

Supporting Information (Tables S1_0.00001 - S17_0.00001)

Quantum-mechanical LSERs for the concentration-dependent adsorption of aromatic organic compounds by activated carbon: Applications and a comparison with CNTs

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Tables-(for models developed using *ab-initio* quantum-mechanical descriptors and LSER adsorbate descriptors) at adsorbate equilibrium concentration of 0.00001 C_s (mg/L), C_s being adsorbate aqueous solubility

Table S1_0.00001. Computed quantum chemical descriptors: Total energy (E) including Zero point energy (ZPE), dipole moment (d), energies of HOMO and LUMO (E^{HOMO} and E^{LUMO}), mean polarizability (α), Enthalpy (H), Free energy (G), chemical hardness (η), absolute electronegativity (χ), electrophilicity index (ω), and their electron-correlation contribution (CORR), all in atomic units (a.u.) calculated with HF/6-311++G(d,p) and DFT/B3LYP/6-311++G(d,p) levels of theory for 68 different organic compounds along with experimentally observed values of adsorption coefficients at different concentrations for organic compounds and LSER's adsorbate descriptors values employed in the study carried out using linear solvation energy relationship (LSER) by Yu et al. 2015.

Table S2_0.00001. Details of the splitting of data set into training (T) and prediction set (P) through different splitting methods employed along with experimentally observed values of adsorption coefficients at different concentrations for organic compounds.

Table S3_0.00001. Models developed for $\log K_d$ without any splitting method (taking all the compounds in training set) : Values of internal validation parameters for models developed using quantum-mechanical and electron-correlation (CORR) based descriptors.

Table S4_0.00001. Models developed for $\log K_d$, but employing splitting method taking training set and prediction set in a ratio of 3:1. Values of internal and external validation parameters for models developed using quantum-mechanical and electron-correlation (CORR) based descriptors.

Table S5_0.00001. Same as Table S4_0.00001, but employing splitting method taking training set and prediction set in a ratio of 2:1.

Table S6_0.00001. Same as Table S5_0.00001, but employing splitting method taking training set and prediction set in a ratio of 1:1.

Table S7_0.00001. Same as Table S3_0.00001 but for models developed using the descriptors reported in the work of Yu et al., 2015.

Table S8_0.00001. Same as Table S4_0.00001 but for models developed using the descriptors employed in the work of Yu et al., 2015.

Table S9_0.00001. Same as Table S5_0.00001 but for models developed using the descriptors employed in the work of Yu et al., 2015.

Table S10_0.00001. Same as Table S6_0.00001 but for models developed using the descriptors employed in the work of Yu et al., 2015.

Table S11_0.00001. Same as Table S3_0.00001 but for models developed using combined quantum mechanical descriptors and LSER's adsorbate descriptors.

Table S12_0.00001. Same as Table S4_0.00001 but for models developed using combined quantum mechanical descriptors and LSER's adsorbate descriptors.

Table S13_0.00001. Same as Table S5_0.00001 but for models developed using combined quantum mechanical descriptors and LSER's adsorbate descriptors.

Table S14_0.00001. Same as Table S6_0.00001 but for models developed using combined quantum mechanical descriptors and LSER's adsorbate descriptors.

Table S15_0.00001. Same as Table S4_0.00001 but using splitting employed as in Yu et al., 2015.

Table S16_0.00001. Same as Table S8_0.00001 but using splitting employed as in Yu et al., 2015.

Table S17_0.00001. Same as Table S11_0.00001 but using splitting employed as in Yu et al., 2015.

Table S1. 0.00001. Computed quantum chemical descriptors* Total energy (E), absolute Zero point energy (ZPE), dipole moment (μ), energies of HOMO and LUMO (E_{HOMO} and E_{LUMO}), mean polarizability (α), Enthalpy (H), Free energy (G), chemical hardness (η), absolute electronegativity (χ), electrophilicity index (ω), and their electron-correlation contribution (CORR), all in atomic units (a.u.) calculated with HF/6-311++G(d,p) and DFT(B3LYP/6-311++G(d,p)) levels of theory for 68 different organic compounds along with experimentally observed values of adsorption coefficients at different concentrations for organic compounds and LSER's adsorbate descriptors values employed in the study carried out using linear solvation energy relationship (LSER) by Yu et al. 2015[†].

| ID No. | Name of compounds | Quantum-mechanical descriptors | | | | | | | | | | | | | LSER's adsorbate descrip | | | | | | | | | | | | | | | | |
|--------|----------------------|--------------------------------|-------------------|-------------------|--------------------------------------|-------------------|-------------------|--------------------------------------|-------------------|-------------------|--------------------------------------|-------------------|-------------------|--------------------------------------|--------------------------|-------------------|--------------------------------------|-------------------|-------------------|--------------------------------------|------------|-------------|------------|-------------|-------------|------------|-------------|-------------|------------|-------------|----------|
| | | log K _{ow} | E _{HOMO} | E _{LUMO} | E _{HOMO} -E _{LUMO} | E _{HOMO} | E _{LUMO} | E _{HOMO} -E _{LUMO} | E _{HOMO} | E _{LUMO} | E _{HOMO} -E _{LUMO} | E _{HOMO} | E _{LUMO} | E _{HOMO} -E _{LUMO} | E _{HOMO} | E _{LUMO} | E _{HOMO} -E _{LUMO} | E _{HOMO} | E _{LUMO} | E _{HOMO} -E _{LUMO} | R | P | A | B | V | | | | | | |
| 1 | Benzene | -332.211239 | -330.650633 | -325.087873 | 0.100909 | 0.106485 | -0.004923 | 0.07815 | 0.07383 | 0.04232 | 0.07815 | 0.07383 | 0.04232 | -332.205991 | -330.645291 | -325.087873 | 0.100909 | 0.106485 | -0.004923 | 0.07815 | 0.07383 | 0.04232 | 0.07815 | 0.07383 | 0.04232 | 0.07815 | 0.07383 | 0.04232 | | | |
| 2 | Toluene | -271.511477 | -269.667506 | -1.844141 | 0.127224 | 0.135335 | -0.008111 | 0.1581468 | 0.1563732 | -0.007184 | 0.1581468 | 0.1563732 | -0.007184 | -271.504221 | -269.661928 | -1.844141 | 0.127224 | 0.135335 | -0.008111 | 0.1581468 | 0.1563732 | -0.007184 | 0.1581468 | 0.1563732 | -0.007184 | 0.1581468 | 0.1563732 | -0.007184 | | | |
| 3 | o-xylene | -310.810725 | -308.682711 | -1.218014 | 0.154995 | 0.163666 | -0.009971 | 0.26582038 | 0.25397904 | 0.01184336 | 0.26582038 | 0.25397904 | 0.01184336 | -310.804421 | -308.674595 | -1.212755 | 0.154995 | 0.163666 | -0.009971 | 0.26582038 | 0.25397904 | 0.01184336 | 0.26582038 | 0.25397904 | 0.01184336 | 0.26582038 | 0.25397904 | 0.01184336 | | | |
| 4 | p-xylene | -310.811812 | -308.684276 | -1.212735 | 0.154315 | 0.16146 | -0.009831 | 0.28204942 | 0.26251034 | 0.02043908 | 0.28204942 | 0.26251034 | 0.02043908 | -310.803997 | -308.676283 | -1.212736 | 0.154315 | 0.16146 | -0.009831 | 0.28204942 | 0.26251034 | 0.02043908 | 0.28204942 | 0.26251034 | 0.02043908 | 0.28204942 | 0.26251034 | 0.02043908 | | | |
| 5 | m-xylene | -310.811996 | -308.684556 | -1.212744 | 0.154315 | 0.16146 | -0.009831 | 0.28204942 | 0.26251034 | 0.02043908 | 0.28204942 | 0.26251034 | 0.02043908 | -310.803997 | -308.676283 | -1.212736 | 0.154315 | 0.16146 | -0.009831 | 0.28204942 | 0.26251034 | 0.02043908 | 0.28204942 | 0.26251034 | 0.02043908 | 0.28204942 | 0.26251034 | 0.02043908 | | | |
| 6 | 2,4-dinitrotoluene | -680.624988 | -676.705803 | -3.919183 | 0.132289 | 0.143306 | -0.011017 | 0.20633466 | 0.1888776 | 0.1255394 | 0.20633466 | 0.1888776 | 0.1255394 | -680.613106 | -676.694252 | -3.918454 | 0.132289 | 0.143306 | -0.011017 | 0.20633466 | 0.1888776 | 0.1255394 | 0.20633466 | 0.1888776 | 0.1255394 | 0.20633466 | 0.1888776 | 0.1255394 | | | |
| 7 | 2-chlorotoluene | -731.144201 | -728.600821 | -2.54338 | 0.11843 | 0.12605 | -0.007662 | 0.6150294 | 0.7117162 | -0.08611236 | 0.6150294 | 0.7117162 | -0.08611236 | -731.136127 | -728.593197 | -2.54293 | 0.11843 | 0.12605 | -0.007662 | 0.6150294 | 0.7117162 | -0.08611236 | 0.6150294 | 0.7117162 | -0.08611236 | 0.6150294 | 0.7117162 | -0.08611236 | | | |
| 8 | Ethylbenzene | -310.806873 | -308.680726 | -1.216147 | 0.156018 | 0.1594058 | -0.009913 | 0.15346534 | 0.1594058 | -0.00994304 | 0.15346534 | 0.1594058 | -0.00994304 | -310.803997 | -308.676283 | -1.212736 | 0.156018 | 0.1594058 | -0.009913 | 0.15346534 | 0.1594058 | -0.00994304 | 0.15346534 | 0.1594058 | -0.00994304 | 0.15346534 | 0.1594058 | -0.00994304 | | | |
| 9 | Chlorobenzene | -691.843688 | -689.583984 | -2.259704 | 0.096061 | 0.096691 | -0.006609 | 0.7319207 | 0.80635198 | -0.07443128 | 0.7319207 | 0.80635198 | -0.07443128 | -691.837348 | -689.613538 | -2.259942 | 0.096061 | 0.096691 | -0.006609 | 0.7319207 | 0.80635198 | -0.07443128 | 0.7319207 | 0.80635198 | -0.07443128 | 0.7319207 | 0.80635198 | -0.07443128 | | | |
| 10 | 1,2-dichlorobenzene | -1151.470773 | -1148.511297 | -2.959476 | 0.081102 | 0.086821 | -0.005719 | 1.04077904 | 1.18499948 | -0.14422004 | 1.04077904 | 1.18499948 | -0.14422004 | -1151.465027 | -1148.506532 | -2.959476 | 0.081102 | 0.086821 | -0.005719 | 1.04077904 | 1.18499948 | -0.14422004 | 1.04077904 | 1.18499948 | -0.14422004 | 1.04077904 | 1.18499948 | -0.14422004 | | | |
| 11 | 1,3-dichlorobenzene | -1151.474718 | -1148.516061 | -2.958653 | 0.081033 | 0.086764 | -0.005707 | 0.68400458 | 0.76276326 | -0.07875868 | 0.68400458 | 0.76276326 | -0.07875868 | -1151.467473 | -1148.512626 | -2.958227 | 0.081033 | 0.086764 | -0.005707 | 0.68400458 | 0.76276326 | -0.07875868 | 0.68400458 | 0.76276326 | -0.07875868 | 0.68400458 | 0.76276326 | -0.07875868 | | | |
| 12 | 1,4-dichlorobenzene | -1161.104448 | -1160.464637 | -3.657711 | 0.071389 | 0.076677 | -0.005288 | 0.00023604 | 0.00023604 | 0.00023604 | 0.00023604 | 0.00023604 | 0.00023604 | -1161.097203 | -1160.457431 | -3.657211 | 0.071389 | 0.076677 | -0.005288 | 0.00023604 | 0.00023604 | 0.00023604 | 0.00023604 | 0.00023604 | 0.00023604 | 0.00023604 | 0.00023604 | 0.00023604 | | | |
| 14 | Bromobenzene | -4156 | -2805.763965 | -2802.444516 | -3.194490 | 0.090038 | 0.096059 | -0.006021 | 0.73247146 | 0.82617934 | -0.09370788 | 0.73247146 | 0.82617934 | -0.09370788 | -4156 | -2805.763965 | -2802.444516 | -3.194490 | 0.090038 | 0.096059 | -0.006021 | 0.73247146 | 0.82617934 | -0.09370788 | 0.73247146 | 0.82617934 | -0.09370788 | 0.73247146 | 0.82617934 | | |
| 15 | Fluorobenzene | 3.11 | -331.48843 | -329.539872 | -1.948558 | 0.091764 | 0.098033 | -0.006269 | 0.68927614 | 0.7163814 | -0.02710326 | 0.68927614 | 0.7163814 | -0.02710326 | 3.11 | -331.48843 | -329.539872 | -1.948558 | 0.091764 | 0.098033 | -0.006269 | 0.68927614 | 0.7163814 | -0.02710326 | 0.68927614 | 0.7163814 | -0.02710326 | 0.68927614 | 0.7163814 | | |
| 16 | Nitrobenzene | 3.519 | -436.772201 | -434.174325 | -2.597876 | 0.102513 | 0.110228 | -0.007745 | 0.93336643 | 0.20474348 | -0.10137918 | 0.93336643 | 0.20474348 | -0.10137918 | 3.519 | -436.772201 | -434.174325 | -2.597876 | 0.102513 | 0.110228 | -0.007745 | 0.93336643 | 0.20474348 | -0.10137918 | 0.93336643 | 0.20474348 | -0.10137918 | 0.93336643 | 0.20474348 | | |
| 17 | 4-chloronitrobenzene | 4.31 | -896.403107 | -893.109398 | -3.297169 | 0.092846 | 0.100205 | -0.007359 | 1.32304354 | 1.31368062 | 0.00936292 | 1.32304354 | 1.31368062 | 0.00936292 | 4.31 | -896.403107 | -893.109398 | -3.297169 | 0.092846 | 0.100205 | -0.007359 | 1.32304354 | 1.31368062 | 0.00936292 | 1.32304354 | 1.31368062 | 0.00936292 | 1.32304354 | 1.31368062 | 0.00936292 | |
| 18 | Styrene | 3.133 | -399.590808 | -397.515599 | -2.082499 | 0.13275 | 0.141424 | -0.008664 | 0.08804337 | 0.06831036 | 0.01774234 | 0.08804337 | 0.06831036 | 0.01774234 | 3.133 | -399.590808 | -397.515599 | -2.082499 | 0.13275 | 0.141424 | -0.008664 | 0.08804337 | 0.06831036 | 0.01774234 | 0.08804337 | 0.06831036 | 0.01774234 | 0.08804337 | 0.06831036 | 0.01774234 | |
| 19 | Biphenyl | -643.242112 | -640.14263 | -3.088082 | 0.180701 | 0.1925 | -0.011799 | 0 | 0 | 0 | -0.23585 | 0.30837 | 0.07252 | -0.0413 | 0.0376 | -0.0789 | 0.180701 | 0.1925 | -0.011799 | 0 | 0 | 0 | -0.23585 | 0.30837 | 0.07252 | -0.0413 | 0.0376 | -0.0789 | 0.180701 | 0.1925 | |
| 20 | Naphthalene | 3.679 | -883.84213 | -883.281783 | -2.560347 | 0.146812 | 0.156555 | -0.009743 | 0 | 0 | 0 | -0.22585 | 0.29441 | 0.06856 | -0.0518 | 0.0384 | -0.08985 | 0.146812 | 0.156555 | -0.009743 | 0 | 0 | 0 | -0.22585 | 0.29441 | 0.06856 | -0.0518 | 0.0384 | -0.08985 | 0.146812 | 0.156555 |
| 21 | Phenanthrene | 5.152 | -539.474942 | -535.915693 | -3.559249 | 0.193543 | 0.20661 | -0.013057 | 0.00581666 | 0.00251776 | 0.00334349 | 0.00581666 | 0.00251776 | 0.00334349 | 5.152 | -539.474942 | -535.915693 | -3.559249 | 0.193543 | 0.20661 | -0.013057 | 0.00581666 | 0.00251776 | 0.00334349 | 0.00581666 | 0.00251776 | 0.00334349 | 0.00581666 | 0.00251776 | 0.00334349 | |
| 22 | Acetophenone | 3.171 | -384.86456 | -382.42178 | -2.44278 | 0.137216 | 0.146651 | -0.009353 | 1.2761896 | 1.31340524 | 0.00772564 | 1.2761896 | 1.31340524 | 0.00772564 | 3.171 | -384.86456 | -382.42178 | -2.44278 | 0.137216 | 0.146651 | -0.009353 | 1.2761896 | 1.31340524 | 0.00772564 | 1.2761896 | 1.31340524 | 0.00772564 | 1.2761896 | 1.31340524 | 0.00772564 | |
| 23 | Phenol | 2.58 | -307.454784 | -305.528876 | -1.925908 | 0.111143 | 0.111143 | -0.007202 | 0.4544428 | 0.6673026 | 0.23489 | 0.4544428 | 0.6673026 | 0.23489 | 2.58 | -307.454784 | -305.528876 | -1.925908 | 0.111143 | 0.111143 | -0.007202 | 0.4544428 | 0.6673026 | 0.23489 | 0.4544428 | 0.6673026 | 0.23489 | 0.4544428 | 0.6673026 | 0.23489 | |
| 24 | 4-ethylphenol | 3.325 | -386.049891 | -383.558386 | -2.491305 | 0.159968 | 0.170585 | -0.010617 | 0.5670861 | 0.60017104 | -0.03308674 | 0.5670861 | 0.60017104 | -0.03308674 | 3.325 | -386.049891 | -383.558386 | -2.491305 | 0.159968 | 0.170585 | -0.010617 | 0.5670861 | 0.60017104 | -0.03308674 | 0.5670861 | 0.60017104 | -0.03308674 | 0.5670861 | 0.60017104 | -0.03308674 | |
| 25 | 4-chlorophenol | 2.727 | -677.086147 | -674.61587 | -2.42546 | 0.094488 | 0.11036 | -0.006818 | 0.90175148 | 0.93227932 | -0.03052784 | 0.90175148 | 0.93227932 | -0.03052784 | 2.727 | -677.086147 | -674.61587 | -2.42546 | 0.094488 | 0.11036 | -0.006818 | 0.90175148 | 0.93227932 | -0.03052784 | 0.90175148 | 0.93227932 | -0.03052784 | 0.90175148 | 0.93227932 | -0.03052784 | |
| 26 | Pentafluorophenol | -2605.586104 | -2600.159837 | -5.426267 | 0.056351 | 0.061377 | -0.005026 | 0.69077106 | 0.73160598 | -0.0408392 | 0.69077106 | 0.73160598 | -0.0408392 | -2605.586104 | -2600.159837 | -5.426267 | 0.056351 | 0.061377 | -0.005026 | 0.69077106 | 0.73160598 | -0.0408392 | 0.69077106 | 0.73160598 | -0.0408392 | 0.69077106 | 0.73160598 | -0.0408392 | 0.69077106 | 0.73160598 | |
| 27 | Perfluorophenol | 2.641 | -803.793196 | -799.929588 | -3.863608 | 0.063737 | 0.069452 | -0.005715 | 0.8450232 | 0.85847664 | -0.01046444 | 0.8450232 | 0.85847664 | -0.01046444 | 2.641 | -803.793196 | -799.929588 | -3.863608 | 0.063737 | 0.069452 | -0.005715 | 0.8450232 | 0.85847664 | -0.01046444 | 0.8450232 | 0.85847664 | -0.01046444 | 0.8450232 | 0.85847664 | -0.01046444 | |
| 28 | 4-nitrophenol | 3.172 | -512.076224 | -509.055032 | -2.962292 | 0.10653 | 0.119625 | -0.008435 | 2.1655488 | 2.16275584 | 0.00279914 | 2.1655488 | 2.16275584 | 0.00279914 | 3.172 | -512.076224 | -509.0550 | | | | | | | | | | | | | | |

Table S2_0.00001. Details of the splitting of data set into training (T) and prediction set (P) through different splitting methods employed along with experimentally observed values of adsorption coefficients at different concentrations for organic compounds.

| ID. No. | Name of compounds | log $K_{d0.00001}$ | Splitting (T:P) | | | | Splitting as in Yu et al. 2015 |
|---------|-----------------------------------|--------------------|-----------------|-----|-----|-----|--------------------------------|
| | | | All Training | 3:1 | 2:1 | 1:1 | |
| 62 | Pyridine | 1.759 | T | T | T | T | T |
| 36 | Hydroquinone | 1.801 | T | T | T | T | T |
| 34 | 4-aminophenol | 2.067 | T | T | T | P | T |
| 46 | Phthalic acid | 2.16 | T | T | P | T | T |
| 35 | Catechol | 2.219 | T | P | T | P | T |
| 60 | dl-phenylalanine | 2.337 | T | T | T | T | P |
| 37 | chlorohydroquinone | 2.354 | T | T | P | P | T |
| 25 | 4-chlorophenol | 2.377 | T | T | T | T | T |
| 1 | Benzene | 2.515 | T | P | T | P | T |
| 31 | 4-methoxyphenol | 2.525 | T | T | P | T | T |
| 23 | Phenol | 2.58 | T | T | T | P | T |
| 27 | Pentafluorophenol | 2.641 | T | T | T | T | P |
| 32 | 4-cresol | 2.65 | T | P | P | P | T |
| 65 | Acetylsalicylic acid | 2.719 | T | T | T | T | P |
| 42 | Benzoic acid | 2.72 | T | T | T | P | T |
| 38 | Aniline | 2.774 | T | T | P | T | T |
| 59 | dl-tyrosine | 2.858 | T | P | T | P | T |
| 41 | Benzaldehyde | 2.865 | T | T | T | T | P |
| 68 | 2,4-methylphenoxy ethanol | 2.965 | T | T | P | P | T |
| 44 | 3-nitrobenzoic acid | 3.031 | T | T | T | T | T |
| 58 | dl-tryptophane | 3.076 | T | P | T | P | T |
| 28 | 4-nitrophenol | 3.083 | T | T | P | T | T |
| 15 | fluorobenzene | 3.11 | T | T | T | P | P |
| 40 | 3-chloro-4-fluoroaniline | 3.131 | T | T | T | T | T |
| 22 | acetophenone | 3.171 | T | P | P | P | P |
| 64 | salicylic acid | 3.174 | T | T | T | T | P |
| 45 | 3,5-dimethoxybenzoic acid | 3.268 | T | T | T | P | T |
| 2 | Toluene | 3.282 | T | T | P | T | P |
| 24 | 4-ethylphenol | 3.325 | T | P | T | P | T |
| 63 | Atrazine | 3.348 | T | T | T | T | T |
| 66 | Atenolol | 3.427 | T | T | P | P | T |
| 55 | Tetracycline | 3.468 | T | T | T | T | T |
| 48 | Anisole | 3.471 | T | P | T | P | T |
| 16 | Nitrobenzene | 3.519 | T | T | P | T | T |
| 43 | 4-chlorobenzoic acid | 3.538 | T | T | T | P | T |
| 3 | o-xylene | 3.558 | T | T | T | T | T |
| 54 | Sulfamethoxazole | 3.638 | T | P | P | P | T |
| 20 | Naphthalene | 3.679 | T | T | T | T | T |
| 51 | Dicamba | 3.735 | T | T | T | P | T |
| 11 | 1,3-dichlorobenzene | 3.736 | T | T | P | T | T |
| 4 | p-xylene | 3.778 | T | P | T | P | P |
| 12 | 1,4 dichlorobenzene | 3.791 | T | T | T | T | T |
| 49 | Diethylphtalate | 3.869 | T | T | P | P | T |
| 5 | m-xylene | 3.871 | T | T | T | T | T |
| 7 | 2-chlorotoluene | 4.009 | T | P | T | P | P |
| 56 | Ciprofloxacin | 4.059 | T | T | P | T | T |
| 29 | 4,6-dinitro-o-cresol | 4.112 | T | T | T | P | T |
| 18 | Styrene | 4.133 | T | T | T | T | T |
| 14 | Bromobenzene | 4.156 | T | P | P | P | T |
| 10 | 1,2-dichlorobenzene | 4.166 | T | T | T | T | T |
| 61 | Carbamazepine | 4.243 | T | T | T | T | T |
| 47 | 2,4,5-trichlorophenoxyacetic acid | 4.283 | T | T | P | T | T |
| 17 | 4-chloronitrobenzene | 4.31 | T | P | T | P | T |
| 50 | Alachlor | 4.63 | T | T | T | T | P |
| 21 | Phenanthrene | 5.152 | T | T | T | T | T |
| 6 | 2,4-dinitrotoluene | . | E* | E* | E* | E* | E* |
| 8 | Ethylbenzene | . | E* | E* | E* | E* | E* |
| 9 | Chlorobenzene | . | E* | E* | E* | E* | E* |
| 13 | 1,3,5-trichlorobenzene | . | E* | E* | E* | E* | E* |
| 19 | Biphenyl | . | E* | E* | E* | E* | E* |
| 26 | Pentachlorophenol | . | E* | E* | E* | E* | E* |
| 30 | 2-phenylphenol | . | E* | E* | E* | E* | E* |
| 33 | 2,3,5-trimethyl phenol | . | E* | E* | E* | E* | E* |
| 39 | 4-iodoaniline | . | E* | E* | E* | E* | E* |
| 52 | Dinoseb | . | E* | E* | E* | E* | E* |
| 53 | Metolachlor | . | E* | E* | E* | E* | E* |
| 57 | Bisphenol A | . | E* | E* | E* | E* | E* |
| 67 | Nalidixic acid | . | E* | E* | E* | E* | E* |

E* compounds whose K_d values were beyond the experimental isotherm range have been excluded in the literature studies, the same is adopted in the present work.

Table S3_0.00001. Models developed for logK_d without any splitting method (taking all the compounds in training set) : Values of internal validation parameters for models developed using quantum-mechanical and electron-correlation (CORR) based descriptors.

| S.No. | α | Size | Variables | R ² | R ² _{adj} | R ² -R ² _{adj} | Δ K | RMSE(tr) | MAE(tr) | RSS(tr) | CCC(tr) | F | Q ² _{loo} | R ² -Q ² _{loo} | RMSE(cv) | MAE(cv) | PRESS(cv) | CCC(cv) | Q ² _{LMO} | R ² _{Yser} | Q ² _{Yser} | R ² _{Xrtd} | Q ² _{Xrtd} | R ² _{Yrtd} | Q ² _{Yrtd} |
|-------|---|------|---|----------------|-------------------------------|---|---------|----------|---------|---------|---------|---------|-------------------------------|---|----------|---------|-----------|---------|-------------------------------|--------------------------------|--------------------------------|--------------------------------|--------------------------------|--------------------------------|--------------------------------|
| 1 | | 5 | E(CORR) ZPE(DFT) ZPE(CORR) η(CORR) ω(DFT) | 0.7099 | 0.6803 | 0.0296 | -0.1068 | 0.3948 | 0.3306 | 8.5734 | 0.8304 | 23.9839 | 0.6237 | 0.0862 | 0.4497 | 0.3756 | 11.1206 | 0.7857 | 65.1172 | 9.2428 | -15.5617 | 9.1193 | -14.6511 | 8.8864 | -16.3663 |
| 2 | | 5 | E(CORR) ZPE(DFT) ZPE(CORR) E ^{HOMO} (CORR) - E ^{LUMO} (CORR) ω(DFT) | 0.7099 | 0.6803 | 0.0296 | -0.1068 | 0.3948 | 0.3306 | 8.5734 | 0.8304 | 23.9839 | 0.6237 | 0.0862 | 0.4497 | 0.3756 | 11.1206 | 0.7857 | 64.9693 | 9.7216 | -14.7772 | 8.6321 | -15.3858 | 9.2069 | -15.7991 |
| 3 | | 5 | E(CORR) ZPE(HF) ZPE(CORR) η(CORR) ω(DFT) | 0.7099 | 0.6803 | 0.0296 | -0.107 | 0.3948 | 0.3306 | 8.5734 | 0.8304 | 23.9839 | 0.6237 | 0.0862 | 0.4497 | 0.3756 | 11.1206 | 0.7857 | 65.1086 | 9.209 | -15.7023 | 9.3591 | -14.4644 | 9.2988 | -15.5221 |
| 4 | | 5 | E(CORR) ZPE(HF) ZPE(CORR) E ^{HOMO} (CORR) - E ^{LUMO} (CORR) ω(DFT) | 0.7099 | 0.6803 | 0.0296 | -0.107 | 0.3948 | 0.3306 | 8.5734 | 0.8304 | 23.9839 | 0.6237 | 0.0862 | 0.4497 | 0.3756 | 11.1206 | 0.7857 | 64.9101 | 9.5935 | -15.1069 | 9.7839 | -13.7781 | 9.3839 | -15.4487 |
| 5 | | 5 | E(CORR) ZPE(DFT) ZPE(HF) E ^{HOMO} (CORR) - E ^{LUMO} (CORR) ω(DFT) | 0.7099 | 0.6803 | 0.0296 | -0.1038 | 0.3948 | 0.3306 | 8.5734 | 0.8304 | 23.9839 | 0.6237 | 0.0862 | 0.4497 | 0.3756 | 11.1206 | 0.7857 | 64.7833 | 9.2419 | -15.4233 | 9.8901 | -13.7567 | 9.0487 | -15.9923 |
| 6 | | 5 | E(CORR) ZPE(DFT) ZPE(HF) E ^{HOMO} (CORR) - E ^{LUMO} (CORR) ω(DFT) | 0.7099 | 0.6803 | 0.0296 | -0.1038 | 0.3948 | 0.3306 | 8.5734 | 0.8304 | 23.9839 | 0.6237 | 0.0862 | 0.4497 | 0.3756 | 11.1206 | 0.7857 | 64.8515 | 9.0753 | -15.6612 | 9.0377 | -14.6942 | 9.0987 | -16.0347 |
| 7 | | 5 | ZPE(DFT) ZPE(CORR) H(CORR) η(CORR) ω(DFT) | 0.7098 | 0.6802 | 0.0296 | -0.1068 | 0.3949 | 0.3306 | 8.5761 | 0.8303 | 23.9732 | 0.6236 | 0.0862 | 0.4497 | 0.3756 | 11.1242 | 0.7856 | 64.9734 | 9.1669 | -15.6172 | 9.3592 | -14.3704 | 8.8037 | -16.362 |
| 8 | | 5 | ZPE(HF) ZPE(CORR) E ^{HOMO} (CORR) - E ^{LUMO} (CORR) H(CORR) ω(DFT) | 0.7098 | 0.6802 | 0.0296 | -0.107 | 0.3949 | 0.3306 | 8.5761 | 0.8303 | 23.9732 | 0.6236 | 0.0862 | 0.4497 | 0.3756 | 11.1242 | 0.7856 | 64.4373 | 8.8931 | -16.1407 | 9.021 | -14.8311 | 8.9972 | -16.2423 |
| 9 | | 5 | ZPE(HF) ZPE(CORR) H(CORR) η(CORR) ω(DFT) | 0.7098 | 0.6802 | 0.0296 | -0.107 | 0.3949 | 0.3306 | 8.5761 | 0.8303 | 23.9732 | 0.6236 | 0.0862 | 0.4497 | 0.3756 | 11.1242 | 0.7856 | 64.9161 | 8.8896 | -15.9374 | 9.2368 | -14.6248 | 9.5284 | -15.2828 |
| 10 | | 5 | ZPE(DFT) ZPE(HF) E ^{HOMO} (CORR) - E ^{LUMO} (CORR) H(CORR) ω(DFT) | 0.7098 | 0.6802 | 0.0296 | -0.1038 | 0.3949 | 0.3306 | 8.5761 | 0.8303 | 23.9732 | 0.6236 | 0.0862 | 0.4497 | 0.3756 | 11.1242 | 0.7856 | 64.6948 | 8.8857 | -15.8941 | 8.8475 | -15.0539 | 9.2507 | -15.4026 |
| 11 | | 4 | ZPE(DFT) ZPE(CORR) E ^{HOMO} (DFT) α(HF) | 0.6497 | 0.6217 | 0.028 | -0.0991 | 0.4339 | 0.3396 | 10.3527 | 0.7877 | 23.1855 | 0.5773 | 0.0724 | 0.4766 | 0.3731 | 12.4918 | 0.7467 | 59.144 | 7.2986 | -13.0375 | 7.1833 | -12.5792 | 7.0842 | -13.534 |
| 12 | | 4 | ZPE(HF) ZPE(CORR) E ^{HOMO} (DFT) α(HF) | 0.6497 | 0.6217 | 0.028 | -0.0993 | 0.4339 | 0.3396 | 10.3527 | 0.7877 | 23.1855 | 0.5773 | 0.0724 | 0.4766 | 0.3731 | 12.4918 | 0.7467 | 58.8665 | 7.5198 | -12.633 | 7.5931 | -11.8271 | 7.7422 | -12.6866 |
| 13 | | 4 | ZPE(DFT) ZPE(HF) E ^{HOMO} (DFT) α(HF) | 0.6497 | 0.6217 | 0.028 | -0.0986 | 0.4339 | 0.3396 | 10.3527 | 0.7877 | 23.1855 | 0.5773 | 0.0724 | 0.4766 | 0.3731 | 12.4918 | 0.7467 | 58.7755 | 7.53 | -12.5705 | 7.6767 | -11.9364 | 7.4449 | -13.2179 |
| 14 | | 4 | ZPE(DFT) ZPE(CORR) α(HF) ω(HF) | 0.6493 | 0.6213 | 0.0281 | -0.0984 | 0.4341 | 0.347 | 10.3648 | 0.7874 | 23.144 | 0.573 | 0.0763 | 0.479 | 0.3828 | 12.6209 | 0.7443 | 58.5903 | 7.6739 | -12.532 | 7.3755 | -12.0944 | 7.6442 | -12.8714 |
| 15 | | 4 | ZPE(HF) ZPE(CORR) α(HF) ω(HF) | 0.6493 | 0.6213 | 0.0281 | -0.0987 | 0.4341 | 0.347 | 10.3648 | 0.7874 | 23.144 | 0.573 | 0.0763 | 0.479 | 0.3828 | 12.6209 | 0.7443 | 58.7079 | 7.4807 | -13.0051 | 7.2817 | -12.4954 | 7.3375 | -13.3411 |
| 16 | | 4 | ZPE(DFT) ZPE(HF) α(HF) ω(HF) | 0.6493 | 0.6213 | 0.0281 | -0.0934 | 0.4341 | 0.347 | 10.3648 | 0.7874 | 23.144 | 0.573 | 0.0763 | 0.479 | 0.3828 | 12.6209 | 0.7443 | 58.8355 | 7.2675 | -13.3952 | 7.5726 | -12.0351 | 7.6818 | -12.6326 |
| 17 | | 4 | ZPE(DFT) ZPE(CORR) E ^{HOMO} (DFT) α(DFT) | 0.6394 | 0.6106 | 0.0288 | -0.1001 | 0.4402 | 0.3484 | 10.6566 | 0.7801 | 22.1679 | 0.5656 | 0.0738 | 0.4831 | 0.3823 | 12.8379 | 0.7372 | 57.508 | 7.3246 | -13.096 | 7.2815 | -12.3443 | 7.733 | -12.4197 |
| 18 | | 4 | ZPE(HF) ZPE(CORR) E ^{HOMO} (DFT) α(DFT) | 0.6394 | 0.6106 | 0.0288 | -0.1004 | 0.4402 | 0.3484 | 10.6566 | 0.7801 | 22.1679 | 0.5656 | 0.0738 | 0.4831 | 0.3823 | 12.8379 | 0.7372 | 57.9299 | 7.5031 | -12.6633 | 7.4847 | -12.2175 | 7.4051 | -12.8064 |
| 19 | | 4 | ZPE(DFT) ZPE(HF) E ^{HOMO} (DFT) α(DFT) | 0.6394 | 0.6106 | 0.0288 | -0.0995 | 0.4402 | 0.3484 | 10.6566 | 0.7801 | 22.1679 | 0.5656 | 0.0738 | 0.4831 | 0.3823 | 12.8379 | 0.7372 | 57.8115 | 7.0095 | -13.5802 | 7.3567 | -12.1256 | 7.4311 | -12.7696 |
| 20 | | 4 | ZPE(HF) ZPE(CORR) α(HF) χ(HF) | 0.6384 | 0.6095 | 0.0289 | -0.097 | 0.4408 | 0.3486 | 10.6863 | 0.7793 | 22.0716 | 0.5592 | 0.0792 | 0.4867 | 0.3848 | 13.027 | 0.7346 | 57.0589 | 7.1157 | -13.4951 | 7.2298 | -12.4658 | 7.3585 | -13.2317 |
| 21 | | 3 | ZPE(HF) ZPE(CORR) α(HF) | 0.5504 | 0.5239 | 0.0264 | -0.2626 | 0.4915 | 0.3922 | 13.2887 | 0.71 | 20.8096 | 0.4677 | 0.0826 | 0.5348 | 0.4241 | 15.7309 | 0.6661 | 48.1096 | 5.4421 | -11.0411 | 5.2106 | -10.3114 | 5.6222 | -10.8632 |
| 22 | | 3 | ZPE(DFT) ZPE(CORR) α(HF) | 0.5504 | 0.5239 | 0.0264 | -0.2621 | 0.4915 | 0.3922 | 13.2887 | 0.71 | 20.8096 | 0.4677 | 0.0826 | 0.5348 | 0.4241 | 15.7309 | 0.6661 | 48.2083 | 5.8782 | -10.3349 | 5.5681 | -10.0654 | 5.3337 | -10.9068 |
| 23 | | 3 | ZPE(DFT) ZPE(HF) α(HF) | 0.5504 | 0.5239 | 0.0264 | -0.2595 | 0.4915 | 0.3922 | 13.2887 | 0.71 | 20.8096 | 0.4677 | 0.0826 | 0.5348 | 0.4241 | 15.7309 | 0.6661 | 47.9778 | 5.4564 | -10.7202 | 5.5556 | -9.8872 | 5.2852 | -10.9109 |
| 24 | | 3 | ZPE(DFT) ZPE(CORR) α(DFT) | 0.5379 | 0.5107 | 0.0272 | -0.264 | 0.4983 | 0.3999 | 13.6584 | 0.6995 | 19.7864 | 0.458 | 0.0799 | 0.5397 | 0.4317 | 16.0185 | 0.6553 | 46.9371 | 5.6018 | -10.8387 | 5.6551 | -9.8209 | 5.4622 | -11.0288 |
| 25 | | 3 | ZPE(HF) ZPE(CORR) α(DFT) | 0.5379 | 0.5107 | 0.0272 | -0.2646 | 0.4983 | 0.3999 | 13.6584 | 0.6995 | 19.7864 | 0.458 | 0.0799 | 0.5397 | 0.4317 | 16.0185 | 0.6553 | 47.2274 | 5.4206 | -11.0988 | 5.4474 | -10.1117 | 6.0359 | -10.1653 |
| 26 | | 3 | ZPE(DFT) ZPE(HF) α(DFT) | 0.5379 | 0.5107 | 0.0272 | -0.2609 | 0.4983 | 0.3999 | 13.6584 | 0.6995 | 19.7864 | 0.458 | 0.0799 | 0.5397 | 0.4317 | 16.0185 | 0.6553 | 46.8824 | 5.1828 | -11.2083 | 5.5081 | -10.0959 | 5.4793 | -10.7478 |
| 27 | | 3 | ZPE(CORR) α(DFT) α(CORR) | 0.5307 | 0.5031 | 0.0276 | -0.2562 | 0.5022 | 0.4073 | 13.8689 | 0.6935 | 19.228 | 0.4346 | 0.0962 | 0.5512 | 0.4428 | 16.7115 | 0.6423 | 45.1312 | 5.425 | -10.9025 | 5.7226 | -9.7634 | 5.5025 | -10.6015 |
| 28 | | 3 | ZPE(CORR) α(HF) α(CORR) | 0.5307 | 0.5031 | 0.0276 | -0.252 | 0.5022 | 0.4073 | 13.8689 | 0.6935 | 19.228 | 0.4346 | 0.0962 | 0.5512 | 0.4428 | 16.7115 | 0.6423 | 45.0607 | 5.4613 | -10.7857 | 5.6572 | -9.9192 | 5.4255 | -10.7347 |
| 29 | | 3 | ZPE(CORR) E ^{HOMO} (DFT) - E ^{LUMO} (DFT) α(HF) | 0.52 | 0.4918 | 0.0282 | -0.1653 | 0.5079 | 0.4231 | 14.1863 | 0.6842 | 18.4174 | 0.4353 | 0.0847 | 0.5509 | 0.4596 | 16.6903 | 0.6342 | 44.6049 | 5.3729 | -10.81 | 5.5987 | -9.8796 | 5.4687 | -10.5711 |
| 30 | | 3 | ZPE(CORR) α(HF) η(DFT) | 0.52 | 0.4918 | 0.0282 | -0.1653 | 0.5079 | 0.4231 | 14.1863 | 0.6842 | 18.4174 | 0.4353 | 0.0847 | 0.5509 | 0.4596 | 16.6903 | 0.6342 | 44.4026 | 5.4433 | -10.9469 | 5.8493 | -9.5808 | 6.0701 | -9.8776 |
| 31 | | 2 | ZPE(CORR) α(HF) | 0.4728 | 0.4525 | 0.0203 | -0.3583 | 0.5323 | 0.4334 | 15.5817 | 0.642 | 23.3169 | 0.3914 | 0.0814 | 0.5719 | 0.4626 | 17.9882 | 0.5981 | 39.6435 | 3.6552 | -8.2876 | 3.7017 | -7.7307 | 3.6889 | -8.3533 |
| 32 | | 2 | ZPE(CORR) α(DFT) | 0.418 | 0.3956 | 0.0224 | -0.3648 | 0.5592 | 0.4567 | 17.2015 | 0.5896 | 18.6728 | 0.3289 | 0.0891 | 0.6005 | 0.4873 | 19.8357 | 0.5395 | 33.4614 | 3.5041 | -8.332 | 3.4506 | -8.1123 | 3.686 | -8.3129 |
| 33 | | 2 | ZPE(HF) α(HF) | 0.3533 | 0.3284 | 0.0249 | -0.3436 | 0.5895 | 0.4785 | 19.1141 | 0.5221 | 14.2028 | 0.234 | 0.1193 | 0.6416 | 0.5116 | 22.6409 | 0.458 | 26.2127 | 3.6117 | -8.3641 | 3.4512 | -8.0635 | 3.8397 | -8.1111 |
| 34 | | 2 | ZPE(DFT) α(HF) | 0.3455 | 0.3203 | 0.0252 | -0.3421 | 0.593 | 0.4811 | 19.3438 | 0.5136 | 13.7254 | 0.2239 | 0.1216 | 0.6458 | 0.5144 | 22.9367 | 0.4484 | 24.3135 | 3.6832 | -8.3339 | 3.4996 | -8.0584 | 3.464 | -8.5296 |
| 35 | | 2 | α(DFT) α(HF) | 0.3386 | 0.3131 | 0.0254 | -0.3435 | 0.5962 | 0.5013 | 19.5491 | 0.5059 | 13.3082 | 0.22 | 0.1185 | 0.6474 | 0.5367 | 23.0522 | 0.4389 | 23.6022 | 3.5981 | -8.4105 | 3.9191 | -7.5795 | 3.7301 | -8.2861 |
| 36 | | 2 | α(DFT) α(CORR) | 0.3386 | 0.3131 | 0.0254 | -0.3586 | 0.5962 | 0.5013 | 19.5491 | 0.5059 | 13.3082 | 0.22 | 0.1185 | 0.6474 | 0.5367 | 23.0522 | 0.4389 | 24.4638 | 3.5705 | -8.3131 | 3.7385 | -7.7599 | 3.7386 | -8.227 |
| 37 | | 2 | α(HF) α(CORR) | 0.3386 | 0.3131 | 0.0254 | -0.3445 | 0.5962 | 0.5013 | 19.5491 | 0.5059 | 13.3082 | 0.22 | 0.1185 | 0.6474 | 0.5367 | 23.0522 | 0.4389 | 24.1393 | 3.4553 | -8.5726 | 3.8004 | -7.6974 | 3.8638 | -7.8998 |
| 38 | | 2 | d(CORR) α(HF) | 0.3048 | 0.278 | 0.0267 | -0.1836 | 0.6112 | 0.5011 | 20.5477 | 0.4672 | 11.3979 | 0.2229 | 0.0818 | 0.6462 | 0.5315 | 22.9666 | 0.4231 | 21.6475 | 3.5893 | -9.2562 | 3.7242 | -7.7945 | 3.5023 | -9.3748 |
| 39 | | 2 | E ^{HOMO} (CORR) α(HF) | 0.2925 | 0.2653 | 0.0272 | 0.0586 | 0.6166 | 0.5053 | 20.9115 | 0.4526 | 10.7472 | 0.1793 | 0.1132 | 0.6641 | 0.5394 | 24.256 | 0.3892 | 19.0024 | 3.5216 | -8.5118 | 3.7439 | -7.7651 | 3.6233 | -8.5543 |
| 40 | | 2 | d(CORR) α(DFT) | 0.2842 | 0.2566 | 0.0275 | -0.1937 | 0.6202 | 0.5078 | 21.1563 | 0.4426 | 10.322 | 0.2045 | 0.0797 | 0.6538 | 0.5379 | 23.5106 | 0.3984 | 19.6241 | 3.8061 | -8.7413 | 4.0131 | -7.5064 | 3.5465 | -9.3295 |
| 41 | | 1 | α(HF) | 0.2126 | 0.1977 | 0.0149 | 0.4611 | 0.6505 | 0.5416 | 23.2727 | 0.3506 | 14.3078 | 0.1012 | 0.1114 | 0.695 | 0.5689 | 26.5652 | 0.2991 | 11.37 | | | | | | |

Table S4_0.00001. Models developed for $\log K_a$, but employing splitting method taking training set and prediction set in a ratio of 3:1. Values of internal and external validation parameters for models developed using quantum-mechanical and electron-correlation (CORR) based descriptors.

| S.No. | Size | Variables | R ² | R ² _{adj} | R ² -R ² _{adj} | ΔK | RMSE(tr) | MAE(tr) | RSS(tr) | CCC(tr) | F | Q ² _{loo} | R ² -Q ² _{loo} | RMSE(cv) | MAE(cv) | PRESS(cv) | CCC(cv) | Q ² _{LMO} | R ² _{Yscr} | Q ² _{Yscr} | R ² _{Ynd} | Q ² _{Ynd} | R ² _{Ynd} | Q ² _{Ynd} | N. ext. OK | RMSE(ext) | MAE(ext) | PRESS(ext) | Q ² _{F1} | Q ² _{F2} | Q ² _{F3} | CCC(ext) | \bar{F}_m^{-2} | ΔF_m^{-2} |
|-------|------|---|----------------|-------------------------------|---|------------|----------|---------|---------|---------|---------|-------------------------------|---|----------|---------|-----------|---------|-------------------------------|--------------------------------|--------------------------------|-------------------------------|-------------------------------|-------------------------------|-------------------------------|------------|-----------|----------|------------|------------------------------|------------------------------|------------------------------|----------|------------------|-------------------|
| 1 | 5 | E(CORR) ZPE(DFT) ZPE(CORR) η (CORR) ω (DFT) | 0.7215 | 0.6829 | 0.0387 | -0.101 | 0.4025 | 0.3388 | 6.8028 | 0.8382 | 18.6564 | 0.6174 | 0.1041 | 0.4717 | 0.3991 | 9.3457 | 0.7835 | 63.6416 | 12.6507 | -21.3815 | 12.7689 | -19.047 | 11.9301 | -22.0056 | 1 | 0.3922 | 0.3205 | 2.0001 | 0.6106 | 0.6072 | 0.7355 | 0.8111 | 0.5807 | 0.078 |
| 2 | 5 | E(CORR) ZPE(DFT) ZPE(CORR) E ^{HOMO} (CORR) - E ^{LUMO} (CORR) ω (DFT) | 0.7215 | 0.6829 | 0.0387 | -0.101 | 0.4025 | 0.3388 | 6.8028 | 0.8382 | 18.6564 | 0.6174 | 0.1041 | 0.4717 | 0.3991 | 9.3457 | 0.7835 | 63.4428 | 12.0232 | -22.8705 | 12.0765 | -20.1562 | 12.0209 | -21.7971 | 1 | 0.3922 | 0.3205 | 2.0001 | 0.6106 | 0.6072 | 0.7355 | 0.8111 | 0.5807 | 0.078 |
| 3 | 5 | E(CORR) ZPE(HF) ZPE(CORR) η (CORR) ω (DFT) | 0.7215 | 0.6829 | 0.0387 | -0.1013 | 0.4025 | 0.3388 | 6.8028 | 0.8382 | 18.6564 | 0.6174 | 0.1041 | 0.4717 | 0.3991 | 9.3457 | 0.7835 | 64.2909 | 13.1233 | -20.3103 | 12.2682 | -19.7893 | 12.426 | -21.3954 | 1 | 0.3922 | 0.3205 | 2.0001 | 0.6106 | 0.6072 | 0.7355 | 0.8111 | 0.5807 | 0.078 |
| 4 | 5 | E(CORR) ZPE(HF) ZPE(CORR) E ^{HOMO} (CORR) - E ^{LUMO} (CORR) ω (DFT) | 0.7215 | 0.6829 | 0.0387 | -0.1013 | 0.4025 | 0.3388 | 6.8028 | 0.8382 | 18.6564 | 0.6174 | 0.1041 | 0.4717 | 0.3991 | 9.3457 | 0.7835 | 63.9427 | 11.9093 | -21.5495 | 12.0322 | -20.2162 | 11.9221 | -22.2733 | 1 | 0.3922 | 0.3205 | 2.0001 | 0.6106 | 0.6072 | 0.7355 | 0.8111 | 0.5807 | 0.078 |
| 5 | 5 | E(CORR) ZPE(DFT) ZPE(HF) E ^{HOMO} (CORR) - E ^{LUMO} (CORR) ω (DFT) | 0.7215 | 0.6829 | 0.0387 | -0.0985 | 0.4025 | 0.3388 | 6.8028 | 0.8382 | 18.6564 | 0.6174 | 0.1041 | 0.4717 | 0.3991 | 9.3457 | 0.7835 | 63.7348 | 12.0224 | -22.0044 | 11.6211 | -20.6703 | 12.7414 | -21.3703 | 1 | 0.3922 | 0.3205 | 2.0001 | 0.6106 | 0.6072 | 0.7355 | 0.8111 | 0.5807 | 0.078 |
| 6 | 5 | E(CORR) ZPE(DFT) ZPE(HF) η (CORR) ω (DFT) | 0.7215 | 0.6829 | 0.0387 | -0.0985 | 0.4025 | 0.3388 | 6.8028 | 0.8382 | 18.6564 | 0.6174 | 0.1041 | 0.4717 | 0.3991 | 9.3457 | 0.7835 | 63.7954 | 12.4603 | -22.0009 | 11.8734 | -20.5557 | 12.5873 | -21.0936 | 1 | 0.3922 | 0.3205 | 2.0001 | 0.6106 | 0.6072 | 0.7355 | 0.8111 | 0.5807 | 0.078 |
| 7 | 5 | ZPE(DFT) ZPE(CORR) H(CORR) η (CORR) ω (DFT) | 0.7215 | 0.6828 | 0.0387 | -0.101 | 0.4025 | 0.3389 | 6.8049 | 0.8382 | 18.6484 | 0.6173 | 0.1041 | 0.4718 | 0.3992 | 9.3486 | 0.7834 | 63.3335 | 12.6345 | -21.3039 | 12.0423 | -20.0519 | 12.3937 | -21.7175 | 1 | 0.3923 | 0.3206 | 2.0008 | 0.6104 | 0.607 | 0.7354 | 0.8111 | 0.5805 | 0.0781 |
| 8 | 5 | ZPE(HF) ZPE(CORR) E ^{HOMO} (CORR) - E ^{LUMO} (CORR) H(CORR) ω (DFT) | 0.7215 | 0.6828 | 0.0387 | -0.101 | 0.4025 | 0.3389 | 6.8049 | 0.8382 | 18.6484 | 0.6173 | 0.1041 | 0.4718 | 0.3992 | 9.3486 | 0.7834 | 63.4128 | 12.0769 | -21.2697 | 12.2914 | -19.864 | 12.3656 | -21.5569 | 1 | 0.3923 | 0.3206 | 2.0008 | 0.6104 | 0.607 | 0.7354 | 0.8111 | 0.5805 | 0.0781 |
| 9 | 5 | ZPE(DFT) ZPE(HF) H(CORR) η (CORR) ω (DFT) | 0.7215 | 0.6828 | 0.0387 | -0.0985 | 0.4025 | 0.3389 | 6.8049 | 0.8382 | 18.6484 | 0.6173 | 0.1041 | 0.4718 | 0.3992 | 9.3486 | 0.7834 | 63.4903 | 12.3443 | -21.5974 | 12.226 | -19.8465 | 12.0377 | -22.2846 | 1 | 0.3923 | 0.3206 | 2.0008 | 0.6104 | 0.607 | 0.7354 | 0.8111 | 0.5805 | 0.0781 |
| 10 | 5 | ZPE(DFT) ZPE(HF) E ^{HOMO} (CORR) - E ^{LUMO} (CORR) H(CORR) ω (DFT) | 0.7215 | 0.6828 | 0.0387 | -0.0985 | 0.4025 | 0.3389 | 6.8049 | 0.8382 | 18.6484 | 0.6173 | 0.1041 | 0.4718 | 0.3992 | 9.3486 | 0.7834 | 63.4426 | 12.0081 | -21.9943 | 12.2986 | -19.7524 | 12.4974 | -21.3723 | 1 | 0.3923 | 0.3206 | 2.0008 | 0.6104 | 0.607 | 0.7354 | 0.8111 | 0.5805 | 0.0781 |
| 11 | 4 | ZPE(DFT) ZPE(HF) E ^{HOMO} (DFT) α (HF) | 0.6711 | 0.6355 | 0.0356 | -0.1063 | 0.4374 | 0.3449 | 8.0349 | 0.8032 | 18.8743 | 0.5792 | 0.0919 | 0.4948 | 0.3919 | 10.2808 | 0.7515 | 58.7228 | 9.6951 | -18.1562 | 9.409 | -17.1677 | 9.5644 | -18.2103 | 0 | 0.4399 | 0.3636 | 2.5156 | 0.5102 | 0.5059 | 0.6673 | 0.6964 | 0.4735 | 0.2958 |
| 12 | 4 | ZPE(DFT) ZPE(HF) E ^{HOMO} (DFT) α (HF) | 0.6711 | 0.6355 | 0.0356 | -0.1068 | 0.4374 | 0.3449 | 8.0349 | 0.8032 | 18.8743 | 0.5792 | 0.0919 | 0.4948 | 0.3919 | 10.2808 | 0.7515 | 58.7495 | 9.7167 | -18.0261 | 9.4719 | -17.0085 | 9.458 | -19.1421 | 0 | 0.4399 | 0.3636 | 2.5156 | 0.5102 | 0.5059 | 0.6673 | 0.6964 | 0.4735 | 0.2958 |
| 13 | 4 | ZPE(HF) ZPE(CORR) E ^{HOMO} (DFT) α (HF) | 0.6711 | 0.6355 | 0.0356 | -0.107 | 0.4374 | 0.3449 | 8.0349 | 0.8032 | 18.8743 | 0.5792 | 0.0919 | 0.4948 | 0.3919 | 10.2808 | 0.7515 | 58.9887 | 9.6033 | -17.9159 | 9.7135 | -16.7209 | 9.3674 | -18.6257 | 0 | 0.4399 | 0.3636 | 2.5156 | 0.5102 | 0.5059 | 0.6673 | 0.6964 | 0.4735 | 0.2958 |
| 14 | 4 | ZPE(DFT) ZPE(CORR) G(DFT) χ (CORR) | 0.668 | 0.6321 | 0.0359 | -0.044 | 0.4395 | 0.357 | 8.1114 | 0.8009 | 18.6091 | 0.5732 | 0.0947 | 0.4982 | 0.4047 | 10.4257 | 0.7461 | 58.4999 | 9.7707 | -18.0491 | 9.7963 | -16.5137 | 9.716 | -17.4611 | 0 | 0.8144 | 0.5557 | 8.6224 | -0.6788 | -0.6934 | -0.1403 | 0.5885 | 0.1918 | 0.4384 |
| 15 | 4 | ZPE(HF) ZPE(CORR) G(DFT) χ (CORR) | 0.668 | 0.6321 | 0.0359 | -0.0351 | 0.4395 | 0.357 | 8.1114 | 0.8009 | 18.6091 | 0.5732 | 0.0947 | 0.4982 | 0.4047 | 10.4257 | 0.7461 | 58.4999 | 9.7167 | -17.786 | 10.131 | -16.1825 | 10.1046 | -17.4517 | 0 | 0.8144 | 0.5557 | 8.6224 | -0.6788 | -0.6934 | -0.1403 | 0.5885 | 0.1918 | 0.4384 |
| 16 | 4 | ZPE(DFT) ZPE(HF) G(DFT) χ (CORR) | 0.668 | 0.6321 | 0.0359 | -0.0275 | 0.4395 | 0.357 | 8.1114 | 0.8009 | 18.6091 | 0.5732 | 0.0947 | 0.4982 | 0.4047 | 10.4257 | 0.7461 | 57.9256 | 10.1505 | -17.5335 | 9.9847 | -16.4269 | 9.9132 | -17.3648 | 0 | 0.8144 | 0.5557 | 8.6224 | -0.6788 | -0.6934 | -0.1403 | 0.5885 | 0.1918 | 0.4384 |
| 17 | 4 | E(DFT) ZPE(DFT) ZPE(CORR) α (HF) | 0.668 | 0.6321 | 0.0359 | 0.0016 | 0.4395 | 0.357 | 8.1114 | 0.8009 | 18.6091 | 0.5732 | 0.0947 | 0.4982 | 0.4047 | 10.4258 | 0.7461 | 58.2357 | 10.4075 | -16.9304 | 9.8354 | -16.6785 | 9.7613 | -17.6623 | 0 | 0.8144 | 0.5557 | 8.6223 | -0.6788 | -0.6934 | -0.1403 | 0.5885 | 0.1918 | 0.4384 |
| 18 | 4 | E(DFT) ZPE(HF) ZPE(CORR) χ (CORR) | 0.668 | 0.6321 | 0.0359 | 0.001 | 0.4395 | 0.357 | 8.1114 | 0.8009 | 18.6091 | 0.5732 | 0.0947 | 0.4982 | 0.4047 | 10.4258 | 0.7461 | 57.9461 | 9.758 | -17.7539 | 9.6065 | -16.8644 | 9.4284 | -18.3829 | 0 | 0.8144 | 0.5557 | 8.6223 | -0.6788 | -0.6934 | -0.1403 | 0.5885 | 0.1918 | 0.4384 |
| 19 | 4 | E(DFT) ZPE(DFT) ZPE(HF) χ (CORR) | 0.668 | 0.6321 | 0.0359 | -0.0276 | 0.4395 | 0.357 | 8.1114 | 0.8009 | 18.6091 | 0.5732 | 0.0947 | 0.4982 | 0.4047 | 10.4258 | 0.7461 | 58.2592 | 9.8911 | -17.5106 | 9.9091 | -16.3876 | 9.4561 | -17.8872 | 0 | 0.8144 | 0.5557 | 8.6223 | -0.6788 | -0.6934 | -0.1403 | 0.5885 | 0.1918 | 0.4384 |
| 20 | 4 | ZPE(DFT) ZPE(HF) H(DFT) χ (CORR) | 0.668 | 0.6321 | 0.0359 | -0.0281 | 0.4395 | 0.357 | 8.1114 | 0.8009 | 18.6091 | 0.5732 | 0.0947 | 0.4982 | 0.4047 | 10.4258 | 0.7461 | 58.7414 | 9.439 | -17.6223 | 9.8232 | -16.5924 | 9.8071 | -17.8456 | 0 | 0.8144 | 0.5557 | 8.6224 | -0.6788 | -0.6934 | -0.1403 | 0.5885 | 0.1918 | 0.4384 |
| 21 | 3 | ZPE(DFT) ZPE(CORR) α (HF) | 0.5709 | 0.537 | 0.0339 | -0.2444 | 0.4996 | 0.3997 | 10.4827 | 0.7269 | 16.853 | 0.4523 | 0.1186 | 0.5644 | 0.4475 | 13.3805 | 0.6647 | 46.3776 | 7.293 | -14.5561 | 7.2728 | -13.4669 | 7.3164 | -14.8663 | 0 | 0.4799 | 0.4004 | 2.9934 | 0.4172 | 0.4121 | 0.6041 | 0.5548 | 0.1686 | 0.5269 |
| 22 | 3 | ZPE(HF) ZPE(CORR) α (HF) | 0.5709 | 0.537 | 0.0339 | -0.2449 | 0.4996 | 0.3997 | 10.4827 | 0.7269 | 16.853 | 0.4523 | 0.1186 | 0.5644 | 0.4475 | 13.3805 | 0.6647 | 46.4578 | 7.3421 | -14.5573 | 7.0089 | -13.7753 | 7.3356 | -14.7109 | 0 | 0.4799 | 0.4004 | 2.9934 | 0.4172 | 0.4121 | 0.6041 | 0.5548 | 0.1686 | 0.5269 |
| 23 | 3 | ZPE(DFT) ZPE(HF) α (HF) | 0.5709 | 0.537 | 0.0339 | -0.2419 | 0.4996 | 0.3997 | 10.4827 | 0.7269 | 16.853 | 0.4523 | 0.1186 | 0.5644 | 0.4475 | 13.3805 | 0.6647 | 46.6267 | 7.5278 | -14.6676 | 7.8158 | -12.7983 | 7.48 | -14.7677 | 0 | 0.4799 | 0.4004 | 2.9934 | 0.4172 | 0.4121 | 0.6041 | 0.5548 | 0.1686 | 0.5269 |
| 24 | 3 | ZPE(CORR) α (HF) α (CORR) | 0.5611 | 0.5265 | 0.0346 | -0.2358 | 0.5053 | 0.4105 | 10.7222 | 0.7189 | 16.1934 | 0.4286 | 0.1325 | 0.5765 | 0.4613 | 13.9587 | 0.6489 | 45.2132 | 6.8681 | -14.8949 | 7.2909 | -13.5653 | 6.9378 | -14.9886 | 0 | 0.5067 | 0.4233 | 3.3375 | 0.3502 | 0.3445 | 0.5586 | 0.5008 | 0.1314 | 0.51 |
| 25 | 3 | ZPE(CORR) α (DFT) α (CORR) | 0.5611 | 0.5265 | 0.0346 | -0.2406 | 0.5053 | 0.4105 | 10.7222 | 0.7189 | 16.1934 | 0.4286 | 0.1325 | 0.5765 | 0.4613 | 13.9587 | 0.6489 | 45.0602 | 7.1464 | -14.7005 | 7.5108 | -13.2974 | 7.2794 | -14.6327 | 0 | 0.5067 | 0.4233 | 3.3375 | 0.3502 | 0.3445 | 0.5586 | 0.5008 | 0.1314 | 0.51 |
| 26 | 3 | ZPE(CORR) E ^{HOMO} (DFT) - E ^{LUMO} (DFT) α (HF) | 0.5609 | 0.5262 | 0.0347 | -0.1489 | 0.5054 | 0.4064 | 10.7276 | 0.7187 | 16.1791 | 0.446 | 0.1149 | 0.5677 | 0.4561 | 13.5352 | 0.6546 | 45.2513 | 7.3529 | -14.5582 | 7.5887 | -13.1371 | 7.5296 | -13.8843 | 0 | 0.5293 | 0.4652 | 3.6426 | 0.2908 | 0.2846 | 0.5183 | 0.5094 | 0.1927 | 0.3287 |
| 27 | 3 | ZPE(CORR) α (HF) η (DFT) | 0.5609 | 0.5262 | 0.0347 | -0.1489 | 0.5054 | 0.4064 | 10.7276 | 0.7187 | 16.1791 | 0.446 | 0.1149 | 0.5677 | 0.4561 | 13.5352 | 0.6546 | 45.3029 | 7.2903 | -14.631 | 7.5534 | -13.1507 | 7.3496 | -14.412 | 0 | 0.5293 | 0.4652 | 3.6426 | 0.2908 | 0.2846 | 0.5183 | 0.5094 | 0.1927 | 0.3287 |
| 28 | 3 | ZPE(HF) ZPE(CORR) α (DFT) | 0.5554 | 0.5203 | 0.0351 | -0.2475 | 0.5085 | 0.4103 | 10.8617 | 0.7141 | 15.8228 | 0.4434 | 0.112 | 0.569 | 0.458 | 13.5974 | 0.6528 | 44.6701 | 7.2683 | -15.2218 | 7.0298 | -13.8136 | 7.6691 | -14.4226 | 0 | 0.4794 | 0.402 | 2.9871 | 0.4184 | 0.4133 | 0.605 | 0.5599 | 0.1814 | 0.5139 |
| 29 | 3 | ZPE(DFT) ZPE(CORR) α (DFT) | 0.5554 | 0.5203 | 0.0351 | -0.2469 | 0.5085 | 0.4103 | 10.8617 | 0.7141 | 15.8228 | 0.4434 | 0.112 | 0.569 | 0.458 | 13.5974 | 0.6528 | 45.6351 | 7.8378 | -14.0287 | 7.4086 | -13.3629 | 7.2141 | -14.5982 | 0 | 0.4794 | 0.402 | 2.9871 | 0.4184 | 0.4133 | 0.605 | 0.5599 | 0.1814 | 0.5139 |
| 30 | 3 | ZPE(DFT) ZPE(HF) α (DFT) | 0.5554</ | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |

Table S5_0.00001. Same as Table S4_0.00001, but employing splitting method taking training set and prediction set in a ratio of 2:1.

| S.No. | Size | Variables | R ² | R ² _{adj} | R ² _{adj} | ΔK | RMSE(tr) | MAE(tr) | RSS(tr) | CCC(tr) | F | Q ² _{loo} | R ² _{loo} | RMSE(cv) | MAE(cv) | PRESS(cv) | CCC(cv) | Q ² _{LMO} | R ² _{Yser} | Q ² _{Yser} | R ² _{Xnd} | Q ² _{Xnd} | R ² _{Ynd} | Q ² _{Ynd} | N. ext. OK | RMSE(ext) | MAE(ext) | PRESS(ext) | Q ² _{F1} | Q ² _{F2} | Q ² _{F3} | CCC(ext) | \bar{r}_m^{-2} | Δr_m^{-2} |
|-------|------|---|----------------|-------------------------------|-------------------------------|------------|----------|---------|---------|---------|---------|-------------------------------|-------------------------------|----------|---------|-----------|---------|-------------------------------|--------------------------------|--------------------------------|-------------------------------|-------------------------------|-------------------------------|-------------------------------|------------|-----------|----------|------------|------------------------------|------------------------------|------------------------------|----------|------------------|-------------------|
| 1 | 5 | E(CORR) ZPE(HF) ZPE(CORR) η (CORR) ω (DFT) | 0.6994 | 0.6524 | 0.047 | -0.1141 | 0.4259 | 0.3713 | 6.8926 | 0.8231 | 14.8905 | 0.5746 | 0.1248 | 0.5066 | 0.4439 | 9.7543 | 0.7581 | 58.7894 | 13.5007 | -28.5493 | 13.07 | -22.7821 | 13.6851 | -27.5776 | 1 | 0.3498 | 0.2885 | 2.0802 | 0.6861 | 0.6861 | 0.7972 | 0.8156 | 0.5602 | 0.2542 |
| 2 | 5 | E(CORR) ZPE(DFT) ZPE(CORR) E ^{HOMO} (CORR) - E ^{LUMO} (CORR) ω (DFT) | 0.6994 | 0.6524 | 0.047 | -0.1141 | 0.4259 | 0.3713 | 6.8926 | 0.8231 | 14.8905 | 0.5746 | 0.1248 | 0.5066 | 0.4439 | 9.7543 | 0.7581 | 58.2355 | 13.8621 | -27.3025 | 13.4892 | -22.6938 | 14.1804 | -25.8462 | 1 | 0.3498 | 0.2885 | 2.0802 | 0.6861 | 0.6861 | 0.7972 | 0.8156 | 0.5602 | 0.2542 |
| 3 | 5 | E(CORR) ZPE(DFT) ZPE(CORR) η (CORR) ω (DFT) | 0.6994 | 0.6524 | 0.047 | -0.1138 | 0.4259 | 0.3713 | 6.8926 | 0.8231 | 14.8905 | 0.5746 | 0.1248 | 0.5066 | 0.4439 | 9.7543 | 0.7581 | 58.6739 | 13.4295 | -28.324 | 13.2945 | -22.7774 | 13.2393 | -28.1255 | 1 | 0.3498 | 0.2885 | 2.0802 | 0.6861 | 0.6861 | 0.7972 | 0.8156 | 0.5602 | 0.2542 |
| 4 | 5 | E(CORR) ZPE(DFT) ZPE(CORR) E ^{HOMO} (CORR) - E ^{LUMO} (CORR) ω (DFT) | 0.6994 | 0.6524 | 0.047 | -0.1138 | 0.4259 | 0.3713 | 6.8926 | 0.8231 | 14.8905 | 0.5746 | 0.1248 | 0.5066 | 0.4439 | 9.7543 | 0.7581 | 58.3423 | 13.7048 | -27.7207 | 13.5901 | -22.627 | 13.7603 | -26.5969 | 1 | 0.3498 | 0.2885 | 2.0802 | 0.6861 | 0.6861 | 0.7972 | 0.8156 | 0.5602 | 0.2542 |
| 5 | 5 | E(CORR) ZPE(DFT) ZPE(HF) η (CORR) ω (DFT) | 0.6994 | 0.6524 | 0.047 | -0.1106 | 0.4259 | 0.3713 | 6.8926 | 0.8231 | 14.8905 | 0.5746 | 0.1248 | 0.5066 | 0.4439 | 9.7543 | 0.7581 | 58.2311 | 13.1211 | -29.1676 | 13.4354 | -22.7458 | 13.4034 | -28.5498 | 1 | 0.3498 | 0.2885 | 2.0802 | 0.6861 | 0.6861 | 0.7972 | 0.8156 | 0.5602 | 0.2542 |
| 6 | 5 | E(CORR) ZPE(DFT) ZPE(HF) E ^{HOMO} (CORR) - E ^{LUMO} (CORR) ω (DFT) | 0.6994 | 0.6524 | 0.047 | -0.1106 | 0.4259 | 0.3713 | 6.8926 | 0.8231 | 14.8905 | 0.5746 | 0.1248 | 0.5066 | 0.4439 | 9.7543 | 0.7581 | 58.5393 | 13.0274 | -28.495 | 13.9051 | -21.7697 | 13.1778 | -28.2369 | 1 | 0.3498 | 0.2885 | 2.0802 | 0.6861 | 0.6861 | 0.7972 | 0.8156 | 0.5602 | 0.2542 |
| 7 | 5 | ZPE(HF) ZPE(CORR) H(CORR) η (CORR) ω (DFT) | 0.6993 | 0.6523 | 0.047 | -0.1141 | 0.4259 | 0.3713 | 6.8945 | 0.8231 | 14.8847 | 0.5745 | 0.1248 | 0.5067 | 0.4439 | 9.757 | 0.758 | 58.2163 | 13.4627 | -28.1743 | 13.4239 | -22.8206 | 13.6385 | -27.7106 | 1 | 0.3499 | 0.2885 | 2.0812 | 0.6859 | 0.6859 | 0.7971 | 0.8155 | 0.5601 | 0.2543 |
| 8 | 5 | ZPE(DFT) ZPE(CORR) E ^{HOMO} (CORR) - E ^{LUMO} (CORR) H(CORR) ω (DFT) | 0.6993 | 0.6523 | 0.047 | -0.1138 | 0.4259 | 0.3713 | 6.8945 | 0.8231 | 14.8847 | 0.5745 | 0.1248 | 0.5067 | 0.4439 | 9.757 | 0.758 | 58.9074 | 13.4819 | -27.8492 | 13.6272 | -22.3031 | 14.131 | -25.9847 | 1 | 0.3499 | 0.2885 | 2.0812 | 0.6859 | 0.6859 | 0.7971 | 0.8155 | 0.5601 | 0.2543 |
| 9 | 5 | ZPE(DFT) ZPE(HF) E ^{HOMO} (CORR) - E ^{LUMO} (CORR) H(CORR) ω (DFT) | 0.6993 | 0.6523 | 0.047 | -0.1106 | 0.4259 | 0.3713 | 6.8945 | 0.8231 | 14.8847 | 0.5745 | 0.1248 | 0.5067 | 0.4439 | 9.757 | 0.758 | 58.5875 | 13.5362 | -28.6325 | 13.1295 | -22.9828 | 13.3185 | -28.1352 | 1 | 0.3499 | 0.2885 | 2.0812 | 0.6859 | 0.6859 | 0.7971 | 0.8155 | 0.5601 | 0.2543 |
| 10 | 5 | ZPE(DFT) ZPE(HF) H(CORR) η (CORR) ω (DFT) | 0.6993 | 0.6523 | 0.047 | -0.1106 | 0.4259 | 0.3713 | 6.8945 | 0.8231 | 14.8847 | 0.5745 | 0.1248 | 0.5067 | 0.4439 | 9.757 | 0.758 | 58.3224 | 13.9496 | -27.4532 | 13.3275 | -22.6948 | 13.3053 | -28.1273 | 1 | 0.3499 | 0.2885 | 2.0812 | 0.6859 | 0.6859 | 0.7971 | 0.8155 | 0.5601 | 0.2543 |
| 11 | 4 | ZPE(HF) ZPE(CORR) G(DFT) χ (CORR) | 0.6388 | 0.595 | 0.0438 | -0.0228 | 0.4669 | 0.3847 | 8.2827 | 0.7796 | 14.5885 | 0.5208 | 0.118 | 0.5377 | 0.4439 | 10.9877 | 0.7138 | 52.8757 | 10.9691 | -20.9463 | 10.9691 | -18.6427 | 10.3692 | -21.7084 | 0 | 0.6665 | 0.4167 | 7.552 | -0.1397 | -0.1397 | 0.2638 | 0.637 | 0.3367 | 0.2751 |
| 12 | 4 | ZPE(DFT) ZPE(CORR) G(DFT) χ (CORR) | 0.6388 | 0.595 | 0.0438 | -0.0226 | 0.4669 | 0.3847 | 8.2827 | 0.7796 | 14.5885 | 0.5208 | 0.118 | 0.5377 | 0.4439 | 10.9877 | 0.7138 | 52.4147 | 11.1502 | -20.8962 | 10.5094 | -18.8505 | 10.7178 | -21.6423 | 0 | 0.6665 | 0.4167 | 7.552 | -0.1397 | -0.1397 | 0.2638 | 0.637 | 0.3367 | 0.2751 |
| 13 | 4 | ZPE(DFT) ZPE(HF) G(DFT) χ (CORR) | 0.6388 | 0.595 | 0.0438 | 0.009 | 0.4669 | 0.3847 | 8.2827 | 0.7796 | 14.5885 | 0.5208 | 0.118 | 0.5377 | 0.4439 | 10.9877 | 0.7138 | 52.8596 | 10.4637 | -22.4286 | 10.6748 | -18.9776 | 10.2064 | -22.5022 | 0 | 0.6665 | 0.4167 | 7.552 | -0.1397 | -0.1397 | 0.2638 | 0.637 | 0.3367 | 0.2751 |
| 14 | 4 | E(DFT) ZPE(HF) ZPE(CORR) χ (CORR) | 0.6388 | 0.595 | 0.0438 | -0.0078 | 0.4669 | 0.3847 | 8.2828 | 0.7796 | 14.5884 | 0.5208 | 0.118 | 0.5377 | 0.4439 | 10.9877 | 0.7138 | 52.7263 | 10.4449 | -22.279 | 10.2272 | -19.3854 | 11.1201 | -20.6001 | 0 | 0.6665 | 0.4167 | 7.5519 | -0.1397 | -0.1397 | 0.2638 | 0.637 | 0.3367 | 0.2751 |
| 15 | 4 | E(DFT) ZPE(DFT) ZPE(CORR) χ (CORR) | 0.6388 | 0.595 | 0.0438 | -0.0064 | 0.4669 | 0.3847 | 8.2828 | 0.7796 | 14.5884 | 0.5208 | 0.118 | 0.5377 | 0.4439 | 10.9877 | 0.7138 | 52.8191 | 11.3223 | -20.7125 | 10.2021 | -19.4649 | 10.3681 | -21.93 | 0 | 0.6665 | 0.4167 | 7.5519 | -0.1397 | -0.1397 | 0.2638 | 0.637 | 0.3367 | 0.2751 |
| 16 | 4 | E(DFT) ZPE(DFT) ZPE(HF) χ (CORR) | 0.6388 | 0.595 | 0.0438 | -0.0182 | 0.4669 | 0.3847 | 8.2828 | 0.7796 | 14.5884 | 0.5208 | 0.118 | 0.5377 | 0.4439 | 10.9877 | 0.7138 | 52.7581 | 10.4442 | -21.7192 | 10.7233 | -18.8949 | 11.0744 | -21.089 | 0 | 0.6665 | 0.4167 | 7.5519 | -0.1397 | -0.1397 | 0.2638 | 0.637 | 0.3367 | 0.2751 |
| 17 | 4 | ZPE(HF) ZPE(CORR) H(DFT) χ (CORR) | 0.6388 | 0.595 | 0.0438 | -0.0228 | 0.4669 | 0.3847 | 8.2828 | 0.7796 | 14.5884 | 0.5208 | 0.118 | 0.5377 | 0.4439 | 10.9877 | 0.7138 | 52.7402 | 10.9989 | -20.7231 | 10.6749 | -19.0057 | 10.8167 | -21.4814 | 0 | 0.6665 | 0.4167 | 7.5519 | -0.1397 | -0.1397 | 0.2638 | 0.637 | 0.3367 | 0.2751 |
| 18 | 4 | ZPE(DFT) ZPE(CORR) H(DFT) χ (CORR) | 0.6388 | 0.595 | 0.0438 | -0.0226 | 0.4669 | 0.3847 | 8.2828 | 0.7796 | 14.5884 | 0.5208 | 0.118 | 0.5377 | 0.4439 | 10.9877 | 0.7138 | 52.9748 | 11.0905 | -20.5355 | 11.0158 | -18.5412 | 10.8671 | -21.9345 | 0 | 0.6665 | 0.4167 | 7.5519 | -0.1397 | -0.1397 | 0.2638 | 0.637 | 0.3367 | 0.2751 |
| 19 | 4 | ZPE(DFT) ZPE(HF) H(DFT) χ (CORR) | 0.6388 | 0.595 | 0.0438 | 0.009 | 0.4669 | 0.3847 | 8.2828 | 0.7796 | 14.5884 | 0.5208 | 0.118 | 0.5377 | 0.4439 | 10.9877 | 0.7138 | 52.853 | 10.8523 | -20.9804 | 11.5922 | -17.314 | 11.0174 | -21.2615 | 0 | 0.6665 | 0.4167 | 7.5519 | -0.1397 | -0.1397 | 0.2638 | 0.637 | 0.3367 | 0.2751 |
| 20 | 4 | ZPE(HF) ZPE(CORR) G(HF) χ (CORR) | 0.6387 | 0.5949 | 0.0438 | -0.0225 | 0.4669 | 0.3847 | 8.284 | 0.7795 | 14.5849 | 0.5207 | 0.118 | 0.5378 | 0.4439 | 10.9899 | 0.7138 | 53.124 | 11.4612 | -20.6418 | 11.2517 | -17.997 | 10.3498 | -21.9586 | 0 | 0.6671 | 0.4169 | 7.5649 | -0.1416 | -0.1417 | 0.2625 | 0.6367 | 0.3363 | 0.2754 |
| 21 | 3 | ZPE(HF) ZPE(CORR) α (HF) | 0.5235 | 0.4814 | 0.042 | -0.2639 | 0.5362 | 0.4429 | 10.9268 | 0.6872 | 12.4488 | 0.3495 | 0.1739 | 0.6265 | 0.5089 | 14.9152 | 0.6003 | 38.483 | 7.9074 | -18.7154 | 8.1641 | -14.8713 | 8.22 | -17.8142 | 1 | 0.3755 | 0.2813 | 2.3964 | 0.6384 | 0.6383 | 0.7664 | 0.7572 | 0.4113 | 0.3332 |
| 22 | 3 | ZPE(DFT) ZPE(CORR) α (HF) | 0.5235 | 0.4814 | 0.042 | -0.2632 | 0.5362 | 0.4429 | 10.9268 | 0.6872 | 12.4488 | 0.3495 | 0.1739 | 0.6265 | 0.5089 | 14.9152 | 0.6003 | 38.0272 | 7.9957 | -18.3142 | 8.4952 | -14.3971 | 8.2163 | -17.8579 | 1 | 0.3755 | 0.2813 | 2.3964 | 0.6384 | 0.6383 | 0.7664 | 0.7572 | 0.4113 | 0.3332 |
| 23 | 3 | ZPE(DFT) ZPE(HF) α (HF) | 0.5235 | 0.4814 | 0.042 | -0.2603 | 0.5362 | 0.4429 | 10.9268 | 0.6872 | 12.4488 | 0.3495 | 0.1739 | 0.6265 | 0.5089 | 14.9152 | 0.6003 | 38.7741 | 7.9863 | -18.6584 | 8.056 | -15.0373 | 7.9449 | -18.5554 | 1 | 0.3755 | 0.2813 | 2.3964 | 0.6384 | 0.6383 | 0.7664 | 0.7572 | 0.4113 | 0.3332 |
| 24 | 3 | ZPE(CORR) α (HF) η (DFT) | 0.5185 | 0.476 | 0.0425 | -0.1754 | 0.539 | 0.454 | 11.0399 | 0.6829 | 12.2053 | 0.3482 | 0.1703 | 0.6271 | 0.5237 | 14.9452 | 0.5904 | 37.2689 | 8.4363 | -18.4363 | 8.3246 | -14.832 | 8.1013 | -17.1782 | 0 | 0.4406 | 0.3658 | 3.3006 | 0.5019 | 0.5019 | 0.6782 | 0.741 | 0.4152 | 0.0678 |
| 25 | 3 | ZPE(CORR) E ^{HOMO} (DFT) - E ^{LUMO} (DFT) α (HF) | 0.5185 | 0.476 | 0.0425 | -0.1754 | 0.539 | 0.454 | 11.0399 | 0.6829 | 12.2053 | 0.3482 | 0.1703 | 0.6271 | 0.5237 | 14.9452 | 0.5904 | 37.0675 | 8.0309 | -18.5389 | 7.7589 | -15.4206 | 8.0596 | -18.0769 | 0 | 0.4406 | 0.3658 | 3.3006 | 0.5019 | 0.5019 | 0.6782 | 0.741 | 0.4152 | 0.0678 |
| 26 | 3 | ZPE(HF) ZPE(CORR) α (DFT) | 0.5148 | 0.472 | 0.0428 | -0.2663 | 0.5411 | 0.45 | 11.1252 | 0.6797 | 12.0248 | 0.3395 | 0.1753 | 0.6313 | 0.5173 | 15.1449 | 0.5907 | 36.4018 | 8.2138 | -17.3004 | 8.0367 | -15.0007 | 8.1503 | -17.5551 | 1 | 0.39 | 0.3029 | 2.5857 | 0.6098 | 0.6098 | 0.7479 | 0.7517 | 0.432 | 0.3151 |
| 27 | 3 | ZPE(DFT) ZPE(CORR) α (DFT) | 0.5148 | 0.472 | 0.0428 | -0.2656 | 0.5411 | 0.45 | 11.1252 | 0.6797 | 12.0248 | 0.3395 | 0.1753 | 0.6313 | 0.5173 | 15.1449 | 0.5907 | 37.7503 | 8.3323 | -18.2237 | 7.8453 | -15.329 | 7.6875 | -18.2025 | 1 | 0.39 | 0.3029 | 2.5857 | 0.6098 | 0.6098 | 0.7479 | 0.7517 | 0.432 | 0.3151 |
| 28 | 3 | ZPE(DFT) ZPE(HF) α (DFT) | 0.5148 | 0.472 | 0.0428 | -0.262 | 0.5411 | 0.45 | 11.1252 | 0.6797 | 12.0248 | 0.3395 | 0.1753 | 0.6313 | 0.5173 | 15.1449 | 0.5907 | 37.5291 | 7.9941 | -18.0662 | 7.9894 | -15.0349 | 8.2794 | -17.3167 | 1 | 0.39 | 0.3029 | 2.5857 | 0.6098 | 0.6098 | 0.7479 | 0.7517 | 0.432 | 0.3151 |
| 29 | 3 | ZPE(CORR) α (HF) α (CORR) | 0.51 | 0.4667 | 0.0432 | -0.2557 | 0.5438 | 0.4565 | 11.2362 | 0.6755 | 11.7941 | 0.3282 | 0.1817 | 0.6367 | 0.5244 | 15.4035 | 0.5844 | 36.4498 | 8.5607 | -16.6746 | 7.8887 | -15.3134 | 8.034 | -17.4785 | 1 | 0.4046 | 0.3114 | 2.7833 | 0.58 | 0.5799 | 0.7287 | 0.7021 | 0.3324 | 0.3806 |
| 30 | 3 | ZPE(CORR) α (DFT) α (HF) | 0.51 | 0.4667 | 0.0432 | -0.2526 | 0.5438 | 0.4565 | 11.2362 | 0.6755 | | | | | | | | | | | | | | | | | | | | | | | | |

Table S6_0.00001. Same as Table S5_0.00001, but employing splitting method taking training set and prediction set in a ratio of 1:1.

| S.No. | Size | Variables | R ² | R ² _{adj} | R ² -R ² _{adj} | ΔK | RMSE(tr) | MAE(tr) | RSS(tr) | CCC(tr) | F | Q ² _{loo} | R ² -Q ² _{loo} | RMSE(cv) | MAE(cv) | PRESS(cv) | CCC(cv) | Q ² _{LMO} | R ² _{Yscr} | Q ² _{Yscr} | R ² _{Xmdl} | Q ² _{Xmdl} | R ² _{Ymdl} | Q ² _{Ymdl} | N. ext. OK | RMSE(ext) | MAE(ext) | PRESS(ext) | Q ² _{F1} | Q ² _{F2} | Q ² _{F3} | CCC(ext) | \bar{F}_α^{-2} | Δr_α^{-2} |
|-------|------|--|----------------|-------------------------------|---|---------|----------|---------|---------|---------|---------|-------------------------------|---|----------|---------|-----------|---------|-------------------------------|--------------------------------|--------------------------------|--------------------------------|--------------------------------|--------------------------------|--------------------------------|------------|-----------|----------|------------|------------------------------|------------------------------|------------------------------|----------|-----------------------|------------------------|
| 1 | 5 | E(CORR) ZPE(HF) ZPE(CORR) E ^{HOMO} (CORR) ω(DFT) | 0.8216 | 0.7828 | 0.0388 | -0.0143 | 0.3412 | 0.2828 | 3.3755 | 0.9021 | 21.1825 | 0.7351 | 0.0865 | 0.4157 | 0.351 | 5.0114 | 0.8575 | 71.6236 | 18.2832 | -44.007 | 18.9133 | -29.6661 | 18.133 | -43.2418 | 0 | 0.5284 | 0.4277 | 7.26 | 0.3174 | 0.3174 | 0.572 | 0.7049 | 0.3819 | 0.1671 |
| 2 | 5 | E(CORR) ZPE(DFT) ZPE(CORR) E ^{HOMO} (CORR) ω(DFT) | 0.8216 | 0.7828 | 0.0388 | -0.0134 | 0.3412 | 0.2828 | 3.3755 | 0.9021 | 21.1825 | 0.7351 | 0.0865 | 0.4157 | 0.351 | 5.0114 | 0.8575 | 71.7465 | 17.5569 | -45.2693 | 17.5137 | -32.4797 | 17.3905 | -46.1542 | 0 | 0.5284 | 0.4277 | 7.26 | 0.3174 | 0.3174 | 0.572 | 0.7049 | 0.3819 | 0.1671 |
| 3 | 5 | E(CORR) ZPE(DFT) ZPE(HF) E ^{HOMO} (CORR) ω(DFT) | 0.8216 | 0.7828 | 0.0388 | -0.0143 | 0.3412 | 0.2828 | 3.3755 | 0.9021 | 21.1825 | 0.7351 | 0.0865 | 0.4157 | 0.351 | 5.0114 | 0.8575 | 71.3739 | 17.5882 | -44.334 | 17.4598 | -32.2051 | 17.2257 | -45.4165 | 0 | 0.5284 | 0.4277 | 7.26 | 0.3174 | 0.3174 | 0.572 | 0.7049 | 0.3819 | 0.1671 |
| 4 | 5 | ZPE(HF) ZPE(CORR) E ^{HOMO} (CORR) H(CORR) ω(DFT) | 0.8215 | 0.7827 | 0.0388 | -0.0143 | 0.3412 | 0.2829 | 3.3768 | 0.902 | 21.1733 | 0.735 | 0.0865 | 0.4158 | 0.351 | 5.0131 | 0.8574 | 71.2278 | 18.2848 | -43.1328 | 18.0879 | -31.3438 | 17.6108 | -44.211 | 0 | 0.5285 | 0.4277 | 7.261 | 0.3173 | 0.3173 | 0.5719 | 0.7048 | 0.3818 | 0.167 |
| 5 | 5 | ZPE(DFT) ZPE(CORR) E ^{HOMO} (CORR) H(CORR) ω(DFT) | 0.8215 | 0.7827 | 0.0388 | -0.0134 | 0.3412 | 0.2829 | 3.3768 | 0.902 | 21.1733 | 0.735 | 0.0865 | 0.4158 | 0.351 | 5.0131 | 0.8574 | 71.3169 | 18.3339 | -41.9306 | 17.7131 | -31.7501 | 17.3952 | -46.7406 | 0 | 0.5285 | 0.4277 | 7.261 | 0.3173 | 0.3173 | 0.5719 | 0.7048 | 0.3818 | 0.167 |
| 6 | 5 | ZPE(DFT) ZPE(HF) E ^{HOMO} (CORR) H(CORR) ω(DFT) | 0.8215 | 0.7827 | 0.0388 | -0.0037 | 0.3412 | 0.2829 | 3.3768 | 0.902 | 21.1733 | 0.735 | 0.0865 | 0.4158 | 0.351 | 5.0131 | 0.8574 | 71.5342 | 18.2868 | -44.9288 | 18.585 | -30.3231 | 17.3999 | -47.8397 | 0 | 0.5285 | 0.4277 | 7.261 | 0.3173 | 0.3173 | 0.5719 | 0.7048 | 0.3818 | 0.167 |
| 7 | 5 | ZPE(HF) ZPE(CORR) E ^{HOMO} (CORR) G(CORR) ω(DFT) | 0.8211 | 0.7822 | 0.0389 | -0.0144 | 0.3417 | 0.2844 | 3.3854 | 0.9017 | 21.1072 | 0.7338 | 0.0872 | 0.4167 | 0.3535 | 5.0359 | 0.8568 | 71.3167 | 17.8739 | -45.3121 | 17.9329 | -31.9056 | 18.0242 | -43.3196 | 0 | 0.5284 | 0.4277 | 7.2597 | 0.3174 | 0.3174 | 0.572 | 0.7054 | 0.3824 | 0.1688 |
| 8 | 5 | ZPE(DFT) ZPE(CORR) E ^{HOMO} (CORR) G(CORR) ω(DFT) | 0.8211 | 0.7822 | 0.0389 | -0.0135 | 0.3417 | 0.2844 | 3.3854 | 0.9017 | 21.1072 | 0.7338 | 0.0872 | 0.4167 | 0.3535 | 5.0359 | 0.8568 | 70.8731 | 18.5237 | -42.5207 | 17.4129 | -32.2074 | 17.5809 | -42.6924 | 0 | 0.5284 | 0.4277 | 7.2597 | 0.3174 | 0.3174 | 0.572 | 0.7054 | 0.3824 | 0.1688 |
| 9 | 5 | ZPE(DFT) ZPE(HF) E ^{HOMO} (CORR) G(CORR) ω(DFT) | 0.8211 | 0.7822 | 0.0389 | -0.0038 | 0.3417 | 0.2844 | 3.3854 | 0.9017 | 21.1072 | 0.7338 | 0.0872 | 0.4167 | 0.3535 | 5.0359 | 0.8568 | 71.0417 | 18.1107 | -44.7897 | 17.2011 | -32.484 | 17.7704 | -44.1313 | 0 | 0.5284 | 0.4277 | 7.2597 | 0.3174 | 0.3174 | 0.572 | 0.7054 | 0.3824 | 0.1688 |
| 10 | 5 | ZPE(DFT) ZPE(HF) α(HF) G(DFT) χ(CORR) | 0.7945 | 0.7499 | 0.0447 | -0.0602 | 0.3661 | 0.3093 | 3.8874 | 0.8855 | 17.788 | 0.7166 | 0.078 | 0.43 | 0.3755 | 5.3627 | 0.8405 | 68.1401 | 18.2941 | -39.0059 | 18.07 | -31.9936 | 17.5676 | -40.4375 | 0 | 0.6202 | 0.4554 | 10.0003 | 0.0598 | 0.0597 | 0.4104 | 0.6569 | 0.3075 | 0.2768 |
| 11 | 4 | E(CORR) ZPE(HF) ZPE(CORR) χ(CORR) | 0.7721 | 0.7341 | 0.038 | -0.1186 | 0.3856 | 0.3274 | 4.3123 | 0.8714 | 20.3241 | 0.676 | 0.0961 | 0.4598 | 0.3947 | 6.1301 | 0.8184 | 64.8524 | 14.5837 | -27.7052 | 15.1808 | -24.6656 | 14.6279 | -28.9785 | 0 | 0.5856 | 0.4703 | 8.9162 | 0.1617 | 0.1617 | 0.4744 | 0.6679 | 0.3257 | 0.2253 |
| 12 | 4 | E(CORR) ZPE(DFT) ZPE(CORR) χ(CORR) | 0.7721 | 0.7341 | 0.038 | -0.1184 | 0.3856 | 0.3274 | 4.3123 | 0.8714 | 20.3241 | 0.676 | 0.0961 | 0.4598 | 0.3947 | 6.1301 | 0.8184 | 64.5116 | 15.1483 | -27.5371 | 14.741 | -25.968 | 14.3473 | -29.1758 | 0 | 0.5856 | 0.4703 | 8.9162 | 0.1617 | 0.1617 | 0.4744 | 0.6679 | 0.3257 | 0.2253 |
| 13 | 4 | ZPE(HF) ZPE(DFT) ZPE(HF) χ(CORR) | 0.7721 | 0.7341 | 0.038 | -0.1054 | 0.3856 | 0.3274 | 4.3123 | 0.8714 | 20.3241 | 0.676 | 0.0961 | 0.4598 | 0.3947 | 6.1301 | 0.8184 | 65.4675 | 13.7931 | -30.0255 | 14.2443 | -26.296 | 14.5709 | -28.7653 | 0 | 0.5856 | 0.4703 | 8.9162 | 0.1617 | 0.1617 | 0.4744 | 0.6679 | 0.3257 | 0.2253 |
| 14 | 4 | ZPE(HF) ZPE(CORR) H(CORR) χ(CORR) | 0.772 | 0.734 | 0.038 | -0.1186 | 0.3857 | 0.3275 | 4.3135 | 0.8713 | 20.3167 | 0.6759 | 0.0961 | 0.4598 | 0.3947 | 6.1317 | 0.8184 | 64.8571 | 14.6596 | -27.6535 | 14.1777 | -26.2033 | 14.3977 | -28.2991 | 0 | 0.5856 | 0.4703 | 8.9175 | 0.1616 | 0.1615 | 0.4743 | 0.6678 | 0.3255 | 0.2252 |
| 15 | 4 | ZPE(DFT) ZPE(CORR) H(CORR) χ(CORR) | 0.772 | 0.734 | 0.038 | -0.1116 | 0.3857 | 0.3275 | 4.3135 | 0.8713 | 20.3167 | 0.6759 | 0.0961 | 0.4598 | 0.3947 | 6.1317 | 0.8184 | 64.7711 | 14.5347 | -28.8677 | 14.0593 | -26.4292 | 14.5191 | -29.7355 | 0 | 0.5856 | 0.4703 | 8.9175 | 0.1616 | 0.1615 | 0.4743 | 0.6678 | 0.3255 | 0.2252 |
| 16 | 4 | ZPE(DFT) ZPE(HF) H(CORR) χ(CORR) | 0.772 | 0.734 | 0.038 | -0.1156 | 0.3857 | 0.3275 | 4.3135 | 0.8713 | 20.3167 | 0.6759 | 0.0961 | 0.4598 | 0.3947 | 6.1317 | 0.8184 | 64.8463 | 13.9281 | -29.6472 | 14.0567 | -26.2942 | 13.9254 | -29.5922 | 0 | 0.5856 | 0.4703 | 8.9175 | 0.1616 | 0.1615 | 0.4743 | 0.6678 | 0.3255 | 0.2252 |
| 17 | 4 | ZPE(HF) ZPE(CORR) G(CORR) χ(CORR) | 0.7718 | 0.7337 | 0.038 | -0.1187 | 0.3859 | 0.3289 | 4.3184 | 0.8712 | 20.2871 | 0.675 | 0.0967 | 0.4604 | 0.3967 | 6.1481 | 0.8179 | 64.4941 | 14.4116 | -28.5231 | 14.1935 | -26.2209 | 14.5709 | -28.5635 | 0 | 0.5855 | 0.4703 | 8.9139 | 0.1619 | 0.1619 | 0.4745 | 0.6684 | 0.3263 | 0.2266 |
| 18 | 4 | ZPE(DFT) ZPE(CORR) G(CORR) χ(CORR) | 0.7718 | 0.7337 | 0.038 | -0.1185 | 0.3859 | 0.3289 | 4.3184 | 0.8712 | 20.2871 | 0.675 | 0.0967 | 0.4604 | 0.3967 | 6.1481 | 0.8179 | 64.648 | 13.8679 | -28.9616 | 14.7089 | -25.2977 | 14.427 | -28.4301 | 0 | 0.5855 | 0.4703 | 8.9139 | 0.1619 | 0.1619 | 0.4745 | 0.6684 | 0.3263 | 0.2266 |
| 19 | 4 | ZPE(DFT) ZPE(HF) G(CORR) χ(CORR) | 0.7718 | 0.7337 | 0.038 | -0.1157 | 0.3859 | 0.3289 | 4.3184 | 0.8712 | 20.2871 | 0.675 | 0.0967 | 0.4604 | 0.3967 | 6.1481 | 0.8179 | 65.2833 | 13.717 | -29.5882 | 14.2045 | -25.8382 | 14.6318 | -28.5694 | 0 | 0.5855 | 0.4703 | 8.9139 | 0.1619 | 0.1619 | 0.4745 | 0.6684 | 0.3263 | 0.2266 |
| 20 | 4 | ZPE(HF) ZPE(CORR) G(DFT) χ(CORR) | 0.7643 | 0.725 | 0.0393 | -0.0583 | 0.3922 | 0.3374 | 4.4597 | 0.8664 | 19.4542 | 0.6712 | 0.093 | 0.4631 | 0.4023 | 6.2201 | 0.8159 | 65.3408 | 14.8932 | -27.3871 | 13.5912 | -26.8001 | 13.3111 | -31.7884 | 0 | 0.783 | 0.5222 | 15.939 | -0.4986 | -0.4986 | 0.0603 | 0.5761 | 0.2153 | 0.3724 |
| 21 | 3 | ZPE(DFT) ZPE(HF) α(HF) | 0.6976 | 0.6613 | 0.0363 | -0.2556 | 0.4442 | 0.3737 | 5.7211 | 0.8219 | 19.2251 | 0.6054 | 0.0922 | 0.5074 | 0.4337 | 7.4661 | 0.7733 | 56.9151 | 10.4915 | -23.4584 | 10.707 | -20.6775 | 10.4252 | -25.141 | 0 | 0.5661 | 0.4295 | 8.3326 | 0.2166 | 0.2165 | 0.5088 | 0.5519 | 0.184 | 0.0831 |
| 22 | 3 | ZPE(HF) ZPE(CORR) α(HF) | 0.6976 | 0.6613 | 0.0363 | -0.2607 | 0.4442 | 0.3737 | 5.7211 | 0.8219 | 19.2251 | 0.6054 | 0.0922 | 0.5074 | 0.4337 | 7.4661 | 0.7733 | 57.7006 | 10.5075 | -23.8387 | 11.1833 | -19.9972 | 10.5008 | -23.9776 | 0 | 0.5661 | 0.4295 | 8.3326 | 0.2166 | 0.2165 | 0.5088 | 0.5519 | 0.184 | 0.0831 |
| 23 | 3 | ZPE(DFT) ZPE(CORR) α(HF) | 0.6976 | 0.6613 | 0.0363 | -0.26 | 0.4442 | 0.3737 | 5.7211 | 0.8219 | 19.2251 | 0.6054 | 0.0922 | 0.5074 | 0.4337 | 7.4661 | 0.7733 | 57.1882 | 10.3523 | -24.4497 | 11.2985 | -19.5574 | 10.5316 | -23.8364 | 0 | 0.5661 | 0.4295 | 8.3326 | 0.2166 | 0.2165 | 0.5088 | 0.5519 | 0.184 | 0.0831 |
| 24 | 3 | ZPE(HF) ZPE(CORR) α(DFT) | 0.6784 | 0.6398 | 0.0386 | -0.2635 | 0.458 | 0.3832 | 6.0842 | 0.8084 | 17.5801 | 0.5856 | 0.0928 | 0.5199 | 0.4389 | 7.8394 | 0.756 | 54.5315 | 10.1203 | -25.1089 | 10.7719 | -20.4545 | 11.0645 | -23.7152 | 0 | 0.5658 | 0.4324 | 8.3237 | 0.2174 | 0.2174 | 0.5093 | 0.5459 | 0.1776 | 0.0922 |
| 25 | 3 | ZPE(DFT) ZPE(CORR) α(DFT) | 0.6784 | 0.6398 | 0.0386 | -0.2628 | 0.458 | 0.3832 | 6.0842 | 0.8084 | 17.5801 | 0.5856 | 0.0928 | 0.5199 | 0.4389 | 7.8394 | 0.756 | 53.5829 | 10.7889 | -23.3766 | 10.4184 | -21.3181 | 11.0332 | -23.7139 | 0 | 0.5658 | 0.4324 | 8.3237 | 0.2174 | 0.2174 | 0.5093 | 0.5459 | 0.1776 | 0.0922 |
| 26 | 3 | ZPE(DFT) ZPE(HF) α(DFT) | 0.6784 | 0.6398 | 0.0386 | -0.2579 | 0.458 | 0.3832 | 6.0842 | 0.8084 | 17.5801 | 0.5856 | 0.0928 | 0.5199 | 0.4389 | 7.8394 | 0.756 | 53.9504 | 10.5989 | -23.9136 | 11.4157 | -20.2831 | 10.9128 | -24.004 | 0 | 0.5658 | 0.4324 | 8.3237 | 0.2174 | 0.2174 | 0.5093 | 0.5459 | 0.1776 | 0.0922 |
| 27 | 3 | ZPE(CORR) α(HF) H(CORR) | 0.6153 | 0.5692 | 0.0462 | -0.2448 | 0.5009 | 0.4034 | 7.2775 | 0.7619 | 13.3312 | 0.4556 | 0.1597 | 0.5959 | 0.48 | 10.2995 | 0.689 | 45.0532 | 10.7054 | -24.1459 | 10.5279 | -20.8446 | 10.945 | -23.5321 | 0 | 0.5634 | 0.4731 | 8.253 | 0.224 | 0.224 | 0.5135 | 0.5376 | 0.18 | 0.1186 |
| 28 | 3 | E(CORR) ZPE(CORR) α(HF) | 0.6153 | 0.5691 | 0.0462 | -0.2448 | 0.501 | 0.4034 | 7.2783 | 0.7618 | 13.3289 | 0.4556 | 0.1597 | 0.596 | 0.48 | 10.3005 | 0.689 | 45.1027 | 10.5293 | -24.5083 | 11.0467 | -19.9709 | 10.6989 | -24.806 | 0 | 0.5634 | 0.4731 | 8.2526 | 0.2241 | 0.2241 | 0.5135 | 0.5376 | 0.18 | 0.1186 |
| 29 | 3 | ZPE(CORR) α(HF) G(CORR) | 0.6152 | 0.5691 | 0.0462 | -0.245 | 0.501 | 0.4032 | 7.2797 | 0.7618 | 13.3245 | 0.4554 | 0.1599 | 0.5961 | 0.4798 | 10.3041 | 0.6887 | 44.9807 | 10.9759 | -23.9275 | 10.0475 | -21.3123 | 10.8943 | -23.1538 | 0 | 0.5634 | 0.473 | 8.2522 | 0.2241 | 0.2241 | 0.5135 | 0.5373 | 0.1798 | 0.1192 |
| 30 | 3 | ZPE(CORR) d(CORR) α(HF) | 0.6006 | 0.5526 | 0.0479 | -0.2083 | 0.5105 | 0.4002 | 7.5574 | 0.7504 | 12.5287 | 0.4675 | 0.1331 | 0.5894 | 0.4715 | 10.0748 | 0.6695 | 41.7918 | 10.7827 | -35.9978 | 11.4902 | -19.6926 | 10.4223 | -34.871 | 0 | 0.5793 | 0.4765 | 8.7248 | 0.1797 | 0.1797 | 0. | | | |

Table S7_0.00001. Same as Table_S3_0.00001 but for models developed using the descriptors reported in the work of Yu et al., 2015.

| S.No. | Size | Variables | R ² | R ² _{adj} | R ² -R ² _{adj} | Δ K | RMSE(tr) | MAE(tr) | RSS(tr) | CCC(tr) | F | Q ² _{loo} | R ² -Q ² _{loo} | RMSE(cv) | MAE(cv) | PRESS(cv) | CCC(cv) | Q ² _{LMO} | R ² _{Yscr} | Q ² _{Yscr} | R ² _{Xrnd} | Q ² _{Xrnd} | R ² _{Yrnd} | Q ² _{Yrnd} |
|-------|------|-----------|----------------|-------------------------------|---|---------|----------|---------|---------|---------|---------|-------------------------------|---|----------|---------|-----------|---------|-------------------------------|--------------------------------|--------------------------------|--------------------------------|--------------------------------|--------------------------------|--------------------------------|
| 1 | 5 | R P A B V | 0.8311 | 0.8139 | 0.0172 | -0.0453 | 0.3012 | 0.2454 | 4.991 | 0.9078 | 48.2333 | 0.7811 | 0.05 | 0.343 | 0.2792 | 6.4689 | 0.8824 | 79.3132 | 8.9774 | -16.4235 | 9.7771 | -13.9022 | 9.0472 | -16.4678 |
| 2 | 4 | R A B V | 0.8298 | 0.8161 | 0.0136 | -0.0439 | 0.3025 | 0.2442 | 5.0317 | 0.907 | 60.9224 | 0.7887 | 0.0411 | 0.337 | 0.2721 | 6.2464 | 0.8864 | 79.363 | 7.4308 | -13.687 | 7.6945 | -11.8117 | 7.2528 | -13.438 |
| 3 | 4 | P A B V | 0.8141 | 0.7992 | 0.0149 | -0.0666 | 0.3161 | 0.2583 | 5.4957 | 0.8975 | 54.724 | 0.7582 | 0.0559 | 0.3605 | 0.2904 | 7.1468 | 0.8685 | 77.4326 | 7.2098 | -12.924 | 7.3071 | -12.2727 | 7.5648 | -12.8393 |
| 4 | 4 | R P B V | 0.8094 | 0.7941 | 0.0152 | -0.1857 | 0.32 | 0.2634 | 5.6337 | 0.8947 | 53.0773 | 0.7663 | 0.0431 | 0.3544 | 0.2931 | 6.9081 | 0.8735 | 77.0241 | 7.5329 | -13.1559 | 7.316 | -12.2445 | 7.5197 | -13.3901 |
| 5 | 3 | R B V | 0.8094 | 0.7982 | 0.0112 | -0.24 | 0.3201 | 0.2633 | 5.6339 | 0.8946 | 72.1825 | 0.7747 | 0.0347 | 0.348 | 0.2873 | 6.6599 | 0.878 | 77.4703 | 5.5327 | -11.0291 | 5.5008 | -10.0936 | 5.6709 | -10.96 |
| 6 | 3 | A B V | 0.7934 | 0.7813 | 0.0122 | -0.0731 | 0.3332 | 0.265 | 6.1054 | 0.8848 | 65.2945 | 0.7399 | 0.0535 | 0.3739 | 0.293 | 7.6871 | 0.8569 | 75.434 | 5.471 | -11.022 | 5.4493 | -10.115 | 5.6406 | -10.5084 |
| 7 | 3 | P B V | 0.7893 | 0.7769 | 0.0124 | -0.2656 | 0.3365 | 0.2754 | 6.227 | 0.8823 | 63.6883 | 0.7428 | 0.0465 | 0.3718 | 0.3018 | 7.6027 | 0.8587 | 75.026 | 5.5425 | -10.5841 | 5.2538 | -10.2351 | 5.6389 | -10.4907 |
| 8 | 2 | B V | 0.7775 | 0.7689 | 0.0086 | -0.3864 | 0.3458 | 0.2786 | 6.5772 | 0.8748 | 90.8333 | 0.7357 | 0.0417 | 0.3768 | 0.3002 | 7.8104 | 0.8537 | 73.9577 | 4.0925 | -8.2993 | 3.8979 | -7.5791 | 3.6236 | -8.8202 |
| 9 | 4 | R P A V | 0.6151 | 0.5843 | 0.0308 | -0.0474 | 0.4548 | 0.3601 | 11.3759 | 0.7617 | 19.976 | 0.5252 | 0.0899 | 0.5051 | 0.3994 | 14.0338 | 0.7096 | 54.9942 | 7.2491 | -13.2557 | 7.464 | -12.0713 | 7.7194 | -12.6503 |
| 10 | 3 | R A V | 0.6084 | 0.5854 | 0.023 | -0.0245 | 0.4587 | 0.3634 | 11.5738 | 0.7565 | 26.412 | 0.5387 | 0.0697 | 0.4979 | 0.3944 | 13.6345 | 0.7172 | 54.9798 | 5.5161 | -11.2688 | 5.5284 | -10.0282 | 5.6263 | -10.5991 |
| 11 | 3 | P A V | 0.5934 | 0.5695 | 0.0239 | -0.0563 | 0.4674 | 0.3698 | 12.0164 | 0.7448 | 24.8129 | 0.5339 | 0.0595 | 0.5005 | 0.3981 | 13.7759 | 0.7111 | 54.0602 | 5.4262 | -10.6039 | 5.3204 | -10.1849 | 5.4799 | -10.4352 |
| 12 | 2 | A V | 0.5933 | 0.5777 | 0.0156 | 0.0196 | 0.4675 | 0.3699 | 12.0192 | 0.7448 | 37.9344 | 0.5497 | 0.0436 | 0.4919 | 0.3911 | 13.3084 | 0.7201 | 54.7321 | 3.7277 | -7.9639 | 4.0672 | -7.4124 | 3.647 | -8.3 |
| 13 | 4 | R P A B | 0.5625 | 0.5275 | 0.035 | -0.0846 | 0.4849 | 0.3967 | 12.9312 | 0.72 | 16.0699 | 0.4788 | 0.0836 | 0.5292 | 0.4344 | 15.4033 | 0.6674 | 49.3723 | 7.3493 | -13.3476 | 7.242 | -12.3156 | 7.4934 | -13.6681 |
| 14 | 3 | R A B | 0.5329 | 0.5054 | 0.0275 | -0.1009 | 0.501 | 0.4048 | 13.8053 | 0.6953 | 19.395 | 0.4619 | 0.071 | 0.5378 | 0.4364 | 15.9047 | 0.6517 | 47.3184 | 5.4526 | -11.1519 | 5.7516 | -9.7499 | 5.3174 | -11.5726 |
| 15 | 3 | R P A | 0.5324 | 0.5049 | 0.0275 | -0.0909 | 0.5013 | 0.3984 | 13.8205 | 0.6948 | 19.3549 | 0.4583 | 0.074 | 0.5395 | 0.4308 | 16.0087 | 0.6473 | 47.5191 | 5.5917 | -10.8657 | 5.5331 | -10.0238 | 5.9921 | -10.0494 |
| 16 | 2 | R A | 0.524 | 0.5057 | 0.0183 | -0.0626 | 0.5058 | 0.4062 | 14.0684 | 0.6877 | 28.6217 | 0.4703 | 0.0537 | 0.5335 | 0.4301 | 15.6559 | 0.6565 | 46.5514 | 3.7959 | -8.3574 | 3.6731 | -7.7437 | 3.746 | -8.0141 |
| 17 | 3 | P A B | 0.5145 | 0.4859 | 0.0286 | -0.1558 | 0.5108 | 0.4167 | 14.3496 | 0.6794 | 18.0143 | 0.4403 | 0.0742 | 0.5484 | 0.4494 | 16.5433 | 0.6337 | 44.9178 | 5.77 | -10.3822 | 5.8288 | -9.6327 | 5.5761 | -10.5436 |
| 18 | 2 | P A | 0.4908 | 0.4712 | 0.0196 | -0.1797 | 0.5231 | 0.4098 | 15.0497 | 0.6584 | 25.0602 | 0.4422 | 0.0485 | 0.5475 | 0.4305 | 16.4846 | 0.6272 | 43.6238 | 3.4469 | -8.5113 | 3.7308 | -7.7363 | 4.0268 | -7.9544 |
| 19 | 2 | A B | 0.3312 | 0.3055 | 0.0257 | -0.257 | 0.5995 | 0.4738 | 19.7666 | 0.4976 | 12.8757 | 0.2695 | 0.0617 | 0.6265 | 0.499 | 21.5893 | 0.4525 | 26.9969 | 3.6518 | -8.5745 | 3.7346 | -7.7364 | 3.7136 | -8.5733 |
| 20 | 3 | R P V | 0.3257 | 0.286 | 0.0397 | -0.2437 | 0.602 | 0.5046 | 19.9301 | 0.4913 | 8.2102 | 0.156 | 0.1697 | 0.6735 | 0.555 | 24.9456 | 0.3873 | 21.1471 | 5.682 | -10.7637 | 5.7778 | -9.6836 | 5.4878 | -10.7847 |
| 21 | 3 | R P B | 0.2973 | 0.2559 | 0.0413 | -0.2658 | 0.6145 | 0.5055 | 20.7698 | 0.4583 | 7.191 | 0.208 | 0.0892 | 0.6524 | 0.54 | 23.4068 | 0.3891 | 20.846 | 5.3122 | -11.4584 | 5.1499 | -10.4862 | 5.5076 | -11.1557 |
| 22 | 2 | R B | 0.2853 | 0.2578 | 0.0275 | -0.3681 | 0.6197 | 0.4962 | 21.1241 | 0.4439 | 10.3774 | 0.2226 | 0.0627 | 0.6463 | 0.5211 | 22.9768 | 0.3959 | 20.1362 | 3.6122 | -9.0142 | 3.6919 | -7.8103 | 3.8815 | -8.4896 |
| 23 | 2 | P V | 0.2808 | 0.2531 | 0.0277 | -0.3542 | 0.6217 | 0.5142 | 21.2568 | 0.4385 | 10.1503 | 0.1858 | 0.095 | 0.6615 | 0.5466 | 24.0635 | 0.3827 | 19.2346 | 3.8844 | -8.1119 | 3.4291 | -8.1349 | 3.8273 | -8.0186 |
| 24 | 1 | A | 0.2047 | 0.1897 | 0.015 | 0.4524 | 0.6538 | 0.5259 | 23.5065 | 0.3398 | 13.6385 | 0.1238 | 0.0808 | 0.6862 | 0.5488 | 25.896 | 0.2856 | 13.2471 | 1.8122 | -5.8113 | 1.8797 | -5.6996 | 1.7815 | -5.943 |
| 25 | 2 | P B | 0.1906 | 0.1594 | 0.0311 | -0.4349 | 0.6595 | 0.5605 | 23.9233 | 0.3201 | 6.121 | 0.1013 | 0.0893 | 0.6949 | 0.5932 | 26.5613 | 0.2557 | 9.4238 | 3.6447 | -8.7085 | 3.9951 | -7.3774 | 3.7875 | -8.4037 |
| 26 | 2 | R V | 0.1596 | 0.1273 | 0.0323 | -0.299 | 0.672 | 0.5537 | 24.8376 | 0.2753 | 4.9386 | -0.0034 | 0.1631 | 0.7343 | 0.5953 | 29.657 | 0.1795 | 4.9777 | 3.8185 | -8.588 | 3.6775 | -7.8708 | 3.5516 | -8.8782 |
| 27 | 1 | V | 0.1556 | 0.1397 | 0.0159 | 0.3945 | 0.6736 | 0.5575 | 24.9567 | 0.2693 | 9.7662 | 0.0583 | 0.0973 | 0.7114 | 0.5837 | 27.8314 | 0.2209 | 6.9045 | 1.6964 | -6.1858 | 1.7364 | -5.8995 | 1.8053 | -6.1273 |
| 28 | 2 | R P | 0.1284 | 0.0949 | 0.0335 | -0.3957 | 0.6844 | 0.5506 | 25.7606 | 0.2276 | 3.8301 | -0.001 | 0.1294 | 0.7334 | 0.5882 | 29.5863 | 0.1312 | 2.8801 | 3.8099 | -8.5182 | 3.5588 | -7.92 | 3.6856 | -8.4187 |
| 29 | 1 | R | 0.0829 | 0.0655 | 0.0173 | 0.2878 | 0.702 | 0.5813 | 27.1067 | 0.153 | 4.7878 | -0.012 | 0.0948 | 0.7374 | 0.608 | 29.909 | 0.101 | -0.3303 | 1.6519 | -6.5873 | 1.8686 | -5.6992 | 1.7415 | -6.4807 |
| 30 | 1 | P | 0.0259 | 0.0076 | 0.0184 | 0.1611 | 0.7235 | 0.5979 | 28.7887 | 0.0506 | 1.4114 | -0.0326 | 0.0586 | 0.7449 | 0.6185 | 30.52 | 0.0002 | -4.5584 | 1.7331 | -6.1738 | 1.8294 | -5.7901 | 1.9497 | -5.8606 |
| 31 | 1 | B | 0.0016 | -0.0173 | 0.0188 | 0.0398 | 0.7325 | 0.6032 | 29.5085 | 0.0032 | 0.0842 | -0.0629 | 0.0645 | 0.7558 | 0.6255 | 31.4152 | -0.0537 | -7.4861 | 1.9408 | -6.6562 | 1.7112 | -5.9308 | 1.8042 | -6.4515 |

Table S8_0.00001. Same as Table S4_0.00001 but for models developed using the descriptors employed in the work of Yu et al., 2015.

| S.No. | Size | Variables | R ² | R ² _{adj} | R ² -R ² _{adj} | ΔK | RMSE(tr) | MAE(tr) | RSS(tr) | CCC(tr) | F | Q ² _{loo} | R ² -Q ² _{loo} | RMSE(cv) | MAE(cv) | PRESS(cv) | CCC(cv) | Q ² _{LMO} | R ² _{scr} | Q ² _{scr} | R ² _{xrnd} | Q ² _{xrnd} | R ² _{vrnd} | Q ² _{vrnd} | N. ext. | OK | RMSE(ext) | MAE(ext) | PRESS(ext) | Q ² _{F1} | Q ² _{F2} | Q ² _{F3} | CCC(ext) | F _m ² | Δr _v ² |
|-------|------|-----------|----------------|-------------------------------|---|---------|----------|---------|---------|---------|---------|-------------------------------|---|----------|---------|-----------|---------|-------------------------------|-------------------------------|-------------------------------|--------------------------------|--------------------------------|--------------------------------|--------------------------------|---------|--------|-----------|----------|------------|------------------------------|------------------------------|------------------------------|----------|-----------------------------|------------------------------|
| 1 | 5 | R P A B V | 0.8775 | 0.8605 | 0.017 | -0.0377 | 0.2669 | 0.215 | 2.9923 | 0.9348 | 51.5825 | 0.8219 | 0.0556 | 0.3218 | 0.258 | 4.3503 | 0.9067 | 83.0624 | 12.5735 | -22.3551 | 11.8823 | -20.2138 | 11.5502 | -23.7038 | 1 | 0.4078 | 0.3368 | 2.1622 | 0.579 | 0.5754 | 0.7141 | 0.7696 | 0.5848 | 0.133 | |
| 2 | 4 | R A B V | 0.8758 | 0.8624 | 0.0134 | -0.0917 | 0.2687 | 0.2177 | 3.033 | 0.9338 | 65.2562 | 0.83 | 0.0459 | 0.3145 | 0.254 | 4.1532 | 0.9108 | 83.4273 | 9.5364 | -19.0966 | 9.8537 | -16.3703 | 10.3478 | -18.1634 | 1 | 0.4064 | 0.3271 | 2.1468 | 0.582 | 0.5784 | 0.7161 | 0.7643 | 0.5785 | 0.1832 | |
| 3 | 4 | P A B V | 0.8563 | 0.8408 | 0.0155 | -0.0589 | 0.2891 | 0.2323 | 3.5105 | 0.9226 | 55.1221 | 0.7856 | 0.0707 | 0.3532 | 0.275 | 5.2385 | 0.8863 | 80.4867 | 9.1345 | -19.1138 | 10.2222 | -15.9196 | 9.4876 | -18.6409 | 1 | 0.4117 | 0.3449 | 2.2039 | 0.5709 | 0.5672 | 0.7085 | 0.7752 | 0.6105 | 0.0729 | |
| 4 | 4 | R P B V | 0.8561 | 0.8406 | 0.0156 | -0.184 | 0.2893 | 0.2363 | 3.5152 | 0.9225 | 55.0356 | 0.8103 | 0.0458 | 0.3322 | 0.2733 | 4.6345 | 0.8999 | 80.6989 | 9.5269 | -19.1922 | 10.0678 | -16.0717 | 9.9593 | -19.3303 | 0 | 0.4218 | 0.343 | 2.3124 | 0.5498 | 0.5459 | 0.6942 | 0.7313 | 0.5443 | 0.2585 | |
| 5 | 3 | R B V | 0.856 | 0.8447 | 0.0114 | -0.2347 | 0.2894 | 0.2364 | 3.5169 | 0.9224 | 75.3211 | 0.8186 | 0.0375 | 0.3248 | 0.2666 | 4.432 | 0.9042 | 81.1743 | 7.1077 | -16.4327 | 7.2092 | -13.4724 | 7.4037 | -15.9509 | 0 | 0.4216 | 0.3442 | 2.3108 | 0.5501 | 0.5462 | 0.6944 | 0.7326 | 0.5494 | 0.256 | |
| 6 | 3 | A B V | 0.8324 | 0.8192 | 0.0132 | -0.0567 | 0.3122 | 0.2468 | 4.0937 | 0.9086 | 62.9231 | 0.7557 | 0.0767 | 0.377 | 0.2863 | 5.9684 | 0.8691 | 77.4614 | 6.8869 | -15.2296 | 7.0766 | -13.7278 | 7.1904 | -14.7386 | 1 | 0.4098 | 0.3263 | 2.1829 | 0.575 | 0.5713 | 0.7113 | 0.7533 | 0.5868 | 0.2396 | |
| 7 | 3 | P B V | 0.8286 | 0.8151 | 0.0135 | -0.2683 | 0.3157 | 0.2595 | 4.1864 | 0.9063 | 61.2502 | 0.7686 | 0.06 | 0.3669 | 0.2956 | 5.6529 | 0.876 | 77.4518 | 7.5989 | -14.6022 | 7.6356 | -12.9957 | 7.3865 | -14.9926 | 0 | 0.4188 | 0.3345 | 2.2797 | 0.5561 | 0.5523 | 0.6985 | 0.743 | 0.5981 | 0.2272 | |
| 8 | 2 | B V | 0.8172 | 0.8078 | 0.0094 | -0.3823 | 0.3261 | 0.2643 | 4.4653 | 0.8994 | 87.1843 | 0.758 | 0.0593 | 0.3752 | 0.295 | 5.9131 | 0.8696 | 76.0632 | 5.1643 | -11.511 | 4.6575 | -10.7543 | 4.6645 | -12.3565 | 0 | 0.4224 | 0.3427 | 2.3195 | 0.5484 | 0.5445 | 0.6933 | 0.7255 | 0.5367 | 0.2582 | |
| 9 | 4 | R P A V | 0.6349 | 0.5955 | 0.0395 | -0.0361 | 0.4608 | 0.3609 | 8.9186 | 0.7767 | 16.0877 | 0.5172 | 0.1178 | 0.5299 | 0.4153 | 11.7955 | 0.709 | 54.4683 | 9.4286 | -18.5 | 9.6551 | -16.6787 | 9.3759 | -18.3371 | 0 | 0.4406 | 0.3556 | 2.5233 | 0.5087 | 0.5044 | 0.6663 | 0.6755 | 0.3633 | 0.3339 | |
| 10 | 3 | R A V | 0.6252 | 0.5957 | 0.0296 | -0.0051 | 0.4669 | 0.3572 | 9.1552 | 0.7694 | 21.1334 | 0.5327 | 0.0926 | 0.5214 | 0.3992 | 11.417 | 0.7171 | 54.7278 | 7.1338 | -15.5295 | 6.8596 | -14.1408 | 7.5837 | -14.3434 | 0 | 0.4354 | 0.3732 | 2.4648 | 0.5201 | 0.5159 | 0.674 | 0.7016 | 0.3921 | 0.2473 | |
| 11 | 3 | P A V | 0.6068 | 0.5757 | 0.031 | -0.0444 | 0.4782 | 0.3698 | 9.6063 | 0.7553 | 19.5462 | 0.5308 | 0.076 | 0.5224 | 0.4074 | 11.4627 | 0.7121 | 53.6019 | 7.6477 | -13.9829 | 7.1757 | -13.7985 | 7.4386 | -14.2446 | 0 | 0.436 | 0.3608 | 2.4711 | 0.5189 | 0.5147 | 0.6732 | 0.696 | 0.3972 | 0.2802 | |
| 12 | 2 | A V | 0.6068 | 0.5866 | 0.0202 | 0.051 | 0.4782 | 0.3699 | 9.6063 | 0.7553 | 30.0906 | 0.5544 | 0.0523 | 0.5091 | 0.3963 | 10.8849 | 0.7251 | 54.0788 | 4.8074 | -11.8297 | 4.4374 | -10.916 | 5.0209 | -11.0202 | 0 | 0.4361 | 0.3609 | 2.472 | 0.5187 | 0.5145 | 0.6731 | 0.6956 | 0.3968 | 0.2814 | |
| 13 | 4 | R P A B | 0.5956 | 0.5519 | 0.0437 | -0.0755 | 0.485 | 0.3812 | 9.8788 | 0.7466 | 13.625 | 0.4952 | 0.1004 | 0.5419 | 0.4286 | 12.3326 | 0.684 | 50.3507 | 9.5143 | -19.3633 | 9.2253 | -17.4427 | 9.7899 | -18.7786 | 0 | 0.5034 | 0.453 | 3.2941 | 0.3586 | 0.353 | 0.5644 | 0.6772 | 0.3235 | 0.0178 | |
| 14 | 3 | P A B | 0.5517 | 0.5163 | 0.0354 | -0.1479 | 0.5107 | 0.4113 | 10.9525 | 0.7111 | 15.5868 | 0.4597 | 0.092 | 0.5606 | 0.455 | 13.1997 | 0.6549 | 45.8881 | 7.6789 | -14.3664 | 7.1249 | -13.5608 | 7.509 | -14.8182 | 0 | 0.5398 | 0.465 | 3.788 | 0.2625 | 0.256 | 0.499 | 0.6628 | 0.3085 | 0.1024 | |
| 15 | 3 | R P A | 0.5486 | 0.513 | 0.0356 | -0.0769 | 0.5124 | 0.3865 | 11.0271 | 0.7085 | 15.3955 | 0.4507 | 0.0979 | 0.5653 | 0.4295 | 13.4198 | 0.6463 | 46.4882 | 6.997 | -15.3133 | 7.2056 | -13.7121 | 7.4405 | -14.7939 | 0 | 0.4676 | 0.4235 | 2.8426 | 0.4465 | 0.4417 | 0.6241 | 0.6757 | 0.3255 | 0.1416 | |
| 16 | 3 | R A B | 0.5466 | 0.5108 | 0.0358 | -0.0816 | 0.5136 | 0.4009 | 11.0776 | 0.7068 | 15.2675 | 0.4532 | 0.0933 | 0.5639 | 0.4435 | 13.3573 | 0.65 | 45.8038 | 7.98 | -15.3768 | 7.0543 | -13.7589 | 7.1108 | -15.9191 | 0 | 0.459 | 0.4136 | 2.7391 | 0.4667 | 0.4621 | 0.6378 | 0.6622 | 0.3129 | 0.2373 | |
| 17 | 2 | R A | 0.5362 | 0.5124 | 0.0238 | -0.0298 | 0.5194 | 0.4035 | 11.3317 | 0.698 | 22.5399 | 0.4642 | 0.072 | 0.5583 | 0.4359 | 13.0895 | 0.6567 | 45.2338 | 5.0521 | -11.4212 | 4.9047 | -10.45 | 4.9155 | -11.8144 | 0 | 0.4599 | 0.4102 | 2.7493 | 0.4647 | 0.4601 | 0.6364 | 0.6598 | 0.3104 | 0.2402 | |
| 18 | 2 | P A | 0.5076 | 0.4823 | 0.0253 | -0.1738 | 0.5352 | 0.3955 | 12.0297 | 0.6734 | 20.1004 | 0.4464 | 0.0612 | 0.5675 | 0.4204 | 13.5242 | 0.6342 | 43.4506 | 4.7957 | -11.7948 | 5.0242 | -10.3793 | 4.9691 | -11.4168 | 0 | 0.4913 | 0.4415 | 3.138 | 0.389 | 0.3837 | 0.585 | 0.6733 | 0.3202 | 0.0406 | |
| 19 | 3 | R P V | 0.4107 | 0.3642 | 0.0465 | -0.2276 | 0.5855 | 0.4976 | 14.397 | 0.5822 | 8.8271 | 0.195 | 0.2156 | 0.6843 | 0.5669 | 19.6648 | 0.4592 | 25.6713 | 6.9003 | -15.0706 | 7.0804 | -13.6761 | 7.4142 | -14.2438 | 0 | 0.6642 | 0.5292 | 5.7358 | -0.1168 | -0.1265 | 0.2415 | 0.0894 | -0.0024 | 0.0242 | |
| 20 | 2 | P V | 0.3451 | 0.3115 | 0.0336 | -0.3364 | 0.6172 | 0.5181 | 15.999 | 0.5131 | 10.2757 | 0.2302 | 0.1149 | 0.6691 | 0.5616 | 18.8054 | 0.4488 | 22.862 | 4.8279 | -10.8925 | 5.0159 | -10.2839 | 4.5796 | -11.4657 | 0 | 0.6456 | 0.5103 | 5.4179 | -0.0549 | -0.0641 | 0.2835 | 0.1193 | -0.0076 | 0.0682 | |
| 21 | 2 | A B | 0.3234 | 0.2887 | 0.0347 | -0.2471 | 0.6274 | 0.4847 | 16.5299 | 0.4887 | 9.3195 | 0.2318 | 0.0916 | 0.6685 | 0.5218 | 18.768 | 0.4235 | 22.5376 | 4.7916 | -11.9053 | 4.6949 | -10.6612 | 4.8677 | -12.0075 | 0 | 0.5001 | 0.4419 | 3.2518 | 0.3669 | 0.3614 | 0.57 | 0.5567 | 0.1948 | 0.2986 | |
| 22 | 3 | R P B | 0.3144 | 0.2603 | 0.0541 | -0.2639 | 0.6315 | 0.5207 | 16.7487 | 0.4784 | 5.8091 | 0.188 | 0.1264 | 0.6872 | 0.5747 | 19.837 | 0.3876 | 17.9995 | 7.1191 | -15.7584 | 7.6209 | -13.0781 | 7.4187 | -15.5549 | 0 | 0.5695 | 0.5029 | 4.2163 | 0.1791 | 0.1719 | 0.4424 | 0.3866 | 0.0679 | 0.2288 | |
| 23 | 2 | R B | 0.3003 | 0.2644 | 0.0359 | -0.3578 | 0.638 | 0.5075 | 17.0942 | 0.4619 | 8.3681 | 0.204 | 0.0963 | 0.6804 | 0.5481 | 19.4456 | 0.3957 | 18.7577 | 4.9584 | -12.6557 | 5.1157 | -10.1795 | 5.0355 | -12.5334 | 0 | 0.5651 | 0.4923 | 4.1513 | 0.1917 | 0.1847 | 0.451 | 0.3257 | 0.0255 | 0.3416 | |
| 24 | 2 | R V | 0.1996 | 0.1585 | 0.041 | -0.2642 | 0.6823 | 0.563 | 19.5539 | 0.3328 | 4.8626 | -0.0647 | 0.2643 | 0.7869 | 0.6265 | 26.01 | 0.2038 | 3.5919 | 4.6186 | -12.2283 | 4.8117 | -10.4832 | 4.9547 | -11.7702 | 0 | 0.6457 | 0.5378 | 5.4206 | -0.0554 | -0.0646 | 0.2831 | 0.0746 | -0.012 | 0.0582 | |
| 25 | 1 | V | 0.1986 | 0.1785 | 0.02 | 0.4456 | 0.6828 | 0.5636 | 19.5786 | 0.3314 | 9.9113 | 0.0589 | 0.1397 | 0.7399 | 0.6009 | 22.9918 | 0.2686 | 7.7132 | 2.2781 | -8.3683 | 2.1928 | -7.9082 | 2.5942 | -7.8325 | 0 | 0.6494 | 0.5412 | 5.4831 | -0.0676 | -0.0769 | 0.2749 | 0.0685 | -0.0086 | 0.0429 | |
| 26 | 2 | P B | 0.1964 | 0.1552 | 0.0412 | -0.4399 | 0.6837 | 0.5827 | 19.631 | 0.3284 | 4.7669 | 0.0924 | 0.104 | 0.7266 | 0.622 | 22.1716 | 0.2474 | 5.4438 | 5.0035 | -12.2108 | 4.8061 | -10.5829 | 5.5798 | -11.0349 | 0 | 0.5989 | 0.5081 | 4.6625 | 0.0922 | 0.0843 | 0.3834 | 0.3828 | 0.0692 | 0.1409 | |
| 27 | 1 | A | 0.1876 | 0.1673 | 0.0203 | 0.4331 | 0.6874 | 0.5454 | 19.8476 | 0.3159 | 9.2349 | 0.0602 | 0.1274 | 0.7394 | 0.5796 | 22.959 | 0.2358 | 6.2587 | 2.4389 | -7.7173 | 2.3091 | -7.7446 | 2.3485 | -7.9215 | 0 | 0.5308 | 0.4617 | 3.6627 | 0.2869 | 0.2807 | 0.5156 | 0.464 | 0.1125 | 0.3119 | |
| 28 | 2 | R P | 0.1675 | 0.1249 | 0.0427 | -0.3694 | 0.6958 | 0.5516 | 20.3366 | 0.287 | 3.9248 | -0.0302 | 0.1978 | 0.7741 | 0.6076 | 25.1687 | 0.1662 | 1.9903 | 4.8555 | -11.7888 | 4.9933 | -10.3592 | 4.8512 | -11.6079 | 0 | 0.6476 | 0.5477 | 5.4523 | -0.0616 | -0.0708 | 0.2789 | -0.0148 | -0.0017 | 0.0052 | |
| 29 | 1 | R | 0.1182 | 0.0961 | 0.022 | 0.3438 | 0.7162 | 0.5885 | 21.5426 | 0.2114 | 5.361 | -0.0499 | 0.1681 | 0.7815 | 0.6311 | 25.6498 | 0.1432 | -2.8034 | 2.6647 | -8.4483 | 2.3443 | -7.8265 | 2.4937 | -8.5931 | 0 | 0.6604 | 0.5688 | 5.67 | -0.104 | -0.1136 | 0.2502 | 0.0073 | -0.0001 | 0.0005 | |
| 30 | 1 | P | 0.0398 | 0.0157 | 0.024 | 0.1994 | 0.7474 | 0.6153 | 23.4587 | 0.0765 | 1.6559 | -0.0485 | 0.0883 | 0.781 | 0.6472 | 25.6151 | 0.0154 | -7.1104 | 2.5255 | -8.394 | 2.349 | -7.7512 | 2.3073 | -8.6939 | 0 | 0.6457 | 0.549 | 5.4206 | -0.0554 | -0.0646 | 0.2831 | 0.0131 | -0.001 | 0.0034 | |
| 31 | 1 | B | 0.0001 | -0.0249 | 0.025 | 0.0109 | 0.7626 | 0.6219 | 24.4269 | 0.0002 | 0.0048 | -0.0738 | 0.0739 | 0.7903 | 0.6485 | 26.2327 | -0.0711 | -10.6785 | 2.4069 | -9.0955 | 2.2497 | -7.7933 | 2.4026 | -9.5734 | 0 | 0.6305 | 0.5358 | 5.1682 | -0.0063 | -0.015 | 0.3165 | -0.0058 | -4.2626 | 8.6473 | |

Table S9_0.00001. Same as Table S5_0.00001 but for models developed using the descriptors employed in the work of Yu et al., 2015.

| S.No. | Size | Variables | R ² | R ² _{adj} | R ² -R ² _{adj} | ΔK | RMSE(tr) | MAE(tr) | RSS(tr) | CCC(tr) | F | Q ² _{loo} | R ² -Q ² _{loo} | RMSE(cv) | MAE(cv) | PRESS(cv) | CCC(cv) | Q ² _{LMO} | R ² _{Yscr} | Q ² _{Yscr} | R ² _{Xrnd} | Q ² _{Xrnd} | R ² _{Yrnd} | Q ² _{Yrnd} | N. ext. OK | RMSE(ext) | MAE(ext) | PRESS(ext) | Q ² _{F1} | Q ² _{F2} | Q ² _{F3} | CCC(ext) | \bar{r}_m^2 | Δr _m ² |
|-------|------|-----------|----------------|-------------------------------|---|---------|----------|---------|---------|---------|---------|-------------------------------|---|----------|---------|-----------|---------|-------------------------------|--------------------------------|--------------------------------|--------------------------------|--------------------------------|--------------------------------|--------------------------------|------------|-----------|----------|------------|------------------------------|------------------------------|------------------------------|----------|---------------|------------------------------|
| 1 | 5 | R P A B V | 0.8261 | 0.7989 | 0.0272 | -0.0475 | 0.3239 | 0.268 | 3.9871 | 0.9048 | 30.4053 | 0.7152 | 0.111 | 0.4146 | 0.3355 | 6.5313 | 0.8508 | 74.1165 | 13.2473 | -28.9095 | 13.8699 | -22.0244 | 13.8389 | -28.2042 | 5 | 0.2539 | 0.2011 | 1.0956 | 0.8347 | 0.8347 | 0.8932 | 0.9033 | 0.6925 | 0.1629 |
| 2 | 4 | R A B V | 0.8254 | 0.8043 | 0.0212 | -0.0464 | 0.3246 | 0.2654 | 4.003 | 0.9044 | 39.0057 | 0.7345 | 0.0909 | 0.4002 | 0.3213 | 6.0874 | 0.8606 | 75.2172 | 10.7164 | -24.8636 | 9.9398 | -19.8376 | 10.5769 | -24.7975 | 5 | 0.2569 | 0.2011 | 1.1222 | 0.8306 | 0.8306 | 0.8906 | 0.8996 | 0.6785 | 0.169 |
| 3 | 4 | R P B V | 0.8175 | 0.7954 | 0.0221 | -0.1792 | 0.3319 | 0.2772 | 4.1848 | 0.8996 | 36.9529 | 0.7234 | 0.0941 | 0.4085 | 0.3347 | 6.3422 | 0.855 | 74.0719 | 10.7481 | -24.0347 | 10.7685 | -18.7238 | 11.1248 | -23.6113 | 4 | 0.294 | 0.2307 | 1.4699 | 0.7782 | 0.7782 | 0.8567 | 0.8663 | 0.6223 | 0.2098 |
| 4 | 3 | R B V | 0.8175 | 0.8014 | 0.0161 | -0.2569 | 0.3319 | 0.277 | 4.1851 | 0.8996 | 50.7585 | 0.7418 | 0.0756 | 0.3947 | 0.3238 | 5.9197 | 0.8646 | 74.6951 | 8.0874 | -20.1491 | 8.1339 | -15.08 | 8.0678 | -20.6539 | 4 | 0.2941 | 0.2304 | 1.4704 | 0.7781 | 0.7781 | 0.8567 | 0.866 | 0.6209 | 0.2103 |
| 5 | 4 | P A B V | 0.815 | 0.7925 | 0.0224 | -0.0758 | 0.3342 | 0.2798 | 4.243 | 0.898 | 36.3327 | 0.7012 | 0.1138 | 0.4246 | 0.3425 | 6.8514 | 0.841 | 73.4853 | 10.926 | -22.7757 | 10.3416 | -19.2756 | 10.9888 | -22.4676 | 5 | 0.2805 | 0.2119 | 1.338 | 0.7981 | 0.7981 | 0.8696 | 0.8897 | 0.716 | 0.1716 |
| 6 | 3 | A B V | 0.8041 | 0.7868 | 0.0173 | -0.0859 | 0.3438 | 0.2746 | 4.4924 | 0.8914 | 46.5116 | 0.6995 | 0.1046 | 0.4258 | 0.3279 | 6.8911 | 0.8391 | 72.3943 | 8.4719 | -19.2618 | 7.8407 | -15.142 | 7.8341 | -20.4729 | 4 | 0.3131 | 0.2426 | 1.6665 | 0.7485 | 0.7485 | 0.8375 | 0.8611 | 0.6492 | 0.1725 |
| 7 | 3 | P B V | 0.8034 | 0.7861 | 0.0173 | -0.2547 | 0.3444 | 0.2874 | 4.5076 | 0.891 | 46.3168 | 0.7043 | 0.0992 | 0.4224 | 0.3392 | 6.7811 | 0.8428 | 72.3511 | 8.355 | -18.3356 | 8.2401 | -14.6591 | 8.3219 | -18.6263 | 4 | 0.3197 | 0.2454 | 1.7372 | 0.7378 | 0.7378 | 0.8306 | 0.8525 | 0.6308 | 0.1919 |
| 8 | 2 | B V | 0.7964 | 0.7848 | 0.0116 | -0.3662 | 0.3505 | 0.2859 | 4.6685 | 0.8867 | 68.4497 | 0.7118 | 0.0846 | 0.417 | 0.3279 | 6.6093 | 0.8458 | 72.8327 | 5.6122 | -14.8567 | 4.7794 | -12.3277 | 5.3139 | -14.9393 | 3 | 0.3363 | 0.2621 | 1.9223 | 0.7099 | 0.7099 | 0.8126 | 0.8359 | 0.5954 | 0.1919 |
| 9 | 4 | R P A V | 0.6226 | 0.5768 | 0.0457 | -0.0541 | 0.4772 | 0.3797 | 8.6537 | 0.7674 | 13.6095 | 0.4385 | 0.1841 | 0.5821 | 0.4579 | 12.8744 | 0.6711 | 50.4197 | 10.9386 | -22.1954 | 10.9666 | -18.3188 | 10.7853 | -21.9312 | 1 | 0.4163 | 0.3413 | 2.9459 | 0.5554 | 0.5554 | 0.7128 | 0.7587 | 0.4572 | 0.1487 |
| 10 | 3 | R A V | 0.6109 | 0.5766 | 0.0343 | -0.0347 | 0.4845 | 0.3833 | 8.9212 | 0.7585 | 17.7955 | 0.4606 | 0.1504 | 0.5705 | 0.4464 | 12.3689 | 0.6841 | 50.1007 | 8.3183 | -17.8922 | 7.9638 | -15.1593 | 8.0147 | -18.2335 | 1 | 0.4124 | 0.3494 | 2.8908 | 0.5637 | 0.5637 | 0.7182 | 0.7746 | 0.4936 | 0.1083 |
| 11 | 3 | P A V | 0.6085 | 0.574 | 0.0345 | -0.0721 | 0.486 | 0.3845 | 8.9762 | 0.7566 | 17.6168 | 0.4818 | 0.1267 | 0.5592 | 0.4421 | 11.8819 | 0.6924 | 51.2804 | 8.4224 | -17.0848 | 8.5039 | -14.3986 | 8.1311 | -17.1039 | 0 | 0.4441 | 0.3665 | 3.3529 | 0.494 | 0.494 | 0.6731 | 0.7467 | 0.4406 | 0.0611 |
| 12 | 2 | A V | 0.6062 | 0.5837 | 0.0225 | -0.0045 | 0.4874 | 0.3844 | 9.029 | 0.7548 | 26.9412 | 0.5114 | 0.0949 | 0.543 | 0.4276 | 11.2042 | 0.708 | 51.8864 | 5.9748 | -12.8927 | 6.0318 | -10.935 | 5.1432 | -14.6641 | 0 | 0.4339 | 0.3634 | 3.2008 | 0.517 | 0.5169 | 0.688 | 0.7588 | 0.4653 | 0.0652 |
| 13 | 4 | R P A B | 0.5496 | 0.495 | 0.0546 | -0.0913 | 0.5213 | 0.4297 | 10.3283 | 0.7093 | 10.0652 | 0.4127 | 0.1369 | 0.5953 | 0.494 | 13.4673 | 0.6215 | 42.8478 | 10.5432 | -23.6252 | 10.8937 | -18.5546 | 10.9373 | -23.649 | 1 | 0.3977 | 0.336 | 2.6889 | 0.5942 | 0.5942 | 0.7379 | 0.7444 | 0.4282 | 0.3151 |
| 14 | 3 | R A B | 0.5267 | 0.4849 | 0.0418 | -0.1087 | 0.5344 | 0.4273 | 10.8534 | 0.6899 | 12.6097 | 0.4086 | 0.1181 | 0.5974 | 0.4745 | 13.5605 | 0.6168 | 41.2551 | 8.2883 | -19.276 | 7.6724 | -15.4404 | 8.0831 | -19.1416 | 1 | 0.4236 | 0.3528 | 3.0505 | 0.5396 | 0.5396 | 0.7026 | 0.6853 | 0.3267 | 0.3658 |
| 15 | 3 | R P A | 0.516 | 0.4733 | 0.0427 | -0.0996 | 0.5404 | 0.4387 | 11.0975 | 0.6807 | 12.0831 | 0.3921 | 0.1239 | 0.6056 | 0.4962 | 13.938 | 0.6011 | 40.4123 | 8.1178 | -17.5035 | 8.1615 | -14.9988 | 9.0151 | -15.8386 | 1 | 0.4043 | 0.312 | 2.7789 | 0.5806 | 0.5806 | 0.7291 | 0.7406 | 0.4307 | 0.3131 |
| 16 | 2 | R A | 0.5118 | 0.4839 | 0.0279 | -0.0622 | 0.5427 | 0.4381 | 11.1937 | 0.6771 | 18.3471 | 0.4263 | 0.0855 | 0.5884 | 0.4782 | 13.1551 | 0.628 | 41.4435 | 5.2333 | -13.6188 | 5.0836 | -12.0853 | 5.9681 | -12.869 | 1 | 0.4137 | 0.3313 | 2.9101 | 0.5608 | 0.5608 | 0.7163 | 0.7154 | 0.3803 | 0.3374 |
| 17 | 3 | P A B | 0.4915 | 0.4466 | 0.0449 | -0.1808 | 0.5539 | 0.4537 | 11.6604 | 0.659 | 10.9527 | 0.3628 | 0.1287 | 0.6201 | 0.5115 | 14.6104 | 0.5808 | 37.189 | 7.6546 | -20.4981 | 7.8586 | -15.4874 | 7.5387 | -19.1898 | 1 | 0.4041 | 0.3358 | 2.7761 | 0.5811 | 0.581 | 0.7294 | 0.7615 | 0.4755 | 0.2362 |
| 18 | 2 | P A | 0.4686 | 0.4383 | 0.0304 | -0.2163 | 0.5662 | 0.4458 | 12.1835 | 0.6382 | 15.4346 | 0.3939 | 0.0748 | 0.6048 | 0.4781 | 13.8985 | 0.589 | 38.0806 | 5.5036 | -12.883 | 5.3138 | -11.7771 | 5.1988 | -13.6763 | 1 | 0.4189 | 0.3308 | 2.9834 | 0.5498 | 0.5497 | 0.7092 | 0.7481 | 0.4568 | 0.2194 |
| 19 | 3 | R P V | 0.3799 | 0.3252 | 0.0547 | -0.2538 | 0.6117 | 0.4887 | 14.2174 | 0.5507 | 6.9445 | 0.0787 | 0.3012 | 0.7456 | 0.576 | 21.1241 | 0.3875 | 19.3575 | 8.346 | -17.4312 | 8.3141 | -14.8423 | 7.9435 | -18.223 | 0 | 0.5937 | 0.5439 | 5.9918 | 0.0958 | 0.0957 | 0.4159 | 0.3718 | 0.0536 | 0.1347 |
| 20 | 3 | R P B | 0.3676 | 0.3118 | 0.0558 | -0.2601 | 0.6178 | 0.4988 | 14.5014 | 0.5375 | 6.5865 | 0.2491 | 0.1185 | 0.6731 | 0.5547 | 17.2183 | 0.4557 | 23.6876 | 8.8138 | -18.9314 | 8.2674 | -14.9157 | 7.6381 | -20.3924 | 0 | 0.6256 | 0.5185 | 6.6526 | -0.004 | -0.004 | 0.3515 | 0.3012 | 0.028 | 0.0888 |
| 21 | 2 | R B | 0.3597 | 0.3231 | 0.0366 | -0.3579 | 0.6216 | 0.4861 | 14.6817 | 0.5291 | 9.8306 | 0.286 | 0.0737 | 0.6564 | 0.5221 | 16.3713 | 0.4777 | 25.4437 | 5.1574 | -16.9128 | 5.2974 | -11.8392 | 5.4993 | -15.6546 | 0 | 0.6337 | 0.5121 | 6.8278 | -0.0304 | -0.0304 | 0.3344 | 0.2536 | 0.0152 | 0.08 |
| 22 | 2 | P V | 0.3329 | 0.2948 | 0.0381 | -0.3712 | 0.6344 | 0.5073 | 15.2958 | 0.4995 | 8.7334 | 0.1511 | 0.1818 | 0.7157 | 0.564 | 19.4645 | 0.4132 | 18.093 | 5.4208 | -13.8549 | 5.3867 | -11.698 | 5.2176 | -13.7227 | 0 | 0.611 | 0.5451 | 6.3471 | 0.0422 | 0.0421 | 0.3842 | 0.3987 | 0.0659 | 0.0926 |
| 23 | 2 | A B | 0.3221 | 0.2833 | 0.0387 | -0.2746 | 0.6396 | 0.5013 | 15.5446 | 0.4872 | 8.3135 | 0.2132 | 0.1088 | 0.689 | 0.5473 | 18.0401 | 0.413 | 21.1152 | 5.2849 | -15.5371 | 5.4441 | -11.61 | 5.161 | -16.3445 | 0 | 0.5038 | 0.4088 | 4.3151 | 0.3488 | 0.3488 | 0.5793 | 0.5867 | 0.2231 | 0.2526 |
| 24 | 2 | P B | 0.2144 | 0.1695 | 0.0449 | -0.4383 | 0.6885 | 0.5823 | 18.0124 | 0.3531 | 4.7769 | -0.0104 | 0.2249 | 0.7808 | 0.6496 | 23.1687 | 0.2362 | 2.5585 | 5.3204 | -15.0477 | 5.7896 | -11.0775 | 5.476 | -15.0439 | 0 | 0.6002 | 0.5289 | 6.1238 | 0.0758 | 0.0758 | 0.403 | 0.3406 | 0.0399 | 0.1323 |
| 25 | 1 | A | 0.2082 | 0.1862 | 0.022 | 0.4563 | 0.6912 | 0.5441 | 18.156 | 0.3446 | 9.4642 | 0.0742 | 0.1339 | 0.7474 | 0.5817 | 21.2273 | 0.2635 | 9.2741 | 2.5866 | -8.857 | 2.7006 | -8.5251 | 2.7407 | -8.5409 | 0 | 0.5612 | 0.4834 | 5.3543 | 0.192 | 0.1919 | 0.478 | 0.346 | 0.0348 | 0.3023 |
| 26 | 2 | R P | 0.1687 | 0.1212 | 0.0475 | -0.4061 | 0.7082 | 0.5532 | 19.0612 | 0.2887 | 3.5512 | -0.0071 | 0.1758 | 0.7796 | 0.6113 | 23.0926 | 0.1647 | 1.553 | 5.6308 | -13.2769 | 5.2035 | -11.9651 | 5.4052 | -13.876 | 0 | 0.646 | 0.5476 | 7.0935 | -0.0705 | -0.0705 | 0.3085 | 0.0385 | -0.0024 | 0.0108 |
| 27 | 2 | R V | 0.1492 | 0.1006 | 0.0486 | -0.3211 | 0.7165 | 0.6014 | 19.5083 | 0.2596 | 3.0687 | -0.234 | 0.3832 | 0.8629 | 0.6886 | 28.2938 | 0.093 | -8.822 | 5.1635 | -13.937 | 5.4142 | -11.7212 | 5.1191 | -14.6303 | 0 | 0.5631 | 0.4391 | 5.3899 | 0.1866 | 0.1866 | 0.4746 | 0.3775 | 0.0539 | 0.2751 |
| 28 | 1 | V | 0.1426 | 0.1188 | 0.0238 | 0.3777 | 0.7193 | 0.6082 | 19.6588 | 0.2496 | 5.9888 | -0.115 | 0.2576 | 0.8202 | 0.6659 | 25.5657 | 0.1677 | -4.4428 | 2.3061 | -10.6067 | 2.8823 | -8.2786 | 2.5624 | -9.9752 | 0 | 0.5596 | 0.4458 | 5.3228 | 0.1967 | 0.1967 | 0.4811 | 0.3549 | 0.0377 | 0.3321 |
| 29 | 1 | R | 0.0764 | 0.0508 | 0.0257 | 0.2765 | 0.7465 | 0.6255 | 21.1767 | 0.142 | 2.9791 | -0.1031 | 0.1795 | 0.8158 | 0.6755 | 25.2922 | 0.0656 | -9.1568 | 2.7419 | -10.2579 | 2.6315 | -8.6394 | 2.8239 | -10.0602 | 0 | 0.591 | 0.4822 | 5.9379 | 0.1039 | 0.1038 | 0.4211 | 0.1677 | -0.074 | 0.3531 |
| 30 | 1 | P | 0.0114 | -0.0161 | 0.0275 | 0.1065 | 0.7724 | 0.6386 | 22.6688 | 0.0225 | 0.4134 | -0.0726 | 0.0839 | 0.8045 | 0.6701 | 24.5928 | -0.0507 | -11.2694 | 2.7985 | -9.408 | 2.6376 | -8.6028 | 2.6439 | -9.8669 | 0 | 0.6035 | 0.503 | 6.191 | 0.0657 | 0.0657 | 0.3965 | 0.0825 | -0.2826 | 0.7325 |
| 31 | 1 | B | 0.0101 | -0.0174 | 0.0275 | 0.1006 | 0.7728 | 0.6314 | 22.697 | 0.02 | 0.3683 | -0.1757 | 0.1858 | 0.8423 | 0.6841 | 26.9578 | -0.0618 | -14.5517 | 2.4182 | -12.1582 | 2.7698 | -8.4893 | 2.8134 | -11.0791 | 0 | 0.6388 | 0.5523 | 6.9374 | -0.0469 | -0.047 | 0.3237 | -0.0326 | -0.0685 | 0.1669 |

Table S10_0.00001. Same as Table S6_0.00001 but for models developed using the descriptors employed in the work of Yu et al., 2015.

| S.No. | Size | Variables | R ² | R ² _{adj} | R ² -R ² _{adj} | ΔK | RMSE(tr) | MAE(tr) | RSS(tr) | CCC(tr) | F | Q ² _{loo} | R ² -Q ² _{loo} | RMSE(cv) | MAE(cv) | PRESS(cv) | CCC(cv) | Q ² _{LMO} | R ² _{Yscr} | Q ² _{Yscr} | R ² _{Xrnd} | Q ² _{Xrnd} | R ² _{Yrnd} | Q ² _{Yrnd} | N. ext. OK | RMSE(ext) | MAE(ext) | PRESS(ext) | Q ² _{F1} | Q ² _{F2} | Q ² _{F3} | CCC(ext) | \bar{r}_m^2 | Δr _m ² |
|-------|------|-----------|----------------|-------------------------------|---|---------|----------|---------|---------|---------|---------|-------------------------------|---|----------|---------|-----------|---------|-------------------------------|--------------------------------|--------------------------------|--------------------------------|--------------------------------|--------------------------------|--------------------------------|------------|-----------|----------|------------|------------------------------|------------------------------|------------------------------|----------|---------------|------------------------------|
| 1 | 5 | R P A B V | 0.8904 | 0.8665 | 0.0238 | -0.0578 | 0.2674 | 0.2087 | 2.0742 | 0.942 | 37.3587 | 0.7897 | 0.1006 | 0.3704 | 0.2853 | 3.978 | 0.896 | 80.5492 | 18.4105 | -40.4724 | 18.6558 | -30.6319 | 17.6189 | -40.653 | 1 | 0.3631 | 0.2892 | 3.4288 | 0.6776 | 0.6776 | 0.7979 | 0.8417 | 0.6494 | 0.0546 |
| 2 | 4 | R A B V | 0.8887 | 0.8702 | 0.0185 | -0.0578 | 0.2694 | 0.2087 | 2.1052 | 0.9411 | 47.923 | 0.8085 | 0.0803 | 0.3535 | 0.2725 | 3.6237 | 0.9043 | 81.3031 | 14.3276 | -35.1721 | 14.4179 | -25.9702 | 14.6791 | -33.0041 | 1 | 0.3594 | 0.2893 | 3.3584 | 0.6842 | 0.6842 | 0.802 | 0.8386 | 0.646 | 0.0071 |
| 3 | 4 | R P B V | 0.8693 | 0.8475 | 0.0218 | -0.1894 | 0.292 | 0.2331 | 2.4723 | 0.9301 | 39.9153 | 0.7932 | 0.0761 | 0.3673 | 0.2962 | 3.912 | 0.896 | 77.1797 | 14.4763 | -33.5307 | 14.576 | -25.7901 | 14.4844 | -33.9759 | 1 | 0.3774 | 0.3032 | 3.7035 | 0.6518 | 0.6518 | 0.7817 | 0.813 | 0.5998 | 0.0839 |
| 4 | 3 | R B V | 0.869 | 0.8533 | 0.0157 | -0.2587 | 0.2923 | 0.2349 | 2.4785 | 0.9299 | 55.2789 | 0.8029 | 0.0661 | 0.3586 | 0.2896 | 3.7284 | 0.9008 | 77.7828 | 10.4837 | -29.0037 | 11.2817 | -19.9344 | 11.2299 | -26.5134 | 1 | 0.3782 | 0.303 | 3.7185 | 0.6504 | 0.6504 | 0.7808 | 0.8149 | 0.6016 | 0.0619 |
| 5 | 4 | P A B V | 0.8564 | 0.8324 | 0.0239 | -0.091 | 0.3061 | 0.2433 | 2.7173 | 0.9226 | 35.7762 | 0.7134 | 0.143 | 0.4324 | 0.3204 | 5.4231 | 0.8528 | 73.9582 | 14.3035 | -29.8877 | 14.0116 | -26.3401 | 14.0671 | -29.4393 | 3 | 0.3577 | 0.276 | 3.3271 | 0.6872 | 0.6872 | 0.8039 | 0.8578 | 0.6762 | 0.1734 |
| 6 | 3 | A B V | 0.8322 | 0.8121 | 0.0201 | -0.0986 | 0.3308 | 0.2696 | 3.1742 | 0.9084 | 41.3373 | 0.691 | 0.1412 | 0.449 | 0.3417 | 5.8464 | 0.8389 | 72.051 | 10.484 | -26.1723 | 10.7905 | -20.7487 | 10.7472 | -24.5016 | 1 | 0.3518 | 0.265 | 3.218 | 0.6974 | 0.6974 | 0.8103 | 0.845 | 0.6439 | 0.0092 |
| 7 | 3 | P B V | 0.8149 | 0.7927 | 0.0222 | -0.2672 | 0.3475 | 0.2903 | 3.5022 | 0.898 | 36.685 | 0.6881 | 0.1267 | 0.4511 | 0.359 | 5.9002 | 0.8368 | 69.4912 | 10.6227 | -24.3912 | 10.8197 | -20.3697 | 10.6557 | -24.9874 | 5 | 0.3402 | 0.2613 | 3.01 | 0.717 | 0.717 | 0.8226 | 0.8537 | 0.6732 | 0.0246 |
| 8 | 2 | B V | 0.8054 | 0.7904 | 0.015 | -0.3934 | 0.3564 | 0.2982 | 3.6827 | 0.8922 | 53.787 | 0.6897 | 0.1156 | 0.4499 | 0.3568 | 5.8701 | 0.8364 | 67.6489 | 7.4213 | -20.6384 | 7.1541 | -15.7532 | 7.0842 | -20.973 | 3 | 0.3462 | 0.2639 | 3.1158 | 0.7071 | 0.707 | 0.8163 | 0.8393 | 0.6449 | 0.1206 |
| 9 | 4 | R P A V | 0.6555 | 0.5981 | 0.0574 | -0.0623 | 0.4741 | 0.3823 | 6.5183 | 0.7919 | 11.4152 | 0.4749 | 0.1805 | 0.5853 | 0.4732 | 9.9341 | 0.6941 | 49.6789 | 14.1444 | -31.8174 | 13.8883 | -26.442 | 14.1542 | -30.7623 | 0 | 0.4573 | 0.356 | 5.4369 | 0.4888 | 0.4888 | 0.6795 | 0.6869 | 0.355 | 0.2182 |
| 10 | 3 | P A V | 0.6279 | 0.5833 | 0.0446 | -0.0931 | 0.4927 | 0.3841 | 7.0395 | 0.7714 | 14.0637 | 0.5182 | 0.1097 | 0.5606 | 0.4435 | 9.115 | 0.7151 | 51.7557 | 10.2524 | -25.6314 | 11.0031 | -20.3371 | 10.9962 | -22.4271 | 0 | 0.4614 | 0.3738 | 5.5362 | 0.4795 | 0.4795 | 0.6736 | 0.7119 | 0.3762 | 0.0951 |
| 11 | 3 | R A V | 0.6279 | 0.5833 | 0.0447 | -0.0459 | 0.4927 | 0.3736 | 7.0399 | 0.7714 | 14.0622 | 0.4726 | 0.1553 | 0.5866 | 0.4475 | 9.9784 | 0.689 | 48.7097 | 10.7136 | -26.1793 | 10.741 | -20.3047 | 10.247 | -26.9123 | 1 | 0.4276 | 0.353 | 4.7548 | 0.5529 | 0.5529 | 0.7197 | 0.7526 | 0.4465 | 0.1059 |
| 12 | 2 | A V | 0.6204 | 0.5912 | 0.0292 | -0.0352 | 0.4977 | 0.3777 | 7.1827 | 0.7657 | 21.2427 | 0.543 | 0.0774 | 0.546 | 0.4202 | 8.6465 | 0.7242 | 51.5873 | 7.037 | -18.4194 | 7.496 | -15.3344 | 7.1305 | -18.5561 | 1 | 0.4412 | 0.3635 | 5.0614 | 0.5241 | 0.5241 | 0.7016 | 0.7433 | 0.426 | 0.0707 |
| 13 | 4 | R P A B | 0.6105 | 0.5456 | 0.0649 | -0.0995 | 0.5041 | 0.3943 | 7.3689 | 0.7582 | 9.4049 | 0.4252 | 0.1853 | 0.6124 | 0.4788 | 10.8756 | 0.6495 | 43.566 | 14.0491 | -34.279 | 14.4662 | -25.7842 | 13.9449 | -33.6645 | 0 | 0.5055 | 0.4265 | 6.6436 | 0.3754 | 0.3753 | 0.6083 | 0.6955 | 0.3557 | 0.0441 |
| 14 | 3 | R A B | 0.5724 | 0.5211 | 0.0513 | -0.1097 | 0.5282 | 0.3791 | 8.0898 | 0.7281 | 11.1558 | 0.4135 | 0.1589 | 0.6186 | 0.4383 | 11.0967 | 0.6382 | 41.4863 | 11.1548 | -27.9833 | 11.1273 | -20.3768 | 10.5154 | -27.3978 | 0 | 0.4915 | 0.4365 | 6.2803 | 0.4095 | 0.4095 | 0.6298 | 0.6356 | 0.289 | 0.201 |
| 15 | 3 | R P A | 0.5374 | 0.4819 | 0.0555 | -0.1082 | 0.5494 | 0.4151 | 8.7528 | 0.6991 | 9.6796 | 0.3619 | 0.1755 | 0.6452 | 0.4936 | 12.0724 | 0.5901 | 37.251 | 10.6875 | -25.6331 | 10.3468 | -20.8162 | 10.5999 | -25.5202 | 0 | 0.4495 | 0.3826 | 5.2522 | 0.5062 | 0.5062 | 0.6904 | 0.696 | 0.3707 | 0.2322 |
| 16 | 2 | R A | 0.5361 | 0.5004 | 0.0357 | -0.0649 | 0.5501 | 0.4175 | 8.7767 | 0.698 | 15.0236 | 0.4181 | 0.118 | 0.6161 | 0.472 | 11.009 | 0.6334 | 38.5491 | 6.9523 | -20.9476 | 6.8934 | -16.138 | 7.0544 | -19.7602 | 0 | 0.4552 | 0.3912 | 5.3863 | 0.4936 | 0.4936 | 0.6825 | 0.6786 | 0.3504 | 0.2691 |
| 17 | 3 | P A B | 0.5265 | 0.4697 | 0.0568 | -0.1928 | 0.5558 | 0.458 | 8.9579 | 0.6898 | 9.2671 | 0.3196 | 0.207 | 0.6663 | 0.5483 | 12.8735 | 0.5696 | 30.2095 | 10.7179 | -24.1617 | 10.6918 | -20.6247 | 11.2905 | -23.0682 | 0 | 0.5049 | 0.4182 | 6.6283 | 0.3768 | 0.3768 | 0.6092 | 0.7288 | 0.4045 | 0.1623 |
| 18 | 3 | R P V | 0.5023 | 0.4426 | 0.0597 | -0.2534 | 0.5698 | 0.4955 | 9.4155 | 0.6687 | 8.4118 | 0.2096 | 0.2927 | 0.7181 | 0.6053 | 14.9538 | 0.5065 | 25.4907 | 10.8745 | -24.4219 | 10.1967 | -21.6141 | 10.6018 | -25.743 | 0 | 0.6707 | 0.5286 | 11.695 | -0.0996 | -0.0996 | 0.3105 | 0.2134 | 0.0084 | 0.0522 |
| 19 | 2 | P A | 0.4732 | 0.4327 | 0.0405 | -0.254 | 0.5863 | 0.4311 | 9.9671 | 0.6424 | 11.6767 | 0.37 | 0.1032 | 0.6411 | 0.4766 | 11.9196 | 0.5773 | 33.6794 | 7.3622 | -18.6376 | 7.056 | -15.9257 | 6.7366 | -18.5416 | 0 | 0.4549 | 0.3797 | 5.3793 | 0.4942 | 0.4942 | 0.6829 | 0.7333 | 0.4056 | 0.043 |
| 20 | 3 | R P B | 0.4253 | 0.3563 | 0.069 | -0.2719 | 0.6123 | 0.4707 | 10.8734 | 0.5968 | 6.1666 | 0.2973 | 0.128 | 0.6771 | 0.5332 | 13.2945 | 0.5237 | 24.1523 | 10.309 | -26.7463 | 10.059 | -21.5191 | 10.9951 | -27.6797 | 0 | 0.6505 | 0.5628 | 11.0027 | -0.0345 | -0.0345 | 0.3514 | 0.3841 | 0.0626 | 0.0564 |
| 21 | 2 | R B | 0.4212 | 0.3767 | 0.0445 | -0.3842 | 0.6145 | 0.4652 | 10.9504 | 0.5928 | 9.4607 | 0.3336 | 0.0876 | 0.6594 | 0.5106 | 12.6086 | 0.5473 | 27.0733 | 7.55 | -23.9562 | 7.1695 | -15.9231 | 7.4536 | -21.6149 | 0 | 0.6509 | 0.5608 | 11.0151 | -0.0357 | -0.0357 | 0.3506 | 0.3456 | 0.0459 | 0.0689 |
| 22 | 2 | P V | 0.418 | 0.3732 | 0.0448 | -0.3805 | 0.6162 | 0.5289 | 11.0115 | 0.5895 | 9.3362 | 0.2852 | 0.1327 | 0.6829 | 0.5911 | 13.5228 | 0.5206 | 23.514 | 7.2984 | -18.3007 | 7.0274 | -15.837 | 7.0015 | -17.9043 | 0 | 0.6668 | 0.5284 | 11.5605 | -0.0869 | -0.0869 | 0.3185 | 0.2767 | 0.0215 | 0.0578 |
| 23 | 2 | A B | 0.3185 | 0.2661 | 0.0524 | -0.2821 | 0.6668 | 0.5034 | 12.8937 | 0.4831 | 6.0756 | 0.16 | 0.1585 | 0.7403 | 0.5702 | 15.8932 | 0.3789 | 13.428 | 6.8193 | -20.1071 | 7.02 | -16.0066 | 7.2186 | -20.7179 | 0 | 0.516 | 0.4424 | 6.9239 | 0.349 | 0.349 | 0.5918 | 0.5548 | 0.1908 | 0.2722 |
| 24 | 2 | R P | 0.2599 | 0.203 | 0.0569 | -0.3978 | 0.6949 | 0.5341 | 14.0023 | 0.4126 | 4.5653 | 0.0237 | 0.2363 | 0.7981 | 0.6154 | 18.4722 | 0.2766 | 3.9308 | 6.7891 | -19.3828 | 6.9206 | -16.1042 | 6.6113 | -20.1339 | 0 | 0.6993 | 0.5845 | 12.7149 | -0.1955 | -0.1955 | 0.2504 | -0.0283 | -0.0008 | 0.0035 |
| 25 | 1 | A | 0.1824 | 0.1522 | 0.0303 | 0.4271 | 0.7303 | 0.5532 | 15.4677 | 0.3086 | 6.0255 | -0.0227 | 0.2052 | 0.8168 | 0.6088 | 19.3499 | 0.1905 | -2.7228 | 3.8643 | -11.4573 | 3.7407 | -11.1657 | 3.676 | -11.7958 | 0 | 0.5564 | 0.4975 | 8.0487 | 0.2432 | 0.2432 | 0.5255 | 0.3791 | 0.0455 | 0.3873 |
| 26 | 2 | P B | 0.1626 | 0.0982 | 0.0644 | -0.4643 | 0.7391 | 0.6519 | 15.8436 | 0.2797 | 2.5239 | -0.0758 | 0.2384 | 0.8378 | 0.7415 | 20.3545 | 0.1172 | -19.583 | 7.2971 | -19.9215 | 6.8585 | -16.3677 | 7.0288 | -20.989 | 0 | 0.5679 | 0.4737 | 8.3861 | 0.2115 | 0.2115 | 0.5056 | 0.4725 | 0.1165 | 0.1748 |
| 27 | 2 | R V | 0.1528 | 0.0876 | 0.0652 | -0.3157 | 0.7435 | 0.611 | 16.0292 | 0.2651 | 2.3441 | -0.3503 | 0.503 | 0.9386 | 0.731 | 25.5463 | 0.0405 | -21.2093 | 7.3185 | -19.0252 | 7.2445 | -15.7411 | 7.3663 | -19.2442 | 0 | 0.5833 | 0.495 | 8.8469 | 0.1682 | 0.1682 | 0.4784 | 0.2638 | -0.0311 | 0.3871 |
| 28 | 1 | V | 0.1519 | 0.1205 | 0.0314 | 0.3897 | 0.7438 | 0.6133 | 16.0458 | 0.2637 | 4.8357 | -0.0938 | 0.2456 | 0.8447 | 0.6795 | 20.6934 | 0.1708 | -10.7734 | 3.5994 | -13.4817 | 3.5091 | -11.4492 | 3.5663 | -12.7869 | 0 | 0.5858 | 0.4968 | 8.9232 | 0.161 | 0.161 | 0.4739 | 0.2529 | -0.0369 | 0.3852 |
| 29 | 1 | R | 0.1032 | 0.07 | 0.0332 | 0.3213 | 0.7649 | 0.6349 | 16.9669 | 0.1871 | 3.1075 | -0.1885 | 0.2917 | 0.8805 | 0.7102 | 22.4855 | 0.0921 | -17.8297 | 3.6415 | -13.5993 | 3.748 | -11.2461 | 3.5821 | -14.5365 | 0 | 0.6249 | 0.5233 | 10.1544 | 0.0453 | 0.0453 | 0.4014 | 0.1152 | -0.0328 | 0.1583 |
| 30 | 1 | P | 0.0109 | -0.0257 | 0.0366 | 0.1044 | 0.8033 | 0.6607 | 18.7134 | 0.0216 | 0.2975 | -0.0947 | 0.1056 | 0.8451 | 0.7021 | 20.7119 | -0.0726 | -17.43 | 3.3657 | -14.1804 | 3.5667 | -11.4362 | 3.4868 | -13.3939 | 0 | 0.6254 | 0.5247 | 10.1694 | 0.0439 | 0.0438 | 0.4005 | 0.0543 | -0.2473 | 0.6098 |
| 31 | 1 | B | 0.0013 | -0.0357 | 0.037 | 0.0359 | 0.8072 | 0.6585 | 18.8953 | 0.0026 | 0.0348 | -0.1424 | 0.1437 | 0.8633 | 0.7134 | 21.6131 | -0.1056 | -29.2634 | 3.5196 | -15.3571 | 3.7142 | -11.1873 | 3.285 | -16.5771 | 0 | 0.6389 | 0.5408 | 10.6143 | 0.002 | 0.002 | 0.3742 | 0.0029 | -0.0363 | 0.0772 |

Table S11_0.00001. Same as Table S3_0.00001 but for models developed using combined quantum mechanical descriptors and LSER's adsorbate descriptors.

| S.No. | Size | Variables | R ² | R ² _{adj} | R ² -R ² _{adj} | Δ K | RMSE(tr) | MAE(tr) | RSS(tr) | CCC(tr) | F | Q ² _{loo} | R ² -Q ² _{loo} | RMSE(ev) | MAE(ev) | PRESS(ev) | CCC(ev) | Q ² _{LMO} | R ² _{Yscr} | Q ² _{Yscr} | R ² _{Xrnd} | Q ² _{Xrnd} | R ² _{Yrnd} | Q ² _{Yrnd} |
|-------|-------|------------------------------|----------------|-------------------------------|---|---------|----------|---------|---------|---------|----------|-------------------------------|---|----------|---------|-----------|---------|-------------------------------|--------------------------------|--------------------------------|--------------------------------|--------------------------------|--------------------------------|--------------------------------|
| 1 | 5 B | ZPE(HF) α(HF) H(HF) ω(DFT) | 0.8556 | 0.8409 | 0.0147 | -0.0126 | 0.2785 | 0.2217 | 4.2665 | 0.9222 | 58.0876 | 0.8234 | 0.0323 | 0.3081 | 0.2473 | 5.2205 | 0.9063 | 82.3196 | 9.2122 | -18.0583 | 9.364 | -14.3543 | 9.011 | -18.5372 |
| 2 | 5 B | E(HF) ZPE(HF) α(HF) ω(DFT) | 0.8556 | 0.8409 | 0.0147 | -0.0058 | 0.2785 | 0.2217 | 4.2665 | 0.9222 | 58.0875 | 0.8234 | 0.0323 | 0.3081 | 0.2473 | 5.2205 | 0.9063 | 82.4216 | 9.3903 | -16.4927 | 8.9558 | -14.8896 | 9.0947 | -17.2981 |
| 3 | 5 B | ZPE(HF) α(HF) G(HF) ω(DFT) | 0.8556 | 0.8409 | 0.0147 | -0.0126 | 0.2785 | 0.2217 | 4.2665 | 0.9222 | 58.0875 | 0.8234 | 0.0323 | 0.3081 | 0.2473 | 5.2205 | 0.9063 | 82.3447 | 9.4113 | -17.9045 | 9.3193 | -14.3879 | 9.6208 | -16.9113 |
| 4 | 5 B | ZPE(HF) α(HF) H(DFT) ω(DFT) | 0.8556 | 0.8409 | 0.0147 | -0.0128 | 0.2785 | 0.2217 | 4.2671 | 0.9222 | 58.0785 | 0.8234 | 0.0323 | 0.3081 | 0.2473 | 5.2209 | 0.9062 | 82.54 | 9.3874 | -17.2651 | 9.5261 | -14.3058 | 9.1842 | -17.9715 |
| 5 | 5 B | E(DFT) ZPE(HF) α(HF) ω(DFT) | 0.8556 | 0.8409 | 0.0147 | -0.006 | 0.2785 | 0.2217 | 4.2671 | 0.9222 | 58.0784 | 0.8234 | 0.0323 | 0.3081 | 0.2473 | 5.2209 | 0.9062 | 82.3834 | 9.3961 | -17.2179 | 9.4528 | -14.3505 | 9.436 | -17.2076 |
| 6 | 5 B | ZPE(DFT) α(HF) H(HF) ω(DFT) | 0.8556 | 0.8409 | 0.0147 | -0.013 | 0.2785 | 0.2219 | 4.2671 | 0.9222 | 58.0777 | 0.8234 | 0.0323 | 0.3081 | 0.2475 | 5.2205 | 0.9063 | 82.3237 | 9.5238 | -17.5711 | 8.9747 | -14.931 | 9.3463 | -17.0965 |
| 7 | 5 B | E(HF) ZPE(DFT) α(HF) ω(DFT) | 0.8556 | 0.8409 | 0.0147 | -0.0051 | 0.2785 | 0.2219 | 4.2671 | 0.9222 | 58.0777 | 0.8234 | 0.0323 | 0.3081 | 0.2475 | 5.2205 | 0.9063 | 82.4287 | 8.6797 | -18.2082 | 9.6327 | -13.9091 | 9.2275 | -17.8922 |
| 8 | 5 B | ZPE(DFT) α(HF) G(HF) ω(DFT) | 0.8556 | 0.8409 | 0.0147 | -0.013 | 0.2785 | 0.2219 | 4.2671 | 0.9222 | 58.0776 | 0.8234 | 0.0323 | 0.3081 | 0.2475 | 5.2205 | 0.9063 | 82.4211 | 9.3437 | -17.2644 | 9.1287 | -14.7113 | 8.9337 | -18.365 |
| 9 | 5 B | ZPE(DFT) α(HF) H(DFT) ω(DFT) | 0.8556 | 0.8409 | 0.0147 | -0.0132 | 0.2786 | 0.2219 | 4.2677 | 0.9222 | 58.0689 | 0.8234 | 0.0323 | 0.3081 | 0.2475 | 5.221 | 0.9062 | 82.5254 | 9.2568 | -17.9588 | 9.3693 | -14.4337 | 9.3347 | -17.9458 |
| 10 | 5 B | E(DFT) ZPE(DFT) α(HF) ω(DFT) | 0.8556 | 0.8409 | 0.0147 | -0.0054 | 0.2786 | 0.2219 | 4.2677 | 0.9222 | 58.0689 | 0.8234 | 0.0323 | 0.3081 | 0.2475 | 5.221 | 0.9062 | 82.4033 | 9.6273 | -17.0431 | 8.8338 | -15.1454 | 8.8855 | -17.7591 |
| 11 | 4 A B | α(DFT) G(DFT) | 0.8427 | 0.8301 | 0.0126 | 0.0568 | 0.2907 | 0.2322 | 4.6494 | 0.9146 | 66.9611 | 0.8087 | 0.034 | 0.3206 | 0.2556 | 5.6529 | 0.8966 | 81.2269 | 7.2029 | -14.57 | 7.7298 | -11.8073 | 7.1488 | -15.0545 |
| 12 | 4 A B | α(DFT) G(HF) | 0.8427 | 0.8301 | 0.0126 | 0.057 | 0.2908 | 0.2322 | 4.6495 | 0.9146 | 66.9591 | 0.8087 | 0.034 | 0.3206 | 0.2556 | 5.6529 | 0.8966 | 81.0198 | 7.2075 | -14.6334 | 7.0132 | -12.6962 | 7.3901 | -14.4989 |
| 13 | 4 A B | E(HF) α(DFT) | 0.8427 | 0.8301 | 0.0126 | 0.0571 | 0.2908 | 0.2322 | 4.6495 | 0.9146 | 66.9591 | 0.8087 | 0.034 | 0.3206 | 0.2556 | 5.6529 | 0.8966 | 81.2104 | 7.3324 | -14.2897 | 7.5168 | -12.1001 | 7.1676 | -15.0708 |
| 14 | 4 A B | α(DFT) H(HF) | 0.8427 | 0.8301 | 0.0126 | 0.0571 | 0.2908 | 0.2322 | 4.6495 | 0.9146 | 66.9591 | 0.8087 | 0.034 | 0.3206 | 0.2556 | 5.6529 | 0.8966 | 81.1743 | 7.3723 | -14.6163 | 7.2829 | -12.2511 | 7.5303 | -14.7383 |
| 15 | 4 A B | α(HF) G(DFT) | 0.841 | 0.8283 | 0.0127 | 0.062 | 0.2923 | 0.2322 | 4.698 | 0.9137 | 66.1382 | 0.8093 | 0.0317 | 0.3201 | 0.2545 | 5.636 | 0.8972 | 81.0572 | 7.5696 | -14.7107 | 7.2765 | -12.361 | 7.559 | -14.1057 |
| 16 | 4 A B | E(DFT) α(HF) | 0.841 | 0.8283 | 0.0127 | 0.062 | 0.2923 | 0.2322 | 4.698 | 0.9137 | 66.1381 | 0.8093 | 0.0317 | 0.3201 | 0.2545 | 5.636 | 0.8972 | 81.0187 | 7.3729 | -14.0706 | 7.4222 | -12.106 | 7.4395 | -14.2605 |
| 17 | 4 A B | α(HF) H(DFT) | 0.841 | 0.8283 | 0.0127 | 0.062 | 0.2923 | 0.2322 | 4.698 | 0.9137 | 66.1381 | 0.8093 | 0.0317 | 0.3201 | 0.2545 | 5.636 | 0.8972 | 81.224 | 7.421 | -14.6799 | 7.3817 | -12.1841 | 7.0671 | -14.694 |
| 18 | 4 A B | α(HF) G(HF) | 0.841 | 0.8283 | 0.0127 | 0.0622 | 0.2923 | 0.2322 | 4.6984 | 0.9137 | 66.131 | 0.8093 | 0.0317 | 0.3201 | 0.2545 | 5.6365 | 0.8972 | 80.9622 | 7.2805 | -14.7264 | 7.1913 | -12.3563 | 7.3962 | -14.4851 |
| 19 | 4 A B | E(HF) α(HF) | 0.841 | 0.8283 | 0.0127 | 0.0622 | 0.2923 | 0.2322 | 4.6984 | 0.9137 | 66.131 | 0.8093 | 0.0317 | 0.3201 | 0.2545 | 5.6365 | 0.8972 | 81.0574 | 7.2636 | -13.8287 | 7.4784 | -11.9683 | 7.6702 | -13.5742 |
| 20 | 4 A B | α(HF) H(HF) | 0.841 | 0.8283 | 0.0127 | 0.0622 | 0.2923 | 0.2322 | 4.6984 | 0.9137 | 66.131 | 0.8093 | 0.0317 | 0.3201 | 0.2545 | 5.6365 | 0.8972 | 81.1865 | 7.197 | -14.5109 | 7.3825 | -12.1452 | 7.5722 | -14.1719 |
| 21 | 3 B | α(HF) G(HF) | 0.8226 | 0.8122 | 0.0104 | -0.0616 | 0.3087 | 0.2511 | 5.2423 | 0.9027 | 78.8438 | 0.7953 | 0.0274 | 0.3317 | 0.2718 | 6.0508 | 0.8888 | 79.3255 | 5.2646 | -12.1232 | 5.2372 | -10.3206 | 5.4628 | -11.4633 |
| 22 | 3 B | E(HF) α(HF) | 0.8226 | 0.8122 | 0.0104 | -0.0616 | 0.3087 | 0.2511 | 5.2423 | 0.9027 | 78.8437 | 0.7953 | 0.0274 | 0.3317 | 0.2718 | 6.0508 | 0.8888 | 79.2389 | 5.4707 | -11.7586 | 5.43 | -10.0544 | 5.6589 | -12.1434 |
| 23 | 3 B | α(HF) H(HF) | 0.8226 | 0.8122 | 0.0104 | -0.0616 | 0.3087 | 0.2511 | 5.2423 | 0.9027 | 78.8437 | 0.7953 | 0.0274 | 0.3317 | 0.2718 | 6.0508 | 0.8888 | 78.98 | 5.5956 | -11.9023 | 5.3094 | -10.2686 | 5.2861 | -11.807 |
| 24 | 3 B | α(HF) G(DFT) | 0.8226 | 0.8122 | 0.0104 | -0.0623 | 0.3087 | 0.2511 | 5.2423 | 0.9027 | 78.8432 | 0.7953 | 0.0274 | 0.3317 | 0.2718 | 6.0511 | 0.8888 | 78.9704 | 5.2489 | -11.7116 | 5.7525 | -9.7798 | 5.4463 | -12.1245 |
| 25 | 3 B | E(DFT) α(HF) | 0.8226 | 0.8122 | 0.0104 | -0.0623 | 0.3087 | 0.2511 | 5.2423 | 0.9027 | 78.8432 | 0.7953 | 0.0274 | 0.3317 | 0.2718 | 6.0511 | 0.8888 | 79.041 | 5.4972 | -11.4816 | 5.5604 | -9.9507 | 5.6268 | -11.8759 |
| 26 | 3 B | α(HF) H(DFT) | 0.8226 | 0.8122 | 0.0104 | -0.0623 | 0.3087 | 0.2511 | 5.2423 | 0.9027 | 78.8432 | 0.7953 | 0.0274 | 0.3317 | 0.2718 | 6.0511 | 0.8888 | 79.1114 | 5.6063 | -11.6946 | 5.3268 | -10.1908 | 5.6146 | -11.8787 |
| 27 | 3 B | α(HF) w(HF) | 0.8203 | 0.8097 | 0.0106 | -0.0852 | 0.3108 | 0.2497 | 5.3117 | 0.9013 | 77.5924 | 0.7882 | 0.0321 | 0.3374 | 0.2715 | 6.2609 | 0.8851 | 78.6687 | 5.5565 | -10.5766 | 5.6684 | -9.8096 | 5.4173 | -10.6125 |
| 28 | 3 B | α(DFT) H(HF) | 0.8203 | 0.8097 | 0.0106 | -0.0652 | 0.3108 | 0.2566 | 5.3121 | 0.9013 | 77.5847 | 0.7868 | 0.0334 | 0.3384 | 0.2804 | 6.3001 | 0.8838 | 78.525 | 5.39 | -11.9745 | 5.3943 | -10.2041 | 5.6555 | -11.4769 |
| 29 | 3 B | α(HF) ω(DFT) | 0.8197 | 0.8091 | 0.0106 | -0.0915 | 0.3113 | 0.2477 | 5.3297 | 0.9009 | 77.2724 | 0.7874 | 0.0323 | 0.338 | 0.2687 | 6.2838 | 0.8846 | 78.5995 | 5.1159 | -11.3097 | 5.6503 | -9.8571 | 5.4377 | -10.9608 |
| 30 | 3 B | ELUMO(HF) α(HF) | 0.8187 | 0.8081 | 0.0107 | -0.1717 | 0.3121 | 0.2517 | 5.358 | 0.9003 | 76.775 | 0.7871 | 0.0316 | 0.3383 | 0.2733 | 6.2934 | 0.8847 | 78.6223 | 5.7644 | -10.5549 | 5.504 | -9.9898 | 5.5432 | -10.937 |
| 31 | 2 B | α(DFT) | 0.8062 | 0.7987 | 0.0075 | -0.3609 | 0.3227 | 0.261 | 5.7279 | 0.8927 | 108.1576 | 0.7753 | 0.0309 | 0.3475 | 0.2801 | 6.6423 | 0.8774 | 77.2682 | 3.6268 | -8.7513 | 3.6921 | -7.7965 | 4.1373 | -7.9516 |
| 32 | 2 B | α(HF) | 0.8039 | 0.7963 | 0.0075 | -0.3489 | 0.3246 | 0.2621 | 5.7964 | 0.8913 | 106.5719 | 0.7745 | 0.0294 | 0.3481 | 0.2806 | 6.6646 | 0.8771 | 77.1099 | 3.4876 | -8.8932 | 3.9033 | -7.5771 | 3.7341 | -8.3744 |
| 33 | 2 B | V | 0.7775 | 0.7689 | 0.0086 | -0.3864 | 0.3458 | 0.2786 | 6.5772 | 0.8748 | 90.8333 | 0.7357 | 0.0417 | 0.3768 | 0.3002 | 7.8104 | 0.8537 | 73.8961 | 3.9593 | -8.4216 | 3.6482 | -7.8054 | 3.7838 | -8.3206 |
| 34 | 2 A | E(CORR) | 0.6663 | 0.6535 | 0.0128 | -0.0469 | 0.4235 | 0.324 | 9.863 | 0.7997 | 51.9114 | 0.6262 | 0.0401 | 0.4482 | 0.3439 | 11.0481 | 0.7778 | 63.1803 | 3.7906 | -8.077 | 3.6687 | -7.8873 | 3.7547 | -8.116 |
| 35 | 2 A | G(CORR) | 0.6663 | 0.6534 | 0.0128 | -0.0472 | 0.4235 | 0.3243 | 9.8631 | 0.7997 | 51.9103 | 0.6262 | 0.0401 | 0.4482 | 0.3442 | 11.0481 | 0.7778 | 63.0536 | 3.6744 | -8.2492 | 3.6017 | -7.9411 | 3.6238 | -8.2859 |
| 36 | 2 A | H(CORR) | 0.6663 | 0.6534 | 0.0128 | -0.0469 | 0.4235 | 0.324 | 9.8635 | 0.7997 | 51.9076 | 0.6262 | 0.0401 | 0.4482 | 0.3439 | 11.0486 | 0.7778 | 63.0818 | 3.5532 | -8.3906 | 3.4953 | -8.0766 | 3.5333 | -8.4475 |
| 37 | 2 A | α(HF) | 0.6307 | 0.6165 | 0.0142 | 0.08 | 0.4455 | 0.3559 | 10.9138 | 0.7736 | 44.4102 | 0.5876 | 0.0431 | 0.4708 | 0.3772 | 12.1885 | 0.7495 | 58.2455 | 3.5171 | -8.6368 | 3.5781 | -7.9698 | 3.7361 | -8.0079 |
| 38 | 2 A | α(DFT) | 0.6288 | 0.6145 | 0.0143 | 0.057 | 0.4466 | 0.3554 | 10.9709 | 0.7721 | 44.0433 | 0.5858 | 0.043 | 0.4718 | 0.3766 | 12.2408 | 0.7481 | 58.1714 | 3.9752 | -7.8969 | 3.5099 | -8.0793 | 3.7709 | -8.0747 |
| 39 | 2 A | V | 0.5933 | 0.5777 | 0.0156 | 0.0196 | 0.4675 | 0.3699 | 12.0192 | 0.7448 | 37.9344 | 0.5497 | 0.0436 | 0.4919 | 0.3911 | 13.3084 | 0.7201 | 54.4296 | 3.5498 | -8.7549 | 3.5549 | -7.9668 | 3.6639 | -8.2305 |
| 40 | 2 A | α(CORR) | 0.5786 | 0.5624 | 0.0162 | -0.0651 | 0.4759 | 0.3776 | 12.4545 | 0.7331 | 35.6999 | 0.5303 | 0.0483 | 0.5024 | 0.3993 | 13.8811 | 0.7063 | 53.1923 | 3.5469 | -8.3486 | 3.6452 | -7.8343 | 3.6156 | -8.1383 |
| 41 | 1 | α(HF) | 0.2126 | 0.1977 | 0.0149 | 0.4611 | 0.6505 | 0.5416 | 23.2727 | 0.3506 | 14.3078 | 0.1012 | 0.1114 | 0.695 | 0.5689 | 26.5652 | 0.2991 | 11.2279 | 1.7364 | -6.1046 | 1.9031 | -5.681 | 1.7903 | -6.2162 |
| 42 | 1 | A | 0.2047 | 0.1897 | 0.015 | 0.4524 | 0.6538 | 0.5259 | 23.5065 | 0.3398 | 13.6385 | 0.1238 | 0.0808 | 0.6862 | 0.5488 | 25.896 | 0.2856 | 13.3642 | 2.0134 | -5.6518 | 1.7906 | -5.7406 | 1.8629 | -5.7942 |
| 43 | 1 | G(DFT) | 0.2 | 0.1849 | 0.0151 | 0.4472 | 0.6557 | 0.5202 | 23.6449 | 0.3333 | 13.2483 | 0.1369 | 0.0631 | 0.681 | 0.5415 | 25.5085 | 0.305 | 13.9912 | 1.7944 | -6.0994 | 1.7847 | -5.8458 | 1.652 | -6.4468 |
| 44 | 1 | E(DFT) | 0.2 | 0.1849 | 0.01 | | | | | | | | | | | | | | | | | | | |

Table S12_0.00001. Same as Table S4_0.00001 but for models developed using combined quantum mechanical descriptors and LSER's adsorbate descriptors.

| S.No. | Size | Variables | R ² | R ² _{adj} | R ² -R ² _{adj} | ΔK | RMSE(tr) | MAE(tr) | RSS(tr) | CCC(tr) | F | Q ² _{loo} | R ² -Q ² _{loo} | RMSE(ev) | MAE(ev) | PRESS(ev) | CCC(ev) | Q ² _{LMO} | R ² _{Yscr} | Q ² _{Yscr} | R ² _{Xrd} | Q ² _{Xrd} | R ² _{Yrd} | Q ² _{Yrd} | N. ext. OK | RMSE(ext) | MAE(ext) | PRESS(ext) | Q ² _{F1} | Q ² _{F2} | Q ² _{F3} | CCC(ext) | F _m ² | Δ r _m ² |
|-------|------|---|----------------|-------------------------------|---|---------|----------|---------|---------|---------|----------|-------------------------------|---|----------|---------|-----------|---------|-------------------------------|--------------------------------|--------------------------------|-------------------------------|-------------------------------|-------------------------------|-------------------------------|------------|-----------|----------|------------|------------------------------|------------------------------|------------------------------|----------|-----------------------------|-------------------------------|
| 1 | 5 | B E(HF) ZPE(CORR) E ^{LUMO} (DFT) - E ^{LUMO} (DFT) H(HF) | 0.9054 | 0.8922 | 0.0131 | -0.0549 | 0.2346 | 0.1792 | 2.3116 | 0.9503 | 68.8908 | 0.8657 | 0.0397 | 0.2795 | 0.212 | 3.2817 | 0.9306 | 87.2035 | 12.3805 | -22.7052 | 11.5451 | -20.9251 | 12.1784 | -23.035 | 0 | 0.6942 | 0.419 | 6.2655 | -0.2199 | -0.2305 | 0.1714 | 0.6632 | 0.2785 | 0.4023 |
| 2 | 5 | B E(HF) ZPE(CORR) H(HF) η(DFT) | 0.9054 | 0.8922 | 0.0131 | -0.0549 | 0.2346 | 0.1792 | 2.3116 | 0.9503 | 68.8908 | 0.8657 | 0.0397 | 0.2795 | 0.212 | 3.2817 | 0.9306 | 87.3107 | 12.3685 | -22.2561 | 12.445 | -19.3818 | 12.5242 | -22.069 | 0 | 0.6942 | 0.419 | 6.2655 | -0.2199 | -0.2305 | 0.1714 | 0.6632 | 0.2785 | 0.4023 |
| 3 | 5 | B E(HF) ZPE(CORR) E ^{LUMO} (CORR) H(HF) | 0.905 | 0.8918 | 0.0132 | -0.032 | 0.2351 | 0.1926 | 2.3213 | 0.9501 | 68.5729 | 0.8666 | 0.0384 | 0.2786 | 0.2273 | 3.2592 | 0.9309 | 87.8045 | 11.9721 | -22.2937 | 12.2597 | -19.9169 | 12.0043 | -22.3587 | 0 | 0.7802 | 0.4745 | 7.9138 | -0.5408 | -0.5542 | -0.0466 | 0.6323 | 0.2209 | 0.4558 |
| 4 | 5 | B E(HF) ZPE(CORR) E ^{LUMO} (DFT) H(HF) | 0.9048 | 0.8916 | 0.0132 | -0.0329 | 0.2353 | 0.193 | 2.3258 | 0.95 | 68.427 | 0.8654 | 0.0394 | 0.2798 | 0.2285 | 3.289 | 0.9303 | 87.7846 | 12.6701 | -21.733 | 11.9437 | -20.3509 | 12.2176 | -22.1422 | 0 | 0.7787 | 0.4685 | 7.8829 | -0.5348 | -0.5482 | -0.0425 | 0.6331 | 0.223 | 0.4539 |
| 5 | 5 | B E(HF) ZPE(CORR) H(HF) χ(CORR) | 0.9026 | 0.8891 | 0.0135 | -0.0182 | 0.238 | 0.192 | 2.3791 | 0.9488 | 66.7332 | 0.861 | 0.0416 | 0.2843 | 0.2271 | 3.3951 | 0.9281 | 87.3853 | 12.4579 | -22.0361 | 11.8732 | -20.5198 | 12.37 | -22.0413 | 0 | 0.7442 | 0.4604 | 7.2004 | -0.4019 | -0.4141 | 0.0478 | 0.6436 | 0.2442 | 0.4313 |
| 6 | 5 | B E(HF) ZPE(CORR) H(HF) ω(DFT) | 0.9014 | 0.8877 | 0.0137 | -0.035 | 0.2395 | 0.194 | 2.4086 | 0.9481 | 65.8293 | 0.8626 | 0.0388 | 0.2827 | 0.2269 | 3.3575 | 0.9288 | 87.4026 | 12.5024 | -21.7834 | 11.8962 | -20.4699 | 12.0554 | -22.818 | 0 | 0.793 | 0.4699 | 8.1756 | -0.5918 | -0.6057 | -0.0812 | 0.6263 | 0.2178 | 0.4564 |
| 7 | 5 | B E(HF) ZPE(CORR) H(HF) η(CORR) | 0.9004 | 0.8866 | 0.0138 | -0.0414 | 0.2407 | 0.197 | 2.4333 | 0.9476 | 65.0866 | 0.8623 | 0.0381 | 0.283 | 0.2324 | 3.3646 | 0.9285 | 87.2184 | 12.4551 | -21.6473 | 12.2286 | -19.9826 | 12.2447 | -22.3009 | 0 | 0.8161 | 0.4902 | 8.6575 | -0.6856 | -0.7003 | -0.1449 | 0.619 | 0.2 | 0.4757 |
| 8 | 5 | B E(HF) ZPE(CORR) E ^{LUMO} (CORR) - E ^{LUMO} (CORR) H(HF) | 0.9004 | 0.8866 | 0.0138 | -0.0414 | 0.2407 | 0.197 | 2.4333 | 0.9476 | 65.0866 | 0.8623 | 0.0381 | 0.283 | 0.2324 | 3.3646 | 0.9285 | 87.1907 | 12.3759 | -22.7603 | 12.4054 | -19.7746 | 12.2777 | -21.7835 | 0 | 0.8161 | 0.4902 | 8.6575 | -0.6856 | -0.7003 | -0.1449 | 0.619 | 0.2 | 0.4757 |
| 9 | 5 | A B d(CORR) α(DFT) ω(DFT) | 0.8965 | 0.8821 | 0.0144 | 0.011 | 0.2454 | 0.1948 | 2.5288 | 0.9454 | 62.3556 | 0.8605 | 0.036 | 0.2848 | 0.2277 | 3.4078 | 0.9267 | 86.0949 | 12.0725 | -24.8031 | 12.5755 | -19.3911 | 11.8599 | -24.5044 | 0 | 0.4845 | 0.3758 | 3.0516 | 0.4059 | 0.4007 | 0.5964 | 0.7347 | 0.5333 | 0.1461 |
| 10 | 5 | P B E ^{LUMO} (CORR) α(DFT) ω(DFT) | 0.8931 | 0.8782 | 0.0148 | -0.1186 | 0.2494 | 0.207 | 2.6117 | 0.9435 | 60.148 | 0.8618 | 0.0313 | 0.2836 | 0.2381 | 3.3768 | 0.9278 | 85.8355 | 12.1045 | -23.1189 | 12.3415 | -19.7741 | 12.1412 | -22.5562 | 0 | 0.4492 | 0.3663 | 2.6231 | 0.4893 | 0.4848 | 0.6531 | 0.7315 | 0.5468 | 0.0907 |
| 11 | 4 | P B α(HF) ω(DFT) | 0.8825 | 0.8698 | 0.0127 | -0.1242 | 0.2615 | 0.2229 | 2.8712 | 0.9376 | 69.4553 | 0.8499 | 0.0326 | 0.2955 | 0.2525 | 3.668 | 0.9214 | 84.67 | 9.6471 | -19.36 | 9.9586 | -16.2517 | 9.6349 | -19.4944 | 0 | 0.4638 | 0.3814 | 2.7964 | 0.4555 | 0.4508 | 0.6302 | 0.7128 | 0.5557 | 0.1255 |
| 12 | 4 | B d(CORR) α(HF) ω(HF) | 0.8824 | 0.8697 | 0.0127 | -0.0694 | 0.2615 | 0.2208 | 2.8719 | 0.9376 | 69.4351 | 0.8537 | 0.0287 | 0.2917 | 0.2387 | 3.5731 | 0.9232 | 84.7825 | 9.746 | -18.9813 | 9.7371 | -16.709 | 9.8767 | -18.4492 | 0 | 0.4647 | 0.3747 | 2.8077 | 0.4533 | 0.4486 | 0.6287 | 0.7363 | 0.5625 | 0.0316 |
| 13 | 4 | P B α(DFT) ω(DFT) | 0.8824 | 0.8697 | 0.0127 | -0.1292 | 0.2615 | 0.2203 | 2.8721 | 0.9375 | 69.4295 | 0.8488 | 0.0336 | 0.2966 | 0.2521 | 3.694 | 0.9207 | 84.4736 | 9.7461 | -18.4182 | 9.8226 | -16.3779 | 9.5136 | -20.0169 | 0 | 0.4708 | 0.3889 | 2.8814 | 0.439 | 0.4341 | 0.6189 | 0.7106 | 0.5609 | 0.098 |
| 14 | 4 | B E ^{LUMO} (DFT) α(DFT) ω(DFT) | 0.8816 | 0.8688 | 0.0128 | -0.1179 | 0.2624 | 0.2057 | 2.8928 | 0.9371 | 68.8665 | 0.8533 | 0.0283 | 0.2921 | 0.2296 | 3.5846 | 0.9228 | 84.6308 | 9.68 | -20.3936 | 9.5391 | -16.9931 | 9.4562 | -20.1909 | 1 | 0.413 | 0.3456 | 2.2176 | 0.5682 | 0.5645 | 0.7067 | 0.763 | 0.5894 | 0.1483 |
| 15 | 4 | B d(CORR) E ^{LUMO} (HF) α(HF) | 0.8807 | 0.8678 | 0.0129 | -0.1091 | 0.2634 | 0.2019 | 2.9148 | 0.9366 | 68.2766 | 0.853 | 0.0277 | 0.2924 | 0.227 | 3.5913 | 0.9229 | 84.6099 | 9.7467 | -19.7493 | 9.9337 | -16.3141 | 9.6609 | -20.2575 | 0 | 0.4505 | 0.3614 | 2.6381 | 0.4864 | 0.4819 | 0.6511 | 0.7352 | 0.5471 | 0.0575 |
| 16 | 4 | B d(CORR) α(DFT) ω(DFT) | 0.88 | 0.8671 | 0.013 | -0.0792 | 0.2642 | 0.2069 | 2.931 | 0.9362 | 67.8487 | 0.8485 | 0.0315 | 0.2969 | 0.2332 | 3.7014 | 0.9203 | 84.0613 | 10.3131 | -19.4368 | 9.3573 | -17.1504 | 9.7563 | -20.3365 | 0 | 0.4786 | 0.3731 | 2.9784 | 0.4201 | 0.4151 | 0.6061 | 0.7252 | 0.5545 | 0.0479 |
| 17 | 4 | B d(CORR) E ^{LUMO} (HF) α(DFT) | 0.8799 | 0.8669 | 0.013 | -0.1134 | 0.2643 | 0.2061 | 2.9346 | 0.9361 | 67.7543 | 0.8507 | 0.0292 | 0.2947 | 0.2336 | 3.6473 | 0.9216 | 84.108 | 9.584 | -20.0651 | 9.6563 | -16.7313 | 9.1976 | -20.3286 | 0 | 0.4691 | 0.38 | 2.8603 | 0.4431 | 0.4382 | 0.6217 | 0.725 | 0.5311 | 0.0013 |
| 18 | 4 | B d(CORR) α(DFT) χ(DFT) | 0.8796 | 0.8666 | 0.013 | -0.083 | 0.2646 | 0.2108 | 2.9409 | 0.936 | 67.5894 | 0.8493 | 0.0303 | 0.2962 | 0.2379 | 3.6822 | 0.9206 | 84.2119 | 9.5874 | -19.1878 | 9.5333 | -16.8243 | 9.6374 | -19.4079 | 0 | 0.4872 | 0.3883 | 3.0859 | 0.3992 | 0.3939 | 0.5919 | 0.7201 | 0.5475 | 0.0693 |
| 19 | 4 | B E ^{LUMO} (CORR) α(HF) ω(DFT) | 0.8794 | 0.8664 | 0.013 | -0.1126 | 0.2648 | 0.2096 | 2.9452 | 0.9359 | 67.4757 | 0.849 | 0.0304 | 0.2964 | 0.2356 | 3.6891 | 0.9208 | 84.4049 | 10.1447 | -17.7892 | 9.9959 | -16.303 | 9.541 | -19.798 | 1 | 0.4006 | 0.3318 | 2.0865 | 0.5937 | 0.5902 | 0.7241 | 0.7672 | 0.6122 | 0.2281 |
| 20 | 4 | B d(CORR) E ^{LUMO} (DFT) α(DFT) | 0.8788 | 0.8657 | 0.0131 | -0.0647 | 0.2655 | 0.2129 | 2.9603 | 0.9355 | 67.0849 | 0.8482 | 0.0306 | 0.2962 | 0.2341 | 3.7087 | 0.9201 | 83.8608 | 10.2064 | -19.1367 | 9.6533 | -16.6475 | 9.9321 | -19.6153 | 0 | 0.4796 | 0.3904 | 2.9904 | 0.4178 | 0.4127 | 0.6045 | 0.7235 | 0.5406 | 0.0489 |
| 21 | 3 | B α(HF) ω(DFT) | 0.8681 | 0.8577 | 0.0104 | -0.1119 | 0.277 | 0.2241 | 3.2215 | 0.9294 | 83.3885 | 0.8365 | 0.0316 | 0.3084 | 0.2499 | 3.9934 | 0.9136 | 83.4331 | 7.8584 | -14.5884 | 7.3501 | -13.421 | 7.3536 | -15.6945 | 0 | 0.4248 | 0.3449 | 2.3461 | 0.5432 | 0.5392 | 0.6895 | 0.7463 | 0.6163 | 0.2251 |
| 22 | 3 | B α(HF) ω(HF) | 0.8678 | 0.8574 | 0.0104 | -0.2567 | 0.2773 | 0.2306 | 3.2297 | 0.9292 | 83.1446 | 0.833 | 0.0348 | 0.3117 | 0.2588 | 4.0805 | 0.9117 | 82.6482 | 7.1958 | -15.2379 | 7.4077 | -13.333 | 7.3261 | -15.0585 | 0 | 0.4209 | 0.3374 | 2.3025 | 0.5517 | 0.5478 | 0.6897 | 0.7462 | 0.6104 | 0.2277 |
| 23 | 3 | B α(DFT) ω(DFT) | 0.8665 | 0.8559 | 0.0105 | -0.119 | 0.2787 | 0.2268 | 3.2618 | 0.9285 | 82.2014 | 0.8308 | 0.0357 | 0.3137 | 0.2554 | 4.134 | 0.9104 | 82.6218 | 7.0428 | -15.8893 | 7.4386 | -13.1312 | 7.2642 | -15.3102 | 0 | 0.4349 | 0.3507 | 2.4591 | 0.5212 | 0.517 | 0.6748 | 0.7375 | 0.6123 | 0.1975 |
| 24 | 3 | B E ^{LUMO} (HF) α(HF) | 0.8662 | 0.8556 | 0.0106 | -0.1638 | 0.279 | 0.2263 | 3.2685 | 0.9283 | 82.0088 | 0.8314 | 0.0348 | 0.3131 | 0.2546 | 4.1185 | 0.9109 | 82.6604 | 7.2381 | -15.1371 | 7.2738 | -13.4543 | 7.3606 | -15.3166 | 0 | 0.4192 | 0.3307 | 2.284 | 0.5553 | 0.5514 | 0.698 | 0.7365 | 0.5577 | 0.2513 |
| 25 | 3 | B α(HF) χ(HF) | 0.8654 | 0.8548 | 0.0106 | -0.0836 | 0.2798 | 0.2324 | 3.2887 | 0.9278 | 81.4262 | 0.8296 | 0.0358 | 0.3148 | 0.2609 | 4.1626 | 0.9099 | 82.67 | 7.2249 | -15.3726 | 7.2415 | -13.5438 | 6.9063 | -15.635 | 0 | 0.4205 | 0.3396 | 2.2992 | 0.5523 | 0.5484 | 0.6959 | 0.7452 | 0.6048 | 0.2299 |
| 26 | 3 | B α(HF) χ(DFT) | 0.8649 | 0.8543 | 0.0107 | -0.0501 | 0.2803 | 0.2307 | 3.2993 | 0.9276 | 81.1252 | 0.831 | 0.034 | 0.3135 | 0.258 | 4.1291 | 0.9105 | 82.6878 | 6.8935 | -15.5272 | 7.6544 | -13.0466 | 7.6446 | -14.3003 | 0 | 0.4254 | 0.3436 | 2.3531 | 0.5418 | 0.5379 | 0.6888 | 0.7395 | 0.603 | 0.2298 |
| 27 | 3 | B E ^{LUMO} (CORR) - E ^{LUMO} (DFT) α(HF) | 0.8634 | 0.8526 | 0.0108 | -0.1095 | 0.2819 | 0.2315 | 3.3374 | 0.9267 | 80.0538 | 0.8297 | 0.0337 | 0.3147 | 0.2587 | 4.1603 | 0.9097 | 82.3448 | 7.2558 | -15.2188 | 7.1749 | -13.6555 | 7.5039 | -14.8976 | 0 | 0.4299 | 0.3478 | 2.4024 | 0.5322 | 0.5282 | 0.6823 | 0.7386 | 0.6162 | 0.2255 |
| 28 | 3 | B α(HF) η(CORR) | 0.8634 | 0.8526 | 0.0108 | -0.1095 | 0.2819 | 0.2315 | 3.3374 | 0.9267 | 80.0538 | 0.8297 | 0.0337 | 0.3147 | 0.2587 | 4.1603 | 0.9097 | 82.5463 | 7.1521 | -15.4353 | 7.4419 | -13.294 | 7.2799 | -15.2286 | 0 | 0.4299 | 0.3478 | 2.4024 | 0.5322 | 0.5282 | 0.6823 | 0.7386 | 0.6162 | 0.2255 |
| 29 | 3 | B E ^{LUMO} (DFT) α(HF) | 0.8633 | 0.8525 | 0.0108 | -0.1331 | 0.282 | 0.2306 | 3.3406 | 0.9266 | 79.9657 | 0.8284 | 0.0348 | 0.3159 | 0.2583 | 4.191 | 0.9092 | 82.5648 | 7.1784 | -15.9073 | 7.2693 | -13.5373 | 7.5654 | -15.0359 | 0 | 0.4276 | 0.345 | 2.3772 | 0.5371 | 0.5331 | 0.6856 | 0.7459 | 0.5967 | 0.2324 |
| 30 | 3 | B E ^{LUMO} (HF) α(HF) | 0.8632 | 0.8524 | 0.0108 | -0.0969 | 0.2821 | 0.2336 | 3.342 | 0.9266 | 79.9253 | 0.8269 | 0.0363 | 0.3173 | 0.2621 | 4.2292 | 0.9084 | 82.4634 | 7.6826 | -14.5433 | 7.6058 | -13.1316 | 7.2978 | -15.0542 | 0 | 0.4204 | 0.3415 | 2.2981 | 0.5526 | 0.5487 | 0.6961 | 0.7435 | 0.5966 | 0.2332 |
| 31 | 2 | B α(DFT) | 0.8555 | 0.848 | 0.0074 | -0.3563 | 0.29 | 0.2391 | 3.5312 | 0.9221 | 115.4071 | 0.81 | | | | | | | | | | | | | | | | | | | | | | |

Table S13_0.00001. Same as Table S5_0.00001 but for models developed using combined quantum mechanical descriptors and LSER's adsorbate descriptors.

| S.No. | Size | Variables | R ² | R ² _{adj} | R ² -R ² _{adj} | ΔK | RMSE(tr) | MAE(tr) | RSS(tr) | CCC(tr) | F | Q ² _{loo} | R ² -Q ² _{loo} | RMSE(ev) | MAE(ev) | PRESS(ev) | CCC(ev) | Q ² _{LMO} | R ² _{Yser} | Q ² _{Yser} | R ² _{Xmd} | Q ² _{Xmd} | R ² _{Yrd} | Q ² _{Yrd} | N. ext. | OK | RMSE(ext) | MAE(ext) | PRESS(ext) | Q ² _{F1} | Q ² _{F2} | Q ² _{F3} | CCC(ext) | \bar{r}_m^2 | Δr ² _m |
|-------|------|---|----------------|-------------------------------|---|---------|----------|---------|---------|---------|---------|-------------------------------|---|----------|---------|-----------|---------|-------------------------------|--------------------------------|--------------------------------|-------------------------------|-------------------------------|-------------------------------|-------------------------------|---------|--------|-----------|----------|------------|------------------------------|------------------------------|------------------------------|----------|---------------|------------------------------|
| 1 | 5 | B E(HF) ZPE(CORR) E ^{HOMO} (DFT) - E ^{LUMO} (DFT) H(HF) | 0.8712 | 0.8511 | 0.0201 | -0.0533 | 0.2788 | 0.2096 | 2.9532 | 0.9312 | 43.2904 | 0.8102 | 0.061 | 0.3384 | 0.2517 | 4.3517 | 0.9012 | 81.5652 | 13.2986 | -28.5919 | 13.3082 | -22.6028 | 13.4998 | -27.5197 | 0 | 0.6207 | 0.3237 | 6.5493 | 0.0116 | 0.0116 | 0.3615 | 0.708 | 0.3986 | 0.3328 | |
| 2 | 5 | B E(HF) ZPE(CORR) H(HF) η(DFT) | 0.8712 | 0.8511 | 0.0201 | -0.0533 | 0.2788 | 0.2096 | 2.9532 | 0.9312 | 43.2904 | 0.8102 | 0.061 | 0.3384 | 0.2517 | 4.3517 | 0.9012 | 81.4779 | 14.1732 | -27.6126 | 12.4831 | -23.8284 | 13.3786 | -28.0914 | 0 | 0.6207 | 0.3237 | 6.5493 | 0.0116 | 0.0116 | 0.3615 | 0.708 | 0.3986 | 0.3328 | |
| 3 | 5 | B E(DFT) ZPE(CORR) H(DFT) η(DFT) | 0.8636 | 0.8423 | 0.0213 | -0.053 | 0.2868 | 0.2184 | 3.1265 | 0.9268 | 40.5371 | 0.798 | 0.0656 | 0.3491 | 0.2631 | 4.6312 | 0.8942 | 80.5725 | 13.5811 | -28.2406 | 13.4748 | -22.7927 | 14.1273 | -27.3889 | 0 | 0.5937 | 0.3312 | 5.9913 | 0.0958 | 0.0958 | 0.4159 | 0.7199 | 0.4175 | 0.3212 | |
| 4 | 5 | P B V E ^{HOMO} (HF) - E ^{LUMO} (HF) ω(DFT) | 0.8551 | 0.8325 | 0.0226 | -0.1099 | 0.2957 | 0.2307 | 3.3221 | 0.9219 | 37.7725 | 0.8025 | 0.0526 | 0.3452 | 0.2705 | 4.5284 | 0.8952 | 79.5254 | 13.7446 | -30.2953 | 13.3363 | -22.6207 | 13.6865 | -29.5307 | 1 | 0.408 | 0.3175 | 2.8297 | 0.573 | 0.5729 | 0.7241 | 0.7382 | 0.4375 | 0.2533 | |
| 5 | 5 | P B V η(HF) ω(DFT) | 0.8551 | 0.8325 | 0.0226 | -0.1099 | 0.2957 | 0.2307 | 3.3221 | 0.9219 | 37.7725 | 0.8025 | 0.0526 | 0.3452 | 0.2705 | 4.5284 | 0.8952 | 79.6371 | 13.4636 | -30.6221 | 13.429 | -22.782 | 13.276 | -31.9619 | 1 | 0.408 | 0.3175 | 2.8297 | 0.573 | 0.5729 | 0.7241 | 0.7382 | 0.4375 | 0.2533 | |
| 6 | 5 | P B V E ^{HOMO} (HF) ω(DFT) | 0.8546 | 0.8319 | 0.0227 | -0.1145 | 0.2962 | 0.2317 | 3.3332 | 0.9216 | 37.6258 | 0.8018 | 0.0528 | 0.3458 | 0.2722 | 4.5442 | 0.8948 | 79.4247 | 13.4731 | -30.1421 | 13.8076 | -21.9734 | 13.1149 | -32.2139 | 1 | 0.4071 | 0.3177 | 2.8178 | 0.5748 | 0.5747 | 0.7253 | 0.7412 | 0.4437 | 0.2442 | |
| 7 | 5 | R B α(HF) χ(DFT) ω(DFT) | 0.854 | 0.8312 | 0.0228 | -0.0973 | 0.2968 | 0.2341 | 3.348 | 0.9212 | 37.4305 | 0.7984 | 0.0556 | 0.3488 | 0.2758 | 4.6226 | 0.8929 | 79.3651 | 13.1398 | -30.0422 | 13.6076 | -22.5132 | 13.2665 | -29.9821 | 1 | 0.3492 | 0.2782 | 2.0735 | 0.6871 | 0.6871 | 0.7979 | 0.8164 | 0.5717 | 0.2249 | |
| 8 | 5 | B V d(DFT) χ(DFT) ω(DFT) | 0.8525 | 0.8294 | 0.0231 | -0.0994 | 0.2984 | 0.232 | 3.3829 | 0.9204 | 36.9785 | 0.7998 | 0.0526 | 0.3475 | 0.2727 | 4.5893 | 0.8937 | 79.3366 | 13.7697 | -28.8409 | 13.384 | -22.7656 | 13.7966 | -28.7655 | 1 | 0.3987 | 0.3289 | 2.7027 | 0.5921 | 0.5921 | 0.7365 | 0.7512 | 0.4662 | 0.256 | |
| 9 | 5 | B V d(HF) χ(DFT) ω(DFT) | 0.8516 | 0.8284 | 0.0232 | -0.0967 | 0.2992 | 0.2312 | 3.4029 | 0.9198 | 36.7238 | 0.7985 | 0.0531 | 0.3487 | 0.2707 | 4.6209 | 0.8931 | 79.3022 | 13.4817 | -30.545 | 13.1401 | -22.8782 | 13.533 | -29.8945 | 1 | 0.3802 | 0.3205 | 2.5622 | 0.6133 | 0.6133 | 0.7502 | 0.7634 | 0.4864 | 0.2684 | |
| 10 | 5 | P B ELUMO(HF) α(HF) ω(DFT) | 0.8509 | 0.8276 | 0.0233 | -0.0821 | 0.3 | 0.2412 | 3.4192 | 0.9194 | 36.5185 | 0.7987 | 0.0522 | 0.3485 | 0.2801 | 4.6162 | 0.8934 | 79.5638 | 13.7566 | -30.3723 | 13.1486 | -22.7465 | 13.3959 | -31.2315 | 3 | 0.3204 | 0.2448 | 1.7448 | 0.7367 | 0.7367 | 0.8299 | 0.8356 | 0.5577 | 0.2471 | |
| 11 | 4 | B V χ(DFT) ω(DFT) | 0.8461 | 0.8275 | 0.0187 | -0.1214 | 0.3047 | 0.2449 | 3.5282 | 0.9167 | 45.3657 | 0.7932 | 0.0529 | 0.3532 | 0.2853 | 4.7418 | 0.8899 | 79.0839 | 10.889 | -24.5721 | 11.1565 | -18.2896 | 10.4955 | -24.9163 | 1 | 0.3422 | 0.2772 | 1.9907 | 0.6996 | 0.6996 | 0.8059 | 0.8146 | 0.5489 | 0.256 | |
| 12 | 4 | B E ^{LUMO} (CORR) α(HF) ω(DFT) | 0.8392 | 0.8197 | 0.0195 | -0.107 | 0.3115 | 0.2615 | 3.6881 | 0.9125 | 43.0408 | 0.792 | 0.0472 | 0.3543 | 0.2983 | 4.7695 | 0.889 | 78.1258 | 10.7225 | -23.7315 | 10.9466 | -18.5141 | 11.0591 | -24.7002 | 4 | 0.2676 | 0.1887 | 1.2174 | 0.8163 | 0.8163 | 0.8813 | 0.8829 | 0.6138 | 0.1957 | |
| 13 | 4 | B E ^{LUMO} (DFT) α(HF) ω(DFT) | 0.8377 | 0.8181 | 0.0197 | -0.1078 | 0.3129 | 0.2622 | 3.7206 | 0.9117 | 42.5934 | 0.7885 | 0.0492 | 0.3572 | 0.2995 | 4.8489 | 0.8869 | 77.9568 | 10.8934 | -25.0554 | 11.2916 | -17.8735 | 11.2536 | -24.8406 | 4 | 0.2741 | 0.2029 | 1.2768 | 0.8073 | 0.8073 | 0.8755 | 0.8766 | 0.6075 | 0.2001 | |
| 14 | 4 | B E ^{LUMO} (CORR) α(DFT) ω(DFT) | 0.8377 | 0.8181 | 0.0197 | -0.1125 | 0.3129 | 0.2608 | 3.7209 | 0.9117 | 42.5882 | 0.7898 | 0.0479 | 0.3561 | 0.2992 | 4.8194 | 0.8876 | 77.6957 | 10.6803 | -24.4236 | 10.9851 | -18.5272 | 11.1817 | -24.4243 | 4 | 0.2701 | 0.1919 | 1.2401 | 0.8128 | 0.8128 | 0.8791 | 0.8865 | 0.6491 | 0.1863 | |
| 15 | 4 | P B α(HF) ω(DFT) | 0.8375 | 0.8178 | 0.0197 | -0.111 | 0.3132 | 0.26 | 3.7265 | 0.9116 | 42.5127 | 0.7867 | 0.0507 | 0.3587 | 0.2986 | 4.8899 | 0.886 | 78.1008 | 11.1374 | -24.5032 | 10.8698 | -18.8225 | 11.5455 | -24.0568 | 3 | 0.3117 | 0.2359 | 1.6518 | 0.7507 | 0.7507 | 0.839 | 0.8439 | 0.5744 | 0.2355 | |
| 16 | 4 | B E ^{LUMO} (DFT) α(DFT) ω(DFT) | 0.8372 | 0.8175 | 0.0197 | -0.1133 | 0.3134 | 0.2584 | 3.733 | 0.9114 | 42.4245 | 0.7898 | 0.0474 | 0.3561 | 0.2925 | 4.8193 | 0.8872 | 77.6866 | 10.9254 | -25.502 | 10.6622 | -19.0678 | 11.0958 | -24.2609 | 4 | 0.2682 | 0.1927 | 1.2225 | 0.8155 | 0.8155 | 0.8808 | 0.8869 | 0.6469 | 0.1845 | |
| 17 | 4 | P B E ^{LUMO} (HF) α(DFT) | 0.8356 | 0.8156 | 0.0199 | -0.143 | 0.315 | 0.2506 | 3.7703 | 0.9104 | 41.9231 | 0.7807 | 0.0549 | 0.3638 | 0.2916 | 5.029 | 0.8833 | 77.7326 | 11.0573 | -23.121 | 10.7078 | -18.6731 | 10.6396 | -24.8522 | 4 | 0.31 | 0.2359 | 1.6332 | 0.7535 | 0.7535 | 0.8408 | 0.8564 | 0.6234 | 0.2169 | |
| 18 | 4 | P B α(DFT) ω(DFT) | 0.8353 | 0.8153 | 0.02 | -0.1154 | 0.3153 | 0.2546 | 3.7733 | 0.9102 | 41.8301 | 0.7848 | 0.0549 | 0.3603 | 0.2905 | 4.9333 | 0.8845 | 77.5755 | 10.5988 | -25.5667 | 10.7642 | -18.8496 | 10.8972 | -24.4521 | 4 | 0.3042 | 0.2337 | 1.5728 | 0.6826 | 0.6826 | 0.8467 | 0.8578 | 0.617 | 0.2166 | |
| 19 | 4 | B α(DFT) η(CORR) ω(DFT) | 0.8342 | 0.8141 | 0.0201 | -0.1095 | 0.3163 | 0.264 | 3.8022 | 0.9096 | 41.5022 | 0.7807 | 0.0535 | 0.3638 | 0.305 | 5.0293 | 0.8825 | 77.5072 | 10.4581 | -24.0819 | 10.9081 | -18.7011 | 10.7462 | -22.8544 | 4 | 0.2906 | 0.1962 | 1.4357 | 0.7833 | 0.7833 | 0.86 | 0.8675 | 0.6223 | 0.2064 | |
| 20 | 4 | B E ^{HOMO} (CORR) - E ^{LUMO} (CORR) α(DFT) ω(DFT) | 0.8342 | 0.8141 | 0.0201 | -0.103 | 0.3163 | 0.264 | 3.8022 | 0.9096 | 41.5022 | 0.7807 | 0.0535 | 0.3638 | 0.305 | 5.0293 | 0.8825 | 77.7082 | 10.9565 | -23.9086 | 10.5986 | -19.0109 | 10.7515 | -23.9543 | 4 | 0.2906 | 0.1962 | 1.4357 | 0.7833 | 0.7833 | 0.86 | 0.8675 | 0.6223 | 0.2064 | |
| 21 | 3 | B α(HF) ω(DFT) | 0.8249 | 0.8095 | 0.0154 | -0.1339 | 0.325 | 0.2734 | 4.014 | 0.9041 | 53.4063 | 0.7748 | 0.0502 | 0.3686 | 0.3103 | 5.1641 | 0.8786 | 77.0302 | 7.9089 | -20.3403 | 8.1686 | -14.8245 | 8.0961 | -18.9459 | 4 | 0.2812 | 0.1939 | 1.3442 | 0.7971 | 0.7971 | 0.869 | 0.8747 | 0.6224 | 0.2017 | |
| 22 | 3 | B E ^{LUMO} (HF) α(DFT) | 0.8246 | 0.8091 | 0.0155 | -0.1868 | 0.3253 | 0.2689 | 4.0218 | 0.9039 | 53.28 | 0.7748 | 0.0498 | 0.3686 | 0.304 | 5.1639 | 0.8791 | 76.3649 | 8.0764 | -20.1114 | 8.4742 | -14.5399 | 7.9048 | -20.3721 | 4 | 0.299 | 0.2254 | 1.5193 | 0.7707 | 0.7707 | 0.8519 | 0.8681 | 0.6512 | 0.203 | |
| 23 | 3 | B E ^{LUMO} (HF) α(HF) | 0.8245 | 0.809 | 0.0155 | -0.1802 | 0.3255 | 0.273 | 4.0251 | 0.9038 | 53.2272 | 0.7735 | 0.0509 | 0.3697 | 0.3096 | 5.1924 | 0.8786 | 76.9051 | 7.839 | -19.909 | 8.238 | -14.8302 | 8.3099 | -20.0688 | 4 | 0.283 | 0.2062 | 1.3614 | 0.7945 | 0.7945 | 0.8673 | 0.8749 | 0.6251 | 0.2027 | |
| 24 | 3 | B α(DFT) ω(DFT) | 0.8236 | 0.808 | 0.0156 | -0.1414 | 0.3263 | 0.2705 | 4.0448 | 0.9033 | 52.9128 | 0.7719 | 0.0517 | 0.371 | 0.308 | 5.2307 | 0.8768 | 76.2998 | 8.244 | -18.6979 | 7.9473 | -15.3074 | 7.7768 | -19.9677 | 5 | 0.2896 | 0.2043 | 1.4254 | 0.7849 | 0.7849 | 0.861 | 0.8741 | 0.653 | 0.1974 | |
| 25 | 3 | B α(HF) ω(HF) | 0.8223 | 0.8066 | 0.0157 | -0.0996 | 0.3275 | 0.2759 | 4.0752 | 0.9025 | 52.4338 | 0.7708 | 0.0515 | 0.3719 | 0.314 | 5.2561 | 0.8765 | 76.2342 | 8.1527 | -18.3975 | 7.7578 | -15.6253 | 8.3018 | -19.0629 | 5 | 0.2712 | 0.192 | 1.2499 | 0.8114 | 0.8114 | 0.8782 | 0.8877 | 0.6591 | 0.1842 | |
| 26 | 3 | B E(DFT) α(HF) | 0.8205 | 0.8047 | 0.0158 | -0.1307 | 0.3291 | 0.2759 | 4.1155 | 0.9014 | 51.8088 | 0.7684 | 0.0521 | 0.3738 | 0.3144 | 5.3105 | 0.8756 | 75.9787 | 8.1872 | -18.7167 | 7.8372 | -15.5303 | 7.869 | -19.3006 | 5 | 0.2671 | 0.2146 | 1.2127 | 0.817 | 0.817 | 0.8818 | 0.906 | 0.7508 | 0.0698 | |
| 27 | 3 | B α(HF) H(DFT) | 0.8205 | 0.8047 | 0.0158 | -0.1307 | 0.3291 | 0.2759 | 4.1155 | 0.9014 | 51.8088 | 0.7684 | 0.0521 | 0.3738 | 0.3144 | 5.3105 | 0.8756 | 76.0384 | 8.1509 | -18.0684 | 8.6073 | -14.4896 | 8.0359 | -18.6179 | 5 | 0.2671 | 0.2146 | 1.2127 | 0.817 | 0.817 | 0.8818 | 0.906 | 0.7508 | 0.0698 | |
| 28 | 3 | B α(HF) G(HF) | 0.8205 | 0.8047 | 0.0158 | -0.1302 | 0.3291 | 0.2759 | 4.1156 | 0.9014 | 51.8079 | 0.7684 | 0.0521 | 0.3738 | 0.3144 | 5.3104 | 0.8756 | 75.9325 | 7.9453 | -20.005 | 8.2747 | -14.8299 | 7.9937 | -19.6039 | 5 | 0.2671 | 0.2147 | 1.213 | 0.8169 | 0.8169 | 0.8818 | 0.906 | 0.7508 | 0.0696 | |
| 29 | 3 | B E(HF) α(HF) | 0.8205 | 0.8047 | 0.0158 | -0.1302 | 0.3291 | 0.2759 | 4.1156 | 0.9014 | 51.8079 | 0.7684 | 0.0521 | 0.3738 | 0.3144 | 5.3104 | 0.8756 | 75.9702 | 8.2122 | -18.3996 | 7.6877 | -15.5022 | 7.9685 | -18.8915 | 5 | 0.2671 | 0.2147 | 1.213 | 0.8169 | 0.8169 | 0.8818 | 0.906 | 0.7508 | 0.0696 | |
| 30 | 3 | B α(HF) H(HF) | 0.8205 | 0.8047 | 0.0158 | -0.1302 | 0.3291 | 0.2759 | 4.1156 | 0.9014 | 51.8079 | 0.7684 | 0.0521 | 0.3738 | 0.3144 | 5.3104 | 0.8756 | 76.1711 | 7.8895 | -18.3717 | 8.4403 | -14.7179 | 8.01 | -18.515 | 5 | 0.2671 | 0.2147 | 1.213 | 0.8169 | 0.8169 | 0.8818 | 0.906 | 0.7508 | 0.0696 | |
| 31 | 2 | B α(DFT) | 0.8146 | 0.804 | 0.0106 | -0.3333 | 0.3345 | 0.2764 | 4.252 | 0.8978 | 76.8708 | 0.7665 | 0.0481 | 0.3754 | 0.308 | | | | | | | | | | | | | | | | | | | | |

Table S14_0.00001. Same as Table S6_0.00001 but for models developed using combined quantum mechanical descriptors and LSER's adsorbate descriptors.

| S.No. | Size | Variables | R ² | R ² _{adj} | R ² -R ² _{adj} | ΔK | RMSE(tr) | MAE(tr) | RSS(tr) | CCC(tr) | F | Q ² _{loo} | R ² -Q ² _{loo} | RMSE(cv) | MAE(cv) | PRESS(cv) | CCC(cv) | Q ² _{LMO} | R ² _{Yser} | Q ² _{Yser} | R ² _{Xmdl} | Q ² _{Xmdl} | R ² _{Ymdl} | Q ² _{Ymdl} | N. ext. OK | RMSE(ext) | MAE(ext) | PRESS(ext) | Q ² _{F1} | Q ² _{F2} | Q ² _{F3} | CCC(ext) | F _m ² | Δr _m ² |
|-------|------|---|----------------|-------------------------------|---|---------|----------|---------|---------|---------|---------|-------------------------------|---|----------|---------|-----------|---------|-------------------------------|--------------------------------|--------------------------------|--------------------------------|--------------------------------|--------------------------------|--------------------------------|------------|-----------|----------|------------|------------------------------|------------------------------|------------------------------|----------|-----------------------------|------------------------------|
| 1 | 5 | B E ^{HOMO} (DFT) α(DFT) χ(DFT) ω(DFT) | 0.9076 | 0.8875 | 0.0201 | -0.109 | 0.2455 | 0.1995 | 1.7479 | 0.9516 | 45.19 | 0.8616 | 0.046 | 0.3005 | 0.249 | 2.6182 | 0.9289 | 85.2613 | 17.6368 | -48.7991 | 17.6489 | -32.4564 | 17.9837 | -47.3159 | 1 | 0.3961 | 0.3091 | 4.0797 | 0.6164 | 0.6164 | 0.7595 | 0.8185 | 0.614 | 0.1042 |
| 2 | 5 | B α(DFT) η(DFT) χ(DFT) ω(DFT) | 0.9076 | 0.8875 | 0.0201 | -0.0964 | 0.2455 | 0.1995 | 1.7479 | 0.9516 | 45.19 | 0.8616 | 0.046 | 0.3005 | 0.249 | 2.6182 | 0.9289 | 85.3453 | 18.0206 | -46.527 | 17.8285 | -31.8995 | 18.7497 | -45.5363 | 1 | 0.3961 | 0.3091 | 4.0797 | 0.6164 | 0.6164 | 0.7595 | 0.8185 | 0.614 | 0.1042 |
| 3 | 5 | B E ^{HOMO} (DFT) α(DFT) χ(DFT) ω(DFT) | 0.9076 | 0.8875 | 0.0201 | -0.1139 | 0.2455 | 0.1995 | 1.7479 | 0.9516 | 45.19 | 0.8616 | 0.046 | 0.3005 | 0.249 | 2.6182 | 0.9289 | 85.2881 | 17.4821 | -47.8233 | 18.0612 | -30.9502 | 17.3733 | -50.579 | 1 | 0.3961 | 0.3091 | 4.0797 | 0.6164 | 0.6164 | 0.7595 | 0.8185 | 0.614 | 0.1042 |
| 4 | 5 | B E ^{HOMO} (DFT) - E ^{LUMO} (DFT) α(DFT) χ(DFT) ω(DFT) | 0.9076 | 0.8875 | 0.0201 | -0.0964 | 0.2455 | 0.1995 | 1.7479 | 0.9516 | 45.19 | 0.8616 | 0.046 | 0.3005 | 0.249 | 2.6182 | 0.9289 | 85.2743 | 18.5831 | -44.1477 | 16.4121 | -33.8494 | 17.7461 | -47.2033 | 1 | 0.3961 | 0.3091 | 4.0797 | 0.6164 | 0.6164 | 0.7595 | 0.8185 | 0.614 | 0.1042 |
| 5 | 5 | B E ^{LUMO} (DFT) E ^{HOMO} (DFT) - E ^{LUMO} (DFT) α(DFT) ω(DFT) | 0.9076 | 0.8875 | 0.0201 | -0.0919 | 0.2455 | 0.1995 | 1.7479 | 0.9516 | 45.19 | 0.8616 | 0.046 | 0.3005 | 0.249 | 2.6182 | 0.9289 | 85.6133 | 17.9262 | -46.2637 | 18.0625 | -31.7756 | 17.9347 | -47.5375 | 1 | 0.3961 | 0.3091 | 4.0797 | 0.6164 | 0.6164 | 0.7595 | 0.8185 | 0.614 | 0.1042 |
| 6 | 5 | B E ^{LUMO} (DFT) α(DFT) η(DFT) ω(DFT) | 0.9076 | 0.8875 | 0.0201 | -0.0919 | 0.2455 | 0.1995 | 1.7479 | 0.9516 | 45.19 | 0.8616 | 0.046 | 0.3005 | 0.249 | 2.6182 | 0.9289 | 85.0364 | 18.3072 | -46.6632 | 18.101 | -31.2717 | 18.1865 | -45.7218 | 1 | 0.3961 | 0.3091 | 4.0797 | 0.6164 | 0.6164 | 0.7595 | 0.8185 | 0.614 | 0.1042 |
| 7 | 5 | B E ^{HOMO} (DFT) E ^{LUMO} (DFT) α(DFT) ω(DFT) | 0.9076 | 0.8875 | 0.0201 | -0.1051 | 0.2455 | 0.1995 | 1.7479 | 0.9516 | 45.19 | 0.8616 | 0.046 | 0.3005 | 0.249 | 2.6182 | 0.9289 | 85.1978 | 18.6684 | -45.0322 | 17.7805 | -32.133 | 18.0532 | -45.9819 | 1 | 0.3961 | 0.3091 | 4.0797 | 0.6164 | 0.6164 | 0.7595 | 0.8185 | 0.614 | 0.1042 |
| 8 | 5 | B E ^{HOMO} (DFT) α(DFT) η(DFT) ω(DFT) | 0.9076 | 0.8875 | 0.0201 | -0.0935 | 0.2455 | 0.1995 | 1.7479 | 0.9516 | 45.19 | 0.8616 | 0.046 | 0.3005 | 0.249 | 2.6182 | 0.9289 | 85.0057 | 17.6077 | -48.713 | 17.7979 | -32.5271 | 17.6497 | -48.4866 | 1 | 0.3961 | 0.3091 | 4.0797 | 0.6164 | 0.6164 | 0.7595 | 0.8185 | 0.614 | 0.1042 |
| 9 | 5 | B E ^{HOMO} (DFT) E ^{HOMO} (DFT) - E ^{LUMO} (DFT) α(DFT) ω(DFT) | 0.9076 | 0.8875 | 0.0201 | -0.0935 | 0.2455 | 0.1995 | 1.7479 | 0.9516 | 45.19 | 0.8616 | 0.046 | 0.3005 | 0.249 | 2.6182 | 0.9289 | 85.4646 | 18.0907 | -45.7406 | 17.6917 | -32.4664 | 18.3322 | -48.1409 | 1 | 0.3961 | 0.3091 | 4.0797 | 0.6164 | 0.6164 | 0.7595 | 0.8185 | 0.614 | 0.1042 |
| 10 | 5 | B d(CORR) E ^{LUMO} (CORR) α(HF) ω(DFT) | 0.9074 | 0.8873 | 0.0201 | -0.0919 | 0.2458 | 0.196 | 1.7522 | 0.9514 | 45.0679 | 0.8612 | 0.0462 | 0.3009 | 0.2428 | 2.6265 | 0.9291 | 84.7172 | 18.5078 | -63.2778 | 18.0925 | -31.7254 | 17.7294 | -58.6101 | 2 | 0.3822 | 0.298 | 3.7975 | 0.643 | 0.643 | 0.7761 | 0.8321 | 0.6594 | 0.1151 |
| 11 | 4 | B E ^{LUMO} (CORR) α(HF) ω(DFT) | 0.9034 | 0.8873 | 0.0161 | -0.1078 | 0.251 | 0.209 | 1.8275 | 0.9493 | 56.117 | 0.856 | 0.0475 | 0.3066 | 0.2586 | 2.7253 | 0.9264 | 84.8119 | 14.456 | -32.1275 | 14.2264 | -26.1895 | 14.1478 | -31.8255 | 2 | 0.3742 | 0.2922 | 3.6407 | 0.6577 | 0.6577 | 0.7854 | 0.8383 | 0.6652 | 0.1108 |
| 12 | 4 | B E ^{LUMO} (DFT) α(HF) ω(DFT) | 0.9006 | 0.884 | 0.0166 | -0.1041 | 0.2546 | 0.2161 | 1.8803 | 0.9477 | 54.3707 | 0.8574 | 0.0433 | 0.3051 | 0.2638 | 2.6988 | 0.9265 | 84.8869 | 14.0208 | -35.4103 | 14.3847 | -25.8476 | 14.7567 | -32.8279 | 2 | 0.3755 | 0.288 | 3.6665 | 0.6553 | 0.6553 | 0.7838 | 0.8367 | 0.6618 | 0.1067 |
| 13 | 4 | B E ^{LUMO} (DFT) α(DFT) ω(DFT) | 0.9003 | 0.8837 | 0.0166 | -0.1096 | 0.255 | 0.2114 | 1.8863 | 0.9475 | 54.1801 | 0.8538 | 0.0465 | 0.3088 | 0.2604 | 2.7656 | 0.9244 | 84.1771 | 14.0451 | -36.0728 | 14.3048 | -25.6389 | 14.6959 | -32.9763 | 2 | 0.3808 | 0.2896 | 3.7697 | 0.6456 | 0.6456 | 0.7778 | 0.8357 | 0.6591 | 0.1384 |
| 14 | 4 | B E ^{LUMO} (CORR) α(DFT) ω(DFT) | 0.9002 | 0.8836 | 0.0166 | -0.1131 | 0.2552 | 0.2047 | 1.8883 | 0.9475 | 54.1149 | 0.8424 | 0.0578 | 0.3207 | 0.256 | 2.9823 | 0.9191 | 83.9255 | 14.9707 | -30.4406 | 13.9883 | -26.2321 | 14.4365 | -32.0814 | 2 | 0.38 | 0.2978 | 3.755 | 0.6469 | 0.6469 | 0.7786 | 0.8362 | 0.6599 | 0.1373 |
| 15 | 4 | A B α(HF) ω(DFT) | 0.8989 | 0.882 | 0.0169 | -0.1029 | 0.2569 | 0.2095 | 1.9136 | 0.9467 | 53.32 | 0.8355 | 0.0634 | 0.3276 | 0.2635 | 3.1127 | 0.915 | 83.9283 | 14.2011 | -30.0682 | 13.6872 | -27.1043 | 14.3935 | -30.9414 | 2 | 0.3757 | 0.2981 | 3.6703 | 0.6549 | 0.6549 | 0.7836 | 0.8412 | 0.6705 | 0.152 |
| 16 | 4 | P B α(HF) ω(DFT) | 0.8952 | 0.8777 | 0.0175 | -0.1191 | 0.2615 | 0.2171 | 1.9827 | 0.9447 | 51.2536 | 0.8456 | 0.0496 | 0.3173 | 0.2668 | 2.9205 | 0.9204 | 83.4428 | 14.2295 | -32.8377 | 13.9275 | -26.5335 | 14.012 | -32.9946 | 1 | 0.3913 | 0.3208 | 3.9817 | 0.6256 | 0.6256 | 0.7653 | 0.8229 | 0.6459 | 0.1026 |
| 17 | 4 | B α(HF) χ(DFT) ω(DFT) | 0.8925 | 0.8745 | 0.0179 | -0.1124 | 0.2649 | 0.2106 | 2.0344 | 0.9432 | 49.7991 | 0.8289 | 0.0636 | 0.3341 | 0.2646 | 3.2375 | 0.9126 | 83.1509 | 14.7319 | -34.6114 | 14.3316 | -25.5858 | 13.7234 | -35.6689 | 1 | 0.3858 | 0.2948 | 3.8697 | 0.6362 | 0.6362 | 0.7719 | 0.8202 | 0.6217 | 0.0401 |
| 18 | 4 | B α(HF) η(CORR) ω(DFT) | 0.8918 | 0.8738 | 0.018 | -0.0875 | 0.2657 | 0.2193 | 2.0469 | 0.9428 | 49.4576 | 0.8359 | 0.0559 | 0.3272 | 0.2703 | 3.1044 | 0.9159 | 83.2603 | 14.7743 | -31.0322 | 14.664 | -25.6514 | 14.7369 | -32.3586 | 1 | 0.3774 | 0.2962 | 3.7031 | 0.6518 | 0.6518 | 0.7817 | 0.8288 | 0.6466 | 0.0478 |
| 19 | 4 | B E ^{HOMO} (CORR) - E ^{LUMO} (CORR) α(HF) ω(DFT) | 0.8918 | 0.8738 | 0.018 | -0.0875 | 0.2657 | 0.2193 | 2.0469 | 0.9428 | 49.4576 | 0.8359 | 0.0559 | 0.3272 | 0.2703 | 3.1044 | 0.9159 | 83.553 | 14.8812 | -30.4129 | 14.0337 | -32.3399 | 14.5542 | -31.6457 | 1 | 0.3774 | 0.2962 | 3.7031 | 0.6518 | 0.6518 | 0.7817 | 0.8288 | 0.6466 | 0.0478 |
| 20 | 3 | B α(HF) ω(DFT) | 0.8869 | 0.8733 | 0.0136 | -0.1571 | 0.2716 | 0.2243 | 2.14 | 0.9401 | 65.3421 | 0.831 | 0.0558 | 0.332 | 0.2704 | 3.1965 | 0.9131 | 82.6119 | 10.5536 | -26.4101 | 10.5783 | -20.8845 | 10.4849 | -26.3281 | 1 | 0.3792 | 0.2958 | 3.7392 | 0.6484 | 0.6484 | 0.7796 | 0.8305 | 0.6492 | 0.0781 |
| 21 | 3 | B E ^{LUMO} (HF) α(HF) | 0.8847 | 0.8709 | 0.0138 | -0.1842 | 0.2742 | 0.2277 | 2.1808 | 0.9388 | 63.9613 | 0.8085 | 0.0762 | 0.3535 | 0.2807 | 3.6231 | 0.9024 | 81.2767 | 10.7744 | -24.7552 | 11.0021 | -20.1666 | 10.8444 | -25.8284 | 1 | 0.3727 | 0.2803 | 3.6114 | 0.6605 | 0.6604 | 0.7871 | 0.8291 | 0.6470 | 0.0138 |
| 22 | 3 | B E ^{LUMO} (DFT) α(HF) ω(DFT) | 0.8818 | 0.8677 | 0.0142 | -0.1249 | 0.2776 | 0.2312 | 2.2354 | 0.9372 | 62.1983 | 0.8184 | 0.0634 | 0.3442 | 0.2799 | 3.4351 | 0.9067 | 81.5355 | 10.4465 | -24.5642 | 10.9416 | -20.3407 | 10.7579 | -24.6077 | 1 | 0.3786 | 0.2929 | 3.7259 | 0.6497 | 0.6497 | 0.7803 | 0.8268 | 0.6309 | 0.04 |
| 23 | 3 | B E ^{LUMO} (CORR) α(HF) | 0.8806 | 0.8663 | 0.0143 | -0.1235 | 0.2791 | 0.2319 | 2.2593 | 0.9365 | 61.4493 | 0.8164 | 0.0642 | 0.3461 | 0.2807 | 3.4735 | 0.9057 | 80.7728 | 10.4147 | -25.9292 | 10.3485 | -21.1737 | 10.5558 | -26.0148 | 1 | 0.3789 | 0.2933 | 3.7321 | 0.6491 | 0.6491 | 0.78 | 0.8254 | 0.6339 | 0.0301 |
| 24 | 3 | B α(HF) χ(DFT) | 0.8805 | 0.8662 | 0.0143 | -0.0986 | 0.2792 | 0.2363 | 2.2603 | 0.9365 | 61.4201 | 0.8148 | 0.0657 | 0.3476 | 0.2864 | 3.5034 | 0.9046 | 81.6027 | 10.5665 | -24.4158 | 10.5253 | -20.9968 | 10.7263 | -25.7534 | 1 | 0.3744 | 0.2939 | 3.6452 | 0.6573 | 0.6573 | 0.7851 | 0.831 | 0.6476 | 0.0446 |
| 25 | 3 | B α(HF) η(CORR) | 0.8801 | 0.8657 | 0.0144 | -0.0805 | 0.2797 | 0.2319 | 2.2683 | 0.9362 | 61.1748 | 0.8178 | 0.0623 | 0.3447 | 0.2795 | 3.4467 | 0.9061 | 80.9518 | 10.9935 | -25.0758 | 11.0553 | -20.1474 | 10.534 | -26.3596 | 1 | 0.3763 | 0.2919 | 3.6813 | 0.6539 | 0.6539 | 0.783 | 0.8285 | 0.6394 | 0.0369 |
| 26 | 3 | B E ^{HOMO} (CORR) - E ^{LUMO} (CORR) α(HF) | 0.8801 | 0.8657 | 0.0144 | -0.0805 | 0.2797 | 0.2319 | 2.2683 | 0.9362 | 61.1748 | 0.8178 | 0.0623 | 0.3447 | 0.2795 | 3.4467 | 0.9061 | 80.9376 | 11.3007 | -24.8447 | 10.4671 | -21.0852 | 10.5129 | -26.1614 | 1 | 0.3763 | 0.2919 | 3.6813 | 0.6539 | 0.6539 | 0.783 | 0.8285 | 0.6394 | 0.0369 |
| 27 | 3 | B α(HF) χ(CORR) | 0.8798 | 0.8654 | 0.0144 | -0.1046 | 0.2801 | 0.2324 | 2.2745 | 0.936 | 60.984 | 0.8119 | 0.0679 | 0.3503 | 0.2827 | 3.5583 | 0.9038 | 81.2388 | 10.5835 | -25.74 | 10.4873 | -20.7771 | 10.2707 | -26.2021 | 1 | 0.3803 | 0.2952 | 3.7599 | 0.6465 | 0.6465 | 0.7783 | 0.8211 | 0.6246 | 0.0048 |
| 28 | 4 | B V χ(DFT) ω(DFT) | 0.8776 | 0.8572 | 0.0204 | -0.1255 | 0.2826 | 0.2265 | 2.3152 | 0.9348 | 43.0313 | 0.8281 | 0.0495 | 0.3349 | 0.269 | 3.252 | 0.9099 | 80.3523 | 14.7605 | -35.79 | 14.4651 | -25.7539 | 14.5514 | -34.5008 | 1 | 0.3787 | 0.2956 | 3.7291 | 0.6494 | 0.6494 | 0.7802 | 0.8253 | 0.6122 | 0.0316 |
| 29 | 3 | B α(HF) H(HF) | 0.875 | 0.86 | 0.015 | -0.1553 | 0.2855 | 0.2341 | 2.3646 | 0.9333 | 58.3442 | 0.8068 | 0.0682 | 0.355 | 0.2833 | 3.6549 | 0.9008 | 80.201 | 10.7286 | -25.2862 | 11.0615 | -20.3674 | 10.6101 | -26.7457 | 1 | 0.3566 | 0.281 | 3.3063 | 0.6891 | 0.6891 | 0.8051 | 0.8348 | 0.6438 | 0.07 |
| 30 | 3 | B E(HF) α(HF) | 0.875 | 0.86 | 0.015 | -0.1351 | 0.2855 | 0.2341 | 2.3646 | 0.9333 | 58.3442 | 0.8068 | 0.0682 | 0.355 | 0.2833 | 3.6549 | 0.9008 | 80.0934 | 11.0355 | -26.21 | 9.9873 | -21.5925 | 10.1898 | -25.9545 | 1 | 0.3566 | 0.281 | 3.3063 | 0.6891 | 0.6891 | 0.8051 | 0.8348 | 0.6438 | 0.07 |
| 31 | 2 | B α(HF) | 0.87 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |

Table S15_0.00001. Same as Table S4_0.00001 but using splitting employed as in Yu et al., 2015.

| S.No. | Size | Variables | R ² | R ² _{adj} | R ² -R ² _{adj} | ΔK | RMSE(tr) | MAE(tr) | RSS(tr) | CCC(tr) | F | Q ² _{LMO} | R ² _{Yscr} | Q ² _{Yscr} | R ² _{Yscr} | Q ² _{Xrnt} | R ² _{Yrnt} | Q ² _{Yrnt} | N. ext. OK | RMSE(ext) | MAE(ext) | PRESS(ext) | Q ² _{F1} | Q ² _{F2} | Q ² _{F3} | CCC(ext) | \bar{r}_m^2 | Δr_m^2 | | | | | | |
|-------|------|--|----------------|-------------------------------|---|---------|----------|---------|---------|---------|---------|-------------------------------|--------------------------------|--------------------------------|--------------------------------|--------------------------------|--------------------------------|--------------------------------|------------|-----------|----------|------------|------------------------------|------------------------------|------------------------------|----------|---------------|----------------|--------|--------|--------|--------|---------|--------|
| 1 | 5 | E(CORR) ZPE(HF) ZPE(CORR) E ^{HOMO} (CORR) ω(DFT) | 0.703 | 0.6639 | 0.0391 | -0.0451 | 0.4118 | 0.3312 | 7.4601 | 0.8256 | 17.9878 | 0.6026 | 0.1004 | 0.4763 | 0.3847 | 9.9814 | 0.7706 | 62.1184 | 11.4939 | -20.7465 | 11.9744 | -18.3427 | 11.6071 | -21.1189 | 1 | 0.398 | 0.3619 | 1.7423 | 0.6077 | 0.6064 | 0.7225 | 0.7829 | 0.487 | 0.1327 |
| 2 | 5 | E(CORR) ZPE(DFT) ZPE(CORR) E ^{HOMO} (CORR) ω(DFT) | 0.703 | 0.6639 | 0.0391 | -0.0446 | 0.4118 | 0.3312 | 7.4601 | 0.8256 | 17.9878 | 0.6026 | 0.1004 | 0.4763 | 0.3847 | 9.9814 | 0.7706 | 62.2357 | 11.5142 | -20.3761 | 11.1612 | -19.3108 | 11.6674 | -20.3468 | 1 | 0.398 | 0.3619 | 1.7423 | 0.6077 | 0.6064 | 0.7225 | 0.7829 | 0.487 | 0.1327 |
| 3 | 5 | E(CORR) ZPE(DFT) ZPE(HF) E ^{HOMO} (CORR) ω(DFT) | 0.703 | 0.6639 | 0.0391 | -0.0398 | 0.4118 | 0.3312 | 7.4601 | 0.8256 | 17.9878 | 0.6026 | 0.1004 | 0.4763 | 0.3847 | 9.9814 | 0.7706 | 62.5035 | 10.8707 | -21.625 | 11.0552 | -19.3687 | 11.5623 | -21.4824 | 1 | 0.398 | 0.3619 | 1.7423 | 0.6077 | 0.6064 | 0.7225 | 0.7829 | 0.487 | 0.1327 |
| 4 | 5 | ZPE(HF) ZPE(CORR) E ^{HOMO} (CORR) H(CORR) ω(DFT) | 0.7029 | 0.6638 | 0.0391 | -0.0451 | 0.4118 | 0.3313 | 7.4623 | 0.8255 | 17.9803 | 0.6025 | 0.1004 | 0.4764 | 0.3847 | 9.9845 | 0.7705 | 62.2898 | 11.4328 | -20.747 | 11.2928 | -19.2017 | 11.5083 | -20.7779 | 1 | 0.398 | 0.3619 | 1.7421 | 0.6078 | 0.6064 | 0.7226 | 0.7829 | 0.487 | 0.1326 |
| 5 | 5 | ZPE(DFT) ZPE(CORR) E ^{HOMO} (CORR) H(CORR) ω(DFT) | 0.7029 | 0.6638 | 0.0391 | -0.0446 | 0.4118 | 0.3313 | 7.4623 | 0.8255 | 17.9803 | 0.6025 | 0.1004 | 0.4764 | 0.3847 | 9.9845 | 0.7705 | 62.6247 | 11.9232 | -20.765 | 11.1364 | -19.315 | 11.6875 | -20.7141 | 1 | 0.398 | 0.3619 | 1.7421 | 0.6078 | 0.6064 | 0.7226 | 0.7829 | 0.487 | 0.1326 |
| 6 | 5 | ZPE(DFT) ZPE(HF) E ^{HOMO} (CORR) H(CORR) ω(DFT) | 0.7029 | 0.6638 | 0.0391 | -0.0525 | 0.4118 | 0.3313 | 7.4623 | 0.8255 | 17.9803 | 0.6025 | 0.1004 | 0.4764 | 0.3847 | 9.9845 | 0.7705 | 62.2392 | 11.598 | -20.8165 | 11.7108 | -18.9348 | 11.6147 | -20.7532 | 1 | 0.398 | 0.3619 | 1.7421 | 0.6078 | 0.6064 | 0.7226 | 0.7829 | 0.487 | 0.1326 |
| 7 | 5 | ZPE(HF) ZPE(CORR) E ^{HOMO} (CORR) G(CORR) ω(DFT) | 0.7027 | 0.6636 | 0.0391 | -0.0452 | 0.4119 | 0.332 | 7.466 | 0.8254 | 17.9674 | 0.6026 | 0.1001 | 0.4763 | 0.3855 | 9.9814 | 0.7705 | 62.9543 | 11.3543 | -20.9842 | 11.3196 | -19.1057 | 11.6984 | -20.9251 | 1 | 0.3984 | 0.362 | 1.7456 | 0.607 | 0.6057 | 0.722 | 0.7825 | 0.4862 | 0.1332 |
| 8 | 5 | ZPE(DFT) ZPE(CORR) E ^{HOMO} (CORR) G(CORR) ω(DFT) | 0.7027 | 0.6636 | 0.0391 | -0.0447 | 0.4119 | 0.332 | 7.466 | 0.8254 | 17.9674 | 0.6026 | 0.1001 | 0.4763 | 0.3855 | 9.9814 | 0.7705 | 62.1589 | 11.6425 | -20.5081 | 11.6457 | -19.008 | 11.0822 | -21.5976 | 1 | 0.3984 | 0.362 | 1.7456 | 0.607 | 0.6057 | 0.722 | 0.7825 | 0.4862 | 0.1332 |
| 9 | 5 | ZPE(DFT) ZPE(HF) E ^{HOMO} (CORR) G(CORR) ω(DFT) | 0.7027 | 0.6636 | 0.0391 | -0.0526 | 0.4119 | 0.332 | 7.466 | 0.8254 | 17.9674 | 0.6026 | 0.1001 | 0.4763 | 0.3855 | 9.9814 | 0.7705 | 62.5681 | 11.4285 | -20.6269 | 11.4659 | -19.1559 | 11.8611 | -20.5257 | 1 | 0.3984 | 0.362 | 1.7456 | 0.607 | 0.6057 | 0.722 | 0.7825 | 0.4862 | 0.1332 |
| 10 | 5 | E(CORR) ZPE(DFT) ZPE(CORR) E ^{LUMO} (DFT) η(CORR) | 0.6861 | 0.6448 | 0.0413 | -0.099 | 0.4233 | 0.3408 | 7.8847 | 0.8138 | 16.61 | 0.5934 | 0.0927 | 0.4818 | 0.3899 | 10.2131 | 0.7612 | 60.4446 | 11.546 | -20.1889 | 11.3765 | -19.3386 | 11.897 | -20.0095 | 1 | 0.4079 | 0.3849 | 1.8305 | 0.5879 | 0.5865 | 0.7085 | 0.7791 | 0.4773 | 0.0857 |
| 11 | 4 | ZPE(DFT) ZPE(CORR) α(HF) χ(DFT) | 0.6611 | 0.6263 | 0.0348 | -0.0616 | 0.4399 | 0.3383 | 8.5132 | 0.7959 | 19.0158 | 0.5647 | 0.0963 | 0.4985 | 0.3833 | 10.9321 | 0.744 | 58.3485 | 9.1558 | -16.9116 | 9.2378 | -15.8167 | 9.1992 | -16.9686 | 0 | 0.4547 | 0.4171 | 2.2744 | 0.4879 | 0.4862 | 0.6378 | 0.633 | 0.2764 | 0.3912 |
| 12 | 4 | ZPE(HF) ZPE(CORR) α(HF) χ(DFT) | 0.6611 | 0.6263 | 0.0348 | -0.0618 | 0.4399 | 0.3383 | 8.5132 | 0.7959 | 19.0158 | 0.5647 | 0.0963 | 0.4985 | 0.3833 | 10.9321 | 0.744 | 58.5773 | 9.3328 | -16.5406 | 8.7916 | -16.4228 | 9.5395 | -16.5853 | 0 | 0.4547 | 0.4171 | 2.2744 | 0.4879 | 0.4862 | 0.6378 | 0.633 | 0.2764 | 0.3912 |
| 13 | 4 | ZPE(DFT) ZPE(HF) α(HF) χ(DFT) | 0.6611 | 0.6263 | 0.0348 | -0.058 | 0.4399 | 0.3383 | 8.5132 | 0.7959 | 19.0158 | 0.5647 | 0.0963 | 0.4985 | 0.3833 | 10.9321 | 0.744 | 58.3989 | 8.8192 | -17.735 | 8.9537 | -16.1963 | 9.1976 | -17.4154 | 0 | 0.4547 | 0.4171 | 2.2744 | 0.4879 | 0.4862 | 0.6378 | 0.633 | 0.2764 | 0.3912 |
| 14 | 4 | ZPE(DFT) ZPE(CORR) E ^{HOMO} (CORR) α(HF) | 0.6579 | 0.6228 | 0.0351 | -0.0863 | 0.4419 | 0.3369 | 8.592 | 0.7937 | 18.7521 | 0.5688 | 0.0891 | 0.4961 | 0.3802 | 10.8302 | 0.7438 | 58.5756 | 9.708 | -16.4812 | 9.6114 | -15.2839 | 9.1773 | -17.0917 | 1 | 0.4095 | 0.3662 | 1.8443 | 0.5848 | 0.5833 | 0.7063 | 0.699 | 0.3215 | 0.3952 |
| 15 | 4 | ZPE(HF) ZPE(CORR) E ^{HOMO} (DFT) α(HF) | 0.6579 | 0.6228 | 0.0351 | -0.0865 | 0.4419 | 0.3369 | 8.592 | 0.7937 | 18.7521 | 0.5688 | 0.0891 | 0.4961 | 0.3802 | 10.8302 | 0.7438 | 58.4053 | 9.6459 | -16.6615 | 9.4097 | -15.5753 | 9.3532 | -16.6745 | 1 | 0.4095 | 0.3662 | 1.8443 | 0.5848 | 0.5833 | 0.7063 | 0.699 | 0.3215 | 0.3952 |
| 16 | 4 | ZPE(DFT) ZPE(HF) E ^{HOMO} (DFT) α(HF) | 0.6579 | 0.6228 | 0.0351 | -0.0866 | 0.4419 | 0.3369 | 8.592 | 0.7937 | 18.7521 | 0.5688 | 0.0891 | 0.4961 | 0.3802 | 10.8302 | 0.7438 | 58.5128 | 8.9367 | -17.8254 | 9.7381 | -15.2904 | 9.524 | -16.5453 | 1 | 0.4095 | 0.3662 | 1.8443 | 0.5848 | 0.5833 | 0.7063 | 0.699 | 0.3215 | 0.3952 |
| 17 | 4 | ZPE(DFT) ZPE(CORR) α(HF) ω(HF) | 0.6576 | 0.6225 | 0.0351 | -0.0894 | 0.4421 | 0.3423 | 8.6007 | 0.7934 | 18.7231 | 0.5663 | 0.0913 | 0.4976 | 0.3879 | 10.894 | 0.7423 | 58.4497 | 9.307 | -17.2138 | 9.6007 | -15.3038 | 9.4618 | -17.0232 | 1 | 0.4109 | 0.3727 | 1.8571 | 0.5819 | 0.5805 | 0.7043 | 0.7049 | 0.3526 | 0.3702 |
| 18 | 4 | ZPE(HF) ZPE(CORR) α(HF) ω(HF) | 0.6576 | 0.6225 | 0.0351 | -0.0897 | 0.4421 | 0.3423 | 8.6007 | 0.7934 | 18.7231 | 0.5663 | 0.0913 | 0.4976 | 0.3879 | 10.894 | 0.7423 | 57.9495 | 9.4243 | -16.7888 | 9.4308 | -15.3689 | 9.8202 | -16.3221 | 1 | 0.4109 | 0.3727 | 1.8571 | 0.5819 | 0.5805 | 0.7043 | 0.7049 | 0.3526 | 0.3702 |
| 19 | 4 | ZPE(DFT) ZPE(HF) α(HF) ω(HF) | 0.6576 | 0.6225 | 0.0351 | -0.0853 | 0.4421 | 0.3423 | 8.6007 | 0.7934 | 18.7231 | 0.5663 | 0.0913 | 0.4976 | 0.3879 | 10.894 | 0.7423 | 57.7729 | 10.0513 | -17.2191 | 10.1458 | -14.5922 | 9.4659 | -16.84 | 1 | 0.4109 | 0.3727 | 1.8571 | 0.5819 | 0.5805 | 0.7043 | 0.7049 | 0.3526 | 0.3702 |
| 20 | 4 | ZPE(HF) ZPE(CORR) α(DFT) χ(DFT) | 0.6541 | 0.6186 | 0.0355 | -0.064 | 0.4443 | 0.3468 | 8.6874 | 0.7909 | 18.4388 | 0.5632 | 0.0909 | 0.4994 | 0.3908 | 10.9715 | 0.7403 | 58.0569 | 9.4401 | -16.9457 | 9.2389 | -15.8384 | 9.2013 | -16.8905 | 0 | 0.4689 | 0.4185 | 2.419 | 0.4554 | 0.4535 | 0.6148 | 0.6009 | 0.2388 | 0.4118 |
| 21 | 3 | ZPE(CORR) E ^{HOMO} (DFT) α(HF) | 0.5574 | 0.5242 | 0.0332 | -0.0618 | 0.5027 | 0.395 | 11.117 | 0.7158 | 16.7909 | 0.4492 | 0.1081 | 0.5607 | 0.4003 | 13.8332 | 0.6534 | 46.6735 | 6.8191 | -13.7488 | 6.9274 | -12.818 | 6.683 | -13.673 | 0 | 0.5817 | 0.4996 | 3.7271 | 0.1621 | 0.1592 | 0.4073 | 0.288 | -0.0557 | 0.5469 |
| 22 | 3 | ZPE(HF) ZPE(CORR) α(HF) | 0.5531 | 0.5195 | 0.0335 | -0.271 | 0.5051 | 0.3997 | 11.2255 | 0.7122 | 16.4997 | 0.4535 | 0.0996 | 0.5585 | 0.4418 | 13.7268 | 0.6594 | 46.1093 | 6.9698 | -14.4967 | 6.9063 | -12.7911 | 6.9977 | -13.8952 | 0 | 0.4643 | 0.3823 | 2.3718 | 0.466 | 0.4642 | 0.6223 | 0.5882 | 0.14 | 0.6311 |
| 23 | 3 | ZPE(DFT) ZPE(CORR) α(HF) | 0.5531 | 0.5195 | 0.0335 | -0.2706 | 0.5051 | 0.3997 | 11.2255 | 0.7122 | 16.4997 | 0.4535 | 0.0996 | 0.5585 | 0.4418 | 13.7268 | 0.6594 | 45.7074 | 6.728 | -14.5505 | 6.6353 | -13.1775 | 6.8795 | -13.8701 | 0 | 0.4643 | 0.3823 | 2.3718 | 0.466 | 0.4642 | 0.6223 | 0.5882 | 0.14 | 0.6311 |
| 24 | 3 | ZPE(DFT) ZPE(HF) α(HF) | 0.5531 | 0.5195 | 0.0335 | -0.2694 | 0.5051 | 0.3997 | 11.2255 | 0.7122 | 16.4997 | 0.4535 | 0.0996 | 0.5585 | 0.4418 | 13.7268 | 0.6594 | 45.8266 | 7.2189 | -13.5668 | 6.9346 | -12.8778 | 6.777 | -14.0672 | 0 | 0.4643 | 0.3823 | 2.3718 | 0.466 | 0.4642 | 0.6223 | 0.5882 | 0.14 | 0.6311 |
| 25 | 3 | ZPE(CORR) α(HF) η(HF) | 0.546 | 0.512 | 0.034 | -0.0787 | 0.5091 | 0.4043 | 11.402 | 0.7064 | 16.038 | 0.4362 | 0.1098 | 0.5673 | 0.45 | 14.1604 | 0.6425 | 44.7467 | 7.0856 | -13.1752 | 7.0114 | -12.7268 | 7.0287 | -13.0691 | 0 | 0.6022 | 0.5124 | 3.9887 | 0.102 | 0.0989 | 0.3648 | 0.2371 | -0.0698 | 0.4994 |
| 26 | 3 | ZPE(HF) ZPE(CORR) α(DFT) | 0.5448 | 0.5106 | 0.0341 | -0.2732 | 0.5098 | 0.4067 | 11.4335 | 0.7053 | 15.9569 | 0.4539 | 0.0909 | 0.5583 | 0.4475 | 13.717 | 0.6549 | 45.4872 | 7.3852 | -13.7685 | 7.6352 | -11.9603 | 7.1009 | -13.5194 | 0 | 0.4868 | 0.3962 | 2.6066 | 0.4132 | 0.4111 | 0.5849 | 0.5417 | 0.0499 | 0.7498 |
| 27 | 3 | ZPE(DFT) ZPE(CORR) α(DFT) | 0.5448 | 0.5106 | 0.0341 | -0.2727 | 0.5098 | 0.4067 | 11.4335 | 0.7053 | 15.9569 | 0.4539 | 0.0909 | 0.5583 | 0.4475 | 13.717 | 0.6549 | 45.83 | 6.8335 | -14.0075 | 7.0041 | -12.7404 | 7.2516 | -13.3216 | 0 | 0.4868 | 0.3962 | 2.6066 | 0.4132 | 0.4111 | 0.5849 | 0.5417 | 0.0499 | 0.7498 |
| 28 | 3 | ZPE(DFT) ZPE(HF) α(DFT) | 0.5448 | 0.5106 | 0.0341 | -0.2711 | 0.5098 | 0.4067 | 11.4335 | 0.7053 | 15.9569 | 0.4539 | 0.0909 | 0.5583 | 0.4475 | 13.717 | 0.6549 | 45.3713 | 6.779 | -13.7117 | 6.9732 | -12.7298 | 6.8174 | -14.1184 | 0 | 0.4868 | 0.3962 | 2.6066 | 0.4132 | 0.4111 | 0.5849 | 0.5417 | 0.0499 | 0.7498 |
| 29 | 3 | ZPE(CORR) E ^{HOMO} (DFT) -E ^{LUMO} (DFT) α(HF) | 0.5354 | 0.5005 | 0.0348 | -0.1835 | 0.515 | 0.4194 | 11.6696 | 0.6974 | 15.3645 | 0.4369 | 0.0985 | 0.5669 | 0.4643 | 14.1426 | 0.6417 | 44.1887 | 7.2912 | -13.2848 | 7.0074 | -12.762 | 7.1444 | -13.3441 | 0 | 0.5014 | 0.4349 | 2.7656 | 0.3774 | 0.3752 | 0.5596 | 0.4934 | 0.0046 | 0.7628 |
| 30 | 3 | ZPE(CORR) α(HF) η(DFT) | 0.5354 | 0.5005 | 0.0348 | -0.1835 | 0.515 | 0.4194 | 11.6696 | 0.6974 | 15.3645 | 0.4369 | 0.0985 | 0.5669 | 0.4643 | 14.1426 | 0.6417 | 44.1314 | 6.7786 | -13.8693 | 7.2651 | -12.4697 | 6.5682 | -14.1943 | 0 | 0.5014 | 0.4349 | 2.7656 | 0.3774 | 0.3752 | 0.5596 | 0.4934 | 0.0046 | 0.7628 |
| 31 | 2 | ZPE(CORR) α(HF) | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |

Table S16_0.00001. Same as Table S8_0.00001 but using splitting employed as in Yu et al., 2015.

| S.No. | Size | Variables | R ² | R ² _{adj} | R ² -R ² _{adj} | ΔK | RMSE(tr) | MAE(tr) | RSS(tr) | CCC(tr) | F | Q ² _{loo} | R ² -Q ² _{loo} | RMSE(cv) | MAE(cv) | PRESS(cv) | CCC(cv) | Q ² _{LMO} | R ² _{Yscr} | Q ² _{Yscr} | R ² _{Xrnd} | Q ² _{Xrnd} | R ² _{Yrnd} | Q ² _{Yrnd} | N. ext. OK | RMSE(ext) | MAE(ext) | PRESS(ext) | Q ² _{F1} | Q ² _{F2} | Q ² _{F3} | CCC(ext) | r ² _m | Δ r ² _m |
|-------|------|-----------|----------------|-------------------------------|---|---------|----------|---------|---------|---------|---------|-------------------------------|---|----------|---------|-----------|---------|-------------------------------|--------------------------------|--------------------------------|--------------------------------|--------------------------------|--------------------------------|--------------------------------|------------|-----------|----------|------------|------------------------------|------------------------------|------------------------------|----------|-----------------------------|-------------------------------|
| 1 | 5 | R P A B V | 0.8304 | 0.808 | 0.0223 | -0.0567 | 0.3112 | 0.247 | 4.2608 | 0.9073 | 37.2008 | 0.7601 | 0.0702 | 0.37 | 0.292 | 6.0246 | 0.8703 | 77.7404 | 10.8855 | -22.0465 | 11.3593 | -19.2947 | 10.9341 | -21.8563 | 5 | 0.2998 | 0.2542 | 0.9884 | 0.7775 | 0.7767 | 0.8426 | 0.896 | 0.7444 | 0.0541 |
| 2 | 4 | P A B V | 0.8279 | 0.8103 | 0.0176 | -0.0828 | 0.3134 | 0.249 | 4.3218 | 0.9059 | 46.9137 | 0.7703 | 0.0576 | 0.3621 | 0.2859 | 5.7698 | 0.8746 | 78.0103 | 9.6794 | -15.8621 | 9.4031 | -15.416 | 9.2089 | -16.7213 | 5 | 0.342 | 0.2859 | 1.2866 | 0.7103 | 0.7093 | 0.7951 | 0.8685 | 0.6959 | 0.0681 |
| 3 | 4 | R A B V | 0.8235 | 0.8054 | 0.0181 | -0.0611 | 0.3174 | 0.249 | 4.4323 | 0.9032 | 45.501 | 0.7703 | 0.0532 | 0.3621 | 0.2833 | 5.7693 | 0.8752 | 77.845 | 9.7897 | -16.957 | 8.9422 | -16.2217 | 9.8674 | -16.4032 | 5 | 0.2657 | 0.2115 | 0.7764 | 0.8252 | 0.8246 | 0.8764 | 0.9189 | 0.7986 | 0.0761 |
| 4 | 4 | R P B V | 0.8148 | 0.7958 | 0.019 | -0.1908 | 0.3251 | 0.2648 | 4.6515 | 0.898 | 42.8976 | 0.7617 | 0.0531 | 0.3688 | 0.3016 | 5.9846 | 0.8707 | 76.5358 | 9.036 | -17.8173 | 9.5351 | -15.4033 | 9.7928 | -17.0283 | 5 | 0.3451 | 0.2785 | 1.31 | 0.7051 | 0.7041 | 0.7914 | 0.8636 | 0.6648 | 0.0699 |
| 5 | 3 | P B V | 0.8125 | 0.7985 | 0.0141 | -0.278 | 0.3271 | 0.2666 | 4.7084 | 0.8966 | 57.7936 | 0.7707 | 0.0418 | 0.3618 | 0.2956 | 5.7593 | 0.8745 | 76.7728 | 7.2155 | -13.4256 | 7.0137 | -12.632 | 6.7078 | -14.081 | 1 | 0.3855 | 0.2994 | 1.6344 | 0.632 | 0.6308 | 0.7397 | 0.8351 | 0.6161 | 0.0861 |
| 6 | 3 | R B V | 0.8117 | 0.7976 | 0.0141 | -0.2475 | 0.3279 | 0.2643 | 4.7297 | 0.8961 | 57.4721 | 0.7737 | 0.038 | 0.3594 | 0.2916 | 5.6832 | 0.877 | 76.5452 | 7.3537 | -14.0086 | 7.3716 | -12.2197 | 7.1396 | -13.7148 | 5 | 0.3197 | 0.2593 | 1.1244 | 0.7469 | 0.746 | 0.8209 | 0.8833 | 0.709 | 0.0822 |
| 7 | 3 | A B V | 0.8085 | 0.7942 | 0.0144 | -0.1018 | 0.3306 | 0.2625 | 4.8093 | 0.8941 | 56.3012 | 0.758 | 0.0506 | 0.3717 | 0.2942 | 6.0793 | 0.8661 | 76.2036 | 6.6499 | -14.078 | 7.0448 | -12.7678 | 6.9584 | -14.0893 | 3 | 0.3681 | 0.2657 | 1.4908 | 0.6644 | 0.6632 | 0.7626 | 0.8585 | 0.7088 | 0.1339 |
| 8 | 2 | B V | 0.8009 | 0.7912 | 0.0097 | -0.3975 | 0.3371 | 0.2738 | 5.0001 | 0.8895 | 82.4766 | 0.7665 | 0.0345 | 0.3651 | 0.2968 | 5.8658 | 0.871 | 75.4491 | 4.6756 | -10.7118 | 4.6913 | -9.861 | 4.607 | -11.4133 | 1 | 0.3982 | 0.2896 | 1.7439 | 0.6074 | 0.606 | 0.7223 | 0.8342 | 0.6412 | 0.1364 |
| 9 | 4 | R P A V | 0.6203 | 0.5814 | 0.0389 | -0.0646 | 0.4655 | 0.36 | 9.5361 | 0.7657 | 15.9302 | 0.502 | 0.1183 | 0.5332 | 0.414 | 12.5083 | 0.6971 | 54.0807 | 8.3531 | -18.2307 | 8.9752 | -16.1607 | 9.2866 | -16.865 | 0 | 0.4388 | 0.3914 | 2.1175 | 0.5233 | 0.5216 | 0.6628 | 0.7751 | 0.4774 | 0.0407 |
| 10 | 3 | R A V | 0.6203 | 0.5918 | 0.0285 | -0.0529 | 0.4656 | 0.36 | 9.5371 | 0.7657 | 21.7814 | 0.5308 | 0.0895 | 0.5175 | 0.402 | 11.7846 | 0.7154 | 54.7354 | 6.5414 | -14.5436 | 6.7409 | -12.9502 | 7.2821 | -13.55 | 0 | 0.4417 | 0.3942 | 2.1464 | 0.5167 | 0.5151 | 0.6582 | 0.7721 | 0.4722 | 0.0405 |
| 11 | 3 | P A V | 0.6077 | 0.5782 | 0.0294 | -0.0817 | 0.4732 | 0.3625 | 9.8542 | 0.756 | 20.6512 | 0.5287 | 0.0789 | 0.5187 | 0.4005 | 11.8364 | 0.7117 | 54.2658 | 6.4173 | -14.1472 | 6.6471 | -13.1759 | 7.0435 | -13.4194 | 0 | 0.4708 | 0.4355 | 2.4377 | 0.4512 | 0.4493 | 0.6118 | 0.7474 | 0.4517 | 0.0223 |
| 12 | 2 | A V | 0.6022 | 0.5828 | 0.0194 | -0.0345 | 0.4765 | 0.3651 | 9.9903 | 0.7518 | 31.0393 | 0.5419 | 0.0603 | 0.5114 | 0.3937 | 11.5058 | 0.7176 | 54.2741 | 4.5759 | -10.7859 | 4.731 | -9.8216 | 4.6803 | -10.3398 | 0 | 0.4462 | 0.4151 | 2.1902 | 0.5069 | 0.5052 | 0.6512 | 0.7747 | 0.5152 | 0.0146 |
| 13 | 4 | R P A B | 0.5959 | 0.5544 | 0.0415 | -0.0941 | 0.4803 | 0.3766 | 10.1508 | 0.7468 | 14.3751 | 0.499 | 0.0969 | 0.5348 | 0.4219 | 12.5839 | 0.6856 | 51.4985 | 9.9924 | -16.9649 | 9.4218 | -15.6652 | 9.5288 | -17.1211 | 0 | 0.5134 | 0.4536 | 2.8998 | 0.3471 | 0.3449 | 0.5382 | 0.6386 | 0.2727 | 0.0731 |
| 14 | 3 | R P A | 0.5681 | 0.5357 | 0.0324 | -0.1066 | 0.4965 | 0.3753 | 10.847 | 0.7246 | 17.5408 | 0.4838 | 0.0843 | 0.5428 | 0.4138 | 12.9648 | 0.6701 | 49.6947 | 6.9321 | -14.4623 | 6.9682 | -12.6379 | 6.989 | -14.2592 | 0 | 0.5343 | 0.4739 | 3.1404 | 0.293 | 0.2905 | 0.4999 | 0.6427 | 0.2692 | 0.0009 |
| 15 | 3 | P A B | 0.5584 | 0.5253 | 0.0331 | -0.1691 | 0.5021 | 0.3932 | 11.092 | 0.7166 | 16.8588 | 0.4722 | 0.0862 | 0.5489 | 0.4314 | 13.2566 | 0.6652 | 48.851 | 7.0667 | -13.9864 | 6.6957 | -13.1643 | 6.6958 | -13.8859 | 0 | 0.5542 | 0.501 | 3.3787 | 0.2393 | 0.2367 | 0.4619 | 0.579 | 0.1985 | 0.0774 |
| 16 | 3 | R A B | 0.557 | 0.5238 | 0.0332 | -0.1189 | 0.5029 | 0.398 | 11.1258 | 0.7155 | 16.7671 | 0.4747 | 0.0823 | 0.5476 | 0.437 | 13.1941 | 0.6653 | 47.3276 | 7.2606 | -13.6416 | 6.909 | -12.8918 | 7.0045 | -14.6564 | 0 | 0.5041 | 0.4231 | 2.7952 | 0.3707 | 0.3685 | 0.5548 | 0.6624 | 0.3126 | 0.047 |
| 17 | 2 | R A | 0.5511 | 0.5292 | 0.0219 | -0.094 | 0.5062 | 0.3935 | 11.276 | 0.7106 | 25.1629 | 0.4913 | 0.0598 | 0.5389 | 0.422 | 12.7771 | 0.6748 | 48.154 | 4.681 | -11.2735 | 4.4026 | -10.2504 | 4.4701 | -11.072 | 0 | 0.5141 | 0.4449 | 2.9072 | 0.3455 | 0.3432 | 0.537 | 0.6617 | 0.3008 | 0.0119 |
| 18 | 2 | P A | 0.536 | 0.5134 | 0.0226 | -0.2001 | 0.5147 | 0.3829 | 11.6541 | 0.6979 | 23.6816 | 0.4786 | 0.0574 | 0.5456 | 0.4075 | 13.096 | 0.6626 | 47.8756 | 4.7524 | -10.3969 | 4.676 | -9.9624 | 4.0224 | -11.3373 | 0 | 0.5702 | 0.5065 | 3.577 | 0.1947 | 0.1919 | 0.4303 | 0.5903 | 0.2117 | 0.0279 |
| 19 | 2 | A B | 0.3375 | 0.3052 | 0.0323 | -0.2913 | 0.615 | 0.4631 | 16.6404 | 0.5046 | 10.4424 | 0.2621 | 0.0754 | 0.649 | 0.4927 | 18.5331 | 0.4488 | 27.6641 | 4.6147 | -11.1669 | 4.8277 | -9.7979 | 4.8077 | -10.507 | 0 | 0.5474 | 0.5068 | 3.296 | 0.2579 | 0.2554 | 0.4751 | 0.5885 | 0.2324 | 0.1527 |
| 20 | 3 | R P B | 0.332 | 0.2819 | 0.0501 | -0.2655 | 0.6175 | 0.5326 | 16.7778 | 0.4985 | 6.627 | 0.2149 | 0.1171 | 0.6694 | 0.5801 | 19.7184 | 0.4109 | 19.8497 | 6.8712 | -14.8127 | 6.9266 | -12.7514 | 6.5488 | -15.4208 | 0 | 0.6156 | 0.4349 | 4.1681 | 0.0616 | 0.0584 | 0.3362 | 0.2373 | -0.1012 | 0.6127 |
| 21 | 2 | R B | 0.3131 | 0.2796 | 0.0335 | -0.3682 | 0.6262 | 0.5306 | 17.2521 | 0.4769 | 9.3453 | 0.2302 | 0.0829 | 0.6629 | 0.5653 | 19.3353 | 0.4178 | 19.9728 | 4.2551 | -12.0102 | 5.0452 | -9.542 | 4.4021 | -11.9741 | 0 | 0.607 | 0.3893 | 4.0528 | 0.0876 | 0.0844 | 0.3546 | 0.2922 | -0.0458 | 0.5964 |
| 22 | 3 | R P V | 0.2661 | 0.2111 | 0.055 | -0.2499 | 0.6472 | 0.5595 | 18.4324 | 0.4204 | 4.8353 | 0.0234 | 0.2427 | 0.7466 | 0.6307 | 24.5281 | 0.2759 | 9.9571 | 6.8394 | -14.1676 | 6.8388 | -12.819 | 6.8801 | -14.3019 | 1 | 0.3785 | 0.2923 | 1.5758 | 0.6452 | 0.644 | 0.749 | 0.7341 | 0.3167 | 0.4232 |
| 23 | 2 | P B | 0.2406 | 0.2036 | 0.037 | -0.4298 | 0.6584 | 0.5619 | 19.0734 | 0.3879 | 6.4954 | 0.137 | 0.1036 | 0.7019 | 0.6028 | 21.6755 | 0.3165 | 11.3341 | 4.7168 | -11.0684 | 4.8337 | -9.6901 | 4.5737 | -11.2678 | 0 | 0.6695 | 0.5691 | 4.9305 | -0.1101 | -0.1139 | 0.2148 | 0.0153 | -0.0004 | 0.0017 |
| 24 | 2 | P V | 0.2344 | 0.1971 | 0.0373 | -0.3626 | 0.6611 | 0.5653 | 19.2292 | 0.3798 | 6.2767 | 0.0963 | 0.1382 | 0.7183 | 0.6119 | 22.6991 | 0.3046 | 10.7331 | 4.4478 | -10.7708 | 4.4162 | -10.227 | 4.778 | -10.3849 | 0 | 0.4353 | 0.3033 | 2.0847 | 0.5306 | 0.529 | 0.668 | 0.664 | 0.2673 | 0.4292 |
| 25 | 1 | A | 0.186 | 0.1666 | 0.0194 | 0.4312 | 0.6817 | 0.5409 | 20.4463 | 0.3136 | 9.594 | 0.0796 | 0.1064 | 0.7249 | 0.571 | 23.1181 | 0.2427 | 8.6932 | 2.241 | -7.4573 | 2.2997 | -7.3771 | 2.282 | -7.3869 | 0 | 0.5336 | 0.4656 | 3.1319 | 0.2949 | 0.2925 | 0.5012 | 0.449 | 0.0297 | 0.5817 |
| 26 | 2 | R V | 0.1444 | 0.1027 | 0.0417 | -0.3218 | 0.6988 | 0.5843 | 21.4891 | 0.2524 | 3.4607 | -0.0627 | 0.2071 | 0.7788 | 0.6381 | 26.6904 | 0.1438 | 0.0673 | 4.8194 | -10.7085 | 4.4224 | -10.1867 | 4.8509 | -10.7672 | 0 | 0.5527 | 0.438 | 3.36 | 0.2435 | 0.2409 | 0.4649 | 0.3443 | -0.0122 | 0.4754 |
| 27 | 1 | V | 0.1422 | 0.1218 | 0.0204 | 0.3771 | 0.6997 | 0.5871 | 21.5442 | 0.2491 | 6.9648 | 0.0169 | 0.1253 | 0.7491 | 0.6222 | 24.6917 | 0.1923 | 2.2899 | 2.3422 | -7.8277 | 2.41 | -7.2394 | 2.4276 | -7.5608 | 0 | 0.558 | 0.443 | 3.4245 | 0.229 | 0.2264 | 0.4546 | 0.3143 | -0.0478 | 0.5226 |
| 28 | 2 | R P | 0.1273 | 0.0848 | 0.0426 | -0.3943 | 0.7058 | 0.5957 | 21.9187 | 0.2259 | 2.9911 | -0.0575 | 0.1848 | 0.7769 | 0.65 | 26.5598 | 0.0933 | -1.512 | 4.6861 | -10.8419 | 4.7105 | -9.8163 | 4.5564 | -10.9676 | 0 | 0.5975 | 0.3904 | 3.9267 | 0.1159 | 0.1129 | 0.3747 | 0.2288 | -0.1814 | 0.7644 |
| 29 | 1 | R | 0.0896 | 0.0679 | 0.0217 | 0.2993 | 0.7209 | 0.6086 | 22.8665 | 0.1645 | 4.1333 | -0.0376 | 0.1272 | 0.7696 | 0.6452 | 26.0601 | 0.099 | -2.7621 | 2.3458 | -8.1333 | 2.5664 | -6.9832 | 2.3818 | -8.077 | 0 | 0.6234 | 0.4713 | 4.275 | 0.0375 | 0.0342 | 0.3192 | 0.0913 | -0.1703 | 0.4988 |
| 30 | 1 | P | 0.0356 | 0.0126 | 0.023 | 0.1886 | 0.742 | 0.6201 | 24.2238 | 0.0687 | 1.5484 | -0.0403 | 0.0758 | 0.7706 | 0.648 | 26.1279 | 0.0089 | -5.7429 | 2.3181 | -7.96 | 2.468 | -7.0675 | 2.2393 | -7.8368 | 0 | 0.6456 | 0.5145 | 4.585 | -0.0323 | -0.0358 | 0.2698 | -0.0128 | -0.0051 | 0.0135 |
| 31 | 1 | B | 0.0016 | -0.0221 | 0.0238 | 0.0404 | 0.7549 | 0.6271 | 25.0759 | 0.0033 | 0.0686 | -0.0779 | 0.0795 | 0.7844 | 0.656 | 27.0724 | -0.0659 | -10.2346 | 2.4203 | -8.0319 | 2.3392 | -7.306 | 2.4127 | -8.2906 | 0 | 0.6351 | 0.5076 | 4.4375 | 0.0009 | -0.0025 | 0.2933 | 0.0037 | -0.0825 | 0.1742 |

Table S17_0.00001. Same as Table S11_0.00001 but using splitting employed as in Yu et al., 2015.

| S.No. | Size | Variables | R ² | R ² _{adj} | R ² -R ² _{adj} | ΔK | RMSE(tr) | MAE(tr) | RSS(tr) | CCC(tr) | F | Q ² _{loo} | R ² -Q ² _{loo} | RMSE(ev) | MAE(ev) | PRESS(ev) | CCC(ev) | Q ² _{LMO} | R ² _{Yser} | Q ² _{Yser} | R ² _{Xmdl} | Q ² _{Xmdl} | R ² _{Ymdl} | Q ² _{Ymdl} | N. ext. OK | RMSE(ext) | MAE(ext) | PRESS(ext) | Q ² _{F1} | Q ² _{F2} | Q ² _{F3} | CCC(ext) | \bar{r}_m^2 | Δr_m^2 |
|-------|------|--|----------------|-------------------------------|---|---------|----------|---------|---------|---------|---------|-------------------------------|---|----------|---------|-----------|---------|-------------------------------|--------------------------------|--------------------------------|--------------------------------|--------------------------------|--------------------------------|--------------------------------|------------|-----------|----------|------------|------------------------------|------------------------------|------------------------------|----------|---------------|----------------|
| 1 | 5 | B V H(HF) η(CORR) ω(DFT) | 0.8636 | 0.8456 | 0.018 | -0.0325 | 0.2791 | 0.2194 | 3.4267 | 0.9268 | 48.1064 | 0.8223 | 0.0413 | 0.3185 | 0.2553 | 4.4645 | 0.9046 | 82.6174 | 11.5853 | -23.4915 | 11.3161 | -19.2526 | 11.4759 | -23.8653 | 0 | 0.4333 | 0.3243 | 2.0652 | 0.535 | 0.5334 | 0.6711 | 0.8333 | 0.579 | 0.2301 |
| 2 | 5 | B V E ^{HOMO} (CORR) - E ^{LUMO} (CORR) H(HF) ω(DFT) | 0.8636 | 0.8456 | 0.018 | -0.0325 | 0.2791 | 0.2194 | 3.4267 | 0.9268 | 48.1064 | 0.8223 | 0.0413 | 0.3185 | 0.2553 | 4.4645 | 0.9046 | 82.7514 | 11.7598 | -22.47 | 11.7538 | -18.7971 | 11.5901 | -22.9967 | 0 | 0.4333 | 0.3243 | 2.0652 | 0.535 | 0.5334 | 0.6711 | 0.8333 | 0.579 | 0.2301 |
| 3 | 5 | B V E(HF) η(CORR) ω(DFT) | 0.8636 | 0.8456 | 0.018 | -0.0325 | 0.2791 | 0.2194 | 3.4267 | 0.9268 | 48.1064 | 0.8223 | 0.0413 | 0.3185 | 0.2553 | 4.4645 | 0.9046 | 82.577 | 11.23 | -24.5279 | 11.7791 | -18.6654 | 11.6717 | -23.3822 | 0 | 0.4333 | 0.3243 | 2.0652 | 0.535 | 0.5334 | 0.6711 | 0.8333 | 0.579 | 0.2301 |
| 4 | 5 | B V E(HF) E ^{HOMO} (CORR) - E ^{LUMO} (CORR) ω(DFT) | 0.8636 | 0.8456 | 0.018 | -0.0325 | 0.2791 | 0.2194 | 3.4267 | 0.9268 | 48.1064 | 0.8223 | 0.0413 | 0.3185 | 0.2553 | 4.4645 | 0.9046 | 82.5225 | 11.6191 | -22.8548 | 11.9363 | -18.2628 | 11.6697 | -23.7489 | 0 | 0.4333 | 0.3243 | 2.0652 | 0.535 | 0.5334 | 0.6711 | 0.8333 | 0.579 | 0.2301 |
| 5 | 5 | B ZPE(CORR) α(HF) H(HF) ω(DFT) | 0.8619 | 0.8438 | 0.0182 | 0.002 | 0.2807 | 0.2182 | 3.4681 | 0.9258 | 47.4412 | 0.8252 | 0.0367 | 0.3159 | 0.2486 | 4.3899 | 0.9073 | 82.4558 | 11.9945 | -22.851 | 10.9811 | -19.5489 | 11.167 | -23.4882 | 5 | 0.2876 | 0.2313 | 0.9096 | 0.7952 | 0.7945 | 0.8551 | 0.8978 | 0.7336 | 0.0246 |
| 6 | 5 | B E(HF) ZPE(CORR) α(HF) ω(DFT) | 0.8619 | 0.8438 | 0.0182 | 0.002 | 0.2807 | 0.2182 | 3.4681 | 0.9258 | 47.4412 | 0.8252 | 0.0367 | 0.3159 | 0.2486 | 4.3899 | 0.9073 | 82.3293 | 11.4621 | -23.0423 | 11.6086 | -18.8663 | 11.1761 | -23.976 | 5 | 0.2876 | 0.2313 | 0.9096 | 0.7952 | 0.7945 | 0.8551 | 0.8978 | 0.7336 | 0.0246 |
| 7 | 5 | B ZPE(CORR) α(HF) G(HF) ω(DFT) | 0.8619 | 0.8438 | 0.0182 | 0.002 | 0.2807 | 0.2182 | 3.4681 | 0.9258 | 47.4412 | 0.8252 | 0.0367 | 0.3159 | 0.2486 | 4.3899 | 0.9073 | 82.2919 | 11.1695 | -23.0674 | 11.4614 | -18.9204 | 11.2999 | -23.3668 | 5 | 0.2876 | 0.2313 | 0.9096 | 0.7952 | 0.7945 | 0.8551 | 0.8978 | 0.7336 | 0.0246 |
| 8 | 5 | B ZPE(CORR) α(HF) H(DFT) ω(DFT) | 0.8619 | 0.8437 | 0.0182 | 0.0018 | 0.2808 | 0.2182 | 3.4683 | 0.9258 | 47.4383 | 0.8252 | 0.0367 | 0.3159 | 0.2486 | 4.3897 | 0.9073 | 82.2832 | 11.8994 | -22.2672 | 11.713 | -18.6854 | 11.2856 | -23.3207 | 5 | 0.2877 | 0.2314 | 0.9104 | 0.795 | 0.7943 | 0.855 | 0.8977 | 0.7334 | 0.0246 |
| 9 | 5 | B E(DFT) ZPE(CORR) α(HF) ω(DFT) | 0.8619 | 0.8437 | 0.0182 | 0.0018 | 0.2808 | 0.2182 | 3.4683 | 0.9258 | 47.4383 | 0.8252 | 0.0367 | 0.3159 | 0.2486 | 4.3897 | 0.9073 | 82.2665 | 11.7567 | -22.8752 | 11.2826 | -19.2871 | 11.3618 | -23.3684 | 5 | 0.2877 | 0.2314 | 0.9104 | 0.795 | 0.7943 | 0.855 | 0.8977 | 0.7334 | 0.0246 |
| 10 | 5 | B ZPE(CORR) α(HF) G(DFT) ω(DFT) | 0.8619 | 0.8437 | 0.0182 | 0.0018 | 0.2808 | 0.2182 | 3.4683 | 0.9258 | 47.4382 | 0.8252 | 0.0367 | 0.3159 | 0.2486 | 4.3897 | 0.9073 | 82.1363 | 11.832 | -22.24 | 11.4018 | -19.1995 | 11.2565 | -23.2435 | 5 | 0.2877 | 0.2314 | 0.9104 | 0.795 | 0.7943 | 0.855 | 0.8977 | 0.7334 | 0.0246 |
| 11 | 4 | B V η(CORR) ω(DFT) | 0.8386 | 0.822 | 0.0166 | -0.1104 | 0.3035 | 0.2347 | 4.0539 | 0.9122 | 50.6584 | 0.8019 | 0.0367 | 0.3363 | 0.2623 | 4.9749 | 0.8927 | 79.6351 | 8.8935 | -18.0625 | 9.3548 | -15.6734 | 9.1305 | -18.1914 | 1 | 0.4134 | 0.2945 | 1.8796 | 0.5768 | 0.5754 | 0.7007 | 0.8394 | 0.6389 | 0.2036 |
| 12 | 4 | B V E ^{HOMO} (CORR) - E ^{LUMO} (CORR) ω(DFT) | 0.8386 | 0.822 | 0.0166 | -0.1104 | 0.3035 | 0.2347 | 4.0539 | 0.9122 | 50.6584 | 0.8019 | 0.0367 | 0.3363 | 0.2623 | 4.9749 | 0.8927 | 79.7684 | 9.5576 | -17.2336 | 9.583 | -15.2517 | 9.1701 | -17.3865 | 1 | 0.4134 | 0.2945 | 1.8796 | 0.5768 | 0.5754 | 0.7007 | 0.8394 | 0.6389 | 0.2036 |
| 13 | 4 | B E(DFT) ZPE(CORR) α(DFT) | 0.8362 | 0.8194 | 0.0168 | -0.0562 | 0.3058 | 0.2429 | 4.1152 | 0.9108 | 49.7578 | 0.7996 | 0.0365 | 0.3382 | 0.2735 | 5.0322 | 0.8927 | 79.4377 | 8.9868 | -19.4268 | 9.1134 | -15.9393 | 9.6106 | -18.5371 | 5 | 0.2843 | 0.2431 | 0.8893 | 0.7998 | 0.7991 | 0.8584 | 0.9031 | 0.7431 | 0.0352 |
| 14 | 4 | B ZPE(CORR) α(DFT) H(DFT) | 0.8362 | 0.8194 | 0.0168 | -0.0562 | 0.3058 | 0.2429 | 4.1152 | 0.9108 | 49.7578 | 0.7996 | 0.0365 | 0.3382 | 0.2735 | 5.0322 | 0.8927 | 79.1835 | 9.6434 | -19.2085 | 9.4699 | -15.3748 | 9.9704 | -19.8554 | 5 | 0.2843 | 0.2431 | 0.8893 | 0.7998 | 0.7991 | 0.8584 | 0.9031 | 0.7431 | 0.0352 |
| 15 | 4 | B ZPE(CORR) α(DFT) G(DFT) | 0.8362 | 0.8194 | 0.0168 | -0.0562 | 0.3058 | 0.2429 | 4.1152 | 0.9108 | 49.7578 | 0.7996 | 0.0365 | 0.3382 | 0.2735 | 5.0323 | 0.8927 | 79.266 | 9.688 | -19.3689 | 9.4564 | -15.6115 | 9.25 | -19.5098 | 5 | 0.2843 | 0.2431 | 0.8893 | 0.7998 | 0.7991 | 0.8584 | 0.9031 | 0.7431 | 0.0352 |
| 16 | 4 | B ZPE(CORR) α(DFT) H(HF) | 0.8361 | 0.8193 | 0.0168 | -0.0558 | 0.3058 | 0.2429 | 4.1157 | 0.9108 | 49.7511 | 0.7996 | 0.0365 | 0.3382 | 0.2735 | 5.033 | 0.8927 | 79.2129 | 9.3614 | -19.6646 | 9.7253 | -15.0835 | 9.3707 | -19.3548 | 5 | 0.2842 | 0.243 | 0.8883 | 0.8 | 0.7993 | 0.8585 | 0.9032 | 0.7434 | 0.0351 |
| 17 | 4 | B E(HF) ZPE(CORR) α(DFT) | 0.8361 | 0.8193 | 0.0168 | -0.0558 | 0.3058 | 0.2429 | 4.1157 | 0.9108 | 49.7511 | 0.7996 | 0.0365 | 0.3382 | 0.2735 | 5.033 | 0.8927 | 79.4495 | 8.9157 | -20.4585 | 9.178 | -15.9637 | 9.3834 | -20.264 | 5 | 0.2842 | 0.243 | 0.8883 | 0.8 | 0.7993 | 0.8585 | 0.9032 | 0.7434 | 0.0351 |
| 18 | 4 | B ZPE(CORR) α(DFT) G(HF) | 0.8361 | 0.8193 | 0.0168 | -0.0558 | 0.3058 | 0.2429 | 4.1157 | 0.9108 | 49.7511 | 0.7996 | 0.0365 | 0.3382 | 0.2735 | 5.033 | 0.8927 | 79.2198 | 9.2835 | -19.7658 | 9.0925 | -15.7744 | 9.3453 | -20.1361 | 5 | 0.2842 | 0.243 | 0.8883 | 0.8 | 0.7993 | 0.8585 | 0.9032 | 0.7434 | 0.0351 |
| 19 | 4 | B ELUMO(HF) α(HF) G(HF) | 0.8326 | 0.8155 | 0.0172 | -0.0237 | 0.3091 | 0.2435 | 4.2039 | 0.9087 | 48.5024 | 0.7985 | 0.0341 | 0.3391 | 0.2722 | 5.0608 | 0.8907 | 79.0514 | 9.0714 | -19.5674 | 9.4364 | -15.5405 | 9.283 | -19.1972 | 5 | 0.2549 | 0.2215 | 0.7147 | 0.8391 | 0.8385 | 0.8862 | 0.9119 | 0.7695 | 0.1371 |
| 20 | 4 | B E(HF) ELUMO(HF) α(HF) | 0.8326 | 0.8155 | 0.0172 | -0.0237 | 0.3091 | 0.2435 | 4.2039 | 0.9087 | 48.5024 | 0.7985 | 0.0341 | 0.3391 | 0.2722 | 5.0608 | 0.8907 | 79.2123 | 9.4139 | -18.4032 | 9.1394 | -15.8559 | 9.0777 | -19.1748 | 5 | 0.2549 | 0.2215 | 0.7147 | 0.8391 | 0.8385 | 0.8862 | 0.9119 | 0.7695 | 0.1371 |
| 21 | 3 | B α(DFT) G(DFT) | 0.8177 | 0.804 | 0.0137 | -0.0499 | 0.3226 | 0.2643 | 4.5795 | 0.8997 | 59.7955 | 0.7828 | 0.0349 | 0.3521 | 0.292 | 5.4563 | 0.8814 | 77.4014 | 7.2747 | -14.632 | 7.2099 | -12.4911 | 6.9792 | -15.1976 | 5 | 0.264 | 0.2258 | 0.7667 | 0.8274 | 0.8268 | 0.8779 | 0.8997 | 0.7103 | 0.1604 |
| 22 | 3 | B E(DFT) α(DFT) | 0.8177 | 0.804 | 0.0137 | -0.0499 | 0.3226 | 0.2643 | 4.5795 | 0.8997 | 59.7955 | 0.7828 | 0.0349 | 0.3521 | 0.292 | 5.4563 | 0.8814 | 77.4576 | 7.1279 | -15.4278 | 6.8716 | -12.7698 | 6.5851 | -16.0043 | 5 | 0.264 | 0.2258 | 0.7667 | 0.8274 | 0.8268 | 0.8779 | 0.8997 | 0.7103 | 0.1604 |
| 23 | 3 | B α(DFT) H(DFT) | 0.8177 | 0.804 | 0.0137 | -0.0499 | 0.3226 | 0.2643 | 4.5795 | 0.8997 | 59.7955 | 0.7828 | 0.0349 | 0.3521 | 0.292 | 5.4563 | 0.8814 | 77.1826 | 7.6128 | -14.1059 | 6.6243 | -13.2917 | 7.0515 | -15.0646 | 5 | 0.264 | 0.2258 | 0.7667 | 0.8274 | 0.8268 | 0.8779 | 0.8997 | 0.7103 | 0.1604 |
| 24 | 3 | B α(DFT) G(HF) | 0.8177 | 0.804 | 0.0137 | -0.0492 | 0.3226 | 0.2643 | 4.5796 | 0.8997 | 59.7932 | 0.7828 | 0.0349 | 0.3521 | 0.292 | 5.4564 | 0.8814 | 77.4457 | 7.2541 | -15.2267 | 6.5193 | -13.28 | 7.3167 | -14.536 | 5 | 0.2639 | 0.2257 | 0.7662 | 0.8275 | 0.8269 | 0.878 | 0.8998 | 0.7104 | 0.1603 |
| 25 | 3 | B α(HF) G(DFT) | 0.8169 | 0.8031 | 0.0137 | -0.0467 | 0.3233 | 0.2581 | 4.5996 | 0.8992 | 59.4756 | 0.7871 | 0.0298 | 0.3487 | 0.2816 | 5.3486 | 0.8842 | 77.7386 | 7.0909 | -15.0915 | 7.0698 | -12.5915 | 6.7686 | -15.4454 | 5 | 0.248 | 0.2244 | 0.6764 | 0.8477 | 0.8472 | 0.8923 | 0.9143 | 0.7551 | 0.1403 |
| 26 | 3 | B E(DFT) α(HF) | 0.8169 | 0.8031 | 0.0137 | -0.0467 | 0.3233 | 0.2581 | 4.5996 | 0.8992 | 59.4756 | 0.7871 | 0.0298 | 0.3487 | 0.2816 | 5.3486 | 0.8842 | 77.773 | 6.8804 | -15.9993 | 7.0256 | -12.6007 | 7.0223 | -15.3026 | 5 | 0.248 | 0.2244 | 0.6764 | 0.8477 | 0.8472 | 0.8923 | 0.9143 | 0.7551 | 0.1403 |
| 27 | 3 | B α(HF) H(DFT) | 0.8169 | 0.8031 | 0.0137 | -0.0467 | 0.3233 | 0.2581 | 4.5996 | 0.8992 | 59.4755 | 0.7871 | 0.0298 | 0.3487 | 0.2816 | 5.3486 | 0.8842 | 77.3993 | 7.057 | -14.7461 | 6.6316 | -13.1098 | 7.0602 | -15.5971 | 5 | 0.248 | 0.2244 | 0.6764 | 0.8477 | 0.8472 | 0.8923 | 0.9143 | 0.7551 | 0.1403 |
| 28 | 3 | B α(HF) G(HF) | 0.8169 | 0.8031 | 0.0137 | -0.046 | 0.3233 | 0.2581 | 4.6 | 0.8992 | 59.4692 | 0.787 | 0.0298 | 0.3487 | 0.2816 | 5.349 | 0.8842 | 77.6333 | 7.152 | -15.1923 | 7.3101 | -12.4373 | 6.8845 | -15.3045 | 5 | 0.2479 | 0.2244 | 0.6759 | 0. | | | | | |