# Supporting Information for:

# Variable van der Waals radii derived from a hybrid Gaussian charge distribution model for continuum-solvent electrostatic calculations

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Table S2: Experimental and calculated hydration free energies (from the QM/PB/SA model ) for the four representative molecules (in kcal/mol).

| molecule | model | $G_{el}$ | $G_{np}$ | $G_{sol}$ | exptl |
|---|---|---|---|---|---|
| $H_2O$ | Bondi | −5.45 | 0.74 | −4.71 | −6.30 |
| | GM | −5.46 | 0.74 | −4.72 | |
| | HGM | −6.22 | 0.72 | −5.50 | |
| acetic acid | Bondi | -8.94 | 1.19 | -7.75 | −6.70 |
| | GM | -9.24 | 1.19 | −8.05 | |
| | HGM | -7.64 | 1.20 | -6.44 | |
| 4-cresol | Bondi | -5.81 | 1.65 | −4.16 | −6.13 |
| | GM | -6.34 | 1.69 | −4.65 | |
| | HGM | -8.01 | 1.63 | -6.38 | |
| 9-methyl-guanine | Bondi | -21.21 | 1.97 | −19.24 | −22.4 |
| | GM | -11.52 | 1.20 | −10.32 | |
| | HGM | -25.34 | 1.96 | -23.38 | |

Table S3: The coordinates and vdW radii of the four representative molecules.

$H_2O$

| | x | y | z | radii |
|---|---|---|---|---|
| O | 0.000000 | 0.122365 | 0.000000 | 1.559 |
| H | 0.765428 | -0.489461 | 0.000000 | 1.124 |
| H | -0.765428 | -0.489461 | 0.000000 | 1.124 |

acetic acid

| | x | y | z | radii |
|---|---|---|---|---|
| O | 0.654978 | 1.214927 | -0.000169 | 1.586 |
| C | -1.408960 | -0.108295 | -0.000014 | 1.692 |
| C | 0.092270 | 0.129760 | -0.000069 | 1.683 |
| O | 0.782277 | -1.063725 | 0.000182 | 1.461 |
| H | -1.700611 | -0.692730 | 0.888123 | 1.163 |
| H | -1.700489 | -0.694439 | -0.887049 | 1.188 |
| H | -1.932591 | 0.855939 | -0.000924 | 1.202 |
| H | 1.735780 | -0.807180 | 0.000243 | 1.054 |

4-cresol

| | x | y | z | radii |
|---|---|---|---|---|
| O | -2.834177 | -0.096304 | 0.006228 | 1.432 |
| C | 0.667816 | -1.206005 | -0.007317 | 1.691 |
| C | -0.733132 | -1.230014 | -0.001109 | 1.718 |
| C | 1.391339 | 0.008855 | -0.008214 | 1.667 |
| C | -1.451723 | -0.017239 | 0.002871 | 1.716 |
| C | 0.651660 | 1.208254 | -0.007504 | 1.750 |
| C | -0.754225 | 1.205396 | -0.001144 | 1.735 |
| C | 2.912373 | 0.016071 | 0.009846 | 1.678 |
| H | -3.190318 | 0.817859 | 0.007292 | 1.017 |
| H | 1.213689 | -2.155650 | -0.013250 | 1.187 |
| H | -1.284979 | -2.173325 | -0.003347 | 1.120 |
| H | 1.179938 | 2.167514 | -0.013191 | 1.177 |
| H | -1.306120 | 2.152787 | -0.003712 | 1.182 |
| H | 3.311526 | -0.232862 | 1.011019 | 1.202 |
| H | 3.313579 | 1.005526 | -0.264624 | 1.120 |
| H | 3.331508 | -0.723327 | -0.694603 | 1.211 |

9-methyl-guanine

| | x | y | z | radii |
|---|---|---|---|---|
| N | -2.531731 | -2.068992 | 0.075426 | 1.580 |
| O | -1.673422 | 2.539367 | 0.014878 | 1.572 |
| C | 2.759647 | -1.631966 | 0.018597 | 1.686 |
| N | 1.949917 | -0.410402 | -0.005569 | 1.363 |
| C | 0.564230 | -0.346962 | -0.003317 | 1.684 |
| C | 0.250468 | 1.027725 | -0.010037 | 1.778 |
| C | 2.389716 | 0.916529 | -0.009634 | 1.692 |
| N | 1.406600 | 1.802615 | -0.013622 | 1.651 |
| N | -0.273855 | -1.428143 | -0.014327 | 1.597 |
| C | -1.553140 | -1.078357 | -0.000772 | 1.664 |
| C | -1.140371 | 1.430450 | 0.000479 | 1.711 |
| N | -1.984763 | 0.234731 | 0.003952 | 1.584 |
| H | -3.393464 | -1.891792 | -0.444176 | 1.039 |
| H | -2.145241 | -2.995697 | -0.112405 | 0.994 |
| H | 3.506618 | -1.612270 | -0.790744 | 1.210 |
| H | 2.084365 | -2.485661 | -0.128331 | 1.225 |
| H | 3.276738 | -1.743305 | 0.986174 | 1.239 |
| H | 3.453129 | 1.154161 | -0.012791 | 1.223 |
| H | -2.981304 | 0.446451 | 0.090326 | 0.998 |