Supporting Information for

Assessing Physicochemical Properties of Drug Molecules via Microsolvation Measurements with Differential Mobility Spectrometry

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METHODS

RRCK cell permeability & pKa/pKb measurements

In vitro cell permeability using MDCKII cells was performed using the protocol described by Di and coworkers. Briefly, a drug compound is placed on the exterior of a lipid bilayer. After incubating at 37 °C for 1.5 hours, the apical (donor) and basal (receiver) sides of the membrane were isolated and analyzed for drug compound content by using an established LC-MS/MS workflow. Drug concentrations from both sides were compared to the concentration of the original dosing, with permeability values ($P_{App}$) calculated using the following equation:

$$P_{App} \left( \frac{cm}{s} \right) = \frac{1}{\text{[Momolayer Surface Area]} \times \text{[Apical Conc.} \text{t=0]} \times \frac{dM_r}{dt}}$$

where Apical Conc.\text{t=0} is the concentration in the donor at the beginning of the permeability experiment, $M_r$ is the mass of compound appearing in the basal side as a function of time, and $dM_r/dt$ is the flux of the compound across the monolayer.

Experimental determination of pKa. We employed the method of Wan and coworkers to determine the experimental pKa values for the drug molecules in this study.

References

1. Di L, Whitney-Pickett C, Umland JP, Zhang H, Zhang X, Gebhard DF, et al. Development of a new permeability assay using low-efflux MDCKII cells. J Pharm Sci 2011, 100, 4974-4985.

2. Wan H, Holmen AG, Wang Y, Lindberg W, Englund M, Nagard MB, et al. High-throughput screening of pKa values of pharmaceuticals by pressure-assisted capillary electrophoresis and mass spectrometry. Rapid Commun Mass Spectrom 2003, 17, 2639-2648.
Table S1. Data for the twenty-two 2-methylquinolin-8-ol derivatives examined in this study, including DMS results, calculated solvent (methanol) binding energies, experimentally determined pKa, pKb, and cell permeability values (Papp values), and sigma parameters.

| Substitution | CV at SV=4000V (V) | SV at CV_{min} (V) | pKa | pKb | P_{App} (10^{-6} cm/s) | Sigma (σ⁺) Values |
|--------------|--------------------|--------------------|-----|-----|------------------------|------------------|
| 5-methoxy    | -14.2              | 3364               | 10.60 | 5.40 | 2.15                   | -0.78            |
| 6-methoxy    | -21.2              | 3639               | 9.40  | 5.60 | 0.44                   | 0.05             |
| 7-methoxy    | -0.8               | 2749               | n/a  | 5.30 | 3.40                   | -0.78            |
| 5-methyl     | -18.7              | 3523               | 10.50 | 5.70 | 0.55                   | -0.31            |
| 6-methyl     | -20.6              | 3561               | 10.00 | 5.70 | 0.81                   | -0.07            |
| 7-methyl     | -6.0               | 3002               | 10.70 | 5.60 | 4.14                   | -0.31            |
| H            | -25.2              | 3631               | 9.60  | 5.60 | 3.35                   | 0.00             |
| 5-bromo      | -25.7              | 3956               | 9.20  | 4.50 | ~0                     | 0.15             |
| 6-bromo      | -29.1              | 4066               | 9.10  | 4.60 | 0.15                   | 0.41             |
| 7-bromo      | -6.5               | 3103               | 8.60  | 4.30 | 4.10                   | 0.15             |
| 5-chloro     | -27.3              | 3921               | 9.20  | 4.50 | 2.27                   | 0.23             |
| 6-chloro     | -30.7              | 4035               | 8.90  | 4.70 | 1.41                   | 0.37             |
| 7-chloro     | -10.2              | 3210               | 8.65  | 4.40 | 9.85                   | 0.23             |
| 5-fluoro     | -28.1              | 3809               | 9.40  | 4.60 | ~0                     | -0.07            |
| 6-fluoro     | -32.7              | 4020               | 8.90  | 4.90 | ~0                     | 0.35             |
| 7-fluoro     | -23.4              | 3614               | 9.00  | 4.90 | 2.57                   | -0.07            |
| 5-nitro      | -31.5              | 4352               | 6.55  | 2.70 | 3.86                   | 0.66             |
| 6-nitro      | -33.8              | 4479               | 8.30  | 3.80 | 1.73                   | 0.71             |
| 7-nitro      | -15.9              | 3530               | 6.65  | 2.20 | 4.60                   | 0.66             |
| 5-cyano      | -33.2              | 4264               | 7.60  | 3.60 | 2.36                   | 0.78             |
| 6-cyano      | -35.6              | 4368               | 8.60  | 4.10 | 1.20                   | 0.56             |
| 7-cyano      | -33.0              | 4217               | 7.10  | 2.30 | 2.91                   | 0.78             |
Table S2. Multiple reaction monitoring (MRM) signal channels monitored for each substituted 2-methylquinolin-8-ol species.

| Substitution | MRM Channels (Q1 → Q3) | Collision Energy (Lab) (eV) | Declustering Potential (DP) (eV) |
|--------------|------------------------|----------------------------|----------------------------------|
| 5-methoxy    | 190 → 93               | 60.0                       | 65.0                             |
| 6-methoxy    |                        |                            |                                  |
| 7-methoxy    |                        |                            |                                  |
| 5-methyl     | 174 → 128              | 45.0                       | 130.0                            |
| 6-methyl     |                        |                            |                                  |
| 7-methyl     | H                      | 160 → 115                  | 43.0                             |
|              |                        |                            | 35.0                             |
| H            |                        |                            |                                  |
| 5-bromo      | 238 → 113              | 85.0                       | 85.0                             |
| 6-bromo      |                        |                            |                                  |
| 7-bromo      |                        |                            |                                  |
| 5-chloro     | 194 → 130              | 55.0                       | 200.0                            |
| 6-chloro     |                        |                            |                                  |
| 7-chloro     |                        |                            |                                  |
| 5-fluoro     | 178 → 133              | 45.0                       | 100.0                            |
| 6-fluoro     |                        |                            |                                  |
| 7-fluoro     |                        |                            |                                  |
| 5-nitro      | 205 → 130              | 32.0                       | 120.0                            |
| 6-nitro      |                        |                            |                                  |
| 7-nitro      |                        |                            |                                  |
| 5-cyano      | 185 → 140              | 30.0                       | 75.0                             |
| 6-cyano      |                        |                            |                                  |
| 7-cyano      |                        |                            |                                  |
Table S3. DMS-based CV shifts, van der Waals (VDW) radii, cell permeabilities, pKas, and pKbs, for the various 7-substituted 2-methylquinolin-8-ols. As microsolvation energies increase (more negative CV shifts), $P_{app}$ is reduced for –CN and –F substituents, the smaller van der waals radii allows increased clustering at the 7-position, likewise, clustering is reduced for congeners with larger van der waals radii (e.g. Cl, Me and Br). Removal of the methoxy (OMe) and nitro (NO₂) group’s data from any comparisons of the CV shifts to the other experimental properties (e.g., CV vs. pKa) shows improved correlations (see Figure S4), revealing an alternative mechanism (potentially intramolecular hydrogen bonding) during the microsolvation event.

| 7-Substitution | CV/V | (VDW radii) (Å) | Cell Permeability ($10^{-6}$ cm s⁻¹) | pKa | pKb |
|----------------|------|----------------|-------------------------------------|-----|-----|
| F              | -23.4| 1.47           | 2.6                                 | 9   | 4.9 |
| CN             | -33.0| 1.51           | 2.9                                 | 7.1 | 2.3 |
| OMe            | -0.8 | 1.52           | 3.4                                 | 5.3 |     |
| NO₂            | -15.9| 1.61           | 4.6                                 | 6.65| 2.2 |
| Cl             | -10.2| 1.73           | 4.0                                 | 8.65| 4.4 |
| Me             | -6.0 | 1.8            | 4.1                                 | 10.7| 5.6 |
| Br             | -6.5 | 1.86           | 4.1                                 | 8.6 | 4.3 |
Figure S1. Exploded schematic diagram of the DMS-MS instrumentation used in this study.
Figure S2. CV traces for all twenty-two 2-methylquinolin-8-ol species as measured at SV = 4000 V in the presence of methanol vapor. The influence of both functional group (different colors) and their substitution position (inset structures in each plot) is evident from these data.
Figure S3. Plots showing the correlation between RRCK-based cell permeabilities (bar graphs) and CV shifts (line graphs) as a function of substitution position for the fluoro-, nitro-, methyl-, and bromo-substituted 2-methylquinolin-8-ols.
Figure S4. (Left) Plots showing the correlations between CV and various experimental parameters for the 7-substituted 2-methylquinolin-8-ol species. (Right) Note that the correlations improve when the nitro (NO$_2$) data points are excluded from the comparison, hinting at an alternative microsolvation mechanism at play.
**Figure S5.** Plot comparing the correlations between calculated microsolvation energy (x-axis) with the measured CV values at SV = 4000V (blue diamonds), the CV at a measured minimum value (green triangles), and the SV at the measured CV minimum value (SV@CV$_{min}$) (red squares). The strong correlations with these three experimental measurements with calculated binding energy supports the use of any of these values as experimental measures of microsolvation energy, with SV@CV$_{min}$ employed in this study. These data represent a subset of the entire cohort of 22 compounds studied, substituted in either the 5- or 6-position.
Figure S6. Substituent van der Waals radii plotted against the difference in relative isomer energy ($E_{\text{OH-bound}} - E_{\text{NH-bound}}$) for the 7-substituted 2-methylquinolin-8-ol halogen derivatives bound to water. The line of best fit through the halogen series is plotted in red.

Figure S7. Substituent van der Waals radii plotted against the difference in relative isomer energy ($E_{\text{OH-bound}} - E_{\text{NH-bound}}$) for all of the 7-substituted 2-methylquinolin-8-ol derivatives bound to water that were studied in this work. The line of best fit through the halogen series is plotted in red.
**Figure S8.** Substituent van der Waals radii plotted against the difference in relative isomer energy ($E_{\text{OH-bound}} - E_{\text{NH-bound}}$) for the 7-substituted 2-methylquinolin-8-ol halogen derivatives bound to methanol. The line of best fit through the halogen series is plotted in red.

![Graph showing van der Waals radii vs. isomer energy difference for halogen derivatives.]

**Figure S9.** Substituent van der Waals radii plotted against the difference in relative isomer energy ($E_{\text{OH-bound}} - E_{\text{NH-bound}}$) for all of the 7-substituted 2-methylquinolin-8-ol derivatives bound to methanol that were studied in this work. The line of best fit through the halogen series is plotted in red.

![Graph showing van der Waals radii vs. isomer energy difference for all substituents.]

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### Thermochemical Data for 2-methylquinolin-8-ol Ion-Solvent Clusters

| Water      | $E_0$ (hartree) | $\Delta H^o$ (hartree) | $\Delta G^o$ (hartree) | $S^o$ (kcal/mol) | $E_{\text{Binding}}$ (kcal/mol) | $E_{\text{relative}}$ (kcal/mol) |
|------------|----------------|------------------------|------------------------|-----------------|-------------------------------|---------------------------------|
| OH-bound   | -593.291654    | -593.277399            | -593.332568            | 116.113         | 15.45                         | 0.00                            |
| NH-bound   | -593.288719    | -593.274207            | -593.329123            | 115.582         | 13.69                         | 1.84                            |
| Methanol   |                |                        |                        |                 |                               |                                 |
| OH-bound   | -632.573393    | -632.557869            | -632.617549            | 125.608         | 17.8                          | 0.00                            |
| NH-bound   | -632.570066    | -632.554424            | -632.613547            | 124.435         | 15.73                         | 2.09                            |

Calculations were conducted at the B3LYP/6-311++G(d,p) level of theory at $T = 298$ K and employed the GD3 empirical dispersion correction.

### Thermochemical Data for 5-substituted 2-methylquinolin-8-ol Ion-Solvent Clusters

| Water      | $E_0$ (hartree) | $\Delta H^o$ (hartree) | $\Delta G^o$ (hartree) | $S^o$ (kcal/mol) | $E_{\text{Binding}}$ (kcal/mol) | $E_{\text{relative}}$ (kcal/mol) |
|------------|----------------|------------------------|------------------------|-----------------|-------------------------------|---------------------------------|
| 5-F        |                |                        |                        |                 |                               |                                 |
| OH-bound   | -692.561137    | -692.546021            | -692.603057            | 120.043         | 15.78                         | 0.00                            |
| NH-bound   | -692.558363    | -692.542943            | -692.599978            | 120.04          | 14.09                         | 1.74                            |
| 5-Cl       |                |                        |                        |                 |                               |                                 |
| OH-bound   | -1052.91946    | -1052.90398            | -1052.9623             | 122.734         | 15.85                         | 0.00                            |
| NH-bound   | -1052.91614    | -1052.90038            | -1052.95861            | 122.548         | 13.86                         | 2.08                            |
| 5-Br       |                |                        |                        |                 |                               |                                 |
| OH-bound   | -3166.84072    | -3166.82495            | -3166.88466            | 125.669         | 15.83                         | 0.00                            |
| NH-bound   | -3166.83732    | -3166.82127            | -3166.88095            | 125.617         | 13.78                         | 2.13                            |
| 5-OMe      |                |                        |                        |                 |                               |                                 |
| OH-bound   | -707.822961    | -707.806862            | -707.865385            | 123.171         | 14.63                         | 0.00                            |
| NH-bound   | -707.820805    | -707.803518            | -707.865312            | 130.057         | 13.44                         | 1.35                            |
| 5-Me       |                |                        |                        |                 |                               |                                 |
| OH-bound   | -632.595715    | -632.580639            | -632.636626            | 117.835         | 15.09                         | 0.00                            |
| NH-bound   | -632.593083    | -632.576889            | -632.635686            | 123.747         | 13.48                         | 1.65                            |
| 5-NO$_2$   |                |                        |                        |                 |                               |                                 |
| OH-bound   | -797.839238    | -797.82328             | -797.882244            | 124.101         | 17.32                         | 0.00                            |
| NH-bound   | -797.834275    | -797.817161            | -797.878854            | 129.843         | 14.16                         | 3.11                            |
| 5-CN       |                |                        |                        |                 |                               |                                 |
| OH-bound   | -685.550266    | -685.534236            | -685.593339            | 124.392         | 16.84                         | 0.00                            |
| NH-bound   | -685.54621     | -685.529867            | -685.589137            | 124.745         | 14.26                         | 2.55                            |

| Methanol   |                |                        |                        |                 |                               |                                 |
| OH-bound   | -731.842948    | -731.826548            | -731.888136            | 129.623         | 18.17                         | 0.00                            |
| NH-bound   | -731.839818    | -731.823265            | -731.884545            | 128.976         | 16.2                          | 1.96                            |

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Calculations were conducted at the B3LYP/6-311++G(d,p) level of theory at $T = 298$ K and employed the GD3 empirical dispersion correction.

### Thermochemical Data for 6-substituted 2-methylquinolin-8-ol Ion-Solvent Clusters

| Water | $E_0$ (hartree) | $\Delta H^\circ$ (hartree) | $\Delta G^\circ$ (hartree) | $S^\circ$ (kcal/mol) | $E_{binding}$ (kcal/mol) | $E_{relative}$ (kcal/mol) |
|-------|----------------|---------------------------|---------------------------|---------------------|-------------------------|---------------------------|
| 6-F   |                |                           |                           |                     |                         |                           |
| OH-bound | -692.563654   | -692.549445              | -692.603722              | 114.235             | 16.44                   | 0.00                      |
| NH-bound | -692.559931   | -692.544547              | -692.601485              | 119.836             | 13.92                   | 2.34                      |
| 6-Cl  |                |                           |                           |                     |                         |                           |
| OH-bound | -1052.92068   | -1052.9052               | -1052.96337              | 122.429             | 16.18                   | 0.00                      |
| NH-bound | -1052.917     | -1052.90122              | -1052.95947              | 122.595             | 13.91                   | 2.31                      |
| 6-Br  |                |                           |                           |                     |                         |                           |
| OH-bound | -3166.84176   | -3166.82599              | -3166.88562              | 125.499             | 16.09                   | 0.00                      |
| NH-bound | -3166.83816   | -3166.82211              | -3166.88173              | 125.5               | 13.89                   | 2.26                      |
| 6-OMe |                |                           |                           |                     |                         |                           |
| OH-bound | -707.822667   | -707.805769              | -707.866525              | 127.872             | 15.32                   | 0.00                      |
| NH-bound | -707.819369   | -707.802093              | -707.863206              | 128.623             | 13.18                   | 2.07                      |
| 6-Me  |                |                           |                           |                     |                         |                           |
| OH-bound | -632.597916   | -632.581804              | -632.641323              | 125.269             | 15.09                   | 0.00                      |
| NH-bound | -632.595254   | -632.578892              | -632.638071              | 124.551             | 13.49                   | 1.67                      |
| 6-NO$_2$ |               |                           |                           |                     |                         |                           |
| OH-bound | -797.841599   | -797.824691              | -797.886666              | 130.437             | 17.1                    | 0.00                      |
| NH-bound | -797.837553   | -797.820399              | -797.882258              | 130.193             | 14.6                    | 2.54                      |
Calculations were conducted at the B3LYP/6-311++G(d,p) level of theory at T = 298 K and employed the GD3 empirical dispersion correction.

### Thermochemical Data for 7-substituted 2-methylquinolin-8-ol Ion-Solvent Clusters

| Water   | $E_0$ (hartree) | $\Delta H^0$ (hartree) | $\Delta G^0$ (hartree) | $S^\circ$ (kcal/mol) | $E_{\text{Binding}}$ (kcal/mol) | $E_{\text{relative}}$ (kcal/mol) |
|---------|-----------------|------------------------|------------------------|----------------------|-------------------------------|-------------------------------|
| 7-F     |                 |                        |                        |                      |                               |                               |
| OH-bound| -692.561612     | -692.546517            | -692.603874            | 120.718              | 15.64                         | 0.00                          |
| NH-bound| -692.559706     | -692.545228            | -692.599815            | 114.888              | 13.72                         | 1.20                          |
| 7-Cl    |                 |                        |                        |                      |                               |                               |
| OH-bound| -1052.91895     | -1052.90328            | -1052.96282            | 125.313              | 14.07                         | 0.00                          |
| NH-bound| -1052.91963     | -1052.904              | -1052.96197            | 122.005              | 14.08                         | -0.42                         |
| 7-Br    |                 |                        |                        |                      |                               |                               |
| OH-bound| -3166.84002     | -3166.82405            | -3166.88505            | 128.373              | 13.58                         | 0.00                          |
| NH-bound| -3166.84128     | -3166.82617            | -3166.88346            | 120.582              | 13.36                         | -0.79                         |
|                  | OH-bound     | NH-bound     |                  |                  |
|------------------|--------------|--------------|------------------|------------------|
| 7-OMe            | -707.822641  | -707.80622   | -707.86634       | 126.535          | 12.39 | 0.00 |
|                  | -707.824925  | -707.807901  | -707.868965      | 128.519          | 13.71 | -1.43 |
| 7-Me             | -632.596409  | -632.580893  | -632.639553      | 123.462          | 13.79 | 0.00 |
|                  | -632.595214  | -632.579603  | -632.636765      | 120.308          | 12.58 | 0.75 |
| 7-NO₂            | -797.839009  | -797.822314  | -797.884278      | 130.415          | 13.43 | 0.00 |
|                  | -797.845166  | -797.8286    | -797.888643      | 126.37           | 15.2  | -3.86 |
| 7-CN             | -685.551926  | -685.536359  | -685.594166      | 121.666          | 19.06 | 0.00 |
|                  | -685.54731   | -685.531124  | -685.590014      | 123.945          | 14.71 | 2.90 |

|                  | ΔH° (hartree) | ΔG° (hartree) | S° (kcal/mol) | E_{Binding} (kcal/mol) | E_{relative} (kcal/mol) |
|------------------|---------------|---------------|---------------|------------------------|-------------------------|
| Methanol         | ΔH° (hartree) | ΔG° (hartree) | S° (kcal/mol) | E_{Binding} (kcal/mol) | E_{relative} (kcal/mol) |
| 7-F              | -731.843443   | -731.827052   | 130.419       | 18.11                  | 0.00                    |
|                  | -731.841636   | -731.825151   | 128.964       | 16.3                   | 1.13                    |
| 7-Cl             | -1092.20056   | -1092.18367   | 135.263       | 16.49                  | 0.00                    |
|                  | -1092.2011    | -1092.1843    | 131.282       | 16.14                  | -0.34                   |
| 7-Br             | -3206.1216    | -3206.1044    | 138.894       | 16.01                  | 0.00                    |
|                  | -3206.12315   | -3206.10605   | 134.425       | 15.91                  | -0.97                   |
| 7-OMe            | -747.103825   | -747.085436   | 140.989       | 14.65                  | 0.00                    |
|                  | -747.10621    | -747.087973   | 137.229       | 15.74                  | -1.50                   |
| 7-Me             | -671.877662   | -671.860369   | 134.505       | 16.34                  | 0.00                    |
|                  | -671.876838   | -671.859263   | 134.648       | 14.96                  | 0.52                    |
| 7-NO₂            | -837.120443   | -837.102583   | 137.204       | 20.24                  | 0.00                    |
|                  | -837.12695    | -837.109135   | 136.815       | 17.48                  | -4.08                   |
| 7-CN             | -724.834287   | -724.817296   | 131.963       | 21.95                  | 0.00                    |
|                  | -724.829265   | -724.811882   | 133.228       | 16.91                  | 3.15                    |

Calculations were conducted at the B3LYP/6-311++G(d,p) level of theory at T = 298 K and employed the GD3 empirical dispersion correction.
**XYZ Coordinates of 2-Methylquinolin-8-ol Ion-Solvent Clusters**

**Proton-bound 2-methylquinolin-8-ol and water (OH bound)**

| Atom           | X         | Y         | Z         | Charge |
|----------------|-----------|-----------|-----------|--------|
| C(Fragment=1)  | -2.349714 | -0.955028 | 0.000113  | 0.000000 |
| C(Fragment=1)  | -0.185899 | 0.082159  | 0.000035  | 0.000000 |
| C(Fragment=1)  | -0.758779 | 1.378622  | -0.000029 | 0.000000 |
| C(Fragment=1)  | -2.173201 | 1.454798  | 0.000000  | 0.000000 |
| C(Fragment=1)  | -2.949875 | 0.317615  | 0.000097  | 0.000000 |
| C(Fragment=1)  | 1.214847  | -0.111739 | 0.000070  | 0.000000 |
| C(Fragment=1)  | 0.102276  | 2.500083  | -0.000082 | 0.000000 |
| H(Fragment=1)  | -2.645511 | 2.431046  | -0.000070 | 0.000000 |
| H(Fragment=1)  | -4.030081 | 0.379055  | 0.000159  | 0.000000 |
| C(Fragment=1)  | 1.465405  | 2.302790  | -0.000680 | 0.000000 |
| C(Fragment=1)  | 2.027426  | 1.007831  | 0.000090  | 0.000000 |
| C(Fragment=1)  | -3.138408 | -2.224850 | -0.001740 | 0.000000 |
| H(Fragment=1)  | -3.786595 | -2.261850 | 0.879370  | 0.000000 |
| H(Fragment=1)  | -3.782591 | -2.263816 | -0.882615 | 0.000000 |
| H(Fragment=1)  | -2.500025 | -3.109434 | 0.002205  | 0.000000 |
| N(Fragment=1)  | -1.014300 | -1.015091 | 0.000103  | 0.000000 |
| O(Fragment=1)  | 1.622263  | -1.395899 | 0.000150  | 0.000000 |
| H(Fragment=1)  | 2.603589  | -1.477869 | 0.000177  | 0.000000 |
| H(Fragment=1)  | 3.103077  | 0.878297  | 0.000020  | 0.000000 |
| H(Fragment=1)  | 2.132384  | 3.155708  | -0.000112 | 0.000000 |
| H(Fragment=1)  | -0.547559 | -1.919767 | 0.000162  | 0.000000 |
| H(Fragment=1)  | -0.319669 | 3.497062  | -0.000129 | 0.000000 |
| O(Fragment=2)  | 4.334131  | -1.501957 | -0.000054 | 0.000000 |
| H(Fragment=2)  | 4.848275  | -1.765489 | -0.771579 | 0.000000 |
| H(Fragment=2)  | 4.849179  | -1.765136 | 0.770987  | 0.000000 |
Proton-bound 2-methylquinolin-8-ol and water (NH bound)

\begin{verbatim}
C(Fragment=1)  1.68506100 -1.10427500 -0.01920200
c(Fragment=1)  -0.40767400  0.05705200 -0.00424700
C(Fragment=1)  -1.12660400 -1.16840400  0.00853800
C(Fragment=1)  -0.36936800 -2.36486700  0.00550800
C(Fragment=1)   1.00534100 -2.33564800 -0.0138100
C(Fragment=1)  -1.10267800 -2.39555000  0.01212500
C(Fragment=1)  -2.54101300 -1.13867000  0.01966200
H(Fragment=1)  -0.89219700 -3.31493500  0.01309400
H(Fragment=1)   1.58400300 -3.24942100  0.31881000
C(Fragment=1)  -3.19813800  0.06346900  0.01633400
C(Fragment=1)  -2.48213800  1.27822700  0.00672100
C(Fragment=1)   3.17724300 -0.99534400  0.00734300
H(Fragment=1)   3.52764300 -0.81535900  1.01439800
H(Fragment=1)   3.63112400 -1.92021000 -0.36099500
H(Fragment=1)   3.51827600 -0.16823600  0.63157100
N(Fragment=1)   0.96634700  0.02338300  0.01633400
O(Fragment=1)   0.34145700  2.41964000  0.03325000
H(Fragment=1)  -0.90155100  2.20494300  0.07323500
H(Fragment=1)  -3.02329700  2.21865100 -0.00606200
H(Fragment=1)  -4.28042900  0.09524400  0.02495000
H(Fragment=1)  -1.48661900  0.91607700  0.00781600
H(Fragment=1)  -3.08775800 -2.07833200  0.02987400
O(Fragment=2)   2.61436400  2.30712400  0.02813700
H(Fragment=2)   3.53555000  2.54971000  0.16735600
H(Fragment=2)   2.11412600  3.12870000 -0.01671100
\end{verbatim}

\begin{figure}
\centering
\includegraphics[width=0.5\textwidth]{proton-bound.png}
\caption{Proton-bound 2-methylquinolin-8-ol and water (NH bound).}
\end{figure}
Proton-bound 2-methylquinolin-8-ol and methanol (OH bound)

C(Fragment=1)  2.59254200  -1.20776800  0.03510400
C(Fragment=1)  0.60974100   0.14009300 -0.05843700
C(Fragment=1)  1.36307500  1.33519700  0.05735100
C(Fragment=1)  2.76896400  1.19882500  0.16316800
C(Fragment=1)  3.36945800 -0.04050400  0.15264400
C(Fragment=1) -0.80034800  0.15539500 -0.17020400
C(Fragment=1)  0.67659600  2.57112800  0.05955400
C(Fragment=1)  3.37692500  2.09235500  0.25362200
C(Fragment=1)  4.44368000 -0.14121800  0.23343500
C(Fragment=1) -0.69654600  2.57815800 -0.05123800
C(Fragment=1) -1.43863700  1.38353100 -0.16578800
C(Fragment=1)  3.18569600 -2.57983400  0.01504700
C(Fragment=1)  3.87835300 -2.67465400 -0.82549600
C(Fragment=1)  3.75729500 -2.75315800  0.93058600
C(Fragment=1)  2.42643500 -3.35822300 -0.07230100
C(Fragment=1)  1.26699000 -1.06721800  0.06325300
C(Fragment=1) -1.38877200 -1.04989700 -0.27109400
C(Fragment=1) -2.37491100 -0.98173300 -0.35648600
C(Fragment=1) -2.51795300  1.41431200 -0.25399900
C(Fragment=1) -1.23043600  3.52064200 -0.05170300
C(Fragment=1)  0.67356500 -1.88989600 -0.15045400
C(Fragment=1)  1.23706400  3.49317900  0.14712000
O(Fragment=2)  4.02371800 -0.75316000 -0.43300500
H(Fragment=2)  4.50547100 -0.93073100 -1.24794500
C(Fragment=2)  4.87970600 -0.99315400  0.70545700
H(Fragment=2)  5.20791400 -2.03493100  0.73860700
H(Fragment=2)  4.28500500 -0.77596700  1.59162400
H(Fragment=2)  5.74564400 -0.32773700  0.68300300
Proton-bound 2-methylquinolin-8-ol and methanol (NH bound)

C (Fragment=1)  -0.86619800  1.69257900  0.08615300
C (Fragment=1)   0.71911300 -0.09700100  0.02782100
C (Fragment=1)  1.80147000  0.81857200  0.06600100
C (Fragment=1)  1.48488500  2.19916300  0.07500000
C (Fragment=1)  0.18195400  2.62838300 -0.02782100
C (Fragment=1)  0.96905600 -1.48943300  0.06712800
C (Fragment=1)  3.12547600  0.32578600  0.13572200
H (Fragment=1)  2.29181100  2.92047800  0.14534800
C (Fragment=1)   0.06111200  3.68247800 -0.00370700
C (Fragment=1)  3.34673500 -1.03070100  0.10708100
C (Fragment=1)  2.27215600 -1.93740000  0.00282200
C (Fragment=1)  0.96905600 -1.48943300  0.06712800
C (Fragment=1)  3.12547600  0.32578600  0.13572200
H (Fragment=1)  2.29181100  2.92047800  0.14534800
XYZ Coordinates of 5-substituted Ion-Solvent Clusters

Proton-bound 5-Bromo-2-methylquinolin-8-ol and water (OH bound)

C(Fragment=1)  -1.31102100  2.73498700  0.00005100
C(Fragment=1)  -0.97910900  0.35605900  0.00003200
C(Fragment=1)  0.43303900  0.50696500  0.00001200
C(Fragment=1)  0.93086500  1.83329300  0.00002100
C(Fragment=1)  0.08274900  2.91769100  0.00005000
C(Fragment=1) -1.60688000  -0.91021900  0.00004100
C(Fragment=1)  1.22046100  -0.67661600  -0.00001200
H(Fragment=1)  2.00259700  1.98898600  0.00001500
H(Fragment=1)  0.47318700  3.92669000  0.00006700
C(Fragment=1)  0.60350300  -1.90932800  -0.00000800
C(Fragment=1) -0.79965200  -2.03180600  0.00002000
C(Fragment=1) -2.28227600  3.87061200  -0.00010700
H(Fragment=1) -2.12069600  4.49896000  0.87981200
H(Fragment=1) -2.12290900  3.92669000  0.00006700
C(Fragment=1) -3.29408800  1.83329300  0.00002100
O(Fragment=1) -2.95360000  -0.89197400  0.00010300
H(Fragment=1) -3.34091800  -1.79799600  0.00007000
H(Fragment=1) -1.25475000  -3.01487800  0.00002800
Br(Fragment=1)  3.12249400  -0.58186500  -0.00016000
H(Fragment=1)  1.20540800  -2.80878800  -0.00001900
H(Fragment=1) -2.77401500  1.30726500  0.00006700
O(Fragment=2)  -3.89422600  -3.43254300  -0.00006400
H(Fragment=2) -4.30511100  -3.83905400  -0.77152000
H(Fragment=2) -4.30510900  -3.83947600  0.77117100
Proton-bound 5-Bromo-2-methylquinolin-8-ol and water (NH bound)

| Atom Type    | X         | Y         | Z         | x         | y         | z         |
|--------------|-----------|-----------|-----------|-----------|-----------|-----------|
| C (Fragment=1) | 2.07041700 | -1.66961600 | -0.01877500 |       |           |           |
| C (Fragment=1) | 0.85369600 | 0.39441900 | -0.00808200 |       |           |           |
| C (Fragment=1) | -0.39154300 | -0.29675700 | -0.00388400 |       |           |           |
| C (Fragment=1) | -0.33982900 | -1.71166100 | -0.00904000 |       |           |           |
| C (Fragment=1) | 0.86030500 | -2.38266100 | -0.01920600 |       |           |           |
| C (Fragment=1) | 0.90170800 | 1.80784200 | -0.01293900 |       |           |           |
| C (Fragment=1) | -1.58967900 | 0.47206200 | 0.00176900 |       |           |           |
| H (Fragment=1) | -1.26853100 | -2.26828600 | -0.00795100 |       |           |           |
| H (Fragment=1) | 0.89100300 | -3.46372300 | -0.02751200 |       |           |           |
| C (Fragment=1) | -1.52429000 | 1.84646900 | 0.00077900 |       |           |           |
| C (Fragment=1) | -0.28348400 | 2.51049600 | -0.00762700 |       |           |           |
| C (Fragment=1) | 3.41276600 | -2.32941800 | -0.00383900 |       |           |           |
| H (Fragment=1) | 3.84060100 | -2.27922100 | 1.00268400 |       |           |           |
| H (Fragment=1) | 3.32702500 | -3.37809600 | -0.28432000 |       |           |           |
| H (Fragment=1) | 4.10252500 | -1.83176600 | -0.68763100 |       |           |           |
| N (Fragment=1) | 2.01924900 | -0.33367900 | -0.01222100 |       |           |           |
| O (Fragment=1) | 2.13879300 | 2.37751600 | -0.02491000 |       |           |           |
| H (Fragment=1) | 2.07009800 | 3.33963400 | -0.02754500 |       |           |           |
| H (Fragment=1) | -0.26678900 | 3.59518400 | -0.01079000 |       |           |           |
| Br (Fragment=1) | -3.29498300 | -0.37403200 | 0.01004300 |       |           |           |
| H (Fragment=1) | -2.43386400 | 2.43237500 | 0.00508900 |       |           |           |
| H (Fragment=1) | 2.92020700 | 0.17296100 | -0.00150700 |       |           |           |
| O (Fragment=2) | 4.61451200 | 0.75729800 | 0.03704600 |       |           |           |
| H (Fragment=2) | 5.52202800 | 0.46331600 | 0.16726700 |       |           |           |
| H (Fragment=2) | 4.63853800 | 1.71893000 | -0.00576600 |       |           |           |
Proton-bound 5-Bromo-2-methylquinolin-8-ol and methanol (OH bound)

|          | X1       | Y1       | Z1     |
|----------|----------|----------|--------|
| C(Fragment=1) | -0.27596600 | 3.13778200 | 0.04492100 |
| C(Fragment=1) | 0.40528000  | 0.83819400 | -0.08246500 |
| C(Fragment=1) | -0.93942200 | 0.38750700 | -0.00743300 |
| C(Fragment=1) | -1.93945900 | 1.38559600 | 0.09618900  |
| C(Fragment=1) | -1.61720200 | 2.72382500 | 0.12192600  |
| C(Fragment=1) | 1.50058300  | -0.04953800 | -0.18874600 |
| C(Fragment=1) | -1.16467300 | -1.01542900 | -0.04303300 |
| H(Fragment=1) | -2.97709300 | 1.08125900 | 0.15576500  |
| H(Fragment=1) | -2.38866200 | 3.47821500 | 0.20113400  |
| C(Fragment=1) | -0.09438100 | -1.87797800 | -0.14833900 |
| C(Fragment=1) | 1.23019500  | -1.40508000 | -0.22105100 |
| C(Fragment=1) | 0.13682600  | 4.57387100 | 0.06657500  |
| H(Fragment=1) | -0.32540800 | 5.10693300 | -0.76853900 |
| H(Fragment=1) | -0.21059900 | 5.04751100 | 0.98859000  |
| H(Fragment=1) | 1.21877200  | 4.69562600 | -0.00008700 |
| N(Fragment=1) | 0.65938300  | 2.18886800 | -0.05202000 |
| O(Fragment=1) | 2.71444900  | 0.52556300 | -0.24812800 |
| H(Fragment=1) | 3.44439600  | -0.14268900 | -0.33172400 |
| H(Fragment=1) | 2.05080600  | -2.10713300 | -0.30546000 |
| Br(Fragment=1) | -2.93103800 | -1.72183500 | 0.05236000  |
| H(Fragment=1) | -0.26918100 | -2.94570400 | -0.17648800 |
| H(Fragment=1) | 1.64276300  | 2.44724600 | -0.11089500 |
| O(Fragment=2) | 4.57734900  | -1.35317400 | -0.40989400 |
| H(Fragment=2) | 5.07961600  | -1.49885800 | -1.21875700 |
| C(Fragment=2) | 5.37443800  | -1.72477900 | 0.73669000  |
| H(Fragment=2) | 6.28028200  | -1.11694100 | 0.79917300  |
| H(Fragment=2) | 4.75771400  | -1.54173600 | 1.61544900  |
| H(Fragment=2) | 5.63556900  | -2.78453200 | 0.69613900  |
Proton-bound 5-Bromo-2-methylquinolin-8-ol and methanol (NH bound)

C  -1.68939400   1.73284800   0.13508300
C   -0.52364100  -0.35796400   0.08970500
C    0.73652600   0.30250600   0.03116600
C    0.71966700  1.71908100   0.03145900
C   -0.46190000  2.41714300   0.08862900
C   -0.60258700 -1.76993400   0.11686100
C    1.91493300 -0.49398700  -0.01644800
H    1.66076600  2.25288500   0.00016000
C    0.56485500 -2.50081800   0.07013200
C   -3.00724900  2.43977300   0.16446300
H    2.90949300  3.39845100   0.67418500
H   -3.33596700  2.64377100  -0.86042000
H   -3.77235600  1.84210100   0.65906100
N   -1.67336200  0.39665200   0.12894500
O   -1.84998600 -2.30980000   0.19449900
H   -1.80675800 -3.27319700   0.17721900
H    0.52280900 -3.58463100   0.08996200
Br   3.63825900  0.31155200  -0.10256200
H    2.71384800 -2.47338400  -0.03556800
H   -2.59369200 -0.09081900   0.14670700
O   -4.28398800 -0.54708900   0.26425100
H   -4.32779100 -1.42283600   0.66189200
C   -5.36119100  0.39216200  -0.68053000
H   -6.32980500 -0.49384500  -0.18558300
H   -5.27944800  0.61424300  -1.08953500
H   -5.28068900 -1.11629500  -1.49580300
Proton-bound 5-Chloro-2-methylquinolin-8-ol and water (OH bound)

| Atom    | X    | Y    | Z    |
|---------|------|------|------|
| C(Fragment=1) | 1.46352300 | 2.33016500 | 0.00016500 |
| C(Fragment=1) | -0.10357500 | 0.51006200 | -0.00037600 |
| C(Fragment=1) | 2.26936500 | 0.05177100 | 0.00035700 |
| C(Fragment=1) | 2.52241200 | 1.40505200 | 0.00045400 |
| C(Fragment=1) | -1.46741500 | 0.14045600 | -0.00076100 |
| C(Fragment=1) | 0.57968600 | -1.82027600 | -0.00053000 |
| C(Fragment=1) | 0.94415100 | -0.44724100 | 0.00003600 |
| C(Fragment=1) | 2.26936500 | 0.05177100 | -0.00037600 |
| C(Fragment=1) | -0.10357500 | 0.51006200 | -0.00037600 |
| C(Fragment=1) | 2.26936500 | 0.05177100 | 0.00035700 |
| C(Fragment=1) | 2.52241200 | 1.40505200 | 0.00045400 |
| C(Fragment=1) | -1.46741500 | 0.14045600 | -0.00076100 |
| H(Fragment=1) | 3.09330300 | -0.65103000 | 0.00059600 |
| H(Fragment=1) | 3.53742300 | 1.77957000 | 0.00077500 |
| C(Fragment=1) | -0.75080300 | -1.77748000 | -0.00037000 |
| H(Fragment=1) | -1.77182600 | -1.20798900 | -0.00073100 |
| C(Fragment=1) | 1.67473700 | 3.80945900 | 0.00029400 |
| H(Fragment=1) | 2.25175600 | 4.10307200 | 0.88124200 |
| H(Fragment=1) | 2.25179500 | 4.10321300 | -0.88058700 |
| H(Fragment=1) | 0.73486900 | 4.36308500 | 0.00030900 |
| N(Fragment=1) | 0.21765400 | 1.84692900 | -0.00025600 |
| O(Fragment=1) | -2.34687600 | 1.16081600 | -0.00129600 |
| H(Fragment=1) | -3.28165300 | 0.84965000 | 0.00043400 |
| H(Fragment=1) | -0.57484800 | 2.48635600 | -0.00043500 |
| H(Fragment=1) | -1.01868900 | -3.22642200 | -0.00044100 |
| H(Fragment=1) | -2.80964800 | -1.51843800 | -0.00116400 |
| Cl(Fragment=1) | 1.81067900 | -3.05390000 | 0.00022400 |
| O(Fragment=2) | -4.87222100 | 0.17740100 | 0.00171400 |
| H(Fragment=2) | -5.44679100 | 0.21853500 | -0.77122200 |
| H(Fragment=2) | -5.45139000 | 0.21221600 | 0.77147900 |
Proton-bound 5-Chloro-2-methylquinolin-8-ol and water (NH bound)

| Atom (Fragment=1) | X-coordinate | Y-coordinate | Z-coordinate |
|-------------------|--------------|--------------|--------------|
| C                  | 1.66540900   | -1.59152900  | -0.01907900  |
| C                  | 0.26626700   | 0.35316000   | -0.00715900  |
| C                  | -0.90791700  | -0.45086800  | -0.00077400  |
| C                  | -0.73102000  | -1.85510800  | -0.00554300  |
| C                  | 0.52563400   | -2.41311800  | -0.01751200  |
| C                  | 0.18055900   | 1.76467400   | -0.01290500  |
| C                  | -2.17200000  | 0.20170700   | 0.00636800   |
| H                  | -1.60587700  | -2.49297900  | -0.00282400  |
| H                  | 0.65597800   | -3.48673700  | -0.02585100  |
| C                  | -2.23906400  | 1.57525600   | 0.00461100   |
| C                  | -1.06617700  | 2.35235600   | -0.00618200  |
| C                  | 3.06204300   | -2.12683400  | -0.00484700  |
| H                  | 3.47576700   | -2.05769200  | 1.00654000   |
| H                  | 3.07382300   | -3.17363100  | -0.30479000  |
| H                  | 3.70896100   | -1.55599000  | -0.67293800  |
| N                  | 1.49334500   | -0.26560100  | -0.01275400  |
| O                  | 1.35837700   | 2.44893400   | -0.02746400  |
| H                  | 1.19894600   | 3.40023200   | -0.02946000  |
| H                  | 2.34456000   | 0.32106700   | -0.00278400  |
| H                  | -3.20302400  | 2.06671400   | 0.00998200   |
| H                  | -1.15146400  | 3.43374700   | -0.01009500  |
| Cl                 | -3.64242600  | -0.73157500  | 0.01652900   |
| O                  | 3.97383200   | 1.06373400   | 0.03482400   |
| H                  | 4.90468900   | 0.85862700   | 0.17052200   |
| H                  | 3.90540400   | 2.02311900   | -0.01076900  |
Proton-bound 5-Chloro-2-methylquinolinol-8-ol and methanol (OH bound)

| Atom (Fragment=1) | x          | y          | z          |
|-------------------|------------|------------|------------|
| C                 | 1.78179700 | 2.36492400 | 0.04115900 |
| C                 | 0.26925900 | 0.50322100 | -0.07597800|
| C                 | 1.33891100 | -0.42570900| 0.00907100 |
| C                 | 2.64606900 | 0.10896100 | 0.11207000 |
| C                 | 2.86180900 | 1.46867000 | 0.12796000 |
| C                 | -1.08120400| 0.09923600 | -0.18269400|
| C                 | 1.01188800 | -1.80765700| -0.01664600|
| H                 | 3.48608200 | 0.57127800 | 0.17893100 |
| H                 | 3.86324400 | 1.87046700 | 0.20669600 |
| C                 | 0.30467900 | -2.19986800| -0.12226000|
| C                 | 1.34783400 | 1.25775500 | -0.20500900|
| C                 | 1.95256100 | 3.84947900 | 0.05215500 |
| H                 | 2.45047200 | 4.16031600 | 0.97447500 |
| H                 | 2.58869500 | 4.15741300 | -0.78194500|
| H                 | 1.00993000 | 4.37721700 | -0.02364800|
| N                 | 0.55346300 | 1.84801600 | -0.05509900|
| O                 | -1.98422000| 1.09320600 | -0.25229800|
| H                 | -2.91325000| 0.75284300 | -0.33696600|
| H                 | -0.25466600| 2.46433400 | -0.12079900|
| H                 | -0.54363300| -3.25535100| -0.14233400|
| H                 | -2.37402700| -1.59404100| -0.28954400|
| Cl                | 2.27132000 | -3.00869900| 0.08411900 |
| O                 | -4.42202600| 0.06344000 | -0.41645200|
| H                 | -4.93783300| 0.11263700 | -1.22841200|
| C                 | -5.30646800| 0.03273700 | 0.72581200 |
| H                 | -4.67111100| -0.02465400| 1.60848200 |
| H                 | -5.91357300| 0.93977300 | 0.77722600 |
| H                 | -5.95069900| -0.84850500| 0.68967300 |
Proton-bound 5-Chloro-2-methylquinolin-8-ol and methanol (NH bound)

C  -1.20670200  1.72636800  -0.12306500
C   0.06381200  -0.30199200  -0.07314300
C   1.28500500   0.42449500   0.00085500
C   1.19882700   1.83799000   0.00598200
C  -0.01690600   2.47390100  -0.06091600
C   0.06243600  -1.71594400  -0.10587200
C   2.50338300  -0.30684500   0.05766400
H   2.11145300   2.41813700   0.05805800
H  -0.07945700   3.55382600  -0.06568400
C   2.48490800  -1.68189700   0.03508900
C   1.26805000  -2.38221200  -0.04967200
C  -2.55888200   2.36455300  -0.16414000
H  -2.90722100   2.54983000   0.85781800
H  -2.50593400   3.32777600  -0.67194500
H  -3.28748300   1.72907700  -0.66668000
N  -1.12264400   0.39258400  -0.12169000
O  -1.15283900  -2.32304900  -0.19857100
H  -1.05719000  -3.28268200  -0.18301700
H  -2.01685000  -0.14135700  -0.15054800
H   3.41492900  -2.23323000   0.07831800
H   1.28502600  -3.46656000  -0.07373300
Cl  4.02786300   0.53092900   0.15417800
O  -3.67433500  -0.68993800  -0.28636700
H  -3.66373600  -1.56755100  -0.68220200
C  -4.77420900  -0.59174200   0.63978600
H  -4.75292500   0.41778000  1.04871100
H  -5.72741100  -0.74493400   0.12848200
H  -4.66931000  -1.31015900  1.45731400
Proton-bound 5-Cyano-2-methylquinolin-8-ol and water (OH bound)

\[
\begin{array}{cccc}
C(\text{Fragment}=1) & -1.60694700 & -2.16077500 & 0.00016100 \\
C(\text{Fragment}=1) & 0.04816200 & -0.42334200 & -0.00043200 \\
C(\text{Fragment}=1) & -0.94519800 & 0.58019200 & -0.00006100 \\
C(\text{Fragment}=1) & -2.29761200 & 0.15578900 & 0.00035600 \\
C(\text{Fragment}=1) & -2.61855900 & -1.18226200 & 0.00045200 \\
C(\text{Fragment}=1) & 1.43205800 & -0.11330500 & -0.00088800 \\
C(\text{Fragment}=1) & -0.52539100 & 1.94304100 & -0.00009900 \\
H(\text{Fragment}=1) & -3.08355000 & 0.90335100 & 0.00060300 \\
H(\text{Fragment}=1) & -3.65106100 & -1.50579900 & 0.00078300 \\
C(\text{Fragment}=1) & 0.83038000 & 2.23410000 & -0.00048600 \\
C(\text{Fragment}=1) & 1.80316900 & 1.22068000 & -0.00090100 \\
C(\text{Fragment}=1) & -1.89496600 & -3.62656900 & 0.00041900 \\
H(\text{Fragment}=1) & -2.48627000 & -3.89072000 & 0.88183300 \\
H(\text{Fragment}=1) & -2.48810400 & -3.88905300 & -0.87975600 \\
H(\text{Fragment}=1) & -0.98573300 & -4.22912800 & -0.00052700 \\
N(\text{Fragment}=1) & -0.33712400 & -1.74256400 & -0.00029300 \\
O(\text{Fragment}=1) & 2.25925900 & -1.16803400 & -0.00150200 \\
H(\text{Fragment}=1) & 3.21162500 & -0.90485400 & 0.00059400 \\
H(\text{Fragment}=1) & 2.85541000 & 1.47734600 & -0.00142200 \\
H(\text{Fragment}=1) & 1.14901500 & 3.26892900 & -0.00059000 \\
H(\text{Fragment}=1) & 0.41993600 & -2.42352900 & -0.00047900 \\
C(\text{Fragment}=1) & -1.50535000 & 2.97861700 & 0.00017100 \\
N(\text{Fragment}=1) & -2.32905000 & 3.78825700 & 0.00058100 \\
O(\text{Fragment}=2) & 4.81809800 & -0.32904800 & 0.00207200 \\
H(\text{Fragment}=2) & 5.38925500 & -0.39823400 & -0.77161100 \\
H(\text{Fragment}=2) & 5.39535900 & -0.39013800 & 0.77184600 \\
\end{array}
\]
Proton-bound 5-Cyano-2-methylquinolin-8-ol and water (NH bound)

C(Fragment=1)    1.53403000  -1.61131200  -0.02217100
C(Fragment=1)    0.16561000  0.35138800   0.00781000
C(Fragment=1)   -1.01459400  -0.43110100  -0.0009000
C(Fragment=1)   -0.86703400  -1.84002400  -0.00505800
C(Fragment=1)    0.38041500  -2.41643300  -0.01953100
C(Fragment=1)    0.09227900  1.76804900   0.01473100
C(Fragment=1)   -2.27988100  0.22946800   0.00842000
H(Fragment=1)   -1.75547400  -2.46204200  -0.00112000
H(Fragment=1)    0.49545500  -3.49191300  -0.02892000
C(Fragment=1)   -2.32650800  1.61209800   0.00672400
C(Fragment=1)   -1.14741700  2.37494600   0.00601800
C(Fragment=1)    2.92023400  -2.17209400  -0.00879100
H(Fragment=1)    3.18156000  -2.14999900  1.01128700
H(Fragment=1)    2.91710500  -3.20747100  -0.34662300
H(Fragment=1)    3.58791300  -1.58979500  -0.64540600
N(Fragment=1)    1.38449300  -0.28223800  -0.01460100
O(Fragment=1)    1.27369400  2.43297000  -0.03243200
H(Fragment=1)    1.13296200  3.38785500  -0.03442600
H(Fragment=1)   -1.21511400  3.45739000  -0.01050000
H(Fragment=1)   -3.28432800  2.11638400   0.01337900
H(Fragment=1)    2.24577400  0.29147300  -0.00256300
C(Fragment=1)   -3.47642000  -0.54705500  -0.01799900
N(Fragment=1)   -4.42333000  -1.20794800  -0.02569300
O(Fragment=2)    3.88536300   0.99987400   0.04325000
H(Fragment=2)    4.79931500   0.74902400   0.21417600
H(Fragment=2)    3.87335200  1.96006000  -0.02824000
**Proton-bound 5-Cyano-2-methylquinolin-8-ol and methanol (OH bound)**

| Element         | Fragment | X       | Y       | Z       |
|-----------------|----------|---------|---------|---------|
| C (Fragment=1)  | 1        | -1.89152100 | -2.22793800 | 0.04097200 |
| C (Fragment=1)  | 1        | -0.32838300 | -0.41126300 | -0.07423600 |
| C (Fragment=1)  | 1        | -1.36637600 | 0.54251500  | 0.00790200  |
| C (Fragment=1)  | 1        | -2.69236300 | 0.05205200  | 0.10890100  |
| C (Fragment=1)  | 1        | -2.94661800 | -1.30026500 | 0.12508800  |
| C (Fragment=1)  | 1        | 1.03595600  | -0.03608200 | -0.17892400 |
| C (Fragment=1)  | 1        | -1.01420800 | 1.92406300  | -0.01664200 |
| H (Fragment=1)  | 1        | -3.51162000 | 0.75998500  | 0.17366700  |
| H (Fragment=1)  | 1        | -3.95908000 | -1.67409100 | 0.20201900  |
| C (Fragment=1)  | 1        | 0.32226300  | 2.28006900  | -0.12059000 |
| C (Fragment=1)  | 1        | 1.33992000  | 1.31555000  | -0.20114500 |
| C (Fragment=1)  | 1        | -2.10671000 | -3.70622500 | 0.05300700  |
| H (Fragment=1)  | 1        | -2.61533700 | -4.00050200 | 0.97501800  |
| H (Fragment=1)  | 1        | -2.75158700 | -3.99504200 | -0.78131700 |
| H (Fragment=1)  | 1        | -1.17167900 | -4.26298500 | -0.02129200 |
| N (Fragment=1)  | 1        | -0.64763400 | -1.74754200 | -0.05331300 |
| O (Fragment=1)  | 1        | 1.91043900  | -1.04628500 | -0.24654900 |
| H (Fragment=1)  | 1        | 2.85317800  | -0.73239900 | -0.32914300 |
| H (Fragment=1)  | 1        | 2.37554800  | 1.62141600  | -0.28382100 |
| H (Fragment=1)  | 1        | 0.58926500  | 3.32925400  | -0.14034300 |
| H (Fragment=1)  | 1        | 0.14086300  | -2.38894600 | -0.11684000 |
| C (Fragment=1)  | 1        | -2.03973600 | 2.91096800  | 0.06538600  |
| N (Fragment=1)  | 1        | -2.89872300 | 3.68009200  | 0.13414200  |
| O (Fragment=2)  | 2        | 4.36281700  | -0.10306500 | -0.41252900 |
| H (Fragment=2)  | 2        | 4.86972100  | -0.16631400 | 1.22929800  |
| C (Fragment=2)  | 2        | 5.25810600  | -0.09966400 | 0.72331900  |
| H (Fragment=2)  | 2        | 4.63224400  | -0.02450900 | 1.61131200  |
| H (Fragment=2)  | 2        | 5.83829100  | -1.02421100 | 0.76757400  |
| H (Fragment=2)  | 2        | 5.92667300  | 0.76261200  | 0.68105200  |
Proton-bound 5-Cyano-2-methylquinolin-8-ol and methanol (NH bound)

C   -1.01120600  1.84379500  -0.11348200
C    0.12072300 -0.26359800  -0.11229000
C    1.37942700  0.37258600   0.00403100
C    1.39655400  1.78956400   0.06072100
C    0.22828700  2.50545400   0.00339300
C    0.03236200 -1.67795000  -0.17381900
C    2.55713400 -0.43058200   0.05774900
H    2.34844600  2.30145700   0.15017100
H    0.23469400  3.58670200   0.04593100
C    2.44630900 -1.80889000  -0.00505100
C    1.19179700 -2.42686900  -0.11990600
C   -2.29965000  2.59843000  -0.18144500
H   -2.39765000  3.23291600   0.70391900
H   -2.86173000  3.26260200  -1.05061000
H   -3.16284300  1.93963700  -0.24948100
N   -1.01962300  0.50777000  -0.16550900
O   -1.21357600 -2.19489900  -0.28302900
H   -1.18990100  3.15829600  -0.33256600
H    1.13358400 -3.50881900   0.03512200
H    3.33831300 -2.42085900   0.03512200
H   -1.94228000  0.30941000  -0.25139200
C    3.83161500  0.19943300   0.17532100
N    4.84614500  0.74265300   0.27073300
O   -3.67784100 -0.34890400  -0.30316900
H   -4.03885900 -0.74829000  -1.10172400
C   -4.27838400 -0.96693700   0.85344700
H   -3.88255100 -0.44878100   1.72634100
H   -5.36439500 -0.85193300   0.83611800
H   -4.01449900 -2.02588000   0.91565900
Proton-bound 5-Fluoro-2-methylquinolin-8-ol and water (OH bound)

C(Fragment=1)  -2.24342700  -1.37325100  0.00019800
C(Fragment=1)  -0.13622500  -0.22273300  0.00009300
C(Fragment=1)  -0.79226700   1.03335400  0.00001800
C(Fragment=1)  -2.20589600   1.04425600  0.00011700
C(Fragment=1)  -2.91509200  -0.13613500  0.00024300
C(Fragment=1)   1.27150500  -0.33968000  0.00013800
C(Fragment=1)   0.13622500  -2.18687400 -0.00008900
H(Fragment=1)  -2.72202500   1.99686500  0.00012000
H(Fragment=1)  -3.99694900  -0.13585900  0.00036600
C(Fragment=1)   1.38827800   2.09704800  0.00010300
C(Fragment=1)   2.01527300   0.83373200  0.00002600
C(Fragment=1)  -2.96110300  -2.68404200 -0.00044900
H(Fragment=1)  -3.60935200  -2.75408600  0.87708100
H(Fragment=1)  -3.59985400  -2.75813900  0.88467700
H(Fragment=1)  -2.27592300  -3.53275800  0.00512500
N(Fragment=1)  -0.90615700  -1.36180100  0.00017300
O(Fragment=1)   1.75515900  -1.59278600  0.00032900
H(Fragment=1)   1.75510300  -1.61507500 -0.00037400
H(Fragment=1)   3.09662600   0.77051100  0.00004700
H(Fragment=1)   1.98009600   0.30341200 -0.00018000
H(Fragment=1)  -0.39091400  -2.23999800  0.00018400
F(Fragment=1)  -0.58919300   3.38255500 -0.00014200
O(Fragment=2)   4.46711500  -1.51085900 -0.00031500
H(Fragment=2)   4.99835200  -1.74247000  0.77063800
H(Fragment=2)   4.99498800  -1.74445300  0.77173100
**Proton-bound 5-Fluoro-2-methylquinolin-8-ol and water (NH bound)**

| Atom (Fragment=1) | X | Y | Z |
|-------------------|---|---|---|
| C                  | 1.589339900 | -1.43760300 | -0.02127700 |
| C                  | -0.08206600 | 0.27690500 | -0.00678000 |
| C                  | -1.11037600 | -0.70246100 | 0.00361400 |
| C                  | -0.73911600 | -2.06613300 | -0.00027700 |
| C                  | 0.58793500 | -2.42600100 | -0.01586900 |
| C                  | -0.40132000 | 1.65408000 | -0.01401200 |
| C                  | -2.45121000 | -0.25736900 | 0.01265700 |
| H                  | -1.51720300 | -2.81987000 | 0.00554900 |
| H                  | 0.88337000 | -3.46636500 | -0.02431700 |
| C                  | -2.76574700 | 1.07383000 | 0.00974400 |
| C                  | -1.72983300 | 2.02899200 | -0.00458700 |
| C                  | 3.04999700 | -1.75968700 | -0.00726500 |
| H                  | 3.42925400 | -1.70876400 | 1.01890100 |
| H                  | 3.22267200 | -2.76863600 | -0.37972200 |
| H                  | 3.61760200 | -1.05204200 | -0.61292000 |
| N                  | 1.22398400 | -0.15064900 | -0.01524500 |
| O                  | 0.64797100 | 2.52529400 | -0.03266800 |
| H                  | 0.33311800 | 3.43689300 | -0.03902600 |
| H                  | -1.98786200 | 3.08248000 | -0.00944700 |
| H                  | -3.80292400 | 1.38240400 | 0.01674900 |
| H                  | 1.97864900 | 0.55664100 | -0.00630000 |
| F                  | -3.41611300 | -1.18825600 | 0.02324200 |
| O                  | 3.44447800 | 1.56968100 | 0.03530000 |
| H                  | 4.39538900 | 1.53918200 | 0.18290900 |
| H                  | 3.19949600 | 2.49981100 | -0.01158600 |
Proton-bound 5-Fluoro-2-methylquinolin-8-ol and methanol (OH bound)

C(Fragment=1)  -2.34941400  -1.69708600  0.03836200
C(Fragment=1)  -0.49132500  -0.18089600  0.02860700
C(Fragment=1)  -1.36087200   0.93387000  0.13277600
C(Fragment=1)  -2.74868800   0.68583700  0.13766500
C(Fragment=1)  -3.23100600  -0.60406300  0.01368700
C(Fragment=1)   0.90961400  -0.03529400  0.06916900
C(Fragment=1)  -0.77087700   2.21579300  0.01368700
H(Fragment=1)  -3.42672600   1.52749000  0.20858300
H(Fragment=1)  -4.29170800  -0.80164800  0.21694500
C(Fragment=1)   0.58579600   2.37631800  0.03836200
C(Fragment=1)   1.42796700   1.24914700  0.02860700
C(Fragment=1)  -2.81682800  -3.11658400  0.01368700
H(Fragment=1)  -3.38148000  -3.32513400  0.06916900
H(Fragment=1)  -1.99062100  -3.82558800  0.21694500
H(Fragment=1)  -1.04061300  -1.44096200  0.13277600
O(Fragment=1)   1.61043700  -1.18181700  0.20858300
H(Fragment=1)  -2.89350000  -3.28492900 -0.03199800
N(Fragment=1)   -0.37563600  -2.20863600 -0.10137300
F(Fragment=1)  -1.58424300   3.28035600  0.03836200
O(Fragment=2)   4.20012800   -0.61885400  0.13250600
H(Fragment=2)   4.69620000  -0.75138200  0.10137300
H(Fragment=2)   4.46420300   1.60087300  0.20858300
H(Fragment=2)   5.50574800   0.74633100  0.21694500
H(Fragment=2)   5.87280900  -0.02599500  0.69093600
H(Fragment=2)   4.46420300  -0.61265500  1.60087300
H(Fragment=2)   5.50574800  -1.77786700  0.74633100
H(Fragment=2)   5.87280900  -0.02599500  0.69093600
Proton-bound 5-Fluoro-2-methylquinolin-8-ol and methanol (NH bound)

C  -0.99642400  1.71625300  -0.10369000
C   0.39411900  -0.22987900  -0.05050100
C   1.55661800   0.58148600   0.03139300
C   1.39630500   1.98618600   0.04073800
C   0.14182200   2.54220100  -0.03217900
C   0.50449200  -1.63913800  -0.08619700
C   2.81308300  -0.06112400   0.09124800
H   2.27796200   2.61281500   0.10005300
H   0.00644500   3.61537300  -0.03515400
C   2.92463600  -1.42428900   0.06699600
C   1.75954000  -2.21108500  -0.02525000
C  -2.38710900   2.26523800  -0.15325200
H  -2.75951100   2.41252600   0.86638100
H  -2.39316500   3.23618200  -0.64871800
H  -3.06547700   1.58931600  -0.67347700
N  -0.83250800   0.38912000  -0.10429300
O  -0.60528000  -2.34076500  -0.18652300
H  -0.48932000  -3.28979200  -0.17406700
H   1.85637800  -3.29105200   0.05190700
H   3.90225000  -1.88588400   0.11385900
H  -1.69343000  -0.19792800  -0.13880100
F   3.90543900   0.71293500   0.17117600
O  -3.27872900  -0.89146400  -0.28959300
H  -3.16076100  -1.78569500  -0.62656900
C  -4.44937900  -0.83960800   0.54951700
H  -4.54312700   0.18829100   0.89780600
H  -5.34510500  -1.10278700  -0.01778400
H  -4.34669200  -1.50123300   1.41384600
Proton-bound 2,5-Dimethylquinolin-8-ol and water (OH bound)

| Fragment=1 | x  | y  | z   | x  | y  | z   |
|-------------|----|----|-----|----|----|-----|
| C           | -2.17033900 | -1.49905700 | -0.00054100 |
| C           | -0.12223500 | -0.24220100 | -0.00011000 |
| C           | -0.82275100 | 0.99479300 | 0.00011400 |
| C           | -2.23451500 | 0.91542900 | -0.00012000 |
| C           | -2.89371200 | -0.29841900 | -0.00047700 |
| C           | 1.28911100 | -0.30500200 | -0.00010700 |
| C           | -0.08367300 | 2.21568100 | 0.00039400 |
| H           | -2.81657000 | 1.82884100 | -0.00091100 |
| H           | -3.97424300 | -0.34256000 | -0.00071200 |
| C           | 1.29399400 | 2.12042900 | 0.00045000 |
| C           | 1.98240400 | 0.88779500 | 0.00020400 |
| C           | -2.79542500 | -2.85824100 | 0.00046400 |
| H           | -2.49868400 | -3.41914800 | 0.89175400 |
| H           | -3.88134100 | -2.78330400 | -0.01100000 |
| H           | -2.48034300 | -3.42990300 | -0.87748700 |
| N           | -0.83322700 | -1.41625300 | -0.00043800 |
| O           | 1.81814800 | -1.54707300 | -0.00037700 |
| H           | 2.80181900 | -1.53243200 | -0.00045000 |
| H           | 3.06582600 | 0.87068000 | 0.00025000 |
| H           | 1.88397600 | 3.02963700 | 0.00067700 |
| H           | -0.27298300 | -2.26670100 | -0.00060900 |
| C           | -0.78467400 | 3.54893900 | 0.00062100 |
| H           | -1.41850200 | 3.67089800 | -0.88286100 |
| H           | -1.41868800 | 3.67050500 | 0.88402200 |
| H           | -0.06111700 | 4.36400600 | 0.00087600 |
| O           | 4.53345100 | -1.38239400 | -0.00037400 |
| H           | 5.07096900 | -1.59558500 | -0.77144800 |
| H           | 5.07055200 | -1.59629900 | 0.77079400 |
Proton-bound 2,5-Dimethylquinolin-8-ol and water (NH bound)

C(Fragment=1)       1.54994300 -1.49024900  -0.01338700
C(Fragment=1)       -0.05355000  0.29012100   -0.00390100
C(Fragment=1)       -1.13936500  0.63147700   0.00160200
C(Fragment=1)       -0.80356900 -2.00664500  -0.00201900
C(Fragment=1)        0.50689500 -2.42927200  -0.01150300
C(Fragment=1)       -0.29153000  1.68329700  -0.00806700
C(Fragment=1)       -2.48383600 -0.15121300   0.00730700
H(Fragment=1)       -1.59562600 -2.74491800  -0.01767500
H(Fragment=1)        0.75248100 -3.48254400  -0.01767500
C(Fragment=1)       -2.67102200  1.21535500   0.00608900
C(Fragment=1)       -1.59491700  2.12553900  -0.00231400
C(Fragment=1)        2.99835300 -1.86603600  -0.00161700
H(Fragment=1)       -3.42700900 -1.67423000   0.98702800
H(Fragment=1)        3.12205400 -2.92384700  -0.22802800
H(Fragment=1)        3.56050500 -1.27806200  -0.72974300
N(Fragment=1)        1.23327300 -0.19075800  -0.00886700
O(Fragment=1)        0.80523600  2.49599500  -0.01914400
H(Fragment=1)        0.53720100  3.42232800  -0.02311800
H(Fragment=1)       -1.79945700  3.19122000  -0.00494200
H(Fragment=1)       -3.67807600  1.61502900   0.01051600
H(Fragment=1)        2.01502600  0.48406100  -0.00306900
C(Fragment=1)       -3.65110900 -1.10334300   0.01396400
H(Fragment=1)       -3.64918700 -1.74817000  -0.86981200
H(Fragment=1)       -3.63878300 -1.74876900   0.89719100
H(Fragment=1)       -4.59349900 -0.55604600   0.01964100
O(Fragment=2)        3.55148700  1.41314700   0.01923400
H(Fragment=2)        4.50615800  1.33539900   0.11499200
H(Fragment=2)        3.34972300  2.35425300  -0.00883000
Proton-bound 2,5-Dimethylquinolin-8-ol and methanol (OH bound)

C(Fragment=1)  -2.26993400  -1.79957700  0.04105500
C(Fragment=1)  -0.47599900  -0.20695900  -0.07125800
C(Fragment=1)  -1.37432300  0.88910600  0.02443400
C(Fragment=1)  -2.74934800  0.56639300  0.13043900
C(Fragment=1)  -3.18772800  -0.74064500  0.13905500
C(Fragment=1)   0.92092700  2.21748000  0.00849100
C(Fragment=1)  -0.85690700  -0.97410600  0.22045300
C(Fragment=1)  -3.47675800  1.36559200  0.20671600
C(Fragment=1)   0.51328200  2.36090800  0.10228100
C(Fragment=1)   1.39896300  1.26698700  0.19665600
C(Fragment=1)  -2.67895800  -3.23537800  0.03907500
C(Fragment=1)  -3.24687300  -3.46585000  0.94439800
C(Fragment=1)  -3.33057600  -3.43908900  0.81549700
C(Fragment=1)  -1.82253900  -3.91137600  0.01270100
C(Fragment=1)  -0.97401700  1.48777100  0.05759700
C(Fragment=1)   1.65186700  -1.15803400  0.26240900
H(Fragment=1)  -2.62108600  -0.97059800  0.34798900
H(Fragment=1)  -2.46573600  1.43490300  0.28420400
H(Fragment=1)  -0.93705200  3.35844000  0.11851000
H(Fragment=1)   0.27711600  -2.22658000  0.13104300
C(Fragment=1)  -1.77154000  3.41046900  0.10753700
H(Fragment=1)  -2.48722900  3.43935900  0.71957900
H(Fragment=1)  -2.34243800  3.40422400  1.04092500
H(Fragment=1)  -1.19916300  4.33757400  0.07892400
H(Fragment=2)   4.23637100  -0.53722000  0.42288000
H(Fragment=2)   4.74312600  -0.66860200  1.23120600
C(Fragment=2)   5.10560700  -0.64747500  0.72468600
H(Fragment=2)   4.48097500  -0.49041000  1.60296700
H(Fragment=2)   5.56106600  -1.63934400  0.78007200
H(Fragment=2)   5.88227100  0.12018900  0.69557800
**Proton-bound 2,5-Dimethylquinolin-8-ol and methanol (NH bound)**

| Atom (Fragment) | x    | y    | z    |          |          |          |
|-----------------|------|------|------|----------|----------|----------|
| C (Fragment=1)  | -0.98254700 | 1.71781000 | -0.05335700 |
| C (Fragment=1)  | 0.38738200  | -0.24552900 | -0.02272000 |
| C (Fragment=1)  | 1.57809300  | 0.53604600  | 0.01313800  |
| C (Fragment=1)  | 1.41466000  | 1.94229300  | 0.01147200  |
| C (Fragment=1)  | 0.16710500  | 2.52267600  | -0.02535200 |
| C (Fragment=1)  | 0.45654500  | -1.65755300 | -0.03962000 |
| C (Fragment=1)  | 2.85394400  | -0.10380200 | 0.04302900  |
| H (Fragment=1)  | 0.05254100  | 3.59815400  | -0.03267000 |
| C (Fragment=1)  | 2.87455400  | -1.48280500 | 0.03232200  |
| C (Fragment=1)  | 1.69639000  | -2.25462300 | -0.01057100 |
| C (Fragment=1)  | -2.37323700 | 2.27034800  | -0.07011400 |
| H (Fragment=1)  | -2.82449000 | 2.17567600  | 0.92269300  |
| H (Fragment=1)  | -2.36349300 | 3.32551900  | -0.33901400 |
| H (Fragment=1)  | -3.00111400 | 1.72616100  | -0.77551100 |
| N (Fragment=1)  | -0.83070300 | 0.38958600  | -0.04760800 |
| O (Fragment=1)  | -0.72732100 | -2.33595900 | -0.08827200 |
| H (Fragment=1)  | -0.56875000 | -3.28721200 | -0.08669500 |
| H (Fragment=1)  | 1.76987000  | -3.33723500 | -0.02778000 |
| H (Fragment=1)  | 3.82532300  | -2.00191500 | 0.05439300  |
| H (Fragment=1)  | -1.69882800 | -0.18075600 | -0.05474000 |
| C (Fragment=1)  | 4.12776100  | 0.69938900  | 0.08329700  |
| H (Fragment=1)  | 4.22448000  | 1.34442600  | -0.79502500 |
| H (Fragment=1)  | 4.17383600  | 1.33672000  | 0.97126200  |
| H (Fragment=1)  | 4.99630600  | 0.04148000  | 0.10520200  |
| O (Fragment=2)  | -3.28609000 | -0.90921400 | -0.10733700 |
| H (Fragment=2)  | -3.12633000 | -1.85049800 | -0.22864800 |
| C (Fragment=2)  | -4.66505100 | -0.68159900 | 0.23464000  |
| H (Fragment=2)  | -4.78525200 | 0.39146700  | 0.37723800  |
| H (Fragment=2)  | -5.32682300 | -1.00733100 | -0.57187800 |
| H (Fragment=2)  | -4.93012200 | -1.19312700 | 1.16377800  |
Proton-bound 2-Methyl-5-Nitroquinolinol-8-ol and water (OH bound)

| Fragment | C   | H   | O   |
|----------|-----|-----|-----|
| 1        | -0.46472000 | 2.83299900 | 0.00003000 |
| 1        | -0.55669000 | 0.43390400 | -0.00003100 |
| 1        | 0.85658100  | 0.31738600 | 0.00000000 |
| 1        | 1.58449800  | 1.54326700 | 0.00001700 |
| 1        | 0.93788100  | 2.75743000 | 0.00003500 |
| 1        | -1.42734000 | -0.69046800 | -0.00009800 |
| 1        | 1.37655200  | -1.01195100 | 0.00004600 |
| 1        | 2.66253100  | 1.50688600 | 0.00002600 |
| 1        | 1.50620400  | 3.67836100 | 0.00005200 |
| 1        | 0.52748500  | -2.09891300 | -0.00014300 |
| 1        | -0.86657700 | -1.95291900 | 0.00016100 |
| 1        | -1.21679700 | 4.12301900 | 0.00007300 |
| 1        | -0.94524100 | 4.71111200 | 0.88090500 |
| 1        | -0.94493500 | 4.71136100 | -0.88049500 |
| 1        | -2.29747900 | 3.97476800 | -0.0013300 |
| 1        | -1.13664000 | 1.67924900 | -0.0001000 |
| 1        | -2.73436300 | -0.40493500 | -0.00009900 |
| 1        | -3.30318700 | -1.21480000 | 0.00022200 |
| 1        | -2.15519300 | 1.68569000 | -0.00003300 |
| 1        | 0.96208500  | -3.08951500 | -0.00019100 |
| 1        | -1.50757000 | -2.82551800 | -0.00021700 |
| 1        | 2.83323640  | -1.30584300 | 0.00002200 |
| 1        | 3.16417100  | -2.47780700 | -0.00065100 |
| 1        | 3.61283200  | -0.36060400 | 0.00086100 |
| 2        | -4.17295200 | -2.66912800 | 0.00009000 |
| 2        | -4.65503000 | -2.98789000 | -0.77172300 |
| 2        | -4.65499900 | -2.98702500 | 0.77228000 |
Proton-bound 2-Methyl-5-Nitroquinolin-8-ol and water (NH bound)

\[
\begin{align*}
C & : 1.85945500 \quad -1.58403300 \quad -0.03167700 \\
C & : 0.47554700 \quad 0.36774700 \quad 0.01767500 \\
C & : -0.70993700 \quad -0.41553900 \quad 0.00015400 \\
C & : -0.54391800 \quad -1.82713400 \quad -0.05303700 \\
C & : 0.70925400 \quad -2.38992700 \quad -0.06446000 \\
C & : 0.42137500 \quad 1.78731700 \quad 0.05116600 \\
C & : -1.94804600 \quad 0.28748100 \quad -0.00066400 \\
H & : -1.41844800 \quad -2.46010800 \quad -0.07344400 \\
H & : 0.82691300 \quad -3.46469000 \quad -0.09889300 \\
C & : -1.98877500 \quad 1.66079900 \quad 0.00135800 \\
C & : -0.80582300 \quad 2.41413800 \quad 0.03804100 \\
C & : 3.24903000 \quad -2.13501400 \quad -0.05951600 \\
H & : 3.89583700 \quad -1.60428900 \quad 0.64101800 \\
H & : 3.24491400 \quad -3.19470800 \quad 0.19091500 \\
H & : 3.67253400 \quad -2.02390800 \quad -1.06315300 \\
N & : 1.69808500 \quad -0.25779600 \quad 0.00170600 \\
O & : 1.61153500 \quad 2.43134900 \quad 0.09041500 \\
H & : 1.48743800 \quad 3.38858800 \quad 0.10302200 \\
H & : 2.55481700 \quad 0.32253000 \quad 0.00377500 \\
H & : -2.94907500 \quad 2.15887000 \quad -0.01828900 \\
H & : -0.86281500 \quad 3.49669900 \quad 0.05959700 \\
N & : -3.25080200 \quad -0.42026200 \quad 0.00675200 \\
O & : -4.20253700 \quad 0.17140800 \quad -0.46984000 \\
O & : -3.28765600 \quad -1.53679000 \quad 0.50988000 \\
O & : 4.22044600 \quad 0.99287400 \quad -0.01779700 \\
H & : 5.12545400 \quad 0.71258100 \quad -0.19093900 \\
H & : 4.24817400 \quad 1.94910400 \quad 0.09168400
\end{align*}
\]
Proton-bound 2-Methyl-5-Nitroquinolin-8-ol and methanol (OH bound)

| Atoms       | X      | Y      | Z      |
|-------------|--------|--------|--------|
| C(Fragment=1) | -1.23975900 | 2.76592000 | 0.07284100 |
| C(Fragment=1) | -0.06767300 | 0.67710000 | -0.07750500 |
| C(Fragment=1) | -1.26921700 | -0.06876600 | 0.00503200 |
| C(Fragment=1) | -2.47109500 | 0.68254100 | 0.14382200 |
| C(Fragment=1) | -2.44935200 | 2.05752700 | 0.17535000 |
| C(Fragment=1) | 1.21331400 | 0.06964700 | -0.07750500 |
| C(Fragment=1) | -1.13245000 | -1.48568800 | -0.02476800 |
| C(Fragment=1) | 1.26921700 | -0.07750500 | 0.00503200 |
| C(Fragment=1) | 2.47109500 | 0.68254100 | 0.14382200 |
| C(Fragment=1) | 2.44935200 | 2.05752700 | 0.17535000 |
| H(Fragment=1) | -3.41170800 | 0.15771100 | 0.21784600 |
| H(Fragment=1) | -3.36958100 | 2.61723900 | 0.27973800 |
| C(Fragment=1) | 0.10990800 | -2.07527500 | -0.11723800 |
| C(Fragment=1) | 1.28252700 | -1.31171600 | -0.20872500 |
| C(Fragment=1) | -1.16076300 | 4.25714200 | 0.08889400 |
| H(Fragment=1) | -1.71132200 | 4.66634600 | -0.76290400 |
| H(Fragment=1) | -1.62985000 | 4.64552400 | 0.99656600 |
| H(Fragment=1) | -0.13290200 | 4.61962000 | 0.04464100 |
| N(Fragment=1) | -0.11909300 | 2.04923700 | -0.04310700 |
| O(Fragment=1) | 2.24626600 | 0.91315700 | -0.26678200 |
| H(Fragment=1) | 3.12306000 | 0.44227900 | -0.35151800 |
| H(Fragment=1) | 0.78137700 | 2.52047800 | -0.04464100 |
| H(Fragment=1) | 0.16966500 | -3.15569100 | -0.12360000 |
| H(Fragment=1) | 2.24656300 | -1.79653400 | -0.29691900 |
| N(Fragment=1) | -2.30322200 | -2.38811200 | 0.03246900 |
| O(Fragment=1) | -2.10459400 | -3.53478600 | 0.39373000 |
| O(Fragment=1) | -3.39142300 | -1.93283800 | -0.30346400 |
| O(Fragment=2) | 4.49565200 | -0.42812600 | -0.43750900 |
| H(Fragment=2) | 5.00344500 | -0.45400900 | -1.25583400 |
| C(Fragment=2) | 5.37946400 | -0.59075800 | 0.69648400 |
| H(Fragment=2) | 4.75198800 | -0.55809400 | 1.58588600 |
| H(Fragment=2) | 5.88685300 | -1.55642400 | 0.64979400 |
| H(Fragment=2) | 6.11199500 | 0.21837300 | 0.74060100 |
Proton-bound 2-Methyl-5-Nitroquinolin-8-ol and methanol (NH bound)

C  -1.38662900  1.81029400 -0.17827500
C  -0.18838300 -0.25994100 -0.11919200
C   1.05985200  0.40999700 -0.02080300
C   1.02678900  1.83363300 -0.02596300
C  -0.16494500  2.50636100 -0.10260400
C  -0.25994900 -1.67847100 -0.15473800
C   2.22762800 -0.40122400  0.03016000
H   1.95391700  2.38316800  0.03875300
H  -0.18616600  3.58835000 -0.10608100
C   2.14877100 -1.77227500 -0.03160800
C   0.90577700 -2.41447400 -0.11456200
C  -2.69670700  2.52521900 -0.25003000
H  -2.82244400  3.14144500  0.64522500
H  -2.69404400  3.20464900 -1.10696800
H  -3.53873200  1.84178800 -0.33569800
N  -1.35195800  0.47482200 -0.18752600
O  -1.50021700 -2.20969400 -0.23382300
H  -1.46773100 -3.17367900 -0.26675900
H  -2.25929800 -0.03310600 -0.25293600
H   3.06095300 -2.35364500 -0.00903700
H   0.86416500 -3.49750300 -0.14459300
N   3.58257000  0.18466800  0.16263900
O   4.51140300 -0.46711300 -0.28016700
O   3.68065600  1.26789800  0.72698800
O  -3.99706500 -0.44370700 -0.28159300
H  -4.35406400 -0.89189700 -1.05562800
C  -4.59315800 -0.99824800  0.90896200
H  -4.20306200 -0.42621700  1.75026200
H  -5.68019700 -0.89467500  0.88461900
H  -4.32007000 -2.04940100  1.03372200
Proton-bound 2-Methyl-5-methoxyquinolin-8-ol and water (OH bound)

C(Fragment=1)    2.36934500  -1.55766900  0.00098600
C(Fragment=1)    0.18300000  -0.55967000  0.00015400
C(Fragment=1)    0.74422300   0.74193200  0.00089000
C(Fragment=1)    2.14991800   0.84746800  0.00066200
C(Fragment=1)    2.94800500  -0.27935600  0.00126400
C(Fragment=1)   -1.20805800  -0.77850100  0.00012300
C(Fragment=1)   -0.13726000  -1.86401000  0.00020300
H(Fragment=1)    2.59501900   1.83468800  0.00084600
H(Fragment=1)   -4.02671800  -0.19814400  0.00195400
C(Fragment=1)   -1.50250100   1.64151900  0.00033600
C(Fragment=1)   -2.02906600   0.33259200  0.00138000
C(Fragment=1)    3.17580800  -2.81693700  0.00156600
H(Fragment=1)    3.80123200  -2.85708300  0.89737700
H(Fragment=1)    3.84279100  -2.83512700  0.86406900
H(Fragment=1)    2.54999800  -3.71009700  0.02396300
N(Fragment=1)    1.03326500  -1.64097700  0.00059900
O(Fragment=1)   -1.59914400  -2.07537200  0.00032000
H(Fragment=1)   -2.57708200  -2.16572600  0.00058100
H(Fragment=1)   -3.10349200   0.19163500  0.00013800
H(Fragment=1)   -2.19598800  -2.47043000  0.00060600
H(Fragment=1)    0.58081000  -2.55256600  0.00066400
O(Fragment=1)    0.46978900   3.06917800  0.00037400
C(Fragment=1)   -0.33701000   4.25535600  0.00038200
H(Fragment=1)   -0.96065900   4.29999300  0.89701600
H(Fragment=1)    0.36519200   5.08528100  0.00039400
H(Fragment=1)   -0.96066000   4.29998200 -0.89778000
O(Fragment=2)   -4.32880400  -2.19250600  0.00024400
H(Fragment=2)   -4.83241200  -2.47368400  0.77191200
H(Fragment=2)   -4.83747300  -2.47191300  0.76969200
Proton-bound 2-Methyl-5-methoxyquinolin-8-ol and water (NH bound)

| Atom Type       | X      | Y      | Z      |
|-----------------|--------|--------|--------|
| C(Fragment=1)   | 1.81215900 | -1.55360200 | -0.00559600 |
| C(Fragment=1)   | 0.31199600 | 0.31701300 | -0.00152100 |
| C(Fragment=1)   | -0.80940000 | -0.55563200 | -0.00013700 |
| C(Fragment=1)   | -0.56495300 | -1.94332100 | -0.00240900 |
| C(Fragment=1)   | 0.72334600 | -2.43631100 | -0.00610800 |
| C(Fragment=1)   | 0.13658300 | 1.71664300 | -0.00299600 |
| C(Fragment=1)   | -2.12904400 | -0.00229000 | 0.00179900 |
| H(Fragment=1)   | -1.41201200 | -2.61770300 | -0.00230700 |
| H(Fragment=1)   | 0.91252600 | -3.50094900 | -0.00952600 |
| C(Fragment=1)   | -2.27769800 | 1.37132000 | 0.00159600 |
| C(Fragment=1)   | -1.14816900 | 2.21391100 | -0.00122300 |
| C(Fragment=1)   | 3.23993200 | -2.00229500 | 0.00199600 |
| H(Fragment=1)   | 3.72088600 | -1.71662200 | 0.94205900 |
| H(Fragment=1)   | 3.30377300 | -3.08372900 | -0.10458300 |
| H(Fragment=1)   | 3.79658300 | -1.53296600 | -0.81264000 |
| N(Fragment=1)   | 1.56980500 | -0.23587400 | -0.00313600 |
| O(Fragment=1)   | 1.27069200 | 2.48465700 | -0.00712200 |
| H(Fragment=1)   | 1.04120200 | 3.42084600 | -0.00583700 |
| H(Fragment=1)   | -1.30194500 | 3.28811900 | -0.00225400 |
| H(Fragment=1)   | -3.25825300 | 1.82490500 | 0.00298600 |
| H(Fragment=1)   | 2.38782500 | 0.39392200 | 0.00005000 |
| O(Fragment=1)   | -3.12643300 | -0.90467700 | 0.00343900 |
| C(Fragment=1)   | -4.48561100 | -0.44263900 | 0.00447700 |
| H(Fragment=1)   | -4.69471800 | 0.14581500 | -0.89324200 |
| H(Fragment=1)   | -5.09789400 | -1.34082900 | 0.00536400 |
| H(Fragment=1)   | -4.69313800 | 0.14646400 | 0.90213700 |
| O(Fragment=2)   | 3.95239400 | 1.26432000 | 0.00583600 |
| H(Fragment=2)   | 3.77006700 | 2.20975300 | -0.00816800 |
| H(Fragment=2)   | 4.90839900 | 1.16290500 | 0.05142000 |
Proton-bound 2-Methyl-5-methoxyquinolin-8-ol and methanol (OH bound)

\begin{align*}
C(Fragment=1) & : 1.86168600 -2.40565200  0.05229400 \\
C(Fragment=1) & : 0.31202500 -0.57280400 -0.07104300 \\
C(Fragment=1) & : 1.36981200  0.36701200 -0.07104300 \\
C(Fragment=1) & : 2.68213400 -0.13512900  0.12475200 \\
C(Fragment=1) & : 2.92466600 -1.49481400  0.14409600 \\
C(Fragment=1) & : -1.03680500 -0.18120000 -0.17906200 \\
C(Fragment=1) & : 1.05046800  1.75939500 -0.00859700 \\
C(Fragment=1) & : 3.50193500  0.56899200  0.19463300 \\
C(Fragment=1) & : 3.93204700 -1.87953200  0.22914600 \\
C(Fragment=1) & : -0.27649100  2.13542500 -0.11725100 \\
C(Fragment=1) & : -1.30609200  1.17414600 -0.20105300 \\
C(Fragment=1) & : 2.68213400 -3.88860000  0.03796600 \\
C(Fragment=1) & : 2.92466600 -4.19923000 -0.92931800 \\
C(Fragment=1) & : 2.77086000 -4.18427200  0.80613400 \\
C(Fragment=1) & : 1.12039400 -4.42751400  0.20541800 \\
C(Fragment=1) & : 0.62087000 -1.91262000 -0.04791500 \\
C(Fragment=1) & : -1.93866800 -1.18660900 -0.25055400 \\
\end{align*}
Proton-bound 2-Methyl-5-methoxyquinolin-8-ol and methanol (NH bound)

| Atoms | X     | Y     | Z     |
|-------|-------|-------|-------|
| C     | -1.32307800 | 1.72764300 | -0.06159100 |
| C     | 0.03218700  | -0.24776800 | -0.03329300 |
| C     | 1.21488200  | 0.53927300  | 0.00170200  |
| C     | 1.07476800  | 1.94190400  | 0.00102600  |
| C     | -0.17216100 | 2.52853800  | -0.03490800 |
| C     | 0.10657200  | -1.65675100 | -0.05235300 |
| C     | 2.49000800  | -0.10891600 | 0.02928000  |
| H     | 1.96950900  | 2.55107800  | 0.02463900  |
| H     | -0.28256900 | 3.60430500  | -0.04285400 |
| C     | 2.53865700  | -1.48956100 | 0.01682300  |
| C     | 1.35120500  | -2.24670200 | -0.02644700 |
| C     | -2.71148100 | 2.28652400  | -0.07515400 |
| H     | -3.14206000 | 2.23649300  | 0.93021800  |
| H     | -2.70130900 | 3.33012400  | -0.38635600 |
| H     | -3.35637300 | 1.71721400  | -0.74633000 |
| N     | -1.18173200 | 0.39629200  | -0.05577800 |
| O     | -1.07800200 | -2.34306700 | -0.10139900 |
| H     | -0.91499400 | -3.29302900 | -0.09031800 |
| H     | 1.42602900  | -3.32918900 | -0.04118800 |
| H     | 3.48324800  | -2.01356900 | 0.03627500  |
| H     | -2.05284900 | -0.16943400 | -0.06387900 |
| O     | 3.55055100  | 0.71819300  | 0.06443300  |
| C     | 4.87175700  | 0.15783900  | 0.08886600  |
| H     | 5.05731100  | -0.43503700 | -0.81116100 |
| H     | 5.54797100  | 1.00860500  | 0.11366100  |
| H     | 5.01601000  | -0.45429900 | 0.98354800  |
| O     | -3.63706000 | -0.89356000 | -0.16134200 |
| H     | -3.46424600 | -1.82961100 | -0.30497700 |
| C     | -4.97952400 | -0.70547700 | 0.32030200  |
| H     | -5.11588700 | 0.36455800  | 0.47182500  |
| H     | -5.71015200 | -1.05361000 | -0.41423200 |
| H     | -5.13417700 | -1.22069400 | 1.27229200  |
XYZ Coordinates of 6-substituted Ion-Solvent Clusters

Proton-bound 6-Bromo-2-methylquinolin-8-ol and water (OH bound)

| Atom     | X     | Y     | Z     |
|----------|-------|-------|-------|
| C(1)     | -3.6019700000 | -0.4007240000 | -0.0000180000 |
| C(1)     | -1.2728040000 | 0.1607860000 | 0.0000000000 |
| C(1)     | -0.8955780000 | -1.2037430000 | -0.0000050000 |
| C(1)     | -1.9443980000 | -2.1584780000 | -0.0000140000 |
| C(1)     | -3.2636500000 | -1.7668100000 | -0.0000210000 |
| C(1)     | -0.3052530000 | 1.1939460000 | 0.0000110000 |
| C(1)     | 0.4766110000 | -1.5378680000 | 0.0000050000 |
| H(1)     | -1.6937770000 | -3.2134820000 | 0.0000015000 |
| H(1)     | -4.0618400000 | -2.4973160000 | 0.0000028000 |
| C(1)     | 1.4054010000 | -0.5195810000 | 0.0000040000 |
| C(1)     | 1.0314520000 | 0.8427680000 | 0.0000080000 |
| H(1)     | 0.7811010000 | -2.5756110000 | 0.0000090000 |
| C(1)     | -5.0176450000 | 0.0848620000 | 0.0000480000 |
| H(1)     | -5.5427790000 | -0.2943620000 | -0.8806850000 |
| H(1)     | -5.5424280000 | -0.2936530000 | 0.8813060000 |
| H(1)     | -5.0819370000 | 1.1738400000 | -0.0003650000 |
| N(1)     | -2.6061590000 | 0.4889070000 | -0.0000150000 |
| O(1)     | -0.7941290000 | 2.4467830000 | -0.0003600000 |
| H(1)     | -0.0820780000 | 3.1287390000 | -0.0000190000 |
| H(1)     | 1.7867320000 | 1.6180390000 | 0.0000150000 |
| Br(1)    | 3.2595800000 | -0.9373470000 | 0.0000070000 |
| H(1)     | -2.8158320000 | 1.4851790000 | -0.0000160000 |
| O(2)     | 1.2595510000 | 4.2070620000 | 0.0000110000 |
| H(2)     | 1.5137960000 | 4.7258270000 | 0.7716420000 |
| H(2)     | 1.5138330000 | 4.7258850000 | -0.7715690000 |
Proton-bound 6-Bromo-2-methylquinolin-8-ol and water (NH bound)

| Atom          | X   | Y   | Z   | Error |
|---------------|-----|-----|-----|-------|
| C(Fragment=1) | 3.05579500 | -1.07366400 | -0.01623000 |
| C(Fragment=1) | 0.94128000 | 0.04384300  | -0.00912800 |
| C(Fragment=1) | 0.24510000 | -1.19284000 | 0.00139800  |
| C(Fragment=1) | 1.02587200 | -2.37612100 | 0.00140300  |
| C(Fragment=1) | 2.39832000 | -2.31834100 | -0.01050500|
| C(Fragment=1) | 0.21800600 | 1.26133000  | -0.02068100|
| C(Fragment=1) | -1.16797700| -1.20543600 | 0.00719600  |
| H(Fragment=1) | 0.52222100 | -3.33634500 | 0.00728900  |
| H(Fragment=1) | 2.99522700 | -3.22073900 | -0.01566500|
| C(Fragment=1) | -1.84556900| -0.00848800 | 0.00064000  |
| C(Fragment=1) | -1.15971000| 1.22616400  | -0.01446600|
| H(Fragment=1) | -1.69757500| -2.14857100 | 0.01573700  |
| C(Fragment=1) | 4.54540300 | -0.93680000 | 0.00100300  |
| H(Fragment=1) | 5.01713600 | -1.84885400 | -0.36261500|
| H(Fragment=1) | 4.87284700 | -0.09642500 | -0.61259100|
| H(Fragment=1) | 4.89024300 | -0.76355300 | 1.02587800  |
| N(Fragment=1) | 2.31424300 | 0.03910500  | -0.01396700|
| O(Fragment=1) | 0.95255800 | 2.40620900  | -0.03996800|
| H(Fragment=1) | 0.37833500 | 3.18150900  | -0.04732200|
| H(Fragment=1) | -1.72447400| 2.15119400  | -0.02264500|
| Br(Fragment=1) | -3.74362200| 0.01470500  | 0.00916400  |
| H(Fragment=1) | 2.81601100 | 0.94304200  | -0.00513800|
| O(Fragment=2) | 3.91752200 | 2.35172000  | 0.03722000  |
| H(Fragment=2) | 3.41823900 | 3.17320000  | -0.01864100|
| H(Fragment=2) | 4.83602400 | 2.59581700  | 0.19146100  |
Proton-bound 6-Bromo-2-methylquinolin-8-ol and methanol (OH bound)

| Atom (Fragment=1) | X (Å) | Y (Å) | Z (Å) | Atom (Fragment=2) | X (Å) | Y (Å) | Z (Å) |
|-------------------|-------|-------|-------|-------------------|-------|-------|-------|
| C                 | -3.76440100 | -0.06221700 | 0.02904900 | C                  | 1.74520300  | 3.61796500 | -0.43086000 |
| C                 | -1.37349400  | 0.10038800  | -0.05368500 | H                  | 2.02965900  | 4.05168800 | -1.24242400 |
| C                 | -1.22592900  | -1.30241000 | 0.06968900  | H                  | 2.31709500  | 4.28975300 | 0.71350200  |
| C                 | -2.41728100  | -2.06468800 | 0.17369300  | H                  | 1.96407900  | 3.75614000 | 1.59483100  |
| C                 | -3.65353500  | -1.46018000 | 0.15392000  | H                  | 3.40782300  | 4.24467400 | 0.68001200  |
| C                 | -0.25066100  | 0.95595200  | -0.16459700 | H                  | 1.98504900  | 5.32941900 | 0.76473700  |
| C                 | 0.07217000   | -1.85843300 | 0.08217000  | H                  | -2.34413400 | -3.14230300 | 0.26988900  |
| C                 | 1.37349400   | 0.10038800  | -0.05368500 | H                  | -4.56077700 | -2.04446600 | 0.23313900  |
| C                 | 1.15445000   | -1.01205500 | -0.02819400 | H                  | 0.20241000  | -2.92791100 | 0.17608900  |
| C                 | 1.00983400   | 0.38741600  | -0.15182100 | H                  | -5.07803500 | 0.65010400  | -0.00005300 |
| C                 | 2.41728100   | -2.06468800 | 0.17369300  | H                  | -5.63648000 | 0.44174000  | 0.91640600  |
| H                 | -3.76440100  | -0.06221700 | 0.02904900  | H                  | -4.96152700 | 1.73041700  | -0.09684400 |
| H                 | -1.37349400  | 0.10038800  | -0.05368500 | H                  | -5.67992900 | 0.28940800  | -0.83847500 |
| N                 | -2.63381400  | 0.64462000  | -0.06729000 | H                  | -2.63381400 | 0.64462000  | -0.06729000 |
| O                 | -0.52472600  | 2.26596200  | -0.27316300 | H                  | -0.52472600 | 2.26596200  | -0.27316300 |
| C                 | 0.97267000   | 2.81802500  | -0.35662200 | H                  | 0.29726700  | 2.81802500  | -0.35662200 |
| H                 | 1.88062400   | 1.02390300  | -0.24028100 | H                  | 1.88062400  | 1.02390300  | -0.24028100 |
| Br                | 2.91491800   | -1.73008500 | -0.01542200 | H                  | 2.67458300  | 1.65785000  | -0.15951000 |
| O                 | 1.74520300   | 3.61796500  | -0.43086000 | H                  | 2.02965900  | 4.05168800  | -1.24242400 |
| C                 | 2.31709500   | 4.28975300  | 0.71350200  | H                  | 2.31709500  | 4.28975300  | 0.71350200  |
| H                 | 1.96407900   | 3.75614000  | 1.59483100  | H                  | 1.96407900  | 3.75614000  | 1.59483100  |
| H                 | 3.40782300   | 4.24467400  | 0.68001200  | H                  | 1.98504900  | 5.32941900  | 0.76473700  |
Proton-bound 6-Bromo-2-methylquinolin-8-ol and methanol (NH bound)

| Atom      | Fragment | X       | Y       | Z       |
|-----------|----------|---------|---------|---------|
| C         | Fragment=1 | -2.6416900 | 1.55038700 | -0.06932100 |
| C         | Fragment=1 | -0.66562100 | 0.20920300 | -0.10363100 |
| C         | Fragment=1 | 0.16051200 | 1.35287000 | 0.04340900 |
| C         | Fragment=1 | -0.48566600 | 2.61293300 | 0.13211800 |
| C         | Fragment=1 | -1.85293500 | 2.70856600 | 0.07640700 |
| C         | Fragment=1 | -0.17979300 | -1.07610600 | -0.20132000 |
| C         | Fragment=1 | 1.56431300 | 1.20624200 | 0.09416500 |
| C         | Fragment=1 | 0.11946500 | 3.50563400 | 0.24444400 |
| C         | Fragment=1 | -2.34986400 | 3.66754000 | 0.14230600 |
| C         | Fragment=1 | 2.10748400 | -0.05450200 | -0.00192200 |
| C         | Fragment=1 | 1.29312000 | -1.19749000 | -0.14973500 |
| H         | Fragment=1 | 2.19299700 | 2.07929600 | 0.20634200 |
| C         | Fragment=1 | -4.13730600 | 1.61676200 | -0.12327100 |
| H         | Fragment=1 | -4.44646900 | 2.32957200 | -0.89200300 |
| H         | Fragment=1 | -4.58578800 | 0.64740000 | -0.33222000 |
| H         | Fragment=1 | -4.52068200 | 1.98842100 | 0.83198400 |
| N         | Fragment=1 | -2.03226800 | 0.36491200 | -0.15187000 |
| O         | Fragment=1 | -0.93623900 | -2.12041000 | -0.34337700 |
| H         | Fragment=1 | -0.45798300 | -2.95584900 | -0.40535400 |
| H         | Fragment=1 | 1.75209200 | -2.17646700 | -0.22394100 |
| Br        | Fragment=1 | 3.99068200 | -0.28924400 | 0.06196700 |
| H         | Fragment=1 | -2.62724200 | -0.48290600 | -0.25816300 |
| O         | Fragment=2 | -3.98251500 | -1.63471900 | -0.36251100 |
| H         | Fragment=2 | -3.99305200 | -2.92058000 | -1.14077500 |
| C         | Fragment=2 | -4.27924000 | -2.42420700 | 0.80679100 |
| H         | Fragment=2 | -4.30993100 | -1.73565500 | 1.65049300 |
| H         | Fragment=2 | -5.25314700 | -2.90965800 | 0.71183700 |
| H         | Fragment=2 | -3.50254400 | -3.17262300 | 0.98426100 |
Proton-bound 6-Chloro-2-methylquinolin-8-ol and water (OH bound)

C(Fragment=1)  3.09993300  0.11503700  0.00012000
C(Fragment=1)  0.70234400  0.15876400  0.00013500
C(Fragment=1)  0.62899800 -1.25515500  0.00016000
C(Fragment=1)  1.85971900 -1.96028800  0.00002800
C(Fragment=1)  3.06282300 -1.29245600  0.00032000
C(Fragment=1) -0.46582300  0.95878800  0.00022000
C(Fragment=1) -0.63766600 -1.87802900  0.00003300
H(Fragment=1)  1.84342000 -3.04451700  0.00037700
H(Fragment=1)  4.00012200 -1.83303100  0.00033300
C(Fragment=1) -1.76390900 -1.08396700  0.00002200
C(Fragment=1) -1.69429200  0.32681500  0.00011000
H(Fragment=1) -0.71644800 -2.95663700  0.00009100
C(Fragment=1)  4.37490800  0.89479500  0.00032700
H(Fragment=1)  4.97169300  0.63528900  0.87814800
H(Fragment=1)  4.96705300  0.64154700  0.88382400
H(Fragment=1)  4.20220300  1.97190500  0.00389700
N(Fragment=1)  1.93313600  0.76751400  0.00019700
O(Fragment=1) -0.25958600  2.28730000  0.00036000
H(Fragment=1) -1.10240200  2.79915300  0.00037300
H(Fragment=1)  1.92228700  1.78556800  0.00032300
Cl(Fragment=1) -3.33892900 -1.82276800  0.00008700
H(Fragment=1) -2.60274600  0.91529800  0.00053000
O(Fragment=2) -2.64594000  3.55929000  0.00029000
H(Fragment=2) -3.00600000  4.01051400  0.77200000
H(Fragment=2) -3.00734900  4.01082200  0.77094500
Proton-bound 6-Chloro-2-methylquinolin-8-ol and water (NH bound)

| Atom      | Fragment | X          | Y          | Z          | Energy   |
|-----------|----------|------------|------------|------------|----------|
| C         | 1        | -2.42068600| -1.07715400| 0.01776000 |          |
| C         | 1        | -0.30903100| 0.04554600 | 0.00824300 |          |
| C         | 1        | 0.39043600 | -1.18935200| -0.00359800|          |
| C         | 1        | -0.38749400| -2.37464800| -0.00281000|          |
| C         | 1        | -1.76038800| -2.32022700| 0.01098000 |          |
| C         | 1        | 0.41082500 | 1.26541900 | 0.01945500 |          |
| C         | 1        | 1.80278300 | -1.19859000| -0.01124000|          |
| H         | 1        | 0.11848000 | -1.18935200| -0.00358900|          |
| C         | 1        | 0.39043600 | -1.18935200| -0.00358900|          |
| H         | 1        | 0.38749400 | -2.37464800| -0.00281000|          |
| C         | 1        | 1.76038800 | -2.32022700| 0.01098000 |          |
| C         | 1        | 2.47602000 | 0.00046500 | -0.00510000|          |
| C         | 1        | 1.78813400 | 1.23370700 | 0.01142100 |          |
| H         | 1        | 2.33995300 | -2.13740800| -0.02078400|          |
| C         | 1        | -3.91070400| -0.94474200| 0.00233500 |          |
| H         | 1        | -4.25784300| -0.78009600| -1.02320200|          |
| H         | 1        | -4.37895600| -1.85574700| 0.37310500 |          |
| H         | 1        | -4.23972700| -0.10117600| 0.61059200 |          |
| N         | 1        | -1.68204400| 0.03734500 | 0.01472700 |          |
| O         | 1        | -0.32676300| 2.40783500 | 0.04039200 |          |
| H         | 1        | 0.24480500 | 3.18511700 | 0.04707200 |          |
| H         | 1        | -2.18609100| 0.94012200 | 0.00617700 |          |
| Cl        | 1        | 4.21309500 | 0.02797000 | -0.01514400|          |
| H         | 1        | 2.35588600 | 2.15690600 | 0.01931900 |          |
| O         | 2        | -3.29290800| 2.34452400 | -0.03722300|          |
| H         | 2        | -4.21236000| 2.58206700 | -0.19610300|          |
| H         | 2        | -2.79995900| 3.16965400 | 0.02086400 |          |
Proton-bound 6-Chloro-2-methylquinolin-8-ol and methanol (OH bound)

C(Fragment=1)  -3.20326800 -0.86555300  0.03082600
C(Fragment=1)  -0.91173700 -0.16481500 -0.05436100
C(Fragment=1)  -1.27392000  1.19860200  0.06629800
C(Fragment=1)  -2.65893700  1.48070000  0.17027200
C(Fragment=1)  -3.59812600  0.48039000  0.15303090
C(Fragment=1)   0.44259100 -0.56439800 -0.16511400
C(Fragment=1)  -0.26021700  2.18079900  0.07623100
H(Fragment=1)  -2.97504100  2.51905100  0.07623100
H(Fragment=1)  -4.65404700  0.70290000  0.23231800
C(Fragment=1)  1.05220400  1.77496700 -0.03380000
C(Fragment=1)  1.41684400  0.41608600 -0.15467200
H(Fragment=1) -0.51418200  3.22802200  0.16770400
H(Fragment=1) -4.17656200 -1.99949600  0.00451600
H(Fragment=1) -4.77211900 -2.00209700  0.92129500
H(Fragment=1) -4.86796200 -1.87879800 -0.83377300
H(Fragment=1) -3.68259500 -2.96746800 -0.09059200
N(Fragment=1) -1.89507200 -1.12273700 -0.06559400
O(Fragment=1)  0.65354000 -1.88557900 -0.27133600
H(Fragment=1)  1.61862800 -2.10870200 -0.35484700
H(Fragment=1) -1.57186900 -2.08408400 -0.15603100
Cl(Fragment=1) 2.32416800  2.96267800 -0.02562000
H(Fragment=1)  2.45899900  0.13759500 -0.24239600
O(Fragment=2)  3.25320200 -2.33966400 -0.43073400
H(Fragment=2)  3.67337400 -2.64072500 -1.24456000
C(Fragment=2)  4.02827200 -2.77463300  0.71019400
H(Fragment=2)  3.51197600 -2.40344100  1.59435000
H(Fragment=2)  4.08186600 -3.86498200  0.75524700
H(Fragment=2)  5.03387100 -2.34980200  0.67733400
Proton-bound 6-Chloro-2-methylquinolin-8-ol and methanol (NH bound)

C  -1.94262100  1.60683000  -0.07178000
C   -0.03376000  0.16750200  -0.09459600
C    0.84803600  1.26777300   0.05852800
C    0.26566900  2.55906200   0.14481100
C    -1.09440900  2.72339300   0.08112200
C     0.48755300  -1.14607600  -0.18758900
C     2.24183700   1.05151100   0.11792100
H     0.91415700   3.42011400   0.26852000
C    -1.54277900   3.70614400   0.14582400
C     2.72052400   -0.23489000   0.02474000
C     1.85168700  -1.33626200  -0.12762200
H     2.91711200   1.88843000   0.23493000
C    -3.42930700   1.74310000  -0.13339000
H    -3.79498800   2.22400000   0.73373000
H    -3.69251300   2.41571100  -0.97191200
H    -3.93209700   0.79669500  -0.27829000
N    -1.39076700   0.39201400  -0.15216000
O    -0.41966200  -2.14572000  -0.32359000
H     0.01593100  -3.00319700   0.26386800
H    -2.02745200   -0.42424000   0.26852000
Cl    4.43043100  -0.53790100   0.09383700
H     2.26717100  -2.33457500  -0.19305000
O    -3.43885400  -1.57062700  -0.35827000
H    -3.53612400  -2.03433100  -1.15797000
C    -3.73066400  -2.32615700   0.79192000
H    -3.66515400  -1.67629100   1.66373400
H    -4.74144100  -2.73586500   0.73154600
H    -3.00291000  -3.13557300   0.89304500
Proton-bound 6-Cyano-2-methylquinolin-8-ol and water (OH bound)

C(Fragment=1)  -3.00556800  0.15297500  0.00009000
C(Fragment=1)  -0.60721900  0.12532700  0.00015000
C(Fragment=1)  -0.58011400  -1.28968200  -0.00030000
C(Fragment=1)  -1.83068200  -1.95916300  -0.00013800
C(Fragment=1)  -3.01277300  -1.25533100  -0.00063000
C(Fragment=1)   0.58269400  0.89414900  0.00030800
C(Fragment=1)   0.66792100  -1.94799900  -0.00060000
H(Fragment=1)  -1.84604300  -3.04346700  -0.00022800
H(Fragment=1)  -3.96647900  -1.76634700  -0.00114000
H(Fragment=1)   1.82762100  -1.19511100  0.00003400
H(Fragment=1)   1.79163600   0.22704200  0.00021500
H(Fragment=1)   0.71177500  -3.02910800  -0.00152000
H(Fragment=1)  -4.25580800   0.97042500  -0.00252000
H(Fragment=1)  -4.85532300   0.73289900  -0.88379000
H(Fragment=1)  -4.85955200   0.72747900   0.87834400
H(Fragment=1)  -4.05189900   2.04193700  -0.00347700
N(Fragment=1)  -1.81952200   0.77094300  -0.00022200
O(Fragment=1)   0.41144100   2.22597800  -0.00045000
H(Fragment=1)  -1.26825700   2.71681200  -0.00035200
H(Fragment=1)   2.71513600   0.79223900  -0.00027700
H(Fragment=1)  -1.77831000   1.78854200  -0.00042400
C(Fragment=1)   3.10306800  -1.84129600  -0.00046000
N(Fragment=1)   4.13581300  -2.35628100  -0.00010100
O(Fragment=2)   2.83051300   3.41544100  -0.00037500
H(Fragment=2)   3.21382000   3.84757900  -0.77256800
H(Fragment=2)   3.21491800   3.84783000   0.77082500
Proton-bound 6-Cyano-2-methylquinolin-8-ol and water (NH bound)

C(Fragment=1)    2.29972500 -1.07541300 -0.01684400
C(Fragment=1)    0.18801200  0.04735500 -0.00728100
C(Fragment=1)   -0.50779800 -1.18914500  0.00374000
C(Fragment=1)    0.26887700 -2.37508900  0.00284000
C(Fragment=1)   1.64170000 -2.31973600 -0.01064400
C(Fragment=1)   -0.52961100  1.26998800 -0.01800000
C(Fragment=1)   -1.91957200 -1.19617800  0.01096400
H(Fragment=1)   -0.23749700 -3.33393200  0.00932400
C(Fragment=1)   -2.60351300  0.00426500  0.00525500
C(Fragment=1)  -1.90580400  1.23935500 -0.01040900
H(Fragment=1)  -2.45466300 -2.13675200  0.02008900
C(Fragment=1)   3.78888600 -0.94091200 -0.00262600
H(Fragment=1)  -1.73081000  0.73925900  1.01770800
H(Fragment=1)   4.25998200 -1.86296300 -0.34038300
H(Fragment=1)  -4.11708900 -0.11733900  0.63841100
N(Fragment=1)   1.56069300  0.04010000  0.01333200
O(Fragment=1)   -0.21263300  2.40737000 -0.03795700
H(Fragment=1)  -0.35311400  3.73543000 -0.00187300
H(Fragment=1)  -4.70029000  2.16506900  0.00179320
H(Fragment=1)  -2.06616700  0.94355100 -0.00462300
C(Fragment=1)  -4.03393400  0.02047200  0.00313840
N(Fragment=1)  -5.18768100  0.04222400  0.00206500
O(Fragment=2)   3.18157100  2.33166500  0.19346100
H(Fragment=2)  -2.70999900  3.16876000 -0.02957400
H(Fragment=2)  -4.10644600  2.54808500  0.19393800
Proton-bound 6-Cyano-2-methylquinolin-8-ol and methanol (OH bound)

| Atom     | X       | Y       | Z       |
|----------|---------|---------|---------|
| C(Fragment=1) | 3.12708600 | -0.86632500 | 0.03148600 |
| C(Fragment=1) | 0.85337000 | -0.10817000 | -0.05377800 |
| C(Fragment=1) | 1.25365300 | 1.24434400 | 0.06299500 |
| C(Fragment=1) | 2.64540400 | 1.49850300 | 0.16506800 |
| C(Fragment=1) | 3.55822000 | 0.46917900 | 0.14980400 |
| C(Fragment=1) | -0.51031400 | -0.47814400 | -0.16262000 |
| C(Fragment=1) | 0.26400700 | 2.25002300 | 0.07097300 |
| H(Fragment=1) | 2.98694400 | 2.52370400 | 0.25604000 |
| C(Fragment=1) | 4.61975300 | 0.66364600 | 0.22744500 |
| C(Fragment=1) | -1.06713800 | 1.88377900 | -0.03692100 |
| C(Fragment=1) | -1.45972600 | 0.52553900 | -0.15415900 |
| H(Fragment=1) | 0.54719000 | 3.29049700 | 0.15977700 |
| C(Fragment=1) | 4.07059400 | -2.02425600 | 0.00761300 |
| H(Fragment=1) | 4.76488100 | -1.92132600 | -0.83079600 |
| H(Fragment=1) | 4.66645000 | -2.03801100 | 0.92423100 |
| C(Fragment=1) | 3.55313000 | -2.97996300 | -0.08507600 |
| N(Fragment=1) | 1.81230800 | -1.09112600 | -0.06321300 |
| O(Fragment=1) | 0.74965000 | -0.74965000 | -1.79306000 | -0.26459700 |
| H(Fragment=1) | -1.72114600 | -1.99609800 | -0.34874000 |
| H(Fragment=1) | -2.50787000 | 0.26865600 | -0.24047900 |
| H(Fragment=1) | 1.46463300 | -2.04452200 | -0.15074300 |
| C(Fragment=1) | -2.08622800 | 2.88912000 | -0.03052600 |
| N(Fragment=1) | -2.91545000 | 3.69173500 | -0.02527600 |
| O(Fragment=2) | -3.35311600 | -2.17482300 | -0.43114300 |
| H(Fragment=2) | -3.77833900 | -2.45499800 | -1.24884300 |
| C(Fragment=2) | -4.15375500 | -2.57807400 | 0.70371500 |
| H(Fragment=2) | -4.25539000 | -3.66499200 | 0.74442500 |
| H(Fragment=2) | -3.62830700 | -2.23282000 | 1.59271100 |
| H(Fragment=2) | -5.13883700 | -2.10862000 | 0.66348900 |
Proton-bound 6-Cyano-2-methylquinolin-8-ol and methanol (NH bound)

C    -1.81148800  1.60691800  -0.06854000
C     0.08699200  0.15377200  -0.09137400
C     0.97340100  1.25004100  0.06016800
C     0.40175400  2.54615500  0.14592300
C    -0.95699300  2.71918800  0.08310700
C     0.59650000 -1.16583700 -0.18340700
C     2.36464300  1.02203000  0.11873400
H     1.05695100  3.40232300  0.26210900
H    -1.39981800  3.70441800  0.14740100
C     2.84488400 -0.27091300  0.02702600
C     1.95807800 -1.36627000 -0.12421000
H     3.04396200  1.85645800  0.23421900
C    -3.29620900  1.76340900 -0.14101000
H    -3.65544300  2.25757700  0.76630800
H    -3.55319800  2.41381800 -0.98210000
H    -3.80808100  0.81033900 -0.25733300
N    -1.26852200  0.38703000 -0.14834300
O    -0.32085800 -2.15397200 -0.32606800
H     0.10290300 -3.01798600 -0.35497400
H     2.36251700 -2.36969500 -0.19338100
H    -1.91274600 -0.42535400 -0.25970700
C     4.25175700 -0.52413100  0.08425700
N     5.38509500 -0.73663600  0.12981200
O    -3.32729000 -1.48761800 -0.35497400
H    -3.45484000 -1.99522100 -1.16349300
C    -3.62995900 -2.32033600  0.78319000
H    -2.93008100 -3.15677500  0.85619700
H    -3.52773800 -1.69143800  1.66735800
H    -4.65537500 -2.69265000  0.73105600
Proton-bound 6-Fluoro-2-methylquinolin-8-ol and water (OH bound)

\[
\begin{align*}
\text{C(Fragment=1)} & : 2.73850900 \quad -0.62865800 \quad -0.00111600 \\
\text{C(Fragment=1)} & : 0.39872100 \quad -0.09551500 \quad -0.00025500 \\
\text{C(Fragment=1)} & : 0.66747800 \quad 1.29681400 \quad -0.00136900 \\
\text{C(Fragment=1)} & : 2.03022100 \quad 1.68300200 \quad -0.00078900 \\
\text{C(Fragment=1)} & : 3.03927100 \quad 0.74411500 \quad -0.00111600 \\
\text{C(Fragment=1)} & : -0.92873300 \quad -0.59532900 \quad -0.00018800 \\
\text{C(Fragment=1)} & : -0.41239500 \quad 2.20723000 \quad 0.00027400 \\
\text{H(Fragment=1)} & : 2.27640400 \quad 2.73901100 \quad -0.00104900 \\
\text{H(Fragment=1)} & : 4.07762600 \quad 1.04655800 \quad -0.00204200 \\
\text{C(Fragment=1)} & : -1.68295600 \quad 1.69013000 \quad 0.00051400 \\
\text{C(Fragment=1)} & : -1.96910100 \quad 0.31217000 \quad 0.00029900 \\
\text{H(Fragment=1)} & : -0.25052200 \quad 3.27652900 \quad 0.00034000 \\
\text{C(Fragment=1)} & : 3.76893600 \quad -1.71311300 \quad 0.00208300 \\
\text{H(Fragment=1)} & : 4.77202800 \quad -1.29166400 \quad -0.03078700 \\
\text{H(Fragment=1)} & : 3.68296800 \quad -2.32430500 \quad 0.90562900 \\
\text{H(Fragment=1)} & : 3.64329200 \quad -2.37076900 \quad -0.86305700 \\
\text{N(Fragment=1)} & : 1.44637400 \quad -0.98060600 \quad -0.00079700 \\
\text{O(Fragment=1)} & : -1.04481100 \quad -1.93349500 \quad -0.00053700 \\
\text{H(Fragment=1)} & : -1.98622100 \quad -2.22975800 \quad -0.00030200 \\
\text{H(Fragment=1)} & : -2.99939700 \quad -0.02045700 \quad 0.00047600 \\
\text{H(Fragment=1)} & : 1.19123600 \quad -1.96655200 \quad -0.00094000 \\
\text{F(Fragment=1)} & : -2.72893000 \quad 2.52407200 \quad 0.00093000 \\
\text{O(Fragment=2)} & : -3.66022300 \quad -2.59366200 \quad -0.00023000 \\
\text{H(Fragment=2)} & : -4.11587200 \quad -2.94955300 \quad 0.77119600 \\
\text{H(Fragment=2)} & : -4.11522000 \quad -2.94926100 \quad -0.77217900 \\
\end{align*}
\]
Proton-bound 6-Fluoro-2-methylquinolin-8-ol and water (NH bound)

|   |   |   |   |   |
|---|---|---|---|---|
| C | 2.05050100 | -1.08201000 | -0.02094700 |
| C | -0.05821500 | 0.04718100 | -0.00785900 |
| C | -0.76216600 | -1.18644100 | 0.00696900 |
| C | 0.01331300 | -2.37367800 | 0.00574000 |
| C | 1.38585100 | -2.32316700 | -0.01150000 |
| C | -0.77057600 | 1.27322300 | -0.01946100 |
| C | -2.17434400 | -1.19221400 | 0.01757500 |
| H | -0.49514000 | -3.33126000 | 0.01475700 |
| H | 1.97698500 | -3.22904600 | -0.01800400 |
| C | -2.82203500 | 0.01468100 | 0.01109100 |
| C | -2.14799900 | 1.24846900 | -0.00843900 |
| H | -2.73333700 | -2.11817200 | 0.02927700 |
| C | 3.54116900 | -0.95595100 | -0.00860200 |
| H | 4.00372700 | -1.86176300 | -0.39902600 |
| H | 3.87209900 | -0.10230600 | -0.60126200 |
| H | 3.89276700 | -0.81428900 | 1.01886700 |
| N | 1.31534000 | 0.03399700 | -0.01714300 |
| O | -0.02628600 | 2.40962900 | -0.04394800 |
| H | -0.59158100 | 3.19146900 | -0.05223800 |
| H | -2.73146400 | 2.16186200 | -0.01632400 |
| H | 1.82216200 | 0.93525500 | -0.00857600 |
| F | -4.15758000 | 0.05132000 | 0.02129000 |
| O | 2.94298000 | 2.33143900 | 0.04168400 |
| H | 3.86391900 | 2.55475300 | 0.21245300 |
| H | 2.46415200 | 3.16453400 | -0.02082300 |
| Fragment  | x  | y  | z  | x  | y  | z  |
|-----------|----|----|----|----|----|----|
| C(Fragment=1) | -2.83547000 | -1.18659400 | 0.03247700 |
| C(Fragment=1) | -0.71932500 | -0.06149300 | -0.05528000 |
| C(Fragment=1) | -1.33511700 | 1.20920400 | 0.06325600 |
| C(Fragment=1) | -2.74979200 | 1.22614200 | 0.16756300 |
| C(Fragment=1) | -3.47954000 | 0.05996800 | 0.15269300 |
| C(Fragment=1) | 0.68765300 | -0.20036200 | -0.16633300 |
| C(Fragment=1) | -0.52803600 | 2.36689700 | 0.07081200 |
| H(Fragment=1) | -3.25745100 | 2.17978000 | 0.26008400 |
| H(Fragment=1) | -4.55849600 | 0.07743500 | 0.23220300 |
| C(Fragment=1) | 0.83013400 | 2.19860100 | -0.03971300 |
| C(Fragment=1) | 1.45868900 | 0.94659600 | -0.15815600 |
| H(Fragment=1) | -0.95692100 | 3.35571900 | 0.15933300 |
| C(Fragment=1) | -3.57485000 | -2.48536000 | 0.00897900 |
| H(Fragment=1) | -4.15682900 | -2.60071700 | 0.92722700 |
| H(Fragment=1) | -4.27842500 | -2.49958500 | -0.82770800 |
| H(Fragment=1) | -2.90552600 | -3.34144800 | -0.08683700 |
| N(Fragment=1) | -1.50284700 | -1.18916200 | -0.06426600 |
| O(Fragment=1) | 1.14330000 | -1.45712900 | -0.27007400 |
| H(Fragment=1) | 2.13371400 | -1.49435800 | -0.35382700 |
| H(Fragment=1) | 2.53636500 | 0.89201500 | -0.24433700 |
| H(Fragment=1) | -1.00244200 | -2.07150500 | -0.15334000 |
| F(Fragment=1) | 1.62364500 | 3.27621500 | -0.03660400 |
| O(Fragment=2) | 3.78076500 | -1.40805000 | -0.42988400 |
| H(Fragment=2) | 4.24626800 | -1.61795500 | -1.24662800 |
| C(Fragment=2) | 4.62218600 | -1.70683300 | 0.70694000 |
| H(Fragment=2) | 4.04700300 | -1.44853000 | 1.59488800 |
| H(Fragment=2) | 4.87646100 | -2.76891600 | 0.73820000 |
| H(Fragment=2) | 5.53169800 | -1.10290500 | 0.68026700 |
Proton-bound 6-Fluoro-2-methylquinolin-8-ol and methanol (NH bound)

C  -1.46195600  1.68110000  -0.07827900
C   0.33113300  0.09888200  -0.08400000
C   1.29476000  1.12927500   0.07295500
C   0.81168800  2.46157100   0.15202800
C  -0.53092400  2.72945500   0.07834400
C   0.74615800  0.00079265  -0.10943100
C   2.67742200  0.80758200   0.14305000
H   1.52330600  3.27074700   0.27201900
C  -0.90255400  1.37840000   0.08400000
C   3.02411200  1.71245300   0.05489300
C   1.09060600  3.75095400   0.10041000
H   2.74262600  0.13274900   0.26294900
C  -2.93226800  1.94147200  -0.16239800
H  -3.26485200  2.45718800   0.74261000
H  -3.13776700  2.60811800  -1.00474100
H  -3.50784400  1.02604700  -0.28442500
N  -1.00451100  0.42788400  -0.15180200
O  -0.23629200  2.17205000  -0.31890500
H   0.12836400  3.06774800  -0.38510400
H   2.44906200  2.57186800  -0.16247900
H  -1.70142000  0.33710700  -0.26641600
F   4.31419800  0.85645300   0.11705000
O  -3.19474800  1.30565400  -0.36625600
H  -3.34424600  1.81462100  -1.17001500
C  -3.55448400  2.10547500   0.77829900
H  -3.42392300  1.47278600  1.65565700
H  -4.59916500  2.41936200   0.72127500
H  -2.90435900  2.97975600   0.86774300

![Proton-bound 6-Fluoro-2-methylquinolin-8-ol and methanol (NH bound)](image)
Proton-bound 2,6-Dimethylquinolin-8-ol and water (OH bound)

C (Fragment=1) 2.78352400 0.54887800 -0.00004900
C (Fragment=1) 0.42772300 0.10025400 -0.00003900
C (Fragment=1) 0.64473300 -1.29899600 0.00000900
C (Fragment=1) 1.99234200 -1.73510100 0.00005800
C (Fragment=1) 3.03522800 -0.83487000 0.00001900
C (Fragment=1) -0.88011100 0.63842400 -0.00006000
C (Fragment=1) -0.47429800 -2.16192400 0.00001100
H (Fragment=1) 2.19171000 -2.79967500 0.00010200
H (Fragment=1) 4.06322400 -1.17243200 0.00005500
C (Fragment=1) -1.75575500 -1.64534700 -0.00004200
C (Fragment=1) -1.94607900 -0.23805800 -0.00005700
H (Fragment=1) -0.31164300 -3.23288800 0.00004700
C (Fragment=1) 3.87137000 1.57466200 0.00007000
H (Fragment=1) 4.50455100 1.44843900 0.88224500
H (Fragment=1) 4.50707000 1.44597600 -0.87991700
H (Fragment=1) 3.48002000 2.59299300 -0.00193100
N (Fragment=1) 1.50739700 0.94877800 -0.00008700
O (Fragment=1) -0.95162900 1.98505300 -0.00011400
H (Fragment=1) -1.88008900 2.31083800 -0.00006400
H (Fragment=1) -2.95236400 0.16649000 -0.00006800
H (Fragment=1) 1.28760000 1.94260600 -0.00005000
C (Fragment=1) -2.96628700 -2.54013300 0.00002900
H (Fragment=1) -3.58633000 -2.35040000 0.88094200
H (Fragment=1) -3.58657300 -2.35021400 -0.88066800
H (Fragment=1) -2.68846900 -3.59433000 -0.00011400
O (Fragment=2) -3.55247700 2.78336100 0.00010200
H (Fragment=2) -3.97493500 3.17858300 -0.77081700
H (Fragment=2) -3.97454600 3.17852800 0.77126100
Proton-bound 2,6-Dimethylquinolin-8-ol and water (NH bound)

| Atom          | X   | Y   | Z   |
|---------------|-----|-----|-----|
| C(Fragment=1) | 2.08945000 | -1.08348000 | -0.01705700 |
| C(Fragment=1) | -0.01944600 | 0.04554600 | -0.00582800 |
| C(Fragment=1) | -0.72333600 | -1.18689400 | 0.00494900 |
| C(Fragment=1) | 0.05144500 | -2.37206900 | 0.00290600 |
| C(Fragment=1) | 1.42618600 | -2.32323700 | -0.01093500 |
| C(Fragment=1) | -0.74012400 | 1.26330900 | -0.01470600 |
| C(Fragment=1) | -2.13730300 | -1.18337600 | 0.01268400 |
| H(Fragment=1) | -0.45692900 | -3.32993800 | 0.00884100 |
| H(Fragment=1) | 2.01710800 | -3.22919100 | -0.01736100 |
| H(Fragment=1) | -2.83825200 | 0.00403300 | 0.00818700 |
| H(Fragment=1) | -2.11620100 | 1.22552900 | -0.00654100 |
| H(Fragment=1) | -2.66167200 | -2.13136700 | 0.02128700 |
| C(Fragment=1) | 3.58011500 | -0.95212100 | -0.00163500 |
| H(Fragment=1) | 3.92644600 | -0.76281400 | 1.01973300 |
| H(Fragment=1) | 4.04853600 | -1.87131500 | -0.35117100 |
| H(Fragment=1) | 3.91045000 | -0.12278200 | -0.62881000 |
| N(Fragment=1) | 1.35358000 | 0.03344800 | -0.01328600 |
| O(Fragment=1) | -0.00127900 | 2.40959800 | -0.03319300 |
| H(Fragment=1) | -0.57798300 | 3.18261600 | -0.04193800 |
| H(Fragment=1) | -2.66836600 | 2.16092400 | -0.01285300 |
| H(Fragment=1) | 1.85939100 | 0.93385800 | -0.00670700 |
| C(Fragment=1) | -4.34250100 | 0.04296900 | 0.01686200 |
| H(Fragment=1) | -4.71045700 | 0.57929000 | 0.89602000 |
| H(Fragment=1) | -4.72108500 | 0.56617900 | -0.86595800 |
| H(Fragment=1) | -4.76978500 | -0.95984300 | 0.02692400 |
| O(Fragment=2) | 2.95679700 | 2.35177500 | 0.02827900 |
| H(Fragment=2) | 3.87174400 | 2.61912800 | 0.16265100 |
| H(Fragment=2) | 2.43320500 | 3.15889000 | -0.01196000 |
Proton-bound 2,6-Dimethylquinolin-8-ol and methanol (OH bound)

| Atoms          | X-Coordinates | Y-Coordinates | Z-Coordinates |
|----------------|---------------|---------------|---------------|
| C(Fragment=1)  | 2.87601900    | -1.15410900  | 0.03077200    |
| C(Fragment=1)  | 0.74036000    | -0.06707200  | -0.05639200   |
| C(Fragment=1)  | 1.33218900    | 1.21353600   | 0.06526200    |
| C(Fragment=1)  | 2.74398900    | 1.25551700   | 0.17062400    |
| C(Fragment=1)  | 3.49699400    | 0.10180000   | 0.15404600    |
| C(Fragment=1)  | -0.66158600   | -0.22062400  | -0.16813300   |
| C(Fragment=1)  | 0.49550100    | 2.35230900   | 0.07340400    |
| H(Fragment=1)  | 3.23460400    | 2.21801200   | 0.26558700    |
| H(Fragment=1)  | 4.57536700    | 0.13865800   | 0.23454300    |
| C(Fragment=1)  | -0.87484000   | 2.21322600   | -0.03658100   |
| C(Fragment=1)  | -1.44310200   | 0.91754100   | -0.16593700   |
| H(Fragment=1)  | 0.94469400    | 3.33366100   | 0.16611700    |
| C(Fragment=1)  | 3.63761200    | -2.44064800  | 0.00504400    |
| H(Fragment=1)  | 4.34230600    | -2.44174800  | -0.83070700   |
| H(Fragment=1)  | 4.21971800    | -2.54956700  | 0.92390200    |
| H(Fragment=1)  | 2.98239300    | -3.30727200  | -0.09408100   |
| N(Fragment=1)  | 1.54267000    | -1.18117800  | -0.06725100   |
| O(Fragment=1)  | -1.09973100   | -1.48915000  | -0.27587800   |
| H(Fragment=1)  | -2.08586200   | -1.54051800  | -0.36033700   |
| H(Fragment=1)  | -2.51847300   | 0.80879800   | -0.24564500   |
| H(Fragment=1)  | 1.05763500    | -2.07149200  | -0.15867300   |
| C(Fragment=1)  | -1.79069800   | 3.40802900   | -0.03287700   |
| H(Fragment=1)  | -2.37149700   | 3.45161100   | -0.95875000   |
| H(Fragment=1)  | -2.50319600   | 3.34575400   | 0.79474000    |
| H(Fragment=1)  | -1.23586200   | 4.34136200   | 0.06519700    |
| O(Fragment=2)  | -3.75838500   | -1.52067700  | -0.43273500   |
| H(Fragment=2)  | -4.21394300   | -1.76768900  | -1.24450600   |
| C(Fragment=2)  | -4.56756500   | -1.87243700  | 0.71015100    |
| H(Fragment=2)  | -4.74685100   | -2.94975900  | 0.74959700    |
| H(Fragment=2)  | -4.00554100   | -1.57019500  | 1.59277000    |
| H(Fragment=2)  | -5.51850200   | -1.33516400  | 0.68961100    |
Proton-bound 2,6-Dimethylquinolin-8-ol and methanol (NH bound)

|   |  X   |  Y   |  Z   |
|---|------|------|------|
|  C | -1.47308200 | 1.62206800 | -0.07055600 |
|  C | 0.35151300  | 0.07841100  | -0.03849600 |
|  C | 1.29557200  | 1.13543100  | 0.04005500  |
|  C | 0.78530200  | 2.45653700  | 0.05841800  |
|  C | -0.56721700 | 2.69621700  | -0.00172700 |
|  C | 0.80574300  | -1.26130600 | -0.08290600 |
|  C | 2.67681300  | 0.83738500  | 0.08840600  |
|  H | 1.48156300  | 3.28600400  | 0.11494500  |
|  C | -0.95683800 | 3.70537500  | 0.00336800  |
|  C | 3.11680800  | -0.46901300 | 0.05532700  |
|  C | 2.15871500  | -1.51146900 | -0.03403000 |
|  H | 3.38535700  | 1.65467400  | 0.14987100  |
|  C | -2.95734900 | 1.81117900  | -0.10727100 |
|  H | -3.35815100 | 1.79455100  | 0.91186500  |
|  H | -3.20662200 | 2.77737200  | -0.54544000 |
|  H | -3.44393200 | 1.02071700  | -0.67915700 |
|  N | -0.98879500 | 0.37605500  | -0.08084400 |
|  O | -0.15139300 | -2.22831500 | -0.17866100 |
|  H | 0.25281200  | -3.10399300 | -0.18280900 |
|  H | 2.50498000  | -2.54046900 | -0.06849800 |
|  H | -1.67924200 | -0.40101600 | -0.11393100 |
|  C | 4.57918300  | -0.82033800 | 0.10612100  |
|  H | 4.79572000  | -1.45030500 | 0.97371900  |
|  H | 4.87377600  | -1.38125900 | -0.78513000 |
|  H | 0.52039320  | 0.07078100  | 0.16887600  |
|  O | -3.03591200 | -1.49140300 | -0.26014200 |
|  H | -2.65982100 | -2.33854700 | -0.52040200 |
|  C | -4.27221500 | -1.70231800 | 0.44726700  |
|  H | -4.11304800 | -2.28568400 | 1.35831300  |
|  H | -4.65357800 | -0.71866900 | 0.71856000  |
|  H | -5.00562800 | -2.20087600 | -0.19108100 |
Proton-bound 2-methyl-6-Nitroquinolin-8-ol and water (OH bound)

C(Fragment=1)  3.29493900  -0.09914100  -0.00006300
C(Fragment=1)  0.91246100   0.17808700  -0.00008000
C(Fragment=1)  0.70817300  -1.22269100   0.00009000
C(Fragment=1)  1.86265700  -2.04584700   0.00011600
C(Fragment=1)  3.12441000  -1.49701300   0.00004200
C(Fragment=1) -0.17011800   1.09247200  -0.00003800
C(Fragment=1) -0.61392100  -1.72015100   0.00014700
H(Fragment=1)  1.73942300  -3.12319500   0.00019200
H(Fragment=1)  4.00594800  -2.12435500   0.00006000
C(Fragment=1) -1.64103700  -0.80950600   0.00010300
C(Fragment=1) -1.45496600   0.58343200   0.00002000
C(Fragment=1)  4.63865700   0.55285100  -0.00013200
H(Fragment=1)  5.20458300   0.23767000  0.88075800
H(Fragment=1)  5.20471900   0.23722500  0.88077000
H(Fragment=1)  4.57292800   1.64156700  -0.00016800
N(Fragment=1)  2.19708400   0.66487800  -0.00008300
O(Fragment=1)  0.16693000   2.39120000  -0.00014000
H(Fragment=1) -0.62293900   2.98524300  -0.00039100
H(Fragment=1)  2.28544000   1.67961400  -0.00016800
H(Fragment=1) -2.31322300   1.24204000  -0.00003000
N(Fragment=1) -3.04676500  -1.32043800   0.00015400
O(Fragment=1) -3.93733600  -0.48643300  -0.00003400
O(Fragment=1) -3.19672400  -2.52983500   0.00022300
H(Fragment=1) -0.81768700  -2.78202400   0.00022000
O(Fragment=2) -2.08334100   3.86092900  -0.00030000
H(Fragment=2) -2.43849400   4.31650200  -0.77203100
H(Fragment=2) -2.43669200   4.31677500  0.77210000
Proton-bound 2-methyl-6-Nitroquinolin-8-ol and water (NH bound)

C      2.65582600   -1.07576700   -0.01616200
C      0.54415500    0.04736400   -0.00762300
C     -0.14958900   -1.19086000    0.00129300
C      0.62605200   -2.37667600    0.00033500
C      1.99912000   -2.32055100   -0.01168700
C     -0.12729750    1.27118500   -0.01782500
C     -1.56300800   -1.20015100    0.00746700
H      0.11886900   -3.33506100    0.00555000
H      2.59508500   -3.22314100   -0.01775000
C     -2.21596300    0.00357700    0.00259100
C      0.62605200   -2.37667600   -0.00033500
C     -1.56300800   -1.20015100    0.00746700
H  4.14472200    -0.94033100   -0.00111300
H      4.48566200   -0.72622000    1.01743800
H     4.61723200   -1.86567300   -0.32742200
H     4.47298300   -0.12346800   -0.64560300
N      1.91687400    0.04022000   -0.01234200
O      0.56836800    2.40826400   -0.03609300
H      0.00149300    3.18957200   -0.03978800
H     2.42290200    0.94388700   -0.00283200
H     2.13649800    2.15179700   -0.01791100
N     -3.70967200    0.01581700    0.00981200
O     -4.25075400    1.10944700    0.00532000
O     -4.27136000   -1.06500800    0.01983900
H     -2.11886700   -2.12793000    0.01523600
O      3.53555900    2.32968500    0.03506000
H     4.46080400    2.54527200    0.19267900
H     3.06486900    3.16726400   -0.03082200
Proton-bound 2-methyl-6-Nitroquinolin-8-ol and methanol (OH bound)

C (Fragment=1)  -3.44108000  0.57364400  0.03168600
C (Fragment=1)  -1.07473600  0.19252600 -0.05313500
C (Fragment=1)  -1.25400200 -1.20720800  0.05967800
C (Fragment=1)  -2.58580200 -1.68336300  0.15953300
C (Fragment=1)  -3.65231400 -0.81402400  0.14593800
C (Fragment=1)   0.21163000  0.77859700 -0.15953300
C (Fragment=1)  -0.11543800 -2.04321800  0.06644700
H (Fragment=1)  -2.75674900 -2.75057400  0.24738100
H (Fragment=1)  -4.66888400 -1.17666300  0.22175000
C (Fragment=1)   1.11676700 -1.44692700 -0.03871100
C (Fragment=1)  -1.31103400 -0.06016400 -0.15235600
C (Fragment=1)  -4.55886700  1.56410500  0.01013200
H (Fragment=1)  -5.22864100  1.35041000 -0.82731100
H (Fragment=1)  -5.14772800  1.48011700  0.92757400
H (Fragment=1)  -4.20292600  2.59094000 -0.08227300
N (Fragment=1)  -2.17976900  1.00833800  0.06099100
O (Fragment=1)   0.23810800  2.11389400  0.25738100
H (Fragment=1)  -1.16659800  2.46078000 -0.33885500
H (Fragment=1)  -1.99041300  2.00573800 -0.14550000
H (Fragment=1)   2.31217800  0.34029500 -0.23650100
N (Fragment=1)   2.33290800 -2.31745200 -0.03042500
O (Fragment=1)   3.41441300 -1.75643600 -0.09972400
O (Fragment=1)   2.15338100 -3.52041500  0.04618400
H (Fragment=1)  -0.20400200 -3.11750900  0.15072300
O (Fragment=2)   2.74709900  2.88383000 -0.42238300
H (Fragment=2)   3.13535400  3.23747300 -1.22976100
C (Fragment=2)   3.53265700  3.28647100  0.72274500
H (Fragment=2)   3.04821500  2.85669200  1.59834300
H (Fragment=2)   4.54912200  2.89485900  0.64658700
H (Fragment=2)   3.55280700  4.37431700  0.81968600
Proton-bound 2-methyl-6-Nitroquinolinol-8-ol and methanol (NH bound)

C  -2.2075400  1.58908400  -0.07370400
C  -0.26995100  0.18835800  -0.09804500
C   0.58475700  1.31126700   0.04444500
C  -0.02105200  2.59134400   0.12656700
C   -1.38455600  2.72586700   0.06893500
C   0.27460100  -1.11830700  -0.18590000
C   1.98385100  1.12397300   0.09828700
H   0.61155500  3.46518300   0.23580200
H   -1.85483100  3.69845500  -0.13051000
C   2.46810700  -0.15465400   0.00932600
C   1.64211400  -1.28141700  -0.13164300
C  -3.69611100   1.70398600  -0.14092000
H  -4.06449800   2.19757600   0.76301000
H  -3.97387700   2.33907600  -0.98717300
H  -4.18235100   0.73631100  -0.24580800
N  -1.63170800   0.38380200  -0.15017400
O  -0.61481700  -2.13186000  -0.31954900
H  -0.16639300  -2.98370600  -0.38718000
H  -2.25440900  -0.44679500  -0.25506400
H   2.09771400  -2.26220200  -0.19537400
N   3.94403000  -0.37382300   0.06436300
O   4.33313400  -1.52760800  -0.01787200
O   4.64630900   0.61435800   0.18073100
H   2.65906200   1.96191200   0.20629500
O  -3.63557700  -1.54613500  -0.34035900
H  -3.75576900  -2.05674400  -1.14815900
C  -3.90896400  -2.38673500   0.80010300
H  -3.81573700  -1.75585500   1.68350600
H  -4.92520700  -2.78416100   0.75481100
H  -3.18804900  -3.20553900   0.86677800
Proton-bound 2-methyl-6-Methoxyquinolin-8-ol and water (OH bound)

C(Fragment=1)  -3.14486300  0.23035500  0.00007300
C(Fragment=1)  -0.74960100  0.13134300  -0.00013200
C(Fragment=1)  -0.75411700  -1.28823900  -0.00002300
C(Fragment=1)  -2.02945300  -1.91678000  0.00006800
C(Fragment=1)  -3.18902200  -1.17892900  0.00009600
C(Fragment=1)   0.46483600   0.85207000  -0.00013200
C(Fragment=1)   0.46504500  -1.97958100   0.00003500
H(Fragment=1)  -2.07861500  -2.99986500  0.00009400
H(Fragment=1)  -4.15669100  -1.66318100  0.00013100
C(Fragment=1)   1.65847200  -1.26669700  -0.00013000
C(Fragment=1)   1.65795200   0.14950000  -0.00035900
H(Fragment=1)   0.49263500  -3.06102100  0.88248600
C(Fragment=1)  -4.37311500   1.08278300  0.00030400
H(Fragment=1)  -4.98313600   0.86176600  -0.87962200
H(Fragment=1)  -4.98087500   0.86447400  0.88248600
H(Fragment=1)  -4.13731300   2.14804700  -0.00162500
N(Fragment=1)  -1.94287500   0.81144200  -0.00005500
O(Fragment=1)   0.34947300   2.19467200  -0.00057200
H(Fragment=1)   1.21738700   2.64851600  0.00002200
H(Fragment=1)   2.58210900   0.71239400  -0.00058400
H(Fragment=1)  -1.87261100   1.82663000  -0.00012600
O(Fragment=1)   2.78350900  -2.00065000  -0.00011700
C(Fragment=1)   4.06499500  -1.35908100  0.00038600
H(Fragment=1)   4.19796700  -0.74847400  0.89826500
H(Fragment=1)   4.79172300  -2.16767700  0.00111800
H(Fragment=1)   4.19897400  -0.74917200  -0.89782400
O(Fragment=2)   2.82048200   3.33937000  0.00042000
H(Fragment=2)   3.15799200   3.81036300  0.77092600
H(Fragment=2)   3.15714200   3.81080500  -0.77019100
**Proton-bound 2-methyl-6-Methoxyquinolin-8-ol and water (NH bound)**

| Atoms (Fragment=1) | X1  | Y1  | Z1  | X2  | Y2  | Z2  |
|--------------------|-----|-----|-----|-----|-----|-----|
| C                  | 2.53836200 | -0.92767200 | -0.02284700 |
| C                  | 0.32996900  | -0.01023200  | 0.00897400   |
| C                  | -0.25591400 | -1.30658600  | 0.00788200   |
| C                  | 0.63628500  | -2.41351200  | 0.00897400   |
| C                  | 1.99533900  | -2.22932800  | -0.00966700  |
| C                  | -0.50518300 | 1.12803100   | -0.02584700  |
| C                  | -1.65079200 | -1.44835400  | 0.01872600   |
| H                  | 0.22377700  | -3.41616100  | 0.02056300   |
| C                  | 0.32996900  | -0.01023200  | 0.00897400   |
| C                  | -0.25591400 | -1.30658600  | 0.00788200   |
| C                  | 0.63628500  | -2.41351200  | 0.00897400   |
| C                  | 1.99533900  | -2.22932800  | -0.00966700  |
| C                  | -0.50518300 | 1.12803100   | -0.02584700  |
| C                  | -1.65079200 | -1.44835400  | 0.01872600   |
| H                  | 0.22377700  | -3.41616100  | 0.02056300   |

![Diagram of the molecule](image-url)
Proton-bound 2-methyl-6-Methoxyquinolin-8-ol and methanol (OH bound)

\[
\begin{array}{cccc}
\text{C(Fragment=1)} & 3.27228900 & -0.79309600 & 0.01789700 \\
\text{C(Fragment=1)} & 0.97731400 & -0.10441200 & -0.05390600 \\
\text{C(Fragment=1)} & 1.32706700 & 1.26494500 & 0.07962900 \\
\text{C(Fragment=1)} & 2.71489500 & 1.55567400 & 0.18276100 \\
\text{C(Fragment=1)} & 3.65807700 & 0.55632000 & 0.15281300 \\
\text{C(Fragment=1)} & -0.37384400 & -0.50186900 & -0.16411900 \\
\text{C(Fragment=1)} & 0.31452500 & 2.23380600 & 0.10149900 \\
\text{H(Fragment=1)} & 3.02642300 & 2.58907800 & 0.28647300 \\
\text{H(Fragment=1)} & 4.71294100 & 0.78428900 & 0.23146000 \\
\text{C(Fragment=1)} & 0.97731400 & -0.10441200 & -0.05390600 \\
\text{C(Fragment=1)} & 1.32706700 & 1.26494500 & 0.07962900 \\
\text{C(Fragment=1)} & 2.71489500 & 1.55567400 & 0.18276100 \\
\text{C(Fragment=1)} & 3.65807700 & 0.55632000 & 0.15281300 \\
\text{C(Fragment=1)} & -0.37384400 & -0.50186900 & -0.16411900 \\
\text{C(Fragment=1)} & 0.31452500 & 2.23380600 & 0.10149900 \\
\text{H(Fragment=1)} & 3.02642300 & 2.58907800 & 0.28647300 \\
\text{H(Fragment=1)} & 4.71294100 & 0.78428900 & 0.23146000 \\
\end{array}
\]

\[
\begin{array}{cccc}
\text{N(Fragment=1)} & 1.96692200 & -1.05613900 & -0.07749800 \\
\text{O(Fragment=1)} & -0.58563000 & -1.82551500 & -0.28398600 \\
\text{H(Fragment=1)} & 1.65010000 & -2.01818900 & -0.17681800 \\
\text{O(Fragment=1)} & -1.92570900 & 2.82661100 & 0.01908600 \\
\text{C(Fragment=1)} & -3.32142400 & 2.52316300 & -0.09290600 \\
\text{H(Fragment=1)} & -3.65424200 & 1.89307200 & 0.73723500 \\
\text{H(Fragment=1)} & -3.38966400 & 0.56261000 & -0.22964700 \\
\text{O(Fragment=2)} & -3.20992800 & -2.29769400 & -0.41999400 \\
\text{H(Fragment=2)} & -3.60912200 & -2.63395800 & -1.22962000 \\
\text{C(Fragment=2)} & -3.90465500 & -2.83668200 & 0.72631300 \\
\text{H(Fragment=2)} & -3.84139900 & -2.42850000 & 1.60749300 \\
\text{H(Fragment=2)} & -4.95161300 & -2.52497500 & 0.72403100 \\
\end{array}
\]

\[
\begin{array}{cccc}
\text{H(Fragment=2)} & -3.83903900 & -3.92723100 & 0.75021500 \\
\end{array}
\]
Proton-bound 2-methyl-6-Methoxyquinolinol-8-ol and methanol (NH bound)

C  2.02255400 -1.49722800 -0.08359100
C  0.00401200 -0.21847800 -0.05849500
C -0.79176200 -1.39299000  0.04747200
C -0.10032000 -2.63487300  0.08238800
C  1.26816000 -2.68579600  0.01245400
C -0.62813100  1.04269900 -0.12156500
C -2.18929200 -1.29415400  0.10496800
H  -0.67560100 -3.55067400  0.15967800
H  1.79318900 -3.63165000  0.03017500
C  -2.79659200 -0.04791500  0.05347900
C  -2.00487900  1.12251900 -0.06407200
H  -2.80472000 -2.18029700  0.18668400
C  3.51843300 -1.49463500 -0.13199900
H  3.92204800 -1.54304900  0.88509700
H  3.87923600 -2.37275100 -0.66880500
H  3.90253700 -0.59672300 -0.61519700
N  1.37380200 -0.33182400 -0.10921000
O  0.18646800  2.12818700 -0.24487900
H  -0.32902100  2.94295200 -0.25567500
H  -2.47390600  2.09685300 -0.11511900
H  1.94847500  0.53312600 -0.15766100
O  -4.13772100 -0.03312100  0.11555200
C  -4.85122400  1.20894800  0.06685500
H  -4.67149600  1.72832300 -0.87923100
H  -5.90233300  0.94046000  0.13680900
H  -4.58298500  1.84936600  0.91245600
O  3.17858900  1.78239700 -0.30241900
H  2.74777700  2.56378100 -0.66380800
C  4.25190700  2.18130900  0.57111900
H  4.70821500  1.26677500  0.94828400
H  5.00663000  2.75238300  0.02505800
H  3.87944500  2.76775600  1.41562900
XYZ Coordinates of 7-substituted Ion-Solvent Clusters

Proton-bound 7-Bromo-2-methylquinolin-8-ol and water (OH bound)

| Atom (Fragment=1) | X       | Y       | Z       |
|-------------------|---------|---------|---------|
| C                 | -3.44643100 | -0.76459600 | -0.00023000 |
| C                 | -1.19215500 | 0.06190900  | -0.00008100 |
| C                 | -1.64327600 | 1.40340100  | 0.00067200  |
| C                 | -3.04185300 | 1.61569200  | 0.00099000  |
| C                 | -3.92427800 | 0.55738500  | 0.00055900  |
| C                 | 0.18252200  | -0.28432000 | -0.00044200 |
| C                 | -0.67716300 | 2.43612100  | 0.00110700  |
| H                 | -3.41765700 | 2.63291900  | 0.00157800  |
| C                 | -4.99366100 | 0.72130900  | 0.00081600  |
| C                 | 0.65753900  | 2.11364300  | 0.00073900  |
| C                 | 1.09108300  | 0.76707900  | -0.00062000 |
| H                 | -0.99492800 | 3.47091700  | 0.00167400  |
| H                 | 1.40639400  | 2.89501200  | 0.00100500  |
| C                 | -4.34981600 | -1.95547400 | -0.00097600 |
| H                 | -4.99799100 | -1.93234400 | 0.87905800  |
| H                 | -4.99535300 | -1.93315900 | -0.88299700 |
| H                 | -3.79667300 | -2.89562500 | 0.00025900  |
| O                 | 0.42383300  | -1.60029300 | -0.00134700 |
| H                 | 1.36795200  | -1.89375100 | -0.00162000 |
| Br                | 2.95894700  | 0.42554700  | -0.00079700 |
| N                 | -2.12168900 | -0.95121800 | -0.00050600 |
| H                 | -1.74111500 | -1.89542800 | 0.00107700  |
| O                 | 2.72188200  | -2.96055100 | 0.00245100  |
| H                 | 2.70069700  | -3.92308400 | 0.00490000  |
| H                 | 3.64825600  | -2.70060600 | 0.00388300  |
Proton-bound 7-Bromo-2-methylquinolin-8-ol and water (NH bound)

C(Fragment=1)  3.17866100 -0.15176800  0.00022400
C(Fragment=1)  0.79109300 -0.33524900  0.00009300
C(Fragment=1)  0.86500100 -1.75164700  0.00015200
C(Fragment=1)  2.15386200 -2.33710100  0.00024900
C(Fragment=1)  3.28392900 -1.55626700  0.00026400
C(Fragment=1) -0.45900900  0.32519300 -0.00006900
C(Fragment=1) -0.33234400 -2.50441800  0.00010600
H(Fragment=1)  2.23876200 -3.41817300  0.00029800
H(Fragment=1)  4.27105100 -1.99923700  0.00031300
C(Fragment=1) -1.54659200 -1.86263500 -0.00008800
C(Fragment=1) -1.60725600 -0.45431500 -0.00010300
H(Fragment=1) -0.28228800 -3.58593500  0.00015800
H(Fragment=1) -2.46956600 -2.42752300 -0.00004100
C(Fragment=1)  4.38841400  0.72700400  0.00020500
H(Fragment=1)  4.99981000  0.50570900  0.87964300
H(Fragment=1)  4.99974100  0.50570200 -0.87928200
H(Fragment=1)  4.13433200  1.78490800  0.00016500
O(Fragment=1) -0.43138600  1.67447900 -0.00019900
H(Fragment=1) -1.33464800  2.02762900 -0.00020500
Br(Fragment=1) -3.29706000  0.42112100 -0.00030300
N(Fragment=1)  1.95859600  0.39856400  0.00016900
H(Fragment=1)  1.88788000  1.43006900 -0.00029000
O(Fragment=2)  2.28356600  3.25794100  0.00024200
H(Fragment=2)  2.06333700  3.79750900 -0.76738800
H(Fragment=2)  2.06654200  3.79800800  0.76843200
Proton-bound 7-Bromo-2-methylquinolin-8-ol and methanol (OH bound)

| Element | X  | Y  | Z  | E   |
|---------|----|----|----|-----|
| C       | 3.46102700 | 1.09567700 | 0.00004300 | 0.00004300 |
| C       | 1.37622700 | -0.09544200 | 0.00002800 | 0.00002800 |
| C       | 2.04499600 | -1.34278000 | -0.00020400 | -0.00020400 |
| C       | 3.45928200 | -1.31862500 | -0.00032300 | -0.00032300 |
| H       | 3.99960000 | -2.25886200 | -0.00051600 | -0.00051600 |
| H       | 5.23459300 | -0.11111900 | -0.00031400 | -0.00031400 |
| C       | -0.10521200 | -2.42464800 | -0.00020800 | -0.00020800 |
| C       | -0.75752100 | -1.16921500 | 0.00005000 | 0.00005000 |
| H       | 1.74943000 | -3.48952900 | -0.00002800 | -0.00002800 |
| H       | -0.71371000 | -3.31968100 | -0.00028600 | -0.00028600 |
| C       | 4.15279500 | 2.42085000 | 0.00034700 | 0.00034700 |
| H       | 4.79317700 | 2.50714300 | 0.88216400 | 0.88216400 |
| H       | 4.79535800 | 2.50646600 | -0.87992500 | -0.87992500 |
| H       | 3.45013300 | 3.25519200 | -0.00082300 | -0.00082300 |
| O       | -0.49126500 | 1.27662600 | 0.00042100 | 0.00042100 |
| H       | -1.47802700 | 1.42407500 | 0.00010900 | 0.00010900 |
| Br      | -2.65683200 | -1.15259000 | 0.00019700 | 0.00019700 |
| N       | 2.12385700 | 1.05815500 | 0.00014300 | 0.00014300 |
| H       | 1.58910700 | 1.92449600 | 0.00031500 | 0.00031500 |
| O       | -2.93286300 | 2.19908200 | -0.00029200 | -0.00029200 |
| H       | -3.77965200 | 1.74356000 | -0.00053400 | -0.00053400 |
| C       | -3.12345900 | 3.62571700 | -0.00049400 | -0.00049400 |
| H       | -3.66066060 | 3.94862900 | 0.89487800 | 0.89487800 |
| H       | -2.13027700 | 4.07268600 | -0.00008400 | -0.00008400 |
| H       | -3.65981400 | 3.94848800 | -0.89639200 | -0.89639200 |
Proton-bound 7-Bromo-2-methylquinolin-8-ol and methanol (NH bound)

C(Fragment=1)  3.00723000 -0.73647000 -0.11613700
C(Fragment=1)  0.61760200 -0.63930900 -0.04566500
C(Fragment=1)  0.53052900 -2.04706300  0.10735800
C(Fragment=1)  1.74410100 -2.77550500  0.14393500
C(Fragment=1)  2.95455100 -2.13615800  0.03441800
C(Fragment=1) -0.55094400  0.15616800 -0.09277100
C(Fragment=1) -0.74293800 -2.65296800  0.21382000
H(Fragment=1)  1.70531300 -3.85301000  0.25972900
H(Fragment=1)  3.88469000 -2.68826800  0.06085700
C(Fragment=1) -1.87700000 -1.87984000  0.16809000
C(Fragment=1) -1.77839800 -0.48216100  0.01534900
H(Fragment=1) -0.81440200 -3.72696300  0.33068300
H(Fragment=1) -2.85711000 -2.33141800  0.24813700
C(Fragment=1)  4.30674700 -0.00548000 -0.23462100
H(Fragment=1)  4.90288800 -0.17257600  0.66724900
H(Fragment=1)  4.87781100 -0.40843800 -1.07550800
H(Fragment=1)  4.16786900  1.06444500 -0.37719300
O(Fragment=1) -0.37884700  1.48765200 -0.24123000
H(Fragment=1) -1.24153000  1.93023300 -0.26982800
Br(Fragment=1) -3.35931900  0.57675100 -0.04767500
N(Fragment=1)  1.85934300 -0.50483000 -0.14980900
H(Fragment=1)  1.91473100  0.98374000 -0.26028700
O(Fragment=2)  2.44404100  2.67640700 -0.37404100
H(Fragment=2)  2.15017500  3.15627100 -1.15568400
C(Fragment=2)  2.24435200  3.50136100  0.79178300
H(Fragment=2)  1.18137300  3.69313600  0.95994900
H(Fragment=2)  2.64591300  2.94706400  1.63960400
H(Fragment=2)  2.78649400  4.44498100  0.69840300
Proton-bound 7-Chloro-2-methylquinolin-8-ol and water (OH bound)

C(Fragment=1)  2.90185400  0.88526500  0.00027200
C(Fragment=1)  0.70113600  -0.07403600  0.00012100
C(Fragment=1)  1.23114800  -1.38694000  -0.00054300
C(Fragment=1)  2.63981000  -1.51511000  -0.00082200
C(Fragment=1)  3.45747500  -0.40549000  -0.00045100
Cl(Fragment=1) -0.69034900  0.18850900  0.00039600
C(Fragment=1)  0.32868700  -2.47604000  -0.00095500
H(Fragment=1)  3.07588100  -2.50800600  -0.00138300
H(Fragment=1)  4.53471800  -0.50583600  -0.00070900
C(Fragment=1)  -1.02285600  -2.34260000  -0.00066100
C(Fragment=1)  -1.53266600  -0.51641000  0.00003300
H(Fragment=1)  0.70831600  -3.48969800  -0.00148100
C(Fragment=1)  3.73292000  -2.12762100  0.00140600
H(Fragment=1)  4.37551200  2.14527900  0.88571900
H(Fragment=1)  4.38451200  2.14113600  -0.87627700
H(Fragment=1)  3.89511900  3.03337800  -0.00037430
N(Fragment=1)  1.56826800  0.99294900  0.00048600
O(Fragment=1)  -1.02196800  1.48428700  0.00112000
H(Fragment=1)  -1.98702100  1.70377200  0.00032000
H(Fragment=1)  1.13290800  1.91317200  0.00094000
Cl(Fragment=1) -1.72902300  -3.05460200  -0.00093300
Cl(Fragment=2) -3.25777200  -0.69215700  0.00054200
O(Fragment=2)  -3.45333100  2.58256300  -0.00164900
H(Fragment=2)  -4.33920700  2.20686200  -0.00216100
H(Fragment=2)  -3.55442300  3.53999000  -0.00145000
Proton-bound 7-Chloro-2-methylquinolin-8-ol and water (NH bound)

| Atom          | X         | Y         | Z         |
|---------------|-----------|-----------|-----------|
| C (Fragment=1)| 2.62352700| 0.32011800| -0.01783000|
| C (Fragment=1)| 0.23061200| 0.27428900| -0.00276300|
| C (Fragment=1)| 0.17164000| 1.69328200| 0.003934000|
| C (Fragment=1)| 2.60076800| 1.72518800| -0.01159000|
| C (Fragment=1)| -0.95280800| -0.49829000| -0.00847700|
| C (Fragment=1)| -1.09143800| 2.33193000| 0.01854400|
| H (Fragment=1)| 1.38175200| 3.47988400| 0.01015200|
| C (Fragment=1)| 3.53981400| 2.26159900| -0.01907500|
| C (Fragment=1)| -2.23934600| 1.58040000| 0.01672400|
| C (Fragment=1)| -2.16668300| 0.17255600| 0.00239800|
| H (Fragment=1)| -1.14187200| 3.41338800| 0.02727800|
| C (Fragment=1)| 3.88837000| -0.47882300| -0.00790400|
| H (Fragment=1)| 4.73654100| 0.14206500| -0.29227800|
| H (Fragment=1)| 4.07359700| -0.86950200| 0.99793000|
| H (Fragment=1)| 3.82233900| -1.32747700| -0.69098700|
| N (Fragment=1)| 1.45950400| -0.34076400| -0.01239800|
| O (Fragment=1)| -0.81953100| 1.84510500| -0.02630700|
| H (Fragment=1)| -1.69455300| -2.26144900| -0.03044000|
| H (Fragment=1)| 1.50155100| -1.37395300| -0.00671100|
| H (Fragment=1)| -3.21429700| 2.05007600| 0.02475800|
| Cl (Fragment=1)| -3.63286700| -0.76898900| -0.00397500|
| O (Fragment=2)| 1.84235300| -3.12530200| 0.02603200|
| H (Fragment=2)| 2.55331400| -3.76454800| 0.13900100|
| H (Fragment=2)| 1.02087100| -3.62666300| -0.00945200|
Proton-bound 7-Chloro-2-methylquinolin-8-ol and methanol (OH bound)

C(Fragment=1)     2.87543500    1.38766200    0.00004400
C(Fragment=1)     0.99310600    -0.10245700    0.00025400
C(Fragment=1)     1.84120700    -1.23616300    -0.00088000
C(Fragment=1)     3.23572500    -0.99985000    -0.00156700
C(Fragment=1)     3.74276100    0.28156400    -0.00113600
C(Fragment=1)    -0.42054300    -0.20070600    0.00099400
C(Fragment=1)     1.24673300    -2.51939900    -0.00134700
H(Fragment=1)     3.91118400    -1.84824000    -0.00248200
H(Fragment=1)     4.80975300    0.46033500    -0.00170100
C(Fragment=1)    -0.12186200    -2.62924600    -0.00063900
C(Fragment=1)    -0.95225000    -1.48557300    0.00056600
H(Fragment=1)     1.87198500    -3.40293000    -0.00222600
C(Fragment=1)     3.36100200    2.80141700    0.00129500
H(Fragment=1)     3.97748100    2.98312900    0.88568700
H(Fragment=1)     3.98740500    2.98152600    -0.87632500
H(Fragment=1)     2.54147600    3.52129100    -0.00388600
N(Fragment=1)     1.55887200    1.15038100    0.00064900
O(Fragment=1)    -1.06868100    0.96667300    -0.00225500
H(Fragment=1)    -2.06736800    0.94180000    0.00056100
H(Fragment=1)     0.90094200    1.92731000    0.00142800
H(Fragment=1)    -0.59551400    -3.60255200    -0.00093000
Cl(Fragment=1)    -2.67648100    -1.71558400    0.00176900
O(Fragment=2)    -3.64249000    1.38993400    -0.00310800
H(Fragment=2)    -4.37359000    0.76529400    -0.00468200
C(Fragment=2)    -4.13155000    2.74414300    -0.00114100
H(Fragment=2)    -3.25583400    3.39160100    0.00024800
H(Fragment=2)    -4.72415400    2.94647600    -0.89678300
H(Fragment=2)    -4.72491500    2.94363400    0.89464100
Proton-bound 7-Chloro-2-methylquinolin-8-ol and methanol (NH bound)

C          -2.15978700  -1.26486300  -0.09668200
C           0.11523800  -0.53128000  -0.02577300
C           0.57829400  -1.87005900   0.07254800
C          -0.39477200  -2.89694700   0.07938200
C          -1.73513000  -2.60311800  -0.03975300
C           1.02878000   0.54682800  -0.06169400
C           1.96947900  -2.11678100   0.15089800
H           -0.06745500   3.92832700   0.15053900
H           -2.48076900  -3.38673500  -0.04623000
C           2.85422100  -1.06799900   0.12691200
C           2.38263600   0.25561300   0.01877100
H           -3.60361600  -0.87844200  -0.16315000
H           -4.18357900  -1.66293500  -0.64930300
H           -3.99791400  -0.75652800   0.85156300
H           -3.74183700   0.05963600  -0.70053300
N          -1.23794600  -0.29545900  -0.09634000
O            0.51727400   1.79427800  -0.17723700
H            1.23451900   2.44575200  -0.17430000
H          -1.57979800   0.68780300  -0.14408100
H           -3.92162800  -1.23633900   0.18599800
Cl          -3.51769500   1.57783400  -0.03120000
O           -2.45004300   2.18653800  -0.31991700
H           -1.83243100   2.83627900  -0.67144800
C           -3.41297900   2.84353000   0.52743500
H           -4.09135100   2.07263200   0.89141000
H           -2.92708500   3.32332300   1.38131500
H           -3.98778400   3.58096300  -0.03760300
Proton-bound 7-Cyano-2-methylquinolin-8-ol and water (OH bound)

| Atom  | x       | y       | z       | Charge | Coordinates |
|-------|---------|---------|---------|--------|-------------|
| C     | -2.81949100 | -0.89077100 | 0.00073300 |        |
| C     | -0.62605500 | 0.07903800 | 0.00026000 |        |
| C     | -1.15514000 | 1.38892200 | -0.00016900 |        |
| C     | -2.56804000 | 1.51303800 | -0.00000100 |        |
| C     | -3.37922500 | 0.40221800 | 0.00054400 |        |
| C     | 0.77055100  | -0.17905200 | 0.00045900 |        |
| C     | -0.25928300 | 2.48532300 | -0.00051700 |        |
| C     | 0.77055100  | -0.17905200 | 0.00045900 |        |
| C     | 1.09158900  | 2.25205200 | -0.00046100 |        |
| C     | 1.61986000  | 0.93097500 | 0.00004000 |        |
| C     | -0.64764500 | 3.49554400 | -0.00082800 |        |
| C     | 1.79007400  | 3.07928800 | -0.00076300 |        |
| C     | -3.64806900 | -2.13364200 | -0.00106600 |        |
| C     | -4.31105800 | -2.14049100 | 0.86819100  |        |
| C     | -4.27993500 | -2.15767800 | -0.89323700 |        |
| C     | -3.03959100 | -3.03864300 | 0.01820300  |        |
| O     | 1.04113000  | 1.46609000 | 0.00010620  |        |
| N     | 2.07837200  | -1.69828700 | 0.00037900  |        |
| N     | -1.48724100 | -0.99166200 | 0.00071600  |        |
| H     | -1.04637600 | -1.91009800 | 0.00105400  |        |
| C     | 3.03153300  | 0.73862700  | 0.00006400  |        |
| N     | 4.17082800  | 0.55159700  | -0.00003600 |        |
| O     | 3.58705700  | -2.30256000 | -0.00063100 |        |
| H     | 3.90504200  | -3.21061100 | -0.00014630 |        |
| H     | 4.35158800  | -1.71193700 | 0.00023000  |        |
Proton-bound 7-Cyano-2-methylquinolin-8-ol and water (NH bound)

| Fragment=1 | C(x)     | C(y)     | C(z)     |
|------------|----------|----------|----------|
|             | 2.51854300 | -0.26587800 | -0.02455700 |
|             | 0.12778800 | -0.27265700 | 0.00620200  |
|             | 0.09382700 | -1.69032800 | 0.01140000  |
|             | 1.33796300 | -2.36949400 | 0.00353700  |
|             | 2.52285200 | -1.67455700 | -0.01534300 |
|             | -1.07489100| 0.47218200 | -0.01174100 |
|             | -1.15434100| -2.35982400 | 0.02611000  |
|             | 1.34301000 | -3.45379600 | 0.01534000  |
|             | 3.47338700 | -2.19081900 | -0.02529300 |
|             | -2.31835100| -1.63657200 | 0.02372000  |
|             | -2.28508600| -0.21865000 | 0.00353700  |
|             | -1.17614700| -3.44205700 | 0.03828000  |
|             | -3.28069600| -2.13180700 | 0.03511300  |
|             | 3.77126800 | 0.55051400 | -0.01622200 |
|             | 4.02412300 | 0.82652400 | 1.01318100  |
|             | 4.60353600 | -0.02290300 | -0.4295700  |
|             | 3.65157800 | 1.46758200 | -0.59407700 |
|             | -0.96934800| 1.81700600 | -0.03710800 |
|             | -1.84407000| 2.23546000 | -0.04022400 |
|             | 1.34298300 | 0.36983200 | -0.01649100 |
|             | 1.36211200 | 1.40537800 | -0.00742500 |
|             | -3.47996200| 0.55956100 | -0.00414100 |
|             | -4.38998200| 1.27193800 | -0.01173600 |
|             | 1.66821400 | 3.15712500 | 0.04051300  |
|             | 2.37186600 | 3.79136400 | 0.21366800  |
|             | 0.85204600 | 3.66385900 | -0.02854700 |
Proton-bound 7-Cyano-2-methylquinolin-8-ol and methanol (OH bound)

| Atom (Fragment=1) | X (Å)  | Y (Å)  | Z (Å)  | E (kcal/mol) |
|-------------------|--------|--------|--------|--------------|
| C                  | -2.85462800 | -1.34214600 | 0.00017800 |
| C                  | -0.95610400  | 0.12308800  | 0.00007300  |
| C                  | -1.78233200  | 1.26896600  | -0.00005000 |
| C                  | -3.18389400  | 1.05219900  | -0.00002000 |
| C                  | -3.70669400  | -0.22020700 | 0.00011600  |
| C                  | 0.46309100   | 0.12308800  | 0.00012600  |
| C                  | -1.17350200  | 2.54718700  | -0.00015400 |
| H                  | -4.77619200  | -0.38448800 | 0.00017300  |
| C                  | 0.19414300   | 2.64129500  | -0.00013100 |
| C                  | 1.02226200   | 1.48429000  | 0.00001600  |
| H                  | -1.79095300  | 3.43604300  | -0.00024100 |
| H                  | 0.67564200   | 3.61105400  | -0.00020600 |
| C                  | -3.36243000  | -2.74708500 | -0.00023700 |
| H                  | -3.99137900  | -2.91593400 | 0.87799900  |
| H                  | -3.98339600  | -2.91809500 | -0.88379700 |
| H                  | -2.55498900  | -3.48035500 | 0.00425000  |
| O                  | 1.09283600   | -0.96542700 | 0.00031700  |
| H                  | 2.10748700   | -0.96416400 | 0.00006100  |
| N                  | -1.53699600  | -1.12170800 | 0.00018600  |
| H                  | -0.88778400  | -1.90695300 | 0.00027200  |
| C                  | 2.43865300   | 1.63681700  | 0.00006600  |
| N                  | 3.58950800   | 1.73072400  | 0.00009800  |
| O                  | 3.64791600   | -1.19173000 | -0.00043700 |
| H                  | 4.23780100   | -0.42742100 | -0.00010700 |
| C                  | 4.38020700   | -2.43090000 | 0.00004200  |
| H                  | 5.00044400   | -2.51279000 | 0.89563900  |
| H                  | 3.64383300   | -3.23331700 | 0.00032000  |
| H                  | 5.00049100   | -2.51341800 | -0.89546200 |
Proton-bound 7-Cyano-2-methylquinolin-8-ol and methanol (NH bound)

| Attrib   | x1   | y1   | z1   | x2   | y2   | z2   |
|----------|------|------|------|------|------|------|
| C(Fragment=1) | 2.20980500 | -1.08736300 | -0.10298700 |
| C(Fragment=1) | -0.11526000 | -0.53631600 | -0.05168100 |
| C(Fragment=1) | -0.47635900 | -1.89844400 | 0.09911100  |
| C(Fragment=1) | 0.57623900  | -2.84863600 | 0.14546600  |
| C(Fragment=1) | 1.88559400  | -2.45296400 | 0.04740100  |
| C(Fragment=1) | -1.11293200 | 0.46516900  | -0.10488800 |
| C(Fragment=1) | -1.84342400 | -2.25414600 | 0.19578000  |
| H(Fragment=1) | 0.33023000  | -3.89843000 | 0.26039200  |
| H(Fragment=1) | 2.69256600  | -3.17309000 | 0.08224600  |
| C(Fragment=1) | -2.80897500 | -1.28234000 | 0.14344900  |
| C(Fragment=1) | -2.44966000 | 0.08071200  | -0.00674600 |
| H(Fragment=1) | -2.11389900 | -3.29603200 | 0.31060700  |
| H(Fragment=1) | -3.85848900 | -1.53694200 | 0.21569200  |
| C(Fragment=1) | 3.62668800  | -0.62516300 | -0.21782000 |
| H(Fragment=1) | 4.19573300  | -0.97150600 | 0.64935800  |
| H(Fragment=1) | 4.08563600  | -1.07624900 | -1.10267100 |
| H(Fragment=1) | 3.70395400  | 0.45784700  | -0.29039700 |
| O(Fragment=1) | -0.69600200 | 1.73780200  | -0.24852300 |
| H(Fragment=1) | -1.44474400 | 2.35270600  | -0.28578100 |
| N(Fragment=1) | 1.21644300  | -0.19475100 | -0.14588900 |
| H(Fragment=1) | 1.47054500  | 0.81134400  | -0.25701300 |
| C(Fragment=1) | -3.43043000 | 1.11477700  | -0.06367300 |
| N(Fragment=1) | -4.15022000 | 2.01871200  | -0.11930900 |
| O(Fragment=2) | 2.30844700  | 2.35977300  | -0.36220000 |
| H(Fragment=2) | 2.21356200  | 2.86928800  | -1.17412700 |
| C(Fragment=2) | 2.22665900  | 3.25036600  | 0.77054500  |
| H(Fragment=2) | 1.24127700  | 3.71899300  | 0.83173600  |
| H(Fragment=2) | 2.38864000  | 2.64163400  | 1.65946200  |
| H(Fragment=2) | 3.00396000  | 4.01575200  | 0.71892400  |
Proton-bound 7-Fluoro-2-methylquinolin-8-ol and water (OH bound)

C(Fragment=1)  -2.63260700  -0.91354700  0.00036800
C(Fragment=1)  -0.43709500   0.05547400  -0.00183000
C(Fragment=1)  -0.97212100  1.36935600  0.00041400
C(Fragment=1)  -2.38151100  1.48897200  0.00105200
C(Fragment=1)  -3.19354000  0.37543200  0.00106000
C(Fragment=1)   0.95192900  -0.19621200 -0.00072400
C(Fragment=1)  -0.07810600  2.46607400  0.00041900
C(Fragment=1)  -2.82360900  2.47924400  0.00158500
H(Fragment=1)  -4.27120100  0.47032100  0.00159600
C(Fragment=1)  -1.27798500  2.23498100  0.00017500
C(Fragment=1)  -1.77015400  0.92195900  0.00079400
H(Fragment=1)  -0.46713000  3.47596400  0.00091200
H(Fragment=1)  -0.07810600  2.46607400  0.00041900
C(Fragment=1)  -3.45870400  2.15902600  0.00082900
H(Fragment=1)  -4.11319000  2.17295400  0.87467400
H(Fragment=1)  -4.09839300  2.18061400  0.88720500
H(Fragment=1)  -2.84770800  3.06259800  0.00055100
O(Fragment=1)  -3.37989800  1.47634900  0.00127600
H(Fragment=1)  -2.32234000  1.61054700  0.00027400
N(Fragment=1)  -1.29839200  1.01639300  0.00015200
H(Fragment=1)  -0.86111300  1.93574300  0.00055100
F(Fragment=1)   3.10127900  0.72859900  0.00152500
O(Fragment=2)   3.94362500  1.98246400  0.00028100
H(Fragment=2)   4.38427700  2.83815300  0.00403900
H(Fragment=2)   4.62703500  1.30452800  0.00045400
**Proton-bound 7-Fluoro-2-methylquinolin-8-ol and water (NH bound)**

| Fragment | X1      | Y1      | Z1     | X2      | Y2      | Z2     |
|----------|---------|---------|--------|---------|---------|--------|
| C        | 2.206189 | -0.674989 | 0.000070 |
| C        | -0.133852 | -0.170160 | -0.000010 |
| C        | -0.468770 | -1.551905 | 0.000043 |
| C        | 0.601322 | -2.478065 | 0.000100 |
| C        | 1.907284 | -2.059070 | 0.000099 |
| C        | -1.145061 | 0.810720 | -0.000106 |
| C        | -1.830028 | -1.938105 | 0.000017 |
| H        | 0.376230 | -3.538902 | 0.000133 |
| H        | 2.727221 | -2.756755 | 0.000122 |
| C        | -2.817044 | -0.980303 | -0.000060 |
| C        | -2.456091 | 0.371171 | -0.000125 |
| H        | -2.084213 | -2.990272 | 0.000055 |
| H        | -3.868918 | -1.236348 | -0.000082 |
| C        | 3.615460 | -0.175645 | 0.000107 |
| H        | 4.138810 | -0.560865 | 0.879817 |
| H        | 4.139145 | -0.561681 | -0.879039 |
| H        | 3.671875 | 0.910975 | -0.000387 |
| O        | -0.786487 | 2.114574 | -0.001980 |
| H        | -1.570695 | 2.680557 | -0.001880 |
| N        | 1.193679 | 0.201026 | 0.000037 |
| H        | 1.420396 | 1.210101 | 0.000092 |
| F        | -3.410525 | 1.319861 | -0.000218 |
| O        | 2.291726 | 2.851066 | 0.000130 |
| H        | 2.234388 | 3.430927 | -0.767632 |
| H        | 2.236363 | 3.430327 | 0.768490 |
Proton-bound 7-Fluoro-2-methylquinolin-8-ol and methanol (OH bound)

C(Fragment=1)  -2.68936300  -1.39313700  -0.00111100
C(Fragment=1)  -0.81411000  -0.10441400  -0.00026900
C(Fragment=1)  -1.66690700  -1.23820600  0.00012600
C(Fragment=1)  -3.06001600  0.99383700  -0.00031400
C(Fragment=1)  -3.56088500 -0.29020000  -0.00108100
C(Fragment=1)   0.59419800  -0.10441400  0.00016800
C(Fragment=1)  -1.66690700  -1.23820600  0.00012600
C(Fragment=1)  -3.06001600  0.99383700  -0.00031400
H(Fragment=1)  -4.62705600  -0.47358700  -0.00165400
C(Fragment=1)   0.28823400  2.64743500  0.00070100
C(Fragment=1)  -1.09911600  1.50347400  0.00016800
H(Fragment=1)  -3.16989600 -2.80844800  -0.00170500
H(Fragment=1)  -2.99771200  0.89951000  -0.00135000
H(Fragment=1)  -3.52562300 -0.02737000  -0.00089000
O(Fragment=1)   3.88843400 -0.77795400  -0.00023200
H(Fragment=2)  -4.20557600 -2.79265600  -0.00100000
H(Fragment=2)  -5.43478500 -1.87112700  -0.89528000
Proton-bound 7-Fluoro-2-methylquinolin-8-ol and methanol (NH bound)

C (Fragment=1)  -1.61866900  1.58109400  -0.09671400
C (Fragment=1)   0.40951000  0.31408900  -0.05795800
C (Fragment=1)  1.18619700  1.49492500   0.09863700
C (Fragment=1)  -0.87951800  2.76983000   0.05739300
C (Fragment=1)  1.03488300  -0.94734900  -0.12168700
C (Fragment=1)  2.59488200  1.39621700   0.19085100
H (Fragment=1)  1.05688600  3.64333900   0.27154000
H (Fragment=1)  0.49028500  2.72630000   0.15304100
H (Fragment=1)  0.87951800  2.76983000   0.05739300
H (Fragment=1)  1.03488300  2.76983000   0.05739300
C (Fragment=1)  3.20401100  0.16495500   0.12860300
C (Fragment=1)  2.41370000  -0.97886000  -0.02596100
H (Fragment=1)  3.18413000  2.29640200   0.19505200
H (Fragment=1)  4.27822900   0.04828400  -0.12168700
C (Fragment=1)  -3.11076600  1.58737100  -0.19886000
H (Fragment=1)  -3.53733300  2.00324100   0.71873000
H (Fragment=1)  -3.41914100  2.23989400  -1.02008100
H (Fragment=1)  -3.51809000  0.59121900  -0.36127500
O (Fragment=1)  0.26827600  -2.05302300  -0.27152400
H (Fragment=1)  0.82604400  -2.84218100  -0.30937300
N (Fragment=1)  -0.96129600  0.41672300  -0.14785300
H (Fragment=1)  -1.52238000  -0.45417400  -0.26198900
F (Fragment=1)   2.99519300  -2.19122400  -0.08925100
O (Fragment=2)  -2.79252500  -1.67276700  -0.38560200
H (Fragment=2)  -2.77415600  -2.22802300  -1.17238600
C (Fragment=2)  -3.03867800  -2.49752900   0.77199200
H (Fragment=2)  -2.21683900  -3.19934100   0.93593100
H (Fragment=2)  -3.11030600  -1.82450700   1.62590200
H (Fragment=2)  -3.98134700  -3.03956400   0.66958800
Proton-bound 2,7-Dimethylquinolin-8-ol and water (OH bound)

C(Fragment=1)  2.58891600  -1.00158400  -0.00087800  
C(Fragment=1)  0.45490500  0.10061800  -0.00196000  
C(Fragment=1)  1.07276600  1.37632300  0.00413200  
C(Fragment=1)  2.48610400  1.41069700  0.00761100  
C(Fragment=1)  3.22901300  0.24943700  0.00512700  
C(Fragment=1) -0.94848400  -0.05517100  -0.00610600  
C(Fragment=1)  0.23957900  2.51682500  0.00625000  
C(Fragment=1)  2.98725300  2.37247100  0.01225500  
C(Fragment=1)  4.31050000  0.27754000  0.00772000  
C(Fragment=1)  1.12571500  2.35243700  0.00184400  
C(Fragment=1) -1.75285000  1.08013400  -0.00479700  
H(Fragment=1)  0.68259600  3.50472600  0.01101600  
C(Fragment=1) -1.76365000  3.22864700  0.00303500  
C(Fragment=1)  3.33627300  -2.29674700  -0.00376900  
H(Fragment=1)  3.98328800  -2.35280800  -0.00376900  
H(Fragment=1)  3.97814900  -2.35971200  -0.00376900  
H(Fragment=1)  2.66917800  -3.15988000  -0.00376900  
O(Fragment=1) -1.36299200  -1.34129100  -0.00376900  
H(Fragment=1) -2.33322100  -1.49387100  -0.00376900  
N(Fragment=1)  1.25139400  -2.35971200  -0.00376900  
H(Fragment=1)  0.75616700  -1.91018200  -0.00376900  
C(Fragment=1) -3.25205500  -0.96356500  -0.00376900  
H(Fragment=1) -3.60587700  0.42007200  -0.00376900  
H(Fragment=1) -3.61438800  0.41691800  0.00376900  
H(Fragment=1) -3.71952900  1.94774200  -0.00376900  
O(Fragment=2) -3.93854800  -2.23307800  -0.00376900  
H(Fragment=2) -4.30595900  -2.67470100  0.00376900  
H(Fragment=2) -4.34263700  -2.65322200  -0.00376900
Proton-bound 2,7-Dimethylquinolinol-8-ol and water (NH bound)

C(Fragment=1)  2.24573200  -0.60844900  0.00013600
C(Fragment=1)  -0.11560800  -0.20233700  -0.00000500
C(Fragment=1)  -0.38795400  -1.59531100  -0.00005700
C(Fragment=1)   0.71857100  -2.47708000  -0.00009000
C(Fragment=1)   2.00557000  -1.99572500  0.00007900
C(Fragment=1)  -1.17171600   0.73327900  -0.00068000
C(Fragment=1)  -1.73330400  -2.02589600  -0.00151000
H(Fragment=1)   0.53712900  -3.54627400  -0.00046000
H(Fragment=1)   2.85491400  -2.66597000  0.00110000
C(Fragment=1)  -2.74504200  -1.09580500  -0.00194000
C(Fragment=1)  -2.49019700   0.29608200  -0.00157000
H(Fragment=1)  -1.95229100  -3.08635300  -0.00190000
H(Fragment=1)  -3.77667700  -1.42749300  -0.00263000
C(Fragment=1)   3.63399100  -0.05164700  0.00190000
H(Fragment=1)   4.17314400  -0.41521300  0.87951000
H(Fragment=1)   4.17298800  -0.41471900  -0.87943500
H(Fragment=1)   3.64573900  -1.03626800  0.00046300
O(Fragment=1)  -0.79906100   2.04291700  -0.00036000
H(Fragment=1)  -1.56679600   2.62545000  -0.00081000
N(Fragment=1)   1.19682100   0.22293500  -0.00105000
H(Fragment=1)   1.37876700  -1.23873300  -0.00214000
C(Fragment=1)  -3.61735200   1.29547000  -0.00220000
H(Fragment=1)  -3.58552000  -1.93829300  0.88698200
H(Fragment=1)  -3.58536300  -1.93835700  -0.88737000
H(Fragment=1)  -4.58503300   0.79502200  -0.00324000
O(Fragment=2)  -2.23778700   2.92876700  -0.00256200
H(Fragment=2)   2.17199200   3.50718700  -0.76758000
H(Fragment=2)   2.17330000   3.50720600  0.76820100
Proton-bound 2,7-Dimethylquinolin-8-ol and methanol (OH bound)

C (Fragment=1) -2.75244800 -1.33222700 0.02137200
C (Fragment=1) -0.84349400 0.12514500 0.01857700
C (Fragment=1) -1.67368600 1.27289700 -0.03656100
C (Fragment=1) -3.07906000 1.05992400 -0.06196000
C (Fragment=1) -3.60023200 -0.21288000 -0.03337900
C (Fragment=1) -0.56547400 0.21428200 -0.01857700
C (Fragment=1) -1.67368600 1.27289700 -0.03656100
H (Fragment=1) -3.73185200 1.91872300 -0.10455900
H (Fragment=1) -4.66984800 -0.37399700 -0.05236000
C (Fragment=1) 0.32189500 2.61605300 -0.02337400
C (Fragment=1) 1.15936700 1.47302500 0.04245800
H (Fragment=1) -1.65796900 3.43556300 -0.10786400
H (Fragment=1) 0.79784500 3.58976800 -0.03464500
C (Fragment=1) -3.26256500 -2.73726000 0.06487600
H (Fragment=1) -3.83068900 -2.89858100 0.98539200
H (Fragment=1) -3.94018600 -2.91686300 -0.77320200
H (Fragment=1) -2.45677100 -3.47149500 0.02387400
O (Fragment=1) 1.19970800 -0.97597400 0.12369800
H (Fragment=1) 2.16243300 -0.97674900 -0.10238000
N (Fragment=1) -1.43236800 -1.11763800 0.04317800
H (Fragment=1) -0.78763100 -1.90436200 0.08175500
C (Fragment=1) 2.65353200 1.62034600 0.12559100
H (Fragment=1) 3.03440100 1.16450600 1.04529700
H (Fragment=1) 3.15581300 1.12564800 -0.70918400
H (Fragment=1) 2.94326300 2.67066400 0.12764600
O (Fragment=2) 3.75677100 -1.33709800 -0.57248900
H (Fragment=2) 3.90271900 -1.89445700 -1.34371200
C (Fragment=2) 4.88307200 -1.43830400 0.32200000
H (Fragment=2) 5.79723800 -1.08924100 -0.16418500
H (Fragment=2) 4.66523700 -0.79470400 1.17290400
H (Fragment=2) 5.01512600 -2.46103000 0.67537400
Proton-bound 2,7-Dimethylquinolin-8-ol and methanol (NH bound)

C(Fragment=1)  -1.71270600  1.49913900  -0.10475900
C(Fragment=1)   0.39344900  0.36152600  -0.56872000
C(Fragment=1)   1.08813000  1.58923700  0.10077000
C(Fragment=1)   0.31822200  2.77511500  0.15106700
C(Fragment=1)  -1.05123300  2.73256100  0.04995600
C(Fragment=1)   1.10237600  0.36152600  -0.11703300
C(Fragment=1)  -1.64489000  3.63637500  0.08632700
C(Fragment=1)   3.16550600  1.36110000  0.13535400
C(Fragment=1)   2.48814900  0.84169000  -0.02181700
C(Fragment=1)   3.03718800  2.49892000  0.31672900
C(Fragment=1)   4.24657000  0.35280900  0.20867000
C(Fragment=1)   3.20289000  1.41155200  -0.20710400
C(Fragment=1)   3.65304900  1.75053200  0.73095700
C(Fragment=1)  -3.55765800  2.08209800  -0.99381100
C(Fragment=1)  -3.54379900  0.39957900  -0.41736700
C(Fragment=1)   0.34557600  1.98034100  -0.26948600
C(Fragment=1)   0.89940700  2.76687900  -0.31852200
C(Fragment=1)  -0.98199300  0.37959000  -0.15167500
C(Fragment=1)  -1.48459400  0.52265400  -0.26617100
C(Fragment=1)   3.24348600  2.16598600  -0.08618500
C(Fragment=1)   2.95287100  2.84128200  0.72679800
C(Fragment=1)   3.07299700  2.68476200  -1.03669100
C(Fragment=1)  -3.86240800  2.20343300  0.67050800
### Proton-bound 2-methyl-7-nitroquinolinol-8-ol and water (OH bound)

| Atom          | X         | Y         | Z         |
|---------------|-----------|-----------|-----------|
| C(Fragment=1) | -3.08775500 | 0.79718700 | 0.00001100 |
| C(Fragment=1) | -0.86512200 | -0.10311400 | 0.00002000 |
| C(Fragment=1) | -1.35199700 | -1.42630300 | -0.00008600 |
| C(Fragment=1) | -2.76133600 | -1.59678300 | -0.00014900 |
| C(Fragment=1) | -3.60704400 | -0.51340300 | -0.00010500 |
| C(Fragment=1) | 0.52751000  | 0.21528900  | 0.00008600  |
| C(Fragment=1) | -0.42056500 | -2.49250500 | -0.00013500 |
| H(Fragment=1) | -3.16748800 | -2.60219300 | -0.00023500 |
| H(Fragment=1) | -4.68136100 | -0.64298000 | -0.00015800 |
| C(Fragment=1) | 0.91975800  | -2.21140000 | -0.00006900 |
| C(Fragment=1) | 1.39457400  | -0.87974000 | 0.00005400  |
| C(Fragment=1) | -3.95463800 | 2.01339800  | 0.00015200  |
| H(Fragment=1) | -4.60295600 | 2.00794900  | -0.88032900 |
| H(Fragment=1) | -4.60191200 | 2.00845200  | 0.88141700  |
| H(Fragment=1) | -3.37463100 | 2.93706600  | -0.00044400 |
| N(Fragment=1) | -1.75976100 | 0.93886200  | 0.00006200  |
| O(Fragment=1) | 0.77328500  | 1.51708200  | 0.00017600  |
| H(Fragment=1) | 1.72021300  | 1.81683300  | 0.00008700  |
| H(Fragment=1) | -1.34573200 | 1.87021300  | 0.00013600  |
| H(Fragment=1) | -0.77249800 | -3.51582300 | -0.00022200 |
| H(Fragment=1) | 1.65742500  | -3.00260500 | -0.00010500 |
| N(Fragment=1) | 2.85480500  | -0.68746500 | 0.00014800  |
| O(Fragment=1) | 3.56457000  | -1.67354200 | -0.00016600 |
| O(Fragment=1) | 3.26128200  | 0.47362500  | 0.00050100  |
| O(Fragment=2) | 2.90359800  | 3.13247800  | -0.00046700 |
| H(Fragment=2) | 3.82637000  | 2.85622900  | -0.00035800 |
| H(Fragment=2) | 2.89508300  | 4.09419700  | -0.00075800 |
**Proton-bound 2-methyl-7-nitroquinolin-8-ol and water (NH bound)**

| Atom          | X    | Y    | Z    | Atom          | X    | Y    | Z    |
|---------------|------|------|------|---------------|------|------|------|
| C (Fragment=1) | 2.84633200 | -0.25767100 | -0.02657900 | C (Fragment=1) | 0.45809400 | -0.30622700 | 0.00445000 |
| C (Fragment=1) | 0.44505900 | -1.72016300 | 0.01149300  | C (Fragment=1) | 1.70074000 | -2.38165400 | 0.00681600 |
| C (Fragment=1) | 2.87267900 | -1.66793500 | -0.01599300 | C (Fragment=1) | -0.75366400 | 0.44113900  | -0.01426700 |
| C (Fragment=1) | -0.79467200 | -2.40741900 | 0.02730100  | H (Fragment=1) | 1.72235400 | -3.46569200 | 0.01700900  |
| H (Fragment=1) | 3.83182800 | -2.16839800 | -0.02589000 | C (Fragment=1) | -1.96589500 | -1.69883600 | 0.02478700  |
| C (Fragment=1) | -1.94443600 | -0.28820500 | 0.00286600  | C (Fragment=1) | 4.08775300 | 0.57500600  | -0.01896000 |
| H (Fragment=1) | 4.38528000 | 0.78147200  | 1.01513300  | H (Fragment=1) | 4.90715400 | 0.04062700  | -0.49514000 |
| H (Fragment=1) | 3.93354200 | 1.52729800  | -0.52629700 | N (Fragment=1) | 1.66099800 | 0.35706500  | -0.01854100 |
| O (Fragment=1) | -0.65635800 | 1.76945400  | -0.04213300 | H (Fragment=1) | -1.58364000 | 2.12128700  | -0.04500800 |
| H (Fragment=1) | 1.66112100 | 1.39422800  | -0.00861500 | H (Fragment=1) | -0.80424900 | -3.48958500 | 0.04068600  |
| H (Fragment=1) | -2.92748900 | -2.19414200 | 0.03721400  | N (Fragment=1) | -3.23108900 | 0.42176400  | -0.00396900 |
| O (Fragment=1) | -4.25273300 | -0.22535400 | 0.01353100  | O (Fragment=1) | -3.19539800 | 1.66634900  | -0.02757100 |
| O (Fragment=2) | 1.91657100 | 3.14590100  | 0.05334200  | H (Fragment=2) | 1.07095800 | 3.60424200  | -0.00212600 |
| H (Fragment=2) | 2.58595200 | 3.81785700  | 0.21954100  |
**Proton-bound 2-methyl-7-nitroquinolin-8-ol and methanol (OH bound)**

| Atom         | X       | Y       | Z       |
|--------------|---------|---------|---------|
| C(Fragment=1)| 3.13426900 | 1.20232700 | 0.05410400 |
| C(Fragment=1)| 1.12314900 | -0.10414400 | 0.04016100 |
| C(Fragment=1)| 1.84782700 | -1.30063400 | -0.15029400 |
| C(Fragment=1)| 3.26030000 | -1.19345700 | -0.23229100 |
| C(Fragment=1)| 3.88749900 | 0.02600500 | -0.13152500 |
| C(Fragment=1)| -0.29867900 | -0.06335600 | 0.15045200 |
| C(Fragment=1)| 1.13421300 | -2.51857100 | -0.25337600 |
| C(Fragment=1)| 3.84661700 | 0.10699500 | -0.19306200 |
| C(Fragment=1)| -0.23290200 | -2.50315000 | -0.15524900 |
| C(Fragment=1)| -0.93686500 | -1.29969400 | 0.06629000 |
| C(Fragment=1)| 3.75731900 | 2.55473600 | 0.17337400 |
| H(Fragment=1)| 4.96477000 | 0.10699500 | -0.19306200 |
| H(Fragment=1)| -0.23290200 | -2.50315000 | -0.15524900 |
| H(Fragment=1)| -0.93686500 | -1.29969400 | 0.06629000 |
| H(Fragment=1)| 3.75731900 | 2.55473600 | 0.17337400 |
| H(Fragment=1)| 4.43335200 | 2.57773300 | 1.03258600 |
| H(Fragment=1)| 4.35422500 | 2.77002600 | -0.71688200 |
| H(Fragment=1)| 3.01504100 | 3.34464900 | 0.29458500 |
| N(Fragment=1)| 1.80576900 | 1.08420500 | 0.12687000 |
| O(Fragment=1)| -0.80178400 | 1.15180500 | 0.30621500 |
| H(Fragment=1)| -1.79556100 | 1.28234800 | 0.19796600 |
| H(Fragment=1)| 1.22461700 | 1.91077600 | 0.25993600 |
| H(Fragment=1)| 1.66985840 | -3.44659000 | -0.40553000 |
| H(Fragment=1)| -0.81038600 | -3.41488200 | -0.23544900 |
| N(Fragment=1)| -2.39755700 | -1.40618400 | 0.22788300 |
| O(Fragment=1)| -2.96966600 | -2.28837900 | -0.38358000 |
| O(Fragment=1)| -2.92833900 | -0.60895100 | 0.99587500 |
| O(Fragment=2)| -3.24283800 | 1.78165500 | -0.18952700 |
| H(Fragment=2)| -3.67132000 | 3.09237800 | -0.60417200 |
| C(Fragment=2)| -2.81829700 | 3.56038700 | -1.09343700 |
| H(Fragment=2)| -4.49478000 | 3.01830700 | -1.31788700 |
| H(Fragment=2)| -3.97302800 | 3.69725000 | 0.25476600 |
Proton-bound 2-methyl-7-nitroquinolin-8-ol and methanol (NH bound)

C   2.47638100 -1.10968900 -0.11461200
C   0.14379700 -1.61029700 -0.03349000
C  -0.18954700 -1.97970900  0.07957700
C   0.88202600 -2.91078600  0.08994300
C   2.18230800 -2.48649600 -0.01174700
C  -0.86798100  0.39080600 -0.07670300
C  -1.55118600 -2.36333300  0.17013000
H   0.65736500 -3.96826700  0.17336500
H   3.00240100 -3.19238100 -0.01377900
C  -2.53116300 -1.40796700  0.14293800
C  -2.19184800 -0.04413000  0.01852700
C   3.87753000 -0.59459900 -0.19773400
H   4.30506100 -0.53517600  0.80919000
H   4.49707100 -1.28289700 -0.77408200
H   3.91726400  0.39474100 -0.65179200
N   3.93455700 -0.23884900 -0.11569600
O  -0.47243900  1.65567800 -0.20904600
H  -1.29274300  2.21178500 -0.21229500
H   1.70529900  0.77869300 -0.16934500
H  -1.80484800 -3.41172300  0.25916900
H  -3.57870300 -1.66896600  0.21098300
N  -3.28357600  0.93843300 -0.01493700
O  -4.42425000  0.54389100  0.06715100
O  -2.96852600  2.13801300 -0.12679100
O   2.42594900  2.33475900 -0.32295300
H   1.77743600  2.92371200 -0.72353100
C   3.22601100  3.07339700  0.62354600
H   3.94647600  2.37201500  1.04298100
H   3.76760300  3.87998700  0.12463000
H   2.60960700  3.47948000  1.42980700
Proton-bound 2-methyl-7-methoxyquinolin-8-ol and water (OH bound)

| Atoms | X      | Y      | Z      |
|-------|--------|--------|--------|
| C     | 3.02438600 | -0.70585500 | -0.00214200 |
| C     | 0.73843300  | 0.03552800  | -0.00045000  |
| C     | 1.14682500  | 1.39730300  | 0.00048300   |
| C     | 2.53261400  | 1.65801600  | -0.00308000  |
| C     | 3.45492100  | 0.63017000  | -0.00187400  |
| C     | -0.60942600 | -0.34889400 | -0.00695000  |
| C     | 0.14174300  | 2.38852200  | 0.00148800   |
| H     | 2.87293300  | 2.68780400  | -0.00088000  |
| C     | 4.51749600  | 0.83239100  | -0.00285000  |
| C     | -1.18505800 | 2.02231600  | 0.00155900   |
| C     | -1.57825500 | 0.66199900  | 0.00050800   |
| H     | 0.42139200  | 3.43437900  | 0.00214900   |
| H     | -1.94359300 | 2.79253900  | 0.00240400   |
| C     | 3.97083500  | -1.86377300 | 0.00284000   |
| H     | 4.65525400  | -1.79138600 | -0.84598200  |
| H     | 4.57586600  | -1.84616600 | 0.91348200   |
| H     | 3.45293500  | -2.82243000 | -0.04963000  |
| O     | -0.85311500 | -1.66912900 | -0.00218100  |
| H     | -1.80860700 | -1.91494900 | -0.00134800  |
| N     | 1.70730400  | -0.94489300 | -0.00180300  |
| H     | 1.36447000  | -1.90273200 | -0.00250000  |
| O     | -2.85656800 | 0.23384000  | 0.00058000   |
| C     | -3.92459900 | 1.19503100  | -0.00123000  |
| H     | -3.88769800 | 1.81657700  | -0.89940800  |
| H     | -4.84275300 | 0.61230500  | -0.00239200  |
| H     | -3.89028900 | 1.81696500  | 0.89700200   |
| O     | -3.30057800 | -2.75444500 | 0.00015300   |
| H     | -4.14830500 | -2.30132000 | 0.01089000   |
| H     | -3.48265700 | -3.69947700 | 0.00078200   |
Proton-bound 2-methyl-7-methoxyquinolin-8-ol and water (NH bound)

C  2.67694500  -0.41495700  0.01413200
C  0.28795000  -0.22480400  0.00222100
C  0.15054500  -1.64464400  -0.00551700
C  1.33215300  -2.41384100  -0.00128600
C  2.57428800  -1.81427200  0.01076400
C  -0.84381100  0.59849500  0.00647000
C  -1.14700800  -2.20435800  -0.01296600
H  1.25303300  -3.49551100  0.00501500
H  3.48025500  -2.40446100  0.01776200
C  -2.25661900  -1.39178700  -0.01144600
C  -2.11146200  0.01262300  -0.00108500
H  -1.25882500  -3.28133200  -0.01721100
H  -3.24495800  -1.83009000  -0.01721100
C  3.98503200  0.31190700  -0.00128000
H  4.79824600  -0.35422300  0.28289800
H  4.18881500  0.68966900  -1.00843200
H  3.96856300  1.16563800  0.67873300
O  -0.69092200  1.94940500  0.01936200
H  -1.57241600  2.35210800  0.02179500
N  1.55451100  0.31566000  0.00501500
H  1.65685900  1.34289700  0.00540200
O  -3.12125900  0.90732600  0.00338300
C  -4.48786300  0.45340500  -0.00076100
H  -4.69764600  -0.13814800  0.89350700
H  -5.09252500  1.35650900  0.00527400
H  -4.69646000  -0.12529200  -0.90367500
O  2.00376500  3.09229200  -0.01347600
H  2.68633800  3.76549300  -0.09684500
H  1.15557600  3.54845900  0.00755300
Proton-bound 2-methyl-7-methoxyquinolin-8-ol and methanol (OH bound)

C      3.06119000      -1.20852000      -0.00871500
C      1.02573900       0.06950600      -0.00247300
C      1.75500000      1.28999900      -0.00108100
C      3.16204000      1.20378900      -0.00561500
C      3.80523600      -0.01882000      -0.01067600
C      -0.37624300      0.02254900      -0.00224500
C      1.02239500      2.49661100      0.00182200
H      3.74402300      2.11899300      -0.00699000
C      4.88492200      -0.08206700      -0.01605700
C      -0.35345700      2.46378900      0.00330800
C      -1.06788500      1.24087700      0.00135500
H      1.54828100      3.44286900      0.00262100
H      -0.90096000      3.39588300      0.00579300
C      3.69103900      -2.56480100      0.01829600
H      4.54684300      -2.59893800      0.00578260
H      4.05845100      -2.78174400      0.01263880
H      2.98925300      -3.35093800      0.00666090
O      -0.92962200      -1.19832900      0.00132200
H      -1.92546000      -1.21904100      0.00308000
N      1.72536500      -1.11755900      0.00654000
H      1.15666800      -1.96129000      0.00752300
O      -2.41347700      1.14393100      0.00250300
C      -3.20834800      2.34066400      0.00705500
H      -3.02103200      2.93679300      0.00897000
H      -4.24292200      2.00509800      0.00761300
H      -3.01837100      2.93171800      0.90661000
O      -3.51930000      -1.59683200      0.00114900
H      -4.16376700      -0.88425600      0.00027100
C      -4.16660300      -2.88069800      0.00407900
H      -3.37480400      -3.62833200      0.00425000
H      -4.78148200      -3.01302100      0.89008600
H      -4.77833800      -3.00922600      0.90095700
Proton-bound 2-methyl-7-methoxyquinolin-8-ol and methanol (NH bound)

C  -2.18612500  -1.32157500  -0.00002500
C   0.06259900  -0.49934600  0.00002000
C   0.57498700  -1.83131500  -0.00001400
C  -0.35738600  -2.88850800  -0.00005300
C  -1.71483100  -2.64275200  -0.00005400
C   0.93540600   0.59555700  0.00006600
C   1.97491700  -2.02517900  0.00000500
H   0.00828800  -3.90956900  -0.00008500
H  -2.42995900  -3.45367300  -0.00008000
C   2.82783400   -0.94657200  0.00005700
C   2.31312600   0.36821100  0.00008400
H   2.36945100  -3.03352800  -0.00001500
H   3.89727200  -1.10548900  0.00008100
C  -3.64024000  -0.96527600  0.00003900
H  -4.25791800  -1.86148900  -0.00044800
H  -3.88685800  -0.36985500  0.88318600
H  -3.88675900  -0.36893300  -0.88250500
O   0.43077000   1.85793300  0.00008900
H   1.17451600   2.47922600  0.00009800
N  -1.30150800  -0.31658300  0.00000500
H  -1.68327800   0.64942100  0.00000700
O   3.04843200   1.49991000  0.00016100
C   4.48630300   1.42621500  -0.00022200
H   4.84366200   0.91786500  -0.89886600
H   4.82881600   2.45771100  -0.00033700
H   4.84414300   0.91791600   0.89825900
O  -2.46413300   2.19368000  0.00007300
H  -1.75526500   2.84501700  -0.0000900
C  -3.74683500   2.84223500  -0.00013100
H  -4.50104200   2.05620800  0.00005900
H  -3.87682300   3.45667600   0.89467500
H  -3.87677800   3.45621600  -0.89526100