

Supplementary Information

Anatomy of the Substituent Effect in Complex N-heterocycles

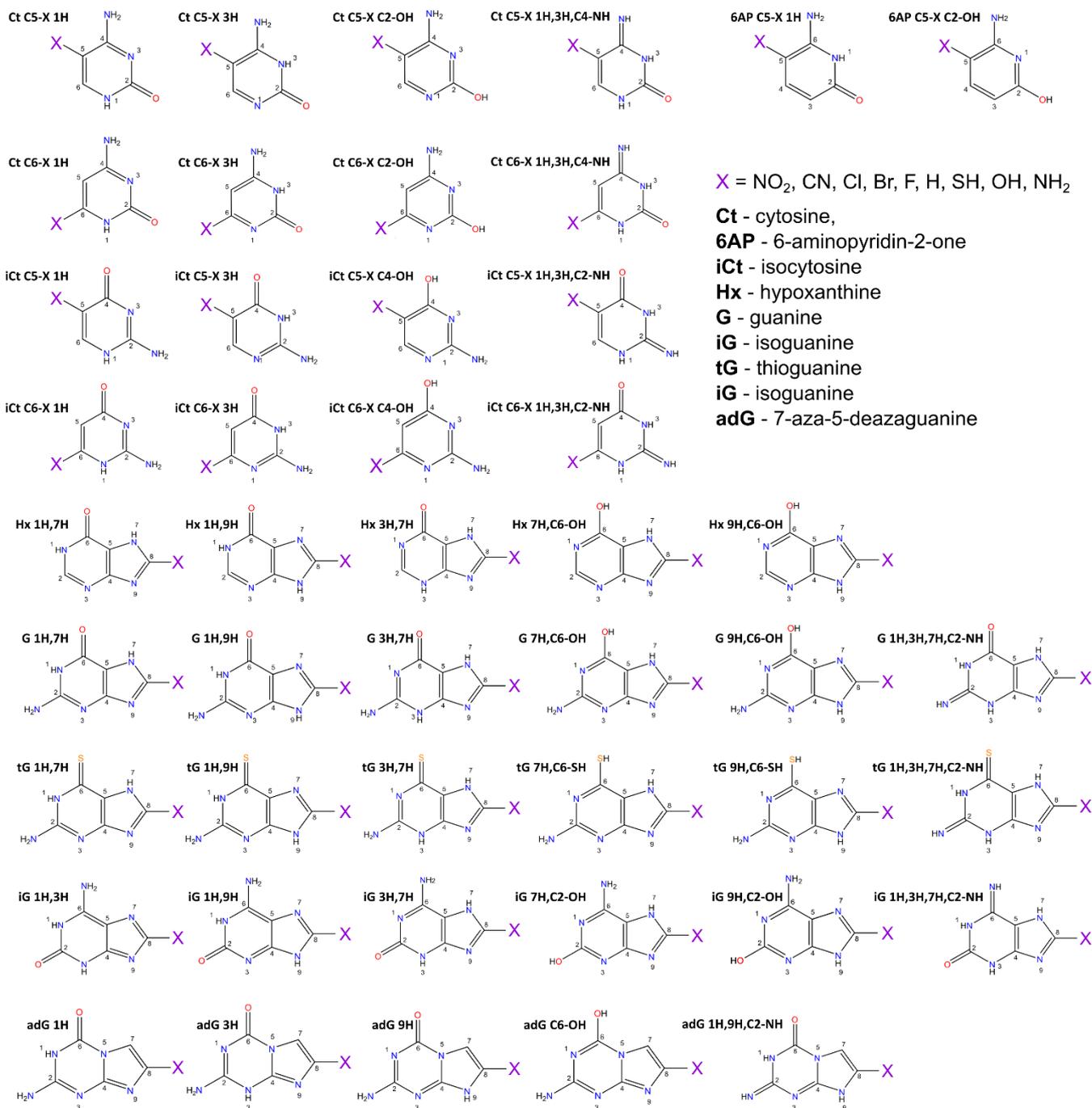
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Scheme S1. Chemical structures of all studied systems.

Table S1. Calculated Gibbs energies, $\Delta G/\text{kcal}\cdot\text{mol}^{-1}$ relative to the lowest energy tautomer for each substituent (green shaded cell in each row).

| Ct C5-X | 1H | 3H | C2-OH | 1H,3H,C4-NH | Ct C6-X | 1H | 3H | C2-OH | 1H,3H,C4-NH | 6-AP C5-X | 1H | C2-OH | |
|----------|-------|-------|-------|-------------|-------------|----------------|---------|-------|-------------|-----------|----------|----------|----------------|
| NO2 | 0.00 | 3.60 | 0.39 | 3.61 | NO2 | 0.73 | 6.54 | 0.00 | 2.18 | NO2 | 0.57 | 0.00 | |
| CN | 0.00 | 4.82 | 0.50 | 2.30 | CN | 1.19 | 6.51 | 0.00 | 2.45 | CN | 2.53 | 0.00 | |
| Br | 0.37 | 7.21 | 0.00 | 1.89 | Br | 1.16 | 4.62 | 0.00 | 2.68 | Br | 3.99 | 0.00 | |
| Cl | 0.08 | 7.37 | 0.00 | 1.51 | Cl | 1.16 | 4.56 | 0.00 | 2.84 | Cl | 4.28 | 0.00 | |
| F | 0.00 | 9.14 | 0.32 | 1.00 | F | 3.23 | 3.91 | 0.00 | 5.55 | F | 5.61 | 0.00 | |
| H | 0.00 | 7.15 | 1.32 | 0.69 | H | 0.00 | 7.15 | 1.32 | 0.69 | H | 3.08 | 0.00 | |
| SH | 0.00 | 5.97 | 0.80 | 1.20 | SH | 2.25 | 3.86 | 0.00 | 3.43 | SH | 2.96 | 0.00 | |
| OH | 3.83 | 12.16 | 3.36 | 0.00 | OH | 4.73 | 2.35 | 0.00 | 6.37 | OH | 5.38 | 0.00 | |
| NH2 | 0.76 | 6.69 | 1.32 | 0.00 | NH2 | 2.70 | 2.70 | 0.00 | 4.79 | NH2 | 3.64 | 0.00 | |
| iCt C5-X | 1H | 3H | C4-OH | 1H,3H,C2-NH | iCt C6-X | 1H | 3H | C4-OH | 1H,3H,C2-NH | | | | |
| NO2 | 16.73 | 5.69 | 0.00 | 12.32 | NO2 | 11.66 | 1.38 | 0.00 | 9.00 | | | | |
| CN | 11.38 | 0.60 | 0.00 | 7.08 | CN | 12.64 | 1.04 | 0.00 | 9.24 | | | | |
| Br | 9.85 | 0.01 | 0.00 | 7.88 | Br | 13.48 | 1.40 | 0.00 | 9.28 | | | | |
| Cl | 9.75 | 0.03 | 0.00 | 7.86 | Cl | 13.84 | 1.57 | 0.00 | 9.48 | | | | |
| F | 9.03 | 0.00 | 0.47 | 7.02 | F | 16.95 | 1.77 | 0.00 | 11.85 | | | | |
| H | 10.45 | 0.49 | 0.00 | 5.55 | H | 10.45 | 0.49 | 0.00 | 5.55 | | | | |
| SH | 8.08 | 0.00 | 1.37 | 6.64 | SH | 14.54 | 1.21 | 0.00 | 9.62 | | | | |
| OH | 5.60 | 0.00 | 3.49 | 6.75 | OH | 17.01 | 2.06 | 0.00 | 13.04 | | | | |
| NH2 | 7.56 | 0.00 | 2.75 | 7.10 | NH2 | 16.91 | 1.02 | 0.00 | 10.65 | | | | |
| G C8-X | 3H,7H | 1H,7H | 1H,9H | 9H,C6-OH | 7H,C6-OH | 1H,3H,7H,C2-NH | Hx C8-X | 3H,7H | 1H,7H | 1H,9H | 9H,C6-OH | 7H,C6-OH | |
| NO2 | 8.30 | 1.51 | 0.00 | 2.45 | 7.03 | 7.73 | NO2 | 8.67 | 0.55 | 0.00 | 7.59 | 9.01 | |
| CN | 7.69 | 1.18 | 0.00 | 2.60 | 7.10 | 7.18 | CN | 8.26 | 0.42 | 0.00 | 7.53 | 9.12 | |
| Br | 7.39 | 0.37 | 0.00 | 2.16 | 5.59 | 6.36 | Br | 8.19 | 0.00 | 0.09 | 6.67 | 7.98 | |
| Cl | 7.35 | 0.24 | 0.00 | 2.13 | 5.37 | 6.24 | Cl | 8.19 | 0.00 | 0.17 | 6.54 | 7.80 | |
| F | 7.48 | 0.00 | 0.19 | 1.91 | 4.73 | 6.31 | F | 8.46 | 0.00 | 0.40 | 6.41 | 7.44 | |
| H | 6.69 | 0.25 | 0.00 | 2.41 | 5.90 | 5.30 | H | 7.70 | 0.00 | 0.19 | 6.66 | 8.20 | |
| SH | 7.24 | 0.00 | 0.18 | 2.23 | 5.07 | 5.78 | SH | 8.44 | 0.00 | 0.39 | 6.83 | 7.59 | |
| OH | 7.95 | 0.00 | 0.78 | 2.28 | 4.36 | 6.33 | OH | 8.89 | 0.00 | 0.71 | 6.63 | 6.86 | |
| NH2 | 7.35 | 0.00 | 1.07 | 2.60 | 4.52 | 5.56 | NH2 | 8.19 | 0.00 | 0.96 | 6.33 | 6.90 | |
| tG C8-x | 3H,7H | 1H,7H | 1H,9H | 9H,C6-SH | 7H,C6-SH | 1H,3H,7H,C2-NH | iG C8-X | 3H,7H | 1H,3H | 1H,9H | 9H,C2-OH | 7H,C2-OH | 1H,3H,7H,C6-NH |
| NO2 | 9.35 | 1.89 | 2.63 | 0.00 | 5.71 | 8.84 | NO2 | 7.12 | 1.65 | 4.71 | 0.00 | 9.24 | 2.19 |
| CN | 8.52 | 1.46 | 2.58 | 0.00 | 5.73 | 8.08 | CN | 7.07 | 0.16 | 4.69 | 0.00 | 9.56 | 1.51 |
| Br | 8.89 | 0.95 | 3.04 | 0.00 | 4.67 | 7.88 | Br | 6.94 | 1.60 | 5.13 | 0.00 | 8.67 | 1.78 |
| Cl | 8.86 | 0.89 | 3.03 | 0.00 | 4.50 | 7.82 | Cl | 6.84 | 1.60 | 5.15 | 0.00 | 8.62 | 1.91 |
| F | 9.26 | 0.77 | 3.36 | 0.00 | 4.09 | 8.11 | F | 7.12 | 0.00 | 5.20 | 0.30 | 8.39 | 2.46 |
| H | 7.90 | 0.61 | 2.80 | 0.00 | 4.71 | 6.70 | H | 6.30 | 3.85 | 5.29 | 0.00 | 8.89 | 0.85 |
| SH | 8.74 | 0.30 | 2.93 | 0.00 | 3.94 | 7.36 | SH | 6.02 | 1.75 | 5.11 | 0.00 | 7.77 | 1.20 |
| OH | 9.56 | 0.25 | 3.35 | 0.00 | 3.26 | 7.86 | OH | 5.43 | 2.27 | 4.63 | 0.00 | 6.42 | 1.22 |
| NH2 | 8.65 | 0.00 | 3.92 | 0.40 | 3.52 | 6.85 | NH2 | 5.25 | 0.00 | 4.57 | 0.20 | 6.69 | 0.70 |
| adG C8-X | 3H | 1H | 9H | C6-OH | 1H,9H,C2-NH | | | | | | | | |
| NO2 | 3.08 | 0.00 | 0.88 | 9.12 | 8.56 | | | | | | | | |
| CN | 2.87 | 0.00 | 0.94 | 9.42 | 8.79 | | | | | | | | |
| Br | 3.39 | 0.00 | 0.60 | 9.29 | 8.25 | | | | | | | | |
| Cl | 3.51 | 0.00 | 0.99 | 9.34 | 8.68 | | | | | | | | |
| F | 3.94 | 0.00 | 3.80 | 9.07 | 11.31 | | | | | | | | |
| H | 5.57 | 2.55 | 0.00 | 12.33 | 7.80 | | | | | | | | |
| SH | 4.87 | 0.82 | 0.00 | 10.02 | 7.61 | | | | | | | | |
| OH | 4.77 | 0.00 | 3.33 | 8.54 | 10.66 | | | | | | | | |
| NH2 | 4.41 | 0.00 | 1.20 | 8.98 | 8.17 | | | | | | | | |

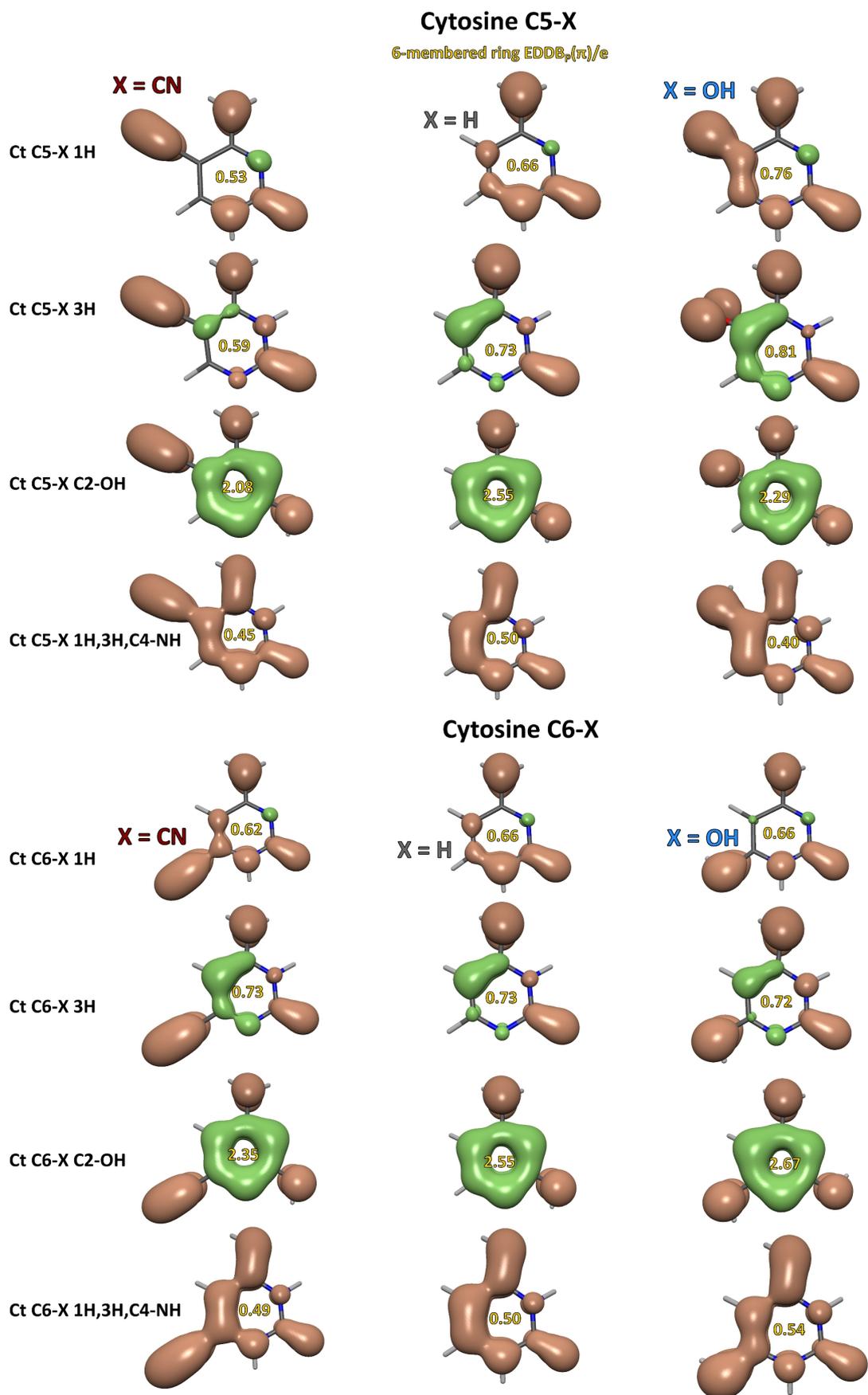
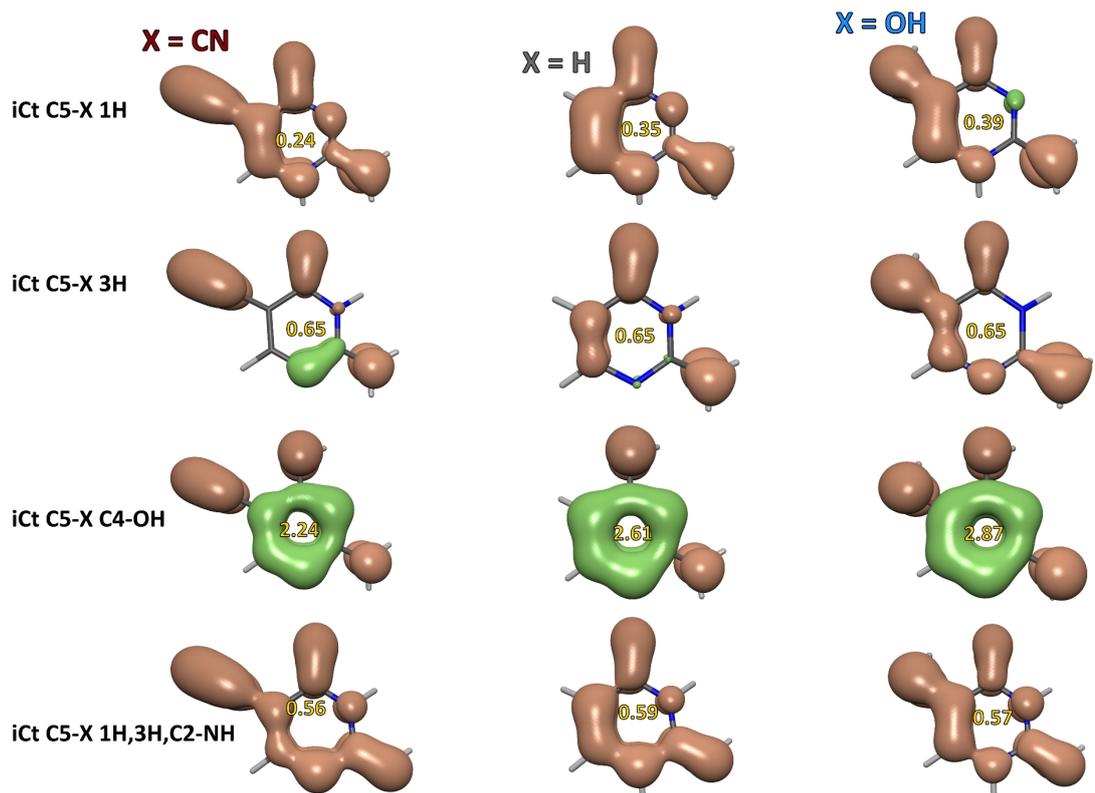


Figure S1. BDF_π maps of selected cytosine derivatives (isovalue = +/-0.015) and EDDB_p(π) populations of cyclically delocalized π -electrons. Green coloring, BDF_π > 0, indicates regions where π -electrons are mostly delocalized, brown localized, BDF_π < 0.

isoCytosine C5-X
6-membered ring EDDB_p(π)/e



isoCytosine C6-X

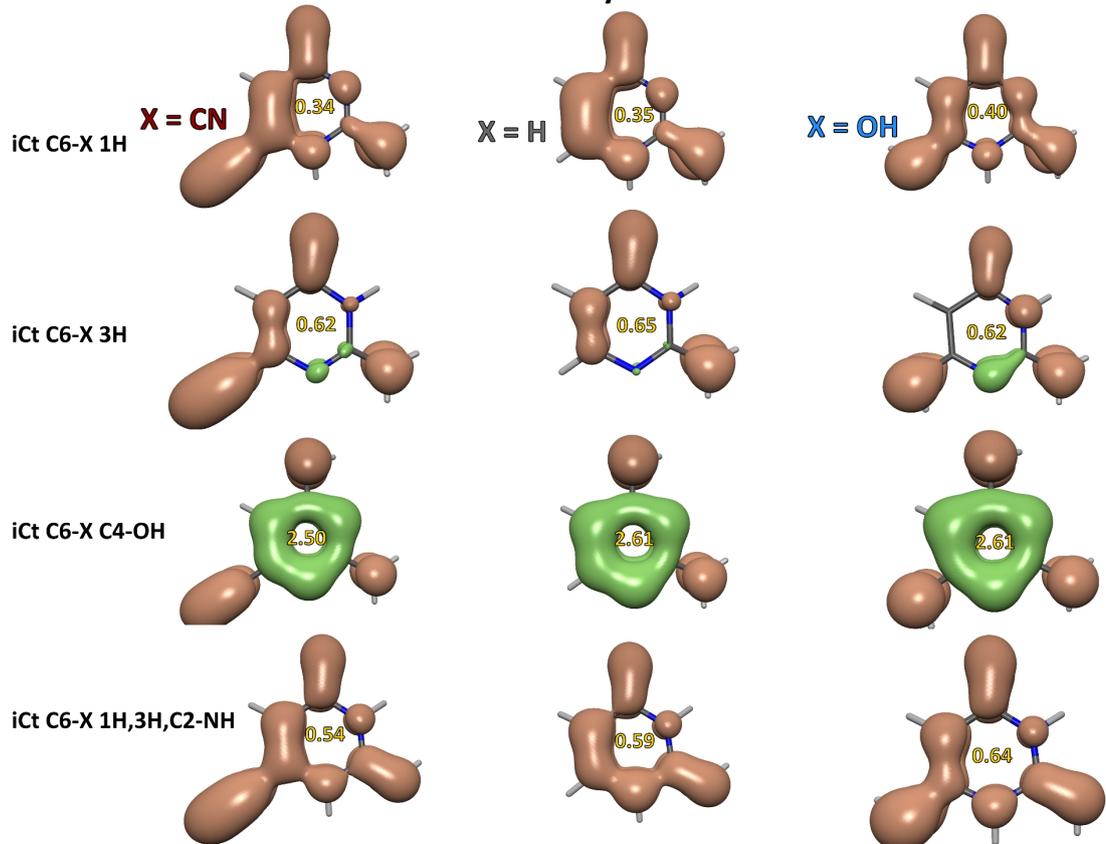


Figure S2. BDF π maps of selected isocytosine derivatives (isovalue = ± 0.015) and EDDB_p(π) populations of cyclically delocalized π -electrons. Green coloring, BDF π > 0, indicates regions where π -electrons are mostly delocalized, brown localized, BDF π < 0.

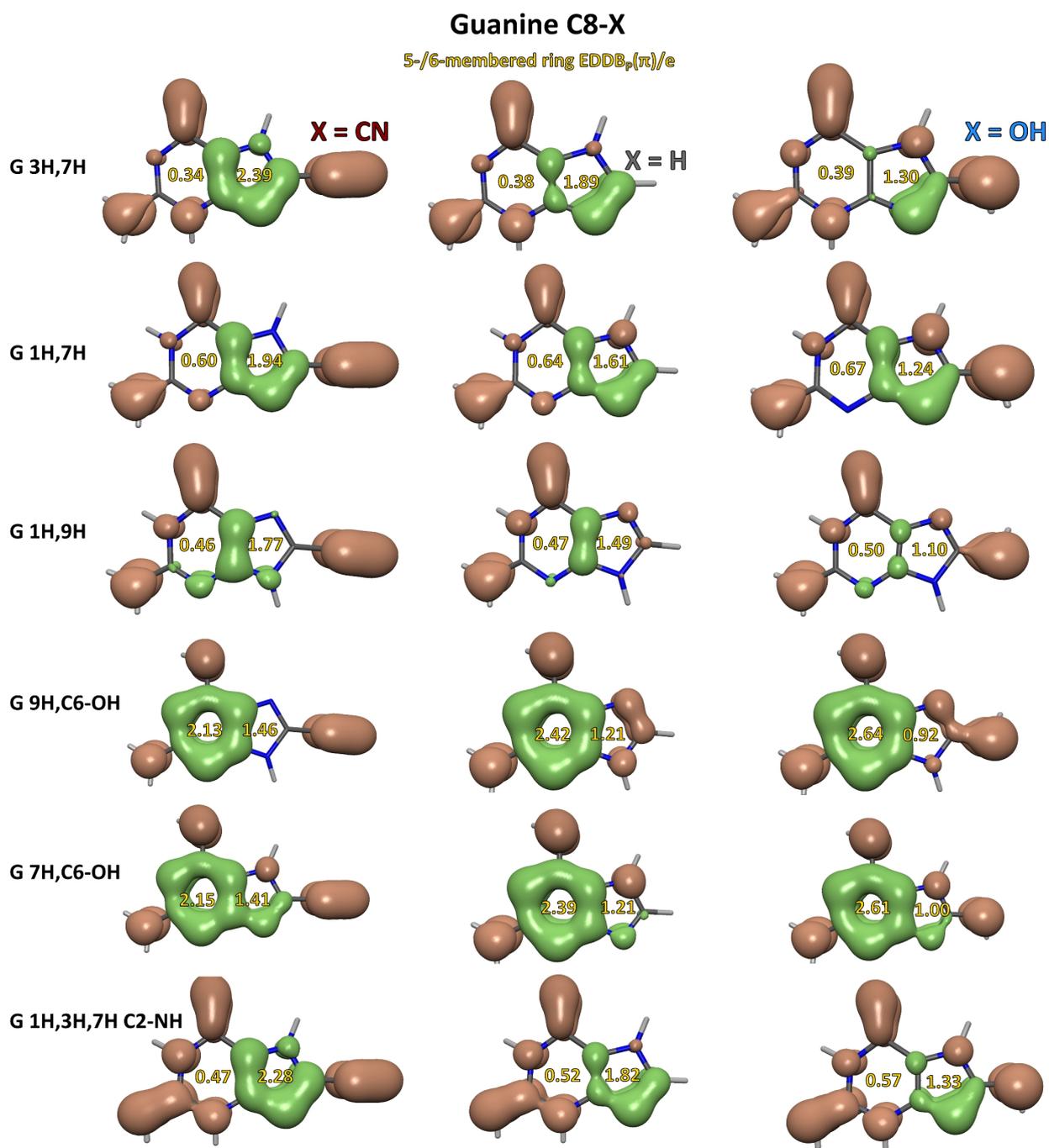


Figure S3. BDF_π maps of selected guanine derivatives (isovalue = ± 0.015) and EDDB_p(π) populations of cyclically delocalized π -electrons. Green coloring, BDF_π > 0, indicates regions where π -electrons are mostly delocalized, brown localized, BDF_π < 0.

Hypoxantine C8-X
5-/6-membered ring EDDB_p(π)/e

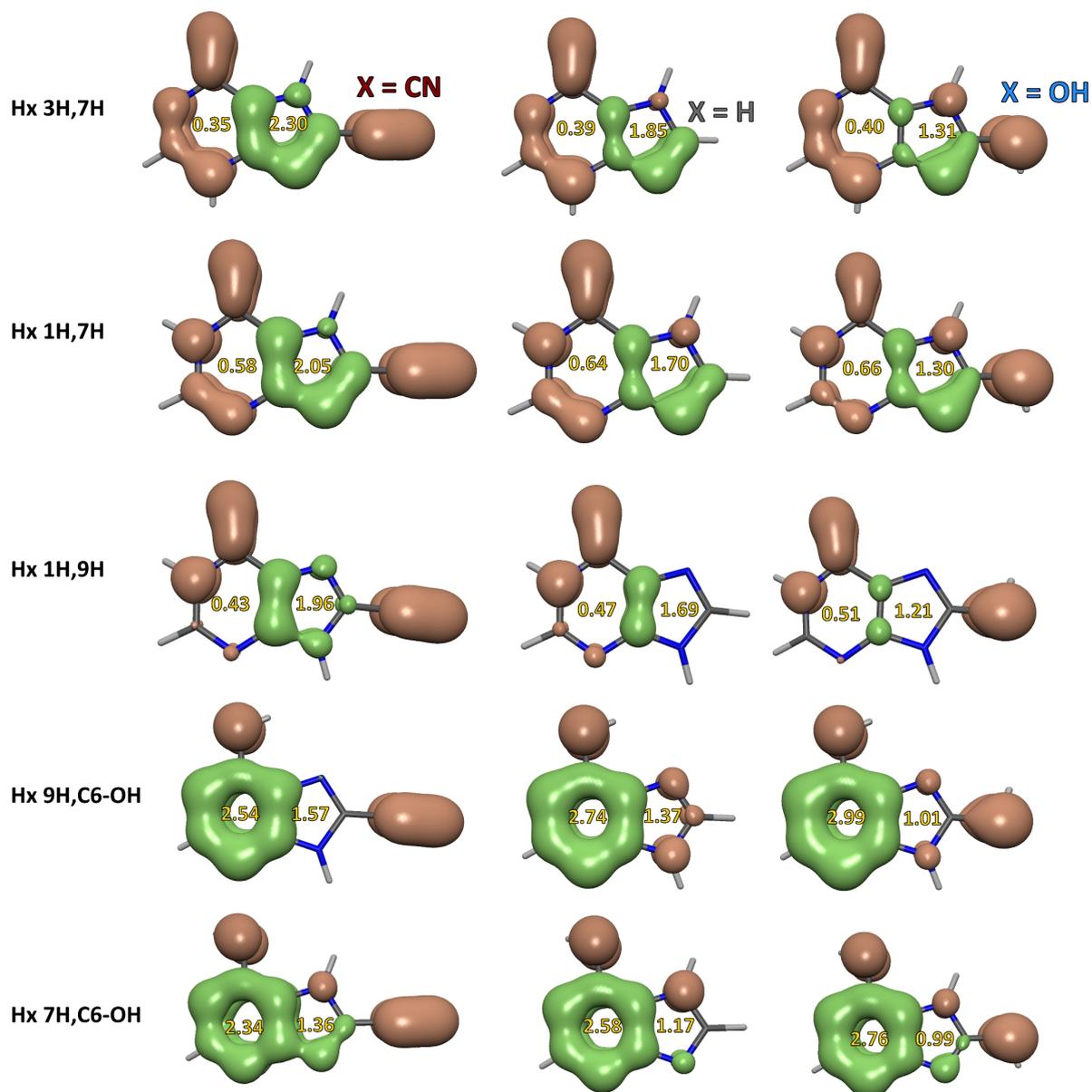


Figure S4. BDF π maps of selected hypoxanthine derivatives (isovalue = ± 0.015) and EDDB_p(π) populations of cyclically delocalized π -electrons. Green coloring, BDF π > 0, indicates regions where π -electrons are mostly delocalized, brown localized, BDF π < 0.

thioGuanine C8-X

5-/6-membered ring EDDB_p(π)/e

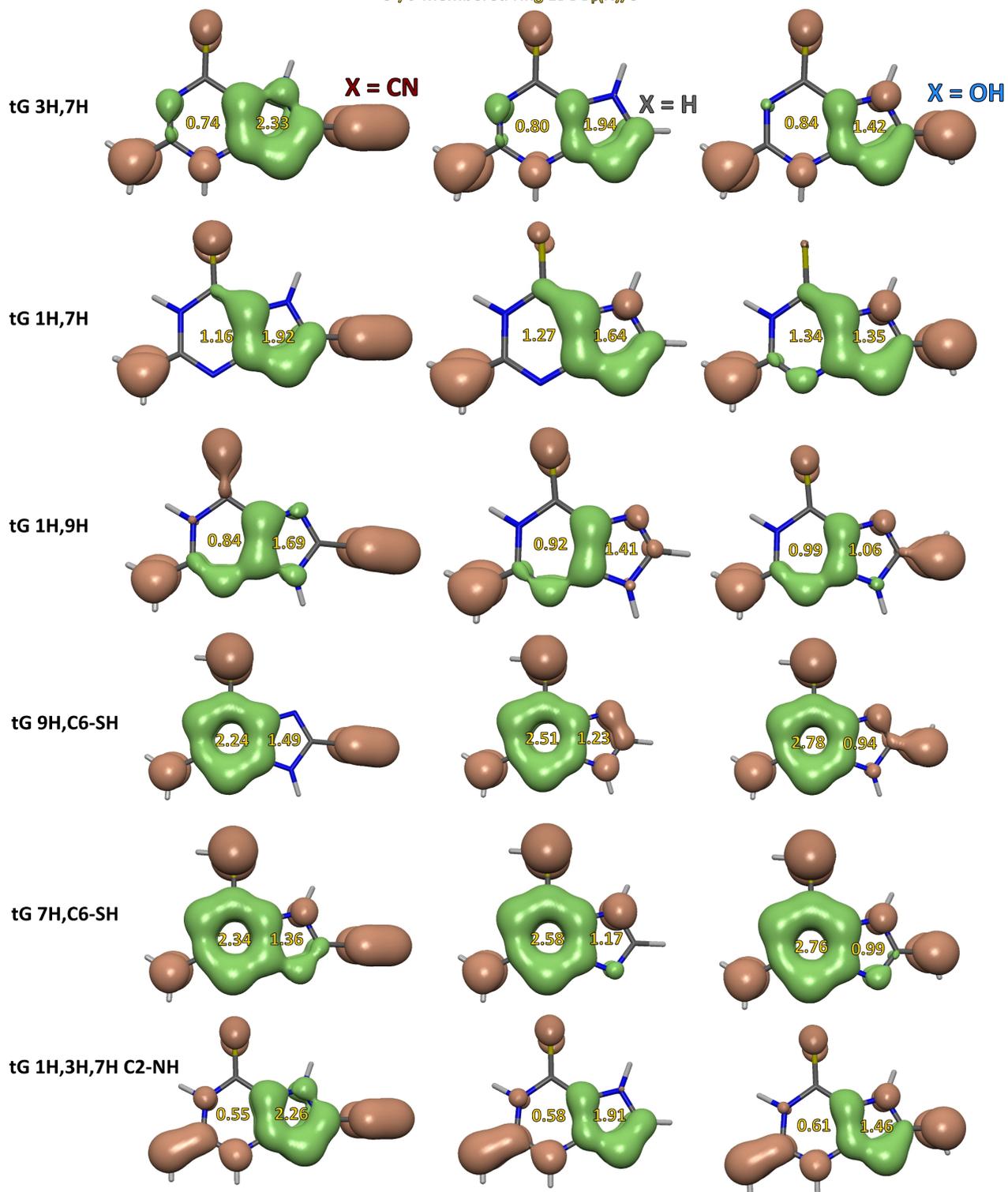


Figure S5. BDF π maps of selected thioguanine derivatives (isovalue = ± 0.015) and EDDB_p(π) populations of cyclically delocalized π -electrons. Green coloring, BDF π > 0, indicates regions where π -electrons are mostly delocalized, brown localized, BDF π < 0.

isoGuanine C8-X

5-/6-membered ring EDDB_r(π)/e

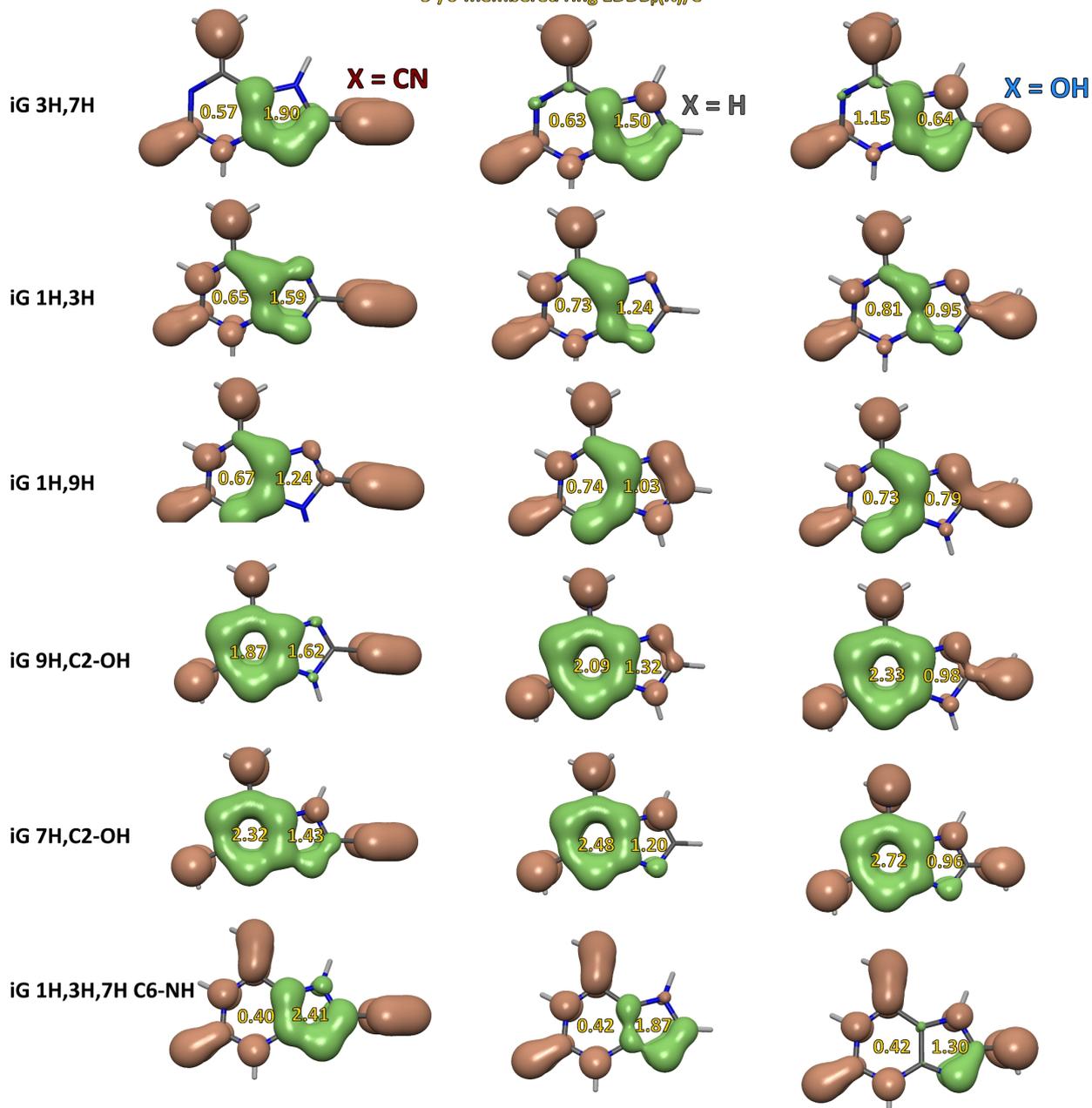


Figure S6. BDF π maps of selected isoguanine derivatives (isovalue = ± 0.015) and EDDB_r(π) populations of cyclically delocalized π -electrons. Green coloring, BDF π > 0, indicates regions where π -electrons are mostly delocalized, brown localized, BDF π < 0.

5-aza-7-deazaGuanine C8-X

5-/6-membered ring EDDB_p(π)/e

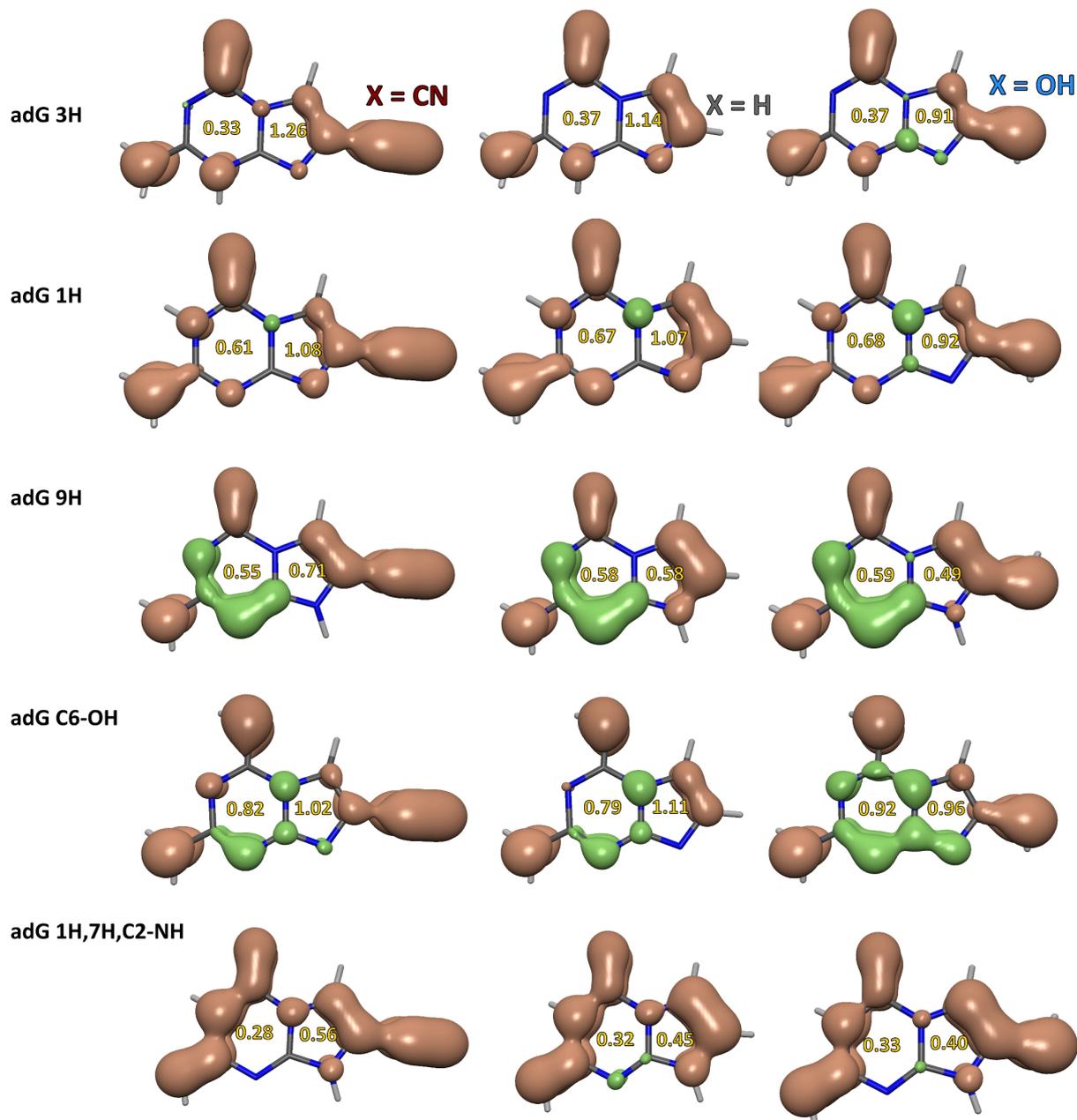


Figure S7. BDF π maps of selected 5-aza-7-deazaguanine derivatives (isovalue = ± 0.015) and EDDB_p(π) populations of cyclically delocalized π -electrons. Green coloring, BDF π > 0, indicates regions where π -electrons are mostly delocalized, brown localized, BDF π < 0.

5-/6-membered ring $\text{EDDB}_p(\pi)/e$

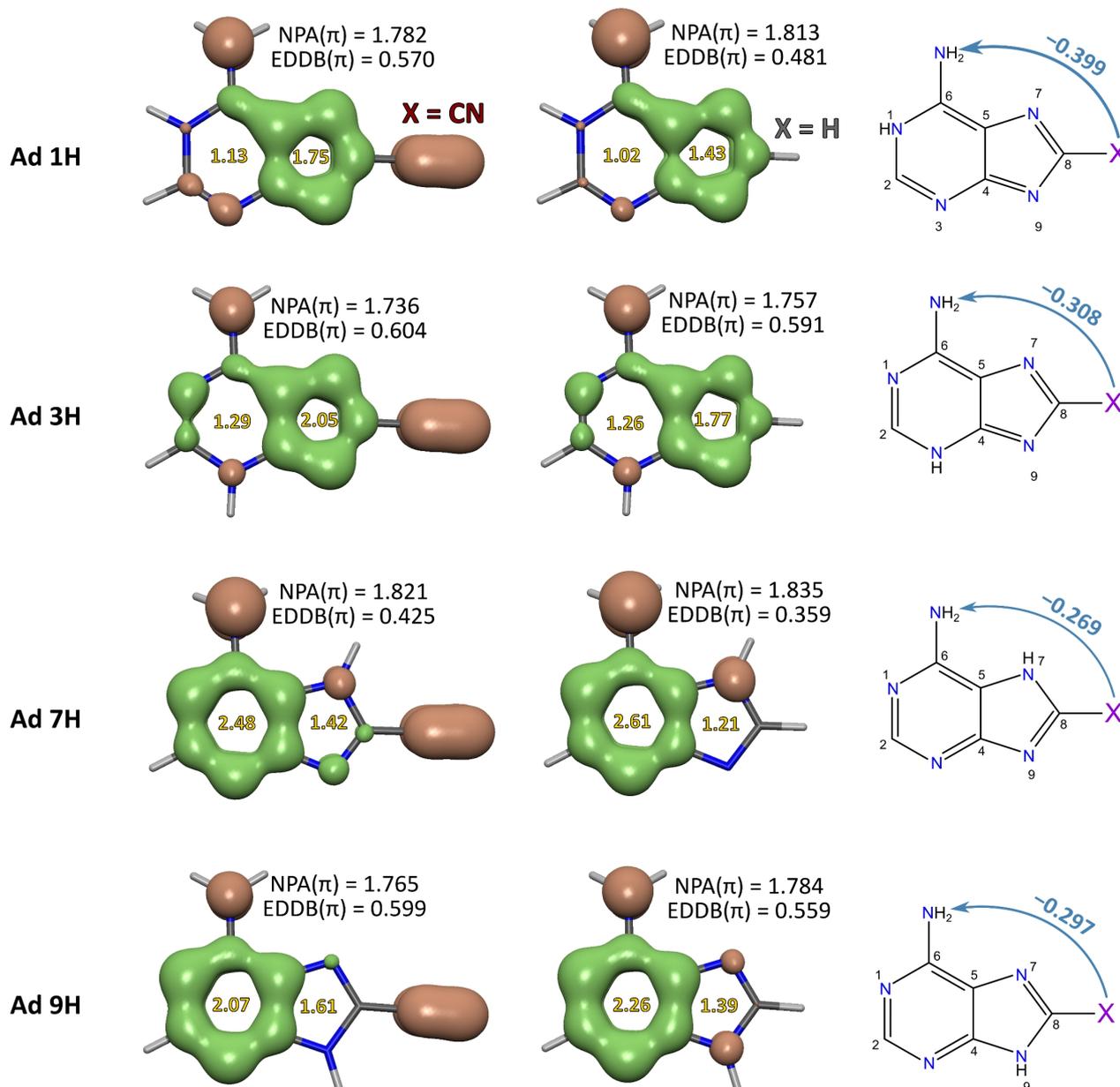


Figure S8. BDF_π maps of selected adenine derivatives (isovalue = ± 0.015) and $\text{EDDB}_p(\pi)$ populations of cyclically delocalized π -electrons. Green coloring, $\text{BDF}_\pi > 0$, indicates regions where π -electrons are mostly delocalized, brown localized, $\text{BDF}_\pi < 0$. In the right column, substituent effect strength above the arrow, calculated from slopes of $\text{cSAR}(\text{NH}_2)$ vs $\text{SAR}(\text{X})$ relations.

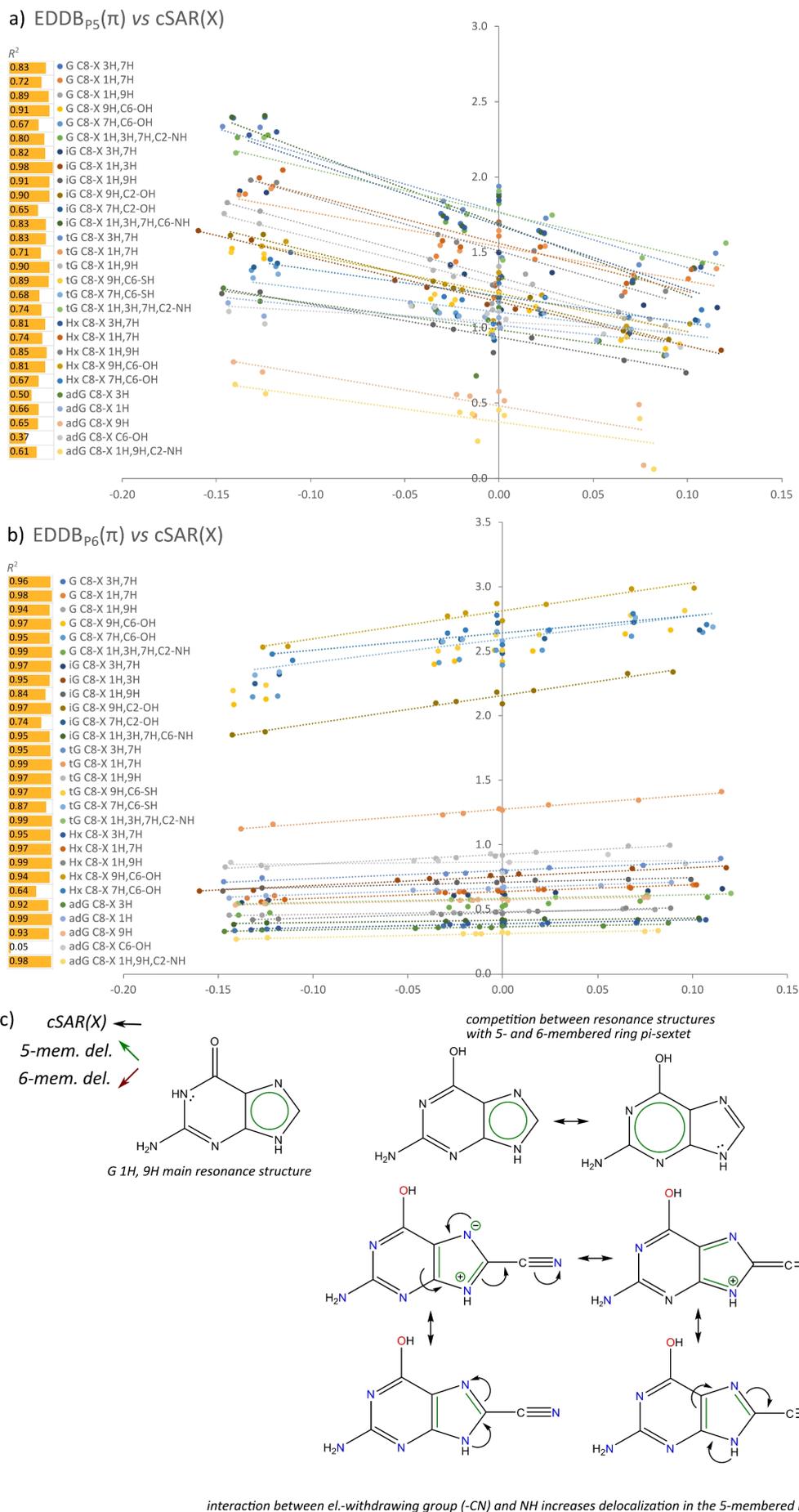


Figure S9. Correlations between cyclic delocalization in (a) five- and (b) six-membered ring, and $cSAR(X)$, i.e. substituent effect on cyclic delocalization. (c) Interpretation of the observed correlations.

Table S2. Substituent effect strength (slopes, a) of X on NH₂ and NH groups calculated from cSAR(X) vs cSAR(NH₂/NH) correlations, and determination coefficients, R^2 of these correlations.

-NH₂

| | a | R^2 |
|----------------|--------|-------|
| 6AP C5-X 1H | -0.498 | 0.964 |
| iCt C5-X C4-OH | -0.476 | 0.945 |
| iCt C5-X 3H | -0.457 | 0.982 |
| iG 1H,3H | -0.444 | 0.983 |
| Ct C5-X 3H | -0.421 | 0.954 |
| 6AP C5-X C2-OH | -0.379 | 0.926 |
| Ct C5-X C2-OH | -0.338 | 0.870 |
| iG 1H,9H | -0.311 | 0.942 |
| Ct C6-X C2-OH | -0.297 | 0.980 |
| Ct C6-X 3H | -0.281 | 0.973 |
| Ct C6-X 1H | -0.247 | 0.949 |
| iG 9H,C2-OH | -0.246 | 0.989 |
| iCt C6-X C4-OH | -0.246 | 0.891 |
| G 9H,C6-OH | -0.241 | 0.986 |
| tG 9H,C6-SH | -0.237 | 0.989 |
| iG 7H,C2-OH | -0.236 | 0.985 |
| iCt C6-X 3H | -0.218 | 0.780 |
| iG 3H,7H | -0.215 | 0.760 |
| G 1H,9H | -0.209 | 0.979 |
| iCt C6-X 1H | -0.207 | 0.844 |
| Ct C5-X 1H | -0.196 | 0.628 |
| iCt C5-X 1H | -0.187 | 0.839 |
| adG C6-OH | -0.183 | 0.980 |
| adG 3H | -0.179 | 0.986 |
| tG 1H,9H | -0.179 | 0.974 |
| G 7H,C6-OH | -0.177 | 0.953 |
| G 3H,7H | -0.173 | 0.989 |
| tG 7H,C6-SH | -0.173 | 0.958 |
| adG 9H | -0.171 | 0.970 |
| tG 3H,7H | -0.167 | 0.996 |
| adG 1H | -0.155 | 0.914 |
| G 1H,7H | -0.140 | 0.916 |
| tG 1H,7H | -0.113 | 0.857 |

=NH

| | a | R^2 |
|----------------------|--------|-------|
| Ct C6 1H,3H,C4-NH | -0.271 | 0.980 |
| iCt C5-X 1H,3H,C2-NH | -0.243 | 0.992 |
| iG 1H,3H,7H,C6-NH | -0.186 | 0.995 |
| iCt C6-X 1H,3H,C2-NH | -0.155 | 0.839 |
| adG 1H,9H,C2-NH | -0.142 | 0.931 |
| G 1H,3H,7H,C2-NH | -0.128 | 0.972 |
| tG 1H,3H,7H,C2-NH | -0.109 | 0.973 |
| Ct C5-X 1H,3H,C4-NH | -0.050 | 0.045 |

Table S3. Substituent effect strength (slopes, a) of X on O/S and OH/SH groups calculated from cSAR(X) vs cSAR(O/OH/S/SH) correlations, and determination coefficients, R^2 of these correlations.

=O

| | a | R^2 |
|--------------------|--------|-------|
| iCt-C6 3H | -0.247 | 0.962 |
| Ct-C5 3H | -0.238 | 0.929 |
| iCt-C6 1H,3H,C2-NH | -0.230 | 0.978 |
| 6AP-C5 1H | -0.227 | 0.950 |
| Ct-C5 1H,3H,C4-NH | -0.226 | 0.948 |
| Ct-C6 3H | -0.208 | 0.931 |
| Ct-C5 1H | -0.204 | 0.972 |
| iCt-C5 1H | -0.201 | 0.902 |
| Hx 1H,7H | -0.193 | 0.996 |
| Hx 3H,7H | -0.191 | 0.995 |
| G 1H,7H | -0.187 | 0.996 |
| iCt-C5 3H | -0.185 | 0.910 |
| Hx 1H,9H | -0.184 | 0.998 |
| iCt-C5 1H,3H,C2-NH | -0.182 | 0.887 |
| iCt-C6 1H | -0.172 | 0.920 |
| G 1H,9H | -0.168 | 0.997 |
| G 1H,3H,7H,C2-NH | -0.152 | 0.993 |
| G 3H,7H | -0.149 | 0.991 |
| Ct-C6 1H | -0.142 | 0.820 |
| adG 1H | -0.139 | 0.985 |
| iG 1H,9H | -0.129 | 0.935 |
| Ct-C6 1H,3H,C4-NH | -0.124 | 0.787 |
| adG 9H | -0.121 | 0.981 |
| iG 3H,7H | -0.120 | 0.894 |
| adG 1H,9H,C2-NH | -0.113 | 0.989 |
| iG 1H,3H | -0.105 | 0.969 |
| adG 3H | -0.105 | 0.958 |
| iG 1H,3H,7H,C6-NH | -0.102 | 0.968 |

=S

| | a | R^2 |
|-------------------|--------|-------|
| tG 1H,7H | -0.315 | 0.997 |
| tG 1H,9H | -0.284 | 0.997 |
| tG 1H,3H,7H,C2-NH | -0.261 | 0.995 |
| tG 3H,7H | -0.254 | 0.994 |

-OH

| | a | R^2 |
|--------------|--------|-------|
| 6AP-C5 C2-OH | -0.280 | 0.961 |
| Ct-C5 C2-OH | -0.259 | 0.958 |
| Hx 9H,C6-OH | -0.204 | 0.997 |
| iCt-C6 C4-OH | -0.189 | 0.977 |
| G 9H,C6-OH | -0.184 | 0.996 |
| Hx 7H,C6-OH | -0.183 | 0.992 |
| iCt-C5 C4-OH | -0.176 | 0.472 |
| G 7H,C6-OH | -0.171 | 0.995 |
| Ct-C6 C2-OH | -0.162 | 0.856 |
| iG 9H,C2-OH | -0.156 | 0.983 |
| iG 7H,C2-OH | -0.127 | 0.963 |
| adG C6-OH | -0.123 | 0.972 |

-SH

| | a | R^2 |
|-------------|--------|-------|
| tG 9H,C6-SH | -0.224 | 0.997 |
| tG 7H,C6-SH | -0.204 | 0.994 |

Table S4. Raw data. Electronic and Gibbs energies in Hartree, relative electronic and Gibbs energies (in kcal/mol) of tautomers (relative to the lowest energy tautomer for each substituent). cSAR(X), cSAR(NH₂/NH) and cSAR(O/OH/S/SH) descriptors of charge transfer onto or from the group. The cSAR table cells are colored proportional to the value; red – lower value and stronger electron withdrawing properties, blue – higher value and stronger donating properties. Populations of cyclically delocalized π electrons in five and six membered rings, EDDB_P(π). d_CX are the bond lengths between the substituted C atom and substituent X, d_CNH₂/d_CNH between C and NH₂/NH group, d_CO/d_COH/d_CS/d_CSH between C and O/OH/S/SH. All bond lengths are in Å.

| Ct C5-X 1H | E/h | G/h | ΔE_{taut} | ΔG_{taut} | cSAR(X) | cSAR(NH ₂) | cSAR(O) | EDDB_P(π) | d_CX | d_CNH ₂ | d_CO |
|---------------------|------------|------------|--------------------------|--------------------------|---------|------------------------|----------|-----------------|-------|--------------------|-------|
| NO ₂ | -597.8125 | -597.7437 | 0.00 | 0.00 | -0.119 | 0.151 | -0.087 | 0.529 | 1.447 | 1.339 | 1.210 |
| CN | -485.8268 | -485.7622 | 0.00 | 0.00 | -0.139 | 0.176 | -0.089 | 0.525 | 1.425 | 1.346 | 1.210 |
| Br | -2966.1989 | -2966.1438 | 0.46 | 0.37 | -0.020 | 0.135 | -0.111 | 0.643 | 1.889 | 1.347 | 1.213 |
| Cl | -852.9444 | -852.8878 | 0.45 | 0.08 | -0.013 | 0.135 | -0.112 | 0.650 | 1.735 | 1.348 | 1.213 |
| F | -492.8248 | -492.7662 | 0.53 | 0.00 | 0.001 | 0.142 | -0.116 | 0.702 | 1.345 | 1.350 | 1.213 |
| H | -393.8320 | -393.7632 | 0.00 | 0.00 | 0.000 | 0.135 | -0.118 | 0.656 | | 1.358 | 1.214 |
| SH | -791.5784 | -791.5121 | 0.00 | 0.00 | 0.001 | 0.116 | -0.111 | 0.607 | 1.773 | 1.351 | 1.213 |
| OH | -468.8555 | -468.7845 | 5.36 | 3.83 | 0.078 | 0.136 | -0.131 | 0.762 | 1.366 | 1.350 | 1.215 |
| NH ₂ | -449.0326 | -448.9482 | 1.23 | 0.76 | 0.067 | 0.117 | -0.127 | 0.682 | 1.427 | 1.346 | 1.215 |
| Ct C5-X 3H | | | ΔE_{taut} | ΔG_{taut} | cSAR(X) | cSAR(NH ₂) | cSAR(O) | EDDB_P(π) | d_CX | d_CNH ₂ | d_CO |
| NO ₂ | -597.8063 | -597.7380 | 3.91 | 3.60 | -0.135 | 0.183 | -0.061 | 0.552 | 1.432 | 1.335 | 1.208 |
| CN | -485.8180 | -485.7545 | 5.51 | 4.82 | -0.154 | 0.206 | -0.070 | 0.592 | 1.423 | 1.345 | 1.209 |
| Br | -2966.1882 | -2966.1329 | 7.15 | 7.21 | -0.024 | 0.135 | -0.094 | 0.711 | 1.887 | 1.356 | 1.211 |
| Cl | -852.9332 | -852.8762 | 7.49 | 7.37 | -0.018 | 0.133 | -0.097 | 0.720 | 1.736 | 1.357 | 1.212 |
| F | -492.8108 | -492.7517 | 9.31 | 9.14 | -0.003 | 0.128 | -0.104 | 0.777 | 1.349 | 1.363 | 1.212 |
| H | -393.8204 | -393.7518 | 7.29 | 7.15 | 0.000 | 0.137 | -0.105 | 0.734 | | 1.366 | 1.213 |
| SH | -791.5687 | -791.5026 | 6.09 | 5.97 | -0.004 | 0.127 | -0.094 | 0.681 | 1.769 | 1.355 | 1.211 |
| OH | -468.8422 | -468.7712 | 13.69 | 12.16 | 0.049 | 0.116 | -0.115 | 0.815 | 1.380 | 1.362 | 1.214 |
| NH ₂ | -449.0234 | -448.9387 | 6.97 | 6.69 | 0.059 | 0.112 | -0.112 | 0.778 | 1.427 | 1.358 | 1.213 |
| Ct C5-X C2-OH | | | ΔE_{taut} | ΔG_{taut} | cSAR(X) | cSAR(NH ₂) | cSAR(OH) | EDDB_P(π) | d_CX | d_CNH ₂ | d_COH |
| NO ₂ | -597.8124 | -597.7431 | 0.05 | 0.39 | -0.126 | 0.167 | 0.237 | 1.870 | 1.447 | 1.337 | 1.329 |
| CN | -485.8264 | -485.7614 | 0.20 | 0.50 | -0.142 | 0.187 | 0.231 | 2.076 | 1.427 | 1.345 | 1.330 |
| Br | -2966.1996 | -2966.1443 | 0.00 | 0.00 | -0.027 | 0.137 | 0.205 | 2.317 | 1.890 | 1.348 | 1.336 |
| Cl | -852.9451 | -852.8879 | 0.00 | 0.00 | -0.018 | 0.135 | 0.203 | 2.339 | 1.736 | 1.336 | 1.349 |
| F | -492.8257 | -492.7657 | 0.00 | 0.32 | -0.001 | 0.135 | 0.195 | 2.467 | 1.345 | 1.354 | 1.338 |
| H | -393.8305 | -393.7611 | 0.97 | 1.32 | 0.000 | 0.133 | 0.197 | 2.554 | | 1.360 | 1.337 |
| SH | -791.5774 | -791.5108 | 0.63 | 0.80 | -0.003 | 0.120 | 0.207 | 2.300 | 1.776 | 1.352 | 1.335 |
| OH | -468.8572 | -468.7853 | 4.29 | 3.36 | 0.074 | 0.125 | 0.177 | 2.286 | 1.365 | 1.356 | 1.342 |
| NH ₂ | -449.0325 | -448.9473 | 1.30 | 1.32 | 0.082 | 0.090 | 0.180 | 2.555 | 1.414 | 1.367 | 1.341 |
| Ct C5-X 1H,3H,C4-NH | | | ΔE_{taut} | ΔG_{taut} | cSAR(X) | cSAR(NH) | cSAR(O) | EDDB_P(π) | d_CX | d_CNH | d_CO |
| NO ₂ | -597.8074 | -597.7380 | 3.19 | 3.61 | -0.115 | -0.059 | -0.065 | 0.432 | 1.453 | 1.274 | 1.209 |
| CN | -485.8243 | -485.7585 | 1.52 | 2.30 | -0.131 | -0.039 | -0.067 | 0.451 | 1.428 | 1.276 | 1.209 |
| Br | -2966.1981 | -2966.1413 | 0.91 | 1.89 | -0.016 | -0.075 | -0.086 | 0.476 | 1.882 | 1.277 | 1.212 |
| Cl | -852.9438 | -852.8855 | 0.81 | 1.51 | -0.009 | -0.074 | -0.087 | 0.475 | 1.728 | 1.277 | 1.212 |
| F | -492.8252 | -492.7646 | 0.32 | 1.00 | 0.003 | -0.065 | -0.091 | 0.504 | 1.337 | 1.278 | 1.212 |
| H | -393.8320 | -393.7621 | 0.01 | 0.69 | 0.000 | -0.072 | -0.092 | 0.503 | | 1.282 | 1.212 |
| SH | -791.5771 | -791.5102 | 0.84 | 1.20 | 0.001 | -0.089 | -0.087 | 0.462 | 1.771 | 1.278 | 1.212 |
| OH | -468.8640 | -468.7906 | 0.00 | 0.00 | 0.034 | -0.043 | -0.104 | 0.404 | 1.343 | 1.285 | 1.214 |
| NH ₂ | -449.0346 | -448.9494 | 0.00 | 0.00 | 0.088 | -0.054 | -0.115 | 0.366 | 1.388 | 1.284 | 1.216 |

| Ct C6-X 1H | | E/h | G/h | ΔE _{taut} | ΔG _{taut} | cSAR(X) | cSAR(NH ₂) | cSAR(O) | EDDB_P(n) | d_CX | d_CNH ₂ | d_CO |
|---------------------|--|------------|------------|--------------------|--------------------|---------|------------------------|---------|-----------|-------|--------------------|-------|
| NO ₂ | | -597.8045 | -597.7386 | 1.40 | 0.73 | -0.101 | 0.170 | -0.088 | 0.591 | 1.477 | 1.351 | 1.209 |
| CN | | -485.8160 | -485.7530 | 1.90 | 1.19 | -0.108 | 0.164 | -0.096 | 0.618 | 1.440 | 1.352 | 1.211 |
| Br | | -2966.1987 | -2966.1441 | 1.75 | 1.16 | -0.025 | 0.150 | -0.102 | 0.616 | 1.881 | 1.355 | 1.211 |
| Cl | | -852.9461 | -852.8899 | 1.85 | 1.16 | -0.017 | 0.149 | -0.104 | 0.624 | 1.722 | 1.355 | 1.212 |
| F | | -492.8366 | -492.7778 | 4.00 | 3.23 | -0.004 | 0.150 | -0.103 | 0.621 | 1.321 | 1.354 | 1.211 |
| H | | -393.8320 | -393.7632 | 0.00 | 0.00 | 0.000 | 0.135 | -0.118 | 0.656 | | 1.358 | 1.214 |
| SH | | -791.5748 | -791.5105 | 3.23 | 2.25 | 0.031 | 0.133 | -0.111 | 0.651 | 1.763 | 1.359 | 1.213 |
| OH | | -468.8716 | -468.7998 | 5.59 | 4.73 | 0.075 | 0.125 | -0.113 | 0.662 | 1.339 | 1.360 | 1.213 |
| NH ₂ | | -449.0456 | -448.9615 | 3.31 | 2.70 | 0.120 | 0.111 | -0.126 | 0.717 | 1.373 | 1.363 | 1.215 |
| Ct C6-X 3H | | | | ΔE _{taut} | ΔG _{taut} | cSAR(X) | cSAR(NH ₂) | cSAR(O) | EDDB_P(n) | d_CX | d_CNH ₂ | d_CO |
| NO ₂ | | -597.7972 | -597.7293 | 5.99 | 6.54 | -0.123 | 0.181 | -0.072 | 0.731 | 1.513 | 1.355 | 1.209 |
| CN | | -485.8084 | -485.7446 | 6.70 | 6.51 | -0.108 | 0.175 | -0.082 | 0.727 | 1.455 | 1.357 | 1.210 |
| Br | | -2966.1936 | -2966.1386 | 4.94 | 4.62 | -0.056 | 0.154 | -0.083 | 0.705 | 1.910 | 1.363 | 1.210 |
| Cl | | -852.9412 | -852.8845 | 4.93 | 4.56 | -0.038 | 0.150 | -0.086 | 0.704 | 1.744 | 1.363 | 1.210 |
| F | | -492.8361 | -492.7767 | 4.28 | 3.91 | -0.014 | 0.149 | -0.088 | 0.692 | 1.329 | 1.363 | 1.210 |
| H | | -393.8204 | -393.7518 | 7.29 | 7.15 | 0.000 | 0.137 | -0.105 | 0.734 | | 1.366 | 1.213 |
| SH | | -791.5735 | -791.5080 | 4.05 | 3.86 | 0.015 | 0.136 | -0.103 | 0.715 | 1.766 | 1.367 | 1.212 |
| OH | | -468.8762 | -468.8036 | 2.70 | 2.35 | 0.060 | 0.129 | -0.110 | 0.724 | 1.336 | 1.368 | 1.213 |
| NH ₂ | | -449.0456 | -448.9615 | 3.31 | 2.70 | 0.127 | 0.109 | -0.126 | 0.717 | 1.363 | 1.373 | 1.215 |
| Ct C6-X C2-OH | | | | ΔE _{taut} | ΔG _{taut} | cSAR(X) | cSAR(NH ₂) | cSAR(O) | EDDB_P(n) | d_CX | d_CNH ₂ | d_COH |
| NO ₂ | | -597.8067 | -597.7398 | 0.00 | 0.00 | -0.129 | 0.178 | 0.232 | 2.320 | 1.495 | 1.349 | 1.331 |
| CN | | -485.8191 | -485.7549 | 0.00 | 0.00 | -0.113 | 0.169 | 0.222 | 2.349 | 1.449 | 1.351 | 1.333 |
| Br | | -2966.2015 | -2966.1460 | 0.00 | 0.00 | -0.052 | 0.153 | 0.218 | 2.467 | 1.897 | 1.355 | 1.334 |
| Cl | | -852.9491 | -852.8917 | 0.00 | 0.00 | -0.037 | 0.150 | 0.216 | 2.501 | 1.735 | 1.355 | 1.334 |
| F | | -492.8430 | -492.7829 | 0.00 | 0.00 | -0.012 | 0.148 | 0.217 | 2.563 | 1.326 | 1.355 | 1.334 |
| H | | -393.8305 | -393.7611 | 0.97 | 1.32 | 0.000 | 0.133 | 0.197 | 2.554 | | 1.360 | 1.337 |
| SH | | -791.5800 | -791.5141 | 0.00 | 0.00 | 0.009 | 0.137 | 0.203 | 2.576 | 1.765 | 1.359 | 1.336 |
| OH | | -468.8805 | -468.8073 | 0.00 | 0.00 | 0.063 | 0.121 | 0.201 | 2.671 | 1.337 | 1.362 | 1.336 |
| NH ₂ | | -449.0509 | -448.9658 | 0.00 | 0.00 | 0.127 | 0.099 | 0.188 | 2.712 | 1.367 | 1.366 | 1.339 |
| Ct C6-X 1H,3H,C4-NH | | | | ΔE _{taut} | ΔG _{taut} | cSAR(X) | cSAR(NH) | cSAR(O) | EDDB_P(n) | d_CX | d_CNH | d_CO |
| NO ₂ | | -597.8042 | -597.7363 | 1.61 | 2.18 | -0.096 | -0.038 | -0.066 | 0.495 | 1.475 | 1.281 | 1.209 |
| CN | | -485.8159 | -485.7510 | 1.95 | 2.45 | -0.105 | -0.043 | -0.073 | 0.494 | 1.438 | 1.281 | 1.210 |
| Br | | -2966.1977 | -2966.1417 | 2.42 | 2.68 | -0.022 | -0.060 | -0.079 | 0.493 | 1.881 | 1.281 | 1.211 |
| Cl | | -852.9449 | -852.8872 | 2.65 | 2.84 | -0.014 | -0.063 | -0.080 | 0.497 | 1.723 | 1.281 | 1.211 |
| F | | -492.8343 | -492.7741 | 5.45 | 5.55 | -0.004 | -0.066 | -0.078 | 0.502 | 1.322 | 1.281 | 1.210 |
| H | | -393.8320 | -393.7621 | 0.01 | 0.69 | 0.000 | -0.072 | -0.092 | 0.503 | | 1.282 | 1.212 |
| SH | | -791.5737 | -791.5086 | 3.91 | 3.43 | 0.032 | -0.076 | -0.086 | 0.476 | 1.771 | 1.282 | 1.212 |
| OH | | -468.8699 | -468.7972 | 6.69 | 6.37 | 0.074 | -0.088 | -0.088 | 0.538 | 1.341 | 1.282 | 1.212 |
| NH ₂ | | -449.0434 | -448.9582 | 4.70 | 4.79 | 0.105 | -0.096 | -0.097 | 0.516 | 1.381 | 1.284 | 1.213 |

| iCt C5-X 1H | E/h | G/h | ΔE_{taut} | ΔG_{taut} | cSAR(X) | cSAR(NH2) | cSAR(O) | EDDB_P(n) | d_CX | d_CNH2 | d_CO |
|----------------------|------------|------------|--------------------------|--------------------------|---------|-----------|---------|-----------|-------|--------|-------|
| NO2 | -597.7855 | -597.7175 | 17.54 | 16.73 | -0.137 | 0.129 | -0.101 | 0.238 | 1.459 | 1.370 | 1.210 |
| CN | -485.8081 | -485.7434 | 11.41 | 11.38 | -0.136 | 0.128 | -0.104 | 0.238 | 1.430 | 1.370 | 1.213 |
| Br | -2966.1824 | -2966.1267 | 10.10 | 9.85 | -0.042 | 0.108 | -0.124 | 0.350 | 1.877 | 1.375 | 1.213 |
| Cl | -852.9274 | -852.8701 | 10.07 | 9.75 | -0.029 | 0.106 | -0.127 | 0.345 | 1.721 | 1.376 | 1.213 |
| F | -492.8092 | -492.7497 | 9.38 | 9.03 | 0.001 | 0.104 | -0.134 | 0.363 | 1.329 | 1.376 | 1.215 |
| H | -393.8158 | -393.7471 | 10.81 | 10.45 | 0.000 | 0.095 | -0.139 | 0.354 | | 1.378 | 1.217 |
| SH | -791.5648 | -791.4989 | 8.19 | 8.08 | -0.019 | 0.105 | -0.121 | 0.333 | 1.756 | 1.376 | 1.223 |
| OH | -468.8553 | -468.7826 | 5.81 | 5.60 | 0.030 | 0.104 | -0.141 | 0.386 | 1.338 | 1.376 | 1.230 |
| NH2 | -449.0255 | -448.9411 | 7.97 | 7.56 | 0.087 | 0.084 | -0.143 | 0.334 | 1.379 | 1.382 | 1.225 |
| iCt C5-X 3H | | | ΔE_{taut} | ΔG_{taut} | cSAR(X) | cSAR(NH2) | cSAR(O) | EDDB_P(n) | d_CX | d_CNH2 | d_CO |
| NO2 | -597.8029 | -597.7351 | 6.62 | 5.69 | -0.154 | 0.176 | -0.104 | 0.634 | 1.454 | 1.351 | 1.210 |
| CN | -485.8256 | -485.7606 | 0.45 | 0.60 | -0.147 | 0.168 | -0.110 | 0.650 | 1.429 | 1.354 | 1.213 |
| Br | -2966.1985 | -2966.1424 | 0.00 | 0.01 | -0.042 | 0.125 | -0.131 | 0.644 | 1.878 | 1.366 | 1.214 |
| Cl | -852.9435 | -852.8856 | 0.00 | 0.03 | -0.028 | 0.119 | -0.132 | 0.645 | 1.723 | 1.367 | 1.214 |
| F | -492.8242 | -492.7641 | 0.00 | 0.00 | 0.002 | 0.104 | -0.135 | 0.653 | 1.332 | 1.372 | 1.214 |
| H | -393.8323 | -393.7629 | 0.50 | 0.49 | 0.000 | 0.114 | -0.146 | 0.648 | | 1.368 | 1.217 |
| SH | -791.5778 | -791.5118 | 0.00 | 0.00 | -0.004 | 0.100 | -0.133 | 0.701 | 1.763 | 1.373 | 1.222 |
| OH | -468.8645 | -468.7915 | 0.00 | 0.00 | 0.052 | 0.074 | -0.151 | 0.655 | 1.347 | 1.381 | 1.226 |
| NH2 | -449.0382 | -448.9531 | 0.00 | 0.00 | 0.102 | 0.058 | -0.149 | 0.696 | 1.385 | 1.385 | 1.224 |
| iCt C5-X C4-OH | | | ΔE_{taut} | ΔG_{taut} | cSAR(X) | cSAR(NH2) | cSAR(O) | EDDB_P(n) | d_CX | d_CNH2 | d_COH |
| NO2 | -597.8134 | -597.7441 | 0.00 | 0.00 | -0.117 | 0.194 | 0.142 | 1.949 | 1.437 | 1.344 | 1.316 |
| CN | -485.8263 | -485.7615 | 0.00 | 0.00 | -0.142 | 0.173 | 0.198 | 2.237 | 1.428 | 1.347 | 1.329 |
| Br | -2966.1984 | -2966.1424 | 0.11 | 0.00 | -0.038 | 0.134 | 0.167 | 2.577 | 1.881 | 1.357 | 1.332 |
| Cl | -852.9432 | -852.8857 | 0.16 | 0.00 | -0.026 | 0.129 | 0.163 | 2.607 | 1.727 | 1.358 | 1.332 |
| F | -492.8234 | -492.7633 | 0.49 | 0.47 | 0.003 | 0.115 | 0.156 | 2.711 | 1.336 | 1.362 | 1.334 |
| H | -393.8331 | -393.7637 | 0.00 | 0.00 | 0.000 | 0.122 | 0.153 | 2.609 | | 1.359 | 1.338 |
| SH | -791.5752 | -791.5096 | 1.65 | 1.37 | -0.013 | 0.129 | 0.159 | 2.561 | 1.771 | 1.357 | 1.336 |
| OH | -468.8581 | -468.7860 | 4.05 | 3.49 | 0.061 | 0.089 | 0.133 | 2.869 | 1.357 | 1.370 | 1.348 |
| NH2 | -449.0336 | -448.9487 | 2.90 | 2.75 | 0.096 | 0.075 | 0.137 | 2.860 | 1.397 | 1.374 | 1.346 |
| iCt C5-X 1H,3H,C2-NH | | | ΔE_{taut} | ΔG_{taut} | cSAR(X) | cSAR(NH) | cSAR(O) | EDDB_P(n) | d_CX | d_CNH | d_CO |
| NO2 | -597.7935 | -597.7245 | 12.48 | 12.32 | -0.140 | -0.007 | -0.083 | 0.579 | 1.454 | 1.275 | 1.208 |
| CN | -485.8160 | -485.7503 | 6.45 | 7.08 | -0.136 | -0.010 | -0.088 | 0.556 | 1.428 | 1.275 | 1.211 |
| Br | -2966.1861 | -2966.1298 | 7.80 | 7.88 | -0.024 | -0.034 | -0.107 | 0.529 | 1.874 | 1.277 | 1.212 |
| Cl | -852.9310 | -852.8732 | 7.85 | 7.86 | -0.014 | -0.036 | -0.109 | 0.520 | 1.720 | 1.277 | 1.212 |
| F | -492.8129 | -492.7529 | 7.10 | 7.02 | 0.003 | -0.040 | -0.112 | 0.563 | 1.332 | 1.278 | 1.213 |
| H | -393.8245 | -393.7549 | 5.38 | 5.55 | 0.000 | -0.042 | -0.123 | 0.590 | | 1.278 | 1.216 |
| SH | -791.5677 | -791.5012 | 6.33 | 6.64 | -0.006 | -0.041 | -0.110 | 0.566 | 1.765 | 1.278 | 1.218 |
| OH | -468.8536 | -468.7808 | 6.87 | 6.75 | 0.041 | -0.051 | -0.123 | 0.575 | 1.350 | 1.279 | 1.224 |
| NH2 | -449.0264 | -448.9418 | 7.38 | 7.10 | 0.079 | -0.062 | -0.120 | 0.536 | 1.395 | 1.281 | 1.221 |

| iCt C6-X 1H | E/h | G/h | ΔE _{taut} | ΔG _{taut} | cSAR(X) | cSAR(NH ₂) | cSAR(O) | EDDB_P(n) | d_CX | d_CNH ₂ | d_CO |
|----------------------|------------|------------|--------------------|--------------------|---------|------------------------|---------|-----------|-------|--------------------|-------|
| NO ₂ | -597.7905 | -597.7234 | 11.65 | 11.66 | -0.100 | 0.137 | -0.114 | 0.325 | 1.471 | 1.366 | 1.215 |
| CN | -485.8015 | -485.7377 | 12.63 | 12.64 | -0.108 | 0.125 | -0.118 | 0.335 | 1.437 | 1.371 | 1.216 |
| Br | -2966.1826 | -2966.1276 | 13.64 | 13.48 | -0.027 | 0.112 | -0.126 | 0.347 | 1.882 | 1.374 | 1.216 |
| Cl | -852.9296 | -852.8730 | 14.01 | 13.84 | -0.018 | 0.111 | -0.128 | 0.352 | 1.724 | 1.374 | 1.216 |
| F | -492.8185 | -492.7594 | 17.29 | 16.95 | -0.006 | 0.110 | -0.128 | 0.357 | 1.325 | 1.374 | 1.215 |
| H | -393.8158 | -393.7471 | 10.81 | 10.45 | 0.000 | 0.095 | -0.139 | 0.354 | | 1.378 | 1.217 |
| SH | -791.5588 | -791.4939 | 15.13 | 14.54 | 0.020 | 0.103 | -0.136 | 0.343 | 1.770 | 1.377 | 1.217 |
| OH | -468.8547 | -468.7830 | 17.80 | 17.01 | 0.070 | 0.098 | -0.147 | 0.397 | 1.344 | 1.377 | 1.217 |
| NH ₂ | -449.0271 | -448.9426 | 17.02 | 16.91 | 0.093 | 0.088 | -0.148 | 0.366 | 1.388 | 1.380 | 1.217 |
| iCt C6-X 3H | | | ΔE _{taut} | ΔG _{taut} | cSAR(X) | cSAR(NH ₂) | cSAR(O) | EDDB_P(n) | d_CX | d_CNH ₂ | d_CO |
| NO ₂ | -597.8074 | -597.7398 | 1.06 | 1.38 | -0.129 | 0.164 | -0.117 | 0.620 | 1.497 | 1.356 | 1.214 |
| CN | -485.8208 | -485.7562 | 0.54 | 1.04 | -0.112 | 0.149 | -0.122 | 0.621 | 1.449 | 1.360 | 1.215 |
| Br | -2966.2024 | -2966.1468 | 1.21 | 1.40 | -0.050 | 0.143 | -0.135 | 0.626 | 1.896 | 1.362 | 1.216 |
| Cl | -852.9499 | -852.8926 | 1.27 | 1.57 | -0.035 | 0.141 | -0.139 | 0.634 | 1.734 | 1.362 | 1.216 |
| F | -492.8435 | -492.7836 | 1.59 | 1.77 | -0.010 | 0.146 | -0.143 | 0.650 | 1.326 | 1.360 | 1.216 |
| H | -393.8323 | -393.7629 | 0.50 | 0.49 | 0.000 | 0.114 | -0.146 | 0.648 | | 1.368 | 1.217 |
| SH | -791.5808 | -791.5152 | 1.30 | 1.21 | 0.010 | 0.127 | -0.149 | 0.624 | 1.765 | 1.365 | 1.217 |
| OH | -468.8796 | -468.8068 | 2.17 | 2.06 | 0.056 | 0.127 | -0.159 | 0.621 | 1.339 | 1.365 | 1.218 |
| NH ₂ | -449.0524 | -448.9679 | 1.16 | 1.02 | 0.124 | 0.109 | -0.177 | 0.669 | 1.366 | 1.369 | 1.220 |
| iCt C6-X C4-OH | | | ΔE _{taut} | ΔG _{taut} | cSAR(X) | cSAR(NH ₂) | cSAR(O) | EDDB_P(n) | d_CX | d_CNH ₂ | d_COH |
| NO ₂ | -597.8090 | -597.7420 | 0.00 | 0.00 | -0.129 | 0.170 | 0.183 | 2.484 | 1.497 | 1.349 | 1.332 |
| CN | -485.8216 | -485.7578 | 0.00 | 0.00 | -0.113 | 0.160 | 0.178 | 2.497 | 1.450 | 1.350 | 1.333 |
| Br | -2966.2043 | -2966.1491 | 0.00 | 0.00 | -0.053 | 0.151 | 0.167 | 2.522 | 1.898 | 1.353 | 1.335 |
| Cl | -852.9519 | -852.8951 | 0.00 | 0.00 | -0.037 | 0.147 | 0.164 | 2.542 | 1.736 | 1.354 | 1.335 |
| F | -492.8460 | -492.7864 | 0.00 | 0.00 | -0.012 | 0.149 | 0.163 | 2.536 | 1.327 | 1.353 | 1.335 |
| H | -393.8331 | -393.7637 | 0.00 | 0.00 | 0.000 | 0.122 | 0.153 | 2.609 | | 1.359 | 1.338 |
| SH | -791.5829 | -791.5171 | 0.00 | 0.00 | 0.010 | 0.130 | 0.155 | 2.587 | 1.765 | 1.358 | 1.337 |
| OH | -468.8831 | -468.8101 | 0.00 | 0.00 | 0.057 | 0.125 | 0.149 | 2.615 | 1.338 | 1.359 | 1.338 |
| NH ₂ | -449.0542 | -448.9695 | 0.00 | 0.00 | 0.122 | 0.107 | 0.134 | 2.577 | 1.366 | 1.363 | 1.341 |
| iCt C6-X 1H,3H,C2-NH | | | ΔE _{taut} | ΔG _{taut} | cSAR(X) | cSAR(NH) | cSAR(O) | EDDB_P(n) | d_CX | d_CNH | d_CO |
| NO ₂ | -597.7956 | -597.7276 | 8.44 | 9.00 | -0.093 | -0.012 | -0.096 | 0.526 | 1.480 | 1.274 | 1.214 |
| CN | -485.8078 | -485.7431 | 8.72 | 9.24 | -0.103 | -0.018 | -0.101 | 0.539 | 1.440 | 1.275 | 1.214 |
| Br | -2966.1900 | -2966.1343 | 8.98 | 9.28 | -0.021 | -0.028 | -0.113 | 0.582 | 1.880 | 1.276 | 1.215 |
| Cl | -852.9374 | -852.8800 | 9.12 | 9.48 | -0.013 | -0.029 | -0.115 | 0.589 | 1.722 | 1.277 | 1.215 |
| F | -492.8274 | -492.7675 | 11.71 | 11.85 | -0.003 | -0.027 | -0.118 | 0.612 | 1.321 | 1.276 | 1.215 |
| H | -393.8245 | -393.7549 | 5.38 | 5.55 | 0.000 | -0.042 | -0.123 | 0.590 | | 1.278 | 1.216 |
| SH | -791.5669 | -791.5018 | 10.05 | 9.62 | 0.034 | -0.036 | -0.128 | 0.618 | 1.764 | 1.278 | 1.216 |
| OH | -468.8617 | -468.7893 | 13.43 | 13.04 | 0.068 | -0.039 | -0.136 | 0.638 | 1.341 | 1.277 | 1.216 |
| NH ₂ | -449.0373 | -448.9526 | 10.64 | 10.65 | 0.113 | -0.050 | -0.147 | 0.654 | 1.377 | 1.279 | 1.218 |

| 6AP C5-X | | | | | | | | | | | | |
|-----------------|------------|------------|--------------------|--------------------|---------|------------------------|---------|-----------|-------|--------------------|-------|--|
| 1H | E/h | G/h | ΔE _{taut} | ΔG _{taut} | cSAR(X) | cSAR(NH ₂) | cSAR(O) | EDDB_P(π) | d_CX | d_CNH ₂ | d_CO | |
| NO ₂ | -581.7989 | -581.7200 | 1.18 | 0.57 | -0.152 | 0.183 | -0.125 | 0.588 | 1.432 | 1.341 | 1.216 | |
| CN | -469.8094 | -469.7331 | 2.52 | 2.53 | -0.156 | 0.184 | -0.134 | 0.620 | 1.424 | 1.361 | 1.217 | |
| Br | -2950.1791 | -2950.1118 | 4.19 | 3.99 | -0.025 | 0.108 | -0.158 | 0.765 | 1.893 | 1.373 | 1.220 | |
| Cl | -836.9243 | -836.8554 | 4.44 | 4.28 | -0.018 | 0.104 | -0.161 | 0.772 | 1.741 | 1.375 | 1.221 | |
| F | -476.8038 | -476.7328 | 5.91 | 5.61 | -0.003 | 0.095 | -0.169 | 0.845 | 1.352 | 1.381 | 1.221 | |
| H | -377.8105 | -377.7300 | 3.20 | 3.08 | 0.000 | 0.112 | -0.168 | 0.788 | | 1.383 | 1.222 | |
| SH | -775.5578 | -775.4803 | 3.18 | 2.96 | -0.007 | 0.108 | -0.158 | 0.727 | 1.775 | 1.369 | 1.220 | |
| OH | -452.8338 | -452.7508 | 5.62 | 5.38 | 0.042 | 0.085 | -0.176 | 0.851 | 1.384 | 1.380 | 1.223 | |
| NH ₂ | -433.0131 | -432.9167 | 3.83 | 3.64 | 0.057 | 0.084 | -0.175 | 0.809 | 1.430 | 1.375 | 1.222 | |
| 6AP C5-X C2-OH | | | | | | | | | | | | |
| | | | | | cSAR(X) | cSAR(NH ₂) | cSAR(O) | EDDB_P(π) | d_CX | d_CNH ₂ | d_COH | |
| NO ₂ | -581.8008 | -581.7209 | 0.00 | 0.00 | -0.141 | 0.163 | 0.168 | 2.105 | 1.447 | 1.344 | 1.337 | |
| CN | -469.8135 | -469.7371 | 0.00 | 0.00 | -0.149 | 0.175 | 0.159 | 2.436 | 1.429 | 1.357 | 1.338 | |
| Br | -2950.1858 | -2950.1181 | 0.00 | 0.00 | -0.031 | 0.113 | 0.132 | 2.913 | 1.897 | 1.365 | 1.344 | |
| Cl | -836.9314 | -836.8622 | 0.00 | 0.00 | -0.021 | 0.110 | 0.129 | 2.938 | 1.742 | 1.366 | 1.344 | |
| F | -476.8132 | -476.7417 | 0.00 | 0.00 | -0.002 | 0.108 | 0.119 | 3.184 | 1.349 | 1.372 | 1.346 | |
| H | -377.8156 | -377.7349 | 0.00 | 0.00 | 0.000 | 0.110 | 0.123 | 3.172 | | 1.377 | 1.345 | |
| SH | -775.5629 | -775.4850 | 0.00 | 0.00 | -0.006 | 0.100 | 0.133 | 2.835 | 1.780 | 1.368 | 1.343 | |
| OH | -452.8428 | -452.7594 | 0.00 | 0.00 | 0.072 | 0.099 | 0.100 | 3.015 | 1.369 | 1.373 | 1.350 | |
| NH ₂ | -433.0192 | -432.9225 | 0.00 | 0.00 | 0.087 | 0.074 | 0.100 | 3.225 | 1.412 | 1.385 | 1.350 | |

| G C8-X | | | | | | | | | | | | |
|-----------------|------------|------------|--------------------|--------------------|---------|------------------------|---------|------------------------|------------------------|-------|--------------------|-------|
| 3H,7H | E/h | G/h | ΔE _{taut} | ΔG _{taut} | cSAR(X) | cSAR(NH ₂) | cSAR(O) | EDDB_P(π) ₅ | EDDB_P(π) ₆ | d_CX | d_CNH ₂ | d_CO |
| NO ₂ | -745.0175 | -744.9334 | 8.74 | 8.30 | -0.141 | 0.130 | -0.137 | 2.394 | 0.337 | 1.448 | 1.368 | 1.218 |
| CN | -633.0333 | -632.9527 | 8.14 | 7.69 | -0.125 | 0.126 | -0.142 | 2.397 | 0.350 | 1.429 | 1.370 | 1.218 |
| Br | -3113.4116 | -3113.3399 | 7.74 | 7.39 | -0.031 | 0.109 | -0.154 | 1.758 | 0.369 | 1.864 | 1.374 | 1.219 |
| Cl | -1000.1591 | -1000.0856 | 7.65 | 7.35 | -0.021 | 0.108 | -0.156 | 1.689 | 0.371 | 1.708 | 1.375 | 1.219 |
| F | -640.0486 | -639.9726 | 7.80 | 7.48 | 0.001 | 0.106 | -0.159 | 1.342 | 0.377 | 1.312 | 1.375 | 1.219 |
| H | -541.0470 | -540.9617 | 6.94 | 6.69 | 0.000 | 0.101 | -0.160 | 1.885 | 0.377 | | 1.377 | 1.220 |
| SH | -938.7902 | -938.7089 | 7.65 | 7.24 | 0.021 | 0.100 | -0.162 | 1.644 | 0.383 | 1.756 | 1.377 | 1.220 |
| OH | -616.0871 | -615.9987 | 8.36 | 7.95 | 0.070 | 0.093 | -0.168 | 1.300 | 0.394 | 1.333 | 1.379 | 1.220 |
| NH ₂ | -596.2586 | -596.1582 | 7.67 | 7.35 | 0.104 | 0.088 | -0.176 | 1.390 | 0.417 | 1.378 | 1.380 | 1.222 |
| G C8-X 1H,7H | | | | | | | | | | | | |
| | | | ΔE _{taut} | ΔG _{taut} | cSAR(X) | cSAR(NH ₂) | cSAR(O) | EDDB_P(π) ₅ | EDDB_P(π) ₆ | d_CX | d_CNH ₂ | d_CO |
| NO ₂ | -745.0290 | -744.9442 | 1.53 | 1.51 | -0.135 | 0.127 | -0.134 | 1.888 | 0.586 | 1.454 | 1.372 | 1.217 |
| CN | -633.0442 | -632.9631 | 1.27 | 1.18 | -0.120 | 0.122 | -0.139 | 1.937 | 0.604 | 1.431 | 1.373 | 1.217 |
| Br | -3113.4233 | -3113.3511 | 0.41 | 0.37 | -0.034 | 0.109 | -0.154 | 1.477 | 0.633 | 1.867 | 1.376 | 1.219 |
| Cl | -1000.1709 | -1000.0970 | 0.26 | 0.24 | -0.023 | 0.109 | -0.156 | 1.438 | 0.637 | 1.710 | 1.376 | 1.219 |
| F | -640.0610 | -639.9845 | 0.00 | 0.00 | -0.003 | 0.110 | -0.161 | 1.203 | 0.646 | 1.313 | 1.376 | 1.219 |
| H | -541.0577 | -540.9720 | 0.23 | 0.25 | 0.000 | 0.099 | -0.160 | 1.609 | 0.643 | | 1.379 | 1.220 |
| SH | -938.8024 | -938.7205 | 0.00 | 0.00 | 0.019 | 0.102 | -0.164 | 1.454 | 0.651 | 1.757 | 1.378 | 1.220 |
| OH | -616.1004 | -616.0114 | 0.00 | 0.00 | 0.067 | 0.100 | -0.172 | 1.236 | 0.669 | 1.333 | 1.378 | 1.221 |
| NH ₂ | -596.2708 | -596.1699 | 0.00 | 0.00 | 0.100 | 0.092 | -0.180 | 1.323 | 0.692 | 1.378 | 1.381 | 1.222 |

| G C8-X 1H,9H | | | ΔE_{taut} | ΔG_{taut} | cSAR(X) | cSAR(NH2) | cSAR(O) | EDDB_P(π)5 | EDDB_P(π)6 | d_CX | d_CNH2 | d_CO |
|-----------------------|------------|------------|--------------------------|--------------------------|---------|-----------|----------|------------------|------------------|-------|--------|-------|
| NO2 | -745.0314 | -744.9466 | 0.00 | 0.00 | -0.144 | 0.145 | -0.101 | 1.829 | 0.455 | 1.449 | 1.364 | 1.210 |
| CN | -633.0462 | -632.9650 | 0.00 | 0.00 | -0.127 | 0.138 | -0.104 | 1.773 | 0.456 | 1.430 | 1.365 | 1.210 |
| Br | -3113.4240 | -3113.3517 | 0.00 | 0.00 | -0.037 | 0.120 | -0.119 | 1.452 | 0.472 | 1.869 | 1.371 | 1.212 |
| Cl | -1000.1713 | -1000.0974 | 0.00 | 0.00 | -0.026 | 0.118 | -0.120 | 1.407 | 0.473 | 1.713 | 1.371 | 1.212 |
| F | -640.0608 | -639.9842 | 0.15 | 0.19 | -0.004 | 0.116 | -0.124 | 1.159 | 0.479 | 1.316 | 1.372 | 1.212 |
| H | -541.0581 | -540.9724 | 0.00 | 0.00 | 0.000 | 0.108 | -0.124 | 1.494 | 0.473 | | 1.374 | 1.213 |
| SH | -938.8022 | -938.7202 | 0.11 | 0.18 | 0.014 | 0.110 | -0.128 | 1.357 | 0.486 | 1.760 | 1.373 | 1.213 |
| OH | -616.0993 | -616.0101 | 0.70 | 0.78 | 0.063 | 0.102 | -0.137 | 1.103 | 0.501 | 1.336 | 1.376 | 1.214 |
| NH2 | -596.2693 | -596.1682 | 0.97 | 1.07 | 0.080 | 0.097 | -0.138 | 1.055 | 0.500 | 1.388 | 1.377 | 1.214 |
| G C8-X 9H,C6-OH | | | ΔE_{taut} | ΔG_{taut} | cSAR(X) | cSAR(NH2) | cSAR(OH) | EDDB_P(π)5 | EDDB_P(π)6 | d_CX | d_CNH2 | d_COH |
| NO2 | -745.0269 | -744.9427 | 2.80 | 2.45 | -0.142 | 0.153 | 0.198 | 1.525 | 2.086 | 1.452 | 1.354 | 1.326 |
| CN | -633.0418 | -632.9608 | 2.81 | 2.60 | -0.125 | 0.145 | 0.195 | 1.461 | 2.126 | 1.431 | 1.356 | 1.327 |
| Br | -3113.4204 | -3113.3482 | 2.23 | 2.16 | -0.036 | 0.123 | 0.179 | 1.194 | 2.402 | 1.869 | 1.362 | 1.330 |
| Cl | -1000.1679 | -1000.0940 | 2.13 | 2.13 | -0.025 | 0.121 | 0.177 | 1.157 | 2.425 | 1.712 | 1.363 | 1.330 |
| F | -640.0580 | -639.9815 | 1.91 | 1.91 | -0.004 | 0.118 | 0.174 | 0.965 | 2.507 | 1.315 | 1.364 | 1.331 |
| H | -541.0543 | -540.9685 | 2.42 | 2.41 | 0.000 | 0.112 | 0.173 | 1.212 | 2.416 | | 1.365 | 1.331 |
| SH | -938.7990 | -938.7169 | 2.12 | 2.23 | 0.016 | 0.111 | 0.168 | 1.111 | 2.504 | 1.758 | 1.365 | 1.332 |
| OH | -616.0969 | -616.0077 | 2.23 | 2.28 | 0.065 | 0.103 | 0.159 | 0.919 | 2.636 | 1.334 | 1.368 | 1.334 |
| NH2 | -596.2669 | -596.1658 | 2.46 | 2.60 | 0.088 | 0.096 | 0.156 | 0.863 | 2.662 | 1.383 | 1.370 | 1.335 |
| G C8-X 7H,C6-OH | | | ΔE_{taut} | ΔG_{taut} | cSAR(X) | cSAR(NH2) | cSAR(OH) | EDDB_P(π)5 | EDDB_P(π)6 | d_CX | d_CNH2 | d_COH |
| NO2 | -745.0195 | -744.9354 | 7.43 | 7.03 | -0.132 | 0.141 | 0.163 | 1.380 | 2.146 | 1.457 | 1.360 | 1.336 |
| CN | -633.0344 | -632.9536 | 7.43 | 7.10 | -0.118 | 0.136 | 0.159 | 1.408 | 2.153 | 1.433 | 1.361 | 1.337 |
| Br | -3113.4145 | -3113.3428 | 5.95 | 5.59 | -0.034 | 0.120 | 0.145 | 1.120 | 2.410 | 1.868 | 1.366 | 1.339 |
| Cl | -1000.1622 | -1000.0888 | 5.73 | 5.37 | -0.023 | 0.119 | 0.143 | 1.098 | 2.435 | 1.711 | 1.366 | 1.340 |
| F | -640.0529 | -639.9770 | 5.06 | 4.73 | -0.003 | 0.120 | 0.140 | 0.953 | 2.509 | 1.312 | 1.366 | 1.340 |
| H | -541.0483 | -540.9630 | 6.16 | 5.90 | 0.000 | 0.109 | 0.139 | 1.211 | 2.394 | | 1.368 | 1.341 |
| SH | -938.7941 | -938.7124 | 5.23 | 5.07 | 0.021 | 0.110 | 0.136 | 1.122 | 2.510 | 1.755 | 1.368 | 1.341 |
| OH | -616.0931 | -616.0044 | 4.58 | 4.36 | 0.068 | 0.106 | 0.129 | 1.002 | 2.613 | 1.331 | 1.369 | 1.342 |
| NH2 | -596.2633 | -596.1627 | 4.71 | 4.52 | 0.105 | 0.098 | 0.121 | 1.044 | 2.648 | 1.375 | 1.371 | 1.344 |
| G C8-X 1H,3H,7H,C2-NH | | | ΔE_{taut} | ΔG_{taut} | cSAR(X) | cSAR(NH) | cSAR(O) | EDDB_P(π)5 | EDDB_P(π)6 | d_CX | d_CNH | d_CO |
| NO2 | -745.0187 | -744.9343 | 7.94 | 7.73 | -0.139 | -0.022 | -0.117 | 2.265 | 0.456 | 1.449 | 1.276 | 1.215 |
| CN | -633.0345 | -632.9535 | 7.36 | 7.18 | -0.123 | -0.026 | -0.122 | 2.277 | 0.472 | 1.429 | 1.276 | 1.216 |
| Br | -3113.4135 | -3113.3415 | 6.57 | 6.36 | -0.028 | -0.038 | -0.135 | 1.701 | 0.518 | 1.863 | 1.278 | 1.217 |
| Cl | -1000.1610 | -1000.0874 | 6.46 | 6.24 | -0.018 | -0.039 | -0.136 | 1.645 | 0.523 | 1.706 | 1.278 | 1.217 |
| F | -640.0505 | -639.9745 | 6.57 | 6.31 | 0.001 | -0.039 | -0.139 | 1.337 | 0.535 | 1.310 | 1.278 | 1.218 |
| H | -541.0493 | -540.9639 | 5.54 | 5.30 | 0.000 | -0.045 | -0.140 | 1.824 | 0.524 | | 1.279 | 1.218 |
| SH | -938.7926 | -938.7113 | 6.17 | 5.78 | 0.024 | -0.045 | -0.143 | 1.623 | 0.543 | 1.755 | 1.279 | 1.218 |
| OH | -616.0899 | -616.0013 | 6.63 | 6.33 | 0.072 | -0.049 | -0.148 | 1.328 | 0.565 | 1.331 | 1.280 | 1.219 |
| NH2 | -596.2616 | -596.1611 | 5.80 | 5.56 | 0.108 | -0.055 | -0.157 | 1.429 | 0.592 | 1.376 | 1.280 | 1.220 |

| iG C8-X | | | | | | | | | | | | | |
|------------------|------------|------------|--------------------------|--------------------------|---------|-----------|----------|------------------|------------------|-------|--------|-------|--|
| 3H,7H | E/h | G/h | ΔE_{taut} | ΔG_{taut} | cSAR(X) | cSAR(NH2) | cSAR(O) | EDDB_P(π)5 | EDDB_P(π)6 | d_CX | d_CNH2 | d_CO | |
| NO2 | -745.0178 | -744.9344 | 7.73 | 7.12 | -0.138 | 0.146 | -0.092 | 1.906 | 0.553 | 1.449 | 1.363 | 1.211 | |
| CN | -633.0320 | -632.9528 | 8.07 | 7.07 | -0.124 | 0.156 | -0.099 | 1.897 | 0.571 | 1.429 | 1.355 | 1.211 | |
| Br | -3113.4122 | -3113.3409 | 7.09 | 6.94 | -0.026 | 0.121 | -0.108 | 1.417 | 0.606 | 1.864 | 1.369 | 1.213 | |
| Cl | -1000.1590 | -1000.0870 | 7.48 | 6.84 | -0.018 | 0.142 | -0.114 | 1.357 | 0.612 | 1.708 | 1.357 | 1.213 | |
| F | -640.0485 | -639.9742 | 8.22 | 7.12 | 0.001 | 0.140 | -0.115 | 1.117 | 0.614 | 1.311 | 1.357 | 1.213 | |
| H | -541.0465 | -540.9626 | 6.91 | 6.30 | 0.000 | 0.137 | -0.119 | 1.502 | 0.629 | | 1.357 | 1.214 | |
| SH | -938.7916 | -938.7106 | 6.23 | 6.02 | 0.028 | 0.111 | -0.115 | 1.367 | 0.628 | 1.755 | 1.372 | 1.214 | |
| OH | -616.0897 | -616.0014 | 5.82 | 5.43 | 0.077 | 0.106 | -0.120 | 1.149 | 0.645 | 1.330 | 1.373 | 1.214 | |
| NH2 | -596.2611 | -596.1605 | 5.43 | 5.25 | 0.116 | 0.097 | -0.124 | 1.135 | 0.661 | 1.374 | 1.374 | 1.215 | |
| iG C8-X 1H,3H | | | ΔE_{taut} | ΔG_{taut} | cSAR(X) | cSAR(NH2) | cSAR(O) | EDDB_P(π)5 | EDDB_P(π)6 | d_CX | d_CNH2 | d_CO | |
| NO2 | -745.0263 | -744.9431 | 2.41 | 1.65 | -0.160 | 0.222 | -0.069 | 1.643 | 0.642 | 1.466 | 1.336 | 1.210 | |
| CN | -633.0440 | -632.9638 | 0.55 | 0.16 | -0.131 | 0.214 | -0.072 | 1.586 | 0.651 | 1.438 | 1.338 | 1.210 | |
| Br | -3113.4209 | -3113.3494 | 1.59 | 1.60 | -0.056 | 0.182 | -0.082 | 1.313 | 0.725 | 1.875 | 1.345 | 1.212 | |
| Cl | -1000.1686 | -1000.0954 | 1.42 | 1.60 | -0.038 | 0.176 | -0.083 | 1.269 | 0.737 | 1.717 | 1.347 | 1.212 | |
| F | -640.0616 | -639.9855 | 0.00 | 0.00 | -0.006 | 0.164 | -0.084 | 1.156 | 0.765 | 1.316 | 1.350 | 1.212 | |
| H | -541.0516 | -540.9665 | 3.71 | 3.85 | 0.000 | 0.167 | -0.090 | 1.237 | 0.728 | | 1.349 | 1.213 | |
| SH | -938.7995 | -938.7174 | 1.26 | 1.75 | 0.008 | 0.149 | -0.088 | 1.122 | 0.775 | 1.756 | 1.354 | 1.213 | |
| OH | -616.0954 | -616.0064 | 2.21 | 2.27 | 0.068 | 0.123 | -0.091 | 0.953 | 0.814 | 1.334 | 1.361 | 1.213 | |
| NH2 | -596.2697 | -596.1688 | 0.00 | 0.00 | 0.118 | 0.100 | -0.099 | 0.851 | 0.823 | 1.369 | 1.367 | 1.214 | |
| iG C8-X 1H,9H | | | ΔE_{taut} | ΔG_{taut} | cSAR(X) | cSAR(NH2) | cSAR(O) | EDDB_P(π)5 | EDDB_P(π)6 | d_CX | d_CNH2 | d_CO | |
| NO2 | -745.0213 | -744.9382 | 5.56 | 4.71 | -0.147 | 0.206 | -0.101 | 1.229 | 0.640 | 1.449 | 1.340 | 1.211 | |
| CN | -633.0360 | -632.9566 | 5.57 | 4.69 | -0.127 | 0.200 | -0.107 | 1.238 | 0.667 | 1.430 | 1.341 | 1.212 | |
| Br | -3113.4148 | -3113.3438 | 5.42 | 5.13 | -0.035 | 0.177 | -0.120 | 1.020 | 0.706 | 1.868 | 1.345 | 1.214 | |
| Cl | -1000.1624 | -1000.0897 | 5.36 | 5.15 | -0.024 | 0.174 | -0.121 | 0.987 | 0.708 | 1.711 | 1.345 | 1.214 | |
| F | -640.0525 | -639.9773 | 5.75 | 5.20 | -0.003 | 0.168 | -0.121 | 0.834 | 0.709 | 1.314 | 1.347 | 1.214 | |
| H | -541.0487 | -540.9642 | 5.52 | 5.29 | 0.000 | 0.171 | -0.129 | 1.028 | 0.736 | | 1.346 | 1.215 | |
| SH | -938.7929 | -938.7121 | 5.40 | 5.11 | 0.017 | 0.162 | -0.127 | 0.932 | 0.726 | 1.758 | 1.347 | 1.215 | |
| OH | -616.0905 | -616.0027 | 5.28 | 4.63 | 0.066 | 0.148 | -0.131 | 0.786 | 0.735 | 1.334 | 1.350 | 1.215 | |
| NH2 | -596.2619 | -596.1615 | 4.90 | 4.57 | 0.099 | 0.120 | -0.133 | 0.703 | 0.730 | 1.379 | 1.362 | 1.216 | |
| iG C8-X 9H,C2-OH | | | ΔE_{taut} | ΔG_{taut} | cSAR(X) | cSAR(NH2) | cSAR(OH) | EDDB_P(π)5 | EDDB_P(π)6 | d_CX | d_CNH2 | d_COH | |
| NO2 | -745.0301 | -744.9457 | 0.00 | 0.00 | -0.143 | 0.182 | 0.214 | 1.615 | 1.853 | 1.450 | 1.342 | 1.335 | |
| CN | -633.0449 | -632.9641 | 0.00 | 0.00 | -0.125 | 0.177 | 0.210 | 1.618 | 1.874 | 1.430 | 1.343 | 1.335 | |
| Br | -3113.4234 | -3113.3520 | 0.00 | 0.00 | -0.035 | 0.158 | 0.195 | 1.309 | 2.097 | 1.868 | 1.346 | 1.339 | |
| Cl | -1000.1709 | -1000.0979 | 0.00 | 0.00 | -0.024 | 0.156 | 0.194 | 1.266 | 2.113 | 1.712 | 1.346 | 1.339 | |
| F | -640.0607 | -639.9851 | 0.59 | 0.30 | -0.003 | 0.151 | 0.192 | 1.038 | 2.182 | 1.315 | 1.348 | 1.340 | |
| H | -541.0575 | -540.9726 | 0.00 | 0.00 | 0.000 | 0.151 | 0.187 | 1.324 | 2.090 | | 1.347 | 1.340 | |
| SH | -938.8015 | -938.7202 | 0.00 | 0.00 | 0.016 | 0.144 | 0.187 | 1.202 | 2.196 | 1.759 | 1.349 | 1.340 | |
| OH | -616.0989 | -616.0101 | 0.00 | 0.00 | 0.066 | 0.129 | 0.182 | 0.978 | 2.329 | 1.335 | 1.353 | 1.342 | |
| NH2 | -596.2694 | -596.1685 | 0.23 | 0.20 | 0.090 | 0.124 | 0.177 | 0.922 | 2.342 | 1.384 | 1.355 | 1.343 | |

| iG C8-X 7H,C2-OH | | | ΔE_{taut} | ΔG_{taut} | cSAR(X) | cSAR(NH2) | cSAR(OH) | EDDB_P(π)5 | EDDB_P(π)6 | d_CX | d_CNH2 | d_COH |
|------------------------|------------|------------|--------------------------|--------------------------|---------|-----------|----------|------------------|------------------|-------|--------|-------|
| NO2 | -745.0152 | -744.9310 | 9.36 | 9.24 | -0.130 | 0.150 | 0.206 | 1.402 | 2.251 | 1.457 | 1.364 | 1.336 |
| CN | -633.0296 | -632.9489 | 9.61 | 9.56 | -0.118 | 0.141 | 0.203 | 1.429 | 2.318 | 1.433 | 1.367 | 1.337 |
| Br | -3113.4100 | -3113.3381 | 8.45 | 8.67 | -0.032 | 0.123 | 0.192 | 1.103 | 2.575 | 1.868 | 1.371 | 1.339 |
| Cl | -1000.1576 | -1000.0842 | 8.32 | 8.62 | -0.022 | 0.122 | 0.191 | 1.079 | 2.594 | 1.711 | 1.371 | 1.339 |
| F | -640.0482 | -639.9722 | 8.44 | 8.39 | -0.003 | 0.118 | 0.192 | 0.917 | 2.719 | 1.313 | 1.372 | 1.339 |
| H | -541.0438 | -540.9585 | 8.59 | 8.89 | 0.000 | 0.114 | 0.185 | 1.198 | 2.482 | | 1.373 | 1.341 |
| SH | -938.7896 | -938.7078 | 7.49 | 7.77 | 0.022 | 0.110 | 0.185 | 1.094 | 2.600 | 1.756 | 1.375 | 1.341 |
| OH | -616.0887 | -615.9998 | 6.40 | 6.42 | 0.069 | 0.103 | 0.182 | 0.964 | 2.724 | 1.331 | 1.376 | 1.341 |
| NH2 | -596.2585 | -596.1582 | 7.09 | 6.69 | 0.104 | 0.090 | 0.175 | 1.052 | 2.664 | 1.376 | 1.379 | 1.343 |
| iG C8-X 1H,3H,7H,C6-NH | | | ΔE_{taut} | ΔG_{taut} | cSAR(X) | cSAR(NH) | cSAR(O) | EDDB_P(π)5 | EDDB_P(π)6 | d_CX | d_CNH | d_CO |
| NO2 | -745.0271 | -744.9422 | 1.89 | 2.19 | -0.142 | -0.055 | -0.077 | 2.398 | 0.386 | 1.447 | 1.280 | 1.210 |
| CN | -633.0429 | -632.9617 | 1.22 | 1.51 | -0.124 | -0.061 | -0.080 | 2.408 | 0.397 | 1.428 | 1.280 | 1.211 |
| Br | -3113.4213 | -3113.3491 | 1.35 | 1.78 | -0.030 | -0.077 | -0.090 | 1.741 | 0.409 | 1.863 | 1.281 | 1.212 |
| Cl | -1000.1688 | -1000.0949 | 1.33 | 1.91 | -0.020 | -0.079 | -0.090 | 1.675 | 0.411 | 1.707 | 1.281 | 1.212 |
| F | -640.0581 | -639.9816 | 2.23 | 2.46 | 0.001 | -0.083 | -0.090 | 1.333 | 0.415 | 1.311 | 1.282 | 1.213 |
| H | -541.0569 | -540.9713 | 0.33 | 0.85 | 0.000 | -0.084 | -0.095 | 1.870 | 0.416 | | 1.282 | 1.213 |
| SH | -938.8001 | -938.7183 | 0.86 | 1.20 | 0.022 | -0.086 | -0.095 | 1.636 | 0.422 | 1.756 | 1.282 | 1.213 |
| OH | -616.0971 | -616.0081 | 1.16 | 1.22 | 0.071 | -0.094 | -0.098 | 1.299 | 0.421 | 1.332 | 1.283 | 1.214 |
| NH2 | -596.2685 | -596.1677 | 0.76 | 0.70 | 0.103 | -0.103 | -0.103 | 1.398 | 0.431 | 1.378 | 1.284 | 1.214 |

| tG C8-X | | | | | | | | | | | | |
|---------------|------------|------------|--------------------------|--------------------------|---------|-----------|---------|------------------|------------------|-------|--------|-------|
| 3H,7H | E/h | G/h | ΔE_{taut} | ΔG_{taut} | cSAR(X) | cSAR(NH2) | cSAR(S) | EDDB_P(π)5 | EDDB_P(π)6 | d_CX | d_CNH2 | d_CS |
| NO2 | -1067.7177 | -1067.6367 | 7.77 | 9.35 | -0.147 | 0.138 | -0.182 | 2.338 | 0.715 | 1.447 | 1.366 | 1.654 |
| CN | -955.7338 | -955.6564 | 7.47 | 8.52 | -0.127 | 0.135 | -0.190 | 2.330 | 0.742 | 1.428 | 1.367 | 1.655 |
| Br | -3436.1123 | -3436.0436 | 8.21 | 8.89 | -0.030 | 0.118 | -0.214 | 1.843 | 0.777 | 1.862 | 1.371 | 1.657 |
| Cl | -1322.8598 | -1322.7895 | 8.30 | 8.86 | -0.019 | 0.117 | -0.216 | 1.782 | 0.782 | 1.706 | 1.372 | 1.657 |
| F | -962.7492 | -962.6763 | 8.82 | 9.26 | 0.001 | 0.115 | -0.221 | 1.464 | 0.793 | 1.310 | 1.372 | 1.657 |
| H | -863.7478 | -863.6656 | 7.60 | 7.90 | 0.000 | 0.112 | -0.222 | 1.937 | 0.801 | | 1.373 | 1.658 |
| SH | -1261.4913 | -1261.4129 | 8.70 | 8.74 | 0.025 | 0.108 | -0.226 | 1.727 | 0.820 | 1.754 | 1.374 | 1.658 |
| OH | -938.7882 | -938.7027 | 9.60 | 9.56 | 0.074 | 0.101 | -0.236 | 1.420 | 0.843 | 1.330 | 1.376 | 1.659 |
| NH2 | -918.9606 | -918.8632 | 8.91 | 8.65 | 0.115 | 0.095 | -0.252 | 1.497 | 0.896 | 1.373 | 1.378 | 1.662 |
| tG C8-X 1H,7H | | | | | | | | | | | | |
| | | | ΔE_{taut} | ΔG_{taut} | cSAR(X) | cSAR(NH2) | cSAR(S) | EDDB_P(π)5 | EDDB_P(π)6 | d_CX | d_CNH2 | d_CS |
| NO2 | -1067.7301 | -1067.6486 | 0.00 | 1.89 | -0.138 | 0.131 | -0.193 | 1.881 | 1.123 | 1.453 | 1.369 | 1.653 |
| CN | -955.7457 | -955.6676 | 0.00 | 1.46 | -0.121 | 0.126 | -0.200 | 1.922 | 1.161 | 1.431 | 1.370 | 1.654 |
| Br | -3436.1254 | -3436.0563 | 0.00 | 0.95 | -0.031 | 0.114 | -0.227 | 1.547 | 1.233 | 1.864 | 1.374 | 1.657 |
| Cl | -1322.8730 | -1322.8022 | 0.00 | 0.89 | -0.021 | 0.114 | -0.230 | 1.513 | 1.245 | 1.708 | 1.374 | 1.657 |
| F | -962.7633 | -962.6899 | 0.00 | 0.77 | -0.002 | 0.118 | -0.238 | 1.294 | 1.282 | 1.311 | 1.373 | 1.658 |
| H | -863.7599 | -863.6773 | 0.00 | 0.61 | 0.000 | 0.105 | -0.235 | 1.645 | 1.266 | | 1.376 | 1.658 |
| SH | -1261.5051 | -1261.4264 | 0.00 | 0.30 | 0.024 | 0.108 | -0.244 | 1.540 | 1.308 | 1.754 | 1.375 | 1.659 |
| OH | -938.8035 | -938.7175 | 0.00 | 0.25 | 0.071 | 0.108 | -0.258 | 1.353 | 1.345 | 1.329 | 1.375 | 1.661 |
| NH2 | -918.9748 | -918.8770 | 0.00 | 0.00 | 0.115 | 0.100 | -0.275 | 1.391 | 1.412 | 1.371 | 1.377 | 1.664 |

| tG C8-X 1H,9H | | | ΔE_{taut} | ΔG_{taut} | cSAR(X) | cSAR(NH2) | cSAR(S) | EDDB_P(π)5 | EDDB_P(π)6 | d_CX | d_CNH2 | d_CS |
|------------------------|------------|------------|--------------------------|--------------------------|---------|-----------|----------|------------------|------------------|-------|--------|-------|
| NO2 | -1067.7289 | -1067.6474 | 0.75 | 2.63 | -0.146 | 0.148 | -0.155 | 1.756 | 0.831 | 1.449 | 1.362 | 1.643 |
| CN | -955.7439 | -955.6658 | 1.15 | 2.58 | -0.127 | 0.141 | -0.161 | 1.693 | 0.842 | 1.429 | 1.364 | 1.644 |
| Br | -3436.1221 | -3436.0529 | 2.04 | 3.04 | -0.035 | 0.125 | -0.186 | 1.381 | 0.897 | 1.867 | 1.368 | 1.647 |
| Cl | -1322.8695 | -1322.7988 | 2.21 | 3.03 | -0.024 | 0.123 | -0.189 | 1.339 | 0.901 | 1.711 | 1.369 | 1.647 |
| F | -962.7590 | -962.6858 | 2.65 | 3.36 | -0.004 | 0.122 | -0.194 | 1.118 | 0.913 | 1.315 | 1.369 | 1.648 |
| H | -863.7563 | -863.6738 | 2.27 | 2.80 | 0.000 | 0.114 | -0.194 | 1.410 | 0.916 | | 1.371 | 1.648 |
| SH | -1261.5010 | -1261.4222 | 2.62 | 2.93 | 0.018 | 0.116 | -0.203 | 1.288 | 0.945 | 1.758 | 1.371 | 1.649 |
| OH | -938.7986 | -938.7126 | 3.11 | 3.35 | 0.066 | 0.110 | -0.217 | 1.062 | 0.990 | 1.334 | 1.372 | 1.651 |
| NH2 | -918.9686 | -918.8707 | 3.86 | 3.92 | 0.088 | 0.104 | -0.221 | 1.015 | 0.998 | 1.384 | 1.374 | 1.652 |
| tG C8-X 9H,C6-SH | | | ΔE_{taut} | ΔG_{taut} | cSAR(X) | cSAR(NH2) | cSAR(SH) | EDDB_P(π)5 | EDDB_P(π)6 | d_CX | d_CNH2 | d_CSH |
| NO2 | -1067.7290 | -1067.6516 | 0.71 | 0.00 | -0.142 | 0.159 | 0.154 | 1.498 | 2.195 | 1.452 | 1.354 | 1.752 |
| CN | -955.7440 | -955.6699 | 1.08 | 0.00 | -0.125 | 0.152 | 0.149 | 1.491 | 2.240 | 1.431 | 1.356 | 1.753 |
| Br | -3436.1231 | -3436.0578 | 1.39 | 0.00 | -0.034 | 0.129 | 0.130 | 1.223 | 2.501 | 1.867 | 1.362 | 1.756 |
| Cl | -1322.8707 | -1322.8036 | 1.47 | 0.00 | -0.024 | 0.127 | 0.128 | 1.186 | 2.528 | 1.711 | 1.362 | 1.756 |
| F | -962.7608 | -962.6911 | 1.57 | 0.00 | -0.004 | 0.124 | 0.125 | 0.983 | 2.626 | 1.313 | 1.363 | 1.757 |
| H | -863.7571 | -863.6782 | 1.74 | 0.00 | 0.000 | 0.119 | 0.123 | 1.235 | 2.510 | | 1.364 | 1.757 |
| SH | -1261.5021 | -1261.4269 | 1.89 | 0.00 | 0.019 | 0.117 | 0.117 | 1.139 | 2.627 | 1.756 | 1.365 | 1.758 |
| OH | -938.8002 | -938.7179 | 2.04 | 0.00 | 0.068 | 0.109 | 0.106 | 0.939 | 2.777 | 1.332 | 1.367 | 1.759 |
| NH2 | -918.9706 | -918.8763 | 2.60 | 0.40 | 0.096 | 0.101 | 0.101 | 0.891 | 2.816 | 1.380 | 1.369 | 1.760 |
| tG C8-X 7H,C6-SH | | | ΔE_{taut} | ΔG_{taut} | cSAR(X) | cSAR(NH2) | cSAR(SH) | EDDB_P(π)5 | EDDB_P(π)6 | d_CX | d_CNH2 | d_CSH |
| NO2 | -1067.7194 | -1067.6425 | 6.70 | 5.71 | -0.131 | 0.143 | 0.121 | 1.332 | 2.315 | 1.458 | 1.359 | 1.761 |
| CN | -955.7342 | -955.6608 | 7.18 | 5.73 | -0.118 | 0.137 | 0.115 | 1.358 | 2.342 | 1.433 | 1.361 | 1.763 |
| Br | -3436.1149 | -3436.0504 | 6.55 | 4.67 | -0.032 | 0.121 | 0.099 | 1.098 | 2.577 | 1.867 | 1.365 | 1.765 |
| Cl | -1322.8627 | -1322.7964 | 6.51 | 4.50 | -0.021 | 0.121 | 0.097 | 1.078 | 2.592 | 1.710 | 1.365 | 1.765 |
| F | -962.7534 | -962.6846 | 6.18 | 4.09 | -0.003 | 0.121 | 0.094 | 0.941 | 2.653 | 1.311 | 1.365 | 1.765 |
| H | -863.7488 | -863.6707 | 6.99 | 4.71 | 0.000 | 0.111 | 0.091 | 1.172 | 2.581 | | 1.368 | 1.766 |
| SH | -1261.4948 | -1261.4206 | 6.47 | 3.94 | 0.024 | 0.112 | 0.088 | 1.097 | 2.659 | 1.754 | 1.367 | 1.766 |
| OH | -938.7942 | -938.7127 | 5.84 | 3.26 | 0.070 | 0.107 | 0.081 | 0.991 | 2.759 | 1.329 | 1.369 | 1.767 |
| NH2 | -918.9647 | -918.8713 | 6.32 | 3.52 | 0.111 | 0.099 | 0.070 | 1.016 | 2.686 | 1.372 | 1.371 | 1.769 |
| tG C8-X 1H,3H,7H,C2-NH | | | ΔE_{taut} | ΔG_{taut} | cSAR(X) | cSAR(NH) | cSAR(S) | EDDB_P(π)5 | EDDB_P(π)6 | d_CX | d_CNH | d_CS |
| NO2 | -1067.7189 | -1067.6375 | 7.05 | 8.84 | -0.140 | -0.015 | -0.158 | 2.159 | 0.544 | 1.449 | 1.275 | 1.650 |
| CN | -955.7349 | -955.6571 | 6.74 | 8.08 | -0.125 | -0.016 | -0.164 | 2.265 | 0.545 | 1.428 | 1.276 | 1.651 |
| Br | -3436.1141 | -3436.0452 | 7.06 | 7.88 | -0.027 | -0.027 | -0.188 | 1.806 | 0.575 | 1.861 | 1.277 | 1.653 |
| Cl | -1322.8617 | -1322.7912 | 7.12 | 7.82 | -0.017 | -0.028 | -0.190 | 1.752 | 0.577 | 1.705 | 1.278 | 1.653 |
| F | -962.7512 | -962.6782 | 7.59 | 8.11 | 0.002 | -0.028 | -0.195 | 1.448 | 0.581 | 1.309 | 1.277 | 1.654 |
| H | -863.7499 | -863.6676 | 6.26 | 6.70 | 0.000 | -0.033 | -0.195 | 1.910 | 0.580 | | 1.278 | 1.654 |
| SH | -1261.4936 | -1261.4151 | 7.22 | 7.36 | 0.028 | -0.034 | -0.202 | 1.746 | 0.595 | 1.753 | 1.278 | 1.655 |
| OH | -938.7910 | -938.7054 | 7.85 | 7.86 | 0.076 | -0.037 | -0.212 | 1.463 | 0.611 | 1.329 | 1.279 | 1.656 |
| NH2 | -918.9634 | -918.8660 | 7.11 | 6.85 | 0.120 | -0.043 | -0.229 | 1.560 | 0.622 | 1.371 | 1.280 | 1.659 |

| Hx C8-X | | | | | | | | | | | |
|------------------|------------|------------|--------------------------|--------------------------|---------|-----------|------------------|------------------|-------|-------|--|
| 3H,7H | E/h | G/h | ΔE_{taut} | ΔG_{taut} | cSAR(X) | cSAR(NH2) | EDDB_P(π)5 | EDDB_P(π)6 | d_CX | d_CO | |
| NO2 | -689.7957 | -689.7269 | 9.10 | 8.67 | -0.133 | -0.118 | 2.282 | 0.339 | 1.451 | 1.215 | |
| CN | -577.8118 | -577.7464 | 8.66 | 8.26 | -0.118 | -0.123 | 2.298 | 0.353 | 1.430 | 1.216 | |
| Br | -3058.1913 | -3058.1350 | 8.52 | 8.19 | -0.028 | -0.140 | 1.726 | 0.384 | 1.862 | 1.217 | |
| Cl | -944.9389 | -944.8809 | 8.54 | 8.19 | -0.018 | -0.141 | 1.667 | 0.387 | 1.706 | 1.218 | |
| F | -584.8285 | -584.7679 | 8.82 | 8.46 | 0.000 | -0.145 | 1.345 | 0.390 | 1.310 | 1.218 | |
| H | -485.8271 | -485.7572 | 8.03 | 7.70 | 0.000 | -0.146 | 1.847 | 0.394 | | 1.218 | |
| SH | -883.5705 | -883.5044 | 8.76 | 8.44 | 0.024 | -0.149 | 1.631 | 0.397 | 1.755 | 1.219 | |
| OH | -560.8678 | -560.7948 | 9.32 | 8.89 | 0.071 | -0.156 | 1.312 | 0.401 | 1.331 | 1.219 | |
| NH2 | -541.0397 | -540.9548 | 8.61 | 8.19 | 0.107 | -0.166 | 1.404 | 0.420 | 1.375 | 1.220 | |
| Hx C8-X 1H,7H | | | ΔE_{taut} | ΔG_{taut} | cSAR(X) | cSAR(O) | EDDB_P(π)5 | EDDB_P(π)6 | d_CX | d_CO | |
| NO2 | -689.8093 | -689.7398 | 0.59 | 0.55 | -0.127 | -0.129 | 1.997 | 0.560 | 1.456 | 1.216 | |
| CN | -577.8248 | -577.7589 | 0.45 | 0.42 | -0.115 | -0.134 | 2.048 | 0.578 | 1.432 | 1.217 | |
| Br | -3058.2049 | -3058.1481 | 0.00 | 0.00 | -0.030 | -0.149 | 1.579 | 0.627 | 1.865 | 1.218 | |
| Cl | -944.9525 | -944.8940 | 0.00 | 0.00 | -0.021 | -0.151 | 1.536 | 0.633 | 1.708 | 1.218 | |
| F | -584.8426 | -584.7814 | 0.00 | 0.00 | -0.002 | -0.154 | 1.279 | 0.644 | 1.311 | 1.218 | |
| H | -485.8399 | -485.7695 | 0.00 | 0.00 | 0.000 | -0.155 | 1.703 | 0.639 | | 1.219 | |
| SH | -883.5845 | -883.5179 | 0.00 | 0.00 | 0.022 | -0.159 | 1.536 | 0.653 | 1.756 | 1.219 | |
| OH | -560.8827 | -560.8089 | 0.00 | 0.00 | 0.068 | -0.166 | 1.295 | 0.664 | 1.331 | 1.220 | |
| NH2 | -541.0534 | -540.9678 | 0.00 | 0.00 | 0.102 | -0.175 | 1.386 | 0.689 | 1.376 | 1.221 | |
| Hx C8-X 1H,9H | | | ΔE_{taut} | ΔG_{taut} | cSAR(X) | cSAR(O) | EDDB_P(π)5 | EDDB_P(π)6 | d_CX | d_CO | |
| NO2 | -689.8102 | -689.7407 | 0.00 | 0.00 | -0.132 | -0.094 | 1.981 | 0.421 | 1.453 | 1.209 | |
| CN | -577.8256 | -577.7596 | 0.00 | 0.00 | -0.118 | -0.097 | 1.964 | 0.426 | 1.431 | 1.209 | |
| Br | -3058.2049 | -3058.1479 | 0.04 | 0.09 | -0.032 | -0.113 | 1.621 | 0.464 | 1.867 | 1.211 | |
| Cl | -944.9523 | -944.8937 | 0.13 | 0.17 | -0.023 | -0.114 | 1.568 | 0.467 | 1.710 | 1.211 | |
| F | -584.8420 | -584.7808 | 0.34 | 0.40 | -0.003 | -0.117 | 1.284 | 0.477 | 1.313 | 1.212 | |
| H | -485.8396 | -485.7692 | 0.17 | 0.19 | 0.000 | -0.118 | 1.690 | 0.469 | | 1.212 | |
| SH | -883.5839 | -883.5172 | 0.34 | 0.39 | 0.018 | -0.123 | 1.510 | 0.487 | 1.758 | 1.213 | |
| OH | -560.8816 | -560.8078 | 0.67 | 0.71 | 0.065 | -0.132 | 1.214 | 0.510 | 1.333 | 1.214 | |
| NH2 | -541.0519 | -540.9663 | 0.97 | 0.96 | 0.088 | -0.134 | 1.245 | 0.512 | 1.383 | 1.214 | |
| Hx C8-X 9H,C6-OH | | | ΔE_{taut} | ΔG_{taut} | cSAR(X) | cSAR(OH) | EDDB_P(π)5 | EDDB_P(π)6 | d_CX | d_COH | |
| NO2 | -689.7979 | -689.7286 | 7.69 | 7.59 | -0.126 | 0.207 | 1.542 | 2.532 | 1.456 | 1.329 | |
| CN | -577.8133 | -577.7476 | 7.66 | 7.53 | -0.113 | 0.203 | 1.571 | 2.540 | 1.432 | 1.329 | |
| Br | -3058.1944 | -3058.1375 | 6.62 | 6.67 | -0.029 | 0.187 | 1.289 | 2.774 | 1.865 | 1.332 | |
| Cl | -944.9420 | -944.8835 | 6.58 | 6.54 | -0.020 | 0.186 | 1.253 | 2.796 | 1.708 | 1.333 | |
| F | -584.8324 | -584.7712 | 6.41 | 6.41 | -0.003 | 0.183 | 1.049 | 2.870 | 1.311 | 1.333 | |
| H | -485.8293 | -485.7589 | 6.66 | 6.66 | 0.000 | 0.181 | 1.369 | 2.738 | | 1.333 | |
| SH | -883.5737 | -883.5070 | 6.73 | 6.83 | 0.023 | 0.175 | 1.215 | 2.865 | 1.755 | 1.335 | |
| OH | -560.8721 | -560.7984 | 6.64 | 6.63 | 0.068 | 0.166 | 1.012 | 2.986 | 1.337 | 1.330 | |
| NH2 | -541.0434 | -540.9577 | 6.33 | 6.33 | 0.101 | 0.161 | 1.026 | 2.991 | 1.375 | 1.337 | |

| Hx C8-X 7H,C6-OH | | | ΔE _{taut} | ΔG _{taut} | cSAR(X) cSAR(OH) | | EDDB_P(π)5 | EDDB_P(π)6 | d_CX | d_COH |
|------------------|------------|------------|--------------------|--------------------|------------------|-------|------------|------------|-------|-------|
| NO2 | -689.7952 | -689.7263 | 9.41 | 9.01 | -0.122 | 0.171 | 1.455 | 2.475 | 1.460 | 1.334 |
| CN | -577.8105 | -577.7451 | 9.47 | 9.12 | -0.111 | 0.166 | 1.499 | 2.430 | 1.434 | 1.335 |
| Br | -3058.1918 | -3058.1354 | 8.20 | 7.98 | -0.029 | 0.152 | 1.208 | 2.642 | 1.866 | 1.338 |
| Cl | -944.9396 | -944.8815 | 8.12 | 7.80 | -0.020 | 0.151 | 1.184 | 2.661 | 1.708 | 1.338 |
| F | -584.8303 | -584.7696 | 7.71 | 7.44 | -0.003 | 0.148 | 1.026 | 2.780 | 1.310 | 1.338 |
| H | -485.8263 | -485.7564 | 8.53 | 8.20 | 0.000 | 0.146 | 1.295 | 2.548 | | 1.339 |
| SH | -883.5720 | -883.5058 | 7.80 | 7.59 | 0.024 | 0.143 | 1.199 | 2.666 | 1.754 | 1.340 |
| OH | -560.8714 | -560.7980 | 7.09 | 6.86 | 0.069 | 0.136 | 1.065 | 2.788 | 1.329 | 1.341 |
| NH2 | -541.0420 | -540.9568 | 7.18 | 6.90 | 0.108 | 0.127 | 1.120 | 2.707 | 1.372 | 1.343 |

| adG C8-X 3H | | | ΔE _{taut} | ΔG _{taut} | cSAR(X) cSAR(NH2) cSAR(O) | | | EDDB_P(π)5 | EDDB_P(π)6 | d_CX | d_CN H2 | d_CO |
|-------------|------------|------------|--------------------|--------------------|---------------------------|-------|--------|------------|------------|-------|---------|-------|
| NO2 | -745.0233 | -744.9401 | 3.44 | 3.08 | -0.147 | 0.154 | -0.039 | 1.263 | 0.328 | 1.449 | 1.354 | 1.204 |
| CN | -633.0409 | -632.9609 | 3.27 | 2.87 | -0.127 | 0.150 | -0.043 | 1.175 | 0.340 | 1.430 | 1.355 | 1.204 |
| Br | -3113.4155 | -3113.3443 | 3.74 | 3.39 | -0.046 | 0.134 | -0.051 | 1.142 | 0.354 | 1.869 | 1.360 | 1.205 |
| Cl | -1000.1620 | -1000.0892 | 3.83 | 3.51 | -0.034 | 0.133 | -0.052 | 1.117 | 0.357 | 1.715 | 1.360 | 1.205 |
| F | -640.0495 | -639.9741 | 4.22 | 3.94 | -0.006 | 0.131 | -0.053 | 1.052 | 0.358 | 1.320 | 1.361 | 1.205 |
| H | -541.0493 | -540.9647 | 4.92 | 5.57 | 0.000 | 0.124 | -0.058 | 1.136 | 0.372 | | 1.362 | 1.206 |
| SH | -938.7920 | -938.7113 | 4.75 | 4.87 | -0.012 | 0.128 | -0.055 | 0.680 | 0.364 | 1.761 | 1.361 | 1.206 |
| OH | -616.0829 | -615.9952 | 5.20 | 4.77 | 0.053 | 0.118 | -0.058 | 0.911 | 0.370 | 1.343 | 1.364 | 1.206 |
| NH2 | -596.2560 | -596.1561 | 4.58 | 4.41 | 0.087 | 0.112 | -0.067 | 0.816 | 0.395 | 1.387 | 1.366 | 1.208 |

| adG C8-X 1H | | | ΔE _{taut} | ΔG _{taut} | cSAR(X) cSAR(NH2) cSAR(O) | | | EDDB_P(π)5 | EDDB_P(π)6 | d_CX | d_CN H2 | d_CO |
|-------------|------------|------------|--------------------|--------------------|---------------------------|-------|--------|------------|------------|-------|---------|-------|
| NO2 | -745.0288 | -744.9450 | 0.00 | 0.00 | -0.144 | 0.141 | -0.033 | 1.168 | 0.587 | 1.453 | 1.364 | 1.204 |
| CN | -633.0461 | -632.9654 | 0.00 | 0.00 | -0.125 | 0.136 | -0.037 | 1.077 | 0.606 | 1.432 | 1.365 | 1.205 |
| Br | -3113.4214 | -3113.3497 | 0.00 | 0.00 | -0.047 | 0.122 | -0.048 | 1.165 | 0.645 | 1.871 | 1.369 | 1.206 |
| Cl | -1000.1681 | -1000.0948 | 0.00 | 0.00 | -0.035 | 0.121 | -0.049 | 1.132 | 0.651 | 1.716 | 1.369 | 1.206 |
| F | -640.0562 | -639.9804 | 0.00 | 0.00 | -0.008 | 0.122 | -0.051 | 1.072 | 0.660 | 1.320 | 1.369 | 1.207 |
| H | -541.0545 | -540.9695 | 1.61 | 2.55 | 0.000 | 0.108 | -0.055 | 1.066 | 0.666 | | 1.373 | 1.207 |
| SH | -938.7988 | -938.7177 | 0.51 | 0.82 | 0.001 | 0.115 | -0.054 | 1.002 | 0.671 | 1.760 | 1.371 | 1.207 |
| OH | -616.0912 | -616.0028 | 0.00 | 0.00 | 0.052 | 0.111 | -0.059 | 0.915 | 0.683 | 1.341 | 1.372 | 1.208 |
| NH2 | -596.2633 | -596.1631 | 0.00 | 0.00 | 0.089 | 0.104 | -0.068 | 0.819 | 0.707 | 1.385 | 1.373 | 1.209 |

| adG C8-X 9H | | | ΔE _{taut} | ΔG _{taut} | cSAR(X) cSAR(NH2) cSAR(O) | | | EDDB_P(π)5 | EDDB_P(π)6 | d_CX | d_CN H2 | d_CO |
|-------------|------------|------------|--------------------|--------------------|---------------------------|-------|--------|------------|------------|-------|---------|-------|
| NO2 | -745.0269 | -744.9436 | 1.14 | 0.88 | -0.141 | 0.169 | -0.085 | 0.771 | 0.535 | 1.431 | 1.345 | 1.209 |
| CN | -633.0438 | -632.9639 | 1.44 | 0.94 | -0.126 | 0.164 | -0.089 | 0.707 | 0.548 | 1.421 | 1.346 | 1.209 |
| Br | -3113.4192 | -3113.3487 | 1.41 | 0.60 | -0.023 | 0.148 | -0.100 | 0.557 | 0.570 | 1.856 | 1.349 | 1.211 |
| Cl | -1000.1653 | -1000.0933 | 1.78 | 0.99 | -0.016 | 0.147 | -0.101 | 0.544 | 0.570 | 1.703 | 1.349 | 1.211 |
| F | -640.0486 | -639.9743 | 4.77 | 3.80 | 0.003 | 0.146 | -0.102 | 0.518 | 0.567 | 1.314 | 1.349 | 1.211 |
| H | -541.0571 | -540.9736 | 0.00 | 0.00 | 0.000 | 0.140 | -0.106 | 0.578 | 0.584 | | 1.350 | 1.212 |
| SH | -938.7996 | -938.7190 | 0.00 | 0.00 | -0.013 | 0.144 | -0.102 | 0.419 | 0.574 | 1.753 | 1.349 | 1.211 |
| OH | -616.0844 | -615.9975 | 4.26 | 3.33 | 0.074 | 0.134 | -0.112 | 0.492 | 0.592 | 1.341 | 1.352 | 1.213 |
| NH2 | -596.2606 | -596.1612 | 1.67 | 1.20 | 0.077 | 0.128 | -0.112 | 0.086 | 0.594 | 1.394 | 1.353 | 1.213 |

| adG C8-X C6-OH | | | | ΔG_{taut} | | | | | | d_CN | d_CO | |
|----------------------|------------|------------|-------|--------------------------|---------|-----------|----------|------------------|------------------|-------|-------|-------|
| | | | | | cSAR(X) | cSAR(NH2) | cSAR(OH) | EDDB_P(π)5 | EDDB_P(π)6 | d_CX | H2 | H |
| NO2 | -745.0130 | -744.9305 | 9.87 | 9.12 | -0.143 | 0.165 | 0.281 | 1.110 | 0.866 | 1.455 | 1.348 | 1.324 |
| CN | -633.0300 | -632.9504 | 10.11 | 9.42 | -0.124 | 0.160 | 0.277 | 1.025 | 0.823 | 1.433 | 1.349 | 1.325 |
| Br | -3113.4059 | -3113.3349 | 9.71 | 9.29 | -0.047 | 0.144 | 0.268 | 1.147 | 0.875 | 1.872 | 1.354 | 1.326 |
| Cl | -1000.1527 | -1000.0799 | 9.66 | 9.34 | -0.034 | 0.143 | 0.267 | 1.137 | 0.877 | 1.716 | 1.354 | 1.326 |
| F | -640.0413 | -639.9659 | 9.35 | 9.07 | -0.007 | 0.142 | 0.266 | 1.094 | 0.930 | 1.319 | 1.354 | 1.327 |
| H | -541.0382 | -540.9539 | 11.84 | 12.33 | 0.000 | 0.137 | 0.260 | 1.107 | 0.788 | | 1.353 | 1.328 |
| SH | -938.7838 | -938.7031 | 9.91 | 10.02 | 0.004 | 0.135 | 0.262 | 1.055 | 0.862 | 1.759 | 1.356 | 1.327 |
| OH | -616.0772 | -615.9892 | 8.77 | 8.54 | 0.055 | 0.130 | 0.258 | 0.959 | 0.923 | 1.339 | 1.357 | 1.328 |
| NH2 | -596.2490 | -596.1488 | 8.98 | 8.98 | 0.096 | 0.119 | 0.249 | 0.872 | 0.853 | 1.381 | 1.360 | 1.330 |
| adG C8-X 1H,9H,C2-NH | | | | ΔG_{taut} | | | | | | d_CN | d_CO | |
| | | | | | cSAR(X) | cSAR(NH) | cSAR(O) | EDDB_P(π)5 | EDDB_P(π)6 | d_CX | H | H |
| NO2 | -745.0154 | -744.9314 | 8.41 | 8.56 | -0.140 | -0.021 | -0.052 | 0.622 | 0.268 | 1.432 | 1.274 | 1.207 |
| CN | -633.0322 | -632.9514 | 8.76 | 8.79 | -0.124 | -0.027 | -0.055 | 0.561 | 0.278 | 1.422 | 1.275 | 1.207 |
| Br | -3113.4082 | -3113.3366 | 8.32 | 8.25 | -0.021 | -0.041 | -0.066 | 0.437 | 0.308 | 1.856 | 1.276 | 1.208 |
| Cl | -1000.1543 | -1000.0810 | 8.65 | 8.68 | -0.014 | -0.041 | -0.067 | 0.426 | 0.310 | 1.702 | 1.276 | 1.209 |
| F | -640.0379 | -639.9623 | 11.48 | 11.31 | 0.003 | -0.041 | -0.067 | 0.417 | 0.314 | 1.313 | 1.276 | 1.209 |
| H | -541.0462 | -540.9611 | 6.81 | 7.80 | 0.000 | -0.049 | -0.070 | 0.453 | 0.320 | | 1.277 | 1.209 |
| SH | -938.7886 | -938.7069 | 6.88 | 7.61 | -0.011 | -0.044 | -0.067 | 0.247 | 0.308 | 1.752 | 1.277 | 1.209 |
| OH | -616.0738 | -615.9859 | 10.88 | 10.66 | 0.075 | -0.051 | -0.077 | 0.397 | 0.331 | 1.339 | 1.277 | 1.210 |
| NH2 | -596.2503 | -596.1501 | 8.16 | 8.17 | 0.082 | -0.055 | -0.078 | 0.061 | 0.336 | 1.390 | 1.278 | 1.210 |