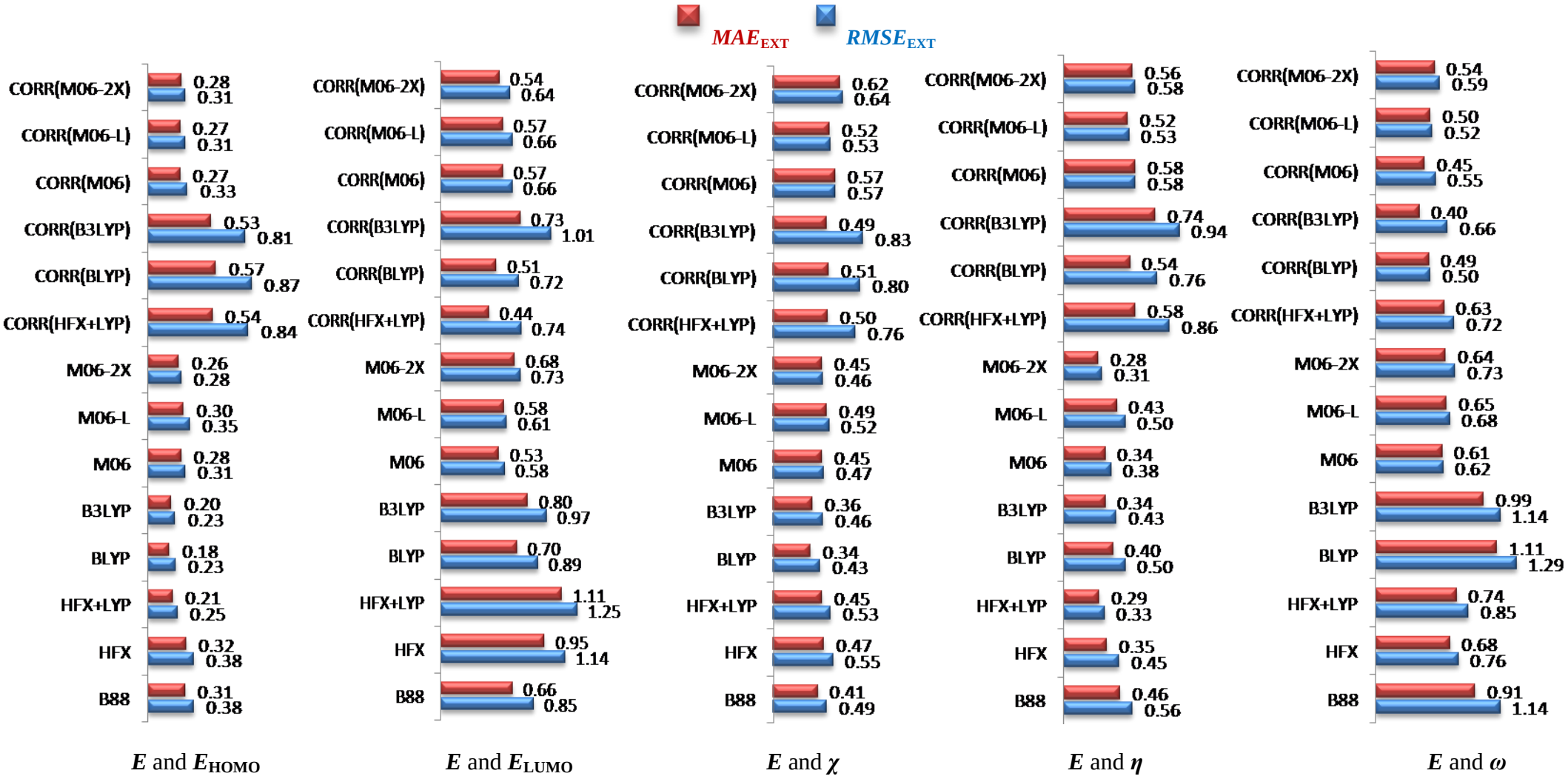


**Figure S1.** Comparison of the mean absolute error (*MAE*) and the root mean square error (*RMSE*) in the external (EXT) predictivity of various models, for the TA98 mutagenicity of nitrated-PAHs, based on the total energy (*E*), energy of the HOMO and the LUMO, absolute electronegativity ($\chi$), chemical hardness ($\eta$) and electrophilicity index ($\omega$) computed through exchange-only methods (HFX, B88), exchange-correlation (XC) methods (HFX+LYP, BLYP, B3LYP, M06, M06-L, M06-2X), and also based on the descriptors incorporating mainly the effect of electron correlation (CORR) from the respective XC methods.

**Figure S2(A).** Williams plots of the Standardized residuals vs Leverage (*h*) for TA100 mutagenicity for best models obtained with Exchange (X) only, Exchange + Correlation (X+C) methods, and effect of the electron-correlation (CORR) of the energies based descriptors with 30% random splitting. Training and prediction set chemicals are represented with open (yellow) and filled (blue) circles, respectively. The encircled values represent ID number of the compounds (refer to Supporting Information Table S1). The vertical (solid) line indicates warning leverage h*, whereas the horizontal (dashed) line specifies standardized residual value of 3.0.

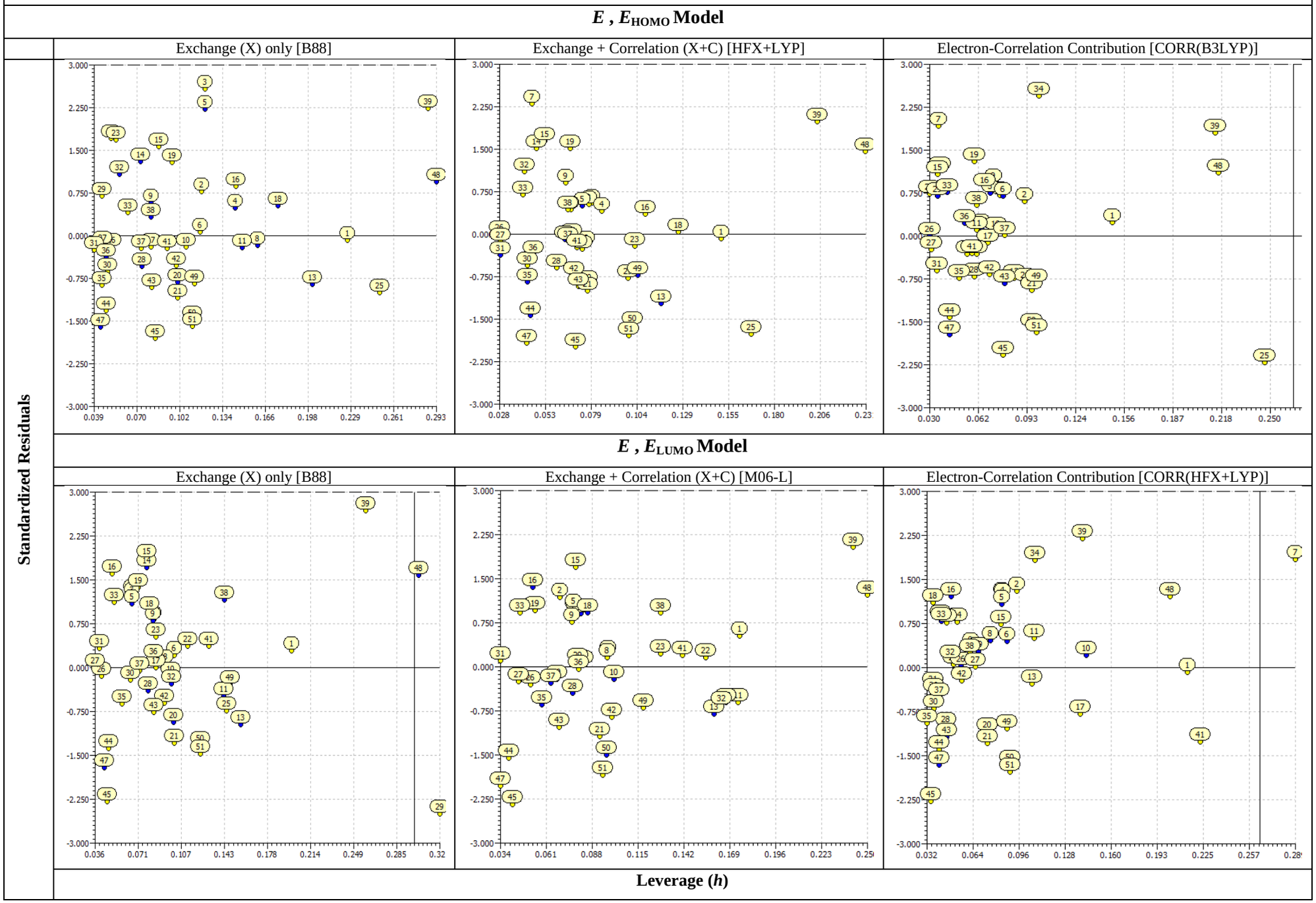

**Figure S2(A) continued…**

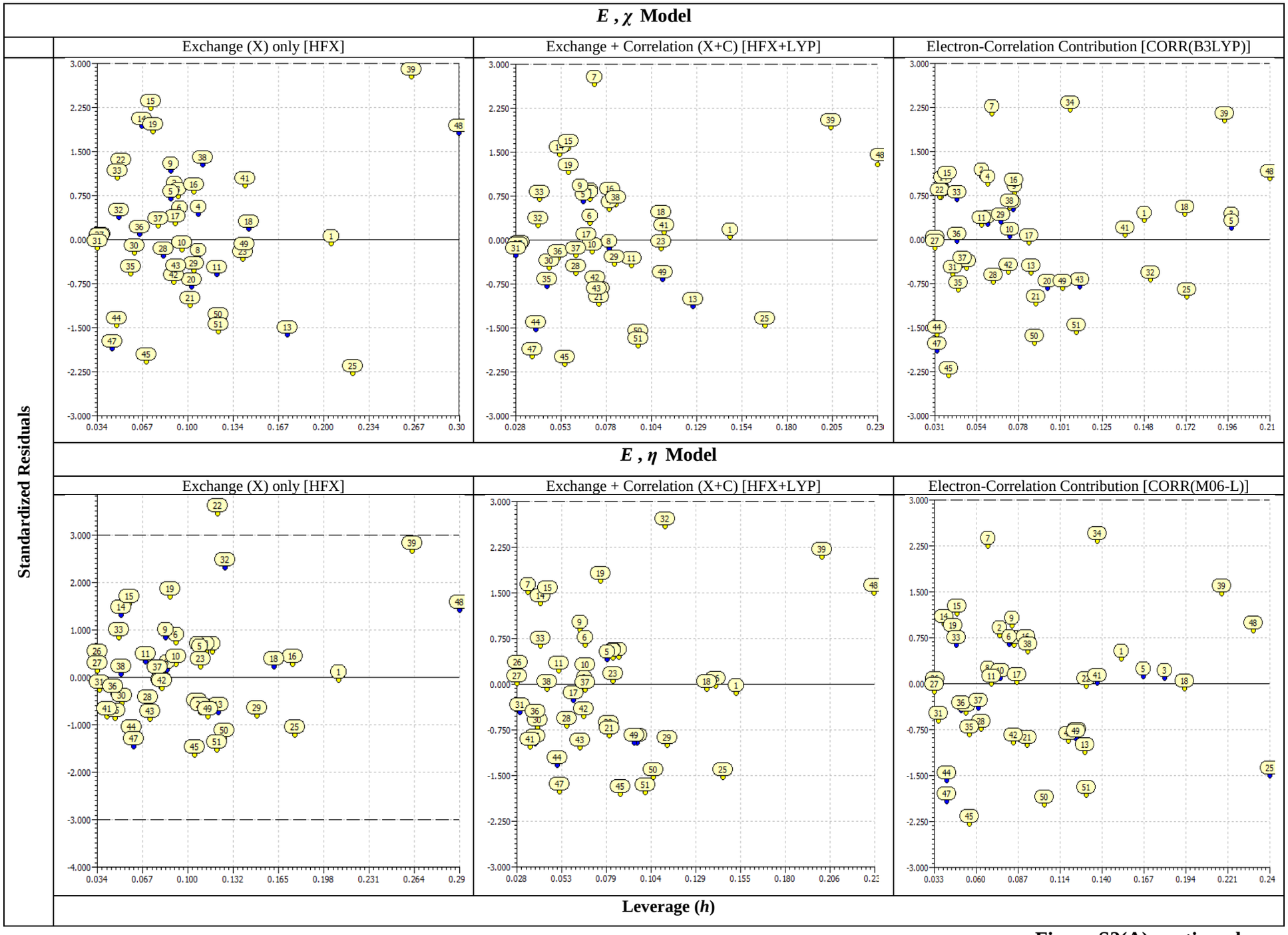


**Figure S2(A) continued…**

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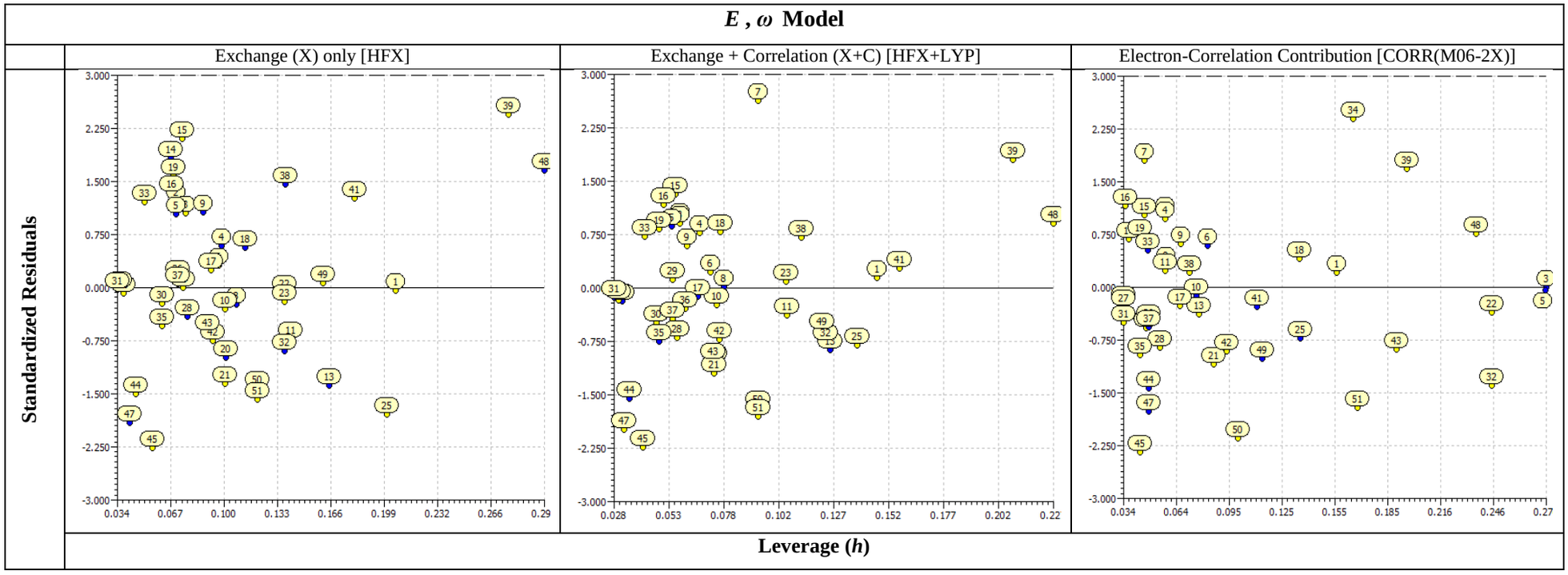
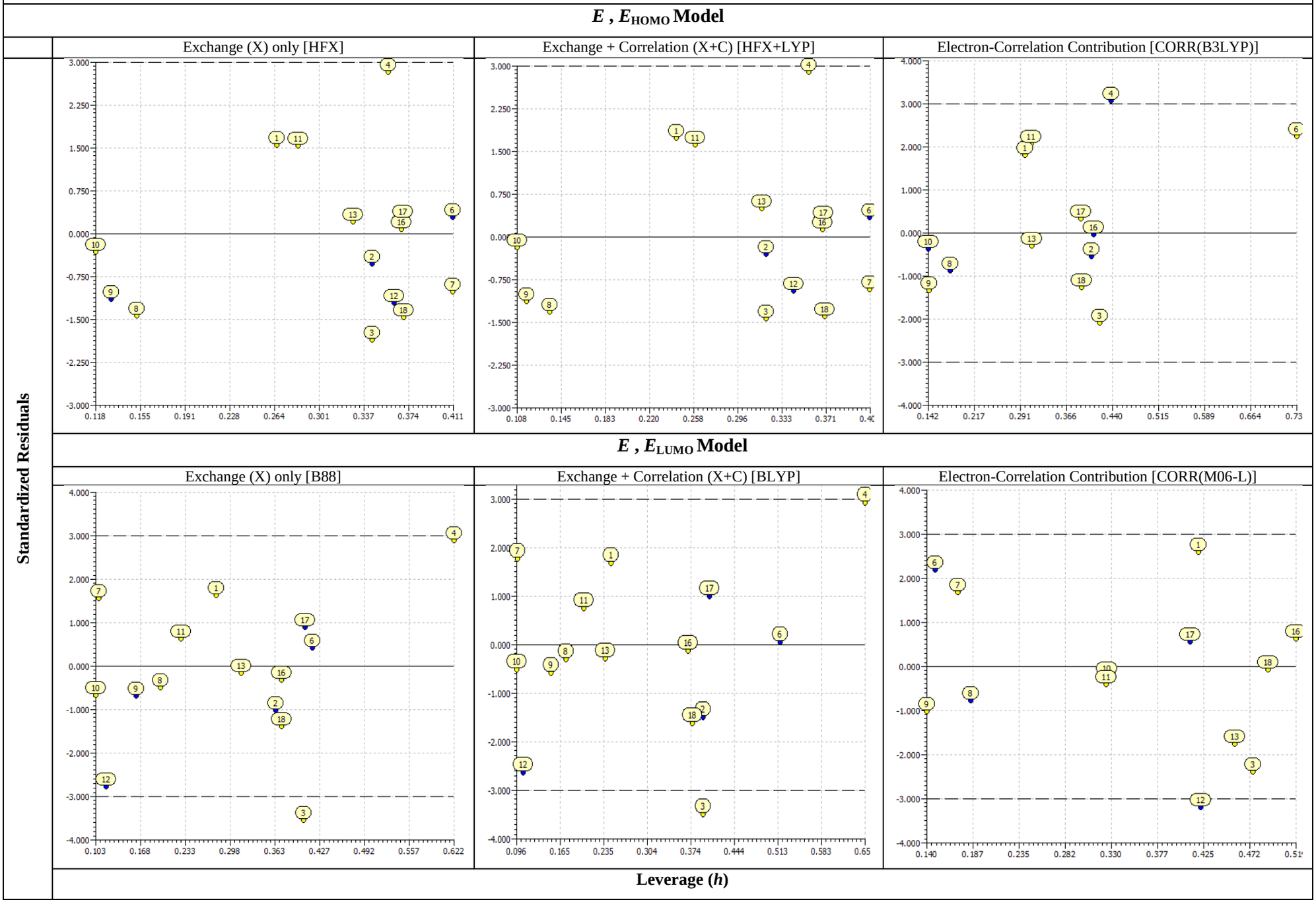


**Figure S2(B).** Williams plots of the Standardized residuals vs Leverage (*h*) for TA98 mutagenicity for best models developed with Exchange (X) only, Exchange + Correlation (X+C) methods, and effect of the electron-correlation (CORR) of the energies based descriptors with 30% random splitting. Training and prediction set chemicals are represented with open (yellow) and filled (blue) circles, respectively. The encircled values represent ID number of the compounds (refer to Supporting Information Table S1). The vertical (solid) line indicates warning leverage h*, whereas the horizontal (dashed) line specifies standardized residual value of 3.0.



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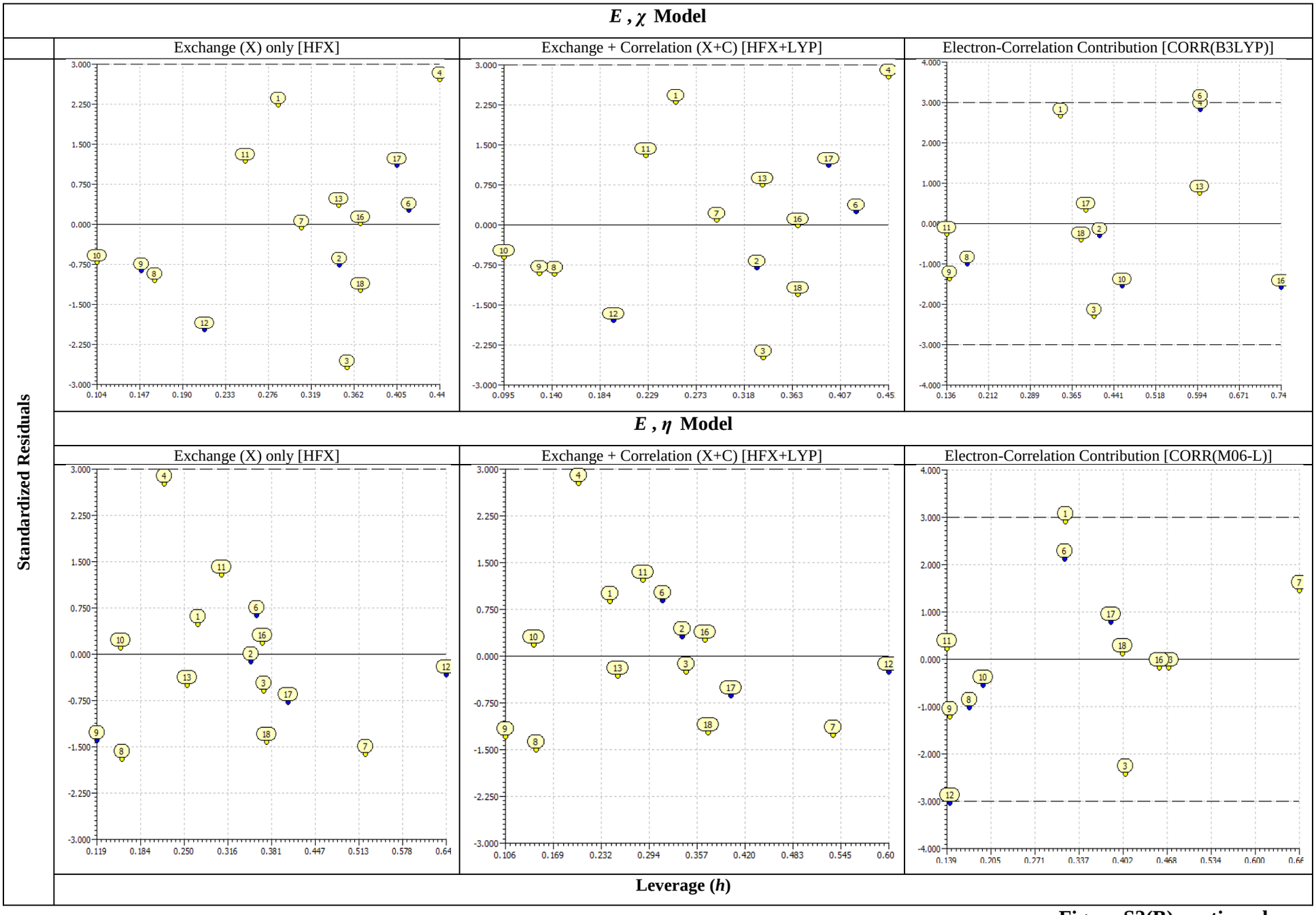



**Figure S2(B) continued…**

**Figure S2(B) continued…**

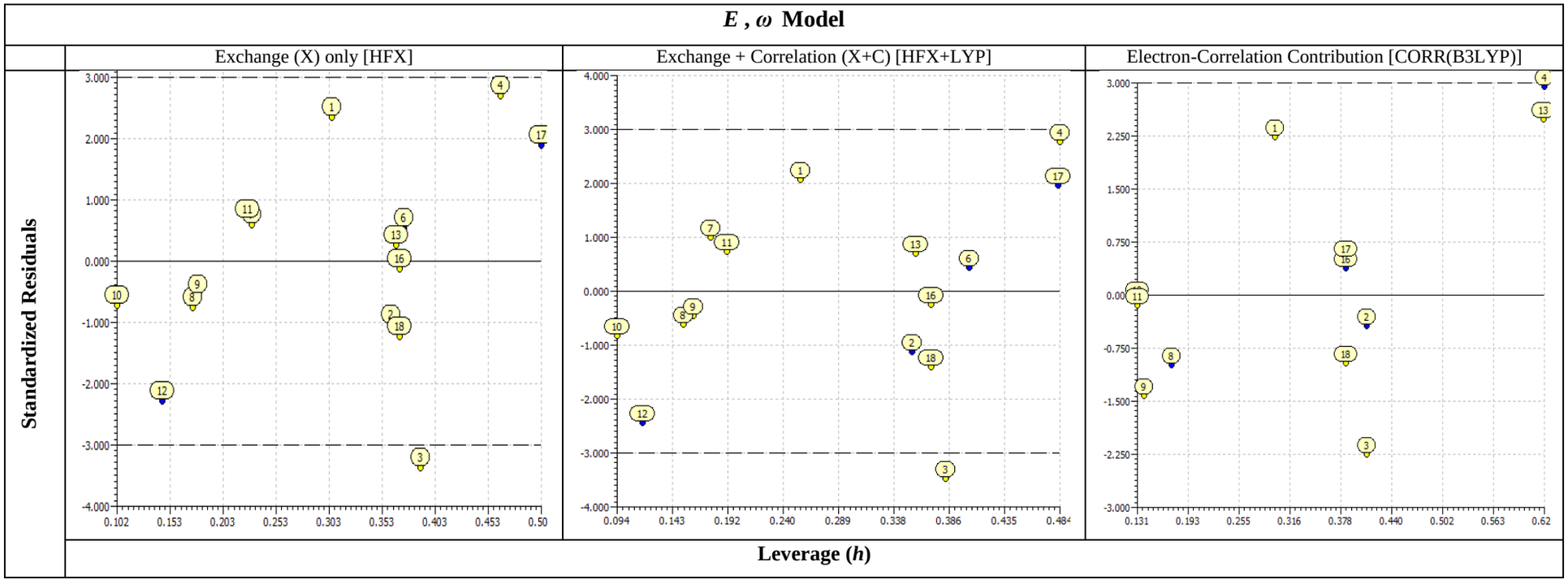
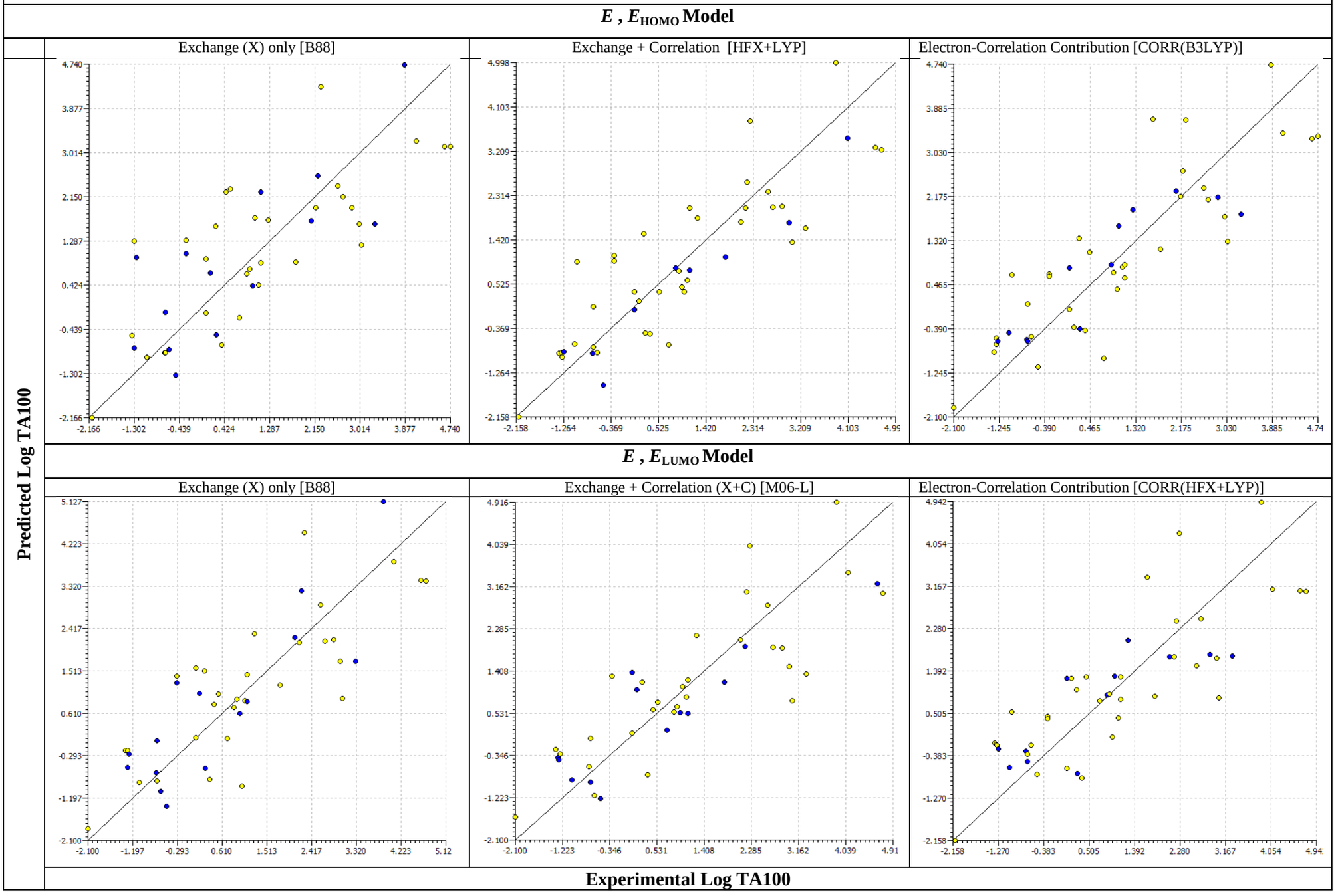


**Figure S3.** (**A**) Scatter plots of the Experimental vs Predicted TA100 Mutagenicity for the best models developed with Exchange (X) only, Exchange + Correlation (X+C) methods, and effect of the electron-correlation (CORR) of the energies based descriptors with 30% random splitting. Training and prediction set chemicals are represented with open (yellow) and filled (blue) circles, respectively.



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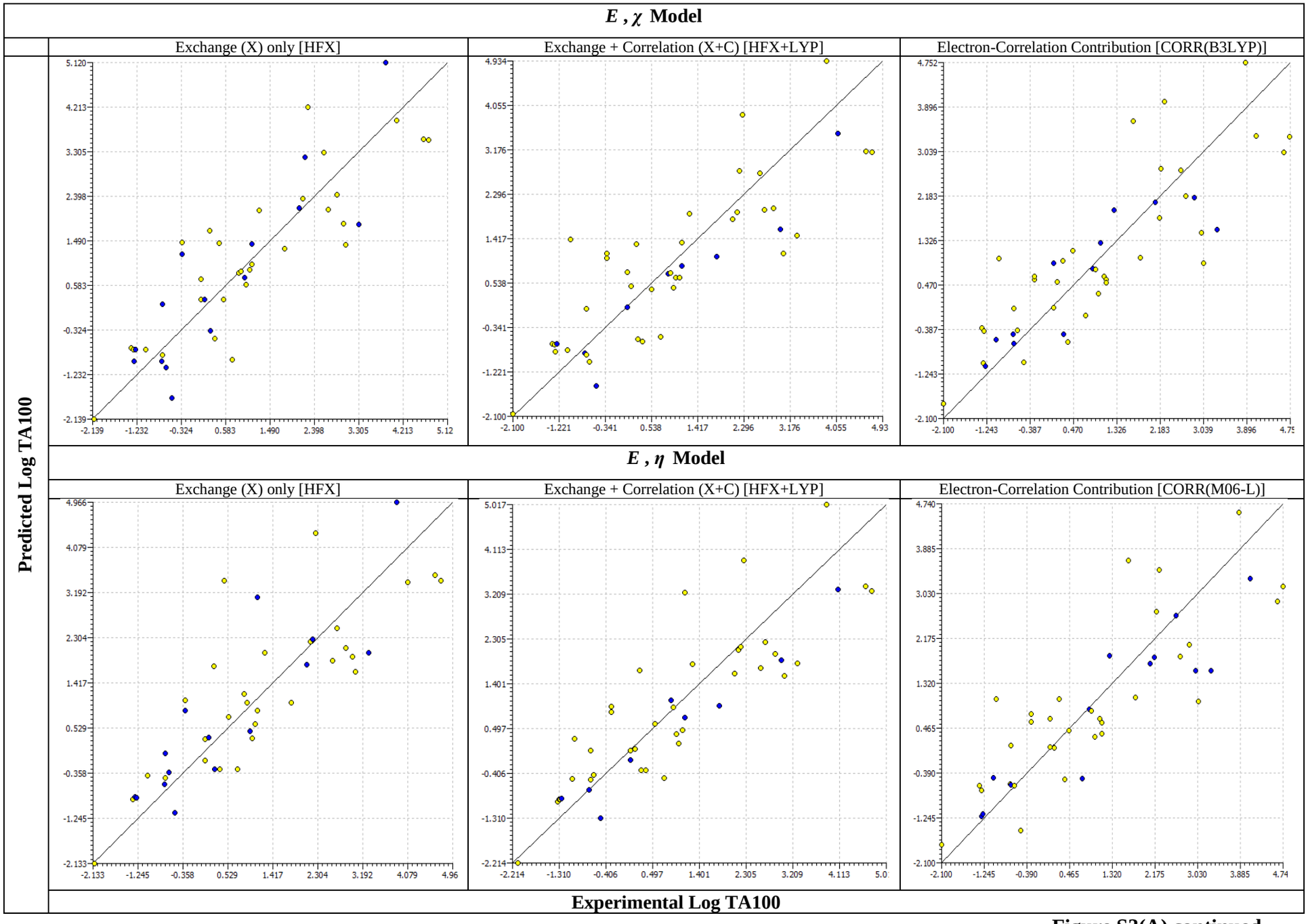


**Figure S3(A) continued…**

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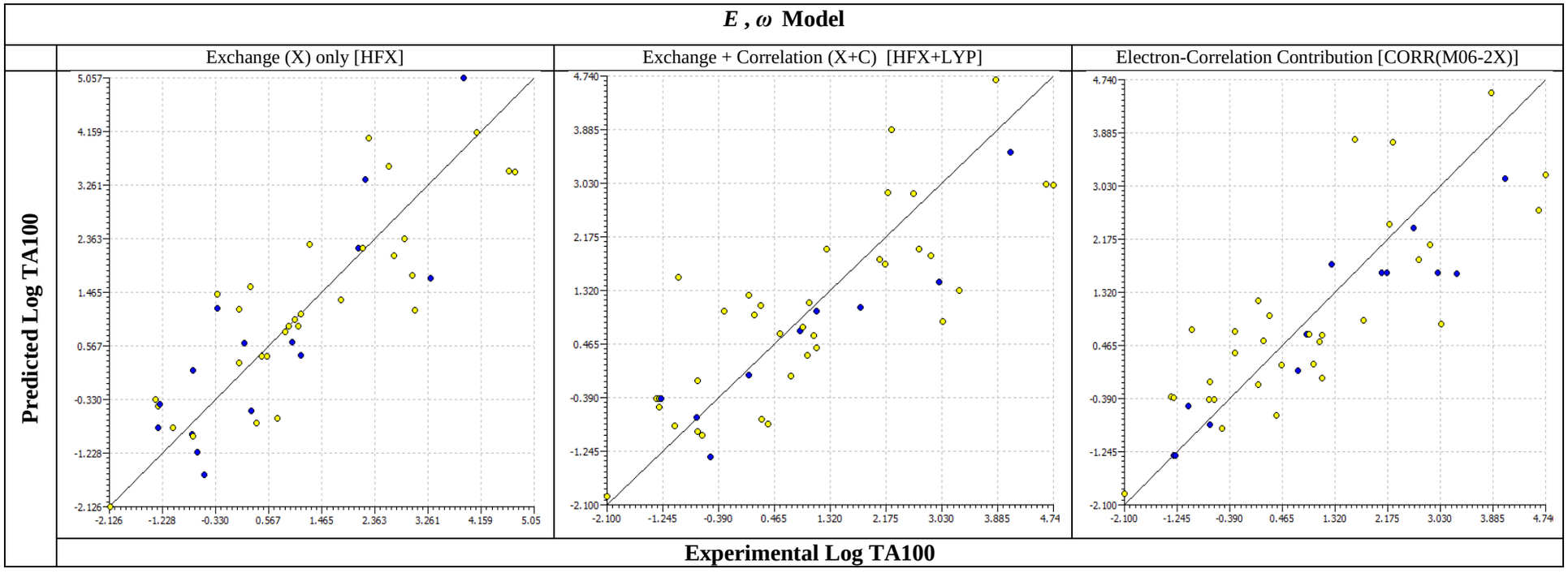
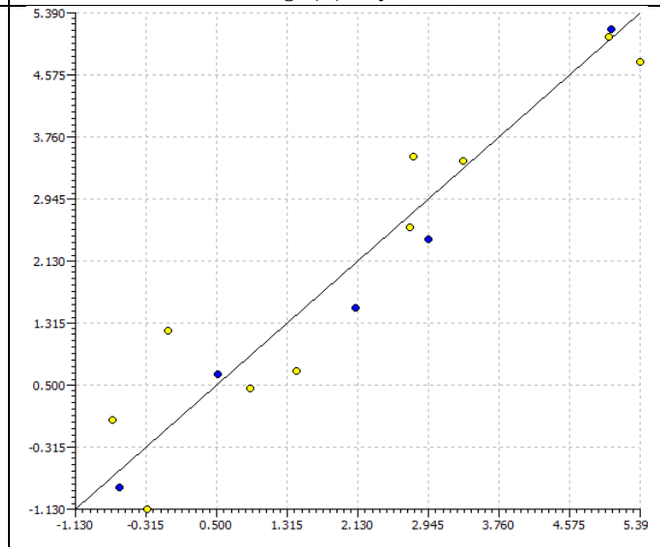
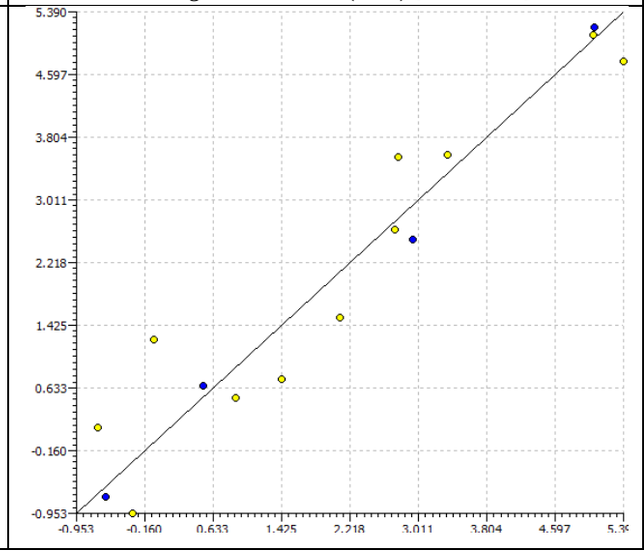
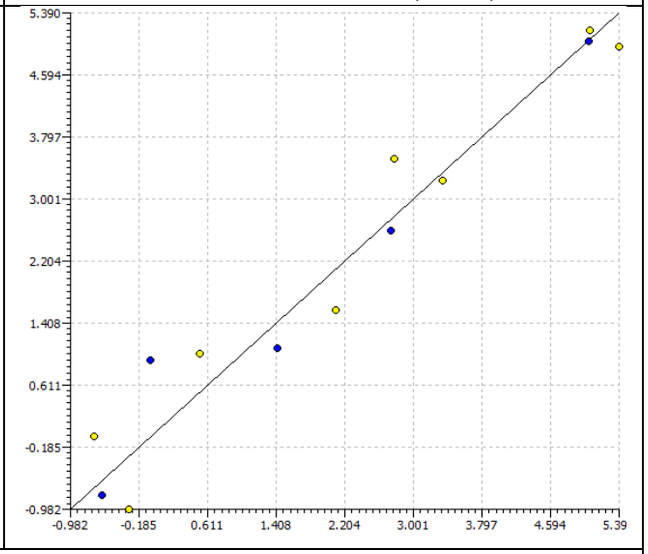
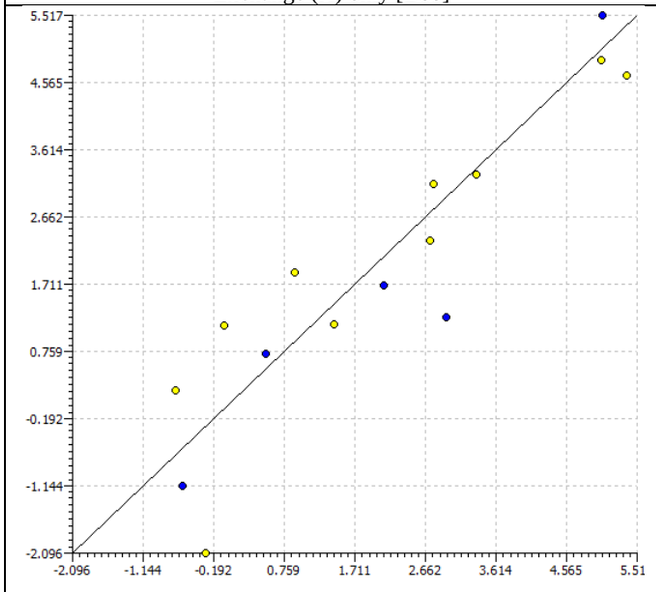
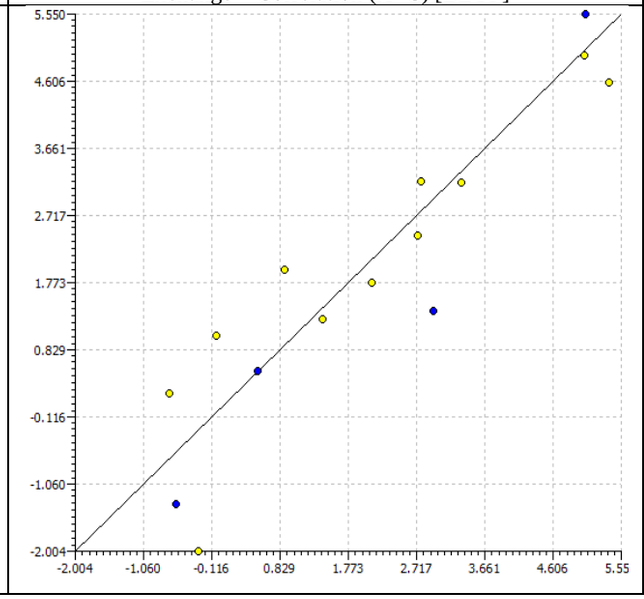
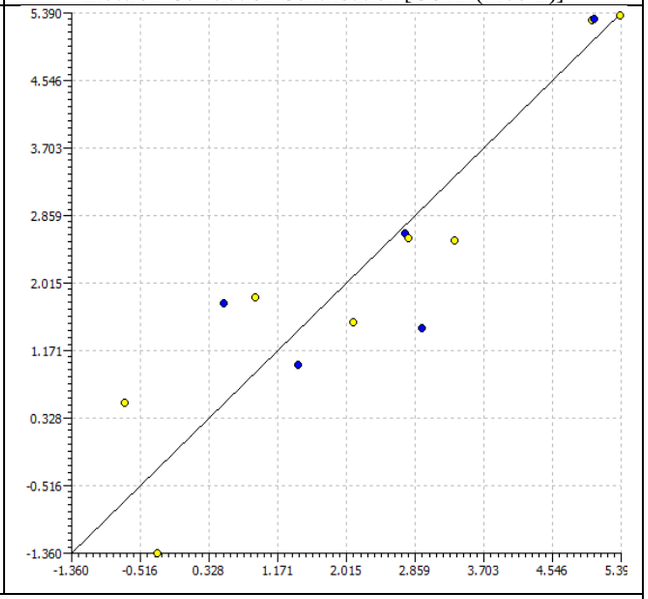


**Figure S3(B).** Scatter plots of the Experimental vs Predicted TA100 Mutagenicity for best models developed with Exchange (X) only, Exchange + Correlation (X+C) methods, and effect of the electron-correlation (CORR) of the energies based descriptors with 30% random splitting. Training and prediction set chemicals are represented with open (yellow) and filled (blue) circles, respectively.

**$E$ , $E_{HOMO}$ Model**

| | Exchange (X) only [HFX] | Exchange + Correlation (X+C) [HFX+LYP] | Electron-Correlation Contribution [CORR(B3LYP)] |
|---|---|---|---|
| **Predicted Log TA98** |  |  |  |

**$E$ , $E_{LUMO}$ Model**

| | Exchange (X) only [B88] | Exchange + Correlation (X+C) [BLYP] | Electron-Correlation Contribution [CORR(M06-L)] |
|---|---|---|---|
| **Predicted Log TA98** |  |  |  |

**Experimental Log TA98**

**Figure S3(B) continued…**

**Figure S3(B) continued…**

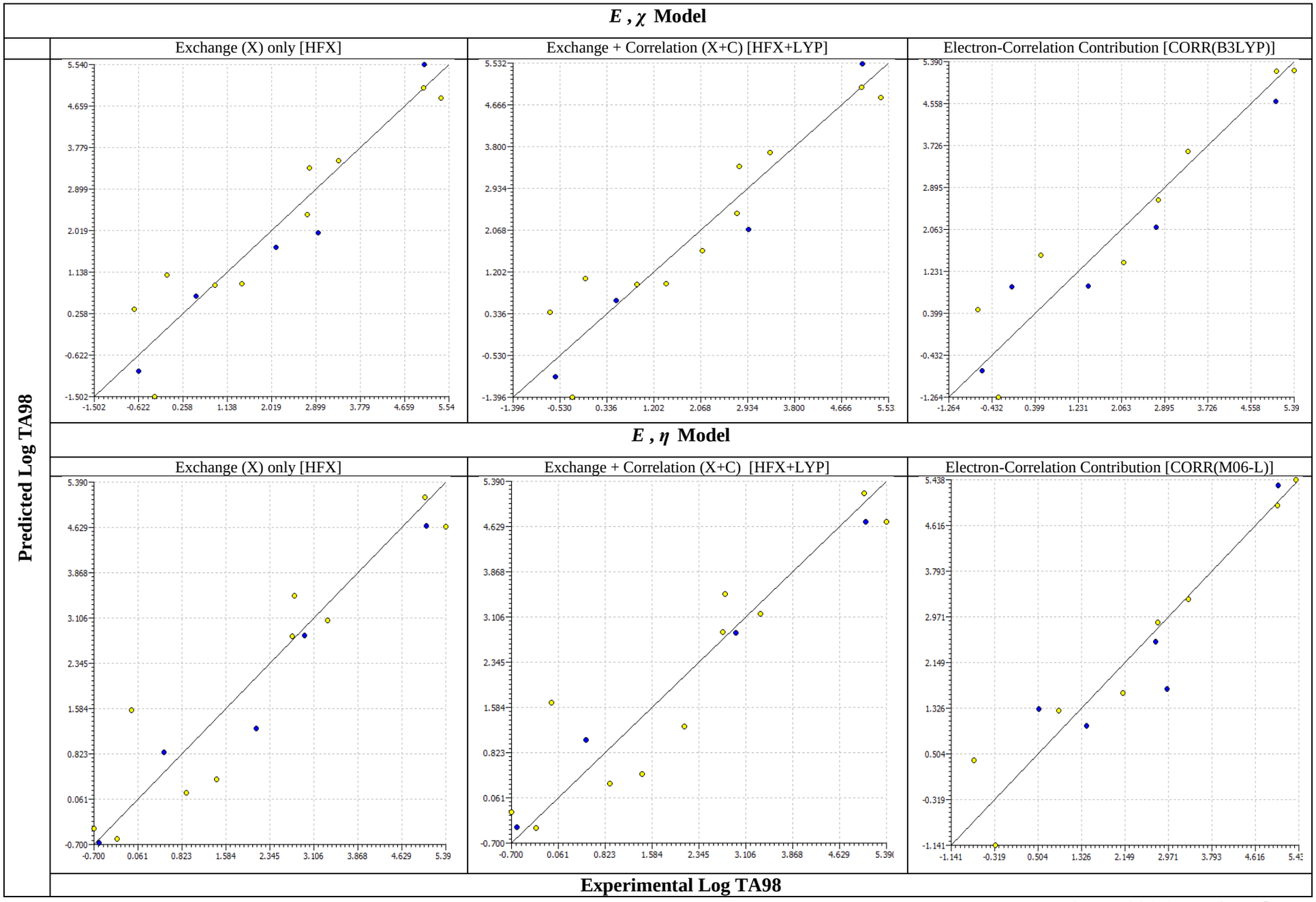



**Figure S3(B) continued…**

**Figure S3(B) continued…**

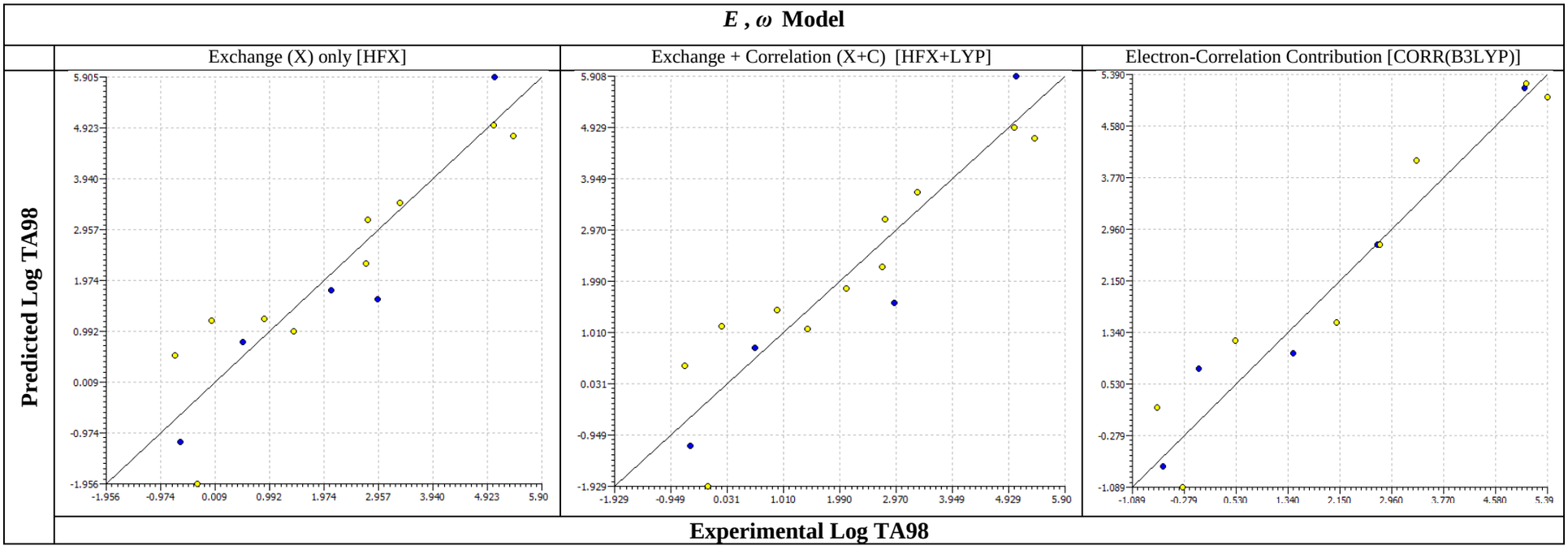


**Table S1.** List of nitrated-PAHs with their mutagenicity expressed as Log TA100 and Log TA98.

| Name of Compound | Chemical ID number | Activity (Log TA100) |
|---|---|---|
| 4-nitrotoulene | 1 | -2.10 |
| 2,6-dinitrotoulene | 2 | -1.34 |
| 3,4-dinitrotoulene | 3 | -1.30 |
| 2,4-dinitrotoulene | 4 | -1.29 |
| 2,3-dinitrotoulene | 5 | -1.26 |
| 6-nitroquinoline | 6 | -1.05 |
| 3-nitrocarbazole | 7 | -1.00 |
| 3,5-dinitrotoulene | 8 | -0.72 |
| 3-methyl-2-nitronaphthalene | 9 | -0.70 |
| 5-nitroquinoline | 10 | -0.70 |
| 2,5-dinitrotoulene | 11 | -0.63 |
| 1,3,6,8-tetranitronaphthalene | 12 | -0.52 |
| 1,3-dinitrobenzene | 13 | -0.51 |
| 2-nitrocarbazole | 14 | -0.30 |
| 4-nitrocarbazole | 15 | -0.30 |
| 2,3,4-trinitrotoulene | 16 | 0.08 |
| 1-methyl-2-nitronaphthalene | 17 | 0.08 |
| 2,4,6-trinitrotoulene | 18 | 0.16 |
| 9-nitroanthracene | 19 | 0.26 |
| 1-nitronaphthlene | 20 | 0.28 |
| 2-nitronaphthlene | 21 | 0.37 |
| 2,3,5-trinitrotoulene | 22 | 0.46 |
| 2,3,6-trinitrotoulene | 23 | 0.55 |
| 6-nitrobenzo[a]pyrene | 24 | 0.71 |
| 1,3,5-trinitrobenzene | 25 | 0.72 |
| 1,3-dinitronaphthlene | 26 | 0.86 |
| 1,5-dinitronaphthlene | 27 | 0.91 |
| 5-nitroacenaphthene | 28 | 0.97 |
| 3,4,5-trinitrotoulene | 29 | 1.01 |
| 2-nitrofluorene | 30 | 1.08 |
| 1,8-dinitronaphthlene | 31 | 1.12 |
| 2,4,5-trinitrotoulene | 32 | 1.12 |
| 2,7-dinitrofluorene | 33 | 1.27 |
| 1-nitrobenzo[e]pyrene | 34 | 1.65 |
| 2-nitrophenanthrene | 35 | 1.79 |
| 7-nitrofluoranthene | 36 | 2.09 |
| 1-nitropyrene | 37 | 2.17 |
| 6-nitrochrysene | 38 | 2.21 |
| 2,4,7-trinitro-9-fluorenone | 39 | 2.27 |
| 2,4,5,7-tetranitro-9-fluorenone | 40 | 2.46 |
| 8-nitrofluoranthene | 41 | 2.60 |
| 2,7-dinitro-9-fluorenone | 42 | 2.69 |
| 2-nitropyrene | 43 | 2.87 |
| 1-nitrofluoranthene | 44 | 3.00 |
| 2-nitroanthracene | 45 | 3.05 |
| 1,3,6,8-tetranitropyrene | 46 | 3.18 |
| 3-nitrofluoranthene | 47 | 3.31 |
| 1,3,6-trinitropyrene | 48 | 3.87 |
| 1,6-dinitropyrene | 49 | 4.09 |
| 1,3-dinitropyrene | 50 | 4.63 |
| 1,8-dinitropyrene | 51 | 4.74 |

| Name of Compound | Chemical ID number | Activity (Log TA98) |
|---|---|---|
| 1-methyl-2-nitronaphthalene | 1 | -0.70 |
| 1-nitronaphthlene | 2 | -0.61 |
| 2-nitronaphthlene | 3 | -0.30 |
| 1,3-dinitronaphthlene | 4 | -0.05 |
| 1,3-dinitrobenzene | 5 | 0.03 |
| 1,5-dinitronaphthlene | 6 | 0.52 |
| 1,8-dinitronaphthlene | 7 | 0.90 |
| 2-nitrofluorene | 8 | 1.43 |
| 2-nitrophenanthrene | 9 | 2.11 |
| 1-nitrofluoranthene | 10 | 2.74 |
| 1-nitropyrene | 11 | 2.78 |
| 2-nitroanthracene | 12 | 2.95 |
| 2-nitropyrene | 13 | 3.35 |
| 1,3,6,8-tetranitropyrene | 14 | 4.99 |
| 1,3,6-trinitropyrene | 15 | 4.99 |
| 1,3-dinitropyrene | 16 | 5.04 |
| 1,6-dinitropyrene | 17 | 5.06 |
| 1,8-dinitropyrene | 18 | 5.39 |

**Table S2a.** Computed value of total energy (*E*) descriptor, (all in a.u., 1a.u.=27.21165eV, 627.50956 kcal/mol) through exchange-only methods (HFX, B88, HF), exchange-correlation (XC) methods (HFX+LYP, BLYP, B3LYP, M06, M06-L, M06-2X), employing 6-311G(d,p) basis set, along with the descriptors incorporating mainly the effect of electron correlation (CORR) from the respective XC methods for 51-nitrated PAHs.

| Name of Compound | $-E_{HFX}$ | $-E_{B88}$ | $-E_{HF}$ | $-E_{HFX+LYP}$ | $-E_{BLYP}$ | $-E_{B3LYP}$ | $-E_{M06}$ | $-E_{M06-L}$ | $-E_{M06-2X}$ | $-E_{CORR(HFX+LYP)}$ | $-E_{CORR(BLYP)}$ | $-E_{CORR(B3LYP)}$ | $-E_{CORR(M06)}$ | $-E_{CORR(M06-L)}$ | $-E_{CORR(M06-2X)}$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 4-nitrotoulene | 473.324 | 473.585 | 473.324 | 475.809 | 476.057 | 476.194 | 475.869 | 476.137 | 475.988 | 2.485 | 2.472 | 2.869 | 2.545 | 2.813 | 2.663 |
| 2,6-dinitrotoulene | 676.827 | 677.298 | 676.828 | 680.148 | 680.599 | 680.733 | 680.318 | 680.668 | 680.458 | 3.321 | 3.301 | 3.905 | 3.490 | 3.841 | 3.631 |
| 3,4-dinitrotoulene | 676.822 | 677.197 | 676.657 | 680.140 | 680.595 | 680.608 | 680.184 | 680.545 | 680.317 | 3.318 | 3.398 | 3.951 | 3.527 | 3.888 | 3.660 |
| 2,4-dinitrotoulene | 676.837 | 677.306 | 676.837 | 680.157 | 680.606 | 680.741 | 680.325 | 680.675 | 680.464 | 3.320 | 3.300 | 3.904 | 3.488 | 3.838 | 3.627 |
| 2,3-dinitrotoulene | 676.820 | 677.192 | 676.654 | 680.139 | 680.491 | 680.605 | 680.183 | 680.544 | 680.316 | 3.319 | 3.299 | 3.951 | 3.529 | 3.890 | 3.662 |
| 6-nitroquinoline | 602.954 | 603.299 | 602.954 | 606.092 | 606.421 | 606.591 | 606.171 | 606.513 | 606.335 | 3.138 | 3.122 | 3.637 | 3.217 | 3.559 | 3.380 |
| 3-nitrocarbazole | 717.765 | 718.134 | 717.765 | 721.591 | 721.941 | 722.154 | 721.655 | 722.074 | 721.864 | 3.826 | 3.807 | 4.389 | 3.890 | 4.308 | 4.099 |
| 3,5-dinitrotoulene | 676.840 | 677.310 | 676.840 | 680.159 | 680.610 | 680.744 | 680.327 | 680.677 | 680.466 | 3.319 | 3.299 | 3.904 | 3.487 | 3.837 | 3.626 |
| 3-methyl-2-nitronaphthalene | 625.999 | 626.306 | 625.999 | 629.376 | 629.666 | 629.865 | 629.422 | 629.793 | 629.600 | 3.378 | 3.360 | 3.866 | 3.424 | 3.794 | 3.602 |
| 5-nitroquinoline | 602.947 | 603.293 | 602.947 | 606.086 | 606.416 | 606.576 | 606.166 | 606.509 | 606.330 | 3.139 | 3.123 | 3.629 | 3.219 | 3.561 | 3.383 |
| 2,5-dinitrotoulene | 676.835 | 677.305 | 676.835 | 680.155 | 680.606 | 680.740 | 680.324 | 680.674 | 680.464 | 3.320 | 3.300 | 3.905 | 3.489 | 3.839 | 3.629 |
| 1,3,6,8-tetranitronaphthalene | 1197.477 | 1198.417 | 1197.477 | 1203.098 | 1204.003 | 1204.169 | 1203.483 | 1204.073 | 1203.709 | 5.621 | 5.586 | 6.692 | 6.006 | 6.596 | 6.232 |
| 1,3-dinitrobenzene | 637.793 | 638.266 | 637.793 | 640.853 | 641.307 | 641.415 | 641.031 | 641.354 | 641.158 | 3.059 | 3.041 | 3.622 | 3.238 | 3.560 | 3.365 |
| 2-nitrocarbazole | 717.763 | 718.133 | 717.763 | 721.589 | 721.940 | 722.153 | 721.654 | 722.072 | 721.863 | 3.826 | 3.807 | 4.390 | 3.891 | 4.310 | 4.100 |
| 4-nitrocarbazole | 717.755 | 718.125 | 717.756 | 721.583 | 721.934 | 722.147 | 721.648 | 722.067 | 721.858 | 3.828 | 3.809 | 4.391 | 3.893 | 4.311 | 4.102 |
| 2,3,4-trinitrotoulene | 880.317 | 881.005 | 880.291 | 884.470 | 885.132 | 885.262 | 884.756 | 885.190 | 884.915 | 4.154 | 4.127 | 4.971 | 4.465 | 4.899 | 4.623 |
| 1-methyl-2-nitronaphthalene | 625.994 | 626.301 | 625.994 | 629.373 | 629.663 | 629.861 | 629.420 | 629.790 | 629.598 | 3.378 | 3.361 | 3.867 | 3.425 | 3.796 | 3.604 |
| 2,4,6-trinitrotoulene | 880.339 | 881.020 | 880.339 | 884.494 | 885.148 | 885.279 | 884.772 | 885.205 | 884.932 | 4.155 | 4.128 | 4.940 | 4.433 | 4.865 | 4.593 |
| 9-nitroanthracene | 739.615 | 739.977 | 739.615 | 743.624 | 743.967 | 744.200 | 743.671 | 744.117 | 743.895 | 4.009 | 3.990 | 4.585 | 4.056 | 4.501 | 4.280 |
| 1-nitronaphthlene | 586.949 | 587.261 | 586.949 | 590.067 | 590.363 | 590.535 | 590.125 | 590.467 | 590.290 | 3.118 | 3.102 | 3.586 | 3.176 | 3.518 | 3.341 |
| 2-nitronaphthlene | 586.957 | 587.268 | 586.957 | 590.074 | 590.370 | 590.542 | 590.131 | 590.474 | 590.296 | 3.117 | 3.102 | 3.584 | 3.173 | 3.516 | 3.339 |
| 2,3,5-trinitrotoulene | 880.167 | 880.918 | 880.167 | 884.329 | 885.144 | 884.876 | 884.641 | 885.085 | 884.794 | 4.162 | 4.226 | 4.709 | 4.474 | 4.918 | 4.627 |
| 2,3,6-trinitrotoulene | 880.323 | 880.910 | 880.324 | 884.478 | 885.137 | 885.149 | 884.635 | 885.079 | 884.789 | 4.155 | 4.227 | 4.825 | 4.311 | 4.755 | 4.465 |
| 6-nitrobenzo[a]pyrene | 968.071 | 968.502 | 968.071 | 973.400 | 973.806 | 974.128 | 973.426 | 974.024 | 973.740 | 5.329 | 5.305 | 6.057 | 5.355 | 5.953 | 5.670 |
| 1,3,5-trinitrobenzene | 841.304 | 841.986 | 841.304 | 845.197 | 845.855 | 845.961 | 845.484 | 845.889 | 845.630 | 3.893 | 3.869 | 4.657 | 4.181 | 4.585 | 4.327 |
| 1,3-dinitronaphthlene | 790.467 | 790.987 | 790.467 | 794.419 | 794.917 | 795.087 | 794.584 | 795.008 | 794.769 | 3.952 | 3.930 | 4.620 | 4.117 | 4.542 | 4.302 |
| 1,5-dinitronaphthlene | 790.460 | 790.981 | 790.460 | 794.413 | 794.912 | 795.081 | 794.579 | 795.003 | 794.765 | 3.953 | 3.931 | 4.621 | 4.119 | 4.543 | 4.305 |
| 5-nitroacenaphthene | 663.873 | 664.187 | 663.873 | 667.468 | 667.763 | 667.977 | 667.509 | 667.902 | 667.702 | 3.595 | 3.577 | 4.104 | 3.636 | 4.029 | 3.829 |
| 3,4,5-trinitrotoulene | 880.319 | 881.039 | 880.102 | 884.472 | 885.134 | 885.281 | 884.756 | 885.190 | 884.913 | 4.153 | 4.095 | 5.179 | 4.655 | 5.089 | 4.812 |
| 2-nitrofluorene | 701.758 | 702.091 | 701.758 | 705.558 | 705.873 | 706.098 | 705.598 | 706.017 | 705.808 | 3.801 | 3.782 | 4.340 | 3.840 | 4.260 | 4.050 |
| 1,8-dinitronaphthlene | 790.452 | 790.972 | 790.452 | 794.405 | 794.903 | 795.073 | 794.573 | 794.998 | 794.760 | 3.954 | 3.931 | 4.621 | 4.121 | 4.547 | 4.308 |
| 2,4,5-trinitrotoulene | 880.163 | 880.916 | 880.163 | 884.324 | 885.140 | 885.152 | 884.637 | 885.082 | 884.790 | 4.161 | 4.225 | 4.990 | 4.474 | 4.919 | 4.627 |
| 2,7-dinitrofluorene | 905.179 | 905.820 | 905.279 | 909.914 | 910.430 | 910.653 | 910.060 | 910.562 | 910.290 | 4.735 | 4.610 | 5.374 | 4.782 | 5.283 | 5.011 |
| 1-nitrobenzo[e]pyrene | 968.070 | 968.499 | 968.070 | 973.400 | 973.804 | 974.127 | 973.426 | 974.023 | 973.742 | 5.330 | 5.305 | 6.057 | 5.356 | 5.953 | 5.672 |
| 2-nitrophenanthrene | 739.640 | 739.995 | 739.640 | 743.650 | 743.985 | 744.220 | 743.691 | 744.136 | 743.915 | 4.010 | 3.990 | 4.580 | 4.051 | 4.496 | 4.275 |
| 7-nitrofluoranthene | 815.381 | 815.767 | 815.381 | 819.815 | 820.180 | 820.695 | 819.855 | 820.350 | 820.110 | 4.435 | 4.413 | 5.315 | 4.475 | 4.970 | 4.730 |
| 1-nitropyrene | 815.402 | 815.786 | 815.402 | 819.838 | 820.202 | 820.461 | 819.877 | 820.372 | 820.132 | 4.437 | 4.416 | 5.060 | 4.475 | 4.971 | 4.730 |
| 6-nitrochrysene | 892.311 | 892.711 | 892.311 | 897.214 | 897.592 | 897.889 | 897.241 | 897.789 | 897.525 | 4.904 | 4.880 | 5.578 | 4.930 | 5.478 | 5.214 |
| 2,4,7-trinitro-9-fluorenone | 1182.494 | 1183.329 | 1182.494 | 1188.212 | 1189.014 | 1189.221 | 1188.512 | 1189.116 | 1188.766 | 5.718 | 5.685 | 6.727 | 6.018 | 6.622 | 6.272 |
| 2,4,5,7-tetranitro-9-fluorenone | 1385.991 | 1387.036 | 1385.991 | 1392.545 | 1393.551 | 1393.755 | 1392.957 | 1393.644 | 1393.233 | 6.554 | 6.514 | 7.764 | 6.966 | 7.653 | 7.242 |
| 8-nitrofluoranthene | 854.433 | 854.812 | 854.433 | 859.126 | 859.483 | 859.770 | 859.152 | 859.673 | 859.420 | 4.694 | 4.671 | 5.337 | 4.719 | 5.241 | 4.988 |
| 2,7-dinitro-9-fluorenone | 978.989 | 979.613 | 978.989 | 983.871 | 984.470 | 984.680 | 984.062 | 984.584 | 984.296 | 4.882 | 4.857 | 5.690 | 5.073 | 5.595 | 5.307 |
| 2-nitropyrene | 815.401 | 815.785 | 815.409 | 819.837 | 820.201 | 820.460 | 819.876 | 820.371 | 820.131 | 4.437 | 4.416 | 5.051 | 4.467 | 4.962 | 4.722 |
| 1-nitrofluoranthene | 815.381 | 815.767 | 815.381 | 819.815 | 820.180 | 820.439 | 819.855 | 820.350 | 820.110 | 4.435 | 4.413 | 5.058 | 4.474 | 4.969 | 4.729 |
| 2-nitroanthracene | 739.630 | 739.990 | 739.630 | 743.638 | 743.979 | 744.212 | 743.682 | 744.127 | 743.905 | 4.008 | 3.989 | 4.583 | 4.052 | 4.498 | 4.275 |
| 1,3,6,8-tetranitropyrene | 1425.925 | 1426.940 | 1425.925 | 1432.867 | 1433.842 | 1434.094 | 1433.233 | 1433.975 | 1433.548 | 6.942 | 6.901 | 8.169 | 7.308 | 8.050 | 7.623 |
| 3-nitrofluoranthene | 815.382 | 815.768 | 815.382 | 819.816 | 820.181 | 820.441 | 819.856 | 820.351 | 820.110 | 4.434 | 4.413 | 5.058 | 4.473 | 4.969 | 4.728 |
| 1,3,6-trinitropyrene | 1222.421 | 1223.225 | 1222.421 | 1228.528 | 1229.298 | 1229.553 | 1228.784 | 1229.443 | 1229.079 | 6.107 | 6.073 | 7.132 | 6.363 | 7.023 | 6.658 |
| 1,6-dinitropyrene | 1018.913 | 1019.506 | 1018.913 | 1024.185 | 1024.750 | 1025.008 | 1024.331 | 1024.908 | 1024.607 | 5.272 | 5.245 | 6.095 | 5.418 | 5.995 | 5.694 |
| 1,3-dinitropyrene | 1018.912 | 1019.506 | 1018.912 | 1024.184 | 1024.751 | 1025.008 | 1024.331 | 1024.908 | 1024.606 | 5.272 | 5.245 | 6.096 | 5.419 | 5.997 | 5.694 |
| 1,8-dinitropyrene | 1018.914 | 1019.507 | 1018.913 | 1024.185 | 1024.752 | 1025.009 | 1024.331 | 1024.910 | 1024.608 | 5.272 | 5.245 | 6.096 | 5.418 | 5.997 | 5.695 |

**Table S2b.** Same as **Table S2a** but for HOMO energy descriptor ($E_{HOMO}$).

| Name of Compound | $-E_{HFex}^{HOMO}$ | $-E_{B88}^{HOMO}$ | $-E_{HF}^{HOMO}$ | $-E_{HFex+LYP}^{HOMO}$ | $-E_{BLYP}^{HOMO}$ | $-E_{B3LYP}^{HOMO}$ | $-E_{M06}^{HOMO}$ | $-E_{M06-L}^{HOMO}$ | $-E_{M06-2X}^{HOMO}$ | $-E_{CORR(HFex+LYP)}^{HOMO}$ | $-E_{CORR(BLYP)}^{HOMO}$ | $E_{CORR(B3LYP)}^{HOMO}$ | $E_{CORR(M06)}^{HOMO}$ | $E_{CORR(M06-L)}^{HOMO}$ | $E_{CORR(M06-2X)}^{HOMO}$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 4-nitrotoulene | 0.363 | 0.199 | 0.363 | 0.397 | 0.233 | 0.278 | 0.289 | 0.252 | 0.329 | 0.034 | 0.034 | 0.085 | 0.074 | 0.112 | 0.035 |
| 2,6-dinitrotoulene | 0.389 | 0.210 | 0.389 | 0.424 | 0.244 | 0.297 | 0.310 | 0.262 | 0.353 | 0.035 | 0.034 | 0.092 | 0.079 | 0.127 | 0.036 |
| 3,4-dinitrotoulene | 0.389 | 0.155 | 0.303 | 0.423 | 0.240 | 0.215 | 0.226 | 0.191 | 0.259 | 0.034 | 0.085 | 0.088 | 0.077 | 0.112 | 0.044 |
| 2,4-dinitrotoulene | 0.393 | 0.215 | 0.393 | 0.428 | 0.250 | 0.304 | 0.315 | 0.268 | 0.356 | 0.035 | 0.035 | 0.089 | 0.078 | 0.125 | 0.037 |
| 2,3-dinitrotoulene | 0.386 | 0.155 | 0.303 | 0.420 | 0.184 | 0.215 | 0.226 | 0.191 | 0.259 | 0.034 | 0.029 | 0.088 | 0.077 | 0.112 | 0.044 |
| 6-nitroquinoline | 0.343 | 0.199 | 0.343 | 0.377 | 0.229 | 0.267 | 0.278 | 0.246 | 0.315 | 0.034 | 0.030 | 0.076 | 0.065 | 0.097 | 0.028 |
| 3-nitrocarbazole | 0.308 | 0.168 | 0.308 | 0.341 | 0.200 | 0.233 | 0.246 | 0.213 | 0.279 | 0.033 | 0.032 | 0.075 | 0.062 | 0.095 | 0.029 |
| 3,5-dinitrotoulene | 0.387 | 0.218 | 0.387 | 0.422 | 0.253 | 0.301 | 0.312 | 0.272 | 0.353 | 0.035 | 0.035 | 0.086 | 0.075 | 0.115 | 0.034 |
| 3-methyl-2-nitronaphthalene | 0.313 | 0.176 | 0.313 | 0.346 | 0.208 | 0.241 | 0.252 | 0.221 | 0.288 | 0.033 | 0.032 | 0.072 | 0.061 | 0.092 | 0.025 |
| 5-nitroquinoline | 0.345 | 0.195 | 0.345 | 0.379 | 0.226 | 0.266 | 0.278 | 0.243 | 0.315 | 0.034 | 0.031 | 0.079 | 0.067 | 0.102 | 0.030 |
| 2,5-dinitrotoulene | 0.385 | 0.216 | 0.386 | 0.420 | 0.251 | 0.301 | 0.311 | 0.269 | 0.353 | 0.035 | 0.035 | 0.085 | 0.075 | 0.117 | 0.033 |
| 1,3,6,8-tetranitronaphthalene | 0.397 | 0.226 | 0.397 | 0.431 | 0.262 | 0.306 | 0.318 | 0.279 | 0.359 | 0.034 | 0.036 | 0.091 | 0.079 | 0.118 | 0.038 |
| 1,3-dinitrobenzene | 0.404 | 0.221 | 0.404 | 0.440 | 0.256 | 0.316 | 0.328 | 0.275 | 0.370 | 0.036 | 0.035 | 0.088 | 0.076 | 0.129 | 0.034 |
| 2-nitrocarbazole | 0.306 | 0.165 | 0.305 | 0.338 | 0.197 | 0.231 | 0.243 | 0.211 | 0.277 | 0.032 | 0.032 | 0.074 | 0.062 | 0.094 | 0.028 |
| 4-nitrocarbazole | 0.300 | 0.161 | 0.301 | 0.333 | 0.192 | 0.226 | 0.238 | 0.206 | 0.272 | 0.033 | 0.031 | 0.075 | 0.063 | 0.095 | 0.029 |
| 2,3,4-trinitrotoulene | 0.416 | 0.222 | 0.396 | 0.451 | 0.255 | 0.309 | 0.322 | 0.274 | 0.371 | 0.035 | 0.033 | 0.087 | 0.074 | 0.122 | 0.025 |
| 1-methyl-2-nitronaphthalene | 0.314 | 0.176 | 0.314 | 0.347 | 0.208 | 0.241 | 0.252 | 0.221 | 0.289 | 0.033 | 0.032 | 0.073 | 0.062 | 0.093 | 0.025 |
| 2,4,6-trinitrotoulene | 0.424 | 0.227 | 0.424 | 0.460 | 0.262 | 0.317 | 0.331 | 0.280 | 0.381 | 0.036 | 0.035 | 0.107 | 0.093 | 0.144 | 0.043 |
| 9-nitroanthracene | 0.287 | 0.158 | 0.287 | 0.319 | 0.190 | 0.221 | 0.232 | 0.202 | 0.266 | 0.032 | 0.032 | 0.066 | 0.055 | 0.085 | 0.021 |
| 1-nitronaphthlene | 0.319 | 0.179 | 0.319 | 0.352 | 0.212 | 0.246 | 0.257 | 0.226 | 0.293 | 0.033 | 0.033 | 0.073 | 0.062 | 0.093 | 0.612 |
| 2-nitronaphthlene | 0.319 | 0.182 | 0.319 | 0.352 | 0.214 | 0.247 | 0.258 | 0.228 | 0.295 | 0.033 | 0.032 | 0.072 | 0.061 | 0.091 | 0.024 |
| 2,3,5-trinitrotoulene | 0.324 | 0.177 | 0.324 | 0.356 | 0.263 | 0.250 | 0.249 | 0.215 | 0.281 | 0.032 | 0.086 | 0.074 | 0.075 | 0.109 | 0.043 |
| 2,3,6-trinitrotoulene | 0.413 | 0.175 | 0.414 | 0.448 | 0.259 | 0.237 | 0.248 | 0.214 | 0.282 | 0.035 | 0.084 | 0.177 | 0.166 | 0.200 | 0.132 |
| 6-nitrobenzo[a]pyrene | 0.275 | 0.152 | 0.275 | 0.307 | 0.185 | 0.214 | 0.224 | 0.196 | 0.257 | 0.032 | 0.033 | 0.061 | 0.051 | 0.079 | 0.018 |
| 1,3,5-trinitrobenzene | 0.442 | 0.237 | 0.442 | 0.478 | 0.272 | 0.336 | 0.352 | 0.292 | 0.399 | 0.036 | 0.035 | 0.106 | 0.090 | 0.150 | 0.043 |
| 1,3-dinitronaphthlene | 0.344 | 0.200 | 0.344 | 0.378 | 0.233 | 0.268 | 0.279 | 0.247 | 0.316 | 0.034 | 0.033 | 0.076 | 0.065 | 0.097 | 0.028 |
| 1,5-dinitronaphthlene | 0.347 | 0.197 | 0.347 | 0.381 | 0.232 | 0.268 | 0.280 | 0.246 | 0.317 | 0.034 | 0.035 | 0.079 | 0.067 | 0.101 | 0.030 |
| 5-nitroacenaphthene | 0.305 | 0.170 | 0.305 | 0.337 | 0.202 | 0.234 | 0.244 | 0.213 | 0.279 | 0.032 | 0.032 | 0.071 | 0.061 | 0.092 | 0.026 |
| 3,4,5-trinitrotoulene | 0.412 | 0.192 | 0.346 | 0.446 | 0.254 | 0.270 | 0.317 | 0.272 | 0.365 | 0.034 | 0.062 | 0.076 | 0.029 | 0.074 | -0.019 |
| 2-nitrofluorene | 0.314 | 0.180 | 0.314 | 0.348 | 0.212 | 0.245 | 0.255 | 0.225 | 0.291 | 0.034 | 0.032 | 0.069 | 0.059 | 0.089 | 0.023 |
| 1,8-dinitronaphthlene | 0.347 | 0.193 | 0.347 | 0.381 | 0.227 | 0.266 | 0.277 | 0.243 | 0.316 | 0.034 | 0.034 | 0.081 | 0.070 | 0.104 | 0.031 |
| 2,4,5-trinitrotoulene | 0.322 | 0.174 | 0.322 | 0.354 | 0.259 | 0.236 | 0.246 | 0.213 | 0.279 | 0.032 | 0.085 | 0.086 | 0.076 | 0.109 | 0.043 |
| 2,7-dinitrofluorene | 0.343 | 0.201 | 0.343 | 0.377 | 0.234 | 0.268 | 0.279 | 0.247 | 0.315 | 0.034 | 0.033 | 0.075 | 0.064 | 0.096 | 0.028 |
| 1-nitrobenzo[e]pyrene | 0.286 | 0.161 | 0.286 | 0.319 | 0.193 | 0.224 | 0.234 | 0.206 | 0.268 | 0.033 | 0.032 | 0.062 | 0.052 | 0.080 | 0.018 |
| 2-nitrophenanthrene | 0.308 | 0.176 | 0.308 | 0.341 | 0.208 | 0.240 | 0.251 | 0.221 | 0.286 | 0.033 | 0.032 | 0.068 | 0.057 | 0.087 | 0.022 |
| 7-nitrofluoranthene | 0.303 | 0.173 | 0.303 | 0.336 | 0.205 | 0.237 | 0.247 | 0.218 | 0.282 | 0.033 | 0.032 | 0.066 | 0.056 | 0.085 | 0.021 |
| 1-nitropyrene | 0.287 | 0.164 | 0.287 | 0.320 | 0.196 | 0.226 | 0.236 | 0.208 | 0.268 | 0.033 | 0.032 | 0.061 | 0.051 | 0.079 | 0.019 |
| 6-nitrochrysene | 0.297 | 0.167 | 0.297 | 0.330 | 0.200 | 0.231 | 0.242 | 0.212 | 0.276 | 0.033 | 0.033 | 0.066 | 0.055 | 0.085 | 0.021 |
| 2,4,7-trinitro-9-fluorenone | 0.382 | 0.216 | 0.382 | 0.416 | 0.250 | 0.299 | 0.311 | 0.266 | 0.349 | 0.034 | 0.034 | 0.083 | 0.071 | 0.116 | 0.033 |
| 2,4,5,7-tetranitro-9-fluorenone | 0.399 | 0.227 | 0.399 | 0.434 | 0.261 | 0.314 | 0.325 | 0.278 | 0.364 | 0.035 | 0.034 | 0.085 | 0.074 | 0.121 | 0.035 |
| 8-nitrofluoranthene | 0.288 | 0.161 | 0.288 | 0.320 | 0.193 | 0.223 | 0.234 | 0.204 | 0.268 | 0.032 | 0.032 | 0.065 | 0.054 | 0.084 | 0.020 |
| 2,7-dinitro-9-fluorenone | 0.362 | 0.205 | 0.363 | 0.397 | 0.238 | 0.284 | 0.295 | 0.254 | 0.332 | 0.035 | 0.033 | 0.079 | 0.068 | 0.109 | 0.031 |
| 2-nitropyrene | 0.284 | 0.162 | 0.284 | 0.316 | 0.194 | 0.223 | 0.234 | 0.206 | 0.267 | 0.032 | 0.032 | 0.061 | 0.050 | 0.078 | 0.017 |
| 1-nitrofluoranthene | 0.305 | 0.173 | 0.305 | 0.338 | 0.205 | 0.237 | 0.248 | 0.218 | 0.284 | 0.033 | 0.032 | 0.068 | 0.057 | 0.087 | 0.021 |
| 2-nitroanthracene | 0.285 | 0.161 | 0.285 | 0.317 | 0.193 | 0.222 | 0.233 | 0.205 | 0.266 | 0.032 | 0.032 | 0.063 | 0.052 | 0.080 | 0.019 |
| 1,3,6,8-tetranitropyrene | 0.352 | 0.206 | 0.352 | 0.386 | 0.242 | 0.277 | 0.287 | 0.256 | 0.322 | 0.034 | 0.036 | 0.075 | 0.065 | 0.096 | 0.030 |
| 3-nitrofluoranthene | 0.307 | 0.175 | 0.307 | 0.340 | 0.207 | 0.239 | 0.250 | 0.220 | 0.286 | 0.033 | 0.032 | 0.068 | 0.057 | 0.087 | 0.021 |
| 1,3,6-trinitropyrene | 0.331 | 0.194 | 0.331 | 0.365 | 0.229 | 0.261 | 0.272 | 0.242 | 0.305 | 0.034 | 0.035 | 0.070 | 0.059 | 0.089 | 0.026 |
| 1,6-dinitropyrene | 0.305 | 0.179 | 0.305 | 0.338 | 0.212 | 0.242 | 0.252 | 0.224 | 0.286 | 0.033 | 0.033 | 0.063 | 0.053 | 0.081 | 0.019 |
| 1,3-dinitropyrene | 0.308 | 0.180 | 0.308 | 0.341 | 0.213 | 0.244 | 0.254 | 0.226 | 0.286 | 0.033 | 0.033 | 0.064 | 0.054 | 0.082 | 0.022 |
| 1,8-dinitropyrene | 0.310 | 0.180 | 0.307 | 0.343 | 0.214 | 0.244 | 0.255 | 0.226 | 0.288 | 0.033 | 0.034 | 0.063 | 0.052 | 0.081 | 0.019 |

**Table S2c.** Same as **Table S2a** but for LUMO energy descriptor ($E_{LUMO}$).

| Name of Compound | $E^{LUMO}_{HFex}$ | $-E^{LUMO}_{B88}$ | $E^{LUMO}_{HF}$ | $E^{LUMO}_{HFex+LYP}$ | $-E^{LUMO}_{BLYP}$ | $-E^{LUMO}_{B3LYP}$ | $-E^{LUMO}_{M06}$ | $-E^{LUMO}_{M06-L}$ | $-E^{LUMO}_{M06-2X}$ | $-E^{LUMO}_{CORR(HFex+LYP)}$ | $-E^{LUMO}_{CORR(BLYP)}$ | $-E^{LUMO}_{CORR(B3LYP)}$ | $-E^{LUMO}_{CORR(M06)}$ | $-E^{LUMO}_{CORR(M06-L)}$ | $-E^{LUMO}_{CORR(M06-2X)}$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 4-nitrotoulene | 0.060 | 0.085 | 0.060 | 0.030 | 0.115 | 0.092 | 0.084 | 0.113 | 0.048 | 0.030 | 0.030 | 0.152 | 0.144 | 0.173 | 0.108 |
| 2,6-dinitrotoulene | 0.040 | 0.100 | 0.040 | 0.006 | 0.133 | 0.111 | 0.103 | 0.132 | 0.068 | 0.034 | 0.033 | 0.151 | 0.143 | 0.172 | 0.108 |
| 3,4-dinitrotoulene | 0.038 | 0.100 | 0.001 | 0.005 | 0.134 | 0.122 | 0.117 | 0.134 | 0.091 | 0.033 | 0.034 | 0.123 | 0.118 | 0.135 | 0.092 |
| 2,4-dinitrotoulene | 0.031 | 0.105 | 0.031 | 0.000 | 0.136 | 0.115 | 0.107 | 0.135 | 0.074 | 0.031 | 0.031 | 0.146 | 0.138 | 0.166 | 0.105 |
| 2,3-dinitrotoulene | 0.039 | 0.100 | 0.002 | 0.006 | 0.131 | 0.122 | 0.117 | 0.134 | 0.091 | 0.033 | 0.031 | 0.124 | 0.119 | 0.136 | 0.093 |
| 6-nitroquinoline | 0.039 | 0.095 | 0.039 | 0.008 | 0.126 | 0.105 | 0.099 | 0.126 | 0.066 | 0.031 | 0.031 | 0.144 | 0.138 | 0.165 | 0.105 |
| 3-nitrocarbazole | 0.069 | 0.074 | 0.069 | 0.040 | 0.104 | 0.082 | 0.075 | 0.102 | 0.040 | 0.029 | 0.030 | 0.151 | 0.144 | 0.171 | 0.109 |
| 3,5-dinitrotoulene | 0.025 | 0.107 | 0.025 | -0.005 | 0.139 | 0.118 | 0.111 | 0.138 | 0.078 | 0.030 | 0.032 | 0.143 | 0.136 | 0.163 | 0.103 |
| 3-methyl-2-nitronaphthalene | 0.052 | 0.084 | 0.052 | 0.019 | 0.115 | 0.094 | 0.087 | 0.115 | 0.054 | 0.033 | 0.031 | 0.146 | 0.139 | 0.167 | 0.106 |
| 5-nitroquinoline | 0.038 | 0.094 | 0.038 | 0.006 | 0.127 | 0.106 | 0.100 | 0.127 | 0.067 | 0.032 | 0.033 | 0.144 | 0.138 | 0.165 | 0.105 |
| 2,5-dinitrotoulene | 0.015 | 0.114 | 0.016 | -0.017 | 0.148 | 0.128 | 0.121 | 0.148 | 0.087 | 0.032 | 0.034 | 0.144 | 0.137 | 0.164 | 0.103 |
| 1,3,6,8-tetranitronaphthalene | -0.021 | 0.135 | -0.021 | -0.053 | 0.168 | 0.153 | 0.147 | 0.171 | 0.120 | 0.032 | 0.033 | 0.132 | 0.126 | 0.150 | 0.099 |
| 1,3-dinitrobenzene | 0.023 | 0.111 | 0.023 | -0.007 | 0.142 | 0.121 | 0.114 | 0.142 | 0.081 | 0.030 | 0.031 | 0.144 | 0.137 | 0.165 | 0.104 |
| 2-nitrocarbazole | 0.047 | 0.082 | 0.047 | 0.017 | 0.112 | 0.092 | 0.086 | 0.112 | 0.054 | 0.030 | 0.030 | 0.139 | 0.133 | 0.159 | 0.101 |
| 4-nitrocarbazole | 0.047 | 0.082 | 0.052 | 0.017 | 0.112 | 0.091 | 0.087 | 0.112 | 0.054 | 0.030 | 0.030 | 0.143 | 0.139 | 0.164 | 0.106 |
| 2,3,4-trinitrotoulene | 0.020 | 0.113 | 0.010 | -0.011 | 0.146 | 0.125 | 0.118 | 0.146 | 0.085 | 0.031 | 0.033 | 0.135 | 0.128 | 0.156 | 0.095 |
| 1-methyl-2-nitronaphthalene | 0.057 | 0.083 | 0.057 | 0.025 | 0.113 | 0.091 | 0.084 | 0.112 | 0.051 | 0.032 | 0.030 | 0.148 | 0.141 | 0.169 | 0.108 |
| 2,4,6-trinitrotoulene | 0.008 | 0.121 | 0.008 | -0.022 | 0.153 | 0.134 | 0.126 | 0.153 | 0.095 | 0.030 | 0.032 | 0.142 | 0.134 | 0.161 | 0.103 |
| 9-nitroanthracene | 0.036 | 0.084 | 0.036 | 0.004 | 0.117 | 0.098 | 0.093 | 0.118 | 0.066 | 0.032 | 0.033 | 0.134 | 0.129 | 0.154 | 0.102 |
| 1-nitronaphthlene | 0.049 | 0.086 | 0.049 | 0.016 | 0.118 | 0.097 | 0.090 | 0.118 | 0.057 | 0.033 | 0.032 | 0.146 | 0.139 | 0.167 | 0.106 |
| 2-nitronaphthlene | 0.045 | 0.088 | 0.045 | 0.015 | 0.118 | 0.098 | 0.091 | 0.118 | 0.059 | 0.030 | 0.030 | 0.143 | 0.136 | 0.163 | 0.104 |
| 2,3,5-trinitrotoulene | -0.027 | 0.126 | -0.027 | -0.058 | 0.154 | 0.169 | 0.145 | 0.162 | 0.118 | 0.031 | 0.028 | 0.142 | 0.118 | 0.135 | 0.091 |
| 2,3,6-trinitrotoulene | 0.000 | 0.122 | 0.001 | -0.034 | 0.160 | 0.146 | 0.141 | 0.159 | 0.115 | 0.034 | 0.038 | 0.147 | 0.142 | 0.160 | 0.116 |
| 6-nitrobenzo[a]pyrene | 0.032 | 0.083 | 0.032 | 0.000 | 0.116 | 0.098 | 0.094 | 0.117 | 0.068 | 0.032 | 0.033 | 0.130 | 0.126 | 0.149 | 0.100 |
| 1,3,5-trinitrobenzene | 0.000 | 0.128 | 0.000 | -0.031 | 0.160 | 0.141 | 0.134 | 0.161 | 0.102 | 0.031 | 0.032 | 0.141 | 0.134 | 0.161 | 0.102 |
| 1,3-dinitronaphthlene | 0.017 | 0.107 | 0.017 | -0.015 | 0.140 | 0.121 | 0.115 | 0.141 | 0.085 | 0.032 | 0.033 | 0.138 | 0.132 | 0.158 | 0.102 |
| 1,5-dinitronaphthlene | 0.022 | 0.104 | 0.022 | -0.011 | 0.138 | 0.119 | 0.112 | 0.139 | 0.081 | 0.033 | 0.034 | 0.141 | 0.134 | 0.161 | 0.103 |
| 5-nitroacenaphthene | 0.051 | 0.082 | 0.051 | 0.019 | 0.113 | 0.093 | 0.086 | 0.112 | 0.054 | 0.032 | 0.031 | 0.144 | 0.137 | 0.163 | 0.105 |
| 3,4,5-trinitrotoulene | 0.016 | 0.145 | -0.005 | -0.017 | 0.149 | 0.131 | 0.126 | 0.152 | 0.094 | 0.033 | 0.004 | 0.126 | 0.121 | 0.147 | 0.089 |
| 2-nitrofluorene | 0.046 | 0.085 | 0.046 | 0.016 | 0.115 | 0.095 | 0.088 | 0.114 | 0.056 | 0.030 | 0.030 | 0.141 | 0.134 | 0.160 | 0.102 |
| 1,8-dinitronaphthlene | 0.029 | 0.095 | 0.029 | -0.001 | 0.126 | 0.108 | 0.102 | 0.128 | 0.073 | 0.030 | 0.031 | 0.137 | 0.131 | 0.157 | 0.102 |
| 2,4,5-trinitrotoulene | -0.027 | 0.124 | -0.027 | -0.059 | 0.159 | 0.150 | 0.145 | 0.163 | 0.119 | 0.032 | 0.035 | 0.123 | 0.118 | 0.136 | 0.092 |
| 2,7-dinitrofluorene | 0.016 | 0.105 | 0.016 | -0.014 | 0.136 | 0.118 | 0.112 | 0.137 | 0.082 | 0.030 | 0.031 | 0.134 | 0.128 | 0.153 | 0.098 |
| 1-nitrobenzo[e]pyrene | 0.042 | 0.083 | 0.042 | 0.011 | 0.114 | 0.094 | 0.088 | 0.115 | 0.060 | 0.031 | 0.031 | 0.136 | 0.130 | 0.157 | 0.102 |
| 2-nitrophenanthrene | 0.043 | 0.087 | 0.043 | 0.012 | 0.117 | 0.097 | 0.091 | 0.117 | 0.059 | 0.031 | 0.030 | 0.140 | 0.134 | 0.160 | 0.102 |
| 7-nitrofluoranthene | 0.037 | 0.086 | 0.037 | 0.007 | 0.116 | 0.097 | 0.091 | 0.117 | 0.063 | 0.030 | 0.030 | 0.134 | 0.128 | 0.154 | 0.100 |
| 1-nitropyrene | 0.031 | 0.088 | 0.031 | 0.000 | 0.119 | 0.102 | 0.097 | 0.120 | 0.068 | 0.031 | 0.031 | 0.133 | 0.128 | 0.151 | 0.099 |
| 6-nitrochrysene | 0.043 | 0.085 | 0.043 | 0.011 | 0.117 | 0.097 | 0.091 | 0.117 | 0.061 | 0.032 | 0.032 | 0.140 | 0.134 | 0.160 | 0.104 |
| 2,4,7-trinitro-9-fluorenone | -0.024 | 0.136 | -0.024 | -0.056 | 0.169 | 0.154 | 0.148 | 0.172 | 0.120 | 0.032 | 0.033 | 0.130 | 0.124 | 0.148 | 0.096 |
| 2,4,5,7-tetranitro-9-fluorenone | -0.040 | 0.148 | -0.040 | -0.073 | 0.182 | 0.167 | 0.161 | 0.185 | 0.135 | 0.033 | 0.034 | 0.127 | 0.121 | 0.145 | 0.095 |
| 8-nitrofluoranthene | 0.059 | 0.083 | 0.059 | 0.029 | 0.113 | 0.091 | 0.084 | 0.112 | 0.048 | 0.030 | 0.030 | 0.150 | 0.143 | 0.171 | 0.107 |
| 2,7-dinitro-9-fluorenone | -0.005 | 0.122 | -0.006 | -0.036 | 0.154 | 0.138 | 0.132 | 0.157 | 0.103 | 0.031 | 0.032 | 0.132 | 0.126 | 0.151 | 0.097 |
| 2-nitropyrene | 0.037 | 0.086 | 0.045 | 0.006 | 0.118 | 0.099 | 0.093 | 0.119 | 0.064 | 0.031 | 0.032 | 0.144 | 0.138 | 0.164 | 0.109 |
| 1-nitrofluoranthene | 0.024 | 0.094 | 0.024 | -0.007 | 0.125 | 0.108 | 0.103 | 0.127 | 0.076 | 0.031 | 0.031 | 0.132 | 0.127 | 0.151 | 0.100 |
| 2-nitroanthracene | 0.030 | 0.091 | 0.030 | 0.000 | 0.121 | 0.103 | 0.098 | 0.123 | 0.070 | 0.030 | 0.030 | 0.133 | 0.128 | 0.153 | 0.100 |
| 1,3,6,8-tetranitropyrene | -0.038 | 0.137 | -0.038 | -0.073 | 0.173 | 0.161 | 0.155 | 0.176 | 0.131 | 0.035 | 0.036 | 0.123 | 0.117 | 0.138 | 0.093 |
| 3-nitrofluoranthene | 0.021 | 0.095 | 0.021 | -0.010 | 0.127 | 0.111 | 0.106 | 0.130 | 0.078 | 0.031 | 0.032 | 0.132 | 0.127 | 0.151 | 0.099 |
| 1,3,6-trinitropyrene | -0.017 | 0.123 | -0.017 | -0.051 | 0.157 | 0.143 | 0.138 | 0.160 | 0.112 | 0.034 | 0.034 | 0.126 | 0.121 | 0.143 | 0.095 |
| 1,6-dinitropyrene | 0.017 | 0.101 | 0.017 | -0.015 | 0.134 | 0.117 | 0.111 | 0.135 | 0.084 | 0.032 | 0.033 | 0.134 | 0.128 | 0.152 | 0.101 |
| 1,3-dinitropyrene | 0.004 | 0.106 | 0.004 | -0.028 | 0.139 | 0.124 | 0.118 | 0.141 | 0.092 | 0.032 | 0.033 | 0.128 | 0.122 | 0.145 | 0.096 |
| 1,8-dinitropyrene | 0.006 | 0.106 | 0.012 | -0.026 | 0.140 | 0.124 | 0.122 | 0.142 | 0.091 | 0.032 | 0.034 | 0.136 | 0.134 | 0.154 | 0.103 |

**Table S2d.** Same as **Table S2a** but for absolute electronegativity descriptor ($\chi$).

| Name of Compound | $\chi_{HFX}$ | $\chi_{B88}$ | $\chi_{HF}$ | $\chi_{HFX+LYP}$ | $\chi_{BLYP}$ | $\chi_{B3LYP}$ | $\chi_{M06}$ | $\chi_{M06-L}$ | $\chi_{M06-2X}$ | $\chi_{CORR(HFX+LYP)}$ | $\chi_{CORR(BLYP)}$ | $\chi_{CORR(B3LYP)}$ | $\chi_{CORR(M06)}$ | $\chi_{CORR(M06-L)}$ | $\chi_{CORR(M06-2X)}$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 4-nitrotoulene | 0.152 | 0.142 | 0.152 | 0.184 | 0.174 | 0.185 | 0.187 | 0.182 | 0.188 | 0.032 | 0.032 | 0.033 | 0.035 | 0.030 | 0.037 |
| 2,6-dinitrotoulene | 0.175 | 0.155 | 0.175 | 0.209 | 0.189 | 0.204 | 0.207 | 0.197 | 0.211 | 0.035 | 0.034 | 0.030 | 0.032 | 0.023 | 0.036 |
| 3,4-dinitrotoulene | 0.176 | 0.128 | 0.151 | 0.209 | 0.187 | 0.169 | 0.171 | 0.163 | 0.175 | 0.034 | 0.060 | 0.018 | 0.020 | 0.012 | 0.024 |
| 2,4-dinitrotoulene | 0.181 | 0.160 | 0.181 | 0.214 | 0.193 | 0.210 | 0.211 | 0.202 | 0.215 | 0.033 | 0.033 | 0.029 | 0.030 | 0.021 | 0.034 |
| 2,3-dinitrotoulene | 0.174 | 0.128 | 0.151 | 0.207 | 0.158 | 0.169 | 0.172 | 0.163 | 0.175 | 0.034 | 0.030 | 0.018 | 0.021 | 0.012 | 0.025 |
| 6-nitroquinoline | 0.152 | 0.147 | 0.152 | 0.185 | 0.178 | 0.186 | 0.188 | 0.186 | 0.191 | 0.033 | 0.031 | 0.034 | 0.036 | 0.034 | 0.039 |
| 3-nitrocarbazole | 0.120 | 0.121 | 0.120 | 0.151 | 0.152 | 0.158 | 0.160 | 0.158 | 0.159 | 0.031 | 0.031 | 0.038 | 0.041 | 0.038 | 0.040 |
| 3,5-dinitrotoulene | 0.181 | 0.163 | 0.181 | 0.214 | 0.196 | 0.210 | 0.211 | 0.205 | 0.215 | 0.033 | 0.034 | 0.029 | 0.030 | 0.024 | 0.034 |
| 3-methyl-2-nitronaphthalene | 0.131 | 0.130 | 0.131 | 0.164 | 0.162 | 0.168 | 0.170 | 0.168 | 0.171 | 0.033 | 0.032 | 0.037 | 0.039 | 0.037 | 0.041 |
| 5-nitroquinoline | 0.154 | 0.145 | 0.154 | 0.187 | 0.177 | 0.186 | 0.189 | 0.185 | 0.191 | 0.033 | 0.032 | 0.033 | 0.035 | 0.031 | 0.038 |
| 2,5-dinitrotoulene | 0.185 | 0.165 | 0.185 | 0.219 | 0.200 | 0.215 | 0.216 | 0.209 | 0.220 | 0.034 | 0.035 | 0.030 | 0.031 | 0.024 | 0.035 |
| 1,3,6,8-tetranitronaphthalene | 0.209 | 0.181 | 0.209 | 0.242 | 0.215 | 0.230 | 0.233 | 0.225 | 0.240 | 0.033 | 0.035 | 0.021 | 0.024 | 0.016 | 0.031 |
| 1,3-dinitrobenzene | 0.191 | 0.166 | 0.191 | 0.224 | 0.199 | 0.219 | 0.221 | 0.209 | 0.225 | 0.033 | 0.033 | 0.028 | 0.031 | 0.018 | 0.035 |
| 2-nitrocarbazole | 0.130 | 0.124 | 0.129 | 0.161 | 0.155 | 0.162 | 0.165 | 0.161 | 0.166 | 0.031 | 0.031 | 0.033 | 0.036 | 0.032 | 0.037 |
| 4-nitrocarbazole | 0.127 | 0.122 | 0.125 | 0.158 | 0.152 | 0.159 | 0.162 | 0.159 | 0.163 | 0.032 | 0.031 | 0.034 | 0.038 | 0.034 | 0.039 |
| 2,3,4-trinitrotoulene | 0.198 | 0.168 | 0.193 | 0.231 | 0.201 | 0.217 | 0.220 | 0.210 | 0.228 | 0.033 | 0.033 | 0.024 | 0.027 | 0.017 | 0.035 |
| 1-methyl-2-nitronaphthalene | 0.129 | 0.130 | 0.129 | 0.161 | 0.161 | 0.166 | 0.168 | 0.166 | 0.170 | 0.033 | 0.031 | 0.038 | 0.040 | 0.038 | 0.041 |
| 2,4,6-trinitrotoulene | 0.208 | 0.174 | 0.208 | 0.241 | 0.208 | 0.226 | 0.229 | 0.217 | 0.238 | 0.033 | 0.034 | 0.018 | 0.021 | 0.009 | 0.030 |
| 9-nitroanthracene | 0.126 | 0.121 | 0.126 | 0.158 | 0.154 | 0.160 | 0.162 | 0.160 | 0.166 | 0.032 | 0.033 | 0.034 | 0.037 | 0.034 | 0.040 |
| 1-nitronaphthlene | 0.135 | 0.133 | 0.135 | 0.168 | 0.165 | 0.172 | 0.174 | 0.172 | -0.118 | 0.033 | 0.033 | 0.037 | 0.039 | 0.037 | -0.253 |
| 2-nitronaphthlene | 0.137 | 0.135 | 0.137 | 0.169 | 0.166 | 0.173 | 0.175 | 0.173 | 0.177 | 0.032 | 0.031 | 0.036 | 0.038 | 0.036 | 0.040 |
| 2,3,5-trinitrotoulene | 0.176 | 0.152 | 0.176 | 0.207 | 0.209 | 0.210 | 0.197 | 0.189 | 0.200 | 0.032 | 0.057 | 0.034 | 0.021 | 0.013 | 0.024 |
| 2,3,6-trinitrotoulene | 0.207 | 0.149 | 0.207 | 0.241 | 0.210 | 0.192 | 0.195 | 0.186 | 0.198 | 0.035 | 0.061 | -0.015 | -0.012 | -0.020 | -0.008 |
| 6-nitrobenzo[a]pyrene | 0.122 | 0.118 | 0.122 | 0.154 | 0.151 | 0.156 | 0.159 | 0.157 | 0.162 | 0.032 | 0.033 | 0.035 | 0.037 | 0.035 | 0.041 |
| 1,3,5-trinitrobenzene | 0.221 | 0.183 | 0.221 | 0.255 | 0.216 | 0.239 | 0.243 | 0.226 | 0.251 | 0.034 | 0.034 | 0.018 | 0.022 | 0.005 | 0.030 |
| 1,3-dinitronaphthlene | 0.164 | 0.154 | 0.164 | 0.197 | 0.187 | 0.195 | 0.197 | 0.194 | 0.201 | 0.033 | 0.033 | 0.031 | 0.034 | 0.031 | 0.037 |
| 1,5-dinitronaphthlene | 0.163 | 0.151 | 0.163 | 0.196 | 0.185 | 0.194 | 0.196 | 0.192 | 0.199 | 0.034 | 0.035 | 0.031 | 0.033 | 0.030 | 0.037 |
| 5-nitroacenaphthene | 0.127 | 0.126 | 0.127 | 0.159 | 0.158 | 0.164 | 0.165 | 0.163 | 0.167 | 0.032 | 0.032 | 0.037 | 0.038 | 0.036 | 0.040 |
| 3,4,5-trinitrotoulene | 0.198 | 0.169 | 0.176 | 0.232 | 0.202 | 0.201 | 0.221 | 0.212 | 0.230 | 0.034 | 0.033 | 0.025 | 0.046 | 0.036 | 0.054 |
| 2-nitrofluorene | 0.134 | 0.133 | 0.134 | 0.166 | 0.164 | 0.170 | 0.172 | 0.169 | 0.174 | 0.032 | 0.031 | 0.036 | 0.038 | 0.035 | 0.040 |
| 1,8-dinitronaphthlene | 0.159 | 0.144 | 0.159 | 0.191 | 0.177 | 0.187 | 0.189 | 0.185 | 0.195 | 0.032 | 0.033 | 0.028 | 0.030 | 0.026 | 0.036 |
| 2,4,5-trinitrotoulene | 0.175 | 0.149 | 0.175 | 0.207 | 0.209 | 0.193 | 0.196 | 0.188 | 0.199 | 0.032 | 0.060 | 0.019 | 0.021 | 0.013 | 0.025 |
| 2,7-dinitrofluorene | 0.164 | 0.153 | 0.164 | 0.196 | 0.185 | 0.193 | 0.196 | 0.192 | 0.198 | 0.032 | 0.032 | 0.030 | 0.032 | 0.029 | 0.035 |
| 1-nitrobenzo[e]pyrene | 0.122 | 0.122 | 0.122 | 0.154 | 0.154 | 0.159 | 0.161 | 0.160 | 0.164 | 0.032 | 0.032 | 0.037 | 0.039 | 0.038 | 0.042 |
| 2-nitrophenanthrene | 0.133 | 0.132 | 0.133 | 0.165 | 0.163 | 0.169 | 0.171 | 0.169 | 0.173 | 0.032 | 0.031 | 0.036 | 0.038 | 0.036 | 0.040 |
| 7-nitrofluoranthene | 0.133 | 0.130 | 0.133 | 0.165 | 0.161 | 0.167 | 0.169 | 0.167 | 0.173 | 0.032 | 0.031 | 0.034 | 0.036 | 0.034 | 0.040 |
| 1-nitropyrene | 0.128 | 0.126 | 0.128 | 0.160 | 0.158 | 0.164 | 0.166 | 0.164 | 0.168 | 0.032 | 0.032 | 0.036 | 0.038 | 0.036 | 0.040 |
| 6-nitrochrysene | 0.127 | 0.126 | 0.127 | 0.160 | 0.159 | 0.164 | 0.167 | 0.165 | 0.168 | 0.033 | 0.033 | 0.037 | 0.040 | 0.038 | 0.041 |
| 2,4,7-trinitro-9-fluorenone | 0.203 | 0.176 | 0.203 | 0.236 | 0.210 | 0.227 | 0.229 | 0.219 | 0.235 | 0.033 | 0.034 | 0.024 | 0.026 | 0.016 | 0.032 |
| 2,4,5,7-tetranitro-9-fluorenone | 0.220 | 0.188 | 0.220 | 0.254 | 0.222 | 0.241 | 0.243 | 0.232 | 0.249 | 0.034 | 0.034 | 0.021 | 0.024 | 0.012 | 0.030 |
| 8-nitrofluoranthene | 0.115 | 0.122 | 0.115 | 0.146 | 0.153 | 0.157 | 0.159 | 0.158 | 0.158 | 0.031 | 0.031 | 0.043 | 0.044 | 0.043 | 0.044 |
| 2,7-dinitro-9-fluorenone | 0.184 | 0.164 | 0.185 | 0.217 | 0.196 | 0.211 | 0.213 | 0.206 | 0.218 | 0.033 | 0.033 | 0.027 | 0.029 | 0.021 | 0.033 |
| 2-nitropyrene | 0.124 | 0.124 | 0.120 | 0.155 | 0.156 | 0.161 | 0.164 | 0.162 | 0.166 | 0.032 | 0.032 | 0.042 | 0.044 | 0.043 | 0.046 |
| 1-nitrofluoranthene | 0.141 | 0.134 | 0.141 | 0.173 | 0.165 | 0.173 | 0.175 | 0.173 | 0.180 | 0.032 | 0.032 | 0.032 | 0.035 | 0.032 | 0.039 |
| 2-nitroanthracene | 0.128 | 0.126 | 0.128 | 0.159 | 0.157 | 0.163 | 0.166 | 0.164 | 0.168 | 0.031 | 0.031 | 0.035 | 0.038 | 0.036 | 0.041 |
| 1,3,6,8-tetranitropyrene | 0.195 | 0.172 | 0.195 | 0.230 | 0.208 | 0.219 | 0.221 | 0.216 | 0.227 | 0.035 | 0.036 | 0.024 | 0.026 | 0.021 | 0.032 |
| 3-nitrofluoranthene | 0.143 | 0.135 | 0.143 | 0.175 | 0.167 | 0.175 | 0.178 | 0.175 | 0.182 | 0.032 | 0.032 | 0.032 | 0.035 | 0.032 | 0.039 |
| 1,3,6-trinitropyrene | 0.174 | 0.159 | 0.174 | 0.208 | 0.193 | 0.202 | 0.205 | 0.201 | 0.209 | 0.034 | 0.035 | 0.028 | 0.031 | 0.027 | 0.035 |
| 1,6-dinitropyrene | 0.144 | 0.140 | 0.144 | 0.177 | 0.173 | 0.180 | 0.181 | 0.179 | 0.185 | 0.033 | 0.033 | 0.036 | 0.037 | 0.035 | 0.041 |
| 1,3-dinitropyrene | 0.152 | 0.143 | 0.152 | 0.185 | 0.176 | 0.184 | 0.186 | 0.183 | 0.189 | 0.033 | 0.033 | 0.032 | 0.034 | 0.031 | 0.037 |
| 1,8-dinitropyrene | 0.152 | 0.143 | 0.148 | 0.185 | 0.177 | 0.184 | 0.189 | 0.184 | 0.190 | 0.033 | 0.034 | 0.037 | 0.041 | 0.037 | 0.042 |

**Table S2e.** Same as **Table S2a** but for chemical hardness descriptor ($\eta$).

| Name of Compound | $\eta_{HFX}$ | $\eta_{B88}$ | $\eta_{HF}$ | $\eta_{HFX+LYP}$ | $\eta_{BLYP}$ | $\eta_{B3LYP}$ | $\eta_{M06}$ | $\eta_{M06-L}$ | $\eta_{M06-2X}$ | $\eta_{CORR(HFX+LYP)}$ | $\eta_{CORR(BLYP)}$ | $\eta_{COR(B3LYP)}$ | $\eta_{CORR(M06)}$ | $\eta_{CORR(M06-L)}$ | $\eta_{CORR(M06-2X)}$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 4-nitrotoulene | 0.423 | 0.114 | 0.423 | 0.427 | 0.118 | 0.186 | 0.205 | 0.139 | 0.280 | 0.004 | 0.004 | 0.237 | 0.070 | 0.061 | 0.073 |
| 2,6-dinitrotoulene | 0.429 | 0.110 | 0.429 | 0.430 | 0.111 | 0.186 | 0.207 | 0.130 | 0.285 | 0.001 | 0.001 | 0.243 | 0.064 | 0.045 | 0.072 |
| 3,4-dinitrotoulene | 0.427 | 0.055 | 0.304 | 0.428 | 0.106 | 0.093 | 0.109 | 0.057 | 0.168 | 0.001 | 0.051 | 0.211 | 0.041 | 0.023 | 0.048 |
| 2,4-dinitrotoulene | 0.424 | 0.110 | 0.424 | 0.428 | 0.114 | 0.189 | 0.208 | 0.133 | 0.282 | 0.004 | 0.004 | 0.235 | 0.061 | 0.042 | 0.069 |
| 2,3-dinitrotoulene | 0.425 | 0.055 | 0.305 | 0.426 | 0.053 | 0.093 | 0.109 | 0.057 | 0.169 | 0.001 | -0.002 | 0.212 | 0.042 | 0.025 | 0.049 |
| 6-nitroquinoline | 0.382 | 0.104 | 0.382 | 0.385 | 0.103 | 0.162 | 0.180 | 0.120 | 0.249 | 0.003 | -0.001 | 0.220 | 0.073 | 0.068 | 0.078 |
| 3-nitrocarbazole | 0.377 | 0.094 | 0.377 | 0.381 | 0.096 | 0.151 | 0.171 | 0.111 | 0.240 | 0.004 | 0.002 | 0.226 | 0.082 | 0.076 | 0.080 |
| 3,5-dinitrotoulene | 0.412 | 0.111 | 0.412 | 0.417 | 0.114 | 0.183 | 0.201 | 0.133 | 0.275 | 0.005 | 0.003 | 0.229 | 0.061 | 0.048 | 0.069 |
| 3-methyl-2-nitronaphthalene | 0.365 | 0.092 | 0.365 | 0.365 | 0.093 | 0.147 | 0.165 | 0.106 | 0.234 | 0.000 | 0.001 | 0.218 | 0.078 | 0.075 | 0.081 |
| 5-nitroquinoline | 0.383 | 0.101 | 0.383 | 0.385 | 0.099 | 0.160 | 0.178 | 0.116 | 0.248 | 0.002 | -0.002 | 0.223 | 0.071 | 0.063 | 0.075 |
| 2,5-dinitrotoulene | 0.400 | 0.102 | 0.402 | 0.403 | 0.103 | 0.173 | 0.190 | 0.121 | 0.266 | 0.003 | 0.001 | 0.229 | 0.062 | 0.047 | 0.070 |
| 1,3,6,8-tetranitronaphthalene | 0.376 | 0.091 | 0.376 | 0.378 | 0.094 | 0.153 | 0.171 | 0.108 | 0.239 | 0.002 | 0.003 | 0.223 | 0.047 | 0.033 | 0.061 |
| 1,3-dinitrobenzene | 0.427 | 0.110 | 0.427 | 0.433 | 0.114 | 0.195 | 0.214 | 0.133 | 0.289 | 0.006 | 0.004 | 0.232 | 0.061 | 0.036 | 0.070 |
| 2-nitrocarbazole | 0.353 | 0.083 | 0.352 | 0.355 | 0.085 | 0.139 | 0.157 | 0.099 | 0.223 | 0.002 | 0.002 | 0.213 | 0.071 | 0.064 | 0.073 |
| 4-nitrocarbazole | 0.347 | 0.079 | 0.353 | 0.350 | 0.080 | 0.135 | 0.151 | 0.093 | 0.218 | 0.003 | 0.001 | 0.218 | 0.076 | 0.069 | 0.077 |
| 2,3,4-trinitrotoulene | 0.436 | 0.109 | 0.406 | 0.440 | 0.109 | 0.184 | 0.203 | 0.128 | 0.286 | 0.004 | 0.000 | 0.222 | 0.054 | 0.033 | 0.070 |
| 1-methyl-2-nitronaphthalene | 0.371 | 0.093 | 0.371 | 0.372 | 0.095 | 0.150 | 0.168 | 0.109 | 0.238 | 0.001 | 0.002 | 0.221 | 0.079 | 0.076 | 0.082 |
| 2,4,6-trinitrotoulene | 0.432 | 0.106 | 0.432 | 0.438 | 0.109 | 0.183 | 0.205 | 0.127 | 0.286 | 0.006 | 0.003 | 0.249 | 0.041 | 0.017 | 0.059 |
| 9-nitroanthracene | 0.323 | 0.074 | 0.323 | 0.323 | 0.073 | 0.123 | 0.139 | 0.084 | 0.200 | 0.000 | -0.001 | 0.200 | 0.074 | 0.069 | 0.080 |
| 1-nitronaphthlene | 0.368 | 0.093 | 0.368 | 0.368 | 0.094 | 0.149 | 0.167 | 0.108 | -0.351 | 0.000 | 0.001 | 0.219 | 0.077 | 0.074 | -0.506 |
| 2-nitronaphthlene | 0.364 | 0.094 | 0.364 | 0.367 | 0.096 | 0.149 | 0.167 | 0.109 | 0.236 | 0.003 | 0.002 | 0.215 | 0.076 | 0.072 | 0.079 |
| 2,3,5-trinitrotoulene | 0.297 | 0.051 | 0.297 | 0.298 | 0.109 | 0.081 | 0.104 | 0.052 | 0.163 | 0.001 | 0.058 | 0.216 | 0.042 | 0.026 | 0.049 |
| 2,3,6-trinitrotoulene | 0.413 | 0.053 | 0.415 | 0.414 | 0.099 | 0.091 | 0.107 | 0.056 | 0.167 | 0.001 | 0.046 | 0.324 | -0.024 | -0.040 | -0.017 |
| 6-nitrobenzo[a]pyrene | 0.307 | 0.069 | 0.307 | 0.307 | 0.069 | 0.116 | 0.131 | 0.079 | 0.188 | 0.000 | 0.000 | 0.191 | 0.075 | 0.070 | 0.082 |
| 1,3,5-trinitrobenzene | 0.442 | 0.109 | 0.442 | 0.447 | 0.112 | 0.195 | 0.218 | 0.131 | 0.297 | 0.005 | 0.003 | 0.247 | 0.043 | 0.011 | 0.059 |
| 1,3-dinitronaphthlene | 0.361 | 0.093 | 0.361 | 0.363 | 0.093 | 0.147 | 0.164 | 0.106 | 0.232 | 0.002 | 0.000 | 0.214 | 0.067 | 0.061 | 0.074 |
| 1,5-dinitronaphthlene | 0.369 | 0.093 | 0.369 | 0.370 | 0.094 | 0.149 | 0.167 | 0.107 | 0.236 | 0.001 | 0.001 | 0.220 | 0.067 | 0.060 | 0.073 |
| 5-nitroacenaphthene | 0.356 | 0.088 | 0.356 | 0.356 | 0.089 | 0.141 | 0.158 | 0.101 | 0.225 | 0.000 | 0.001 | 0.215 | 0.077 | 0.072 | 0.080 |
| 3,4,5-trinitrotoulene | 0.428 | 0.047 | 0.341 | 0.429 | 0.105 | 0.139 | 0.191 | 0.119 | 0.271 | 0.001 | 0.058 | 0.202 | 0.092 | 0.073 | 0.109 |
| 2-nitrofluorene | 0.360 | 0.095 | 0.360 | 0.364 | 0.097 | 0.150 | 0.167 | 0.110 | 0.235 | 0.004 | 0.002 | 0.210 | 0.075 | 0.071 | 0.079 |
| 1,8-dinitronaphthlene | 0.376 | 0.098 | 0.376 | 0.380 | 0.101 | 0.158 | 0.175 | 0.115 | 0.242 | 0.004 | 0.003 | 0.218 | 0.061 | 0.052 | 0.071 |
| 2,4,5-trinitrotoulene | 0.295 | 0.050 | 0.295 | 0.295 | 0.100 | 0.086 | 0.102 | 0.049 | 0.161 | 0.000 | 0.050 | 0.209 | 0.042 | 0.027 | 0.049 |
| 2,7-dinitrofluorene | 0.359 | 0.096 | 0.359 | 0.363 | 0.098 | 0.150 | 0.167 | 0.110 | 0.234 | 0.004 | 0.002 | 0.209 | 0.064 | 0.057 | 0.070 |
| 1-nitrobenzo[e]pyrene | 0.328 | 0.078 | 0.328 | 0.330 | 0.079 | 0.130 | 0.146 | 0.091 | 0.208 | 0.002 | 0.001 | 0.198 | 0.078 | 0.076 | 0.084 |
| 2-nitrophenanthrene | 0.351 | 0.089 | 0.351 | 0.353 | 0.091 | 0.143 | 0.160 | 0.104 | 0.227 | 0.002 | 0.002 | 0.208 | 0.076 | 0.073 | 0.080 |
| 7-nitrofluoranthene | 0.340 | 0.087 | 0.340 | 0.343 | 0.089 | 0.140 | 0.156 | 0.101 | 0.219 | 0.003 | 0.002 | 0.200 | 0.072 | 0.069 | 0.080 |
| 1-nitropyrene | 0.318 | 0.076 | 0.318 | 0.320 | 0.077 | 0.124 | 0.139 | 0.088 | 0.200 | 0.002 | 0.001 | 0.194 | 0.076 | 0.073 | 0.081 |
| 6-nitrochrysene | 0.340 | 0.082 | 0.340 | 0.341 | 0.083 | 0.134 | 0.150 | 0.095 | 0.215 | 0.001 | 0.001 | 0.206 | 0.079 | 0.075 | 0.083 |
| 2,4,7-trinitro-9-fluorenone | 0.358 | 0.080 | 0.358 | 0.360 | 0.081 | 0.145 | 0.163 | 0.094 | 0.229 | 0.002 | 0.001 | 0.213 | 0.053 | 0.033 | 0.063 |
| 2,4,5,7-tetranitro-9-fluorenone | 0.359 | 0.079 | 0.359 | 0.361 | 0.079 | 0.147 | 0.164 | 0.093 | 0.229 | 0.002 | 0.000 | 0.212 | 0.048 | 0.024 | 0.060 |
| 8-nitrofluoranthene | 0.347 | 0.078 | 0.347 | 0.349 | 0.080 | 0.132 | 0.150 | 0.093 | 0.220 | 0.002 | 0.002 | 0.215 | 0.089 | 0.087 | 0.088 |
| 2,7-dinitro-9-fluorenone | 0.357 | 0.083 | 0.357 | 0.361 | 0.084 | 0.146 | 0.163 | 0.098 | 0.228 | 0.004 | 0.001 | 0.211 | 0.058 | 0.042 | 0.066 |
| 2-nitropyrene | 0.321 | 0.076 | 0.329 | 0.322 | 0.076 | 0.124 | 0.140 | 0.087 | 0.202 | 0.001 | 0.000 | 0.205 | 0.088 | 0.086 | 0.092 |
| 1-nitrofluoranthene | 0.329 | 0.079 | 0.329 | 0.331 | 0.080 | 0.129 | 0.145 | 0.090 | 0.208 | 0.002 | 0.001 | 0.200 | 0.070 | 0.064 | 0.078 |
| 2-nitroanthracene | 0.315 | 0.070 | 0.315 | 0.317 | 0.072 | 0.119 | 0.135 | 0.081 | 0.196 | 0.002 | 0.002 | 0.196 | 0.076 | 0.073 | 0.081 |
| 1,3,6,8-tetranitropyrene | 0.314 | 0.069 | 0.314 | 0.313 | 0.069 | 0.116 | 0.132 | 0.080 | 0.192 | -0.001 | 0.000 | 0.198 | 0.053 | 0.042 | 0.063 |
| 3-nitrofluoranthene | 0.328 | 0.080 | 0.328 | 0.330 | 0.080 | 0.128 | 0.145 | 0.090 | 0.208 | 0.002 | 0.000 | 0.200 | 0.070 | 0.064 | 0.078 |
| 1,3,6-trinitropyrene | 0.314 | 0.071 | 0.314 | 0.314 | 0.072 | 0.118 | 0.133 | 0.082 | 0.193 | 0.000 | 0.001 | 0.196 | 0.062 | 0.054 | 0.070 |
| 1,6-dinitropyrene | 0.322 | 0.078 | 0.322 | 0.323 | 0.078 | 0.125 | 0.141 | 0.089 | 0.202 | 0.001 | 0.000 | 0.197 | 0.075 | 0.071 | 0.081 |
| 1,3-dinitropyrene | 0.312 | 0.074 | 0.312 | 0.313 | 0.074 | 0.120 | 0.135 | 0.085 | 0.194 | 0.001 | 0.000 | 0.192 | 0.068 | 0.062 | 0.075 |
| 1,8-dinitropyrene | 0.316 | 0.074 | 0.319 | 0.317 | 0.074 | 0.120 | 0.133 | 0.084 | 0.196 | 0.001 | 0.000 | 0.199 | 0.083 | 0.073 | 0.084 |

**Table S2f.** Same as **Table S2a** but for electrophilicity index descriptor ($\omega$).

| Name of Compound | $\omega_{HFX}$ | $\omega_{B88}$ | $\omega_{HF}$ | $\omega_{HFX+LYP}$ | $\omega_{BLYP}$ | $\omega_{B3LYP}$ | $\omega_{M06}$ | $\omega_{M06-L}$ | $\omega_{M06-2X}$ | $\omega_{CORR(HFX+LYP)}$ | $\omega_{CORR(BLYP)}$ | $-\omega_{CORR(B3LYP)}$ | $\omega_{CORR(M06)}$ | $\omega_{CORR(M06-L)}$ | $\omega_{CORR(M06-2X)}$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 4-nitrotoulene | 0.027 | 0.088 | 0.027 | 0.039 | 0.128 | 0.092 | 0.085 | 0.119 | 0.063 | 0.128 | 0.128 | 0.002 | 0.009 | 0.008 | 0.009 |
| 2,6-dinitrotoulene | 0.035 | 0.109 | 0.035 | 0.051 | 0.160 | 0.112 | 0.103 | 0.150 | 0.078 | 0.613 | 0.578 | 0.002 | 0.008 | 0.006 | 0.009 |
| 3,4-dinitrotoulene | 0.036 | 0.148 | 0.038 | 0.051 | 0.165 | 0.153 | 0.135 | 0.234 | 0.091 | 0.578 | 0.035 | 0.001 | 0.005 | 0.003 | 0.006 |
| 2,4-dinitrotoulene | 0.039 | 0.116 | 0.039 | 0.053 | 0.163 | 0.116 | 0.108 | 0.153 | 0.082 | 0.136 | 0.136 | 0.002 | 0.008 | 0.005 | 0.009 |
| 2,3-dinitrotoulene | 0.035 | 0.148 | 0.037 | 0.050 | 0.234 | 0.153 | 0.136 | 0.233 | 0.091 | 0.578 | -0.225 | 0.001 | 0.005 | 0.003 | 0.006 |
| 6-nitroquinoline | 0.030 | 0.104 | 0.030 | 0.044 | 0.153 | 0.107 | 0.099 | 0.144 | 0.073 | 0.182 | -0.481 | 0.003 | 0.009 | 0.008 | 0.010 |
| 3-nitrocarbazole | 0.019 | 0.078 | 0.019 | 0.030 | 0.120 | 0.082 | 0.075 | 0.112 | 0.053 | 0.120 | 0.240 | 0.003 | 0.010 | 0.010 | 0.010 |
| 3,5-dinitrotoulene | 0.040 | 0.119 | 0.040 | 0.055 | 0.168 | 0.120 | 0.111 | 0.158 | 0.084 | 0.109 | 0.193 | 0.002 | 0.008 | 0.006 | 0.009 |
| 3-methyl-2-nitronaphthalene | 0.023 | 0.092 | 0.023 | 0.037 | 0.140 | 0.095 | 0.087 | 0.133 | 0.062 | - | 0.512 | 0.003 | 0.010 | 0.009 | 0.010 |
| 5-nitroquinoline | 0.031 | 0.103 | 0.031 | 0.045 | 0.157 | 0.108 | 0.100 | 0.147 | 0.074 | 0.272 | -0.256 | 0.002 | 0.009 | 0.008 | 0.009 |
| 2,5-dinitrotoulene | 0.043 | 0.133 | 0.043 | 0.059 | 0.193 | 0.133 | 0.123 | 0.180 | 0.091 | 0.193 | 0.613 | 0.002 | 0.008 | 0.006 | 0.009 |
| 1,3,6,8-tetranitronaphthalene | 0.058 | 0.179 | 0.058 | 0.077 | 0.246 | 0.172 | 0.158 | 0.235 | 0.120 | 0.272 | 0.204 | 0.001 | 0.006 | 0.004 | 0.008 |
| 1,3-dinitrobenzene | 0.042 | 0.125 | 0.042 | 0.058 | 0.174 | 0.122 | 0.114 | 0.163 | 0.088 | 0.091 | 0.136 | 0.002 | 0.008 | 0.005 | 0.009 |
| 2-nitrocarbazole | 0.024 | 0.092 | 0.024 | 0.036 | 0.140 | 0.094 | 0.086 | 0.131 | 0.061 | 0.240 | 0.240 | 0.002 | 0.009 | 0.008 | 0.009 |
| 4-nitrocarbazole | 0.023 | 0.093 | 0.022 | 0.036 | 0.144 | 0.093 | 0.087 | 0.135 | 0.061 | 0.171 | 0.481 | 0.003 | 0.009 | 0.009 | 0.010 |
| 2,3,4-trinitrotoulene | 0.045 | 0.129 | 0.046 | 0.061 | 0.184 | 0.128 | 0.119 | 0.172 | 0.091 | 0.136 | - | 0.001 | 0.007 | 0.004 | 0.009 |
| 1-methyl-2-nitronaphthalene | 0.022 | 0.090 | 0.022 | 0.035 | 0.136 | 0.092 | 0.084 | 0.127 | 0.060 | 0.545 | 0.240 | 0.003 | 0.010 | 0.009 | 0.010 |
| 2,4,6-trinitrotoulene | 0.050 | 0.143 | 0.050 | 0.066 | 0.198 | 0.139 | 0.128 | 0.184 | 0.099 | 0.091 | 0.193 | 0.001 | 0.005 | 0.002 | 0.007 |
| 9-nitroanthracene | 0.024 | 0.099 | 0.024 | 0.038 | 0.161 | 0.103 | 0.095 | 0.152 | 0.069 | - | -0.545 | 0.003 | 0.009 | 0.009 | 0.010 |
| 1-nitronaphthlene | 0.025 | 0.094 | 0.025 | 0.038 | 0.145 | 0.099 | 0.091 | 0.137 | -0.020 | - | 0.545 | 0.003 | 0.010 | 0.009 | -0.063 |
| 2-nitronaphthlene | 0.026 | 0.097 | 0.026 | 0.039 | 0.144 | 0.100 | 0.091 | 0.137 | 0.066 | 0.171 | 0.240 | 0.003 | 0.009 | 0.009 | 0.010 |
| 2,3,5-trinitrotoulene | 0.052 | 0.225 | 0.052 | 0.072 | 0.199 | 0.271 | 0.186 | 0.340 | 0.123 | 0.512 | 0.028 | 0.003 | 0.005 | 0.003 | 0.006 |
| 2,3,6-trinitrotoulene | 0.052 | 0.208 | 0.051 | 0.070 | 0.222 | 0.201 | 0.176 | 0.313 | 0.117 | 0.613 | 0.040 | 0.000 | -0.003 | -0.005 | -0.002 |
| 6-nitrobenzo[a]pyrene | 0.024 | 0.100 | 0.024 | 0.038 | 0.164 | 0.105 | 0.097 | 0.154 | 0.070 | - | - | 0.003 | 0.009 | 0.009 | 0.010 |
| 1,3,5-trinitrobenzene | 0.055 | 0.153 | 0.055 | 0.072 | 0.208 | 0.146 | 0.135 | 0.196 | 0.106 | 0.116 | 0.193 | 0.001 | 0.005 | 0.001 | 0.007 |
| 1,3-dinitronaphthlene | 0.037 | 0.127 | 0.037 | 0.053 | 0.187 | 0.129 | 0.118 | 0.177 | 0.087 | 0.272 | - | 0.002 | 0.008 | 0.008 | 0.009 |
| 1,5-dinitronaphthlene | 0.036 | 0.122 | 0.036 | 0.052 | 0.182 | 0.126 | 0.115 | 0.173 | 0.084 | 0.578 | 0.613 | 0.002 | 0.008 | 0.007 | 0.009 |
| 5-nitroacenaphthene | 0.023 | 0.090 | 0.023 | 0.036 | 0.139 | 0.095 | 0.087 | 0.131 | 0.062 | - | 0.512 | 0.003 | 0.010 | 0.009 | 0.010 |
| 3,4,5-trinitrotoulene | 0.046 | 0.302 | 0.045 | 0.062 | 0.193 | 0.145 | 0.128 | 0.188 | 0.097 | 0.578 | 0.009 | 0.002 | 0.011 | 0.009 | 0.014 |
| 2-nitrofluorene | 0.025 | 0.092 | 0.025 | 0.038 | 0.138 | 0.096 | 0.088 | 0.130 | 0.064 | 0.128 | 0.240 | 0.003 | 0.009 | 0.009 | 0.010 |
| 1,8-dinitronaphthlene | 0.034 | 0.106 | 0.034 | 0.048 | 0.154 | 0.111 | 0.102 | 0.150 | 0.078 | 0.128 | 0.182 | 0.002 | 0.008 | 0.007 | 0.009 |
| 2,4,5-trinitrotoulene | 0.052 | 0.222 | 0.052 | 0.072 | 0.218 | 0.217 | 0.188 | 0.358 | 0.123 | - | 0.036 | 0.001 | 0.005 | 0.003 | 0.006 |
| 2,7-dinitrofluorene | 0.037 | 0.122 | 0.037 | 0.053 | 0.175 | 0.124 | 0.115 | 0.168 | 0.084 | 0.128 | 0.256 | 0.002 | 0.008 | 0.007 | 0.009 |
| 1-nitrobenzo[e]pyrene | 0.023 | 0.095 | 0.023 | 0.036 | 0.149 | 0.097 | 0.089 | 0.141 | 0.065 | 0.256 | 0.512 | 0.003 | 0.010 | 0.010 | 0.011 |
| 2-nitrophenanthrene | 0.025 | 0.097 | 0.025 | 0.038 | 0.145 | 0.099 | 0.091 | 0.138 | 0.065 | 0.256 | 0.240 | 0.003 | 0.010 | 0.009 | 0.010 |
| 7-nitrofluoranthene | 0.026 | 0.096 | 0.026 | 0.039 | 0.145 | 0.100 | 0.092 | 0.139 | 0.068 | 0.171 | 0.240 | 0.003 | 0.009 | 0.009 | 0.010 |
| 1-nitropyrene | 0.026 | 0.104 | 0.026 | 0.040 | 0.161 | 0.108 | 0.099 | 0.154 | 0.071 | 0.256 | 0.512 | 0.003 | 0.010 | 0.009 | 0.010 |
| 6-nitrochrysene | 0.024 | 0.097 | 0.024 | 0.037 | 0.151 | 0.100 | 0.092 | 0.142 | 0.066 | 0.545 | 0.545 | 0.003 | 0.010 | 0.009 | 0.010 |
| 2,4,7-trinitro-9-fluorenone | 0.058 | 0.194 | 0.058 | 0.077 | 0.271 | 0.177 | 0.161 | 0.255 | 0.120 | 0.272 | 0.578 | 0.001 | 0.007 | 0.004 | 0.008 |
| 2,4,5,7-tetranitro-9-fluorenone | 0.067 | 0.223 | 0.067 | 0.089 | 0.311 | 0.197 | 0.181 | 0.289 | 0.135 | 0.289 | - | 0.001 | 0.006 | 0.003 | 0.007 |
| 8-nitrofluoranthene | 0.019 | 0.095 | 0.019 | 0.030 | 0.146 | 0.093 | 0.084 | 0.135 | 0.057 | 0.240 | 0.240 | 0.004 | 0.011 | 0.011 | 0.011 |
| 2,7-dinitro-9-fluorenone | 0.047 | 0.161 | 0.048 | 0.065 | 0.229 | 0.152 | 0.139 | 0.217 | 0.104 | 0.136 | 0.545 | 0.002 | 0.007 | 0.005 | 0.008 |
| 2-nitropyrene | 0.024 | 0.101 | 0.022 | 0.037 | 0.160 | 0.105 | 0.095 | 0.151 | 0.068 | 0.512 | - | 0.004 | 0.011 | 0.011 | 0.012 |
| 1-nitrofluoranthene | 0.030 | 0.113 | 0.030 | 0.045 | 0.170 | 0.115 | 0.106 | 0.165 | 0.078 | 0.256 | 0.512 | 0.003 | 0.009 | 0.008 | 0.010 |
| 2-nitroanthracene | 0.026 | 0.113 | 0.026 | 0.040 | 0.171 | 0.111 | 0.102 | 0.165 | 0.072 | 0.240 | 0.240 | 0.003 | 0.010 | 0.009 | 0.010 |
| 1,3,6,8-tetranitropyrene | 0.061 | 0.213 | 0.061 | 0.084 | 0.312 | 0.207 | 0.185 | 0.294 | 0.134 | -0.613 | - | 0.001 | 0.007 | 0.005 | 0.008 |
| 3-nitrofluoranthene | 0.031 | 0.114 | 0.031 | 0.046 | 0.174 | 0.120 | 0.109 | 0.170 | 0.080 | 0.256 | - | 0.003 | 0.009 | 0.008 | 0.010 |
| 1,3,6-trinitropyrene | 0.048 | 0.177 | 0.048 | 0.069 | 0.259 | 0.173 | 0.157 | 0.247 | 0.113 | - | 0.613 | 0.002 | 0.008 | 0.007 | 0.009 |
| 1,6-dinitropyrene | 0.032 | 0.126 | 0.032 | 0.048 | 0.192 | 0.129 | 0.117 | 0.182 | 0.084 | 0.545 | - | 0.003 | 0.009 | 0.009 | 0.010 |
| 1,3-dinitropyrene | 0.037 | 0.138 | 0.037 | 0.054 | 0.209 | 0.141 | 0.128 | 0.198 | 0.092 | 0.545 | - | 0.003 | 0.009 | 0.008 | 0.009 |
| 1,8-dinitropyrene | 0.037 | 0.138 | 0.034 | 0.054 | 0.212 | 0.141 | 0.134 | 0.202 | 0.092 | 0.545 | - | 0.003 | 0.010 | 0.009 | 0.011 |

Table S3. Compounds in the training set (T), prediction set (P) and excluded set (E), in different types of splitting methods employed[a] for TA100 mutagenicity. Excluded compounds are either response or structural outliers (determined from Williams plot)

| Name of the compound | Activity (log TA100) | Exchange (HFX, B88, HF) only methods | | Exchange+Correlation (HFX+LYP, BLYP, B3LYP) methods | | Exchange+Correlation (Meta functionals, M06, M06-L, M06-2X) methods | | Electron-correlation (CORR(HFX+LYP) , CORR(BLYP) , CORR(B3LYP)) methods | | Electron-correlation (CORR(M06), CORR(M06-L), CORR(M06-2X)) methods | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| | | Activity Sampling (Order splitting) | 30% random splitting | Activity Sampling (Order splitting) | 30% random splitting | Activity Sampling (Order splitting) | 30% random splitting | Activity Sampling (Order splitting) | 30% random splitting | Activity Sampling (Order splitting) | 30% random splitting |
| 4-nitrotoulene | -2.10 | T | T | T | T | T | T | T | T | T | T |
| 2,6-dinitrotoulene | -1.34 | P | T | P | T | P | T | P | T | T | T |
| 3,4-dinitrotoulene | -1.30 | T | T | T | T | T | P | T | T | P | P |
| 2,4-dinitrotoulene | -1.29 | P | P | P | T | P | P | P | T | T | T |
| 2,3-dinitrotoulene | -1.26 | T | P | T | P | T | T | T | P | P | P |
| 6-nitroquinoline | -1.05 | P | T | P | T | P | P | P | P | T | P |
| 3-nitrocarbazole | -1.00 | T | E | T | T | E | E | T | T | P | T |
| 3,5-dinitrotoulene | -0.72 | P | P | P | P | P | T | P | P | T | T |
| 3-methyl-2-nitronaphthalene | -0.70 | T | P | T | T | T | T | T | T | P | T |
| 5-nitroquinoline | -0.70 | P | T | P | T | P | P | P | P | T | P |
| 2,5-dinitrotoulene | -0.63 | T | P | T | T | T | T | T | T | P | T |
| 1,3,6,8-tetranitronaphthalene | -0.52 | E | E | E | E | E | E | E | E | E | E |
| 1,3-dinitrobenzene | -0.51 | P | P | P | P | P | P | P | T | P | T |
| 2-nitrocarbazole | -0.30 | T | P | T | T | T | T | T | T | T | T |
| 4-nitrocarbazole | -0.30 | P | T | P | T | P | T | P | T | P | T |
| 2,3,4-trinitrotoulene | 0.08 | T | T | T | T | T | P | T | P | T | T |
| 1-methyl-2-nitronaphthalene | 0.08 | P | T | P | P | P | T | P | T | P | T |
| 2,4,6-trinitrotoulene | 0.16 | T | P | T | T | T | P | E | T | T | T |
| 9-nitroanthracene | 0.26 | P | T | P | T | P | T | P | T | P | T |
| 1-nitronaphthlene | 0.28 | T | P | T | T | E | E | T | P | E | E |
| 2-nitronaphthlene | 0.37 | P | T | P | T | T | T | P | T | P | T |
| 2,3,5-trinitrotoulene | 0.46 | T | T | T | E | P | T | T | T | T | T |
| 2,3,6-trinitrotoulene | 0.55 | P | T | P | T | T | T | E | E | E | E |
| 6-nitrobenzo[a]pyrene | 0.71 | E | E | E | E | E | E | E | E | E | E |
| 1,3,5-trinitrobenzene | 0.72 | T | T | T | T | T | P | E | T | E | P |
| 1,3-dinitronaphthlene | 0.86 | P | T | P | P | P | T | T | P | T | P |
| 1,5-dinitronaphthlene | 0.91 | T | T | T | T | T | T | P | T | P | T |
| 5-nitroacenaphthene | 0.97 | P | P | P | T | P | P | T | T | T | T |
| 3,4,5-trinitrotoulene | 1.01 | T | T | T | T | T | T | P | P | E | E |
| 2-nitrofluorene | 1.08 | P | T | P | T | P | T | T | T | T | T |
| 1,8-dinitronaphthlene | 1.12 | T | T | T | P | T | T | P | T | P | T |
| 2,4,5-trinitrotoulene | 1.12 | P | P | P | T | P | P | T | T | T | T |
| 2,7-dinitrofluorene | 1.27 | T | T | T | T | T | T | P | P | P | P |
| 1-nitrobenzo[e]pyrene | 1.65 | E | E | E | E | E | E | T | T | T | T |
| 2-nitrophenanthrene | 1.79 | P | T | P | T | T | P | T | P | P | T |
| 7-nitrofluoranthene | 2.09 | T | P | T | T | P | T | T | P | T | P |
| 1-nitropyrene | 2.17 | P | T | P | T | T | P | P | T | P | P |
| 6-nitrochrysene | 2.21 | T | P | T | T | P | T | P | T | T | T |
| 2,4,7-trinitro-9-fluorenone | 2.27 | E | T | E | T | T | T | P | T | P | T |
| 2,4,5,7-tetranitro-9-fluorenone | 2.46 | E | E | E | E | E | E | T | E | T | E |
| 8-nitrofluoranthene | 2.60 | P | T | P | T | P | T | P | T | P | P |
| 2,7-dinitro-9-fluorenone | 2.69 | T | T | T | P | T | T | T | T | T | T |
| 2-nitropyrene | 2.87 | P | T | P | T | P | T | P | P | P | T |
| 1-nitrofluoranthene | 3.00 | T | T | T | P | T | T | T | T | T | P |
| 2-nitroanthracene | 3.05 | P | T | P | T | P | T | P | T | P | T |
| 1,3,6,8-tetranitropyrene | 3.18 | E | E | E | E | E | E | T | E | T | E |
| 3-nitrofluoranthene | 3.31 | T | P | T | T | T | T | P | P | P | P |
| 1,3,6-trinitropyrene | 3.87 | P | P | P | T | E | T | T | T | T | T |
| 1,6-dinitropyrene | 4.09 | T | T | T | P | P | T | P | T | P | P |
| 1,3-dinitropyrene | 4.63 | P | T | P | T | T | P | T | T | T | T |
| 1,8-dinitropyrene | 4.74 | T | T | T | T | T | T | T | T | T | T |
| **Number of Compunds in Training Set** | | 23 | **30** | 23 | 36 | 23 | 31 | 24 | 34 | 24 | 31 |
| **Number of Compunds in Prediction Set** | | 21 | **15** | 22 | 9 | 20 | 13 | 22 | 12 | 21 | 13 |
| **Number of Compunds in External Set** | | 7 | **6** | 6 | 6 | 8 | 7 | 5 | 5 | 6 | 7 |

| [b] Name of the compound | Activity (log TA100) | Electron-correlation (CORR(HFX+LYP) ) method | | [c] Name of the compound | Activity (log TA100) | Electron-correlation (CORR(BLYP) ) method | |
|---|---|---|---|---|---|---|---|
| | | Activity Sampling (Order splitting) | 30% random splitting | | | Activity Sampling (Order splitting) | 30% random splitting |
| 4-nitrotoulene | -2.10 | T | T | 4-nitrotoulene | -2.10 | T | T |
| 2,6-dinitrotoulene | -1.34 | P | T | 2,6-dinitrotoulene | -1.34 | P | T |
| 3,4-dinitrotoulene | -1.30 | T | T | 3,4-dinitrotoulene | -1.30 | T | T |
| 2,4-dinitrotoulene | -1.29 | P | T | 2,4-dinitrotoulene | -1.29 | P | T |
| 2,3-dinitrotoulene | -1.26 | T | P | 2,3-dinitrotoulene | -1.26 | T | P |
| 6-nitroquinoline | -1.05 | P | T | 6-nitroquinoline | -1.05 | E | E |
| 3-nitrocarbazole | -1.00 | T | T | 3-nitrocarbazole | -1.00 | T | T |
| 3,5-dinitrotoulene | -0.72 | P | T | 3,5-dinitrotoulene | -0.72 | P | T |
| 5-nitroquinoline | -0.70 | T | P | 3-methyl-2-nitronaphthalene | -0.70 | T | P |
| 2,5-dinitrotoulene | -0.63 | P | T | 5-nitroquinoline | -0.70 | P | T |
| 1,3,6,8-tetranitronaphthalene | -0.52 | E | E | 2,5-dinitrotoulene | -0.63 | T | E |
| 1,3-dinitrobenzene | -0.51 | T | T | 1,3,6,8-tetranitronaphthalene | -0.52 | E | E |
| 2-nitrocarbazole | -0.30 | P | P | 1,3-dinitrobenzene | -0.51 | P | P |
| 4-nitrocarbazole | -0.30 | T | T | 2-nitrocarbazole | -0.30 | T | T |
| 2,3,4-trinitrotoulene | 0.08 | P | T | 4-nitrocarbazole | -0.30 | P | T |
| 1-methyl-2-nitronaphthalene | 0.08 | T | T | 1-methyl-2-nitronaphthalene | 0.08 | T | T |
| 2,4,6-trinitrotoulene | 0.16 | P | P | 2,4,6-trinitrotoulene | 0.16 | P | P |
| 2-nitronaphthlene | 0.37 | T | T | 9-nitroanthracene | 0.26 | E | E |
| 2,3,5-trinitrotoulene | 0.46 | P | T | 1-nitronaphthlene | 0.28 | T | T |
| 2,3,6-trinitrotoulene | 0.55 | T | T | 2-nitronaphthlene | 0.37 | P | T |
| 1,3,5-trinitrobenzene | 0.72 | P | P | 2,3,5-trinitrotoulene | 0.46 | T | P |
| 1,3-dinitronaphthlene | 0.86 | T | T | 2,3,6-trinitrotoulene | 0.55 | P | T |
| 1,5-dinitronaphthlene | 0.91 | P | T | 1,3,5-trinitrobenzene | 0.72 | T | T |
| 3,4,5-trinitrotoulene | 1.01 | T | T | 1,5-dinitronaphthlene | 0.91 | P | T |
| 2-nitrofluorene | 1.08 | P | P | 5-nitroacenaphthene | 0.97 | T | P |
| 1,8-dinitronaphthlene | 1.12 | T | T | 3,4,5-trinitrotoulene | 1.01 | P | T |
| 2,7-dinitrofluorene | 1.27 | P | T | 2-nitrofluorene | 1.08 | T | T |
| 1-nitrobenzo[e]pyrene | 1.65 | T | T | 1,8-dinitronaphthlene | 1.12 | P | T |
| 2-nitrophenanthrene | 1.79 | P | P | 2,4,5-trinitrotoulene | 1.12 | T | P |
| 7-nitrofluoranthene | 2.09 | T | T | 2,7-dinitrofluorene | 1.27 | P | T |
| 1-nitropyrene | 2.17 | P | T | 1-nitrobenzo[e]pyrene | 1.65 | T | T |
| 6-nitrochrysene | 2.21 | T | T | 2-nitrophenanthrene | 1.79 | P | T |
| 2,4,7-trinitro-9-fluorenone | 2.27 | P | P | 7-nitrofluoranthene | 2.09 | T | P |
| 2,4,5,7-tetranitro-9-fluorenone | 2.46 | E | E | 1-nitropyrene | 2.17 | P | T |
| 8-nitrofluoranthene | 2.60 | T | T | 6-nitrochrysene | 2.21 | T | T |
| 2,7-dinitro-9-fluorenone | 2.69 | P | T | 2,4,7-trinitro-9-fluorenone | 2.27 | P | T |
| 2-nitropyrene | 2.87 | T | P | 8-nitrofluoranthene | 2.60 | T | P |
| 1-nitrofluoranthene | 3.00 | P | T | 2,7-dinitro-9-fluorenone | 2.69 | P | T |
| 2-nitroanthracene | 3.05 | T | T | 1-nitrofluoranthene | 3.00 | T | T |
| 1,3,6,8-tetranitropyrene | 3.18 | E | E | 2-nitroanthracene | 3.05 | P | P |
| 3-nitrofluoranthene | 3.31 | P | P | 1,3,6-trinitropyrene | 3.87 | T | T |
| 1,6-dinitropyrene | 4.09 | T | T | **Number of Compunds in Training Set** | | 20 | 26 |
| 1,3-dinitropyrene | 4.63 | P | P | **Number of Compunds in Prediction Set** | | 18 | 11 |
| 1,8-dinitropyrene | 4.74 | T | T | **Number of Compunds in External Set** | | 3 | 4 |
| **Number of Compunds in Training Set** | | 21 | 29 | | | | |
| **Number of Compunds in Prediction Set** | | 20 | 12 | | | | |
| **Number of Compunds in External Set** | | 3 | 3 | | | | |

[a]Splitting is performed through QSARINS software. Ref.[54]. N. Chirico, E. Papa, S. Kovarich, S. Cassani, P. Gramatica, QSAR Res. Unit in Environ Chem and Ecotox University of Insubria, Varese, Italy,
[b]Data set excluding the compounds with undefined electrophilicity value (-) for CORR(HFX+LYP) method (refer to Supporting Information Table S2f).
[c]Data set excluding the compounds with undefined electrophilicity value (-) for CORR(BLYP) (refer to Supporting Information Table S2f).

**Table S4.** Compounds in the training set (T), prediction set (P) and excluded set (E) in different types of splitting methods employed[a] for TA98 mutagenicity. Excluded compounds are either response or structural outliers (determined from Williams plot).

| *Name of the compound* | Activity (log TA98) | Exchange only (HFX, B88, HF) methods | | Exchange+Correlation (HFX+LYP, BLYP, B3LYP) methods | | Exchange+Correlation (Meta functionals, M06, M06-L, M06-2X) methods | | Electron-correlation (CORR(HFX+LYP) , CORR(BLYP) , CORR(B3LYP)) methods | | Electron-correlation (CORR(M06), CORR(M06-L), CORR(M06-2X)) methods | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| | | *Activity Sampling (Order splitting)* | *30% random splitting* | *Activity Sampling (Order splitting)* | *30% random splitting* | *Activity Sampling (Order splitting)* | *30% random splitting* | *Activity Sampling (Order splitting)* | *30% random splitting* | *Activity Sampling (Order splitting)* | *30% random splitting* |
| 1-methyl-2-nitronaphthalene | -0.70 | T | T | T | T | T | T | T | T | T | T |
| 1-nitronaphthlene | -0.61 | T | P | P | P | E | E | P | T | E | E |
| 2-nitronaphthlene | -0.30 | P | T | T | T | T | P | T | P | T | P |
| 1,3-dinitronaphthlene | -0.05 | T | T | T | T | P | T | P | P | E | T |
| 1,3-dinitrobenzene | 0.03 | E | E | E | E | E | E | E | T | E | E |
| 1,5-dinitronaphthlene | 0.52 | T | P | P | P | P | P | T | T | P | T |
| 1,8-dinitronaphthlene | 0.90 | P | T | T | T | T | T | E | T | T | T |
| 2-nitrofluorene | 1.43 | P | T | T | T | P | T | P | T | P | T |
| 2-nitrophenanthrene | 2.11 | T | P | P | T | T | T | T | T | T | P |
| 1-nitrofluoranthene | 2.74 | T | T | T | T | P | P | P | T | P | P |
| 1-nitropyrene | 2.78 | P | T | T | T | T | T | T | P | T | T |
| 2-nitroanthracene | 2.95 | P | P | P | P | P | T | E | T | P | T |
| 2-nitropyrene | 3.35 | T | T | T | T | T | T | T | T | T | T |
| 1,3,6,8-tetranitropyrene | 4.99 | E | E | E | E | E | E | E | E | E | E |
| 1,3,6-trinitropyrene | 4.99 | T | E | E | E | E | T | E | E | E | E |
| 1,3-dinitropyrene | 5.04 | P | T | T | T | T | P | P | P | T | P |
| 1,6-dinitropyrene | 5.06 | T | P | P | P | P | T | T | T | P | T |
| 1,8-dinitropyrene | 5.39 | T | T | T | T | T | T | T | T | T | T |
| **Number of Compunds in Training Set** | | 10 | 10 | 10 | 11 | 8 | 11 | 8 | 12 | 8 | 10 |
| **Number of Compunds in Prediction Set** | | 6 | 5 | 5 | 4 | 6 | 4 | 5 | 4 | 5 | 4 |
| **Number of Compunds in External Set** | | 2 | 3 | 3 | 3 | 4 | 3 | 5 | 2 | 5 | 4 |

| [d] *Name of the compound* | Activity (log TA98) | Electron-correlation (CORR(HFX+LYP )) method | |
|---|---|---|---|
| | | *Activity Sampling (Order splitting)* | *30% random splitting* |
| 1-methyl-2-nitronaphthalene | -0.70 | T | T |
| 2-nitronaphthlene | -0.30 | T | T |
| 1,3-dinitronaphthlene | -0.05 | P | T |
| 1,3-dinitrobenzene | 0.03 | T | P |
| 1,5-dinitronaphthlene | 0.52 | P | T |
| 1,8-dinitronaphthlene | 0.90 | T | T |
| 2-nitrofluorene | 1.43 | P | T |
| 2-nitrophenanthrene | 2.11 | T | P |
| 1-nitrofluoranthene | 2.74 | P | T |
| 1-nitropyrene | 2.78 | T | T |
| 2-nitroanthracene | 2.95 | P | T |
| 2-nitropyrene | 3.35 | T | P |
| 1,3,6,8-tetranitropyrene | 4.99 | E | E |
| 1,3-dinitropyrene | 5.04 | T | T |
| 1,6-dinitropyrene | 5.06 | P | P |
| 1,8-dinitropyrene | 5.39 | T | T |
| **Number of Compunds in Training Set** | | 9 | 11 |
| **Number of Compunds in Prediction Set** | | 6 | 4 |
| **Number of Compunds in External Set** | | 1 | 1 |

| [e] *Name of the compound* | Activity (log TA98) | Electron-correlation (CORR(BLYP) ) method | |
|---|---|---|---|
| | | *Activity Sampling (Order splitting)* | *30% random splitting* |
| 1-methyl-2-nitronaphthalene | -0.70 | T | T |
| 1-nitronaphthlene | -0.61 | T | T |
| 2-nitronaphthlene | -0.30 | P | T |
| 1,3-dinitrobenzene | 0.03 | T | P |
| 1,5-dinitronaphthlene | 0.52 | P | P |
| 1,8-dinitronaphthlene | 0.90 | T | T |
| 2-nitrofluorene | 1.43 | P | T |
| 2-nitrophenanthrene | 2.11 | T | P |
| 1-nitrofluoranthene | 2.74 | P | P |
| 1-nitropyrene | 2.78 | T | T |
| 2-nitroanthracene | 2.95 | P | T |
| 2-nitropyrene | 3.35 | T | T |
| 1,3,6,8-tetranitropyrene | 4.99 | E | E |
| **Number of Compunds in Training Set** | | 7 | 8 |
| **Number of Compunds in Prediction Set** | | 5 | 4 |
| **Number of Compunds in External Set** | | 0 | 0 |

[a]Splitting is performed through QSARINS software, Ref.[54]. N. Chirico, E. Papa, S. Kovarich, S. Cassani, P. Gramatica, QSAR Res. Unit in Environ Chem and Ecotox University of Insubria, Varese, Italy, 2012 (http://www.qsar.it).
[d]Data set excluding the compounds with undefined electrophilicity value (-) for CORR(HFX+LYP) method (refer to Supporting Information Table S2f).
[e]Data set excluding the compounds with undefined electrophilicity value (-) for CORR(BLYP) (refer to Supporting Information Table S2f).

**Table S5.** Comparison of the key internal and external validation parameters for the models based on the total energy ($E$) and energy of HOMO ($E_{HOMO}$) computed with the Exchange (X) only, Exchange + Correlation (X+C) methods, and with the effect of electron-correlation (CORR) of the descriptors, for modeling TA98 mutagenicity of nitrated-PAHs.

| Model S.No. | Method | Descriptor Employed | Splitting Employed | $R^2$ | $Q^2_{LOO}$ | $R^2$-$Q^2_{LOO}$ | $Q^2_{LMO}$ | $Q^2_{F3}$ | $CCC_{EXT}$ |
|---|---|---|---|---|---|---|---|---|---|
| | | | **Exchange (X) Only** | | | | | | |
| 1. | DFT/B88 | $E_{B88}$ , $E^{HOMO}_{B88}$ | activity sampling | 0.948 | 0.862 | 0.085 | 0.681 | 0.943 | 0.955 |
| 2. | DFT/HFX | $E_{HFX}$ , $E^{HOMO}_{HFX}$ | activity sampling | 0.953 | 0.876 | 0.077 | 0.570 | 0.937 | 0.951 |
| | | | **Exchange + Correlation (X+C)** | | | | | | |
| 3. | HFX + LYP | $E_{HFX\ +\ LYP}$ , $E^{HOMO}_{HFX\ +\ LYP}$ | activity sampling | 0.941 | 0.885 | 0.056 | 0.699 | 0.984 | 0.994 |
| 4. | BLYP | $E_{BLYP}$ , $E^{HOMO}_{BLYP}$ | activity sampling | 0.938 | 0.874 | 0.064 | 0.721 | 0.986 | 0.994 |
| 5. | B3LYP | $E_{B3LYP}$ , $E^{HOMO}_{B3LYP}$ | activity sampling | 0.940 | 0.882 | 0.058 | 0.743 | 0.987 | 0.995 |
| 6. | M06 | $E_{M06}$ , $E^{HOMO}_{M06}$ | activity sampling | 0.963 | 0.912 | 0.051 | 0.244 | 0.910 | 0.922 |
| 7. | M06-L | $E_{M06\text{-}L}$ , $E^{HOMO}_{M06-L}$ | activity sampling | 0.960 | 0.901 | 0.059 | 0.333 | 0.907 | 0.919 |
| 8. | M06-2X | $E_{M06\text{-}2X}$ , $E^{HOMO}_{M06-2X}$ | activity sampling | 0.964 | 0.915 | 0.049 | 0.295 | 0.904 | 0.915 |
| | | | **Electron-Correlation (CORR) only** | | | | | | |
| 9. | CORR(HFX+LYP) | $E_{CORR(HFX+LYP)}$ , $E^{HOMO}_{CORR\ (HFX+LYP)}$ | activity sampling | 0.973 | 0.926 | 0.047 | 0.327 | 0.919 | 0.957 |
| 10. | CORR(BLYP) | $E_{CORR(BLYP)}$ , $E^{HOMO}_{CORR\ (BLYP)}$ | activity sampling | 0.968 | 0.899 | 0.069 | 0.244 | 0.892 | 0.943 |
| 11. | CORR(B3LYP) | $E_{CORR(B3LYP)}$ , $E^{HOMO}_{CORR\ (B3LYP)}$ | activity sampling | 0.975 | 0.942 | 0.033 | 0.486 | 0.950 | 0.971 |
| 12. | CORR(M06) | $E_{CORR(M06)}$ , $E^{HOMO}_{CORR\ (M06)}$ | activity sampling | 0.978 | 0.956 | 0.023 | 0.604 | 0.947 | 0.948 |
| 13. | CORR(M06-L) | $E_{CORR(M06\text{-}L)}$ , $E^{HOMO}_{CORR\ (M06-L)}$ | activity sampling | 0.978 | 0.954 | 0.024 | 0.560 | 0.950 | 0.952 |
| 14. | CORR(M06-2X) | $E_{CORR(M06\text{-}2X)}$ , $E^{HOMO}_{CORR\ (M06-2X)}$ | activity sampling | 0.981 | 0.961 | 0.020 | 0.670 | 0.946 | 0.951 |

**Table S6.** Same as **Table S5** but for the models based on the total electronic energy ($E$) and energy of the LUMO ($E_{\mathrm{LUMO}}$).

| Model S.No. | Method | Descriptor Employed | Splitting Employed | $R^2$ | $Q^2_{\mathrm{LOO}}$ | $R^2$-$Q^2_{\mathrm{LOO}}$ | $Q^2_{\mathrm{LMO}}$ | $Q^2_{\mathrm{F3}}$ | $CCC_{\mathrm{EXT}}$ |
|---|---|---|---|---|---|---|---|---|---|
| | | | **Exchange (X) Only** | | | | | | |
| 1. | DFT/B88 | $E_{\mathrm{B88}}$ , $E^{\mathrm{LUMO}}_{\mathrm{B88}}$ | activity sampling | 0.941 | 0.861 | 0.080 | 0.694 | 0.858 | 0.878 |
| 2. | DFT/HFX | $E_{\mathrm{HFX}}$ , $E^{\mathrm{LUMO}}_{\mathrm{HFX}}$ | activity sampling | 0.860 | 0.660 | 0.200 | 0.120 | 0.733 | 0.762 |
| | | | **Exchange + Correlation (X+C)** | | | | | | |
| 3. | HFX + LYP | $E_{\mathrm{HFX\,+\,LYP}}$ , $E^{\mathrm{LUMO}}_{\mathrm{HFX\,+\,LYP}}$ | activity sampling | 0.886 | 0.711 | 0.175 | 0.542 | 0.588 | 0.872 |
| 4. | BLYP | $E_{\mathrm{BLYP}}$ , $E^{\mathrm{LUMO}}_{\mathrm{BLYP}}$ | activity sampling | 0.927 | 0.823 | 0.104 | - | 0.836 | 0.925 |
| 5. | B3LYP | $E_{\mathrm{B3LYP}}$ , $E^{\mathrm{LUMO}}_{\mathrm{B3LYP}}$ | activity sampling | 0.918 | 0.786 | 0.132 | 0.563 | 0.813 | 0.915 |
| 6. | M06 | $E_{\mathrm{M06}}$ , $E^{\mathrm{LUMO}}_{\mathrm{M06}}$ | activity sampling | 0.793 | 0.556 | 0.237 | 0.083 | 0.912 | 0.959 |
| 7. | M06-L | $E_{\mathrm{M06\text{-}L}}$ , $E^{\mathrm{LUMO}}_{\mathrm{M06-L}}$ | activity sampling | 0.836 | 0.679 | 0.157 | 0.339 | 0.905 | 0.958 |
| 8. | M06-2X | $E_{\mathrm{M06\text{-}2X}}$ , $E^{\mathrm{LUMO}}_{\mathrm{M06-2X}}$ | activity sampling | 0.926 | 0.607 | 0.319 | -0.951 | - | - |
| | | | **Electron-Correlation (CORR) only** | | | | | | |
| 9. | CORR(HFX+LYP) | $E_{\mathrm{CORR(HFX+LYP)}}$ , $E^{\mathrm{LUMO}}_{\mathrm{CORR\,(HFX+LYP)}}$ | activity sampling | 0.992 | 0.986 | 0.006 | 0.667 | 0.839 | 0.924 |
| 10. | CORR(BLYP) | $E_{\mathrm{CORR(BLYP)}}$ , $E^{\mathrm{LUMO}}_{\mathrm{CORR\,(BLYP)}}$ | activity sampling | 0.910 | 0.837 | 0.073 | 0.606 | 0.864 | 0.945 |
| 11. | CORR(B3LYP) | $E_{\mathrm{CORR(B3LYP)}}$ , $E^{\mathrm{LUMO}}_{\mathrm{CORR\,(B3LYP)}}$ | activity sampling | 0.929 | 0.851 | 0.078 | -0.237 | - | - |
| 12. | CORR(M06) | $E_{\mathrm{CORR(M06)}}$ , $E^{\mathrm{LUMO}}_{\mathrm{CORR\,(M06)}}$ | activity sampling | 0.945 | 0.881 | 0.065 | -0.133 | - | - |
| 13. | CORR(M06-L) | $E_{\mathrm{CORR(M06\text{-}L)}}$ , $E^{\mathrm{LUMO}}_{\mathrm{CORR\,(M06-L)}}$ | activity sampling | 0.948 | 0.873 | 0.074 | 0.136 | 0.822 | 0.831 |
| 14. | CORR(M06-2X) | $E_{\mathrm{CORR(M06\text{-}2X)}}$ , $E^{\mathrm{LUMO}}_{\mathrm{CORR\,(M06-2X)}}$ | activity sampling | 0.951 | 0.882 | 0.068 | -0.032 | - | - |

* (-) indicates unstable models, with negative value of corresponding validation parameter.

**Table S7.** Same as **Table S5** but for the models based on the total electronic energy ($E$) and absolute electronegativity ($\chi$).

| Model S.No. | Method | Descriptor Employed | Splitting Employed | $R^2$ | $Q^2_{LOO}$ | $R^2$-$Q^2_{LOO}$ | $Q^2_{LMO}$ | $Q^2_{F3}$ | $CCC_{EXT}$ |
|---|---|---|---|---|---|---|---|---|---|
| | | | **Exchange (X) Only** | | | | | | |
| 1. | DFT/B88 | $E_{B88}$ , $\chi_{B88}$ | activity sampling | 0.951 | 0.873 | 0.078 | 0.557 | 0.945 | 0.954 |
| 2. | DFT/HFX | $E_{HFX}$ , $\chi_{HFX}$ | activity sampling | 0.938 | 0.849 | 0.089 | 0.607 | 0.940 | 0.950 |
| | | | **Exchange + Correlation (X+C)** | | | | | | |
| 3. | HFX + LYP | $E_{HFX + LYP}$ , $\chi_{HFX + LYP}$ | activity sampling | 0.944 | 0.882 | 0.062 | 0.778 | 0.928 | 0.974 |
| 4. | BLYP | $E_{BLYP}$ , $\chi_{BLYP}$ | activity sampling | 0.945 | 0.883 | 0.062 | 0.715 | 0.952 | 0.982 |
| 5. | B3LYP | $E_{B3LYP}$ , $\chi_{B3LYP}$ | activity sampling | 0.918 | 0.786 | 0.132 | 0.563 | 0.813 | 0.915 |
| 6. | M06 | $E_{M06}$ , $\chi_{M06}$ | activity sampling | 0.951 | 0.865 | 0.086 | - | - | - |
| 7. | M06-L | $E_{M06-l}$ , $\chi_{M06-L}$ | activity sampling | 0.913 | 0.803 | 0.110 | 0.425 | 0.932 | 0.971 |
| 8. | M06-2X | $E_{M06-2x}$ , $\chi_{M06-2X}$ | activity sampling | 0.909 | 0.791 | 0.119 | 0.454 | 0.945 | 0.976 |
| | | | **Electron-Correlation (CORR) only** | | | | | | |
| 9. | CORR(HFX+LYP) | $E_{CORR(HFX+LYP)}$ , $\chi_{CORR(HFX+LYP)}$ | activity sampling | 0.992 | 0.986 | 0.006 | 0.667 | 0.839 | 0.924 |
| 10. | CORR(BLYP) | $E_{CORR(BLYP)}$ , $\chi_{CORR(BLYP)}$ | activity sampling | 0.970 | 0.902 | 0.068 | 0.257 | 0.897 | 0.948 |
| 11. | CORR(B3LYP) | $E_{CORR(B3LYP)}$ , $\chi_{CORR(B3LYP)}$ | activity sampling | 0.960 | 0.892 | 0.068 | 0.079 | 0.923 | 0.951 |
| 12. | CORR(M06) | $E_{CORR(M06)}$ , $\chi_{CORR(M06)}$ | activity sampling | 0.967 | 0.923 | 0.045 | 0.274 | 0.878 | 0.883 |
| 13. | CORR(M06-L) | $E_{CORR(M06-L)}$ , $\chi_{CORR(M06-L)}$ | activity sampling | 0.971 | 0.934 | 0.037 | 0.344 | 0.884 | 0.891 |
| 14. | CORR(M06-2X) | $E_{CORR(M06-2X)}$ , $\chi_{CORR(M06-2X)}$ | activity sampling | 0.969 | 0.931 | 0.038 | 0.442 | 0.889 | 0.897 |

* (-) indicates unstable models, with negative value of corresponding validation parameter.

**Table S8.** Same as **Table S5** but for the models based on the total energy ($E$) and chemical hardness ($\eta$).

| Model S.No. | Method | Descriptor Employed | Splitting Employed | $R^2$ | $Q^2_{LOO}$ | $R^2$-$Q^2_{LOO}$ | $Q^2_{LMO}$ | $Q^2_{F3}$ | $CCC_{EXT}$ |
|---|---|---|---|---|---|---|---|---|---|
| | | | **Exchange (X) Only** | | | | | | |
| 1. | DFT/B88 | $E_{B88}$ , $\eta_{B88}$ | activity sampling | 0.909 | 0.786 | 0.124 | 0.491 | 0.746 | 0.847 |
| 2. | DFT/HFX | $E_{HFX}$ , $\eta_{HFX}$ | activity sampling | 0.941 | 0.865 | 0.076 | 0.655 | 0.867 | 0.893 |
| | | | **Exchange + Correlation (X+C)** | | | | | | |
| 3. | HFX + LYP | $E_{HFX + LYP}$ , $\eta_{HFX + LYP}$ | activity sampling | 0.908 | 0.850 | 0.058 | 0.669 | 0.972 | 0.988 |
| 4. | BLYP | $E_{BLYP}$ , $\eta_{BLYP}$ | activity sampling | 0.884 | 0.825 | 0.059 | 0.451 | 0.933 | 0.969 |
| 5. | B3LYP | $E_{B3LYP}$ , $\eta_{B3LYP}$ | activity sampling | 0.895 | 0.838 | 0.057 | 0.476 | 0.952 | 0.979 |
| 6. | M06 | $E_{M06}$ , $\eta_{M06}$ | activity sampling | 0.856 | 0.698 | 0.158 | 0.464 | 0.962 | 0.980 |
| 7. | M06-L | $E_{M06-l}$ , $\eta_{M06-L}$ | activity sampling | 0.836 | 0.655 | 0.182 | 0.374 | 0.935 | 0.965 |
| 8. | M06-2X | $E_{M06-2x}$ , $\eta_{M06-2X}$ | activity sampling | 0.860 | 0.705 | 0.155 | 0.355 | 0.975 | 0.988 |
| | | | **Electron-Correlation (CORR) only** | | | | | | |
| 9. | CORR(HFX+LYP) | $E_{CORR(HFX+LYP)}$ , $\eta_{CORR(HFX+LYP)}$ | activity sampling | 0.904 | 0.842 | 0.062 | 0.542 | 0.807 | 0.922 |
| 10. | CORR(BLYP) | $E_{CORR(BLYP)}$ , $\eta_{CORR(BLYP)}$ | activity sampling | 0.945 | 0.842 | 0.103 | -0.177 | - | - |
| 11. | CORR(B3LYP) | $E_{CORR(B3LYP)}$ , $\eta_{CORR(B3LYP)}$ | activity sampling | 0.928 | 0.842 | 0.086 | 0.690 | 0.766 | 0.908 |
| 12. | CORR(M06) | $E_{CORR(M06)}$ , $\eta_{CORR(M06)}$ | activity sampling | 0.968 | 0.926 | 0.043 | 0.408 | 0.874 | 0.880 |
| 13. | CORR(M06-L) | $E_{CORR(M06-L)}$ , $\eta_{CORR(M06-L)}$ | activity sampling | 0.972 | 0.936 | 0.036 | 0.374 | 0.888 | 0.896 |
| 14. | CORR(M06-2X) | $E_{CORR(M06-2X)}$ , $\eta_{CORR(M06-2X)}$ | activity sampling | 0.969 | 0.929 | 0.040 | 0.367 | 0.887 | 0.894 |

* (-) indicates unstable models, with negative value of corresponding validation parameter.

**Table S9.** Same as **Table S5** but for the models based on the total electronic energy ($E$) and electrophilicity index ($\omega$).

| Model S.No. | Method | Descriptor Employed | Splitting Employed | $R^2$ | $Q^2_{LOO}$ | $R^2$-$Q^2_{LOO}$ | $Q^2_{LMO}$ | $Q^2_{F3}$ | $CCC_{EXT}$ |
|---|---|---|---|---|---|---|---|---|---|
| | | | **Exchange (X) Only** | | | | | | |
| 1. | DFT/B88 | $E_{B88}$ , $\omega_{B88}$ | activity sampling | 0.947 | 0.894 | 0.053 | 0.649 | 0.673 | 0.744 |
| 2. | DFT/HFX | $E_{HFX}$ , $\omega_{HFX}$ | activity sampling | 0.931 | 0.847 | 0.084 | 0.460 | 0.899 | 0.914 |
| | | | **Exchange + Correlation (X+C)** | | | | | | |
| 3. | HFX + LYP | $E_{HFX + LYP}$ , $\omega_{HFX + LYP}$ | activity sampling | 0.932 | 0.842 | 0.090 | 0.682 | 0.810 | 0.937 |
| 4. | BLYP | $E_{BLYP}$ , $\omega_{BLYP}$ | activity sampling | 0.854 | 0.633 | 0.221 | 0.359 | 0.565 | 0.857 |
| 5. | B3LYP | $E_{B3LYP}$ , $\omega_{B3LYP}$ | activity sampling | 0.892 | 0.699 | 0.193 | 0.453 | 0.748 | 0.888 |
| 6. | M06 | $E_{M06}$ , $\omega_{M06}$ | activity sampling | 0.915 | 0.715 | 0.200 | - | - | - |
| 7. | M06-L | $E_{M06-L}$, $\omega_{M06-L}$ | activity sampling | 0.908 | 0.696 | 0.212 | - | - | - |
| 8. | M06-2X | $E_{M06-2X}$ , $\omega_{M06-2X}$ | activity sampling | 0.935 | 0.723 | 0.211 | - | - | - |
| | | | **Electron-Correlation (CORR) only** | | | | | | |
| 9. | CORR(HFX+LYP) | $E_{CORR(HFX+LYP)}$ , $\omega_{CORR(HFX+LYP)}$ | activity sampling | 0.948 | 0.761 | 0.187 | - | - | - |
| 10. | CORR(BLYP) | $E_{CORR(BLYP)}$ , $\omega_{CORR(BLYP)}$ | activity sampling | 0.916 | 0.735 | 0.181 | - | - | - |
| 11. | CORR(B3LYP) | $E_{CORR(B3LYP)}$ , $\omega_{CORR(B3LYP)}$ | activity sampling | 0.972 | 0.924 | 0.049 | 0.158 | 0.962 | 0.978 |
| 12. | CORR(M06) | $E_{CORR(M06)}$ , $\omega_{CORR(M06)}$ | activity sampling | 0.964 | 0.903 | 0.061 | 0.363 | 0.898 | 0.902 |
| 13. | CORR(M06-L) | $E_{CORR(M06-L)}$ , $\omega_{CORR(M06-L)}$ | activity sampling | 0.976 | 0.944 | 0.032 | 0.479 | 0.900 | 0.909 |
| 14. | CORR(M06-2X) | $E_{CORR(M06-2X)}$ , $\omega_{CORR(M06-2X)}$ | activity sampling | 0.970 | 0.932 | 0.038 | 0.380 | 0.881 | 0.886 |

* (-) indicates unstable models, with negative value of corresponding validation parameter.

**Table S10.** Comparison of the key internal and external validation parameters for the models developed with the total energy ($E$), energy of HOMO ($E_{HOMO}$), energy of LUMO ($E_{LUMO}$), absolute electronegativity ($\chi$), chemical hardness ($\eta$) and electrophilicity index ($\omega$) computed with the Hartree-Fock (HF) method, for modeling TA100 mutagenicity and TA98 mutagenicity of nitrated-PAHs.

| Model S.No. | Descriptor Employed | Splitting Employed | $R^2$ | $Q^2_{LOO}$ | $R^2$-$Q^2_{LOO}$ | $Q^2_{LMO}$ | $Q^2_{F3}$ | $CCC_{EXT}$ |
|---|---|---|---|---|---|---|---|---|
| | | | | TA100 mutagenicity | | | | |
| 1. | $E_{HF}$ , $E_{HF}^{HOMO}$ | 30% | 0.743 | 0.668 | 0.075 | 0.643 | 0.707 | 0.841 |
| 2. | $E_{HF}$ , $E_{HF}^{LUMO}$ | 30% | 0.680 | 0.603 | 0.077 | 0.574 | 0.816 | 0.682 |
| 3. | $E_{HF}$ , $\chi_{HF}$ | 30% | 0.778 | 0.711 | 0.067 | 0.692 | 0.731 | 0.859 |
| 4. | $E_{HF}$ , $\eta_{HF}$ | 30% | 0.647 | 0.536 | 0.111 | 0.529 | 0.653 | 0.793 |
| 5. | $E_{HF}$ , $\omega_{HF}$ | 30% | 0.787 | 0.731 | 0.056 | 0.707 | 0.736 | 0.860 |
| | | | | TA98 mutagenicity | | | | |
| 6. | $E_{HF}$ , $E_{HF}^{HOMO}$ | activity sampling | 0.958 | 0.888 | 0.070 | 0.757 | 0.935 | 0.950 |
| 7. | $E_{HF}$ , $E_{HF}^{LUMO}$ | activity sampling | 0.891 | 0.748 | 0.143 | 0.307 | 0.699 | 0.763 |
| 8. | $E_{HF}$ , $\chi_{HF}$ | activity sampling | 0.945 | 0.863 | 0.081 | 0.635 | 0.933 | 0.943 |
| 9. | $E_{HF}$ , $\eta_{HF}$ | activity sampling | 0.942 | 0.860 | 0.082 | 0.615 | 0.750 | 0.852 |
| 10. | $E_{HF}$ , $\omega_{HF}$ | activity sampling | 0.949 | 0.889 | 0.060 | 0.748 | 0.882 | 0.898 |

**Table S11.** Value of internal and external validation parameters of two-descriptor QSAR models, for mutagenicity (LogTA100), developed using exchange (X) only (B88, HFX and HF) based methods through activity sampling (ordered response) splitting method.

| Model | Variables | $Q^2_{LOO}$ | $R^2$-$Q^2_{LOO}$ | $R^2_{adj}$ | $R^2$-$R^2_{adj}$ | $R^2$ | $\Delta K$ | $RMSE_{TR}$ | $RMSE_{CV}$ | $RMSE_{EXT}$ | $F$ | *N. Ext.OK* | $Q^2_{F1}$ | $Q^2_{F2}$ | $Q^2_{F3}$ | $CCC_{TR}$ | $CCC_{CV}$ | $CCC_{EXT}$ | $\bar{r}^2_m$ | $\Delta r^2_m$ | $MAE_{TR}$ | $MAE_{CV}$ | $MAE_{EXT}$ | $RSS_{TR}$ | $PRESS_{CV}$ | $PRESS_{EXT}$ | $R^2_{LMO}$ | $Q^2_{LMO}$ | $R^2_{Yscr}$ | $Q^2_{Yscr}$ | $R^2_{Xrand}$ | $Q^2_{Xrand}$ | $R^2_{Yrand}$ | $Q^2_{Yrand}$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | $E_{HFX}$, $E^{HOMO}_{HFX}$ | 0.7118 | 0.0639 | 0.7533 | 0.0224 | 0.7757 | 0.4230 | 0.8376 | 0.9496 | 0.7738 | 34.5906 | 5 | 0.7561 | 0.7546 | 0.8086 | 0.8737 | 0.8392 | 0.8666 | 0.7010 | 0.0779 | 0.6783 | 0.7793 | 0.6274 | 16.1378 | 20.7390 | 12.5730 | 0.7744 | 0.6258 | 8.4794 | -21.5508 | 9.3239 | -20.3343 | 9.7616 | -19.8615 |
| 2 | $E_{HFX}$, $\eta_{HFX}$ | 0.6852 | 0.0867 | 0.7491 | 0.0228 | 0.7719 | 0.2362 | 0.8448 | 0.9924 | 0.8392 | 33.8353 | 4 | 0.7131 | 0.7113 | 0.7749 | 0.8713 | 0.8254 | 0.8402 | 0.6812 | 0.0915 | 0.6390 | 0.7456 | 0.6984 | 16.4159 | 22.6539 | 14.7905 | 0.7767 | 0.5808 | 9.3805 | -20.9621 | 8.8044 | -21.2567 | 9.8392 | -19.7071 |
| 3 | $E_{HFX}$, $\chi_{HFX}$ | 0.6796 | 0.0755 | 0.7306 | 0.0245 | 0.7551 | 0.1936 | 0.8754 | 1.0012 | 0.8016 | 30.8308 | 5 | 0.7382 | 0.7366 | 0.7946 | 0.8605 | 0.8198 | 0.8559 | 0.6663 | 0.0777 | 0.7157 | 0.8243 | 0.6457 | 17.6238 | 23.0534 | 13.4949 | 0.7568 | 0.6168 | 8.9207 | -20.7981 | 8.5189 | -21.7048 | 8.8984 | -20.8981 |
| 4 | $E_{HF}$, $\omega_{HF}$ | 0.6634 | 0.0777 | 0.7152 | 0.0259 | 0.7411 | 0.0325 | 0.9000 | 1.0263 | 0.8582 | 28.6217 | 1 | 0.6999 | 0.6981 | 0.7646 | 0.8513 | 0.8088 | 0.8298 | 0.6313 | 0.0831 | 0.7356 | 0.8448 | 0.6971 | 18.6319 | 24.2235 | 15.4670 | 0.7433 | 0.5645 | 8.6804 | -21.4844 | 9.1632 | -20.9202 | 9.2232 | -20.6306 |
| 5 | $E_{HFX}$, $\omega_{HFX}$ | 0.6487 | 0.0808 | 0.7024 | 0.0271 | 0.7295 | 0.0172 | 0.9200 | 1.0484 | 0.8708 | 26.9649 | 1 | 0.6911 | 0.6892 | 0.7577 | 0.8436 | 0.7997 | 0.8255 | 0.6163 | 0.0829 | 0.7534 | 0.8647 | 0.7072 | 19.4670 | 25.2796 | 15.9226 | 0.7300 | 0.5577 | 8.7087 | -21.5974 | 9.4434 | -20.3285 | 9.5160 | -20.0754 |
| 6 | $E_{HF}$, $\chi_{HF}$ | 0.6469 | 0.0820 | 0.7018 | 0.0271 | 0.7289 | 0.1386 | 0.9209 | 1.0510 | 0.8490 | 26.8888 | 3 | 0.7063 | 0.7045 | 0.7696 | 0.8432 | 0.7995 | 0.8413 | 0.6156 | 0.0793 | 0.7912 | 0.9107 | 0.6890 | 19.5072 | 25.4064 | 15.1383 | 0.7351 | 0.5388 | 9.1733 | -20.7737 | 8.4604 | -21.6481 | 9.1590 | -20.8695 |
| 7 | $E_{B88}$, $E^{LUMO}_{B88}$ | 0.6215 | 0.0827 | 0.6746 | 0.0296 | 0.7042 | 0.0039 | 0.9620 | 1.0882 | 0.9534 | 23.8095 | 1 | 0.6297 | 0.6274 | 0.7095 | 0.8264 | 0.7804 | 0.7869 | 0.5649 | 0.0916 | 0.7779 | 0.8898 | 0.7843 | 21.2838 | 27.2379 | 19.0886 | 0.7031 | 0.5278 | 9.3865 | -20.4639 | 9.6104 | -20.6987 | 9.4819 | -20.6350 |
| 8 | $E_{HF}$, $E^{HOMO}_{HF}$ | 0.6187 | 0.0863 | 0.6754 | 0.0295 | 0.7049 | 0.3503 | 0.9608 | 1.0923 | 0.8940 | 23.8899 | 1 | 0.6744 | 0.6725 | 0.7446 | 0.8269 | 0.7807 | 0.8242 | 0.5814 | 0.0825 | 0.8225 | 0.9459 | 0.7532 | 21.2333 | 27.4404 | 16.7823 | 0.7094 | 0.5275 | 9.6012 | -20.3977 | 8.8795 | -21.1091 | 9.0659 | -20.9328 |
| 9 | $E_{B88}$, $\chi_{B88}$ | 0.6047 | 0.0878 | 0.6617 | 0.0308 | 0.6924 | 0.0729 | 0.9809 | 1.1122 | 0.9852 | 22.5143 | 0 | 0.6046 | 0.6022 | 0.6898 | 0.8183 | 0.7706 | 0.7889 | 0.5328 | 0.0941 | 0.8245 | 0.9444 | 0.8612 | 22.1317 | 28.4482 | 20.3816 | 0.6990 | 0.4723 | 9.3955 | -20.6414 | 8.5962 | -21.2617 | 9.2430 | -20.9216 |
| 10 | $E_{HF}$, $E^{LUMO}_{HF}$ | 0.5884 | 0.0923 | 0.6488 | 0.0319 | 0.6807 | -0.0106 | 0.9995 | 1.1348 | 1.0153 | 21.3182 | 0 | 0.5800 | 0.5775 | 0.6705 | 0.8100 | 0.7554 | 0.7406 | 0.5497 | 0.1019 | 0.7422 | 0.8465 | 0.8196 | 22.9769 | 29.6209 | 21.6474 | 0.6859 | 0.4761 | 9.0185 | -21.3565 | 8.6193 | -21.0723 | 9.2978 | -21.0592 |
| 11 | $E_{B88}$, $\omega_{B88}$ | 0.5627 | 0.1155 | 0.6460 | 0.0322 | 0.6782 | 0.0757 | 1.0034 | 1.1697 | 1.0247 | 21.0766 | 0 | 0.5722 | 0.5696 | 0.6644 | 0.8083 | 0.7468 | 0.7315 | 0.5445 | 0.0983 | 0.7815 | 0.9211 | 0.8266 | 23.1555 | 31.4702 | 22.0523 | 0.6840 | 0.4408 | 8.2722 | -26.5454 | 9.0316 | -21.1739 | 9.0901 | -23.9524 |
| 12 | $E_{B88}$, $E^{HOMO}_{B88}$ | 0.5593 | 0.1014 | 0.6268 | 0.0339 | 0.6607 | 0.2080 | 1.0303 | 1.1742 | 1.0559 | 19.4724 | 0 | 0.5457 | 0.5430 | 0.6436 | 0.7957 | 0.7392 | 0.7526 | 0.4895 | 0.0997 | 0.8580 | 0.9850 | 0.9222 | 24.4159 | 31.7135 | 23.4145 | 0.6657 | 0.4483 | 9.3778 | -20.4344 | 9.0118 | -20.7525 | 8.9736 | -21.2832 |
| 13 | $E_{HFX}$, $E^{LUMO}_{HFX}$ | 0.5347 | 0.1026 | 0.6010 | 0.0363 | 0.6373 | -0.0427 | 1.0653 | 1.2066 | 1.0967 | 17.5688 | 0 | 0.5100 | 0.5071 | 0.6156 | 0.7785 | 0.7178 | 0.7050 | 0.4733 | 0.1009 | 0.8457 | 0.9679 | 0.8830 | 26.1018 | 33.4839 | 25.2561 | 0.6380 | 0.4174 | 9.1352 | -21.7935 | 9.0360 | -20.7048 | 9.2193 | -21.4392 |
| 14 | $E_{HF}$, $\eta_{HF}$ | 0.5316 | 0.1218 | 0.6187 | 0.0347 | 0.6534 | 0.2451 | 1.0414 | 1.2106 | 1.0393 | 18.8484 | 0 | 0.5599 | 0.5572 | 0.6547 | 0.7903 | 0.7222 | 0.7491 | 0.4994 | 0.0962 | 0.8537 | 0.9928 | 0.8703 | 24.9440 | 33.7087 | 22.6851 | 0.6598 | 0.4211 | 9.3622 | -20.7423 | 9.3999 | -20.4641 | 9.4572 | -20.6024 |
| 15 | $E_{B88}$, $\eta_{B88}$ | 0.5042 | 0.1160 | 0.5822 | 0.0380 | 0.6202 | 0.2183 | 1.0900 | 1.2454 | 1.1716 | 16.3314 | 0 | 0.4408 | 0.4374 | 0.5613 | 0.7656 | 0.6977 | 0.6548 | 0.4273 | 0.1078 | 0.9029 | 1.0424 | 0.9618 | 27.3284 | 35.6752 | 28.8243 | 0.6286 | 0.4003 | 9.4517 | -20.5369 | 8.8553 | -21.5242 | 8.8120 | -21.4746 |

Models are arranged according to $Q^2_{LOO}$ values.

Parameters are obtained through QSARINS software. Ref. [54] N. Chirico, E. Papa, S. Kovarich, S. Cassani, P. Gramatica, QSAR Res. Unit in Environ. Chem. and Ecotox. University of Insubria, Varese, Italy, 2012. (http://www.qsar.it).

$R^2_{adj}$ adjusted $R^2$

*N. Ext.OK* Number of external validation parameters meeting threshold values

$F$ "F-test" statistic value

**Table S12.** Value of internal and external validation parameters of two-descriptor QSAR models, for mutagenicity (LogTA100), developed using exchange (X) only (B88, HFX and HF) based methods through 30% (random) splitting method.

| Model | Variables | $Q^2_{LOO}$ | $R^2$-$Q^2_{LOO}$ | $R^2_{adj}$ | $R^2$-$R^2_{adj}$ | $R^2$ | $\Delta K$ | $RMSE_{TR}$ | $RMSE_{CV}$ | $RMSE_{EXT}$ | $F$ | $N.ExtOK$ | $Q^2_{F1}$ | $Q^2_{F2}$ | $Q^2_{F3}$ | $CCC_{TR}$ | $CCC_{CV}$ | $CCC_{EXT}$ | $\bar{r}^2_m$ | $\Delta r^2_m$ | $MAE_{TR}$ | $MAE_{CV}$ | $MAE_{EXT}$ | $RSS_{TR}$ | $PRESS_{CV}$ | $PRESS_{EXT}$ | $R^2_{LMO}$ | $Q^2_{LMO}$ | $R^2_{Yscr}$ | $Q^2_{Yscr}$ | $R^2_{Xrand}$ | $Q^2_{Xrand}$ | $R^2_{Yrand}$ | $Q^2_{Yrand}$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | $E_{HFX}$, $\chi_{HFX}$ | 0.7346 | 0.0619 | 0.7815 | 0.0151 | 0.7965 | 0.0847 | 0.7759 | 0.8861 | 0.8393 | 52.8549 | 5 | 0.7564 | 0.7187 | 0.7619 | 0.8868 | 0.8550 | 0.8767 | 0.7526 | 0.0429 | 0.6078 | 0.6860 | 0.6867 | 18.0606 | 23.5575 | 10.5672 | 0.8009 | 0.7180 | 7.2607 | -15.0914 | 6.6898 | -15.3408 | 7.1007 | -15.0420 |
| 2 | $E_{HFX}$, $E^{HOMO}_{HFX}$ | 0.7315 | 0.0606 | 0.7767 | 0.0154 | 0.7921 | 0.3632 | 0.7844 | 0.8914 | 0.7958 | 51.4299 | 5 | 0.7810 | 0.7471 | 0.7860 | 0.8840 | 0.8525 | 0.8869 | 0.7626 | 0.0616 | 0.5997 | 0.6760 | 0.6433 | 18.4569 | 23.8356 | 9.5006 | 0.7931 | 0.7194 | 6.6263 | -15.6764 | 6.6681 | -15.5010 | 7.0796 | -15.1925 |
| 3 | $E_{HF}$, $\omega_{HF}$ | 0.7309 | 0.0562 | 0.7714 | 0.0158 | 0.7872 | -0.0998 | 0.7936 | 0.8923 | 0.8836 | 49.9357 | 4 | 0.7300 | 0.6882 | 0.7362 | 0.8809 | 0.8519 | 0.8595 | 0.7126 | 0.0112 | 0.5920 | 0.6643 | 0.7703 | 18.8917 | 23.8839 | 11.7108 | 0.7905 | 0.7037 | 6.3514 | -15.9934 | 7.0228 | -15.0742 | 7.2439 | -15.2148 |
| 4 | $E_{HFX}$, $\omega_{HFX}$ | 0.7197 | 0.0590 | 0.7622 | 0.0164 | 0.7786 | -0.1096 | 0.8094 | 0.9108 | 0.9048 | 47.4775 | 4 | 0.7169 | 0.6730 | 0.7233 | 0.8755 | 0.8453 | 0.8540 | 0.7037 | 0.0223 | 0.6123 | 0.6870 | 0.7939 | 19.6533 | 24.8863 | 12.2811 | 0.7813 | 0.6964 | 7.1440 | -15.3539 | 6.8225 | -15.3359 | 6.3831 | -16.1493 |
| 5 | $E_{HF}$, $\chi_{HF}$ | 0.7109 | 0.0674 | 0.7619 | 0.0164 | 0.7783 | 0.0641 | 0.8100 | 0.9249 | 0.8918 | 47.3911 | 4 | 0.7250 | 0.6824 | 0.7312 | 0.8753 | 0.8410 | 0.8587 | 0.7139 | 0.0346 | 0.6463 | 0.7296 | 0.7300 | 19.6812 | 25.6616 | 11.9292 | 0.7810 | 0.6861 | 7.1613 | -15.4603 | 7.0300 | -15.0703 | 6.5662 | -16.2433 |
| 6 | $E_{HF}$, $E^{HOMO}_{HF}$ | 0.6683 | 0.0746 | 0.7238 | 0.0190 | 0.7429 | 0.3233 | 0.8722 | 0.9907 | 0.9306 | 39.0062 | 3 | 0.7005 | 0.6541 | 0.7073 | 0.8525 | 0.8139 | 0.8412 | 0.6774 | 0.0772 | 0.6847 | 0.7725 | 0.7595 | 22.8241 | 29.4451 | 12.9911 | 0.7518 | 0.6238 | 6.7210 | -15.8855 | 6.7267 | -15.5165 | 7.4222 | -14.6763 |
| 7 | $E_{HFX}$, $\eta_{HFX}$ | 0.6673 | 0.0781 | 0.7265 | 0.0189 | 0.7454 | 0.2594 | 0.8681 | 0.9922 | 0.8312 | 39.5143 | 5 | 0.7611 | 0.7241 | 0.7665 | 0.8541 | 0.8128 | 0.8703 | 0.6953 | 0.0753 | 0.6742 | 0.7595 | 0.6598 | 22.6053 | 29.5356 | 10.3624 | 0.7491 | 0.6390 | 7.1346 | -15.4306 | 7.0321 | -15.2160 | 7.0952 | -15.1003 |
| 8 | $E_{B88}$, $E^{LUMO}_{B88}$ | 0.6404 | 0.0846 | 0.7046 | 0.0204 | 0.7250 | -0.1122 | 0.9021 | 1.0315 | 0.9066 | 35.5904 | 3 | 0.7158 | 0.6718 | 0.7222 | 0.8406 | 0.7970 | 0.8490 | 0.6735 | 0.0816 | 0.7097 | 0.8027 | 0.7831 | 24.4123 | 31.9199 | 12.3288 | 0.7313 | 0.6139 | 6.6037 | -16.0933 | 7.1237 | -14.7420 | 7.1495 | -15.2317 |
| 9 | $E_{B88}$, $\chi_{B88}$ | 0.6400 | 0.0755 | 0.6944 | 0.0211 | 0.7155 | 0.0224 | 0.9175 | 1.0322 | 0.9633 | 33.9544 | 1 | 0.6791 | 0.6294 | 0.6864 | 0.8342 | 0.7940 | 0.8303 | 0.6560 | 0.0858 | 0.7351 | 0.8240 | 0.8161 | 25.2539 | 31.9605 | 13.9193 | 0.7176 | 0.6210 | 7.2325 | -15.2724 | 6.4840 | -15.6382 | 6.3503 | -16.2029 |
| 10 | $E_{HF}$, $E^{LUMO}_{HF}$ | 0.6034 | 0.0766 | 0.6563 | 0.0237 | 0.6800 | -0.1336 | 0.9731 | 1.0833 | 0.9696 | 28.6865 | 0 | 0.6749 | 0.6245 | 0.6823 | 0.8095 | 0.7686 | 0.8156 | 0.6208 | 0.0928 | 0.7348 | 0.8180 | 0.7996 | 28.4074 | 35.2056 | 14.1029 | 0.6846 | 0.5735 | 7.1382 | -15.2424 | 6.7603 | -15.3687 | 6.4490 | -16.1687 |
| 11 | $E_{B88}$, $E^{HOMO}_{B88}$ | 0.5589 | 0.0925 | 0.6256 | 0.0258 | 0.6515 | 0.2458 | 1.0155 | 1.1424 | 0.9841 | 25.2330 | 0 | 0.6651 | 0.6132 | 0.6727 | 0.7890 | 0.7374 | 0.8079 | 0.5932 | 0.0992 | 0.8247 | 0.9234 | 0.8107 | 30.9402 | 39.1528 | 14.5275 | 0.6568 | 0.5253 | 6.8770 | -15.1902 | 6.4536 | -15.7556 | 6.8688 | -15.4849 |
| 12 | $E_{HFX}$, $E^{LUMO}_{HFX}$ | 0.5445 | 0.0824 | 0.5993 | 0.0276 | 0.6269 | -0.1423 | 1.0507 | 1.1609 | 1.0227 | 22.6868 | 0 | 0.6383 | 0.5823 | 0.6466 | 0.7707 | 0.7267 | 0.7858 | 0.5588 | 0.1055 | 0.8249 | 0.9146 | 0.8906 | 33.1172 | 40.4324 | 15.6876 | 0.6299 | 0.5080 | 6.5441 | -16.7207 | 6.8613 | -15.1975 | 7.2964 | -15.6170 |
| 13 | $E_{HF}$, $\eta_{HF}$ | 0.5359 | 0.1113 | 0.6212 | 0.0261 | 0.6473 | 0.2224 | 1.0216 | 1.1718 | 1.0141 | 24.7744 | 0 | 0.6444 | 0.5893 | 0.6525 | 0.7859 | 0.7244 | 0.7931 | 0.5566 | 0.1081 | 0.8250 | 0.9310 | 0.8050 | 31.3109 | 41.1944 | 15.4254 | 0.6495 | 0.5287 | 6.5382 | -16.1358 | 6.6812 | -15.4203 | 6.8262 | -15.2212 |
| 14 | $E_{B88}$, $\omega_{B88}$ | 0.4717 | 0.1708 | 0.6161 | 0.0265 | 0.6426 | -0.0423 | 1.0284 | 1.2502 | 0.9574 | 24.2703 | 0 | 0.6830 | 0.6340 | 0.6902 | 0.7824 | 0.7012 | 0.8044 | 0.5410 | 0.1167 | 0.8388 | 0.9773 | 0.8239 | 31.7288 | 46.8934 | 13.7485 | 0.6552 | 0.4773 | 6.8457 | -17.7301 | 6.6132 | -15.4665 | 7.2000 | -16.7876 |
| 15 | $E_{B88}$, $\eta_{B88}$ | 0.3906 | 0.1475 | 0.5040 | 0.0342 | 0.5382 | 0.1043 | 1.1690 | 1.3428 | 1.0468 | 15.7320 | 0 | 0.6210 | 0.5624 | 0.6297 | 0.6998 | 0.6154 | 0.7455 | 0.4558 | 0.1391 | 0.9990 | 1.1324 | 0.9311 | 40.9964 | 54.0931 | 16.4377 | 0.5480 | 0.3769 | 6.6256 | -15.8523 | 7.0499 | -15.3708 | 6.6508 | -15.9554 |

Models are arranged according to $Q^2_{LOO}$ values.
Parameters are obtained through QSARINS software. Ref. [54] N. Chirico, E. Papa, S. Kovarich, S. Cassani, P. Gramatica, QSAR Res. Unit in Environ. Chem. and Ecotox. University of Insubria, Varese, Italy, 2012. (http://www.qsar.it).

$R^2_{adj}$ adjusted $R^2$

*N. Ext.OK* Number of external validation parameters meeting threshold values

*F* "F-test" statistic value

**Table S13.** Value of internal and external validation parameters of two-descriptor QSAR models, for mutagenicity (LogTA98), developed using exchange (X) only (B88, HFX and HF) based methods through activity sampling (ordered response) splitting method.

| Model | Variables | $Q^2_{LOO}$ | $R^2$-$Q^2_{LOO}$ | $R^2_{adj}$ | $R^2$-$R^2_{adj}$ | $R^2$ | $\Delta K$ | $RMSE_{TR}$ | $RMSE_{CV}$ | $RMSE_{EXT}$ | $F$ | *N. Ext.OK* | $Q^2_{F1}$ | $Q^2_{F2}$ | $Q^2_{F3}$ | $CCC_{TR}$ | $CCC_{CV}$ | $CCC_{EXT}$ | $\bar{r}^2_m$ | $\Delta r^2_m$ | $MAE_{TR}$ | $MAE_{CV}$ | $MAE_{EXT}$ | $RSS_{TR}$ | $PRESS_{CV}$ | $PRESS_{EX}$ | $R^2_{LMO}$ | $Q^2_{LMO}$ | $R^2_{Yscr}$ | $Q^2_{Yscr}$ | $R^2_{Xrand}$ | $Q^2_{Xrand}$ | $R^2_{Yrand}$ | $Q^2_{Yrand}$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | $E_{B88}$ , $\omega_{B88}$ | 0.8940 | 0.0534 | 0.9324 | 0.0150 | 0.9474 | -0.1087 | 0.5225 | 0.7416 | 1.3028 | 63.0304 | 0 | 0.4214 | 0.4171 | 0.6729 | 0.9730 | 0.9484 | 0.7442 | 0.4625 | 0.2217 | 0.4339 | 0.6341 | 1.0414 | 2.7298 | 5.4998 | 10.1835 | 0.9547 | 0.6493 | 22.6515 | -68.8887 | 21.1679 | -70.8873 | 21.8555 | -70.8699 |
| 2 | $E_{HF}$ , $\omega_{HF}$ | 0.8890 | 0.0596 | 0.9340 | 0.0147 | 0.9486 | -0.0834 | 0.5162 | 0.7588 | 0.7827 | 64.6548 | 5 | 0.7912 | 0.7896 | 0.8819 | 0.9736 | 0.9458 | 0.8983 | 0.7128 | 0.0925 | 0.4373 | 0.6427 | 0.6161 | 2.6647 | 5.7580 | 3.6757 | 0.9560 | 0.7476 | 22.0542 | -67.9474 | 23.6261 | -63.6271 | 23.3410 | -65.0586 |
| 3 | $E_{HF}$ , $E^{HOMO}_{HF}$ | 0.8875 | 0.0703 | 0.9457 | 0.0121 | 0.9577 | 0.4671 | 0.4682 | 0.7642 | 0.5799 | 79.3350 | 5 | 0.8853 | 0.8845 | 0.9352 | 0.9784 | 0.9462 | 0.9502 | 0.7636 | 0.0700 | 0.4096 | 0.6353 | 0.5081 | 2.1924 | 5.8397 | 2.0179 | 0.9649 | 0.7565 | 22.2405 | -67.1080 | 23.5371 | -63.1234 | 22.6527 | -64.4347 |
| 4 | $E_{HFX}$ , $E^{HOMO}_{HFX}$ | 0.8761 | 0.0770 | 0.9397 | 0.0134 | 0.9531 | 0.4500 | 0.4932 | 0.8017 | 0.5739 | 71.1738 | 5 | 0.8877 | 0.8869 | 0.9365 | 0.9760 | 0.9409 | 0.9513 | 0.7662 | 0.0685 | 0.4245 | 0.6580 | 0.5013 | 2.4321 | 6.4275 | 1.9759 | 0.9613 | 0.5697 | 22.2525 | -65.4665 | 22.5798 | -64.3062 | 24.6753 | -58.3598 |
| 5 | $E_{B88}$ , $\chi_{B88}$ | 0.8729 | 0.0778 | 0.9365 | 0.0141 | 0.9506 | -0.0244 | 0.5061 | 0.8122 | 0.5322 | 67.4013 | 5 | 0.9035 | 0.9027 | 0.9454 | 0.9747 | 0.9392 | 0.9541 | 0.8169 | 0.0620 | 0.4020 | 0.6113 | 0.5028 | 2.5615 | 6.5961 | 1.6992 | 0.9594 | 0.5569 | 22.5306 | -64.6910 | 21.1065 | -75.4198 | 22.1647 | -67.7708 |
| 6 | $E_{HFX}$ , $\eta_{HFX}$ | 0.8654 | 0.0760 | 0.9246 | 0.0168 | 0.9413 | 0.0651 | 0.5517 | 0.8358 | 0.9202 | 56.1759 | 5 | 0.7113 | 0.7092 | 0.8368 | 0.9698 | 0.9352 | 0.8932 | 0.6965 | 0.1163 | 0.5008 | 0.7432 | 0.7741 | 3.0433 | 6.9850 | 5.0802 | 0.9474 | 0.6552 | 22.7485 | -62.9075 | 21.0681 | -70.4397 | 23.6500 | -65.5799 |
| 7 | $E_{HF}$ , $\chi_{HF}$ | 0.8632 | 0.0814 | 0.9288 | 0.0158 | 0.9446 | -0.0197 | 0.5362 | 0.8426 | 0.5892 | 59.6689 | 5 | 0.8816 | 0.8808 | 0.9331 | 0.9715 | 0.9343 | 0.9427 | 0.7817 | 0.0595 | 0.4565 | 0.6885 | 0.5553 | 2.8750 | 7.0999 | 2.0831 | 0.9533 | 0.6353 | 22.6467 | -63.7464 | 22.3072 | -68.0599 | 21.4049 | -67.6395 |
| 8 | $E_{B88}$ , $E^{HOMO}_{B88}$ | 0.8623 | 0.0853 | 0.9326 | 0.0150 | 0.9476 | 0.2249 | 0.5214 | 0.8453 | 0.5440 | 63.3035 | 5 | 0.8991 | 0.8984 | 0.9430 | 0.9731 | 0.9344 | 0.9553 | 0.7817 | 0.0631 | 0.4120 | 0.6302 | 0.4836 | 2.7186 | 7.1459 | 1.7754 | 0.9574 | 0.6811 | 22.2227 | -62.9682 | 21.0369 | -70.6898 | 23.3120 | -63.7170 |
| 9 | $E_{B88}$ , $E^{LUMO}_{B88}$ | 0.8612 | 0.0815 | 0.9262 | 0.0164 | 0.9426 | -0.0961 | 0.5456 | 0.8488 | 0.8722 | 57.5012 | 5 | 0.7407 | 0.7387 | 0.8534 | 0.9705 | 0.9333 | 0.8720 | 0.6925 | 0.1437 | 0.4027 | 0.6030 | 0.7259 | 2.9772 | 7.2047 | 4.5644 | 0.9526 | 0.6944 | 21.5767 | -67.4983 | 21.4183 | -68.9900 | 21.1444 | -66.5936 |
| 10 | $E_{HF}$ , $\eta_{HF}$ | 0.8597 | 0.0822 | 0.9254 | 0.0166 | 0.9420 | 0.0480 | 0.5488 | 0.8531 | 1.1388 | 56.7945 | 3 | 0.5579 | 0.5546 | 0.7501 | 0.9701 | 0.9327 | 0.8523 | 0.6695 | 0.1342 | 0.4924 | 0.7392 | 0.9910 | 3.0121 | 7.2780 | 7.7807 | 0.9495 | 0.6150 | 22.7995 | -63.2418 | 22.1783 | -73.5844 | 21.7160 | -66.0662 |
| 11 | $E_{HFX}$ , $\chi_{HFX}$ | 0.8486 | 0.0897 | 0.9208 | 0.0176 | 0.9384 | -0.0328 | 0.5654 | 0.8862 | 0.5563 | 53.3046 | 5 | 0.8945 | 0.8937 | 0.9404 | 0.9682 | 0.9274 | 0.9496 | 0.7888 | 0.0585 | 0.4469 | 0.6729 | 0.5339 | 3.1971 | 7.8541 | 1.8566 | 0.9490 | 0.6067 | 21.1746 | -64.9958 | 22.3567 | -67.8936 | 22.7263 | -61.2029 |
| 12 | $E_{HFX}$ , $\omega_{HFX}$ | 0.8471 | 0.0843 | 0.9118 | 0.0196 | 0.9314 | -0.0892 | 0.5966 | 0.8908 | 0.7243 | 47.5212 | 5 | 0.8212 | 0.8199 | 0.8989 | 0.9645 | 0.9259 | 0.9141 | 0.7271 | 0.0886 | 0.4797 | 0.7092 | 0.5765 | 3.5595 | 7.9359 | 3.1472 | 0.9412 | 0.4597 | 22.2852 | -66.8020 | 21.3160 | -68.6635 | 22.5408 | -63.4197 |
| 13 | $E_{B88}$ , $\eta_{B88}$ | 0.7856 | 0.1238 | 0.8835 | 0.0259 | 0.9094 | 0.0511 | 0.6858 | 1.0549 | 1.1478 | 35.1183 | 1 | 0.5509 | 0.5476 | 0.7461 | 0.9525 | 0.8968 | 0.8465 | 0.5636 | 0.1703 | 0.5870 | 0.8661 | 0.9898 | 4.7027 | 11.1276 | 7.9041 | 0.9225 | 0.4913 | 23.3746 | -62.0947 | 22.4306 | -68.1555 | 22.2886 | -64.8389 |
| 14 | $E_{HF}$ , $E^{LUMO}_{HF}$ | 0.7480 | 0.1427 | 0.8594 | 0.0312 | 0.8907 | -0.0977 | 0.7532 | 1.1435 | 1.2496 | 28.5148 | 0 | 0.4677 | 0.4638 | 0.6991 | 0.9422 | 0.8764 | 0.7363 | 0.5216 | 0.1981 | 0.5976 | 0.8857 | 1.0200 | 5.6727 | 13.0771 | 9.3684 | 0.9057 | 0.3073 | 23.9993 | -61.6300 | 21.5777 | -68.3425 | 21.8983 | -65.5037 |
| 15 | $E_{HFX}$ , $E^{LUMO}_{HFX}$ | 0.6597 | 0.2003 | 0.8200 | 0.0400 | 0.8600 | -0.0956 | 0.8523 | 1.3288 | 1.1782 | 21.5007 | 1 | 0.5267 | 0.5232 | 0.7325 | 0.9247 | 0.8328 | 0.7623 | 0.5506 | 0.1900 | 0.7038 | 1.0566 | 0.9473 | 7.2642 | 17.6565 | 8.3295 | 0.8847 | 0.1199 | 22.5905 | -62.4541 | 21.2489 | -71.6427 | 21.2575 | -65.9351 |

Models are arranged according to $Q^2_{LOO}$ values.

Parameters are obtained through QSARINS software. Ref. [54] N. Chirico, E. Papa, S. Kovarich, S. Cassani, P. Gramatica, QSAR Res. Unit in Environ. Chem. and Ecotox. University of Insubria, Varese, Italy, 2012. (http://www.qsar.it).

$R^2_{adj}$ adjusted $R^2$

*N. Ext.OK* Number of external validation parameters meeting threshold values

*F* "F-test" statistic value

**Table S14.** Value of internal and external validation parameters of two-descriptor QSAR models, for mutagenicity (LogTA98), developed using exchange (X) only (B88, HFX and HF) based methods through 30% (random) splitting method.

| Model | Variables | $Q^2_{LOO}$ | $R^2$-$Q^2_{LOO}$ | $R^2_{adj}$ | $R^2$-$R^2_{adj}$ | $R^2$ | $\Delta K$ | $RMSE_{TR}$ | $RMSE_{CV}$ | $RMSE_{EXT}$ | $F$ | N. Ext.OK | $Q^2_{F1}$ | $Q^2_{F2}$ | $Q^2_{F3}$ | $CCC_{TR}$ | $CCC_{CV}$ | $CCC_{EXT}$ | $\bar{r}^2_m$ | $\Delta r^2_m$ | $MAE_{TR}$ | $MAE_{CV}$ | $MAE_{EXT}$ | $RSS_{TR}$ | $PRESS_{CV}$ | $PRESS_{EXT}$ | $R^2_{LMO}$ | $Q^2_{LMO}$ | $R^2_{Yscr}$ | $Q^2_{Yscr}$ | $R^2_{Xrand}$ | $Q^2_{Xrand}$ | $R^2_{Yrand}$ | $Q^2_{Yrand}$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | $E_{HF}$, $E^{HOMO}_{HF}$ | 0.8963 | 0.0542 | 0.9363 | 0.0142 | 0.9505 | 0.3682 | 0.4562 | 0.6601 | 0.3709 | 67.1375 | 5 | 0.9643 | 0.9643 | 0.9672 | 0.9746 | 0.9469 | 0.9826 | 0.8863 | 0.0205 | 0.3858 | 0.5554 | 0.3024 | 2.0808 | 4.3567 | 0.6879 | 0.9541 | 0.7359 | 24.1909 | -56.6951 | 23.1834 | -66.5499 | 22.0206 | -61.7668 |
| 2 | $E_{HFX}$, $E^{HOMO}_{HFX}$ | 0.8917 | 0.0567 | 0.9336 | 0.0147 | 0.9484 | 0.3799 | 0.4656 | 0.6744 | 0.3785 | 64.3175 | 5 | 0.9629 | 0.9628 | 0.9659 | 0.9735 | 0.9445 | 0.9820 | 0.8824 | 0.0220 | 0.3936 | 0.5671 | 0.3204 | 2.1674 | 4.5480 | 0.7163 | 0.9532 | 0.7187 | 22.9371 | -58.4484 | 22.9182 | -67.8165 | 22.4006 | -60.0329 |
| 3 | $E_{HF}$, $\chi_{HF}$ | 0.8878 | 0.0613 | 0.9346 | 0.0145 | 0.9491 | 0.1252 | 0.4623 | 0.6865 | 0.5594 | 65.2636 | 5 | 0.9189 | 0.9188 | 0.9255 | 0.9739 | 0.9425 | 0.9622 | 0.8140 | 0.0475 | 0.3916 | 0.5698 | 0.4661 | 2.1376 | 4.7127 | 1.5648 | 0.9543 | 0.7698 | 23.3206 | -60.1189 | 22.7955 | -65.2709 | 21.4112 | -64.5934 |
| 4 | $E_{HFex}$, $\chi_{HFX}$ | 0.8828 | 0.0651 | 0.9329 | 0.0149 | 0.9478 | 0.0850 | 0.4681 | 0.7017 | 0.5502 | 63.5912 | 5 | 0.9215 | 0.9215 | 0.9279 | 0.9732 | 0.9398 | 0.9644 | 0.8144 | 0.0461 | 0.3842 | 0.5617 | 0.4720 | 2.1908 | 4.9239 | 1.5138 | 0.9532 | 0.7186 | 21.9321 | -61.7354 | 22.2159 | -66.3975 | 21.5205 | -63.3489 |
| 5 | $E_{B88}$, $E^{HOMO}_{B88}$ | 0.8826 | 0.0636 | 0.9309 | 0.0154 | 0.9462 | 0.4568 | 0.4752 | 0.7021 | 0.3764 | 61.5797 | 5 | 0.9633 | 0.9633 | 0.9663 | 0.9724 | 0.9393 | 0.9815 | 0.9066 | 0.0203 | 0.3923 | 0.5776 | 0.3068 | 2.2586 | 4.9299 | 0.7084 | 0.9525 | 0.7535 | 22.0475 | -61.2091 | 21.5975 | -69.0357 | 22.1889 | -61.8658 |
| 6 | $E_{B88}$, $\chi_{B88}$ | 0.8802 | 0.0670 | 0.9322 | 0.0151 | 0.9472 | 0.1505 | 0.4707 | 0.7092 | 0.4902 | 62.8406 | 5 | 0.9377 | 0.9377 | 0.9428 | 0.9729 | 0.9382 | 0.9702 | 0.8392 | 0.0358 | 0.4140 | 0.6134 | 0.4079 | 2.2156 | 5.0293 | 1.2016 | 0.9537 | 0.7526 | 20.9841 | -66.8600 | 23.0754 | -66.5819 | 21.6673 | -65.8154 |
| 7 | $E_{HFX}$, $\eta_{HFX}$ | 0.8692 | 0.0586 | 0.9073 | 0.0206 | 0.9279 | 0.0936 | 0.5504 | 0.7411 | 0.4529 | 45.0176 | 5 | 0.9469 | 0.9468 | 0.9512 | 0.9626 | 0.9327 | 0.9716 | 0.9356 | 0.0264 | 0.4143 | 0.5841 | 0.3548 | 3.0295 | 5.4920 | 1.0255 | 0.9299 | 0.6286 | 21.2630 | -65.4999 | 22.0305 | -68.3950 | 21.7036 | -63.0758 |
| 8 | $E_{HF}$, $\eta_{HF}$ | 0.8529 | 0.0661 | 0.8958 | 0.0232 | 0.9190 | 0.0880 | 0.5834 | 0.7860 | 0.4285 | 39.6891 | 5 | 0.9524 | 0.9524 | 0.9563 | 0.9578 | 0.9243 | 0.9748 | 0.9427 | 0.0264 | 0.4664 | 0.6553 | 0.3259 | 3.4033 | 6.1775 | 0.9182 | 0.9224 | 0.5815 | 22.9847 | -62.0211 | 21.9714 | -69.1585 | 22.7891 | -61.6714 |
| 9 | $E_{HF}$, $\omega_{HF}$ | 0.8515 | 0.0852 | 0.9186 | 0.0181 | 0.9367 | -0.0072 | 0.5156 | 0.7898 | 0.7370 | 51.7953 | 5 | 0.8592 | 0.8591 | 0.8707 | 0.9673 | 0.9241 | 0.9375 | 0.7525 | 0.0765 | 0.4329 | 0.6448 | 0.6180 | 2.6582 | 6.2381 | 2.7159 | 0.9454 | 0.5902 | 21.8853 | -64.0207 | 23.2411 | -67.2532 | 21.7012 | -63.4208 |
| 10 | $E_{B88}$, $\eta_{B88}$ | 0.8478 | 0.0651 | 0.8880 | 0.0249 | 0.9129 | 0.0973 | 0.6047 | 0.7995 | 0.5561 | 36.6929 | 5 | 0.9199 | 0.9198 | 0.9264 | 0.9545 | 0.9206 | 0.9557 | 0.8823 | 0.0526 | 0.4451 | 0.6112 | 0.4586 | 3.6570 | 6.3916 | 1.5464 | 0.9167 | 0.5958 | 22.0327 | -61.6641 | 21.7324 | -69.8288 | 22.1344 | -61.1897 |
| 11 | $E_{HFX}$, $\omega_{HFX}$ | 0.8367 | 0.0969 | 0.9146 | 0.0190 | 0.9336 | -0.0331 | 0.5282 | 0.8282 | 0.7644 | 49.1755 | 5 | 0.8486 | 0.8485 | 0.8609 | 0.9656 | 0.9166 | 0.9364 | 0.7479 | 0.0763 | 0.4338 | 0.6523 | 0.6560 | 2.7904 | 6.8594 | 2.9218 | 0.9441 | 0.6665 | 21.0764 | -65.4603 | 21.8851 | -69.6489 | 22.5857 | -61.8280 |
| 12 | $E_{B88}$, $E^{LUMO}_{B88}$ | 0.8252 | 0.1027 | 0.9073 | 0.0206 | 0.9279 | -0.0376 | 0.5503 | 0.8569 | 0.8481 | 45.0298 | 5 | 0.8136 | 0.8135 | 0.8287 | 0.9626 | 0.9103 | 0.9178 | 0.6996 | 0.0959 | 0.4535 | 0.6887 | 0.6620 | 3.0288 | 7.3430 | 3.5961 | 0.9380 | 0.5603 | 21.8862 | -69.8507 | 23.5395 | -63.3053 | 22.1350 | -67.1439 |
| 13 | $E_{HF}$, $E^{LUMO}_{HF}$ | 0.7377 | 0.1493 | 0.8547 | 0.0323 | 0.8870 | -0.0551 | 0.6889 | 1.0495 | 1.1018 | 27.4691 | 2 | 0.6854 | 0.6852 | 0.7110 | 0.9401 | 0.8652 | 0.8630 | 0.6254 | 0.1425 | 0.5701 | 0.8325 | 0.8985 | 4.7462 | 11.0150 | 6.0694 | 0.8992 | 0.4532 | 21.4773 | -65.7349 | 21.1768 | -66.4496 | 21.2866 | -65.3895 |
| 14 | $E_{B88}$, $\omega_{B88}$ | 0.7064 | 0.1812 | 0.8556 | 0.0321 | 0.8877 | -0.0585 | 0.6869 | 1.1103 | 1.1413 | 27.6559 | 1 | 0.6624 | 0.6622 | 0.6898 | 0.9405 | 0.8521 | 0.8584 | 0.5974 | 0.1467 | 0.5533 | 0.8595 | 0.9116 | 4.7177 | 12.3286 | 6.5130 | 0.9000 | 0.3259 | 20.3550 | -71.7720 | 20.7038 | -71.0775 | 23.5845 | -62.1699 |
| 15 | $E_{HFX}$, $E^{LUMO}_{HFX}$ | 0.6636 | 0.2161 | 0.8454 | 0.0344 | 0.8797 | -0.0646 | 0.7107 | 1.1886 | 1.1444 | 25.5999 | 1 | 0.6606 | 0.6604 | 0.6882 | 0.9360 | 0.8308 | 0.8611 | 0.6205 | 0.1432 | 0.5916 | 0.9281 | 0.9512 | 5.0511 | 14.1276 | 6.5482 | 0.8998 | 0.2864 | 23.0206 | -63.1027 | 22.8256 | -63.6073 | 23.8703 | -63.1084 |

Models are arranged according to $Q^2_{LOO}$ values.

Parameters are obtained through QSARINS software. Ref. [54] N. Chirico, E. Papa, S. Kovarich, S. Cassani, P. Gramatica, QSAR Res. Unit in Environ. Chem. and Ecotox. University of Insubria, Varese, Italy, 2012. (http://www.qsar.it).

$R^2_{adj}$ adjusted $R^2$

*N. Ext.OK* Number of external validation parameters meeting threshold values

*F* "F-test" statistic value

**Table S15.** Value of internal and external validation parameters of two-descriptor QSAR models, for mutagenicity (LogTA100), developed using exchange-correlation (HFX+LYP, BLYP and B3LYP) based methods through activity sampling (ordered response) splitting method.

| Model | Variables | $Q^2_{LOO}$ | $R^2$-$Q^2_{LOO}$ | $R^2_{adj}$ | $R^2$-$R^2_{adj}$ | $R^2$ | $\Delta K$ | $RMSE_{TR}$ | $RMSE_{CV}$ | $RMSE_{EXT}$ | *N. Ext.OK* | $Q^2_{F1}$ | $Q^2_{F2}$ | $Q^2_{F3}$ | $CCC_{TR}$ | $CCC_{CV}$ | $CCC_{EXT}$ | $\overline{r}_m^2$ | $\Delta r_m^2$ | $MAE_{TR}$ | $MAE_{CV}$ | $MAE_{EXT}$ | $RSS_{TR}$ | $PRESS_{CV}$ | $PRESS_{EXT}$ | $R^2_{LMO}$ | $Q^2_{LMO}$ | $R^2_{Yscr}$ | $Q^2_{Yscr}$ | $R^2_{Xrand}$ | $Q^2_{Xrand}$ | $R^2_{Yrand}$ | $Q^2_{Yrand}$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | $E_{HFX+LYP}$, $E^{HOMO}_{HFX+LYP}$ | 0.7102 | 0.0643 | 0.7520 | 0.0225 | 0.7746 | 0.4233 | 0.8398 | 0.9521 | 0.8344 | 5 | 0.7461 | 0.7461 | 0.7775 | 0.8730 | 0.8382 | 0.8787 | 0.7054 | 0.0851 | 0.6806 | 0.7819 | 0.6753 | 16.2222 | 20.8512 | 15.3153 | 0.7775 | 0.6160 | 9.0839 | -20.9894 | 9.2415 | -20.3120 | 8.8312 | -21.1261 |
| 2 | $E_{HFX+LYP}$, $\eta_{HFX+LYP}$ | 0.6867 | 0.0866 | 0.7506 | 0.0227 | 0.7733 | 0.2414 | 0.8422 | 0.9900 | 0.8964 | 5 | 0.7069 | 0.7069 | 0.7432 | 0.8721 | 0.8266 | 0.8583 | 0.6895 | 0.0966 | 0.6402 | 0.7470 | 0.7482 | 16.3144 | 22.5441 | 17.6789 | 0.7765 | 0.5693 | 9.1633 | -20.9206 | 8.5543 | -21.5851 | 8.8513 | -21.2185 |
| 3 | $E_{HFX+LYP}$, $\chi_{HFX+LYP}$ | 0.6745 | 0.0769 | 0.7265 | 0.0249 | 0.7514 | 0.1945 | 0.8819 | 1.0092 | 0.8557 | 5 | 0.7330 | 0.7330 | 0.7660 | 0.8581 | 0.8164 | 0.8719 | 0.6747 | 0.0864 | 0.7212 | 0.8306 | 0.6924 | 17.8894 | 23.4237 | 16.1075 | 0.7563 | 0.5868 | 9.6330 | -20.2007 | 9.3072 | -20.3673 | 8.8481 | -21.5107 |
| 4 | $E_{BLYP}$, $\chi_{BLYP}$ | 0.6442 | 0.0838 | 0.7008 | 0.0272 | 0.7280 | 0.0973 | 0.9225 | 1.0551 | 0.9294 | 2 | 0.6850 | 0.6849 | 0.7239 | 0.8426 | 0.7974 | 0.8519 | 0.6123 | 0.0918 | 0.7629 | 0.8786 | 0.7800 | 19.5737 | 25.6021 | 19.0037 | 0.7308 | 0.5560 | 8.2667 | -22.2341 | 9.2662 | -20.4744 | 9.0706 | -20.9955 |
| 5 | $E_{BLYP}$, $E^{HOMO}_{BLYP}$ | 0.6359 | 0.0938 | 0.7027 | 0.0270 | 0.7297 | 0.2344 | 0.9196 | 1.0674 | 0.9313 | 2 | 0.6837 | 0.6837 | 0.7228 | 0.8437 | 0.7934 | 0.8530 | 0.6145 | 0.0917 | 0.7517 | 0.8725 | 0.7828 | 19.4509 | 26.2039 | 19.0805 | 0.7346 | 0.5412 | 8.7711 | -21.1473 | 8.8202 | -21.2763 | 8.4491 | -21.7246 |
| 6 | $E_{HFX+LYP}$, $\omega_{HFX+LYP}$ | 0.6340 | 0.0842 | 0.6900 | 0.0282 | 0.7182 | 0.0040 | 0.9390 | 1.0701 | 0.9185 | 1 | 0.6923 | 0.6923 | 0.7304 | 0.8360 | 0.7897 | 0.8478 | 0.6205 | 0.0933 | 0.7612 | 0.8726 | 0.7580 | 20.2798 | 26.3393 | 18.5600 | 0.7192 | 0.5506 | 9.6501 | -20.1649 | 8.7927 | -21.1156 | 8.9105 | -21.5348 |
| 7 | $E_{B3LYP}$, $E^{LUMO}_{B3LYP}$ | 0.6212 | 0.0786 | 0.6698 | 0.0300 | 0.6998 | 0.0066 | 0.9691 | 1.0887 | 0.9832 | 0 | 0.6475 | 0.6474 | 0.6910 | 0.8234 | 0.7783 | 0.8203 | 0.5891 | 0.1029 | 0.7415 | 0.8391 | 0.8079 | 21.6027 | 27.2612 | 21.2657 | 0.7047 | 0.4927 | 9.4259 | -20.9756 | 9.1074 | -20.7971 | 9.4459 | -20.8007 |
| 8 | $E_{B3LYP}$, $\chi_{B3LYP}$ | 0.6174 | 0.0872 | 0.6751 | 0.0295 | 0.7046 | 0.0943 | 0.9614 | 1.0941 | 0.9969 | 0 | 0.6376 | 0.6375 | 0.6823 | 0.8267 | 0.7800 | 0.8320 | 0.5857 | 0.0998 | 0.8262 | 0.9494 | 0.8564 | 21.2566 | 27.5318 | 21.8647 | 0.7079 | 0.5223 | 8.9350 | -21.0976 | 8.9309 | -20.9682 | 9.3311 | -20.6773 |
| 9 | $E_{BLYP}$, $E^{LUMO}_{BLYP}$ | 0.6070 | 0.0930 | 0.6700 | 0.0300 | 0.7000 | -0.0065 | 0.9688 | 1.1088 | 0.9637 | 1 | 0.6613 | 0.6613 | 0.7032 | 0.8236 | 0.7717 | 0.8324 | 0.5897 | 0.0976 | 0.7906 | 0.9079 | 0.7992 | 21.5852 | 28.2782 | 20.4313 | 0.7061 | 0.5061 | 8.8386 | -21.4346 | 8.9275 | -21.4680 | 9.6972 | -20.2766 |
| 10 | $E_{B3LYP}$, $\omega_{B3LYP}$ | 0.5935 | 0.0860 | 0.6474 | 0.0321 | 0.6795 | 0.0847 | 1.0014 | 1.1277 | 1.0363 | 0 | 0.6083 | 0.6083 | 0.6567 | 0.8091 | 0.7625 | 0.7897 | 0.5586 | 0.1096 | 0.7666 | 0.8867 | 0.8516 | 23.0659 | 29.2514 | 23.6283 | 0.6772 | 0.4773 | 9.2834 | -29.2417 | 9.4739 | -20.4226 | 8.7891 | -29.2942 |
| 11 | $E_{B3LYP}$, $E^{HOMO}_{B3LYP}$ | 0.5756 | 0.0981 | 0.6411 | 0.0326 | 0.6738 | 0.2485 | 1.0103 | 1.1523 | 1.0680 | 0 | 0.5840 | 0.5840 | 0.6354 | 0.8051 | 0.7512 | 0.8055 | 0.5449 | 0.1073 | 0.8489 | 0.9764 | 0.9253 | 23.4767 | 30.5376 | 25.0934 | 0.6797 | 0.4585 | 9.3052 | -21.0522 | 9.6978 | -20.2786 | 9.3429 | -21.0456 |
| 12 | $E_{BLYP}$, $\omega_{BLYP}$ | 0.5573 | 0.0854 | 0.6069 | 0.0357 | 0.6426 | 0.0078 | 1.0574 | 1.1769 | 1.0841 | 0 | 0.5714 | 0.5713 | 0.6243 | 0.7824 | 0.7298 | 0.7680 | 0.5272 | 0.1135 | 0.8260 | 0.9292 | 0.8941 | 25.7155 | 31.8579 | 25.8565 | 0.6457 | 0.4365 | 8.5693 | -22.7165 | 9.3737 | -20.0531 | 9.1412 | -21.2872 |
| 13 | $E_{HFX+LYP}$, $E^{LUMO}_{HFX+LYP}$ | 0.5289 | 0.1074 | 0.5999 | 0.0364 | 0.6363 | -0.0372 | 1.0667 | 1.2140 | 1.1115 | 0 | 0.5494 | 0.5494 | 0.6051 | 0.7777 | 0.7141 | 0.7681 | 0.5064 | 0.1134 | 0.8464 | 0.9712 | 0.9084 | 26.1716 | 33.8989 | 27.1818 | 0.6420 | 0.4090 | 8.6417 | -22.3318 | 9.0061 | -20.9481 | 8.5792 | -22.2710 |
| 14 | $E_{B3LYP}$, $\eta_{B3LYP}$ | 0.4939 | 0.1350 | 0.5917 | 0.0371 | 0.6289 | 0.2795 | 1.0776 | 1.2584 | 1.1653 | 0 | 0.5048 | 0.5047 | 0.5660 | 0.7721 | 0.6953 | 0.7511 | 0.4819 | 0.1179 | 0.8951 | 1.0462 | 0.9849 | 26.7071 | 36.4215 | 29.8745 | 0.6352 | 0.3820 | 9.3319 | -21.6752 | 8.9937 | -20.8505 | 9.8314 | -20.4240 |
| 15 | $E_{BLYP}$, $\eta_{BLYP}$ | 0.4165 | 0.2857 | 0.6724 | 0.0298 | 0.7022 | 0.2848 | 0.9653 | 1.3511 | 0.9938 | 0 | 0.6399 | 0.6398 | 0.6844 | 0.8251 | 0.6809 | 0.8300 | 0.5849 | 0.1003 | 0.7574 | 0.9498 | 0.8538 | 21.4295 | 41.9882 | 21.7263 | 0.7278 | 0.4099 | 9.3087 | -22.1177 | 8.6959 | -21.4791 | 9.2233 | -22.2913 |

Models are arranged according to $Q^2_{LOO}$ values.

Parameters are obtained through QSARINS software. Ref. [54] N. Chirico, E. Papa, S. Kovarich, S. Cassani, P. Gramatica, QSAR Res. Unit in Environ. Chem. and Ecotox. University of Insubria, Varese, Italy, 2012. (http://www.qsar.it).

$R^2_{adj}$ adjusted $R^2$

*N. Ext.OK* Number of external validation parameters meeting threshold values

*F* "F-test" statistic value

**Table S16.** Value of internal and external validation parameters of two-descriptor QSAR models, for mutagenicity (LogTA100), developed using exchange-correlation (HFX+LYP, BLYP and B3LYP) based methods through 30% (random) splitting method.

| Model | Variables | $Q^2_{LOO}$ | $R^2$-$Q^2_{LOO}$ | $R^2_{adj}$ | $R^2$-$R^2_{adj}$ | $R^2$ | $\Delta K$ | $RMSE_{TR}$ | $RMSE_{CV}$ | $RMSE_{EXT}$ | $F$ | *N. Ext.OK* | $Q^2_{F1}$ | $Q^2_{F2}$ | $Q^2_{F3}$ | $CCC_{TR}$ | $CCC_{CV}$ | $CCC_{EXT}$ | $\bar{r}^2_m$ | $\Delta r^2_m$ | $MAE_{TR}$ | $MAE_{CV}$ | $MAE_{EXT}$ | $RSS_{TR}$ | $PRESS_{CV}$ | $PRESS_{EXT}$ | $R^2_{LMO}$ | $Q^2_{LMO}$ | $R^2_{Yscr}$ | $Q^2_{Yscr}$ | $R^2_{Xrand}$ | $Q^2_{Xrand}$ | $R^2_{Yrand}$ | $Q^2_{Yrand}$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | $E_{BLYP}$ , $\eta_{BLYP}$ | 0.7206 | 0.0530 | 0.7599 | 0.0137 | 0.7736 | 0.1968 | 0.8259 | 0.9175 | 1.6134 | 56.3837 | 0 | 0.0765 | 0.0764 | 0.1360 | 0.8724 | 0.8452 | 0.5029 | 0.1946 | 0.0069 | 0.6561 | 0.7241 | 1.0737 | 24.5558 | 30.3053 | 23.4282 | 0.7774 | 0.7090 | 5.7280 | -12.5098 | 5.8243 | -12.2167 | 5.7656 | -12.3989 |
| 2 | $E_{HFX+LYP}$ , $\eta_{HFX+LYP}$ | 0.7193 | 0.0512 | 0.7566 | 0.0139 | 0.7705 | 0.2638 | 0.8316 | 0.9197 | 0.6273 | 55.3960 | 5 | 0.8604 | 0.8604 | 0.8694 | 0.8704 | 0.8443 | 0.9200 | 0.7929 | 0.0358 | 0.6715 | 0.7382 | 0.5216 | 24.8932 | 30.4511 | 3.5417 | 0.7758 | 0.6967 | 5.8044 | -12.3388 | 5.5544 | -12.5512 | 5.9020 | -12.4195 |
| 3 | $E_{HFX+LYP}$, $E^{HOMO}_{HFX+LYP}$ | 0.7181 | 0.0472 | 0.7511 | 0.0142 | 0.7653 | 0.3512 | 0.8409 | 0.9215 | 0.6402 | 53.8078 | 5 | 0.8546 | 0.8546 | 0.8640 | 0.8671 | 0.8427 | 0.9196 | 0.7642 | 0.0424 | 0.6758 | 0.7404 | 0.4998 | 25.4555 | 30.5727 | 3.6886 | 0.7684 | 0.6975 | 5.7730 | -12.4151 | 5.7259 | -12.3442 | 5.9728 | -12.1645 |
| 4 | $E_{BLYP}$, $E^{HOMO}_{BLYP}$ | 0.6855 | 0.0526 | 0.7222 | 0.0159 | 0.7381 | 0.2347 | 0.8884 | 0.9735 | 1.0451 | 46.4957 | 0 | 0.6125 | 0.6125 | 0.6375 | 0.8493 | 0.8217 | 0.7693 | 0.5721 | 0.0488 | 0.7156 | 0.7842 | 0.7857 | 28.4102 | 34.1162 | 9.8295 | 0.7413 | 0.6640 | 5.4992 | -12.8002 | 5.9906 | -12.1287 | 5.9231 | -12.0892 |
| 5 | $E_{HFX+LYP}$ , $\chi_{HFX+LYP}$ | 0.6813 | 0.0523 | 0.7174 | 0.0161 | 0.7336 | 0.0715 | 0.8960 | 0.9800 | 0.6828 | 45.4273 | 5 | 0.8346 | 0.8346 | 0.8453 | 0.8463 | 0.8190 | 0.9066 | 0.7596 | 0.0483 | 0.7195 | 0.7876 | 0.5311 | 28.9003 | 34.5720 | 4.1958 | 0.7386 | 0.6619 | 5.7890 | -12.4175 | 5.7839 | -12.2668 | 5.8909 | -12.3150 |
| 6 | $E_{BLYP}$ , $\chi_{BLYP}$ | 0.6622 | 0.0548 | 0.6999 | 0.0171 | 0.7171 | 0.0414 | 0.9233 | 1.0088 | 0.8912 | 41.8221 | 4 | 0.7183 | 0.7182 | 0.7364 | 0.8352 | 0.8061 | 0.8298 | 0.7062 | 0.0859 | 0.7464 | 0.8161 | 0.6945 | 30.6868 | 36.6352 | 7.1477 | 0.7218 | 0.6396 | 6.2234 | -11.7809 | 5.6540 | -12.4897 | 5.6782 | -12.3711 |
| 7 | $E_{B3LYP}$ , $\chi_{B3LYP}$ | 0.6363 | 0.0560 | 0.6737 | 0.0186 | 0.6923 | 0.0578 | 0.9628 | 1.0468 | 0.9086 | 37.1276 | 4 | 0.7071 | 0.7071 | 0.7260 | 0.8182 | 0.7883 | 0.8268 | 0.6696 | 0.0890 | 0.7982 | 0.8710 | 0.7412 | 33.3731 | 39.4516 | 7.4307 | 0.6973 | 0.6153 | 6.0531 | -12.2267 | 6.0337 | -12.0689 | 5.5223 | -12.7575 |
| 8 | $E_{HFX+LYP}$ , $\omega_{HFX+LYP}$ | 0.6310 | 0.0565 | 0.6686 | 0.0189 | 0.6875 | -0.0912 | 0.9703 | 1.0544 | 0.7216 | 36.3037 | 5 | 0.8153 | 0.8152 | 0.8272 | 0.8148 | 0.7845 | 0.8910 | 0.7794 | 0.0547 | 0.7965 | 0.8678 | 0.5480 | 33.8938 | 40.0212 | 4.6864 | 0.6930 | 0.6056 | 5.7669 | -12.3057 | 5.6544 | -12.5262 | 5.9757 | -12.3540 |
| 9 | $E_{B3LYP}$, $E^{HOMO}_{B3LYP}$ | 0.6157 | 0.0591 | 0.6550 | 0.0197 | 0.6747 | 0.2897 | 0.9900 | 1.0761 | 1.0253 | 34.2262 | 0 | 0.6271 | 0.6270 | 0.6511 | 0.8058 | 0.7736 | 0.7724 | 0.6125 | 0.1103 | 0.8241 | 0.8987 | 0.8221 | 35.2820 | 41.6890 | 9.4610 | 0.6789 | 0.5937 | 5.4405 | -13.0584 | 5.4296 | -12.6781 | 5.8064 | -12.3999 |
| 10 | $E_{BLYP}$, $E^{LUMO}_{BLYP}$ | 0.6063 | 0.0617 | 0.6480 | 0.0201 | 0.6681 | -0.0932 | 1.0000 | 1.0891 | 0.7427 | 33.2104 | 5 | 0.8043 | 0.8043 | 0.8169 | 0.8010 | 0.7676 | 0.8802 | 0.7981 | 0.0545 | 0.8177 | 0.8915 | 0.5847 | 36.0030 | 42.7007 | 4.9642 | 0.6737 | 0.5759 | 5.9042 | -12.3315 | 5.7791 | -12.2880 | 5.7610 | -12.2556 |
| 11 | $E_{B3LYP}$, $E^{LUMO}_{B3LYP}$ | 0.5835 | 0.0639 | 0.6260 | 0.0214 | 0.6474 | -0.0971 | 1.0307 | 1.1203 | 0.7204 | 30.2957 | 5 | 0.8159 | 0.8158 | 0.8277 | 0.7860 | 0.7509 | 0.8855 | 0.8213 | 0.0432 | 0.8410 | 0.9157 | 0.5506 | 38.2454 | 45.1815 | 4.6713 | 0.6490 | 0.5710 | 5.6929 | -12.4902 | 5.6884 | -12.4562 | 5.4763 | -12.8388 |
| 12 | $E_{B3LYP}$ , $\omega_{B3LYP}$ | 0.5412 | 0.0696 | 0.5872 | 0.0236 | 0.6108 | -0.0681 | 1.0829 | 1.1757 | 0.7637 | 25.8964 | 5 | 0.7931 | 0.7931 | 0.8064 | 0.7584 | 0.7203 | 0.8625 | 0.8768 | 0.0323 | 0.8871 | 0.9670 | 0.5611 | 42.2140 | 49.7654 | 5.2489 | 0.6135 | 0.5165 | 5.6379 | -13.0705 | 5.4357 | -12.7487 | 5.7049 | -12.7142 |
| 13 | $E_{BLYP}$ , $\omega_{BLYP}$ | 0.5262 | 0.0686 | 0.5703 | 0.0246 | 0.5949 | -0.1342 | 1.1048 | 1.1948 | 0.7517 | 24.2270 | 5 | 0.7995 | 0.7995 | 0.8124 | 0.7460 | 0.7070 | 0.8800 | 0.7590 | 0.0507 | 0.8894 | 0.9648 | 0.5735 | 43.9443 | 51.3906 | 5.0859 | 0.5993 | 0.4986 | 5.9825 | -12.4072 | 5.5046 | -12.5163 | 5.8950 | -12.3335 |
| 14 | $E_{B3LYP}$ , $\eta_{B3LYP}$ | 0.5208 | 0.0926 | 0.5900 | 0.0234 | 0.6135 | 0.1973 | 1.0792 | 1.2015 | 1.1270 | 26.1864 | 0 | 0.5494 | 0.5494 | 0.5785 | 0.7604 | 0.7094 | 0.6925 | 0.5371 | 0.0031 | 0.9060 | 0.9981 | 0.8760 | 41.9272 | 51.9724 | 11.4303 | 0.6226 | 0.5008 | 5.7097 | -12.6794 | 5.6244 | -12.6333 | 6.1563 | -12.1235 |
| 15 | $E_{HFX+LYP}$, $E^{LUMO}_{HFX+LYP}$ | 0.5022 | 0.0754 | 0.5521 | 0.0256 | 0.5777 | -0.1044 | 1.1280 | 1.2246 | 0.9171 | 22.5702 | 4 | 0.7016 | 0.7016 | 0.7208 | 0.7323 | 0.6891 | 0.7904 | 0.7816 | 0.0381 | 0.9238 | 1.0038 | 0.7075 | 45.8078 | 53.9915 | 7.5698 | 0.5823 | 0.4722 | 5.4644 | -13.1121 | 5.4830 | -12.8185 | 5.5700 | -12.9921 |

Models are arranged according to $Q^2_{LOO}$ values.
Parameters are obtained through QSARINS software. Ref. [54] N. Chirico, E. Papa, S. Kovarich, S. Cassani, P. Gramatica, QSAR Res. Unit in Environ. Chem. and Ecotox. University of Insubria, Varese, Italy, 2012. (http://www.qsar.it).

$R^2_{adj}$ adjusted $R^2$

*N. Ext.OK* Number of external validation parameters meeting threshold values

*F* "F-test" statistic value

Table S17. Value of internal and external validation parameters of two-descriptor QSAR models, for mutagenicity (LogTA100), developed using meta exchange-correlation functionals (M06, M06-L and M06-2X) based methods through activity sampling (ordered response) splitting method.

| Model | Variables | $Q^2_{LOO}$ | $R^2$-$Q^2_{LOO}$ | $R^2_{adj}$ | $R^2$-$R^2_{adj}$ | $R^2$ | $\Delta K$ | $RMSE_{TR}$ | $RMSE_{CV}$ | $RMSE_{EXT}$ | $F$ | N. Ext.OK | $Q^2_{F1}$ | $Q^2_{F2}$ | $Q^2_{F3}$ | $CCC_{TR}$ | $CCC_{CV}$ | $CCC_{EXT}$ | $\bar{r}^2_m$ | $\Delta r^2_m$ | $MAE_{TR}$ | $MAE_{CV}$ | $MAE_{EXT}$ | $RSS_{TR}$ | $PRESS_{CV}$ | $PRESS_{EXT}$ | $R^2_{LMO}$ | $Q^2_{LMO}$ | $R^2_{Yscr}$ | $Q^2_{Yscr}$ | $R^2_{Xrand}$ | $Q^2_{Xrand}$ | $R^2_{Yrand}$ | $Q^2_{Yrand}$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | $E_{M06-L}, E^{LUMO}_{M06-L}$ | 0.6061 | 0.1087 | 0.6863 | 0.0285 | 0.7148 | -0.1507 | 0.9477 | 1.1138 | 0.8564 | 25.0673 | 3 | 0.704 | 0.6948 | 0.7671 | 0.8337 | 0.7767 | 0.85 | 0.6734 | 0.0428 | 0.7993 | 0.9312 | 0.6423 | 20.6559 | 28.5327 | 14.6669 | 0.7156 | 0.5170 | 8.9048 | -21.3705 | 9.0194 | -20.6567 | 8.8857 | -21.1523 |
| 2 | $E_{M06-2X}, \omega_{M06-2X}$ | 0.5977 | 0.1046 | 0.6726 | 0.0298 | 0.7024 | -0.142 | 0.9682 | 1.1256 | 0.9098 | 23.5971 | 1 | 0.6659 | 0.6555 | 0.7372 | 0.8252 | 0.769 | 0.8243 | 0.6243 | 0.0471 | 0.7889 | 0.9146 | 0.7072 | 21.5598 | 29.1392 | 16.5556 | 0.7070 | 0.5029 | 8.9929 | -21.1497 | 9.034 | -20.8322 | 9.1942 | -21.1689 |
| 3 | $E_{M06}, E^{LUMO}_{M06}$ | 0.5889 | 0.1087 | 0.6673 | 0.0302 | 0.6976 | -0.148 | 0.9759 | 1.1379 | 0.8737 | 23.0655 | 1 | 0.6919 | 0.6823 | 0.7576 | 0.8218 | 0.7634 | 0.8367 | 0.6478 | 0.0861 | 0.8052 | 0.9341 | 0.6765 | 21.9064 | 29.7801 | 15.2679 | 0.6998 | 0.5108 | 9.063 | -20.7371 | 8.9168 | -21.0906 | 9.1405 | -20.9918 |
| 4 | $E_{M06-2X}, \chi_{M06-2X}$ | 0.5591 | 0.118 | 0.6448 | 0.0323 | 0.6771 | -0.0466 | 1.0084 | 1.1784 | 0.7806 | 20.9716 | 5 | 0.7541 | 0.7464 | 0.8065 | 0.8075 | 0.746 | 0.8679 | 0.7086 | 0.0291 | 0.8636 | 1.0032 | 0.6148 | 23.3874 | 31.9369 | 12.1875 | 0.6840 | 0.4634 | 8.8934 | -21.4506 | 9.3654 | -20.5769 | 9.0199 | -21.3408 |
| 5 | $E_{M06-2X}, E^{LUMO}_{M06-2X}$ | 0.5569 | 0.1123 | 0.6361 | 0.0331 | 0.6692 | -0.1455 | 1.0207 | 1.1813 | 0.8955 | 20.2279 | 1 | 0.6763 | 0.6663 | 0.7454 | 0.8018 | 0.74 | 0.8157 | 0.6138 | 0.1117 | 0.8199 | 0.947 | 0.6872 | 23.9628 | 32.0982 | 16.0391 | 0.6733 | 0.4473 | 9.2154 | -20.9118 | 9.3731 | -20.6479 | 9.0196 | -21.3004 |
| 6 | $E_{M06}, \chi_{M06}$ | 0.5565 | 0.1201 | 0.6443 | 0.0323 | 0.6766 | -0.0468 | 1.0092 | 1.1818 | 0.7807 | 20.9211 | 5 | 0.754 | 0.7463 | 0.8065 | 0.8071 | 0.745 | 0.8693 | 0.7113 | 0.0119 | 0.8653 | 1.0077 | 0.6071 | 23.4256 | 32.1243 | 12.1909 | 0.6802 | 0.4656 | 8.912 | -21.6633 | 9.0612 | -20.9569 | 9.1491 | -21.0229 |
| 7 | $E_{M06}, \omega_{M06}$ | 0.5391 | 0.1182 | 0.6231 | 0.0343 | 0.6573 | -0.1084 | 1.0388 | 1.2047 | 0.9293 | 19.1839 | 1 | 0.6515 | 0.6406 | 0.7258 | 0.7933 | 0.7306 | 0.789 | 0.582 | 0.0629 | 0.8344 | 0.9684 | 0.7034 | 24.82 | 33.3823 | 17.2711 | 0.6630 | 0.4273 | 8.9816 | -21.9561 | 9.6895 | -19.909 | 9.2673 | -21.1627 |
| 8 | $E_{M06-L}, \chi_{M06-L}$ | 0.5193 | 0.126 | 0.6099 | 0.0355 | 0.6454 | -0.0467 | 1.0568 | 1.2304 | 0.7946 | 18.197 | 5 | 0.7452 | 0.7372 | 0.7995 | 0.7845 | 0.7174 | 0.8591 | 0.6963 | 0.0024 | 0.9039 | 1.0479 | 0.6405 | 25.6888 | 34.8171 | 12.629 | 0.6537 | 0.3933 | 8.6882 | -21.8218 | 8.9025 | -20.9187 | 9.0413 | -21.0772 |
| 9 | $E_{M06-L}, \omega_{M06-L}$ | 0.4953 | 0.123 | 0.5802 | 0.0382 | 0.6183 | -0.0488 | 1.0963 | 1.2608 | 0.9983 | 16.2015 | 0 | 0.5978 | 0.5852 | 0.6835 | 0.7642 | 0.6981 | 0.7252 | 0.5374 | 0.0578 | 0.9112 | 1.0535 | 0.773 | 27.6452 | 36.5583 | 19.9331 | 0.6187 | 0.4057 | 9.3782 | -22.4399 | 8.7937 | -21.2473 | 8.6473 | -23.5715 |
| 10 | $E_{M06-2X}, E^{HOMO}_{M06-2X}$ | 0.4888 | 0.1367 | 0.588 | 0.0375 | 0.6255 | 0.153 | 1.086 | 1.2689 | 0.8582 | 16.7008 | 2 | 0.7027 | 0.6935 | 0.7661 | 0.7696 | 0.6954 | 0.8249 | 0.6459 | 0.0071 | 0.9022 | 1.0477 | 0.6951 | 27.1282 | 37.0297 | 14.7315 | 0.6371 | 0.3720 | 9.1317 | -20.8141 | 9.5143 | -20.106 | 9.2712 | -21.0597 |
| 11 | $E_{M06}, E^{HOMO}_{M06}$ | 0.484 | 0.1389 | 0.5852 | 0.0377 | 0.6229 | 0.1093 | 1.0897 | 1.2747 | 0.8562 | 16.5212 | 2 | 0.7042 | 0.6949 | 0.7672 | 0.7677 | 0.6924 | 0.8278 | 0.65 | 0.0102 | 0.9101 | 1.0582 | 0.6955 | 27.312 | 37.3733 | 14.6608 | 0.6301 | 0.4248 | 9.1619 | -21.0887 | 9.082 | -20.9086 | 9.532 | -20.3311 |
| 12 | $E_{M06-L}, E^{HOMO}_{M06-L}$ | 0.4349 | 0.1566 | 0.5508 | 0.0408 | 0.5916 | 0.0309 | 1.1341 | 1.334 | 0.8854 | 14.4855 | 1 | 0.6836 | 0.6738 | 0.7511 | 0.7434 | 0.6567 | 0.8063 | 0.6276 | 0.0024 | 0.9396 | 1.0929 | 0.7227 | 29.5827 | 40.9295 | 15.6783 | 0.6033 | 0.3438 | 8.7519 | -21.5956 | 9.1232 | -20.9926 | 8.9122 | -21.3319 |
| 13 | $E_{M06-2X}, \eta_{M06-2X}$ | 0.3856 | 0.1803 | 0.5225 | 0.0434 | 0.5659 | 0.301 | 1.1692 | 1.391 | 0.9948 | 13.0388 | 0 | 0.6006 | 0.5881 | 0.6858 | 0.7228 | 0.6213 | 0.7377 | 0.5452 | 0.0009 | 0.9524 | 1.1162 | 0.8255 | 31.4403 | 44.5033 | 19.7931 | 0.5809 | 0.2967 | 8.7939 | -21.6215 | 9.3398 | -20.5981 | 9.3088 | -20.5606 |
| 14 | $E_{M06}, \eta_{M06}$ | 0.372 | 0.1849 | 0.5126 | 0.0443 | 0.5569 | 0.2925 | 1.1813 | 1.4064 | 1.0036 | 12.5682 | 0 | 0.5935 | 0.5809 | 0.6802 | 0.7154 | 0.6107 | 0.7303 | 0.5405 | 0.0009 | 0.9693 | 1.136 | 0.8309 | 32.0958 | 45.4913 | 20.1428 | 0.5657 | 0.2913 | 9.217 | -21.1696 | 8.9569 | -20.9562 | 8.9464 | -21.4671 |
| 15 | $E_{M06-L}, \eta_{M06-L}$ | 0.3404 | 0.1933 | 0.4871 | 0.0466 | 0.5337 | 0.0672 | 1.2118 | 1.4413 | 1.0351 | 11.4462 | 0 | 0.5676 | 0.5541 | 0.6598 | 0.696 | 0.5836 | 0.6928 | 0.5231 | 0.0422 | 1.0221 | 1.2016 | 0.8467 | 33.775 | 47.7775 | 21.4295 | 0.5483 | 0.2225 | 8.9472 | -21.8243 | 8.6665 | -21.3824 | 9.2377 | -21.4807 |

Models are arranged according to $Q^2_{LOO}$ values.
Parameters are obtained through QSARINS software. Ref. [54] N. Chirico, E. Papa, S. Kovarich, S. Cassani, P. Gramatica, QSAR Res. Unit in Environ. Chem. and Ecotox. University of Insubria, Varese, Italy, 2012. (http://www.qsar.it).

$R^2_{adj}$ adjusted $R^2$

*N. Ext.OK* Number of external validation parameters meeting threshold values

*F* "F-test" statistic value

Table S18. Value of internal and external validation parameters of two-descriptor QSAR models, for mutagenicity (LogTA100), developed using meta exchange-correlation functionals (M06, M06-L and M06-2X) based methods through 30% (random) splitting method.

| Model | Variables | $Q^2_{LOO}$ | $R^2$-$Q^2_{LOO}$ | $R^2_{adj}$ | $R^2$-$R^2_{adj}$ | $R^2$ | $\Delta K$ | $RMSE_{TR}$ | $RMSE_{CV}$ | $RMSE_{EXT}$ | $F$ | *N. Ext.OK* | $Q^2_{F1}$ | $Q^2_{F2}$ | $Q^2_{F3}$ | $CCC_{TR}$ | $CCC_{CV}$ | $CCC_{EXT}$ | $\bar{r}^2_m$ | $\Delta r^2_m$ | $MAE_{TR}$ | $MAE_{CV}$ | $MAE_{EXT}$ | $RSS_{TR}$ | $PRESS_{CV}$ | $PRESS_{EXT}$ | $R^2_{LMO}$ | $Q^2_{LMO}$ | $R^2_{Yscr}$ | $Q^2_{Yscr}$ | $R^2_{Xrand}$ | $Q^2_{Xrand}$ | $R^2_{Yrand}$ | $Q^2_{Yrand}$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | $E_{M06-L}, E^{LUMO}_{M06-L}$ | 0.6457 | 0.059 | 0.6836 | 0.0211 | 0.7047 | -0.1039 | 0.9344 | 1.0235 | 0.7741 | 33.4027 | 5 | 0.8045 | 0.7692 | 0.7973 | 0.8267 | 0.7963 | 0.8539 | 0.7385 | 0.0611 | 0.7329 | 0.8094 | 0.6806 | 27.0677 | 32.4746 | 7.7897 | 0.7072 | 0.6324 | 6.631 | -14.9168 | 6.5415 | -14.9054 | 6.8114 | -14.65 |
| 2 | $E_{M06}, \chi_{M06}$ | 0.645 | 0.0586 | 0.6824 | 0.0212 | 0.7036 | 0.0425 | 0.9361 | 1.0245 | 0.8487 | 33.2288 | 4 | 0.765 | 0.7226 | 0.7563 | 0.826 | 0.7956 | 0.8356 | 0.6982 | 0.0366 | 0.7665 | 0.8447 | 0.6791 | 27.1674 | 32.5369 | 9.3648 | 0.7058 | 0.6239 | 7.0021 | -14.4278 | 6.4345 | -14.9124 | 6.6507 | -14.9168 |
| 3 | $E_{M06-2X}, \omega_{M06-2X}$ | 0.6444 | 0.0573 | 0.6804 | 0.0213 | 0.7017 | -0.0991 | 0.939 | 1.0253 | 0.8381 | 32.9376 | 4 | 0.7708 | 0.7295 | 0.7624 | 0.8247 | 0.795 | 0.8262 | 0.6796 | 0.0736 | 0.7251 | 0.7989 | 0.7122 | 27.3359 | 32.5894 | 9.1321 | 0.7047 | 0.6189 | 6.4535 | -15.2116 | 6.263 | -15.2692 | 6.8421 | -14.8103 |
| 4 | $E_{M06-2X}, \chi_{M06-2X}$ | 0.6391 | 0.0591 | 0.6766 | 0.0216 | 0.6982 | 0.0362 | 0.9447 | 1.033 | 0.8283 | 32.3816 | 4 | 0.7762 | 0.7358 | 0.7679 | 0.8223 | 0.7915 | 0.8418 | 0.7144 | 0.0354 | 0.7836 | 0.8632 | 0.664 | 27.6636 | 33.0781 | 8.9188 | 0.7020 | 0.6082 | 6.5018 | -15.2048 | 6.603 | -14.8244 | 6.6091 | -15.1715 |
| 5 | $E_{M06}, E^{LUMO}_{M06}$ | 0.6355 | 0.0597 | 0.6734 | 0.0218 | 0.6951 | -0.1043 | 0.9493 | 1.0381 | 0.815 | 31.9242 | 4 | 0.7833 | 0.7442 | 0.7753 | 0.8202 | 0.7892 | 0.8358 | 0.6921 | 0.0706 | 0.7311 | 0.805 | 0.697 | 27.9392 | 33.4086 | 8.6348 | 0.6995 | 0.6169 | 6.5893 | -14.9388 | 6.3198 | -15.155 | 6.5335 | -15.1558 |
| 6 | $E_{M06}, \omega_{M06}$ | 0.6198 | 0.0631 | 0.6602 | 0.0227 | 0.6829 | -0.0821 | 0.9682 | 1.0602 | 0.9577 | 30.149 | 1 | 0.7008 | 0.6468 | 0.6898 | 0.8116 | 0.7792 | 0.7711 | 0.5522 | 0.1025 | 0.7574 | 0.8361 | 0.7881 | 29.0626 | 34.844 | 11.9233 | 0.6894 | 0.5835 | 6.521 | -15.6171 | 7.1178 | -14.0682 | 6.9362 | -14.9774 |
| 7 | $E_{M06-L}, \chi_{M06-L}$ | 0.6156 | 0.0637 | 0.6564 | 0.0229 | 0.6793 | 0.0207 | 0.9736 | 1.066 | 0.857 | 29.6611 | 4 | 0.7604 | 0.7172 | 0.7516 | 0.8091 | 0.7755 | 0.8252 | 0.6854 | 0.0722 | 0.797 | 0.8776 | 0.7075 | 29.3874 | 35.2282 | 9.5474 | 0.6817 | 0.5926 | 6.7324 | -14.8209 | 6.2714 | -15.1945 | 6.9439 | -14.6665 |
| 8 | $E_{M06-2X}, E^{LUMO}_{M06-2X}$ | 0.6119 | 0.0623 | 0.6509 | 0.0233 | 0.6742 | -0.1068 | 0.9814 | 1.0712 | 0.87 | 28.9697 | 3 | 0.7531 | 0.7085 | 0.744 | 0.8054 | 0.7727 | 0.8091 | 0.6293 | 0.0848 | 0.75 | 0.8248 | 0.7097 | 29.8602 | 35.5689 | 9.8387 | 0.6771 | 0.5876 | 6.2714 | -15.4525 | 6.6731 | -14.6313 | 6.7733 | -14.9116 |
| 9 | $E_{M06-L}, \omega_{M06-L}$ | 0.5888 | 0.069 | 0.6335 | 0.0244 | 0.6579 | -0.0499 | 1.0057 | 1.1025 | 1.0841 | 26.9231 | 0 | 0.6165 | 0.5473 | 0.6024 | 0.7937 | 0.7585 | 0.7067 | 0.4399 | 0.1277 | 0.8148 | 0.9007 | 0.9221 | 31.3536 | 37.6819 | 15.2798 | 0.6668 | 0.5456 | 6.5828 | -16.1135 | 6.7211 | -14.6945 | 6.5068 | -16.2047 |
| 10 | $E_{M06}, E^{HOMO}_{M06}$ | 0.5881 | 0.0715 | 0.6352 | 0.0243 | 0.6595 | 0.3063 | 1.0033 | 1.1036 | 0.9461 | 27.12 | 1 | 0.708 | 0.6553 | 0.6972 | 0.7948 | 0.7562 | 0.7899 | 0.6135 | 0.0705 | 0.8077 | 0.891 | 0.7751 | 31.2034 | 37.7531 | 11.6363 | 0.6655 | 0.5566 | 6.4845 | -15.3083 | 6.5776 | -14.8402 | 6.3259 | -15.5547 |
| 11 | $E_{M06-2X}, E^{HOMO}_{M06-2X}$ | 0.5831 | 0.0726 | 0.6311 | 0.0246 | 0.6557 | 0.3457 | 1.0089 | 1.1103 | 0.9304 | 26.6599 | 2 | 0.7176 | 0.6666 | 0.7072 | 0.792 | 0.7527 | 0.7946 | 0.6254 | 0.0838 | 0.813 | 0.8975 | 0.7556 | 31.5565 | 38.2123 | 11.2545 | 0.6607 | 0.5602 | 7.2481 | -14.2227 | 6.6043 | -14.7153 | 6.3517 | -15.3904 |
| 12 | $E_{M06-L}, E^{HOMO}_{M06-L}$ | 0.551 | 0.0827 | 0.6076 | 0.0262 | 0.6337 | 0.2823 | 1.0406 | 1.1521 | 0.9651 | 24.2221 | 0 | 0.6962 | 0.6413 | 0.685 | 0.7758 | 0.7302 | 0.769 | 0.5479 | 0.1032 | 0.8266 | 0.9131 | 0.7963 | 33.5692 | 41.1502 | 12.1073 | 0.6405 | 0.5199 | 6.7844 | -14.6291 | 7.0666 | -14.2034 | 6.7418 | -15.101 |
| 13 | $E_{M06-2X}, \eta_{M06-2X}$ | 0.4616 | 0.1262 | 0.5584 | 0.0294 | 0.5878 | 0.1338 | 1.1039 | 1.2616 | 1.0442 | 19.9668 | 0 | 0.6443 | 0.5801 | 0.6312 | 0.7404 | 0.6705 | 0.7137 | 0.4312 | 0.145 | 0.9217 | 1.0399 | 0.884 | 37.7746 | 49.3395 | 14.1748 | 0.5983 | 0.4594 | 6.7489 | -14.9611 | 6.9357 | -14.347 | 6.3502 | -15.6883 |
| 14 | $E_{M06}, \eta_{M06}$ | 0.4527 | 0.1304 | 0.5533 | 0.0298 | 0.5831 | 0.1358 | 1.1102 | 1.272 | 1.0627 | 19.5782 | 0 | 0.6315 | 0.565 | 0.618 | 0.7366 | 0.6644 | 0.7031 | 0.4145 | 0.1505 | 0.932 | 1.0533 | 0.9087 | 38.2118 | 50.1586 | 14.6824 | 0.5971 | 0.4514 | 6.4859 | -15.2957 | 6.7911 | -14.5454 | 6.8381 | -14.8391 |
| 15 | $E_{M06-L}, \eta_{M06-L}$ | 0.4363 | 0.1327 | 0.5383 | 0.0308 | 0.5691 | 0.1038 | 1.1287 | 1.2909 | 1.1237 | 18.4869 | 0 | 0.588 | 0.5137 | 0.5729 | 0.7253 | 0.6507 | 0.6631 | 0.3501 | 0.1788 | 0.9562 | 1.0814 | 1.0061 | 39.4954 | 51.6593 | 16.4154 | 0.5858 | 0.4303 | 6.6439 | -15.3211 | 6.6466 | -14.8362 | 6.4947 | -15.5033 |

Models are arranged according to $Q^2_{LOO}$ values.

Parameters are obtained through QSARINS software. Ref. [54] N. Chirico, E. Papa, S. Kovarich, S. Cassani, P. Gramatica, QSAR Res. Unit in Environ. Chem. and Ecotox. University of Insubria, Varese, Italy, 2012. (http://www.qsar.it).

$R^2_{adj}$ adjusted $R^2$

*N. Ext.OK* Number of external validation parameters meeting threshold values

*F* "F-test" statistic value

**Table S19.** Value of internal and external validation parameters of two-descriptor QSAR models, for mutagenicity (LogTA98), developed using exchange-correlation (HFX+LYP, BLYP and B3LYP) based methods through activity sampling (ordered response) splitting method.

| Model | Variables | $Q^2_{LOO}$ | $R^2$-$Q^2_{LOO}$ | $R^2_{adj}$ | $R^2$-$R^2_{adj}$ | $R^2$ | $\Delta K$ | $RMSE_{TR}$ | $RMSE_{CV}$ | $RMSE_{EXT}$ | $F$ | N. Ext.OK | $Q^2_{F1}$ | $Q^2_{F2}$ | $Q^2_{F3}$ | $CCC_{TR}$ | $CCC_{CV}$ | $CCC_{EXT}$ | $\bar{r}^2_m$ | $\Delta r^2_m$ | $MAE_{TR}$ | $MAE_{CV}$ | $MAE_{EXT}$ | $RSS_{TR}$ | $PRESS_{CV}$ | $PRESS_{EXT}$ | $R^2_{LMO}$ | $Q^2_{LMO}$ | $R^2_{Yscr}$ | $Q^2_{Yscr}$ | $R^2_{Xrand}$ | $Q^2_{Xrand}$ | $R^2_{Yrand}$ | $Q^2_{Yrand}$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | $E_{HFX+LYP}$, $E^{HOMO}_{HFX+LYP}$ | 0.8921 | 0.0561 | 0.9333 | 0.0148 | 0.9481 | 0.3791 | 0.4667 | 0.6732 | 0.3717 | 63.9963 | 5 | 0.9642 | 0.9642 | 0.9671 | 0.9734 | 0.9447 | 0.9826 | 0.8862 | 0.0213 | 0.3952 | 0.5680 | 0.3145 | 2.1777 | 4.5318 | 0.6907 | 0.9528 | 0.7629 | 21.9794 | -61.7079 | 21.7589 | -70.1808 | 22.4744 | -61.4373 |
| 2 | $E_{B3LYP}$, $E^{HOMO}_{B3LYP}$ | 0.8897 | 0.0581 | 0.9329 | 0.0149 | 0.9478 | 0.4409 | 0.4683 | 0.6805 | 0.3691 | 63.5213 | 5 | 0.9647 | 0.9647 | 0.9676 | 0.9732 | 0.9432 | 0.9827 | 0.8879 | 0.0204 | 0.3837 | 0.5550 | 0.3065 | 2.1931 | 4.6312 | 0.6811 | 0.9521 | 0.7383 | 22.1647 | -61.2524 | 22.0663 | -68.2821 | 22.2077 | -61.2150 |
| 3 | $E_{BLYP}$, $\chi_{BLYP}$ | 0.8847 | 0.0653 | 0.9357 | 0.0143 | 0.9500 | 0.1003 | 0.4584 | 0.6959 | 0.4817 | 66.4643 | 5 | 0.9399 | 0.9398 | 0.9448 | 0.9743 | 0.9406 | 0.9720 | 0.8238 | 0.0347 | 0.3879 | 0.5799 | 0.3941 | 2.1009 | 4.8430 | 1.1601 | 0.9574 | 0.7270 | 21.8175 | -67.1722 | 22.0540 | -67.3895 | 20.7748 | -66.5595 |
| 4 | $E_{HFX+LYP}$, $\chi_{HFX+LYP}$ | 0.8831 | 0.0651 | 0.9335 | 0.0148 | 0.9483 | 0.0812 | 0.4661 | 0.7006 | 0.5405 | 64.1557 | 5 | 0.9243 | 0.9242 | 0.9304 | 0.9734 | 0.9401 | 0.9658 | 0.8105 | 0.0443 | 0.3875 | 0.5681 | 0.4707 | 2.1726 | 4.9080 | 1.4609 | 0.9558 | 0.7078 | 21.7435 | -62.2515 | 21.4043 | -70.4791 | 22.1623 | -60.9956 |
| 5 | $E_{BLYP}$, $E^{HOMO}_{BLYP}$ | 0.8814 | 0.0644 | 0.9304 | 0.0155 | 0.9458 | 0.4835 | 0.4770 | 0.7057 | 0.3781 | 61.1130 | 5 | 0.9630 | 0.9629 | 0.9660 | 0.9722 | 0.9387 | 0.9817 | 0.8854 | 0.0203 | 0.3848 | 0.5665 | 0.3002 | 2.2749 | 4.9797 | 0.7147 | 0.9512 | 0.7480 | 20.8031 | -64.4687 | 21.8562 | -68.5860 | 21.4284 | -62.1607 |
| 6 | $E_{B3LYP}$, $\chi_{B3LYP}$ | 0.8794 | 0.0687 | 0.9333 | 0.0148 | 0.9481 | 0.1015 | 0.4669 | 0.7116 | 0.4985 | 63.9202 | 5 | 0.9356 | 0.9356 | 0.9408 | 0.9734 | 0.9380 | 0.9703 | 0.8163 | 0.0373 | 0.3950 | 0.5881 | 0.4116 | 2.1801 | 5.0640 | 1.2423 | 0.9545 | 0.7643 | 23.5082 | -60.1483 | 21.5496 | -70.2395 | 21.5255 | -63.6436 |
| 7 | $E_{HFX+LYP}$, $\eta_{HFX+LYP}$ | 0.8627 | 0.0605 | 0.9013 | 0.0219 | 0.9232 | 0.0925 | 0.5679 | 0.7593 | 0.4647 | 42.0728 | 5 | 0.9440 | 0.9440 | 0.9486 | 0.9601 | 0.9294 | 0.9694 | 0.9431 | 0.0041 | 0.4268 | 0.6012 | 0.3796 | 3.2253 | 5.7655 | 1.0796 | 0.9241 | 0.5293 | 22.3573 | -63.8950 | 21.4242 | -67.5565 | 23.5924 | -58.3102 |
| 8 | $E_{B3LYP}$, $\eta_{B3LYP}$ | 0.8513 | 0.0628 | 0.8896 | 0.0245 | 0.9141 | 0.0957 | 0.6006 | 0.7903 | 0.5406 | 37.2526 | 5 | 0.9243 | 0.9242 | 0.9304 | 0.9551 | 0.9233 | 0.9583 | 0.9095 | 0.0462 | 0.4353 | 0.6074 | 0.4339 | 3.6068 | 6.2455 | 1.4612 | 0.9143 | 0.6270 | 23.9290 | -57.5111 | 22.7135 | -65.9103 | 21.6030 | -65.7885 |
| 9 | $E_{BLYP}$, $\eta_{BLYP}$ | 0.8403 | 0.0633 | 0.8760 | 0.0276 | 0.9035 | 0.0892 | 0.6365 | 0.8190 | 0.5912 | 32.7816 | 5 | 0.9094 | 0.9094 | 0.9168 | 0.9493 | 0.9166 | 0.9490 | 0.8675 | 0.0581 | 0.4487 | 0.6115 | 0.4868 | 4.0512 | 6.7078 | 1.7475 | 0.9057 | 0.5090 | 22.8803 | -62.7192 | 23.5435 | -67.2161 | 22.7790 | -62.8621 |
| 10 | $E_{HFX+LYP}$, $\omega_{HFX+LYP}$ | 0.8363 | 0.0968 | 0.9140 | 0.0191 | 0.9331 | -0.0438 | 0.5301 | 0.8291 | 0.7803 | 48.8159 | 5 | 0.8422 | 0.8421 | 0.8550 | 0.9654 | 0.9166 | 0.9342 | 0.7364 | 0.0790 | 0.4562 | 0.6839 | 0.6484 | 2.8096 | 6.8737 | 3.0443 | 0.9441 | 0.6290 | 21.6940 | -64.7598 | 20.9693 | -72.3987 | 22.7684 | -61.7637 |
| 11 | $E_{BLYP}$, $E^{LUMO}_{BLYP}$ | 0.8230 | 0.1040 | 0.9061 | 0.0209 | 0.9270 | -0.0447 | 0.5537 | 0.8622 | 0.8297 | 44.4478 | 5 | 0.8216 | 0.8215 | 0.8361 | 0.9621 | 0.9090 | 0.9245 | 0.6878 | 0.0904 | 0.4537 | 0.6942 | 0.6379 | 3.0655 | 7.4344 | 3.4416 | 0.9363 | 0.6446 | 21.9277 | -74.3680 | 20.8247 | -68.6930 | 22.4754 | -71.1257 |
| 12 | $E_{B3LYP}$, $E^{LUMO}_{B3LYP}$ | 0.7862 | 0.1319 | 0.8948 | 0.0234 | 0.9182 | -0.0568 | 0.5862 | 0.9475 | 0.8874 | 39.2752 | 5 | 0.7959 | 0.7958 | 0.8125 | 0.9573 | 0.8914 | 0.9150 | 0.6778 | 0.1000 | 0.4712 | 0.7324 | 0.6990 | 3.4362 | 8.9772 | 3.9370 | 0.9330 | 0.4793 | 21.7020 | -70.7957 | 23.9076 | -63.0904 | 21.9027 | -68.1805 |
| 13 | $E_{B3LYP}$, $\omega_{B3LYP}$ | 0.6994 | 0.1926 | 0.8611 | 0.0309 | 0.8920 | -0.0625 | 0.6735 | 1.1236 | 1.0298 | 28.9039 | 4 | 0.7252 | 0.7250 | 0.7475 | 0.9429 | 0.8509 | 0.8879 | 0.6370 | 0.1242 | 0.5435 | 0.8579 | 0.8450 | 4.5361 | 12.6237 | 5.3027 | 0.9057 | 0.3130 | 22.7737 | -64.4224 | 21.9101 | -68.6705 | 22.4299 | -63.9915 |
| 14 | $E_{HFX+LYP}$, $E^{LUMO}_{HFX+LYP}$ | 0.6972 | 0.1906 | 0.8557 | 0.0321 | 0.8878 | -0.0668 | 0.6866 | 1.1277 | 1.1299 | 27.6832 | 1 | 0.6691 | 0.6689 | 0.6960 | 0.9405 | 0.8470 | 0.8696 | 0.6139 | 0.1375 | 0.5644 | 0.8790 | 0.9486 | 4.7136 | 12.7167 | 6.3836 | 0.9033 | 0.4389 | 22.4945 | -62.6439 | 21.8520 | -70.1848 | 21.9754 | -65.0578 |
| 15 | $E_{BLYP}$, $\omega_{BLYP}$ | 0.6171 | 0.2400 | 0.8164 | 0.0408 | 0.8572 | -0.0575 | 0.7745 | 1.2680 | 1.1610 | 21.0035 | 1 | 0.6507 | 0.6504 | 0.6790 | 0.9231 | 0.8080 | 0.8540 | 0.5910 | 0.1498 | 0.6257 | 0.9798 | 0.9607 | 5.9986 | 16.0789 | 6.7400 | 0.8747 | 0.2503 | 21.9825 | -66.6553 | 21.4262 | -70.2615 | 22.0693 | -64.8659 |

Models are arranged according to $Q^2_{LOO}$ values.
Parameters are obtained through QSARINS software. Ref. [54] N. Chirico, E. Papa, S. Kovarich, S. Cassani, P. Gramatica, QSAR Res. Unit in Environ. Chem. and Ecotox. University of Insubria, Varese, Italy, 2012. (http://www.qsar.it).

$R^2_{adj}$ adjusted $R^2$

*N. Ext.OK* Number of external validation parameters meeting threshold values

*F* "F-test" statistic value

**Table S20.** Value of internal and external validation parameters of two-descriptor QSAR models, for mutagenicity (LogTA98), developed using exchange-correlation (HFX+LYP, BLYP and B3LYP) based methods through 30% (random) splitting method.

| Model | Variables | $Q^2_{LOO}$ | $R^2$-$Q^2_{LOO}$ | $R^2_{adj}$ | $R^2$-$R^2_{adj}$ | $R^2$ | $\Delta K$ | $RMSE_{TR}$ | $RMSE_{CV}$ | $RMSE_{EXT}$ | $F$ | *N. Ext.OK* | $Q^2_{F1}$ | $Q^2_{F2}$ | $Q^2_{F3}$ | $CCC_{TR}$ | $CCC_{CV}$ | $CCC_{EXT}$ | $\overline{r}^2_m$ | $\Delta r^2_m$ | $MAE_{TR}$ | $MAE_{CV}$ | $MAE_{EXT}$ | $RSS_{TR}$ | $PRESS_{CV}$ | $PRESS_{EXT}$ | $R^2_{LMO}$ | $Q^2_{LMO}$ | $R^2_{Yscr}$ | $Q^2_{Yscr}$ | $R^2_{Yrand}$ | $Q^2_{Xrand}$ | $R^2_{Yrand}$ | $Q^2_{Yrand}$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | $E_{HFX+LYP}$, $E^{HOMO}_{HFX+LYP}$ | 0.8851 | 0.0558 | 0.9261 | 0.0148 | 0.9409 | 0.3848 | 0.4749 | 0.6624 | 0.2453 | 63.7044 | 5 | 0.9875 | 0.9875 | 0.9842 | 0.9696 | 0.9407 | 0.9938 | 0.9576 | 0.0080 | 0.4089 | 0.5663 | 0.2116 | 2.4813 | 4.8261 | 0.2406 | 0.9434 | 0.6994 | 19.8221 | -53.9691 | 19.8985 | -58.0855 | 21.3591 | -50.4427 |
| 2 | $E_{BLYP}$, $\chi_{BLYP}$ | 0.8826 | 0.0621 | 0.9308 | 0.0138 | 0.9447 | 0.0855 | 0.4596 | 0.6695 | 0.4298 | 68.2891 | 5 | 0.9617 | 0.9616 | 0.9516 | 0.9715 | 0.9391 | 0.9819 | 0.8710 | 0.0224 | 0.3969 | 0.5697 | 0.3362 | 2.3239 | 4.9301 | 0.7391 | 0.9499 | 0.7150 | 20.1971 | -56.0847 | 19.7550 | -58.1195 | 19.6207 | -58.2302 |
| 3 | $E_{B3LYP}$, $E^{HOMO}_{B3LYP}$ | 0.8824 | 0.0576 | 0.9250 | 0.0150 | 0.9400 | 0.4467 | 0.4786 | 0.6701 | 0.2270 | 62.6802 | 5 | 0.9893 | 0.9893 | 0.9865 | 0.9691 | 0.9389 | 0.9947 | 0.9621 | 0.0067 | 0.3970 | 0.5514 | 0.1958 | 2.5194 | 4.9389 | 0.2061 | 0.9452 | 0.7427 | 20.1310 | -53.3814 | 20.5526 | -56.5028 | 19.5937 | -54.0735 |
| 4 | $E_{HFX+LYP}$, $\chi_{HFX+LYP}$ | 0.8822 | 0.0618 | 0.9300 | 0.0140 | 0.9440 | 0.0665 | 0.4624 | 0.6707 | 0.5261 | 67.4389 | 5 | 0.9426 | 0.9425 | 0.9275 | 0.9712 | 0.9392 | 0.9739 | 0.8548 | 0.0318 | 0.3917 | 0.5532 | 0.4492 | 2.3516 | 4.9482 | 1.1073 | 0.9488 | 0.7782 | 19.9449 | -54.7623 | 19.3021 | -57.3220 | 18.2851 | -56.6318 |
| 5 | $E_{B3LYP}$, $\chi_{B3LYP}$ | 0.8782 | 0.0650 | 0.9291 | 0.0142 | 0.9433 | 0.0863 | 0.4655 | 0.6818 | 0.4590 | 66.4853 | 5 | 0.9563 | 0.9563 | 0.9448 | 0.9708 | 0.9370 | 0.9796 | 0.8600 | 0.0253 | 0.4014 | 0.5747 | 0.3648 | 2.3834 | 5.1139 | 0.8428 | 0.9495 | 0.7200 | 20.3673 | -54.2044 | 20.6016 | -55.7319 | 21.6294 | -52.6924 |
| 6 | $E_{BLYP}$, $E^{HOMO}_{BLYP}$ | 0.8738 | 0.0639 | 0.9221 | 0.0156 | 0.9377 | 0.4762 | 0.4877 | 0.6940 | 0.2318 | 60.2189 | 5 | 0.9889 | 0.9888 | 0.9859 | 0.9679 | 0.9342 | 0.9944 | 0.9596 | 0.0066 | 0.4123 | 0.5801 | 0.1841 | 2.6160 | 5.2985 | 0.2149 | 0.9435 | 0.7206 | 21.1418 | -51.2546 | 20.9238 | -54.5191 | 20.9746 | -51.8951 |
| 7 | $E_{HFX+LYP}$, $\eta_{HFX+LYP}$ | 0.8498 | 0.0582 | 0.8850 | 0.0230 | 0.9080 | 0.0862 | 0.5926 | 0.7572 | 0.3264 | 39.4896 | 5 | 0.9779 | 0.9779 | 0.9721 | 0.9518 | 0.9215 | 0.9875 | 0.8822 | 0.0140 | 0.4534 | 0.6032 | 0.2858 | 3.8628 | 6.3073 | 0.4261 | 0.9078 | 0.6691 | 19.6280 | -57.3645 | 19.1549 | -57.7598 | 19.5265 | -56.9078 |
| 8 | $E_{HFX+LYP}$, $\omega_{HFX+LYP}$ | 0.8416 | 0.0903 | 0.9148 | 0.0170 | 0.9319 | -0.0530 | 0.5101 | 0.7777 | 0.8520 | 54.7039 | 5 | 0.8495 | 0.8493 | 0.8099 | 0.9647 | 0.9191 | 0.9372 | 0.7556 | 0.0686 | 0.4373 | 0.6369 | 0.7376 | 2.8617 | 6.6529 | 2.9036 | 0.9402 | 0.6822 | 19.7244 | -56.0226 | 20.7992 | -56.2872 | 19.3957 | -56.9965 |
| 9 | $E_{B3LYP}$, $\eta_{B3LYP}$ | 0.8379 | 0.0574 | 0.8691 | 0.0262 | 0.8953 | 0.0874 | 0.6322 | 0.7868 | 0.4263 | 34.2066 | 5 | 0.9623 | 0.9623 | 0.9524 | 0.9448 | 0.9146 | 0.9785 | 0.8313 | 0.0288 | 0.4662 | 0.6068 | 0.3403 | 4.3970 | 6.8094 | 0.7271 | 0.8956 | 0.4757 | 21.5021 | -54.5061 | 21.7267 | -51.5034 | 21.0012 | -54.4140 |
| 10 | $E_{BLYP}$, $E^{LUMO}_{BLYP}$ | 0.8301 | 0.0947 | 0.9060 | 0.0188 | 0.9248 | -0.0540 | 0.5359 | 0.8055 | 0.8933 | 49.1816 | 5 | 0.8346 | 0.8343 | 0.7910 | 0.9609 | 0.9123 | 0.9297 | 0.7032 | 0.0784 | 0.4316 | 0.6376 | 0.6994 | 3.1589 | 7.1369 | 3.1917 | 0.9305 | 0.6301 | 20.2387 | -59.4732 | 20.4010 | -57.3591 | 19.5696 | -62.9501 |
| 11 | $E_{BLYP}$, $\eta_{BLYP}$ | 0.8245 | 0.0592 | 0.8546 | 0.0291 | 0.8837 | 0.0804 | 0.6664 | 0.8185 | 0.5047 | 30.3885 | 5 | 0.9472 | 0.9471 | 0.9333 | 0.9382 | 0.9065 | 0.9692 | 0.7889 | 0.0423 | 0.4787 | 0.6107 | 0.4025 | 4.8852 | 7.3697 | 1.0189 | 0.8858 | 0.4507 | 21.0491 | -54.0528 | 20.3026 | -57.9467 | 20.1140 | -54.8191 |
| 12 | $E_{B3LYP}$, $E^{LUMO}_{B3LYP}$ | 0.7951 | 0.1217 | 0.8960 | 0.0208 | 0.9168 | -0.0654 | 0.5636 | 0.8844 | 0.9713 | 44.0727 | 5 | 0.8044 | 0.8041 | 0.7529 | 0.9566 | 0.8958 | 0.9184 | 0.6891 | 0.0886 | 0.4432 | 0.6673 | 0.7978 | 3.4946 | 8.6038 | 3.7738 | 0.9269 | 0.6311 | 18.8755 | -60.0352 | 18.6105 | -60.7592 | 20.0680 | -60.2992 |
| 13 | $E_{HFX+LYP}$, $E^{LUMO}_{HFX+LYP}$ | 0.7112 | 0.1747 | 0.8573 | 0.0285 | 0.8859 | -0.0748 | 0.6601 | 1.0500 | 1.2549 | 31.0498 | 1 | 0.6735 | 0.6731 | 0.5875 | 0.9395 | 0.8541 | 0.8717 | 0.6298 | 0.1230 | 0.5245 | 0.7907 | 1.1104 | 4.7930 | 12.1280 | 6.2993 | 0.8947 | 0.5419 | 20.5400 | -56.4358 | 20.5850 | -55.5373 | 19.9968 | -58.9030 |
| 14 | $E_{B3LYP}$, $\omega_{B3LYP}$ | 0.7089 | 0.1819 | 0.8635 | 0.0273 | 0.8908 | -0.0707 | 0.6457 | 1.0542 | 1.1402 | 32.6340 | 3 | 0.7305 | 0.7301 | 0.6595 | 0.9423 | 0.8556 | 0.8901 | 0.6459 | 0.1117 | 0.5089 | 0.7823 | 0.9923 | 4.5857 | 12.2256 | 5.2004 | 0.9024 | 0.4876 | 20.3042 | -57.3648 | 20.4722 | -56.7230 | 18.6994 | -60.2581 |
| 15 | $E_{BLYP}$, $\omega_{BLYP}$ | 0.6329 | 0.2212 | 0.8176 | 0.0365 | 0.8541 | -0.0659 | 0.7465 | 1.1839 | 1.2882 | 23.4074 | 1 | 0.6560 | 0.6555 | 0.5654 | 0.9213 | 0.8150 | 0.8569 | 0.6026 | 0.1354 | 0.5849 | 0.8891 | 1.1097 | 6.1295 | 15.4177 | 6.6379 | 0.8668 | 0.3586 | 19.7015 | -60.8864 | 21.2735 | -54.7731 | 19.1376 | -60.2717 |

Models are arranged according to $Q^2_{LOO}$ values.

Parameters are obtained through QSARINS software. Ref. [54] N. Chirico, E. Papa, S. Kovarich, S. Cassani, P. Gramatica, QSAR Res. Unit in Environ. Chem. and Ecotox. University of Insubria, Varese, Italy, 2012. (http://www.qsar.it).

$R^2_{adj}$ adjusted $R^2$

*N. Ext.OK* Number of external validation parameters meeting threshold values

*F* "F-test" statistic value

**Table S21.** Value of internal and external validation parameters of two-descriptor QSAR models, for mutagenicity (LogTA98), developed using meta exchange-correlation functionals (M06, M06-L and M06-2X) based methods through activity sampling (ordered response) splitting method.

| Model | Variables | $Q^2_{LOO}$ | $R^2$-$Q^2_{LOO}$ | $R^2_{adj}$ | $R^2$-$R^2_{adj}$ | $R^2$ | $\Delta K$ | $RMSE_{TR}$ | $RMSE_{CV}$ | $RMSE_{EXT}$ | $F$ | N. Ext.OK | $Q^2_{F1}$ | $Q^2_{F2}$ | $Q^2_{F3}$ | $CCC_{TR}$ | $CCC_{CV}$ | $CCC_{EXT}$ | $\bar{r}_m^2$ | $\Delta r_m^2$ | $MAE_{TR}$ | $MAE_{CV}$ | $MAE_{EXT}$ | $RSS_{TR}$ | $PRESS_{CV}$ | $PRESS_{EXT}$ | $R^2_{LMO}$ | $Q^2_{LMO}$ | $R^2_{Yscr}$ | $Q^2_{Yscr}$ | $R^2_{Xvand}$ | $Q^2_{Xvand}$ | $R^2_{Yvand}$ | $Q^2_{Yvand}$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | $E_{M06}$, $\eta_{M06}$ | 0.9376 | 0.0294 | 0.9539 | 0.0132 | 0.9671 | 0.0922 | 0.3856 | 0.5308 | 0.8451 | 73.4735 | 4 | 0.7584 | 0.7546 | 0.8419 | 0.9833 | 0.9681 | 0.8524 | 0.5745 | 0.1954 | 0.306 | 0.4597 | 0.6485 | 1.1893 | 2.2536 | 4.2849 | 0.9665 | 0.4282 | 27.7949 | -111.7891 | 28.2131 | -109.2969 | 28.3554 | -106.8579 |
| 2 | $E_{M06-L}$, $\eta_{M06-L}$ | 0.9338 | 0.0322 | 0.9523 | 0.0136 | 0.966 | 0.0992 | 0.3922 | 0.5469 | 0.901 | 70.9336 | 3 | 0.7253 | 0.7211 | 0.8203 | 0.9827 | 0.966 | 0.8365 | 0.5489 | 0.2102 | 0.312 | 0.4754 | 0.6781 | 1.2304 | 2.393 | 4.8705 | 0.9665 | 0.4517 | 27.9991 | -103.9355 | 29.1644 | -103.9607 | 29.0461 | -98.2654 |
| 3 | $E_{M06-2X}$, $\eta_{M06-2X}$ | 0.9255 | 0.0391 | 0.9503 | 0.0142 | 0.9645 | 0.0812 | 0.4004 | 0.5803 | 0.8164 | 67.9586 | 4 | 0.7745 | 0.771 | 0.8525 | 0.9819 | 0.9618 | 0.8638 | 0.5971 | 0.1827 | 0.3433 | 0.5338 | 0.622 | 1.2824 | 2.6937 | 3.9987 | 0.9667 | 0.4467 | 29.4742 | -94.3226 | 29.123 | -106.5453 | 28.8858 | -95.8147 |
| 4 | $E_{M06-2X}$, $E^{HOMO}_{M06-2X}$ | 0.9154 | 0.0488 | 0.9498 | 0.0143 | 0.9642 | 0.3813 | 0.4024 | 0.6182 | 0.6584 | 67.2372 | 5 | 0.8533 | 0.8511 | 0.9041 | 0.9817 | 0.9569 | 0.9154 | 0.7345 | 0.1167 | 0.361 | 0.5729 | 0.5509 | 1.2956 | 3.0576 | 2.6008 | 0.9669 | 0.2947 | 28.3913 | -94.96 | 28.2176 | -107.765 | 29.0638 | -90.382 |
| 5 | $E_{M06}$, $E^{HOMO}_{M06}$ | 0.912 | 0.051 | 0.9482 | 0.0148 | 0.963 | 0.4472 | 0.409 | 0.6306 | 0.6381 | 65.03 | 5 | 0.8622 | 0.8601 | 0.9099 | 0.9811 | 0.9552 | 0.9221 | 0.7564 | 0.1082 | 0.3621 | 0.5745 | 0.5332 | 1.338 | 3.181 | 2.4428 | 0.9665 | 0.2437 | 29.3185 | -89.4435 | 29.5409 | -107.8017 | 28.1431 | -92.6082 |
| 6 | $E_{M06-L}$, $E^{HOMO}_{M06-L}$ | 0.9007 | 0.0589 | 0.9435 | 0.0161 | 0.9596 | 0.4873 | 0.4271 | 0.6698 | 0.6469 | 59.4245 | 5 | 0.8584 | 0.8562 | 0.9074 | 0.9794 | 0.9497 | 0.9194 | 0.747 | 0.1118 | 0.3755 | 0.598 | 0.537 | 1.4591 | 3.5886 | 2.5106 | 0.9630 | 0.3326 | 29.892 | -84.3877 | 28.2755 | -110.5739 | 28.6256 | -90.1226 |
| 7 | $E_{M06-2X}$, $X_{M06-2X}$ | 0.8869 | 0.0709 | 0.9409 | 0.0169 | 0.9578 | 0.0975 | 0.4367 | 0.7148 | 0.6766 | 56.7217 | 5 | 0.8451 | 0.8427 | 0.8987 | 0.9784 | 0.9432 | 0.9139 | 0.7736 | 0.1141 | 0.3855 | 0.6288 | 0.6009 | 1.5257 | 4.0872 | 2.7467 | 0.9620 | 0.0473 | 29.9173 | -84.8367 | 28.1887 | -108.8898 | 28.409 | -90.3705 |
| 8 | $E_{M06}$, $X_{M06}$ | 0.8653 | 0.0857 | 0.9314 | 0.0196 | 0.951 | 0.0841 | 0.4705 | 0.78 | 0.6957 | 48.5188 | 5 | 0.8362 | 0.8337 | 0.8929 | 0.9749 | 0.9327 | 0.9107 | 0.7692 | 0.1183 | 0.4241 | 0.6922 | 0.6077 | 1.771 | 4.8678 | 2.9044 | 0.9568 | -0.1088 | 28.285 | -87.7112 | 29.086 | -105.774 | 28.0153 | -87.1623 |
| 9 | $E_{M06-L}$, $X_{M06-L}$ | 0.8644 | 0.0861 | 0.9306 | 0.0198 | 0.9504 | 0.0934 | 0.4732 | 0.7828 | 0.6626 | 47.9485 | 5 | 0.8514 | 0.8491 | 0.9028 | 0.9746 | 0.9325 | 0.9176 | 0.7791 | 0.1103 | 0.4172 | 0.6784 | 0.576 | 1.791 | 4.9021 | 2.6344 | 0.9569 | 0.0372 | 28.7003 | -86.8684 | 29.0013 | -107.4807 | 28.7019 | -85.8066 |
| 10 | $E_{M06-L}$, $E^{LUMO}_{M06-L}$ | 0.7279 | 0.2013 | 0.9009 | 0.0283 | 0.9292 | -0.0166 | 0.5655 | 1.1087 | 0.873 | 32.8217 | 5 | 0.7421 | 0.7381 | 0.8313 | 0.9633 | 0.8789 | 0.8602 | 0.6618 | 0.0803 | 0.4757 | 0.8531 | 0.7203 | 2.558 | 9.8346 | 4.5731 | 0.9414 | -0.7682 | 27.9867 | -100.0206 | 29.8237 | -104.964 | 27.5712 | -98.7785 |
| 11 | $E_{M06-2X}$, $\omega_{M06-2X}$ | 0.7232 | 0.2113 | 0.9083 | 0.0262 | 0.9345 | -0.0224 | 0.544 | 1.1183 | 0.9597 | 35.6573 | 1 | 0.6884 | 0.6835 | 0.7961 | 0.9661 | 0.8781 | 0.834 | 0.6064 | 0.0805 | 0.4353 | 0.8082 | 0.8368 | 2.3679 | 10.0041 | 5.5256 | 0.9503 | -0.7994 | 28.4668 | -96.7516 | 29.2101 | -104.6621 | 29.1888 | -93.7139 |
| 12 | $E_{M06}$, $\omega_{M06}$ | 0.7146 | 0.2 | 0.8805 | 0.0342 | 0.9146 | -0.0158 | 0.621 | 1.1355 | 1.1443 | 26.7821 | 1 | 0.5569 | 0.55 | 0.7101 | 0.9554 | 0.8719 | 0.7491 | 0.4609 | 0.2018 | 0.5243 | 0.937 | 0.9638 | 3.0856 | 10.3153 | 7.8571 | 0.9247 | -0.7434 | 28.4578 | -113.1536 | 29.5066 | -103.8563 | 28.8376 | -111.896 |
| 13 | $E_{M06-L}$, $\omega_{M06-L}$ | 0.6956 | 0.2123 | 0.871 | 0.0368 | 0.9079 | -0.0152 | 0.6451 | 1.1727 | 1.2723 | 24.642 | 0 | 0.4523 | 0.4437 | 0.6417 | 0.9517 | 0.8692 | 0.6739 | 0.3532 | 0.25 | 0.5378 | 0.9653 | 1.0343 | 3.3289 | 11.0024 | 9.7132 | 0.9141 | -0.9541 | 29.4002 | -132.8891 | 29.0162 | -108.4973 | 28.6865 | -134.2754 |
| 14 | $E_{M06}$, $E^{LUMO}_{M06}$ | 0.6909 | 0.2308 | 0.8904 | 0.0313 | 0.9217 | -0.0185 | 0.5948 | 1.1817 | 1.005 | 29.42 | 1 | 0.6582 | 0.6529 | 0.7764 | 0.9592 | 0.8644 | 0.8114 | 0.5658 | 0.1462 | 0.5068 | 0.9364 | 0.8591 | 2.8306 | 11.1708 | 6.0607 | 0.9357 | -1.1518 | 28.0177 | -106.0502 | 27.4887 | -113.4558 | 29.3138 | -104.1459 |
| 15 | $E_{M06-2X}$, $E^{LUMO}_{M06-2X}$ | 0.607 | 0.319 | 0.8963 | 0.0296 | 0.926 | -0.0247 | 0.5784 | 1.3325 | 1.0272 | 31.2611 | 1 | 0.643 | 0.6375 | 0.7665 | 0.9616 | 0.8405 | 0.8049 | 0.5513 | 0.0901 | 0.472 | 0.9372 | 0.8735 | 2.6762 | 14.2045 | 6.3304 | 0.9429 | -0.9509 | 29.6514 | -103.5237 | 30.5324 | -101.0151 | 26.6299 | -110.496 |

Models are arranged according to $Q^2_{LOO}$ values.

Parameters are obtained through QSARINS software. Ref. [54] N. Chirico, E. Papa, S. Kovarich, S. Cassani, P. Gramatica, QSAR Res. Unit in Environ. Chem. and Ecotox. University of Insubria, Varese, Italy, 2012. (http://www.qsar.it).

$R^2_{adj}$ adjusted $R^2$

*N. Ext.OK* Number of external validation parameters meeting threshold values

*F* "F-test" statistic value

**Table S22**. Value of internal and external validation parameters of two-descriptor QSAR models, for mutagenicity (LogTA98), developed using meta exchange-correlation functionals (M06, M06-L and M06-2X) based methods through 30% (random) splitting method.

| Model | Variables | $Q^2_{LOO}$ | $R^2$-$Q^2_{LOO}$ | $R^2_{adj}$ | $R^2$-$R^2_{adj}$ | $R^2$ | $\Delta K$ | $RMSE_{TR}$ | $RMSE_{CV}$ | $RMSE_{EXT}$ | $F$ | *N. Ext.OK* | $Q^2_{F1}$ | $Q^2_{F2}$ | $Q^2_{F3}$ | $CCC_{TR}$ | $CCC_{CV}$ | $CCC_{EXT}$ | $\bar{r}^2_m$ | $\Delta r^2_m$ | $MAE_{TR}$ | $MAE_{CV}$ | $MAE_{EXT}$ | $RSS_{TR}$ | $PRESS_{CV}$ | $PRESS_{EXT}$ | $R^2_{LMO}$ | $Q^2_{LMO}$ | $R^2_{Yscr}$ | $Q^2_{Yscr}$ | $R^2_{Xrand}$ | $Q^2_{Xrand}$ | $R^2_{Yrand}$ | $Q^2_{Yrand}$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | $E_{M06-L}$, $\chi_{M06-L}$ | 0.8029 | 0.1097 | 0.8908 | 0.0218 | 0.9126 | -0.0994 | 0.5821 | 0.8743 | 0.515 | 41.7915 | 5 | 0.9428 | 0.9386 | 0.9316 | 0.9543 | 0.9051 | 0.971 | 0.7986 | 0.0278 | 0.478 | 0.6885 | 0.4896 | 3.7267 | 8.4085 | 1.061 | 0.9225 | 0.4249 | 20.7231 | -57.8864 | 19.7506 | -57.2044 | 19.9462 | -60.7468 |
| 2 | $E_{M06}$, $E^{HOMO}_{M06}$ | 0.7966 | 0.117 | 0.8919 | 0.0216 | 0.9135 | 0.2004 | 0.5791 | 0.8883 | 0.31 | 42.2546 | 5 | 0.9793 | 0.9777 | 0.9752 | 0.9548 | 0.9015 | 0.9888 | 0.9073 | 0.0078 | 0.5292 | 0.7718 | 0.281 | 3.6894 | 8.679 | 0.3845 | 0.9236 | 0.6483 | 20.2452 | -57.6463 | 19.5393 | -57.3815 | 19.6521 | -57.8741 |
| 3 | $E_{M06-L}$, $E^{HOMO}_{M06-L}$ | 0.7952 | 0.1174 | 0.8907 | 0.0219 | 0.9126 | 0.1423 | 0.5824 | 0.8913 | 0.3531 | 41.744 | 5 | 0.9731 | 0.9711 | 0.9678 | 0.9543 | 0.9007 | 0.9855 | 0.8954 | 0.0119 | 0.5286 | 0.7682 | 0.295 | 3.7306 | 8.7384 | 0.4988 | 0.9238 | 0.6750 | 19.8096 | -57.7607 | 20.4369 | -56.3584 | 19.124 | -60.238 |
| 4 | $E_{M06-2X}$, $\chi_{M06-2X}$ | 0.7907 | 0.1185 | 0.8865 | 0.0227 | 0.9092 | -0.0934 | 0.5934 | 0.9009 | 0.4607 | 40.06 | 5 | 0.9542 | 0.9508 | 0.9453 | 0.9524 | 0.899 | 0.9758 | 0.8378 | 0.0179 | 0.499 | 0.7225 | 0.452 | 3.8732 | 8.9288 | 0.8489 | 0.9196 | 0.4544 | 20.0443 | -58.6461 | 20.2271 | -57.4871 | 19.5866 | -59.1815 |
| 5 | $E_{M06-2X}$, $E^{HOMO}_{M06-2X}$ | 0.7854 | 0.1248 | 0.8876 | 0.0225 | 0.9101 | 0.2822 | 0.5904 | 0.9124 | 0.2758 | 40.5031 | 5 | 0.9836 | 0.9824 | 0.9804 | 0.9529 | 0.8965 | 0.991 | 0.9216 | 0.0048 | 0.5441 | 0.7967 | 0.2611 | 3.8346 | 9.1571 | 0.3043 | 0.9199 | 0.5766 | 20.2852 | -56.762 | 20.2144 | -56.5654 | 19.9734 | -57.6441 |
| 6 | $E_{M06}$, $\chi_{M06}$ | 0.7813 | 0.1209 | 0.8777 | 0.0245 | 0.9022 | -0.0981 | 0.6159 | 0.921 | 0.4729 | 36.8954 | 5 | 0.9518 | 0.9482 | 0.9423 | 0.9486 | 0.894 | 0.9753 | 0.8178 | 0.0233 | 0.4927 | 0.7082 | 0.4476 | 4.1729 | 9.3311 | 0.8947 | 0.9132 | 0.4133 | 20.2397 | -59.3655 | 20.3822 | -57.6207 | 20.1287 | -59.5271 |
| 7 | $E_{M06-2X}$, $\omega_{M06-2X}$ | 0.7121 | 0.1341 | 0.8078 | 0.0384 | 0.8462 | -0.1409 | 0.7722 | 1.0566 | 0.7292 | 22.0146 | 5 | 0.8853 | 0.8768 | 0.8629 | 0.9167 | 0.8547 | 0.9391 | 0.7623 | 0.0483 | 0.5371 | 0.7703 | 0.6395 | 6.5598 | 12.2811 | 2.127 | 0.8577 | 0.0407 | 20.0714 | -61.6787 | 20.5407 | -54.9415 | 20.3017 | -61.3724 |
| 8 | $E_{M06-2X}$, $\eta_{M06-2X}$ | 0.705 | 0.1545 | 0.8244 | 0.0351 | 0.8595 | 0.1217 | 0.7382 | 1.0697 | 0.3096 | 24.4702 | 5 | 0.9793 | 0.9778 | 0.9753 | 0.9244 | 0.8565 | 0.9875 | 0.8573 | 0.0171 | 0.6652 | 0.9419 | 0.2801 | 5.994 | 12.5874 | 0.3834 | 0.8729 | 0.3548 | 20.2079 | -56.909 | 20.4296 | -55.1677 | 19.4959 | -58.4826 |
| 9 | $E_{M06}$, $\eta_{M06}$ | 0.6983 | 0.1576 | 0.8199 | 0.036 | 0.8559 | 0.1282 | 0.7475 | 1.0817 | 0.3832 | 23.7615 | 5 | 0.9683 | 0.966 | 0.9621 | 0.9224 | 0.8536 | 0.9802 | 0.8243 | 0.0261 | 0.6705 | 0.95 | 0.3381 | 6.1471 | 12.8713 | 0.5873 | 0.8679 | 0.4637 | 20.5301 | -55.4222 | 18.9807 | -59.4511 | 20.5426 | -56.2351 |
| 10 | $E_{M06-L}$, $E^{LUMO}_{M06-L}$ | 0.6791 | 0.157 | 0.7952 | 0.041 | 0.8361 | -0.1355 | 0.7972 | 1.1156 | 0.6062 | 20.4115 | 5 | 0.9207 | 0.9149 | 0.9053 | 0.9108 | 0.841 | 0.9583 | 0.7895 | 0.0309 | 0.5808 | 0.8088 | 0.5794 | 6.9906 | 13.6894 | 1.4697 | 0.8481 | 0.3388 | 19.0538 | -70.3668 | 20.0604 | -58.4087 | 21.0157 | -65.4341 |
| 11 | $E_{M06-L}$, $\eta_{M06-L}$ | 0.6546 | 0.1818 | 0.7955 | 0.0409 | 0.8364 | 0.1379 | 0.7965 | 1.1574 | 0.5017 | 20.4533 | 5 | 0.9457 | 0.9417 | 0.9351 | 0.9109 | 0.833 | 0.9653 | 0.7744 | 0.0482 | 0.7001 | 0.994 | 0.4346 | 6.9787 | 14.7354 | 1.007 | 0.8519 | 0.3739 | 19.4985 | -61.362 | 19.7692 | -56.9152 | 20.278 | -58.6698 |
| 12 | $E_{M06}$, $E^{LUMO}_{M06}$ | 0.5557 | 0.2372 | 0.7411 | 0.0518 | 0.7929 | -0.1318 | 0.8963 | 1.3127 | 0.5836 | 15.3127 | 5 | 0.9265 | 0.9211 | 0.9122 | 0.8845 | 0.7745 | 0.9591 | 0.8453 | 0.0274 | 0.6606 | 0.9816 | 0.533 | 8.8362 | 18.9564 | 1.3625 | 0.8152 | 0.0829 | 20.5617 | -63.9972 | 19.6951 | -58.4899 | 20.5158 | -65.3048 |
| 13 | $E_{M06-2X}$, $E^{LUMO}_{M06-2X}$ | 0.5184 | 0.2645 | 0.7286 | 0.0543 | 0.7829 | -0.1317 | 0.9176 | 1.3668 | 0.732 | 14.4237 | 5 | 0.8844 | 0.8759 | 0.8619 | 0.8782 | 0.7548 | 0.9321 | 0.8429 | 0.0383 | 0.6927 | 1.0432 | 0.683 | 9.2626 | 20.5485 | 2.1431 | 0.8016 | -0.0577 | 20.0308 | -63.4254 | 19.6596 | -57.2943 | 20.2048 | -64.3493 |
| 14 | $E_{M06}$, $\omega_{M06}$ | 0.5123 | 0.2562 | 0.7107 | 0.0579 | 0.7686 | -0.1303 | 0.9474 | 1.3753 | 0.6217 | 13.2826 | 5 | 0.9166 | 0.9105 | 0.9003 | 0.8691 | 0.7503 | 0.953 | 0.8555 | 0.0396 | 0.7197 | 1.0622 | 0.6105 | 9.8742 | 20.806 | 1.5461 | 0.7869 | -0.2663 | 20.0267 | -62.0108 | 19.7598 | -57.9131 | 19.9072 | -61.7964 |
| 15 | $E_{M06-L}$, $\omega_{M06-L}$ | 0.3121 | 0.4052 | 0.6466 | 0.0707 | 0.7173 | -0.1208 | 1.0471 | 1.6333 | 0.6763 | 10.1494 | 5 | 0.9013 | 0.8941 | 0.8821 | 0.8354 | 0.6628 | 0.9394 | 0.8856 | 0.0487 | 0.8545 | 1.2895 | 0.6522 | 12.0607 | 29.3461 | 1.8297 | 0.7490 | -0.5231 | 19.9278 | -59.3158 | 20.769 | -55.7784 | 20.516 | -58.0956 |

Models are arranged according to $Q^2_{LOO}$ values.

Parameters are obtained through QSARINS software. Ref. [54] N. Chirico, E. Papa, S. Kovarich, S. Cassani, P. Gramatica, QSAR Res. Unit in Environ. Chem. and Ecotox. University of Insubria, Varese, Italy, 2012. (http://www.qsar.it).

$R^2_{adj}$ adjusted $R^2$

*N. Ext.OK* Number of external validation parameters meeting threshold values

*F* "F-test" statistic value

**Table S23.** Value of internal and external validation parameters of two-descriptor QSAR models, for mutagenicity (LogTA100), developed using electron-correlation (CORR(HFX+LYP), CORR(BLYP), CORR(B3LYP)) based methods through activity sampling (ordered response) splitting method.

| Model | Variables | $Q^2_{LOO}$ | $R^2$-$Q^2_{LOO}$ | $R^2_{adj}$ | $R^2$-$R^2_{adj}$ | $R^2$ | $\Delta K$ | $RMSE_{TR}$ | $RMSE_{CV}$ | $RMSE_{EXT}$ | $F$ | *N. Ext.OK* | $Q^2_{F1}$ | $Q^2_{F2}$ | $Q^2_{F3}$ | $CCC_{TR}$ | $CCC_{CV}$ | $CCC_{EXT}$ | $\bar{r}^2_m$ | $\Delta r^2_m$ | $MAE_{TR}$ | $MAE_{CV}$ | $MAE_{EXT}$ | $RSS_{TR}$ | $PRESS_{CV}$ | $PRESS_{EXT}$ | $R^2_{LMO}$ | $Q^2_{LMO}$ | $R^2_{Yscr}$ | $Q^2_{Yscr}$ | $R^2_{Xrand}$ | $Q^2_{Xrand}$ | $R^2_{Yrand}$ | $Q^2_{Yrand}$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | $E_{CORR(B3LYP)}$, $E^{HOMO}_{CORR(B3LYP)}$ | 0.7316 | 0.0638 | 0.7759 | 0.0195 | 0.7954 | 0.2918 | 0.8486 | 0.9720 | 0.6796 | 40.8131 | 5 | 0.8194 | 0.8164 | 0.8687 | 0.8860 | 0.8537 | 0.8979 | 0.7899 | 0.0741 | 0.6628 | 0.7601 | 0.5374 | 17.2837 | 22.6726 | 10.1623 | 0.7983 | 0.7184 | 8.5818 | -19.8806 | 8.8958 | -19.6206 | 8.5980 | -20.3638 |
| 2 | $E_{CORR(B3LYP)}$, $\eta_{CORR(B3LYP)}$ | 0.7140 | 0.0662 | 0.7593 | 0.0209 | 0.7802 | 0.0759 | 0.8795 | 1.0033 | 0.8843 | 37.2770 | 1 | 0.6942 | 0.6892 | 0.7778 | 0.8765 | 0.8433 | 0.8465 | 0.6090 | 0.0998 | 0.6903 | 0.7933 | 0.7837 | 18.5629 | 24.1581 | 17.2038 | 0.7875 | 0.6954 | 8.7341 | -20.7888 | 9.2896 | -19.1411 | 8.7284 | -20.5103 |
| 3 | $E_{CORR(B3LYP)}$, $\omega_{CORR(B3LYP)}$ | 0.7074 | 0.0691 | 0.7552 | 0.0213 | 0.7764 | 0.2506 | 0.8870 | 1.0148 | 0.7811 | 36.4691 | 4 | 0.7614 | 0.7575 | 0.8266 | 0.8742 | 0.8391 | 0.8456 | 0.6957 | 0.1080 | 0.6886 | 0.7902 | 0.6194 | 18.8822 | 24.7146 | 13.4224 | 0.7838 | 0.6829 | 8.6179 | -20.1660 | 8.7765 | -19.7794 | 8.9349 | -19.7431 |
| 4 | $E_{CORR(B3LYP)}$, $\chi_{CORR(B3LYP)}$ | 0.6148 | 0.0941 | 0.6812 | 0.0277 | 0.7090 | 0.2006 | 1.0121 | 1.1643 | 0.8699 | 25.5776 | 3 | 0.7041 | 0.6992 | 0.7850 | 0.8297 | 0.7825 | 0.7957 | 0.6789 | 0.1158 | 0.8110 | 0.9302 | 0.6906 | 24.5826 | 32.5320 | 16.6488 | 0.7217 | 0.5871 | 8.7722 | -20.3955 | 8.8063 | -19.4989 | 8.3950 | -20.6244 |
| 5 | $E_{CORR(HFX+LYP)}$, $E^{HOMO}_{CORR(HFX+LYP)}$ | 0.5811 | 0.1030 | 0.6540 | 0.0301 | 0.6841 | 0.2542 | 1.0545 | 1.2142 | 0.8869 | 22.7332 | 2 | 0.6924 | 0.6874 | 0.7765 | 0.8124 | 0.7608 | 0.8100 | 0.6760 | 0.0995 | 0.8953 | 1.0283 | 0.7326 | 26.6866 | 35.3827 | 17.3041 | 0.6978 | 0.5577 | 8.5996 | -20.1505 | 8.6091 | -19.9511 | 8.9524 | -19.3428 |
| 6 | $E_{CORR(BLYP)}$, $\eta_{CORR(BLYP)}$ | 0.5613 | 0.1018 | 0.6310 | 0.0321 | 0.6631 | 0.2905 | 1.0889 | 1.2426 | 1.0263 | 20.6632 | 1 | 0.5881 | 0.5813 | 0.7007 | 0.7974 | 0.7454 | 0.7027 | 0.5875 | 0.0836 | 0.9167 | 1.0454 | 0.8590 | 28.4592 | 37.0588 | 23.1742 | 0.6749 | 0.3861 | 8.7603 | -20.7541 | 8.7057 | -19.9187 | 8.5276 | -21.3903 |
| 7 | $E_{CORR(BLYP)}$, $E^{HOMO}_{CORR(BLYP)}$ | 0.5598 | 0.1032 | 0.6310 | 0.0321 | 0.6631 | 0.3283 | 1.0889 | 1.2446 | 1.0114 | 20.6643 | 1 | 0.6000 | 0.5934 | 0.7093 | 0.7974 | 0.7445 | 0.7104 | 0.5989 | 0.1029 | 0.9138 | 1.0445 | 0.8385 | 28.4582 | 37.1781 | 22.5061 | 0.6737 | 0.5409 | 9.0654 | -20.4579 | 8.5227 | -20.1933 | 8.8310 | -21.1491 |
| 8 | $E_{CORR(BLYP)}$, $\chi_{CORR(BLYP)}$ | 0.5570 | 0.1053 | 0.6302 | 0.0322 | 0.6624 | 0.3680 | 1.0900 | 1.2486 | 1.0002 | 20.6001 | 1 | 0.6088 | 0.6024 | 0.7158 | 0.7969 | 0.7425 | 0.7170 | 0.6057 | 0.1143 | 0.9169 | 1.0527 | 0.8168 | 28.5170 | 37.4144 | 22.0082 | 0.6747 | 0.5176 | 8.7120 | -21.2602 | 9.1549 | -19.2641 | 8.4688 | -21.1907 |
| 9 | $E_{CORR(HFX+LYP)}$, $\chi_{CORR(HFX+LYP)}$ | 0.5504 | 0.1192 | 0.6381 | 0.0315 | 0.6696 | 0.0980 | 1.0783 | 1.2579 | 0.9148 | 21.2803 | 2 | 0.6728 | 0.6674 | 0.7622 | 0.8021 | 0.7413 | 0.7855 | 0.6690 | 0.0379 | 0.8921 | 1.0368 | 0.7653 | 27.9066 | 37.9781 | 18.4107 | 0.6846 | 0.5373 | 8.6560 | -20.1316 | 8.6377 | -19.7756 | 8.6007 | -20.4133 |
| 10 | $E_{CORR(BLYP)}$, $E^{LUMO}_{CORR(BLYP)}$ | 0.5354 | 0.1162 | 0.6184 | 0.0332 | 0.6516 | 0.0777 | 1.1073 | 1.2787 | 1.0257 | 19.6386 | 1 | 0.5886 | 0.5818 | 0.7011 | 0.7891 | 0.7306 | 0.7090 | 0.5923 | 0.0329 | 0.9385 | 1.0804 | 0.8319 | 29.4267 | 39.2400 | 23.1462 | 0.6662 | 0.5254 | 8.4540 | -20.8180 | 9.1036 | -19.1342 | 8.8774 | -19.8428 |
| 11 | $E_{CORR(HFX+LYP)}$, $\eta_{CORR(HFX+LYP)}$ | 0.5315 | 0.1260 | 0.6249 | 0.0326 | 0.6575 | 0.2027 | 1.0978 | 1.2840 | 1.0298 | 20.1608 | 0 | 0.5854 | 0.5785 | 0.6987 | 0.7934 | 0.7325 | 0.7101 | 0.5982 | 0.0067 | 0.9229 | 1.0718 | 0.8315 | 28.9255 | 39.5683 | 23.3294 | 0.6733 | 0.5461 | 8.6228 | -19.8037 | 8.7390 | -19.6208 | 8.7043 | -20.0552 |
| 12 | $E_{CORR(HFX+LYP)}$, $E^{LUMO}_{CORR(HFX+LYP)}$ | 0.5299 | 0.1298 | 0.6272 | 0.0324 | 0.6596 | 0.1022 | 1.0945 | 1.2863 | 0.9869 | 20.3487 | 1 | 0.6192 | 0.6129 | 0.7232 | 0.7949 | 0.7300 | 0.7332 | 0.6128 | 0.0553 | 0.9256 | 1.0808 | 0.8134 | 28.7494 | 39.7093 | 21.4278 | 0.6779 | 0.5120 | 8.6127 | -20.4149 | 8.2008 | -20.5684 | 8.8164 | -19.9156 |
| 13 | $E_{CORR(B3LYP)}$, $E^{LUMO}_{CORR(B3LYP)}$ | 0.4928 | 0.1407 | 0.5987 | 0.0349 | 0.6336 | 0.0198 | 1.1356 | 1.3360 | 1.0909 | 18.1550 | 0 | 0.5347 | 0.5270 | 0.6618 | 0.7757 | 0.6984 | 0.6598 | 0.5239 | 0.0790 | 0.9535 | 1.1156 | 0.8731 | 30.9503 | 42.8382 | 26.1821 | 0.6513 | 0.4949 | 8.2016 | -21.3063 | 8.7201 | -19.9390 | 8.9866 | -20.4215 |
| 14* | $E_{CORR(BLYP)}$, $\omega_{CORR(BLYP)}$ | 0.6948 | 0.0736 | 0.7412 | 0.0272 | 0.7684 | 0.2315 | 0.7479 | 0.8587 | 0.9434 | 28.2024 | 0 | 0.4828 | 0.4820 | 0.6316 | 0.8690 | 0.8315 | 0.7161 | 0.4592 | 0.0476 | 0.6525 | 0.7582 | 0.7615 | 11.1881 | 14.7457 | 16.0193 | 0.7702 | 0.6389 | 10.5104 | -25.7058 | 11.1067 | -23.6962 | 10.6530 | -25.2916 |
| 15* | $E_{CORR(HFX+LYP)}$, $\omega_{CORR(HFX+LYP)}$ | 0.6213 | 0.1061 | 0.6970 | 0.0303 | 0.7273 | 0.1896 | 0.9478 | 1.1170 | 0.9486 | 24.0054 | 1 | 0.6616 | 0.6616 | 0.7269 | 0.8421 | 0.7833 | 0.7993 | 0.5223 | 0.1645 | 0.7354 | 0.8645 | 0.7866 | 18.8643 | 26.2012 | 17.9951 | 0.7345 | 0.5720 | 10.0636 | -23.0298 | 10.1334 | -23.2785 | 9.5411 | -23.6776 |

*Computed using data set represented with (c) and (b) respectively in Supporting Information Table S3.

Models are arranged according to $Q^2_{LOO}$ values.

Parameters are obtained through QSARINS software. Ref. [54] N. Chirico, E. Papa, S. Kovarich, S. Cassani, P. Gramatica, QSAR Res. Unit in Environ. Chem. and Ecotox. University of Insubria, Varese, Italy, 2012. (http://www.qsar.it).

$R^2_{adj}$ adjusted $R^2$

*N. Ext.OK* Number of external validation parameters meeting threshold values

*F* "F-test" statistic value

**Table S24.** Value of internal and external validation parameters of two-descriptor QSAR models, for mutagenicity (LogTA100), developed using electron-correlation (CORR(HFX+LYP), CORR(BLYP), CORR(B3LYP)) based methods through 30% (random) splitting method.

| Model | Variables | $Q^2_{LOO}$ | $R^2$-$Q^2_{LOO}$ | $R^2_{adj}$ | $R^2$-$R^2_{adj}$ | $R^2$ | $\Delta K$ | $RMSE_{TR}$ | $RMSE_{CV}$ | $RMSE_{EXT}$ | $F$ | *N. Ext.OK* | $Q^2_{F1}$ | $Q^2_{F2}$ | $Q^2_{F3}$ | $CCC_{TR}$ | $CCC_{CV}$ | $CCC_{EXT}$ | $\bar{r}^2_m$ | $\Delta r^2_m$ | $MAE_{TR}$ | $MAE_{CV}$ | $MAE_{EXT}$ | $RSS_{TR}$ | $PRESS_{CV}$ | $PRESS_{EXT}$ | $R^2_{LMO}$ | $Q^2_{LMO}$ | $R^2_{Yscr}$ | $Q^2_{Yscr}$ | $R^2_{Xrand}$ | $Q^2_{Xrand}$ | $R^2_{Yrand}$ | $Q^2_{Yrand}$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | $E_{CORR(B3LYP)}$, $\omega_{CORR(B3LYP)}$ | 0.7300 | 0.0423 | 0.7576 | 0.0147 | 0.7723 | 0.4161 | 0.8490 | 0.9245 | 0.5696 | 52.5632 | 5 | 0.8574 | 0.8463 | 0.8975 | 0.8715 | 0.8495 | 0.9117 | 0.8230 | 0.0489 | 0.7074 | 0.7740 | 0.4538 | 24.5056 | 29.0577 | 3.8934 | 0.7767 | 0.7037 | 5.8120 | -13.7357 | 6.1898 | -13.0184 | 6.2578 | -13.0349 |
| 2 | $E_{CORR(B3LYP)}$, $\eta_{CORR(B3LYP)}$ | 0.7285 | 0.0522 | 0.7666 | 0.0141 | 0.7807 | 0.1350 | 0.8331 | 0.9270 | 0.8462 | 55.1825 | 1 | 0.6852 | 0.6608 | 0.7737 | 0.8769 | 0.8500 | 0.7921 | 0.5166 | 0.1456 | 0.7054 | 0.7806 | 0.7110 | 23.5975 | 29.2155 | 8.5931 | 0.7865 | 0.7093 | 6.0928 | -13.6483 | 6.1851 | -13.0131 | 6.0133 | -13.4949 |
| 3 | $E_{CORR(B3LYP)}$, $E^{HOMO}_{CORR(B3LYP)}$ | 0.7269 | 0.0524 | 0.7650 | 0.0142 | 0.7793 | 0.2428 | 0.8358 | 0.9298 | 0.6599 | 54.7232 | 5 | 0.8085 | 0.7937 | 0.8624 | 0.8759 | 0.8493 | 0.8739 | 0.6864 | 0.0880 | 0.6987 | 0.7739 | 0.5388 | 23.7518 | 29.3930 | 5.2259 | 0.7819 | 0.7144 | 6.0064 | -13.7885 | 6.2754 | -12.9220 | 5.7498 | -13.8372 |
| 4 | $E_{CORR(B3LYP)}$, $\chi_{CORR(B3LYP)}$ | 0.6892 | 0.0502 | 0.7226 | 0.0168 | 0.7394 | 0.3932 | 0.9082 | 0.9918 | 0.6894 | 43.9734 | 5 | 0.7911 | 0.7748 | 0.8498 | 0.8502 | 0.8237 | 0.8616 | 0.7337 | 0.0815 | 0.7519 | 0.8230 | 0.5025 | 28.0449 | 33.4434 | 5.7031 | 0.7411 | 0.6684 | 6.3193 | -13.0769 | 6.1666 | -12.9331 | 6.5960 | -12.6326 |
| 5 | $E_{CORR(BLYP)}$, $\chi_{CORR(BLYP)}$ | 0.6755 | 0.0506 | 0.7085 | 0.0177 | 0.7261 | 0.4132 | 0.9310 | 1.0134 | 0.8213 | 41.1001 | 2 | 0.7034 | 0.6804 | 0.7868 | 0.8414 | 0.8140 | 0.7893 | 0.6028 | 0.1161 | 0.7655 | 0.8373 | 0.6626 | 29.4686 | 34.9151 | 8.0954 | 0.7276 | 0.6541 | 6.0782 | -13.7373 | 6.2074 | -13.0593 | 5.7923 | -14.8742 |
| 6 | $E_{CORR(BLYP)}$, $\eta_{CORR(BLYP)}$ | 0.6755 | 0.0480 | 0.7056 | 0.0178 | 0.7235 | 0.3482 | 0.9355 | 1.0135 | 0.8506 | 40.5513 | 1 | 0.6819 | 0.6572 | 0.7714 | 0.8395 | 0.8135 | 0.7705 | 0.6133 | 0.1132 | 0.7713 | 0.8390 | 0.7241 | 29.7572 | 34.9238 | 8.6831 | 0.7262 | 0.5960 | 5.8767 | -14.3557 | 6.2288 | -12.8752 | 6.1137 | -14.3599 |
| 7 | $E_{CORR(BLYP)}$, $E^{HOMO}_{CORR(BLYP)}$ | 0.6748 | 0.0493 | 0.7063 | 0.0178 | 0.7241 | 0.3775 | 0.9344 | 1.0145 | 0.8271 | 40.6856 | 1 | 0.6993 | 0.6760 | 0.7839 | 0.8400 | 0.8133 | 0.7833 | 0.6153 | 0.1128 | 0.7701 | 0.8403 | 0.6860 | 29.6860 | 34.9897 | 8.2082 | 0.7241 | 0.6025 | 5.9723 | -14.5012 | 6.0097 | -13.2461 | 6.0453 | -13.9386 |
| 8 | $E_{CORR(HFX+LYP)}$, $E^{HOMO}_{CORR(HFX+LYP)}$ | 0.6746 | 0.0551 | 0.7123 | 0.0174 | 0.7297 | 0.2939 | 0.9249 | 1.0148 | 0.7243 | 41.8418 | 4 | 0.7693 | 0.7514 | 0.8342 | 0.8437 | 0.8145 | 0.8428 | 0.7305 | 0.0614 | 0.7938 | 0.8716 | 0.5633 | 29.0875 | 35.0146 | 6.2960 | 0.7310 | 0.6591 | 5.9475 | -13.3280 | 6.3815 | -12.7102 | 6.1515 | -13.2789 |
| 9 | $E_{CORR(HFX+LYP)}$, $\chi_{CORR(HFX+LYP)}$ | 0.6604 | 0.0629 | 0.7055 | 0.0179 | 0.7233 | 0.3913 | 0.9358 | 1.0367 | 0.7951 | 40.5177 | 4 | 0.7220 | 0.7005 | 0.8002 | 0.8394 | 0.8046 | 0.8175 | 0.6626 | 0.0137 | 0.7752 | 0.8547 | 0.6367 | 29.7750 | 36.5435 | 7.5869 | 0.7271 | 0.6611 | 6.0901 | -13.2748 | 6.1081 | -13.2016 | 5.8029 | -13.6337 |
| 10 | $E_{CORR(HFX+LYP)}$, $\eta_{CORR(HFX+LYP)}$ | 0.6595 | 0.0555 | 0.6966 | 0.0184 | 0.7150 | 0.2005 | 0.9497 | 1.0381 | 0.8081 | 38.8916 | 2 | 0.7129 | 0.6907 | 0.7937 | 0.8338 | 0.8042 | 0.7959 | 0.6426 | 0.1059 | 0.8086 | 0.8866 | 0.6448 | 30.6651 | 36.6404 | 7.8356 | 0.7217 | 0.6253 | 6.2968 | -13.0442 | 6.1381 | -13.0603 | 5.8093 | -13.5624 |
| 11 | $E_{CORR(HFX+LYP)}$, $E^{LUMO}_{CORR(HFX+LYP)}$ | 0.6545 | 0.0624 | 0.6986 | 0.0183 | 0.7169 | 0.2128 | 0.9466 | 1.0457 | 0.8553 | 39.2459 | 1 | 0.6784 | 0.6534 | 0.7689 | 0.8351 | 0.8007 | 0.7868 | 0.6044 | 0.0431 | 0.7734 | 0.8536 | 0.6889 | 30.4667 | 37.1805 | 8.7786 | 0.7218 | 0.6418 | 6.0580 | -13.5194 | 5.6578 | -13.6882 | 5.9416 | -13.4927 |
| 12 | $E_{CORR(BLYP)}$, $E^{LUMO}_{CORR(BLYP)}$ | 0.6469 | 0.0627 | 0.6909 | 0.0187 | 0.7097 | 0.1624 | 0.9586 | 1.0571 | 0.9293 | 37.8858 | 1 | 0.6204 | 0.5909 | 0.7272 | 0.8302 | 0.7956 | 0.7566 | 0.5318 | 0.0841 | 0.7960 | 0.8753 | 0.7793 | 31.2429 | 37.9922 | 10.3624 | 0.7145 | 0.6371 | 6.3975 | -12.7487 | 6.2690 | -13.1105 | 6.1649 | -13.1672 |
| 13 | $E_{CORR(B3LYP)}$, $E^{LUMO}_{CORR(B3LYP)}$ | 0.6030 | 0.0936 | 0.6770 | 0.0196 | 0.6966 | 0.0659 | 0.9800 | 1.1209 | 1.0021 | 35.5805 | 0 | 0.5585 | 0.5243 | 0.6827 | 0.8211 | 0.7683 | 0.6961 | 0.4339 | 0.1528 | 0.8235 | 0.9261 | 0.8117 | 32.6529 | 42.7216 | 12.0501 | 0.7078 | 0.6061 | 5.9775 | -13.6795 | 6.0562 | -13.3007 | 5.6018 | -14.7448 |
| 14* | $E_{CORR(BLYP)}$, $\omega_{CORR(BLYP)}$ | 0.6766 | 0.0585 | 0.7120 | 0.0230 | 0.7351 | 0.0959 | 0.7445 | 0.8226 | 1.0635 | 31.9059 | 0 | 0.4638 | 0.4588 | 0.4594 | 0.8473 | 0.8162 | 0.5607 | 0.4721 | 0.1355 | 0.6354 | 0.7097 | 0.8428 | 14.4105 | 17.5914 | 12.4405 | 0.7351 | 0.6273 | 7.9407 | -18.9697 | 8.4925 | -17.3485 | 7.5899 | -18.8297 |
| 15* | $E_{CORR(HFX+LYP)}$, $\omega_{CORR(HFX+LYP)}$ | 0.6627 | 0.0640 | 0.7057 | 0.0210 | 0.7267 | 0.2099 | 0.8787 | 0.9762 | 1.0645 | 34.5727 | 0 | 0.6648 | 0.6607 | 0.5989 | 0.8417 | 0.8055 | 0.7905 | 0.5912 | 0.1370 | 0.6979 | 0.7778 | 0.9469 | 22.3911 | 27.6362 | 13.5990 | 0.7287 | 0.6295 | 7.2501 | -15.6239 | 7.1459 | -15.8096 | 7.5236 | -15.5867 |

*Computed using data set represented with (c) and (b) respectively in Supporting Information Table S3.

Models are arranged according to $Q^2_{LOO}$ values.

Parameters are obtained through QSARINS software. Ref. [54] N. Chirico, E. Papa, S. Kovarich, S. Cassani, P. Gramatica, QSAR Res. Unit in Environ. Chem. and Ecotox. University of Insubria, Varese, Italy, 2012. (http://www.qsar.it).

$R^2_{adj}$ adjusted $R^2$

*N. Ext.OK* Number of external validation parameters meeting threshold values

$F$ "F-test" statistic value

**Table S25.** Value of internal and external validation parameters of two-descriptor QSAR models, for mutagenicity (LogTA98), developed using electron-correlation (CORR(HFX+LYP), CORR(BLYP), CORR(B3LYP)) based methods through activity sampling (ordered response) splitting method.

| Model | Variables | $Q^2_{LOO}$ | $R^2$-$Q^2_{LOO}$ | $R^2_{adj}$ | $R^2$-$R^2_{adj}$ | $R^2$ | $\Delta K$ | $RMSE_{TR}$ | $RMSE_{CV}$ | $RMSE_{EXT}$ | $F$ | N. Ext.OK | $Q^2_{F1}$ | $Q^2_{F2}$ | $Q^2_{F3}$ | $CCC_{TR}$ | $CCC_{CV}$ | $CCC_{EXT}$ | $\bar{r}^2_m$ | $\Delta r^2_m$ | $MAE_{TR}$ | $MAE_{CV}$ | $MAE_{EXT}$ | $RSS_{TR}$ | $PRESS_{CV}$ | $PRESS_{EXT}$ | $R^2_{LMO}$ | $Q^2_{LMO}$ | $R^2_{Yscr}$ | $Q^2_{Yscr}$ | $R^2_{Yrand}$ | $Q^2_{Yrand}$ | $R^2_{Yrand}$ | $Q^2_{Yrand}$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | $E_{CORR(HFX+LYP)}$, $E^{LUMO}_{CORR(HFX+LYP)}$ | 0.9857 | 0.006 | 0.9884 | 0.0033 | 0.9917 | 0.1925 | 0.1967 | 0.2588 | 0.8696 | 300.0248 | 5 | 0.8305 | 0.8174 | 0.8385 | 0.9959 | 0.9928 | 0.9236 | 0.834 | 0.0702 | 0.149 | 0.2045 | 0.7153 | 0.3095 | 0.5357 | 3.7814 | 0.9917 | 0.6673 | 30.568 | -90.9253 | 28.6292 | -114.2375 | 26.0326 | -109.1877 |
| 2 | $E_{CORR(HFX+LYP)}$, $\chi_{CORR(HFX+LYP)}$ | 0.969 | 0.0178 | 0.9815 | 0.0053 | 0.9868 | 0.3371 | 0.2485 | 0.3808 | 0.6743 | 187.0138 | 5 | 0.8981 | 0.8902 | 0.9029 | 0.9934 | 0.9845 | 0.9481 | 0.8655 | 0.0556 | 0.1921 | 0.3014 | 0.5028 | 0.4941 | 1.16 | 2.2737 | 0.9881 | 0.6725 | 31.3447 | -86.6643 | 29.8416 | -102.8297 | 29.9057 | -93.7522 |
| 3 | $E_{CORR(HFX+LYP)}$, $\eta_{CORR(HFX+LYP)}$ | 0.9433 | 0.0255 | 0.9564 | 0.0125 | 0.9688 | 0.1122 | 0.382 | 0.5152 | 1.1211 | 77.7319 | 4 | 0.7184 | 0.6965 | 0.7316 | 0.9842 | 0.9717 | 0.8754 | 0.757 | 0.024 | 0.3003 | 0.4295 | 0.9603 | 1.1672 | 2.1235 | 6.2839 | 0.9682 | 0.4754 | 29.0884 | -104.0019 | 28.1578 | -112.7071 | 27.9369 | -108.8094 |
| 4 | $E_{CORR(B3LYP)}$, $E^{HOMO}_{CORR(B3LYP)}$ | 0.9418 | 0.0333 | 0.9652 | 0.01 | 0.9751 | 0.1537 | 0.3413 | 0.522 | 0.4817 | 97.9877 | 5 | 0.948 | 0.944 | 0.9504 | 0.9874 | 0.9704 | 0.9708 | 0.8963 | 0.0363 | 0.2944 | 0.4691 | 0.3333 | 0.9319 | 2.1801 | 1.1602 | 0.9768 | 0.4862 | 28.8528 | -102.3972 | 30.4638 | -96.361 | 28.4378 | -104.8297 |
| 5 | $E_{CORR(HFX+LYP)}$, $E^{HOMO}_{CORR(HFX+LYP)}$ | 0.9263 | 0.0465 | 0.9619 | 0.0109 | 0.9728 | 0.3776 | 0.3567 | 0.5875 | 0.6179 | 89.4806 | 5 | 0.9144 | 0.9078 | 0.9185 | 0.9862 | 0.9631 | 0.9556 | 0.8738 | 0.0512 | 0.3036 | 0.5149 | 0.4609 | 1.0181 | 2.7617 | 1.9091 | 0.9764 | 0.3271 | 29.4168 | -98.4941 | 29.0534 | -105.5568 | 29.2124 | -100.887 |
| 6 | $E_{CORR(B3LYP)}$, $\omega_{CORR(B3LYP)}$ | 0.9235 | 0.0485 | 0.9608 | 0.0112 | 0.972 | 0.4051 | 0.3621 | 0.5986 | 0.4235 | 86.7637 | 5 | 0.9598 | 0.9567 | 0.9617 | 0.9858 | 0.9617 | 0.9782 | 0.9267 | 0.027 | 0.3116 | 0.5309 | 0.3087 | 1.0491 | 2.8669 | 0.8967 | 0.9754 | 0.1582 | 28.5195 | -100.3837 | 29.2347 | -107.8823 | 27.8915 | -103.8511 |
| 7 | $E_{CORR(BLYP)}$, $\chi_{CORR(BLYP)}$ | 0.9017 | 0.0679 | 0.9573 | 0.0122 | 0.9695 | 0.1141 | 0.3777 | 0.6786 | 0.6948 | 79.5624 | 5 | 0.8918 | 0.8834 | 0.8969 | 0.9845 | 0.9495 | 0.9475 | 0.8864 | 0.0064 | 0.3323 | 0.6047 | 0.5562 | 1.1412 | 3.684 | 2.4139 | 0.9743 | 0.2572 | 28.0261 | -178.0529 | 29.0357 | -106.6961 | 30.4532 | -173.2299 |
| 8 | $E_{CORR(BLYP)}$, $E^{HOMO}_{CORR(BLYP)}$ | 0.8987 | 0.0693 | 0.9551 | 0.0128 | 0.9679 | 0.2028 | 0.3874 | 0.6887 | 0.7105 | 75.4813 | 5 | 0.8869 | 0.8781 | 0.8922 | 0.9837 | 0.9479 | 0.9434 | 0.8627 | 0.0584 | 0.3559 | 0.6309 | 0.5702 | 1.2009 | 3.7949 | 2.5241 | 0.9727 | 0.2441 | 29.9875 | -122.7008 | 28.5371 | -105.595 | 29.9511 | -128.4131 |
| 9 | $E_{CORR(B3LYP)}$, $\chi_{CORR(B3LYP)}$ | 0.8922 | 0.0677 | 0.9439 | 0.016 | 0.9599 | 0.4292 | 0.4332 | 0.7105 | 0.5993 | 59.8744 | 5 | 0.9195 | 0.9133 | 0.9233 | 0.9795 | 0.9451 | 0.9507 | 0.8919 | 0.0462 | 0.3467 | 0.5743 | 0.5298 | 1.5014 | 4.0384 | 1.7958 | 0.9659 | 0.0786 | 29.5733 | -92.1222 | 27.6814 | -106.7811 | 29.5312 | -96.0842 |
| 10 | $E_{CORR(BLYP)}$, $E^{LUMO}_{CORR(BLYP)}$ | 0.8744 | 0.0887 | 0.9485 | 0.0147 | 0.9632 | 0.0589 | 0.4151 | 0.7667 | 0.6419 | 65.4247 | 5 | 0.9077 | 0.9005 | 0.912 | 0.9813 | 0.9357 | 0.9553 | 0.9051 | 0.0075 | 0.3798 | 0.6793 | 0.5335 | 1.3787 | 4.703 | 2.0599 | 0.9688 | 0.0210 | 28.7581 | -113.3556 | 29.682 | -95.7111 | 28.6299 | -120.5318 |
| 11 | $E_{CORR(B3LYP)}$, $\eta_{CORR(B3LYP)}$ | 0.8549 | 0.1049 | 0.9436 | 0.0161 | 0.9597 | 0.087 | 0.4343 | 0.8244 | 0.7223 | 59.5691 | 5 | 0.8831 | 0.874 | 0.8886 | 0.9794 | 0.9286 | 0.9411 | 0.8321 | 0.0593 | 0.3995 | 0.6991 | 0.5685 | 1.5087 | 5.437 | 2.6083 | 0.9649 | 0.0658 | 26.7928 | -100.2076 | 28.451 | -108.2405 | 30.1534 | -89.2488 |
| 12 | $E_{CORR(B3LYP)}$, $E^{LUMO}_{CORR(B3LYP)}$ | 0.8514 | 0.0777 | 0.9007 | 0.0284 | 0.9291 | 0.0695 | 0.5762 | 0.8342 | 0.8242 | 32.7528 | 5 | 0.8478 | 0.836 | 0.8549 | 0.9632 | 0.9242 | 0.9193 | 0.7774 | 0.0885 | 0.4695 | 0.7105 | 0.5564 | 2.6564 | 5.5676 | 3.3966 | 0.9305 | -0.2365 | 28.5725 | -93.5056 | 29.2535 | -101.2577 | 29.4615 | -86.6797 |
| 13 | $E_{CORR(BLYP)}$, $\eta_{CORR(BLYP)}$ | 0.8419 | 0.1027 | 0.9224 | 0.0222 | 0.9446 | 0.0223 | 0.5094 | 0.8603 | 0.6913 | 42.6178 | 5 | 0.8929 | 0.8846 | 0.8979 | 0.9715 | 0.9215 | 0.9434 | 0.8404 | 0.0642 | 0.4344 | 0.7419 | 0.497 | 2.0756 | 5.9212 | 2.3897 | 0.9488 | -0.1774 | 27.8207 | -96.2285 | 27.5899 | -119.1871 | 28.3649 | -93.9013 |
| 14** | $E_{CORR(HFX+LYP)}$, $\omega_{CORR(HFX+LYP)}$ | 0.7610 | 0.1867 | 0.9303 | 0.0174 | 0.9477 | 0.0998 | 0.4869 | 1.0410 | 0.9304 | 54.3871 | 3 | 0.7027 | 0.7026 | 0.8091 | 0.9732 | 0.8728 | 0.8178 | 0.5004 | 0.2375 | 0.4152 | 0.7658 | 0.6919 | 2.1333 | 9.7535 | 5.1935 | 0.9575 | -0.9896 | 24.5289 | -91.8275 | 25.6803 | -80.3081 | 25.1231 | -90.1154 |
| 15** | $E_{CORR(BLYP)}$, $\omega_{CORR(BLYP)}$ | 0.7350 | 0.1805 | 0.8732 | 0.0423 | 0.9155 | 0.1149 | 0.5588 | 0.9895 | 0.8160 | 21.6589 | 1 | 0.5787 | 0.5754 | 0.8198 | 0.9559 | 0.8838 | 0.7169 | 0.6378 | 0.1582 | 0.5075 | 0.9460 | 0.6441 | 2.1861 | 6.8536 | 3.3292 | 0.9129 | -17.3882 | 32.9202 | -204.3347 | 33.6834 | -155.1932 | 31.6185 | -201.5612 |

**Computed using data set represented with (d) and (e) respectively in Supporting Information Table S4.

Models are arranged according to $Q^2_{LOO}$ values.

Parameters are obtained through QSARINS software. Ref. [54] N. Chirico, E. Papa, S. Kovarich, S. Cassani, P. Gramatica, QSAR Res. Unit in Environ. Chem. and Ecotox. University of Insubria, Varese, Italy, 2012. (http://www.qsar.it).

$R^2_{adj}$ adjusted $R^2$

*N. Ext.OK* Number of external validation parameters meeting threshold values

*F* "F-test" statistic value

**Table S26.** Value of internal and external validation parameters of two-descriptor QSAR models, for mutagenicity (LogTA98), developed using electron-correlation (CORR(HFX+LYP), CORR(BLYP), CORR(B3LYP)) based methods through 30% (random) splitting method.

| Model | Variables | $Q^2_{LOO}$ | $R^2$-$Q^2_{LOO}$ | $R^2_{adj}$ | $R^2$-$R^2_{adj}$ | $R^2$ | $\Delta K$ | $RMSE_{TR}$ | $RMSE_{CV}$ | $RMSE_{EXT}$ | $F$ | $N._{Ext.OK}$ | $Q^2_{F1}$ | $Q^2_{F2}$ | $Q^2_{F3}$ | $CCC_{TR}$ | $CCC_{CV}$ | $CCC_{EXT}$ | $\bar{r}^2_m$ | $\Delta r^2_m$ | $MAE_{TR}$ | $MAE_{CV}$ | $MAE_{EXT}$ | $RSS_{TR}$ | $PRESS_{CV}$ | $PRESS_{EXT}$ | $R^2_{LMO}$ | $Q^2_{LMO}$ | $R^2_{Yscr}$ | $Q^2_{Yscr}$ | $R^2_{Xrand}$ | $Q^2_{Xrand}$ | $R^2_{Yrand}$ | $Q^2_{Yrand}$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | $E_{CORR(HFX+LYP)}$, $\chi_{CORR(HFX+LYP)}$ | 0.8736 | 0.0569 | 0.9151 | 0.0154 | 0.9305 | 0.4397 | 0.5149 | 0.6944 | 0.7580 | 60.2690 | 5 | 0.8808 | 0.8807 | 0.8494 | 0.9640 | 0.9341 | 0.9349 | 0.7162 | 0.0843 | 0.4128 | 0.5658 | 0.5025 | 3.1815 | 5.7858 | 2.2984 | 0.9335 | 0.6838 | 17.6814 | -49.8828 | 17.5334 | -50.6731 | 18.9238 | -47.8202 |
| 2 | $E_{CORR(HFX+LYP)}$, $E^{LUMO}_{CORR(HFX+LYP)}$ | 0.8562 | 0.0687 | 0.9082 | 0.0167 | 0.9249 | 0.3625 | 0.5353 | 0.7406 | 0.7399 | 55.4195 | 5 | 0.8865 | 0.8864 | 0.8565 | 0.9610 | 0.9278 | 0.9382 | 0.7201 | 0.0803 | 0.4548 | 0.6264 | 0.4428 | 3.4390 | 6.5826 | 2.1896 | 0.9275 | 0.6527 | 17.8824 | -48.5402 | 17.7493 | -49.9506 | 18.1734 | -49.9844 |
| 3 | $E_{CORR(B3LYP)}$, $\omega_{CORR(B3LYP)}$ | 0.8472 | 0.0644 | 0.8919 | 0.0196 | 0.9116 | 0.2910 | 0.5808 | 0.7636 | 0.6637 | 46.4003 | 5 | 0.9086 | 0.9086 | 0.8845 | 0.9538 | 0.9214 | 0.9517 | 0.7748 | 0.0609 | 0.4535 | 0.6037 | 0.4006 | 4.0483 | 6.9971 | 1.7623 | 0.9138 | 0.6126 | 17.3479 | -50.7034 | 18.5792 | -49.5018 | 18.3787 | -49.7993 |
| 4 | $E_{CORR(HFX+LYP)}$, $\eta_{CORR(HFX+LYP)}$ | 0.8424 | 0.0617 | 0.8828 | 0.0213 | 0.9041 | 0.1990 | 0.6048 | 0.7755 | 0.8583 | 42.4461 | 5 | 0.8472 | 0.8471 | 0.8069 | 0.9497 | 0.9211 | 0.9217 | 0.7318 | 0.0912 | 0.4896 | 0.6551 | 0.5769 | 4.3893 | 7.2160 | 2.9467 | 0.9039 | 0.5415 | 17.0629 | -57.3638 | 17.1314 | -51.2724 | 19.0504 | -53.6329 |
| 5 | $E_{CORR(B3LYP)}$, $\eta_{CORR(B3LYP)}$ | 0.8420 | 0.0859 | 0.9119 | 0.0160 | 0.9279 | 0.0831 | 0.5245 | 0.7764 | 0.9447 | 57.9217 | 5 | 0.8149 | 0.8148 | 0.7661 | 0.9626 | 0.9207 | 0.9084 | 0.6759 | 0.0979 | 0.4262 | 0.5994 | 0.7431 | 3.3011 | 7.2333 | 3.5701 | 0.9322 | 0.6899 | 18.2071 | -51.2352 | 19.0721 | -48.8447 | 18.3919 | -50.2135 |
| 6 | $E_{CORR(BLYP)}$, $E^{LUMO}_{CORR(BLYP)}$ | 0.8370 | 0.0731 | 0.8901 | 0.0200 | 0.9101 | 0.1148 | 0.5858 | 0.7887 | 0.7214 | 45.5462 | 5 | 0.8921 | 0.8920 | 0.8636 | 0.9529 | 0.9150 | 0.9447 | 0.7730 | 0.0656 | 0.4862 | 0.6588 | 0.5139 | 4.1174 | 7.4637 | 2.0817 | 0.9123 | 0.6062 | 18.8179 | -49.4097 | 20.2050 | -46.1911 | 17.5200 | -49.9480 |
| 7 | $E_{CORR(BLYP)}$, $\chi_{CORR(BLYP)}$ | 0.8342 | 0.0798 | 0.8949 | 0.0191 | 0.9140 | 0.2734 | 0.5729 | 0.7955 | 0.7951 | 47.8096 | 5 | 0.8689 | 0.8688 | 0.8343 | 0.9551 | 0.9137 | 0.9313 | 0.7239 | 0.0836 | 0.4589 | 0.6340 | 0.5142 | 3.9393 | 7.5933 | 2.5287 | 0.9191 | 0.6078 | 18.3289 | -48.8464 | 19.2725 | -45.6722 | 17.8342 | -49.6133 |
| 8 | $E_{CORR(BLYP)}$, $\eta_{CORR(BLYP)}$ | 0.8261 | 0.0734 | 0.8772 | 0.0223 | 0.8995 | 0.0519 | 0.6192 | 0.8146 | 0.7560 | 40.2908 | 5 | 0.8815 | 0.8814 | 0.8502 | 0.9471 | 0.9122 | 0.9403 | 0.7927 | 0.0692 | 0.5114 | 0.6884 | 0.5408 | 4.6005 | 7.9622 | 2.2862 | 0.9012 | 0.5336 | 18.3965 | -54.0540 | 17.9292 | -52.1666 | 19.6010 | -49.5501 |
| 9 | $E_{CORR(B3LYP)}$, $\chi_{CORR(B3LYP)}$ | 0.8183 | 0.0751 | 0.8697 | 0.0237 | 0.8934 | 0.3099 | 0.6377 | 0.8326 | 0.8291 | 37.7248 | 5 | 0.8574 | 0.8573 | 0.8199 | 0.9437 | 0.9059 | 0.9229 | 0.7135 | 0.0959 | 0.4918 | 0.6516 | 0.4884 | 4.8801 | 8.3194 | 2.7496 | 0.8958 | 0.5219 | 16.0694 | -54.0524 | 18.2200 | -49.5382 | 17.6263 | -49.5754 |
| 10 | $E_{CORR(B3LYP)}$, $E^{LUMO}_{CORR(B3LYP)}$ | 0.8060 | 0.0821 | 0.8632 | 0.0249 | 0.8880 | 0.0948 | 0.6536 | 0.8604 | 1.0093 | 35.6954 | 5 | 0.7888 | 0.7886 | 0.7331 | 0.9407 | 0.8972 | 0.8972 | 0.6949 | 0.1084 | 0.5492 | 0.7310 | 0.7251 | 5.1265 | 8.8845 | 4.0744 | 0.8888 | 0.4547 | 18.6311 | -46.7816 | 17.5033 | -50.1550 | 20.0132 | -43.9804 |
| 11 | $E_{CORR(B3LYP)}$, $E^{HOMO}_{CORR(B3LYP)}$ | 0.8058 | 0.1123 | 0.8999 | 0.0182 | 0.9181 | 0.1384 | 0.5590 | 0.8609 | 0.8133 | 50.4445 | 5 | 0.8628 | 0.8627 | 0.8267 | 0.9573 | 0.9045 | 0.9270 | 0.6969 | 0.0909 | 0.4169 | 0.6025 | 0.5318 | 3.7503 | 8.8943 | 2.6455 | 0.9259 | 0.5918 | 17.8543 | -50.3190 | 18.5740 | -49.2757 | 18.4400 | -48.8594 |
| 12 | $E_{CORR(BLYP)}$, $E^{HOMO}_{CORR(BLYP)}$ | 0.7845 | 0.1178 | 0.8805 | 0.0217 | 0.9022 | 0.4019 | 0.6108 | 0.9069 | 0.8656 | 41.5279 | 5 | 0.8446 | 0.8445 | 0.8036 | 0.9486 | 0.8917 | 0.9190 | 0.7048 | 0.0966 | 0.4817 | 0.6866 | 0.5659 | 4.4769 | 9.8695 | 2.9974 | 0.9094 | 0.5254 | 19.6301 | -46.1700 | 18.0365 | -49.6408 | 18.5387 | -49.1631 |
| 13 | $E_{CORR(HFX+LYP)}$, $E^{HOMO}_{CORR(HFX+LYP)}$ | 0.7022 | 0.1943 | 0.8735 | 0.0230 | 0.8965 | 0.1876 | 0.6285 | 1.0660 | 0.8352 | 38.9661 | 5 | 0.8553 | 0.8552 | 0.8172 | 0.9454 | 0.8620 | 0.9246 | 0.7274 | 0.0902 | 0.5080 | 0.7665 | 0.5366 | 4.7407 | 13.6364 | 2.7904 | 0.9062 | 0.4129 | 18.7263 | -56.1730 | 18.7885 | -48.3759 | 18.2294 | -56.0729 |
| 14** | $E_{CORR(HFX+LYP)}$, $\omega_{CORR(HFX+LYP)}$ | 0.8190 | 0.0585 | 0.8469 | 0.0306 | 0.8775 | 0.1449 | 0.6932 | 0.8426 | 0.7238 | 28.6553 | 5 | 0.8669 | 0.8443 | 0.8665 | 0.9348 | 0.9038 | 0.9369 | 0.6714 | 0.0846 | 0.5140 | 0.6633 | 0.6290 | 5.2851 | 7.8104 | 2.0953 | 0.8720 | 0.1137 | 21.2369 | -57.1164 | 18.6228 | -59.5211 | 18.8275 | -60.6302 |
| 15** | $E_{CORR(BLYP)}$, $\omega_{CORR(BLYP)}$ | 0.5313 | 0.3321 | 0.8087 | 0.0547 | 0.8634 | 0.1055 | 0.7011 | 1.2985 | 0.5013 | 15.7974 | 5 | 0.7976 | 0.7966 | 0.9301 | 0.9267 | 0.8196 | 0.8790 | 0.7862 | 0.0722 | 0.5608 | 1.0192 | 0.4867 | 3.9321 | 13.4888 | 1.0051 | 0.8741 | -16.8911 | 29.9140 | -146.7222 | 29.3147 | -111.0799 | 28.2766 | -156.3253 |

**Computed using data set represented with (d) and (e) respectively in Supporting Information Table S4.

Models are arranged according to $Q^2_{LOO}$ values.

Parameters are obtained through QSARINS software. Ref. [54] N. Chirico, E. Papa, S. Kovarich, S. Cassani, P. Gramatica, QSAR Res. Unit in Environ. Chem. and Ecotox. University of Insubria, Varese, Italy, 2012. (http://www.qsar.it).

$R^2_{adj}$ adjusted $R^2$

$N._{Ext.OK}$ Number of external validation parameters meeting threshold values

$F$ "F-test" statistic value

**Table S27.** Value of internal and external validation parameters of two-descriptor QSAR models, for mutagenicity (LogTA100), developed using electron-correlation (CORR(M06), CORR(M06-L), CORR(M06-2X)) based methods through activity sampling (ordered response) splitting method.

| Model | Variables | $Q^2_{LOO}$ | $R^2$-$Q^2_{LOO}$ | $R^2_{adj}$ | $R^2$-$R^2_{adj}$ | $R^2$ | $\Delta K$ | $RMSE_{TR}$ | $RMSE_{CV}$ | $RMSE_{EXT}$ | $F$ | *N. Ext.OK* | $Q^2_{F1}$ | $Q^2_{F2}$ | $Q^2_{F3}$ | $CCC_{TR}$ | $CCC_{CV}$ | $CCC_{EXT}$ | $\bar{r}^2_m$ | $\Delta r^2_m$ | $MAE_{TR}$ | $MAE_{CV}$ | $MAE_{EXT}$ | $RSS_{TR}$ | $PRESS_{CV}$ | $PRESS_{EXT}$ | $R^2_{LMO}$ | $Q^2_{LMO}$ | $R^2_{Yscr}$ | $Q^2_{Yscr}$ | $R^2_{Xrand}$ | $Q^2_{Xrand}$ | $R^2_{Yrand}$ | $Q^2_{Yrand}$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | $E_{CORR(M06-L)}$, $E^{HOMO}_{CORR(M06-L)}$ | 0.7274 | 0.0792 | 0.7882 | 0.0184 | 0.8066 | 0.3152 | 0.8304 | 0.9859 | 0.8642 | 43.7948 | 3 | 0.7161 | 0.7124 | 0.7906 | 0.893 | 0.8545 | 0.8111 | 0.5982 | 0.1386 | 0.6279 | 0.7393 | 0.7094 | 16.5513 | 23.3294 | 15.6824 | 0.8157 | 0.7222 | 8.5983 | -20.3654 | 8.4089 | -20.2828 | 8.8788 | -20.0677 |
| 2 | $E_{CORR(M06)}$, $E^{HOMO}_{CORR(M06)}$ | 0.723 | 0.0856 | 0.7904 | 0.0182 | 0.8087 | 0.3042 | 0.826 | 0.9938 | 0.8062 | 44.3782 | 3 | 0.7529 | 0.7497 | 0.8177 | 0.8942 | 0.8529 | 0.8397 | 0.6298 | 0.1259 | 0.6554 | 0.777 | 0.6464 | 16.3754 | 23.7044 | 13.6486 | 0.8191 | 0.7132 | 8.5041 | -20.9155 | 8.4297 | -19.9952 | 8.3211 | -21.124 |
| 3 | $E_{CORR(M06-2X)}$, $E^{HOMO}_{CORR(M06-2X)}$ | 0.6861 | 0.0852 | 0.7495 | 0.0218 | 0.7713 | 0.3115 | 0.9031 | 1.0581 | 0.7464 | 35.405 | 5 | 0.7882 | 0.7855 | 0.8438 | 0.8709 | 0.8287 | 0.8659 | 0.7351 | 0.0946 | 0.7496 | 0.8728 | 0.5921 | 19.5763 | 26.8679 | 11.6993 | 0.7784 | 0.6782 | 8.8287 | -19.4964 | 8.6815 | -19.6684 | 8.3277 | -20.4056 |
| 4 | $E_{CORR(M06-L)}$, $\chi_{CORR(M06-L)}$ | 0.6695 | 0.0904 | 0.7371 | 0.0229 | 0.7599 | 0.241 | 0.9253 | 1.0856 | 0.9136 | 33.2364 | 1 | 0.6826 | 0.6786 | 0.7659 | 0.8636 | 0.8192 | 0.8005 | 0.6188 | 0.102 | 0.7607 | 0.8855 | 0.6909 | 20.547 | 28.2853 | 17.5282 | 0.7694 | 0.6687 | 8.8857 | -19.4851 | 8.7441 | -19.5772 | 8.447 | -20.6445 |
| 5 | $E_{CORR(M06-L)}$, $\eta_{CORR(M06-L)}$ | 0.6694 | 0.0905 | 0.737 | 0.0229 | 0.7599 | 0.2345 | 0.9253 | 1.0857 | 0.9114 | 33.2309 | 1 | 0.6842 | 0.6801 | 0.7671 | 0.8636 | 0.8192 | 0.8027 | 0.6188 | 0.1047 | 0.756 | 0.8802 | 0.6891 | 20.5496 | 28.2921 | 17.4438 | 0.7684 | 0.6552 | 8.391 | -20.3677 | 8.2215 | -20.3838 | 8.5237 | -19.8401 |
| 6 | $E_{CORR(M06-L)}$, $\omega_{CORR(M06-L)}$ | 0.6606 | 0.0938 | 0.7311 | 0.0234 | 0.7544 | 0.2341 | 0.9358 | 1.1001 | 0.9231 | 32.2604 | 1 | 0.676 | 0.6719 | 0.7611 | 0.86 | 0.8141 | 0.7936 | 0.6117 | 0.1147 | 0.7582 | 0.8835 | 0.6849 | 21.016 | 29.0443 | 17.8928 | 0.7641 | 0.6600 | 8.9533 | -19.5899 | 8.57 | -20.1556 | 8.6003 | -20.0929 |
| 7 | $E_{CORR(M06)}$, $\chi_{CORR(M06)}$ | 0.6513 | 0.0953 | 0.7225 | 0.0241 | 0.7466 | 0.1828 | 0.9506 | 1.1152 | 0.9493 | 30.9351 | 1 | 0.6574 | 0.653 | 0.7473 | 0.8549 | 0.8076 | 0.7846 | 0.5909 | 0.0852 | 0.8021 | 0.9337 | 0.7317 | 21.6881 | 29.8475 | 18.9236 | 0.7581 | 0.6389 | 8.6126 | -19.9997 | 8.7449 | -19.6801 | 8.6409 | -20.0249 |
| 8 | $E_{CORR(M06)}$, $\eta_{CORR(M06)}$ | 0.6483 | 0.0968 | 0.7209 | 0.0243 | 0.7452 | 0.1819 | 0.9533 | 1.1199 | 0.9448 | 30.7042 | 1 | 0.6606 | 0.6563 | 0.7497 | 0.854 | 0.8059 | 0.7873 | 0.5942 | 0.0849 | 0.8106 | 0.9439 | 0.7261 | 21.8097 | 30.0983 | 18.7452 | 0.7573 | 0.6307 | 8.7074 | -19.7769 | 8.6103 | -19.9712 | 8.9118 | -19.7475 |
| 9 | $E_{CORR(M06)}$, $\omega_{CORR(M06)}$ | 0.623 | 0.1053 | 0.7024 | 0.0259 | 0.7283 | 0.1965 | 0.9843 | 1.1595 | 0.9104 | 28.1441 | 1 | 0.6849 | 0.6809 | 0.7676 | 0.8428 | 0.7911 | 0.7974 | 0.6325 | 0.086 | 0.8507 | 0.989 | 0.7023 | 23.2546 | 32.2671 | 17.4038 | 0.7384 | 0.6227 | 9.0155 | -19.4652 | 8.7895 | -19.6078 | 9.0004 | -19.8773 |
| 10 | $E_{CORR(M06-2X)}$, $\eta_{CORR(M06-2X)}$ | 0.6188 | 0.1118 | 0.7049 | 0.0257 | 0.7305 | 0.2631 | 0.9803 | 1.166 | 0.88 | 28.4672 | 4 | 0.7055 | 0.7018 | 0.7828 | 0.8443 | 0.79 | 0.8137 | 0.6618 | 0.0493 | 0.8277 | 0.9717 | 0.6909 | 23.0617 | 32.6282 | 16.2639 | 0.7446 | 0.6063 | 8.8405 | -20.0973 | 8.5221 | -20.224 | 8.3951 | -20.8453 |
| 11 | $E_{CORR(M06-2X)}$, $\chi_{CORR(M06-2X)}$ | 0.6152 | 0.1115 | 0.7007 | 0.026 | 0.7267 | 0.2568 | 0.9872 | 1.1714 | 0.8773 | 27.9249 | 4 | 0.7073 | 0.7036 | 0.7842 | 0.8417 | 0.7876 | 0.8137 | 0.6626 | 0.0659 | 0.8317 | 0.976 | 0.6874 | 23.3872 | 32.934 | 16.1639 | 0.7397 | 0.6057 | 8.8554 | -20.2998 | 8.7956 | -19.7671 | 8.7678 | -20.1372 |
| 12 | $E_{CORR(M06-2X)}$, $\omega_{CORR(M06-2X)}$ | 0.6081 | 0.113 | 0.6946 | 0.0266 | 0.7212 | 0.266 | 0.9972 | 1.1822 | 0.8982 | 27.1551 | 2 | 0.6932 | 0.6893 | 0.7738 | 0.838 | 0.7827 | 0.8002 | 0.6532 | 0.074 | 0.8291 | 0.972 | 0.6962 | 23.8653 | 33.5397 | 16.9426 | 0.7334 | 0.5916 | 8.6783 | -19.9128 | 8.995 | -19.4032 | 8.0754 | -21.0687 |
| 13 | $E_{CORR(M06-2X)}$, $E^{LUMO}_{CORR(M06-2X)}$ | 0.5315 | 0.1223 | 0.6208 | 0.033 | 0.6537 | 0.0027 | 1.1112 | 1.2926 | 1.1335 | 19.8246 | 0 | 0.5115 | 0.5053 | 0.6397 | 0.7906 | 0.7276 | 0.644 | 0.5047 | 0.0598 | 0.9233 | 1.0646 | 0.9344 | 29.6343 | 40.0998 | 26.979 | 0.6715 | 0.5171 | 8.8175 | -20.0737 | 8.3812 | -20.1623 | 8.52 | -20.5053 |
| 14 | $E_{CORR(M06-L)}$, $E^{LUMO}_{CORR(M06-L)}$ | 0.5227 | 0.134 | 0.624 | 0.0327 | 0.6567 | -0.002 | 1.1064 | 1.3046 | 1.2451 | 20.0891 | 0 | 0.4106 | 0.4031 | 0.5653 | 0.7928 | 0.7266 | 0.5574 | 0.3797 | 0.0779 | 0.9312 | 1.0896 | 1.0321 | 29.3782 | 40.8468 | 32.5554 | 0.6744 | 0.5009 | 8.561 | -20.8725 | 8.4949 | -19.9891 | 8.2863 | -22.2119 |
| 15 | $E_{CORR(M06)}$, $E^{LUMO}_{CORR(M06)}$ | 0.494 | 0.1452 | 0.6048 | 0.0344 | 0.6392 | -0.0325 | 1.1343 | 1.3434 | 1.2058 | 18.6019 | 0 | 0.4472 | 0.4401 | 0.5923 | 0.7799 | 0.7039 | 0.5859 | 0.4352 | 0.0744 | 0.9476 | 1.1042 | 0.999 | 30.8794 | 43.3104 | 30.5339 | 0.6589 | 0.4860 | 8.5851 | -20.6376 | 8.9148 | -19.2392 | 8.4583 | -21.0518 |

Models are arranged according to $Q^2_{LOO}$ values.

Parameters are obtained through QSARINS software. Ref. [54] N. Chirico, E. Papa, S. Kovarich, S. Cassani, P. Gramatica, QSAR Res. Unit in Environ. Chem. and Ecotox. University of Insubria, Varese, Italy, 2012. (http://www.qsar.it).

$R^2_{adj}$ adjusted $R^2$

*N. Ext.OK* Number of external validation parameters meeting threshold values

*F* "F-test" statistic value

**Table S28.** Value of internal and external validation parameters of two-descriptor QSAR models, for mutagenicity (LogTA100), developed using electron-correlation (CORR(M06), CORR(M06-L), CORR(M06-2X)) based methods through 30% (random) splitting method.

| Model | Variables | $Q^2_{LOO}$ | $R^2$-$Q^2_{LOO}$ | $R^2_{adj}$ | $R^2$-$R^2_{adj}$ | $R^2$ | $\Delta K$ | $RMSE_{TR}$ | $RMSE_{CV}$ | $RMSE_{EXT}$ | $F$ | N. Ext.OK | $Q^2_{F1}$ | $Q^2_{F2}$ | $Q^2_{F3}$ | $CCC_{TR}$ | $CCC_{CV}$ | $CCC_{EXT}$ | $\bar{r}^2_m$ | $\Delta r^2_m$ | $MAE_{TR}$ | $MAE_{CV}$ | $MAE_{EXT}$ | $RSS_{TR}$ | $PRESS_{CV}$ | $PRESS_{EXT}$ | $R^2_{LMO}$ | $Q^2_{LMO}$ | $R^2_{Yscr}$ | $Q^2_{Yscr}$ | $R^2_{Yrand}$ | $Q^2_{Yrand}$ | $R^2_{Yrand}$ | $Q^2_{Yrand}$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | $E_{CORR(M06)}$, $E^{HOMO}_{CORR(M06)}$ | 0.7232 | 0.0543 | 0.7617 | 0.0159 | 0.7775 | 0.2798 | 0.8119 | 0.9056 | 0.7592 | 48.9348 | 5 | 0.8235 | 0.8175 | 0.8055 | 0.8749 | 0.8464 | 0.8892 | 0.8156 | 0.0106 | 0.673 | 0.7509 | 0.585 | 20.4338 | 25.4217 | 7.4932 | 0.7812 | 0.6946 | 6.528 | -15.1181 | 6.7988 | -14.4774 | 6.9398 | -14.6168 |
| 2 | $E_{CORR(M06-L)}$, $E^{HOMO}_{CORR(M06-L)}$ | 0.7216 | 0.0523 | 0.7578 | 0.0161 | 0.774 | 0.2845 | 0.8184 | 0.9082 | 0.849 | 47.9387 | 5 | 0.7794 | 0.7718 | 0.7568 | 0.8726 | 0.8451 | 0.8573 | 0.7515 | 0.0787 | 0.6648 | 0.7402 | 0.6746 | 20.7624 | 25.5704 | 9.3694 | 0.7775 | 0.6937 | 6.7815 | -14.755 | 6.1939 | -15.284 | 6.9448 | -14.5312 |
| 3 | $E_{CORR(M06-2X)}$, $E^{HOMO}_{CORR(M06-2X)}$ | 0.7019 | 0.0575 | 0.7421 | 0.0172 | 0.7593 | 0.2901 | 0.8445 | 0.9399 | 0.6396 | 44.1733 | 5 | 0.8748 | 0.8705 | 0.8619 | 0.8632 | 0.8326 | 0.9264 | 0.8493 | 0.0489 | 0.6967 | 0.7734 | 0.4619 | 22.1063 | 27.3842 | 5.3183 | 0.7622 | 0.6784 | 6.7294 | -14.7926 | 6.7132 | -14.5327 | 6.8356 | -14.6129 |
| 4 | $E_{CORR(M06-L)}$, $\eta_{CORR(M06-L)}$ | 0.6754 | 0.0602 | 0.7168 | 0.0189 | 0.7357 | 0.3326 | 0.885 | 0.9807 | 0.7907 | 38.9602 | 5 | 0.8086 | 0.802 | 0.789 | 0.8477 | 0.8155 | 0.8829 | 0.799 | 0.0726 | 0.7154 | 0.7933 | 0.5677 | 24.2823 | 29.8127 | 8.1281 | 0.7395 | 0.6480 | 6.5491 | -14.7557 | 6.4427 | -14.9318 | 6.433 | -15.1223 |
| 5 | $E_{CORR(M06-L)}$, $\chi_{CORR(M06-L)}$ | 0.6753 | 0.0601 | 0.7165 | 0.0189 | 0.7354 | 0.3367 | 0.8854 | 0.9809 | 0.7992 | 38.9183 | 5 | 0.8044 | 0.7978 | 0.7844 | 0.8476 | 0.8154 | 0.8803 | 0.7937 | 0.0739 | 0.7168 | 0.7948 | 0.5739 | 24.3015 | 29.825 | 8.3039 | 0.7387 | 0.6416 | 6.6108 | -14.7732 | 6.7026 | -14.7912 | 6.53 | -14.8213 |
| 6 | $E_{CORR(M06)}$, $\eta_{CORR(M06)}$ | 0.663 | 0.0617 | 0.705 | 0.0197 | 0.7247 | 0.2685 | 0.9033 | 0.9994 | 0.7982 | 36.8452 | 5 | 0.805 | 0.7983 | 0.785 | 0.8403 | 0.8066 | 0.8815 | 0.7806 | 0.0678 | 0.74 | 0.8196 | 0.5709 | 25.2924 | 30.9598 | 8.2816 | 0.7282 | 0.6256 | 6.8607 | -14.5786 | 6.7568 | -14.529 | 6.5069 | -15.0691 |
| 7 | $E_{CORR(M06)}$, $\chi_{CORR(M06)}$ | 0.662 | 0.0617 | 0.7039 | 0.0197 | 0.7237 | 0.2617 | 0.9049 | 1.0008 | 0.7942 | 36.6623 | 5 | 0.8069 | 0.8003 | 0.7871 | 0.8397 | 0.806 | 0.8826 | 0.7817 | 0.066 | 0.7418 | 0.8215 | 0.5583 | 25.3837 | 31.0503 | 8.2004 | 0.7282 | 0.6216 | 6.6641 | -14.6638 | 6.4698 | -15.0797 | 6.8296 | -14.6233 |
| 8 | $E_{CORR(M06)}$, $\omega_{CORR(M06)}$ | 0.6613 | 0.0648 | 0.7066 | 0.0196 | 0.7261 | 0.2755 | 0.9008 | 1.0018 | 0.8018 | 37.1222 | 5 | 0.8032 | 0.7965 | 0.7831 | 0.8413 | 0.8065 | 0.8818 | 0.7646 | 0.0661 | 0.7559 | 0.8389 | 0.59 | 25.1553 | 31.1107 | 8.3569 | 0.7310 | 0.6292 | 6.8367 | -14.5961 | 6.8001 | -14.572 | 7.0385 | -14.5611 |
| 9 | $E_{CORR(M06-L)}$, $\omega_{CORR(M06-L)}$ | 0.6609 | 0.0648 | 0.7061 | 0.0196 | 0.7257 | 0.3244 | 0.9015 | 1.0024 | 0.7898 | 37.0447 | 5 | 0.809 | 0.8025 | 0.7895 | 0.8411 | 0.8065 | 0.8819 | 0.8079 | 0.0706 | 0.7296 | 0.8103 | 0.5737 | 25.1935 | 31.1497 | 8.1098 | 0.7292 | 0.6409 | 6.4979 | -15.0033 | 6.6576 | -14.5171 | 6.7142 | -14.9102 |
| 10 | $E_{CORR(M06-2X)}$, $\chi_{CORR(M06-2X)}$ | 0.6564 | 0.0667 | 0.7032 | 0.0198 | 0.723 | 0.3365 | 0.9059 | 1.0091 | 0.7164 | 36.5454 | 5 | 0.8429 | 0.8375 | 0.8268 | 0.8392 | 0.8036 | 0.9054 | 0.8173 | 0.0533 | 0.759 | 0.8454 | 0.5295 | 25.4424 | 31.5655 | 6.6715 | 0.7284 | 0.6221 | 6.4501 | -15.47 | 6.4223 | -15.1167 | 6.7822 | -14.9699 |
| 11 | $E_{CORR(M06-2X)}$, $\eta_{CORR(M06-2X)}$ | 0.656 | 0.0668 | 0.7029 | 0.0198 | 0.7227 | 0.3487 | 0.9064 | 1.0097 | 0.7178 | 36.4911 | 5 | 0.8422 | 0.8369 | 0.8261 | 0.839 | 0.8034 | 0.9051 | 0.8154 | 0.0538 | 0.7609 | 0.8471 | 0.5288 | 25.4698 | 31.6022 | 6.6986 | 0.7253 | 0.6259 | 6.3675 | -15.4972 | 6.5863 | -15.0296 | 6.2227 | -15.5397 |
| 12 | $E_{CORR(M06-2X)}$, $\omega_{CORR(M06-2X)}$ | 0.6396 | 0.0698 | 0.6886 | 0.0208 | 0.7093 | 0.3612 | 0.928 | 1.0335 | 0.7395 | 34.1662 | 5 | 0.8326 | 0.8268 | 0.8154 | 0.83 | 0.7924 | 0.896 | 0.832 | 0.0511 | 0.7744 | 0.8616 | 0.5575 | 26.6991 | 33.1097 | 7.1096 | 0.7130 | 0.6059 | 6.6898 | -15.1298 | 6.5104 | -14.7607 | 6.7995 | -14.9874 |
| 13 | $E_{CORR(M06-2X)}$, $E^{LUMO}_{CORR(M06-2X)}$ | 0.5755 | 0.0832 | 0.6343 | 0.0244 | 0.6587 | 0.0378 | 1.0056 | 1.1215 | 0.9235 | 27.0222 | 4 | 0.7389 | 0.73 | 0.7122 | 0.7943 | 0.7465 | 0.8103 | 0.7924 | 0.0762 | 0.8302 | 0.9239 | 0.7376 | 31.3488 | 38.9937 | 11.0877 | 0.6667 | 0.5487 | 6.5367 | -15.3422 | 6.402 | -14.9494 | 6.632 | -14.9778 |
| 14 | $E_{CORR(M06-L)}$, $E^{LUMO}_{CORR(M06-L)}$ | 0.5624 | 0.0938 | 0.6316 | 0.0246 | 0.6561 | 0.0137 | 1.0094 | 1.1387 | 1.0665 | 26.7135 | 0 | 0.6518 | 0.6399 | 0.6161 | 0.7924 | 0.7416 | 0.7254 | 0.5871 | 0.1498 | 0.8563 | 0.9616 | 0.8713 | 31.5865 | 40.1981 | 14.7868 | 0.6651 | 0.5290 | 6.6064 | -15.6886 | 6.7866 | -14.4637 | 6.8157 | -15.2508 |
| 15 | $E_{CORR(M06)}$, $E^{LUMO}_{CORR(M06)}$ | 0.5461 | 0.0972 | 0.6179 | 0.0255 | 0.6434 | -0.0012 | 1.028 | 1.1597 | 1.0389 | 25.2549 | 0 | 0.6696 | 0.6583 | 0.6358 | 0.783 | 0.7267 | 0.7437 | 0.6479 | 0.1244 | 0.864 | 0.9679 | 0.8556 | 32.7601 | 41.6903 | 14.0301 | 0.6506 | 0.5347 | 6.484 | -15.4977 | 6.7901 | -14.4595 | 6.6852 | -15.0387 |

Models are arranged according to $Q^2_{LOO}$ values.

Parameters are obtained through QSARINS software. Ref. [54] N. Chirico, E. Papa, S. Kovarich, S. Cassani, P. Gramatica, QSAR Res. Unit in Environ. Chem. and Ecotox. University of Insubria, Varese, Italy, 2012. (http://www.qsar.it).

$R^2_{adj}$ adjusted $R^2$

*N. Ext.OK* Number of external validation parameters meeting threshold values

$F$ "F-test" statistic value

**Table S29.** Value of internal and external validation parameters of two-descriptor QSAR models, for mutagenicity (LogTA98), developed using electron-correlation (CORR(M06), CORR(M06-L), CORR(M06-2X)) based methods through activity sampling (ordered response) splitting method.

| Model | Variables | $Q^2_{LOO}$ | $R^2$-$Q^2_{LOO}$ | $R^2_{adj}$ | $R^2$-$R^2_{adj}$ | $R^2$ | $\Delta K$ | $RMSE_{TR}$ | $RMSE_{CV}$ | $RMSE_{EXT}$ | $F$ | *N. ExtOK* | $Q^2_{F1}$ | $Q^2_{F2}$ | $Q^2_{F3}$ | $CCC_{TR}$ | $CCC_{CV}$ | $CCC_{EXT}$ | $\bar{r}^2_m$ | $\Delta r^2_m$ | $MAE_{TR}$ | $MAE_{CV}$ | $MAE_{EXT}$ | $RSS_{TR}$ | $PRESS_{CV}$ | $PRESS_{EXT}$ | $R^2_{LMO}$ | $Q^2_{LMO}$ | $R^2_{Yscr}$ | $Q^2_{Yscr}$ | $R^2_{Xrand}$ | $Q^2_{Xrand}$ | $R^2_{Yrand}$ | $Q^2_{Yrand}$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | $E_{CORR(M06-2X)}, E^{HOMO}_{CORR(M06-2X)}$ | 0.9611 | 0.0198 | 0.9733 | 0.0076 | 0.9809 | 0.2325 | 0.2937 | 0.4194 | 0.4926 | 128.4472 | 5 | 0.8998 | 0.8978 | 0.9463 | 0.9904 | 0.9806 | 0.9508 | 0.8575 | 0.0754 | 0.2205 | 0.3249 | 0.42 | 0.69 | 1.4072 | 1.2131 | 0.9819 | 0.6700 | 27.3059 | -109.8418 | 28.4018 | -108.0133 | 29.1242 | -105.3201 |
| 2 | $E_{CORR(M06)}, E^{HOMO}_{CORR(M06)}$ | 0.9559 | 0.0225 | 0.9697 | 0.0086 | 0.9784 | 0.1867 | 0.3125 | 0.4463 | 0.4916 | 113.1597 | 5 | 0.9002 | 0.8982 | 0.9465 | 0.9891 | 0.978 | 0.9484 | 0.8666 | 0.0434 | 0.2566 | 0.3811 | 0.3949 | 0.7812 | 1.5932 | 1.2081 | 0.9792 | 0.6044 | 29.605 | -106.4775 | 29.0671 | -107.032 | 28.6567 | -113 |
| 3 | $E_{CORR(M06-L)}, E^{HOMO}_{CORR(M06-L)}$ | 0.9539 | 0.0238 | 0.9688 | 0.0089 | 0.9777 | 0.1881 | 0.3175 | 0.4563 | 0.4764 | 109.5577 | 5 | 0.9063 | 0.9044 | 0.9498 | 0.9887 | 0.977 | 0.9523 | 0.8764 | 0.0705 | 0.2713 | 0.4095 | 0.3817 | 0.8063 | 1.6657 | 1.1349 | 0.9789 | 0.5603 | 28.4443 | -126.6977 | 29.2881 | -106.2399 | 28.3569 | -119.7613 |
| 4 | $E_{CORR(M06-L)}, \omega_{CORR(M06-L)}$ | 0.9438 | 0.032 | 0.9661 | 0.0097 | 0.9758 | 0.4404 | 0.331 | 0.5039 | 0.6715 | 100.6098 | 5 | 0.8138 | 0.8101 | 0.9002 | 0.9877 | 0.9719 | 0.9094 | 0.7557 | 0.123 | 0.2497 | 0.4003 | 0.5515 | 0.8763 | 2.0312 | 2.2544 | 0.9779 | 0.4794 | 29.0988 | -94.1846 | 27.7599 | -109.4249 | 27.7401 | -100.3493 |
| 5 | $E_{CORR(M06-L)}, \eta_{CORR(M06-L)}$ | 0.9359 | 0.036 | 0.9606 | 0.0113 | 0.9718 | 0.3715 | 0.3567 | 0.5382 | 0.7111 | 86.2733 | 5 | 0.7912 | 0.787 | 0.8881 | 0.9857 | 0.9676 | 0.8958 | 0.7419 | 0.1119 | 0.2466 | 0.3837 | 0.5937 | 1.0178 | 2.3175 | 2.5286 | 0.9749 | 0.3744 | 28.4071 | -98.586 | 29.9315 | -100.8189 | 27.3732 | -101.3424 |
| 6 | $E_{CORR(M06-L)}, \chi_{CORR(M06-L)}$ | 0.9338 | 0.0372 | 0.9594 | 0.0116 | 0.971 | 0.3918 | 0.3621 | 0.547 | 0.7249 | 83.6362 | 5 | 0.7831 | 0.7787 | 0.8837 | 0.9853 | 0.9665 | 0.8911 | 0.7333 | 0.1109 | 0.2523 | 0.3956 | 0.598 | 1.049 | 2.3934 | 2.6271 | 0.9739 | 0.3444 | 29.6038 | -95.005 | 28.0895 | -109.1424 | 29.8759 | -92.1366 |
| 7 | $E_{CORR(M06-2X)}, \omega_{CORR(M06-2X)}$ | 0.932 | 0.0376 | 0.9574 | 0.0122 | 0.9696 | 0.4162 | 0.3707 | 0.5545 | 0.7322 | 79.6938 | 5 | 0.7787 | 0.7742 | 0.8813 | 0.9846 | 0.9656 | 0.8864 | 0.7211 | 0.0729 | 0.3056 | 0.478 | 0.541 | 1.0993 | 2.4593 | 2.6804 | 0.9720 | 0.3794 | 28.7329 | -100.8902 | 28.9748 | -101.9151 | 28.0158 | -102.8402 |
| 8 | $E_{CORR(M06-2X)}, \chi_{CORR(M06-2X)}$ | 0.9308 | 0.038 | 0.9563 | 0.0125 | 0.9688 | 0.4878 | 0.3756 | 0.5593 | 0.7085 | 77.536 | 5 | 0.7928 | 0.7886 | 0.8889 | 0.9841 | 0.9651 | 0.8965 | 0.7389 | 0.0904 | 0.2871 | 0.4424 | 0.5737 | 1.1289 | 2.5021 | 2.5095 | 0.9716 | 0.4423 | 28.7792 | -97.627 | 29.3015 | -107.527 | 29.0874 | -94.9439 |
| 9 | $E_{CORR(M06-2X)}, \eta_{CORR(M06-2X)}$ | 0.9287 | 0.0398 | 0.9559 | 0.0126 | 0.9685 | 0.4364 | 0.3774 | 0.5675 | 0.7146 | 76.7836 | 5 | 0.7891 | 0.7849 | 0.887 | 0.984 | 0.964 | 0.8938 | 0.7376 | 0.1002 | 0.2799 | 0.4302 | 0.5661 | 1.1396 | 2.5767 | 2.5535 | 0.9710 | 0.3673 | 29.2764 | -94.4813 | 27.779 | -111.1206 | 29.375 | -94.7392 |
| 10 | $E_{CORR(M06)}, \eta_{CORR(M06)}$ | 0.9256 | 0.0426 | 0.9556 | 0.0127 | 0.9683 | 0.4757 | 0.3787 | 0.5796 | 0.7536 | 76.246 | 5 | 0.7655 | 0.7608 | 0.8743 | 0.9839 | 0.9625 | 0.8802 | 0.7115 | 0.0929 | 0.2976 | 0.478 | 0.6161 | 1.1474 | 2.6879 | 2.8397 | 0.9714 | 0.4077 | 28.3468 | -95.6521 | 28.0674 | -110.4506 | 29.5381 | -93.032 |
| 11 | $E_{CORR(M06)}, \chi_{CORR(M06)}$ | 0.9226 | 0.0447 | 0.9543 | 0.0131 | 0.9674 | 0.4747 | 0.3839 | 0.5912 | 0.7411 | 74.1171 | 5 | 0.7732 | 0.7686 | 0.8784 | 0.9834 | 0.9609 | 0.8833 | 0.7185 | 0.0825 | 0.2931 | 0.472 | 0.5956 | 1.1793 | 2.7957 | 2.7464 | 0.9710 | 0.2739 | 29.7615 | -90.2826 | 28.193 | -108.2182 | 29.3719 | -92.5418 |
| 12 | $E_{CORR(M06)}, \omega_{CORR(M06)}$ | 0.9032 | 0.0612 | 0.9501 | 0.0142 | 0.9644 | 0.4063 | 0.4011 | 0.6614 | 0.6777 | 67.6918 | 5 | 0.8104 | 0.8066 | 0.8983 | 0.9819 | 0.9514 | 0.9016 | 0.7843 | 0.1195 | 0.2948 | 0.4877 | 0.5544 | 1.2872 | 3.4999 | 2.2963 | 0.9696 | 0.3628 | 28.5542 | -91.4535 | 28.1268 | -108.4975 | 27.707 | -92.6319 |
| 13 | $E_{CORR(M06-2X)}, E^{LUMO}_{CORR(M06-2X)}$ | 0.8823 | 0.0682 | 0.9307 | 0.0198 | 0.9505 | 0.1528 | 0.473 | 0.7293 | 0.8589 | 47.9911 | 1 | 0.6955 | 0.6893 | 0.8367 | 0.9746 | 0.9408 | 0.8449 | 0.623 | 0.0467 | 0.3896 | 0.6139 | 0.6646 | 1.7895 | 4.2555 | 3.6882 | 0.9538 | -0.0319 | 28.4266 | -95.5974 | 28.2882 | -104.9962 | 28.451 | -95.8422 |
| 14 | $E_{CORR(M06)}, E^{LUMO}_{CORR(M06)}$ | 0.8808 | 0.0646 | 0.9235 | 0.0219 | 0.9453 | 0.1002 | 0.4969 | 0.734 | 0.9187 | 43.2416 | 1 | 0.6515 | 0.6445 | 0.8132 | 0.9719 | 0.9403 | 0.8214 | 0.5774 | 0.0483 | 0.4186 | 0.6304 | 0.7235 | 1.9753 | 4.3096 | 4.2201 | 0.9486 | -0.1326 | 28.5311 | -100.8503 | 28.382 | -109.0724 | 28.4172 | -100.3383 |
| 15 | $E_{CORR(M06-L)}, E^{LUMO}_{CORR(M06-L)}$ | 0.8734 | 0.0744 | 0.927 | 0.0209 | 0.9479 | 0.0484 | 0.4854 | 0.7561 | 0.8966 | 45.4447 | 1 | 0.6681 | 0.6614 | 0.822 | 0.9732 | 0.9366 | 0.8308 | 0.5941 | 0.0445 | 0.4056 | 0.6353 | 0.7042 | 1.8845 | 4.5738 | 4.0196 | 0.9520 | 0.1360 | 28.0617 | -91.414 | 29.1216 | -104.2578 | 28.2849 | -91.9444 |

Models are arranged according to $Q^2_{LOO}$ values.

Parameters are obtained through QSARINS software. Ref. [54] N. Chirico, E. Papa, S. Kovarich, S. Cassani, P. Gramatica, QSAR Res. Unit in Environ. Chem. and Ecotox. University of Insubria, Varese, Italy, 2012. (http://www.qsar.it).

$R^2_{adj}$ adjusted $R^2$

*N. ExtOK* Number of external validation parameters meeting threshold values

*F* "F-test" statistic value

**Table S30.** Value of internal and external validation parameters of two-descriptor QSAR models, for mutagenicity (LogTA98), developed using electron-correlation (CORR(M06), CORR(M06-L), CORR(M06-2X)) based methods through activity sampling 30% ( random) splitting method.

| Model | Variables | $Q^2_{LOO}$ | $R^2-Q^2_{LOO}$ | $R^2_{adj}$ | $R^2-R^2_{adj}$ | $R^2$ | $\Delta K$ | $RMSE_{TR}$ | $RMSE_{CV}$ | $RMSE_{EXT}$ | $F$ | *N. Ext.OK* | $Q^2_{F1}$ | $Q^2_{F2}$ | $Q^2_{F3}$ | $CCC_{TR}$ | $CCC_{CV}$ | $CCC_{EXT}$ | $\bar{r}^2_m$ | $\Delta r^2_m$ | $MAE_{TR}$ | $MAE_{CV}$ | $MAE_{EXT}$ | $RSS_{TR}$ | $PRESS_{CV}$ | $PRESS_{EXT}$ | $R^2_{LMO}$ | $Q^2_{LMO}$ | $R^2_{Yscr}$ | $Q^2_{Yscr}$ | $R^2_{Yrand}$ | $Q^2_{Xrand}$ | $R^2_{Yrand}$ | $Q^2_{Yrand}$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | $E_{CORR(M06-2X)}, E^{HOMO}_{CORR(M06-2X)}$ | 0.8891 | 0.0546 | 0.9276 | 0.0161 | 0.9437 | 0.2141 | 0.4696 | 0.659 | 0.3061 | 58.6196 | 5 | 0.9745 | 0.9741 | 0.9761 | 0.971 | 0.9434 | 0.9874 | 0.899 | 0.0141 | 0.3975 | 0.562 | 0.2843 | 2.2053 | 4.3422 | 0.3748 | 0.9462 | 0.7427 | 22.6424 | -59.2023 | 22.1038 | -67.8088 | 22.7615 | -59.8664 |
| 2 | $E_{CORR(M06-L)}, E^{HOMO}_{CORR(M06-L)}$ | 0.8799 | 0.0588 | 0.9211 | 0.0175 | 0.9386 | 0.2153 | 0.4901 | 0.6858 | 0.3138 | 53.5449 | 5 | 0.9732 | 0.9728 | 0.9748 | 0.9684 | 0.9388 | 0.9877 | 0.8535 | 0.018 | 0.3977 | 0.5631 | 0.2669 | 2.4015 | 4.7028 | 0.3938 | 0.9405 | 0.7126 | 22.6056 | -60.9789 | 23.2717 | -64.3708 | 21.9391 | -62.4158 |
| 3 | $E_{CORR(M06)}, E^{HOMO}_{CORR(M06)}$ | 0.8798 | 0.0594 | 0.9219 | 0.0174 | 0.9392 | 0.2166 | 0.4876 | 0.6858 | 0.3258 | 54.1107 | 5 | 0.9711 | 0.9706 | 0.9729 | 0.9687 | 0.9388 | 0.9866 | 0.8489 | 0.0182 | 0.3965 | 0.5594 | 0.2738 | 2.3779 | 4.7032 | 0.4246 | 0.9433 | 0.6687 | 22.1341 | -61.5401 | 21.7539 | -69.0825 | 23.2127 | -59.496 |
| 4 | $E_{CORR(M06)}, \omega_{CORR(M06)}$ | 0.8361 | 0.0768 | 0.888 | 0.0249 | 0.9129 | 0.3879 | 0.5839 | 0.801 | 0.5497 | 36.6812 | 5 | 0.9177 | 0.9164 | 0.9228 | 0.9545 | 0.9134 | 0.965 | 0.7415 | 0.0495 | 0.4704 | 0.6593 | 0.4495 | 3.4094 | 6.4154 | 1.2087 | 0.9177 | 0.5801 | 22.2309 | -61.4706 | 21.8487 | -68.0915 | 22.9083 | -60.7558 |
| 5 | $E_{CORR(M06-L)}, \omega_{CORR(M06-L)}$ | 0.8297 | 0.0644 | 0.8638 | 0.0303 | 0.894 | 0.3397 | 0.644 | 0.8165 | 0.5152 | 29.5338 | 5 | 0.9277 | 0.9266 | 0.9322 | 0.9441 | 0.9114 | 0.9661 | 0.7907 | 0.0326 | 0.4723 | 0.6456 | 0.504 | 4.1471 | 6.666 | 1.0616 | 0.8928 | 0.5006 | 21.938 | -65.0466 | 22.0054 | -68.7132 | 22.4464 | -65.3091 |
| 6 | $E_{CORR(M06-2X)}, \chi_{CORR(M06-2X)}$ | 0.819 | 0.0852 | 0.8768 | 0.0274 | 0.9042 | 0.2938 | 0.6125 | 0.8417 | 0.6359 | 33.0221 | 5 | 0.8898 | 0.8881 | 0.8967 | 0.9497 | 0.907 | 0.9463 | 0.7828 | 0.0366 | 0.486 | 0.6889 | 0.6234 | 3.751 | 7.0844 | 1.6177 | 0.9071 | 0.5675 | 21.9262 | -67.103 | 21.5217 | -69.9175 | 22.9683 | -64.6405 |
| 7 | $E_{CORR(M06-2X)}, \eta_{CORR(M06-2X)}$ | 0.8165 | 0.0786 | 0.865 | 0.03 | 0.895 | 0.2906 | 0.641 | 0.8476 | 0.5799 | 29.843 | 5 | 0.9084 | 0.907 | 0.9141 | 0.9446 | 0.9043 | 0.9573 | 0.7685 | 0.0406 | 0.4835 | 0.6721 | 0.5623 | 4.1086 | 7.1835 | 1.3453 | 0.8943 | 0.4570 | 22.4365 | -64.9872 | 22.298 | -67.0859 | 21.8294 | -67.7045 |
| 8 | $E_{CORR(M06-L)}, \eta_{CORR(M06-L)}$ | 0.8099 | 0.0844 | 0.864 | 0.0302 | 0.8942 | 0.3713 | 0.6434 | 0.8626 | 0.5284 | 29.5934 | 5 | 0.9239 | 0.9228 | 0.9287 | 0.9442 | 0.9009 | 0.9646 | 0.783 | 0.0346 | 0.4931 | 0.6914 | 0.5189 | 4.1396 | 7.4413 | 1.1167 | 0.8978 | 0.5739 | 22.0247 | -65.2178 | 22.6672 | -66.1658 | 21.9127 | -66.4633 |
| 9 | $E_{CORR(M06-L)}, \chi_{CORR(M06-L)}$ | 0.8027 | 0.0823 | 0.8522 | 0.0328 | 0.885 | 0.3618 | 0.6708 | 0.8788 | 0.5297 | 26.9468 | 5 | 0.9235 | 0.9224 | 0.9283 | 0.939 | 0.8963 | 0.9646 | 0.7792 | 0.0358 | 0.5096 | 0.7018 | 0.517 | 4.4995 | 7.7224 | 1.1222 | 0.8827 | 0.5222 | 22.4299 | -63.988 | 22.4202 | -67.0032 | 21.816 | -66.269 |
| 10 | $E_{CORR(M06-2X)}, \omega_{CORR(M06-2X)}$ | 0.7985 | 0.0968 | 0.8654 | 0.0299 | 0.8953 | 0.2566 | 0.6401 | 0.8881 | 0.5891 | 29.9385 | 5 | 0.9054 | 0.904 | 0.9113 | 0.9448 | 0.8976 | 0.9527 | 0.8168 | 0.0318 | 0.4882 | 0.7107 | 0.5444 | 4.0969 | 7.8867 | 1.388 | 0.8965 | 0.5239 | 21.9545 | -72.5352 | 21.6271 | -69.1194 | 22.7447 | -69.239 |
| 11 | $E_{CORR(M06)}, \eta_{CORR(M06)}$ | 0.7958 | 0.0878 | 0.8503 | 0.0333 | 0.8836 | 0.3053 | 0.675 | 0.8941 | 0.5827 | 26.5669 | 5 | 0.9075 | 0.9061 | 0.9132 | 0.9382 | 0.8923 | 0.9548 | 0.7994 | 0.0298 | 0.5312 | 0.7339 | 0.5816 | 4.5563 | 7.9939 | 1.3584 | 0.8842 | 0.4748 | 22.5092 | -63.633 | 22.8636 | -67.0277 | 22.0439 | -65.375 |
| 12 | $E_{CORR(M06)}, \chi_{CORR(M06)}$ | 0.7936 | 0.0859 | 0.8451 | 0.0344 | 0.8795 | 0.3428 | 0.6866 | 0.8987 | 0.5744 | 25.5558 | 5 | 0.9101 | 0.9087 | 0.9157 | 0.9359 | 0.8912 | 0.9578 | 0.7739 | 0.0376 | 0.5247 | 0.7198 | 0.5686 | 4.7149 | 8.0772 | 1.3199 | 0.8804 | 0.5043 | 21.2928 | -66.6456 | 22.8814 | -65.4006 | 22.3948 | -63.6 |
| 13 | $E_{CORR(M06-2X)}, E^{LUMO}_{CORR(M06-2X)}$ | 0.6705 | 0.1492 | 0.7682 | 0.0515 | 0.8197 | 0.2581 | 0.8401 | 1.1357 | 0.6439 | 15.9117 | 5 | 0.887 | 0.8853 | 0.8941 | 0.9009 | 0.8217 | 0.956 | 0.7036 | 0.0647 | 0.664 | 0.9172 | 0.5402 | 7.0573 | 12.8982 | 1.6582 | 0.8271 | 0.0144 | 22.8463 | -66.7218 | 22.6558 | -67.4599 | 22.231 | -68.1258 |
| 14 | $E_{CORR(M06-L)}, E^{LUMO}_{CORR(M06-L)}$ | 0.665 | 0.1531 | 0.7661 | 0.052 | 0.8181 | 0.09 | 0.8438 | 1.1451 | 0.6628 | 15.7427 | 5 | 0.8803 | 0.8785 | 0.8878 | 0.9 | 0.8214 | 0.9548 | 0.7152 | 0.0623 | 0.6627 | 0.8979 | 0.5718 | 7.1193 | 13.1118 | 1.7571 | 0.8230 | 0.1211 | 22.0395 | -66.0791 | 21.3707 | -69.9536 | 22.0005 | -66.2792 |
| 15 | $E_{CORR(M06)}, E^{LUMO}_{CORR(M06)}$ | 0.6506 | 0.1511 | 0.745 | 0.0567 | 0.8016 | 0.1777 | 0.8811 | 1.1695 | 0.663 | 14.1452 | 5 | 0.8802 | 0.8784 | 0.8877 | 0.8899 | 0.8099 | 0.9543 | 0.7029 | 0.0659 | 0.7078 | 0.9499 | 0.5692 | 7.7638 | 13.6769 | 1.7585 | 0.8063 | -0.0129 | 22.0868 | -70.1 | 22.5876 | -66.138 | 22.0817 | -69.3175 |

Models are arranged according to $Q^2_{LOO}$ values.

Parameters are obtained through QSARINS software. Ref. [54] N. Chirico, E. Papa, S. Kovarich, S. Cassani, P. Gramatica, QSAR Res. Unit in Environ. Chem. and Ecotox. University of Insubria, Varese, Italy, 2012. (http://www.qsar.it).

$R^2_{adj}$ adjusted $R^2$

*N. Ext.OK* Number of external validation parameters meeting threshold values

*F* "F-test" statistic value