# Supplementary information: Electrostatic properties of nine fluoroquinolone antibiotics derived directly from their crystal structures

Julian J. Holstein, Christian B. Hübschle and Birger Dittrich*

## Crystallization Conditions

| Structure | Solvent | Method |
|---|---|---|
| enoxacin 1.72 $H_2O$ | water | vapor diffusion with ethanol |
| lomefloxacin 2 $H_2O$ HCl | water | vapor diffusion with acetone |
| nadifloxacin 0.5 $H_2O$ | acetonitrile | slow evaporation |
| norfloxacin 2 $H_2O$ | water | slow evaporation |
| norfloxacin anhydrate | methanol | slow evaporation |
| ofloxacin anhydrate | acetonitrile | slow evaporation |

Table 1: Crystallization conditions of measured fluoroquinolone solvates.

# Refinement Details

For all datasets figures of merit (FOM) are given for three models.

- IAM refinement with SHELXL
- IAM refinement with XD
- invariom refinement with XD

The influence of the weighting scheme was also investigated. For the high-quality datasets of ciprofloxacin, enoxacin, nadifloxacin and ofloxacin anhydrate a weighting scheme of $w = 1/\sigma^2(F_o^2)$ gave the best weighted $R$-factor. A SHELXL-type weighting scheme was used for the other structures. Based on the values $a$ and $b$ (see equation 1) from IAM, refinement weight parameters were manually adjusted for invariom refinement with the program DRKPLOT, which is implemented in the program WINGX (for reference see experimental section of paper). Weighting parameters employed in the refinements are give in the tables below. Rather than having different $\Delta\rho_{min}$ and $\Delta\rho_{max}$ values, we report the range of the residual density features as $|\Delta\rho_{min}|+\Delta\rho_{max}$.

$$w = \frac{1}{\sigma^2(F_o^2) + (aP)2 + bP} \quad \text{with} \quad P = \frac{2F_c^2 + Max(F_o^2, 0)}{3} \tag{1}$$

| | | ciprofloxacin | | | | | |
|---|---|---|---|---|---|---|---|
| **Measurement** | Solvate | 6 $H_2O$ | | | HCl | | |
| | Space group | $P\bar{1}$ | | | $P(2)_1/c$ | | |
| | Temperature | 100 K | | | 100 K | | |
| | $\lambda$ [Å] | 0.71073 | | | 0.7660 | | |
| | Resolution [$\sin\Theta/\lambda$] | 1.16 | | | 0.78 | | |
| | Resolution [$d$] | 0.43 | | | 0.64 | | |
| | | $SHELX$ | $XD_{IAM}$ | $XD_{INV}$ | $SHELX$ | $XD_{IAM}$ | $XD_{INV}$ |
| **Refinement** | weighting a | 0.0580 | 0.0580 | — | 0.0564 | 0.0564 | 0.001 |
| | weighting b | 0.0743 | 0.0743 | — | 1.5709 | 1.5709 | 1.50 |
| | R(F) | 0.0313 | 0.0315 | 0.0205 | 0.0427 | 0.0420 | 0.0339 |
| | $R_{all}$(F) | 0.0391 | 0.0462 | 0.0352 | 0.0463 | 0.0473 | 0.0392 |
| | GoFw | 1.064 | 1.2705 | 2.5770 | 0.926 | 1.0076 | 0.9541 |
| | $\lvert\Delta\rho_{min}\rvert + \Delta\rho_{max}$ | 0.96 | 1.08 | 0.72 | 1.64 | 1.58 | 1.57 |

Table 2: Measurements and structure refinements of ciprofloxacin solvates 6 $H_2O$ and HCl

| | | enoxacin | | | | | |
|---|---|---|---|---|---|---|---|
| **Measurement** | Solvate | 1.7 $H_2O$ | | | 3 $H_2O$ | | |
| | Space group | $P2_1/c$ | | | $P(2)_1/c$ | | |
| | Temperature | 100 K | | | 100 K | | |
| | $\lambda$ [Å] | 0.71073 | | | 0.71073 | | |
| | Resolution [$\sin\Theta/\lambda$] | 1.02 | | | 0.65 | | |
| | Resolution [$d$] | 0.49 | | | 0.77 | | |
| | | $SHELX$ | $XD_{IAM}$ | $XD_{INV}$ | $SHELX$ | $XD_{IAM}$ | $XD_{INV}$ |
| **Refinement** | weighting a | 0.0594 | 0.0594 | — | 0.0526 | 0.0526 | 0.0400 |
| | weighting b | 0.4430 | 0.4430 | — | 0.3952 | 0.3952 | 0.0001 |
| | R(F) | 0.0414 | 0.0376 | 0.0276 | 0.0369 | 0.0346 | 0.0256 |
| | $R_{all}$(F) | 0.0704 | 0.0873 | 0.0782 | 0.0518 | 0.0589 | 0.0500 |
| | GoFw | 1.077 | 1.3574 | 2.8305 | 1.014 | 1.0740 | 1.0829 |
| | $\lvert\Delta\rho_{min}\rvert + \Delta\rho_{max}$ | 1.21 | 1.07 | 0.65 | 0.49 | 0.51 | 0.30 |

Table 3: Measurements and structure refinements of enoxacin solvates 1.7 $H_2O$ and 3 $H_2O$

| | | **norfloxacin** | | | | | |
|---|---|---|---|---|---|---|---|
| **Measurement** | Solvate | 2 $H_2O$ | | | — | | |
| | Space group | $P2_1/c$ | | | $P\bar{1}$ | | |
| | Temperature | 100 K | | | 100 K | | |
| | $\lambda$ [Å] | 0.71073 | | | 1.5418 | | |
| | Resolution [$\sin\Theta/\lambda$] | 0.77 | | | 0.60 | | |
| | Resolution [$d$] | 0.65 | | | 0.84 | | |
| | | $SHELX$ | $XD_{IAM}$ | $XD_{INV}$ | $SHELX$ | $XD_{IAM}$ | $XD_{INV}$ |
| **Refinement** | weighting a | 0.0767 | 0.0767 | 0.04 | 0.1322 | 0.1322 | 0.1322 |
| | weighting b | 0.8569 | 0.8569 | 0.03 | 2.6093 | 2.6093 | 2.6093 |
| | R(F) | 0.0486 | 0.0445 | 0.0337 | 0.0992 | 0.0953 | 0.0937 |
| | $R_{all}$(F) | 0.0957 | 0.1095 | 0.0998 | 0.1062 | 0.1166 | 0.1176 |
| | GoFw | 1.022 | 0.3972 | 0.9315 | 1.102 | 0.4654 | 0.4432 |
| | $\lvert\Delta\rho_{min}\rvert + \Delta\rho_{max}$ | 1.06 | 1.00 | 0.84 | 0.94 | 1.14 | 1.25 |

Table 4: Measurements and structure refinements of Norflocaxin 2 $H_2O$ and Norflocaxin anhydrate

| | | **fleroxacin** | | | **lomefloxacin** | | |
|---|---|---|---|---|---|---|---|
| **Measurement** | Solvate | **$H_2O$ HCl** | | | 2 **$H_2O$ HCl** | | |
| | Space group | $P2_1/c$ | | | $P2_1/c$ | | |
| | Temperature | 298K | | | 100 K | | |
| | $\lambda$ [Å] | 0.71073 | | | 0.80000 | | |
| | Resolution [$\sin\Theta/\lambda$] | 0.60 | | | 0.54 | | |
| | Resolution [$d$] | 0.84 | | | 0.92 | | |
| | | $SHELX$ | $XD_{IAM}$ | $XD_{INV}$ | $SHELX$ | $XD_{IAM}$ | $XD_{INV}$ |
| **Refinement** | weighting a | 0.0585 | 0.0585 | 0.04 | 0.1124 | — | — |
| | weighting b | 0.00 | 0.00 | 0.01 | 3.98 | — | — |
| | R(F) | 0.0380 | 0.0343 | 0.0280 | 0.0706 | 0.0694 | 0.0703 |
| | $R_{all}$(F) | 0.0669 | 0.0818 | 0.0756 | 0.0623 | 0.0722 | 0.0737 |
| | GoFw | 0.956 | 1.0105 | 0.9934 | 1.310 | 3.802 | 3.910 |
| | $\lvert\Delta\rho_{min}\rvert + \Delta\rho_{max}$ | 0.54 | 0.48 | 0.53 | 0.81 | 0.85 | 0.76 |

Table 5: Measurements and structure refinements of fleroxacin $H_2O$ HCl and lomefloxacin 4 $H_2O$ HCl

| | | **sparfloxacin** | | | **moxifloxacin** | | |
|---|---|---|---|---|---|---|---|
| **Measurement** | Solvate | 3 **$H_2O$** | | | **HCl** 0.5 **$H_2O$** 0.5 **$CH_3OH$** 0.5 $CH_3OH$ | | |
| | Space group | $P2_1/n$ | | | $P2_1$ | | |
| | Temperature | 298 K | | | 273 K | | |
| | $\lambda$ [Å] | 1.5418 | | | 0.7107 | | |
| | Resolution [$\sin\Theta/\lambda$] | 0.61 | | | 0.59 | | |
| | Resolution [$d$] | 0.82 | | | 0.84 | | |
| | | *SHELX* | $XD_{IAM}$ | $XD_{INV}$ | *SHELX* | $XD_{IAM}$ | $XD_{INV}$ |
| **Refinement** | weighting a | 0.0394 | 0.0394 | 0.001 | 0.0417 | 0.0417 | 0.03 |
| | weighting b | 1.1263 | 1.1263 | 0.40 | 0.00 | 0.00 | 0.00 |
| | R(F) | 0.0517 | 0.0537 | 0.0478 | 0.0472 | 0.0389 | 0.0375 |
| | $R_{all}$(F) | 0.0615 | 0.0617 | 0.0562 | 0.0815 | 0.0868 | 0.0872 |
| | GoFw | 1.045 | 1.0954 | 1.3203 | 0.863 | 0.9117 | 1.0154 |
| | $\lvert\Delta\rho_{min}\rvert + \Delta\rho_{max}$ | 0.50 | 0.54 | 0.48 | 0.47 | 0.45 | 0.44 |

Table 6: Measurements and structure refinements of sparfloxacin 3 $H_2O$ and moxifloxacin HCl 0.5 $H_2O$ 0.5 $CH_3OH$

| | | **nadifloxacin** | | | **ofloxacin** | | |
|---|---|---|---|---|---|---|---|
| **Measurement** | Solvate | 0.5 **$H_2O$** | | | — | | |
| | Space group | $P2_1/n$ | | | C2/c | | |
| | Temperature | 100 K | | | 100 K | | |
| | $\lambda$ [Å] | 1.5418 | | | 0.5608 | | |
| | Resolution [$\sin\Theta/\lambda$] | 0.62 | | | 0.78 | | |
| | Resolution [$d$] | 0.81 | | | 0.64 | | |
| | | *SHELX* | $XD_{IAM}$ | $XD_{INV}$ | *SHELX* | $XD_{IAM}$ | $XD_{INV}$ |
| **Refinement** | weighting a | 0.0818 | 0.0818 | 0.08 | 0.0722 | 0.0722 | — |
| | weighting b | 2.9411 | 2.9411 | 1.37 | 0.0722 | 3.3730 | — |
| | R(F) | 0.0572 | 0.0571 | 0.0536 | 0.0451 | 0.0458 | 0.0346 |
| | $R_{all}$(F) | 0.0658 | 0.0773 | 0.0747 | 0.0594 | 0.0810 | 0.0701 |
| | GoFw | 1.054 | 0.3517 | 0.4652 | 1.016 | 0.7823 | 2.7286 |
| | $\lvert\Delta\rho_{min}\rvert + \Delta\rho_{max}$ | 1.32 | 1.34 | 1.42 | 1.048 | 1.08 | 0.72 |

Table 7: Measurements and structure refinements of nadifloxacin 0.5 $H_2O$ and ofloxacin anhydrate

## Aspherical scattering factors

Invariom names of scattering factors employed in invariom refinements of twelve fluoroquinolone structures are given below together with corresponding model compounds. Fluoroquinolone structures are sorted alphabetically.

Table 8: Aspherical atomic scattering factors for ciprofloxacin 6 $H_2O$. Invariom names and corresponding model compounds from the invariom database are listed for all atoms.

| **Atom** | **Invariom Name** | **Model Compound** |
|---|---|---|
| F(15) | F@6c | 1-fluorobenzene |
| O(12) | O1.5c[1.5o@6c] | benzoic acid anion |
| O(13) | O1.5c[1.5o@6c] | benzoic acid anion |
| O(14) | O@6c | pyran-4-one ($\gamma$-pyrone) |
| O(2) | O1h1h | water |
| O(3) | O1h1h | water |
| O(4) | O1h1h | water |
| O(5) | O1h1h | water |
| O(6) | O1h1h | water |
| O(7) | O1h1h | water |
| N(1) | 6-N#66c[#66c#6c]#6c[#6c1h]@3c | 1-cyclopropylquinolin-4-one |
| N(20) | N@6c1c1c | *N,N*-dimethylbenzenamine |
| N(23) | N1c1c1h1h | dimethylammonium |
| C(16) | 3-C#3c[#3c1h1h]#3c[#3c1h1h]@6n1h | 1-cyclopropylpyridine-2-one |
| C(18) | 3-C#3c[#3c@6n1h]#3c[#3c1h1h]1h1h | 1-cyclopropylpyridine-2-one |
| C(17) | 3-C#3c[#3c@6n1h]#3c[#3c1h1h]1h1h | 1-cyclopropylpyridine-2-one |
| C(9) | 66-C#6n[#6c@3c]#66c[#6c#6c]#6c[#6c1h] | 1-cyclopropylquinolin-2-one |
| C(2) | 6-C#6n[#66c@3c]#6c[#6c1c]1h | 1-cyclopropyl-3-methylquinolin-4-one |
| C(3) | 6-C#6c[2o#66c]#6c[#6n1h]1c | 3-methylquinolin-4-one |
| C(11) | C1.5o1.5o@6c | benzoic acid anion |
| C(4) | 6-C2o#66c[#66c#6c]#6c[#6c1c] | 3-methyl-chromen-4-one |
| C(10) | 66-C#66c[#6n#6c]#6c[2o#6c]#6c[#6c1h] | quinolin-4-one |
| C(5) | 6-C#66c[#66c#6c]#6c[#6c1f]1h | 2-fluoronaphthalen |
| C(6) | 6-C#6c[#6c1n]#6c[#66c1h]1f | 3-fluoronaphthalen-2-amine |
| C(7) | 6-C#6c[#6c1f]#6c[#66c1h]1n | 3-fluoronaphthalen-2-amine |
| C(21) | C1n1c1h1h | ethylamine |
| C(22) | C1n1c1h1h | ethylamine |
| C(24) | C1n1c1h1h | ethylamine |
| C(25) | C1n1c1h1h | ethylamine |
| C(8) | 6-C#66c[#6n#66c]#6c[#6c1n]1h | 7-aminoquinolin-2-one |
| H(231) | H1n[1c1c1h] | dimethylammonium |
| H(232) | H1n[1c1c1h] | dimethylammonium |
| H(16) | H@3c | cyclopropane |
| H(181) | H@3c | cyclopropane |
| H(182) | H@3c | cyclopropane |
| H(171) | H@3c | cyclopropane |
| H(172) | H@3c | cyclopropane |
| H(2) | H@6c | benzene |
| H(5) | H@6c | benzene |
| H(211) | H1c[1n1c1h] | ethylamine |
| H(212) | H1c[1n1c1h] | ethylamine |
| H(221) | H1c[1n1c1h] | ethylamine |
| H(222) | H1c[1n1c1h] | ethylamine |
| H(241) | H1c[1n1c1h] | ethylamine |
| H(242) | H1c[1n1c1h] | ethylamine |
| H(251) | H1c[1n1c1h] | ethylamine |
| H(252) | H1c[1n1c1h] | ethylamine |

| Atom | Invariom Name | Model Compound |
|---|---|---|
| H(8) | H@6c | benzene |
| H(21) | H1o[1h] | water |
| H(22) | H1o[1h] | water |
| H(31) | H1o[1h] | water |
| H(32) | H1o[1h] | water |
| H(41) | H1o[1h] | water |
| H(42) | H1o[1h] | water |
| H(51) | H1o[1h] | water |
| H(52) | H1o[1h] | water |
| H(61) | H1o[1h] | water |
| H(62) | H1o[1h] | water |
| H(71) | H1o[1h] | water |
| H(72) | H1o[1h] | water |

Table 9: Aspherical atomic scattering factors for ciprofloxacin HCl 1.4 $H_2O$. Invariom names and corresponding model compounds from the invariom database are listed for all atoms.

| Atom | Invariom Name | Model Compound |
|---|---|---|
| Cl-(1) | Cl | chloride |
| F(15) | F@6c | 1-fluorobenzene |
| O(12) | O2c | formaldehyde |
| O(13) | O1c1h | methanol |
| O(14) | O@6c | pyran-4-one ($\gamma$-pyrone) |
| O(2) | O1h1h | water |
| O(31) | O1h1h | water |
| N(1) | 6-N#66c[#66c#6c]#6c[#6c1h]@3c | 1-cyclopropylquinolin-4-one |
| N(20) | N@6c1c1c | *N,N*-dimethylbenzenamine |
| N(23) | N1c1c1h1h | dimethylammonium |
| C(16) | 3-C#3c[#3c1h1h]#3c[#3c1h1h]@6n1h | 1-cyclopropylpyridine-2-one |
| C(18) | 3-C#3c[#3c@6n1h]#3c[#3c1h1h]1h1h | 1-cyclopropylpyridine-2-one |
| C(17) | 3-C#3c[#3c@6n1h]#3c[#3c1h1h]1h1h | 1-cyclopropylpyridine-2-one |
| C(9) | 66-C#6n[#6c@3c]#66c[#6c#6c]#6c[#6c1h] | 1-cyclopropylquinolin-2-one |
| C(2) | 6-C#6n[#66c@3c]#6c[#6c1c]1h | 1-cyclopropyl-3-methylquinolin-4-one |
| C(3) | 6-C#6c[2o#66c]#6c[#6n1h]1c | 3-methylquinolin-4-one |
| C(11) | C2o1o@6c | benzoic acid |
| C(4) | 6-C2o#66c[#66c#6c]#6c[#6c1c] | 3-methyl-chromen-4-one |
| C(10) | 66-C#66c[#6n#6c]#6c[2o#6c]#6c[#6c1h] | quinolin-4-one |
| C(5) | 6-C#66c[#66c#6c]#6c[#6c1f]1h | 2-fluoronaphthalen |
| C(6) | 6-C#6c[#6c1n]#6c[#66c1h]1f | 3-fluoronaphthalen-2-amine |
| C(7) | 6-C#6c[#6c1f]#6c[#66c1h]1n | 3-fluoronaphthalen-2-amine |
| C(21) | C1n1c1h1h | ethylamine |
| C(22) | C1n1c1h1h | ethylamine |
| C(24) | C1n1c1h1h | ethylamine |
| C(25) | C1n1c1h1h | ethylamine |
| C(8) | 6-C#66c[#6n#66c]#6c[#6c1n]1h | 7-aminoquinolin-2-one |
| H(13) | H1o[1c] | methanol |
| H(231) | H1n[1c1c1h] | dimethylammonium |

| Atom | Invariom Name | Model Compound |
|---|---|---|
| H(232) | H1n[1c1c1h] | dimethylammonium |
| H(16) | H@3c | cyclopropane |
| H(181) | H@3c | cyclopropane |
| H(182) | H@3c | cyclopropane |
| H(171) | H@3c | cyclopropane |
| H(172) | H@3c | cyclopropane |
| H(2) | H@6c | benzene |
| H(5) | H@6c | benzene |
| H(211) | H1c[1n1c1h] | ethylamine |
| H(212) | H1c[1n1c1h] | ethylamine |
| H(221) | H1c[1n1c1h] | ethylamine |
| H(222) | H1c[1n1c1h] | ethylamine |
| H(241) | H1c[1n1c1h] | ethylamine |
| H(242) | H1c[1n1c1h] | ethylamine |
| H(251) | H1c[1n1c1h] | ethylamine |
| H(252) | H1c[1n1c1h] | ethylamine |
| H(8) | H@6c | benzene |
| H(21) | H1o[1h] | water |
| H(22) | H1o[1h] | water |
| H(31) | H1o[1h] | water |
| H(32) | H1o[1h] | water |

Table 10: Aspherical atomic scattering factors for enoxacin 1.72 $H_2O$. Invariom names and corresponding model compounds from the invariom database are listed for all atoms.

| Atom | Invariom Name | Model Compound |
|---|---|---|
| F(15) | F@6c | 1-fluorobenzene |
| F(65) | F@6c | 1-fluorobenzene |
| O(12) | O1.5c[1.5o@6c] | benzoic acid anion |
| O(13) | O1.5c[1.5o@6c] | benzoic acid anion |
| O(14) | O@6c | pyran-4-one ($\gamma$-pyrone) |
| O(62) | O1.5c[1.5o@6c] | benzoic acid anion |
| O(63) | O1.5c[1.5o@6c] | benzoic acid anion |
| O(64) | O@6c | pyran-4-one ($\gamma$-pyrone) |
| O(1) | O1h1h | water |
| O(2) | O1h1h | water |
| O(3) | O1h1h | water |
| O(4) | O1h1h | water |
| O(5) | O1h1h | water |
| N(1) | 6-N#66c[#6n#66c]#6c[#6c1h]1c | 1-methyl-1,8-naphthyridin-4-one |
| N(8) | 6-N#66c[#6n#66c]#6c[#6c1n] | 1,8-naphthyridin-2-amine |
| N(20) | N@6c1c1c | *N,N*-dimethylbenzenamine |
| N(23) | N1c1c1h1h | dimethylammonium |
| N(51) | 6-N#66c[#6n#66c]#6c[#6c1h]1c | 1-methyl-1,8-naphthyridin-4-one |
| N(58) | 6-N#66c[#6n#66c]#6c[#6c1n] | 1,8-naphthyridin-2-amine |
| N(70) | N@6c1c1c | *N,N*-dimethylbenzenamine |
| N(73) | N1c1c1h1h | dimethylammonium |
| C(2) | 6-C#6n[#66c1c]#6c[#6c1c]1h | 1,3-dimethylquinolin-4-one |

| Atom | Invariom Name | Model Compound |
|---|---|---|
| C(3) | 6-C#6c[2o#66c]#6c[#6n1h]1c | 3-methylquinolin-4-one |
| C(4) | 6-C2o#66c[#66c#6c]#6c[#6c1c] | 3-methyl-chromen-4-one |
| C(5) | 6-C#66c[#66c#6c]#6c[#6c1f]1h | 2-fluoronaphthalen |
| C(6) | 6-C#6c[#6n1n]#6c[#66c1h]1f | 3-fluoroquinolin-2-amine |
| C(7) | 6-C#6n[#66c]#6c[#6c1f]1n | 3-fluoroquinolin-2-amine |
| C(9) | 66-C#6n[#6c1c]#6n[#6c]#66c[#6c#6c] | 1-methyl-1,8-naphthyridin-4-one |
| C(10) | 66-C#66c[#6n#6n]#6c[2o#6c]#6c[#6c1h] | 1,8-naphthyridin-4-one |
| C(11) | C1.5o1.5o@6c | benzoic acid anion |
| C(16) | C@6n1c1h1h | 1-ethylpylpyridine-2-one |
| C(17) | C1c1h1h1h | ethane |
| C(21) | C1n1c1h1h | ethylamine |
| C(22) | C1n1c1h1h | ethylamine |
| C(24) | C1n1c1h1h | ethylamine |
| C(25) | C1n1c1h1h | ethylamine |
| C(52) | 6-C#6n[#66c1c]#6c[#6c1c]1h | 1,3-dimethylquinolin-4-one |
| C(53) | 6-C#6c[2o#66c]#6c[#6n1h]1c | 3-methylquinolin-4-one |
| C(54) | 6-C2o#66c[#66c#6c]#6c[#6c1c] | 3-methyl-chromen-4-one |
| C(55) | 6-C#66c[#66c#6c]#6c[#6c1f]1h | 2-fluoronaphthalen |
| C(56) | 6-C#6c[#6n1n]#6c[#66c1h]1f | 3-fluoroquinolin-2-amine |
| C(57) | 6-C#6n[#66c]#6c[#6c1f]1n | 3-fluoroquinolin-2-amine |
| C(59) | 66-C#6n[#6c1c]#6n[#6c]#66c[#6c#6c] | 1-methyl-1,8-naphthyridin-4-one |
| C(60) | 66-C#66c[#6n#6n]#6c[2o#6c]#6c[#6c1h] | 1,8-naphthyridin-4-one |
| C(61) | C1.5o1.5o@6c | benzoic acid anion |
| C(66) | C@6n1c1h1h | 1-ethylpylpyridine-2-one |
| C(67) | C1c1h1h1h | ethane |
| C(71) | C1n1c1h1h | ethylamine |
| C(72) | C1n1c1h1h | ethylamine |
| C(74) | C1n1c1h1h | ethylamine |
| C(75) | C1n1c1h1h | ethylamine |
| H(2) | H@6c | benzene |
| H(5) | H@6c | benzene |
| H(161) | H1c[@6n1c1h] | 1-ethylpylpyridine-2-one |
| H(612) | H1c[@6n1c1h] | 1-ethylpylpyridine-2-one |
| H(171) | H1c[1c1h1h] | ethane |
| H(172) | H1c[1c1h1h] | ethane |
| H(173) | H1c[1c1h1h] | ethane |
| H(221) | H1c[1n1c1h] | ethylamine |
| H(222) | H1c[1n1c1h] | ethylamine |
| H(232) | H1n[1c1c1h] | dimethylammonium |
| H(231) | H1n[1c1c1h] | dimethylammonium |
| H(241) | H1c[1n1c1h] | ethylamine |
| H(242) | H1c[1n1c1h] | ethylamine |
| H(251) | H1c[1n1c1h] | ethylamine |
| H(252) | H1c[1n1c1h] | ethylamine |
| H(211) | H1c[1n1c1h] | ethylamine |
| H(212) | H1c[1n1c1h] | ethylamine |
| H(52) | H@6c | benzene |
| H(55) | H@6c | benzene |
| H(661) | H1c[@6n1c1h] | 1-ethylpylpyridine-2-one |
| H(662) | H1c[@6n1c1h] | 1-ethylpylpyridine-2-one |
| H(671) | H1c[1c1h1h] | ethane |

| Atom | Invariom Name | Model Compound |
|---|---|---|
| H(672) | H1c[1c1h1h] | ethane |
| H(673) | H1c[1c1h1h] | ethane |
| H(711) | H1c[1n1c1h] | ethylamine |
| H(712) | H1c[1n1c1h] | ethylamine |
| H(721) | H1c[1n1c1h] | ethylamine |
| H(722) | H1c[1n1c1h] | ethylamine |
| H(731) | H1n[1c1c1h] | dimethylammonium |
| H(732) | H1n[1c1c1h] | dimethylammonium |
| H(741) | H1c[1n1c1h] | ethylamine |
| H(742) | H1c[1n1c1h] | ethylamine |
| H(751) | H1c[1n1c1h] | ethylamine |
| H(752) | H1c[1n1c1h] | ethylamine |
| H(11) | H1o[1h] | water |
| H(12) | H1o[1h] | water |
| H(21) | H1o[1h] | water |
| H(22) | H1o[1h] | water |
| H(31) | H1o[1h] | water |
| H(32) | H1o[1h] | water |
| H(41) | H1o[1h] | water |
| H(42) | H1o[1h] | water |
| H(51) | H1o[1h] | water |
| H(53) | H1o[1h] | water |

Table 11: Aspherical atomic scattering factors for enoxacin 3 $H_2O$. Invariom names and corresponding model compounds from the invariom database are listed for all atoms.

| Atom | Invariom Name | Model Compound |
|---|---|---|
| F(15) | F@6c | 1-fluorobenzene |
| O(14) | O@6c | pyran-4-one ($\gamma$-pyrone) |
| O(12) | O1.5c[1.5o@6c] | benzoic acid anion |
| O(13) | O1.5c[1.5o@6c] | benzoic acid anion |
| O(4) | O1h1h | water |
| O(5) | O1h1h | water |
| O(6) | O1h1h | water |
| N(1) | 6-N#66c[#6n#66c]#6c[#6c1h]1c | 1-methyl-1,8-naphthyridin-4-one |
| N(8) | 6-N#66c[#6n#66c]#6c[#6c1n] | 1,8-naphthyridin-2-amine |
| N(20) | N@6c1c1c | *N,N*-dimethylbenzenamine |
| N(23) | N1c1c1h1h | dimethylammonium |
| C(2) | 6-C#6n[#66c1c]#6c[#6c1c]1h | 1,3-dimethylquinolin-4-one |
| C(3) | 6-C#6c[2o#66c]#6c[#6n1h]1c | 3-methylquinolin-4-one |
| C(4) | 6-C2o#66c[#66c#6c]#6c[#6c1c] | 3-methyl-chromen-4-one |
| C(10) | 66-C#66c[#6n#6n]#6c[2o#6c]#6c[#6c1h] | 1,8-naphthyridin-4-one |
| C(5) | 6-C#66c[#66c#6c]#6c[#6c1f]1h | 2-fluoronaphthalen |
| C(6) | 6-C#6c[#6n1n]#6c[#66c1h]1f | 3-fluoroquinolin-2-amine |
| C(7) | 6-C#6n[#66c]#6c[#6c1f]1n | 3-fluoroquinolin-2-amine |
| C(9) | 66-C#6n[#6c1c]#6n[#6c]#66c[#6c#6c] | 1-methyl-1,8-naphthyridin-4-one |
| C(16) | C@6n1c1h1h | 1-ethylpylpyridine-2-one |
| C(17) | C1c1h1h1h | ethane |

| Atom | Invariom Name | Model Compound |
|---|---|---|
| C(11) | C1.5o1.5o@6c | benzoic acid anion |
| C(25) | C1n1c1h1h | ethylamine |
| C(24) | C1n1c1h1h | ethylamine |
| C(22) | C1n1c1h1h | ethylamine |
| C(21) | C1n1c1h1h | ethylamine |
| H(23A) | H1n[1c1c1h] | dimethylammonium |
| H(23B) | H1n[1c1c1h] | dimethylammonium |
| H(2) | H@6c | benzene |
| H(5) | H@6c | benzene |
| H(16A) | H1c[@6n1c1h] | 1-ethylpylpyridine-2-one |
| H(16B) | H1c[@6n1c1h] | 1-ethylpylpyridine-2-one |
| H(17A) | H1c[1c1h1h] | ethane |
| H(17B) | H1c[1c1h1h] | ethane |
| H(17C) | H1c[1c1h1h] | ethane |
| H(25A) | H1c[1n1c1h] | ethylamine |
| H(25B) | H1c[1n1c1h] | ethylamine |
| H(24A) | H1c[1n1c1h] | ethylamine |
| H(24B) | H1c[1n1c1h] | ethylamine |
| H(22A) | H1c[1n1c1h] | ethylamine |
| H(22B) | H1c[1n1c1h] | ethylamine |
| H(21A) | H1c[1n1c1h] | ethylamine |
| H(21B) | H1c[1n1c1h] | ethylamine |
| H(041) | H1o[1h] | water |
| H(042) | H1o[1h] | water |
| H(051) | H1o[1h] | water |
| H(052) | H1o[1h] | water |
| H(061) | H1o[1h] | water |
| H(062) | H1o[1h] | water |

Table 12: Aspherical atomic scattering factors for fleroxacin $H_2O$ HCl. Invariom names and corresponding model compounds from the invariom database are listed for all atoms.

| Atom | Invariom Name | Model Compound |
|---|---|---|
| Cl-(1) | Cl | chloride |
| F(15) | F@6c | 1-fluorobenzene |
| F(8) | F@6c | 1-fluorobenzene |
| F(17) | F1c | fluoromethane |
| O(13) | O1c1h | methanol |
| O(12) | O2c | formaldehyde |
| O(14) | O@6c | pyran-4-one ($\gamma$-pyrone) |
| O(2) | O1h1h | water |
| N(1) | 6-N#66c[#66c#6c]#6c[#6c1h]1c | 1,3-dimethylquinolin-4-one |
| N(20) | N@6c1c1c | *N,N*-dimethylbenzenamine |
| N(23) | N1c1c1c1h | trimethylammonium |
| C(11) | C2o1o@6c | benzoic acid |
| C(3) | 6-C#6c[2o#66c]#6c[#6n1h]1c | 3-methylquinolin-4-one |
| C(4) | 6-C2o#66c[#66c#6c]#6c[#6c1c] | 3-methyl-chromen-4-one |
| C(10) | 66-C#66c[#6n#6c]#6c[2o#6c]#6c[#6c1h] | quinolin-4-one |
| C(9) | 66-C#6n[#6c1c]#66c[#6c#6c]#6c[#6c1f] | 8-fluoro-1-methylquinolin-2-one |

| Atom | Invariom Name | Model Compound |
|---|---|---|
| C(2) | 6-C#6n[#66c1c]#6c[#6c1c]1h | 1,3-dimethylquinolin-4-one |
| C(16) | C@6n1c1h1h | 1-ethylpylpyridine-2-one |
| C(17) | C1f1c1h1h | fluoroethane |
| C(8) | 6-C#66c[#6n#66c]#6c[#6c1n]1f | 7-amino-8-fluoroquinolin-2-one |
| C(7) | 6-C#6c[#66c1f]#6c[#6c1f]1n | 1,3-difluoronaphthalen-2-amine |
| C(6) | 6-C#6c[#6c1n]#6c[#66c1h]1f | 3-fluoronaphthalen-2-amine |
| C(5) | 6-C#66c[#66c#6c]#6c[#6c1f]1h | 2-fluoronaphthalen |
| C(25) | C1n1c1h1h | ethylamine |
| C(24) | C1n1c1h1h | ethylamine |
| C(19) | C1n1c1h1h | ethylamine |
| C(21) | C1n1c1h1h | ethylamine |
| C(26) | C1n1h1h1h | methylamine |
| H(13) | H1o[1c] | methanol |
| H(23) | H1n[1c1c1c] | trimethylammonium |
| H(2) | H@6c | benzene |
| H(161) | H1c[@6n1c1h] | 1-ethylpylpyridine-2-one |
| H(162) | H1c[@6n1c1h] | 1-ethylpylpyridine-2-one |
| H(171) | H1c[1f1c1h] | fluoroethane |
| H(172) | H1c[1f1c1h] | fluoroethane |
| H(5) | H@6c | benzene |
| H(251) | H1c[1n1c1h] | ethylamine |
| H(252) | H1c[1n1c1h] | ethylamine |
| H(241) | H1c[1n1c1h] | ethylamine |
| H(242) | H1c[1n1c1h] | ethylamine |
| H(191) | H1c[1n1c1h] | ethylamine |
| H(192) | H1c[1n1c1h] | ethylamine |
| H(211) | H1c[1n1c1h] | ethylamine |
| H(212) | H1c[1n1c1h] | ethylamine |
| H(261) | H1c[1n1h1h] | methylamine |
| H(262) | H1c[1n1h1h] | methylamine |
| H(263) | H1c[1n1h1h] | methylamine |
| H(21) | H1o[1h] | water |
| H(22) | H1o[1h] | water |

Table 13: Aspherical atomic scattering factors for lomefloxacin 4 $H_2O$ HCl. Invariom names and corresponding model compounds from the invariom database are listed for all atoms.

| Atom | Invariom Name | Model Compound |
|---|---|---|
| Cl-(1) | Cl | chloride |
| F(17) | F@6c | 1-fluorobenzene |
| F(18) | F@6c | 1-fluorobenzene |
| O(1) | O1h1h | water |
| O(2) | O1h1h | water |
| O(12) | O2c | formaldehyde |
| O(13) | O1c1h | methanol |
| O(14) | O@6c | pyran-4-one ($\gamma$-pyrone) |
| N(1) | 6-N#66c[#66c#6c]#6c[#6c1h]1c | 1,3-dimethylquinolin-4-one |
| N(20) | N@6c1c1c | *N,N*-dimethylbenzenamine |
| N(23A) | N1c1c1h1h | dimethylammonium |

| Atom | Invariom Name | Model Compound |
|---|---|---|
| N(23B) | N1c1c1h1h | dimethylammonium |
| C(2) | 6-C#6n[#66c1c]#6c[#6c1c]1h | 1,3-dimethylquinolin-4-one |
| C(3) | 6-C#6c[2o#66c]#6c[#6n1h]1c | 3-methylquinolin-4-one |
| C(5) | 6-C#66c[#66c#6c]#6c[#6c1f]1h | 2-fluoronaphthalen |
| C(4) | 6-C2o#66c[#66c#6c]#6c[#6c1c] | 3-methyl-chromen-4-one |
| C(6) | 6-C#6c[#6c1n]#6c[#66c1h]1f | 3-fluoronaphthalen-2-amine |
| C(7) | 6-C#6c[#66c1f]#6c[#6c1f]1n | 1,3-difluoronaphthalen-2-amine |
| C(9) | 66-C#6n[#6c1c]#66c[#6c#6c]#6c[#6c1f] | 8-fluoro-1-methylquinolin-2-one |
| C(8) | 6-C#66c[#6n#66c]#6c[#6c1n]1f | 7-amino-8-fluoroquinolin-2-one |
| C(10) | 66-C#66c[#6n#6c]#6c[2o#6c]#6c[#6c1h] | quinolin-4-one |
| C(11) | C2o1o@6c | benzoic acid |
| C(15) | C@6n1c1h1h | 1-ethylpylpyridine-2-one |
| C(16) | C1c1h1h1h | ethane |
| C(21A) | C1n1c1h1h | ethylamine |
| C(22A) | C1n1c1c1h | 2-aminopropane |
| C(24A) | C1n1c1h1h | ethylamine |
| C(25A) | C1n1c1h1h | ethylamine |
| C(26A) | C1c1h1h1h | ethane |
| C(21B) | C1n1c1h1h | ethylamine |
| C(22B) | C1n1c1c1h | 2-aminopropane |
| C(24B) | C1n1c1h1h | ethylamine |
| C(25B) | C1n1c1h1h | ethylamine |
| C(26B) | C1c1h1h1h | ethane |
| H(1A) | H1o[1h] | water |
| H(1B) | H1o[1h] | water |
| H(2A) | H1o[1h] | water |
| H(2B) | H1o[1h] | water |
| H(2) | H@6c | benzene |
| H(5) | H@6c | benzene |
| H(13) | H1o[1c] | methanol |
| H(15A) | H1c[@6n1c1h] | 1-ethylpylpyridine-2-one |
| H(15B) | H1c[@6n1c1h] | 1-ethylpylpyridine-2-one |
| H(16A) | H1c[1c1h1h] | ethane |
| H(16B) | H1c[1c1h1h] | ethane |
| H(16C) | H1c[1c1h1h] | ethane |
| H(23A) | H1n[1c1c1h] | dimethylammonium |
| H(23B) | H1n[1c1c1h] | dimethylammonium |
| H(21A) | H1c[1n1c1h] | ethylamine |
| H(21B) | H1c[1n1c1h] | ethylamine |
| H(22A) | H1c[1n1c1c] | 2-aminopropane |
| H(24C) | H1c[1n1c1h] | ethylamine |
| H(24D) | H1c[1n1c1h] | ethylamine |
| H(25A) | H1c[1n1c1h] | ethylamine |
| H(25C) | H1c[1n1c1h] | ethylamine |
| H(26A) | H1c[1c1h1h] | ethane |
| H(26B) | H1c[1c1h1h] | ethane |
| H(26C) | H1c[1c1h1h] | ethane |
| H(23C) | H1n[1c1c1h] | dimethylammonium |
| H(23D) | H1n[1c1c1h] | dimethylammonium |
| H(21C) | H1c[1n1c1h] | ethylamine |
| H(21D) | H1c[1n1c1h] | ethylamine |

| Atom | Invariom Name | Model Compound |
|---|---|---|
| H(22B) | H1c[1n1c1c] | 2-aminopropane |
| H(24E) | H1c[1n1c1h] | ethylamine |
| H(24F) | H1c[1n1c1h] | ethylamine |
| H(25D) | H1c[1n1c1h] | ethylamine |
| H(25E) | H1c[1n1c1h] | ethylamine |
| H(26D) | H1c[1c1h1h] | ethane |
| H(26E) | H1c[1c1h1h] | ethane |
| H(26F) | H1c[1c1h1h] | ethane |

Table 14: Aspherical atomic scattering factors for moxifloxacin HCl 0.5 $H_2O$ 0.5 $CH_3OH$. Invariom names and corresponding model compounds from the invariom database are listed for all atoms.

| Atom | Invariom Name | Model Compound |
|---|---|---|
| Cl-(1) | Cl | chloride |
| Cl-(2) | Cl | chloride |
| F(15) | F@6c | 1-fluorobenzene |
| F(65) | F@6c | 1-fluorobenzene |
| O(12) | O1c1h | methanol |
| O(13) | O2c | formaldehyde |
| O(14) | O@6c | pyran-4-one ($\gamma$-pyrone) |
| O(19) | O@6c1c | anisole |
| O(63) | O1c1h | methanol |
| O(62) | O2c | formaldehyde |
| O(64) | O@6c | pyran-4-one ($\gamma$-pyrone) |
| O(69) | O@6c1c | anisole |
| O(4) | O1c1h | methanol |
| O(42) | O1h1h | water |
| N(1) | 6-N#66c[#66c#6c]#6c[#6c1h]@3c | 1-cyclopropylquinolin-4-one |
| N(20) | N@6c1c1c | *N,N*-dimethylbenzenamine |
| N(23) | N1c1c1h1h | dimethylammonium |
| N(51) | 6-N#66c[#66c#6c]#6c[#6c1h]@3c | 1-cyclopropylquinolin-4-one |
| N(70) | N@6c1c1c | *N,N*-dimethylbenzenamine |
| N(73) | N1c1c1h1h | dimethylammonium |
| C(2) | 6-C#6n[#66c@3c]#6c[#6c1c]1h | 1-cyclopropyl-3-methylquinolin-4-one |
| C(3) | 6-C#6c[2o#66c]#6c[#6n1h]1c | 3-methylquinolin-4-one |
| C(4) | 6-C2o#66c[#66c#6c]#6c[#6c1c] | 3-methyl-chromen-4-one |
| C(10) | 66-C#66c[#6n#6c]#6c[2o#6c]#6c[#6c1h] | quinolin-4-one |
| C(5) | 6-C#66c[#66c#6c]#6c[#6c1f]1h | 2-fluoronaphthalen |
| C(6) | 6-C#6c[#6c1n]#6c[#66c1h]1f | 3-fluoronaphthalen-2-amine |
| C(7) | 6-C#6c[#6c1f]#6c[#66c1o]1n | 2-amino-3-fluoronaphthalen-1-ol |
| C(8) | 6-C#66c[#6n#66c]#6c[#6c1n]1o | 7-amino-8-hydroxyquinolin-2-one |
| C(9) | 66-C#6n[#6c@3c]#66c[#6c#6c]#6c[#6c1o] | 1-cyclopropyl-8-hydroxy-1,8a-dihydroquinolin-2(3H)-one |
| C(11) | C2o1o@6c | benzoic acid |
| C(16) | 3-C#3c[#3c1h1h]#3c[#3c1h1h]@6n1h | 1-cyclopropylpyridine-2-one |
| C(17) | 3-C#3c[#3c@6n1h]#3c[#3c1h1h]1h1h | 1-cyclopropylpyridine-2-one |
| C(18) | 3-C#3c[#3c@6n1h]#3c[#3c1h1h]1h1h | 1-cyclopropylpyridine-2-one |
| C(19) | C1o1h1h1h | methanol |

| Atom | Invariom Name | Model Compound |
|---|---|---|
| C(21) | C1n1c1h1h | ethylamine |
| C(22) | C1n1c1c1h | 2-aminopropane |
| C(24) | C1n1c1h1h | ethylamine |
| C(25) | C1c1c1h1h | propane |
| C(26) | C1c1c1h1h | propane |
| C(27) | C1c1c1c1h | isobutane |
| C(28) | C1n1c1h1h | ethylamine |
| C(52) | 6-C#6n[#66c@3c]#6c[#6c1c]1h | 1-cyclopropyl-3-methylquinolin-4-one |
| C(53) | 6-C#6c[2o#66c]#6c[#6n1h]1c | 3-methylquinolin-4-one |
| C(54) | 6-C2o#66c[#66c#6c]#6c[#6c1c] | 3-methyl-chromen-4-one |
| C(60) | 66-C#66c[#6n#6c]#6c[2o#6c]#6c[#6c1h] | quinolin-4-one |
| C(55) | 6-C#66c[#66c#6c]#6c[#6c1f]1h | 2-fluoronaphthalen |
| C(56) | 6-C#6c[#6c1n]#6c[#66c1h]1f | 3-fluoronaphthalen-2-amine |
| C(57) | 6-C#6c[#6c1f]#6c[#66c1o]1n | 2-amino-3-fluoronaphthalen-1-ol |
| C(58) | 6-C#66c[#6n#66c]#6c[#6c1n]1o | 7-amino-8-hydroxyquinolin-2-one |
| C(59) | 66-C#6n[#6c@3c]#66c[#6c#6c]#6c[#6c1o] | 1-cyclopropyl-8-hydroxy-1,8a-dihydroquinolin-2(3H)-one |
| C(61) | C2o1o@6c | benzoic acid |
| C(66) | 3-C#3c[#3c1h1h]#3c[#3c1h1h]@6n1h | 1-cyclopropylpyridine-2-one |
| C(67) | 3-C#3c[#3c@6n1h]#3c[#3c1h1h]1h1h | 1-cyclopropylpyridine-2-one |
| C(68) | 3-C#3c[#3c@6n1h]#3c[#3c1h1h]1h1h | 1-cyclopropylpyridine-2-one |
| C(69) | C1o1h1h1h | methanol |
| C(71) | C1n1c1h1h | ethylamine |
| C(72) | C1n1c1c1h | 2-aminopropane |
| C(74) | C1n1c1h1h | ethylamine |
| C(75) | C1c1c1h1h | propane |
| C(76) | C1c1c1h1h | propane |
| C(77) | C1c1c1c1h | isobutane |
| C(78) | C1n1c1h1h | ethylamine |
| C(41) | C1o1h1h1h | methanol |
| H(12) | H1o[1c] | methanol |
| H(23A) | H1n[1c1c1h] | dimethylammonium |
| H(23B) | H1n[1c1c1h] | dimethylammonium |
| H(2) | H@6c | benzene |
| H(5) | H@6c | benzene |
| H(16) | H@3c | cyclopropane |
| H(17A) | H@3c | cyclopropane |
| H(17B) | H@3c | cyclopropane |
| H(18A) | H@3c | cyclopropane |
| H(18B) | H@3c | cyclopropane |
| H(19A) | H1c[1o1h1h] | methanol |
| H(19B) | H1c[1o1h1h] | methanol |
| H(19C) | H1c[1o1h1h] | methanol |
| H(21A) | H1c[1n1c1h] | ethylamine |
| H(21B) | H1c[1n1c1h] | ethylamine |
| H(22A) | H1c[1n1c1c] | 2-aminopropane |
| H(24A) | H1c[1n1c1h] | ethylamine |
| H(24B) | H1c[1n1c1h] | ethylamine |
| H(25A) | H1c[1c1c1h] | propane |
| H(25B) | H1c[1c1c1h] | propane |
| H(26A) | H1c[1c1c1h] | propane |
| H(26B) | H1c[1c1c1h] | propane |

| Atom | Invariom Name | Model Compound |
|---|---|---|
| H(27) | H1c[1c1c1c] | isobutane |
| H(28A) | H1c[1n1c1h] | ethylamine |
| H(28B) | H1c[1n1c1h] | ethylamine |
| H(63) | H1o[1c] | methanol |
| H(73A) | H1n[1c1c1h] | dimethylammonium |
| H(73B) | H1n[1c1c1h] | dimethylammonium |
| H(52) | H@6c | benzene |
| H(55) | H@6c | benzene |
| H(66) | H@3c | cyclopropane |
| H(67A) | H@3c | cyclopropane |
| H(67B) | H@3c | cyclopropane |
| H(68A) | H@3c | cyclopropane |
| H(68B) | H@3c | cyclopropane |
| H(69A) | H1c[1o1h1h] | methanol |
| H(69B) | H1c[1o1h1h] | methanol |
| H(69C) | H1c[1o1h1h] | methanol |
| H(71A) | H1c[1n1c1h] | ethylamine |
| H(71B) | H1c[1n1c1h] | ethylamine |
| H(72) | H1c[1n1c1c] | 2-aminopropane |
| H(74A) | H1c[1n1c1h] | ethylamine |
| H(74B) | H1c[1n1c1h] | ethylamine |
| H(75A) | H1c[1c1c1h] | propane |
| H(75B) | H1c[1c1c1h] | propane |
| H(76A) | H1c[1c1c1h] | propane |
| H(76B) | H1c[1c1c1h] | propane |
| H(77) | H1c[1c1c1c] | isobutane |
| H(78A) | H1c[1n1c1h] | ethylamine |
| H(78B) | H1c[1n1c1h] | ethylamine |
| H(04) | H1o[1c] | methanol |
| H(41A) | H1c[1o1h1h] | methanol |
| H(41B) | H1c[1o1h1h] | methanol |
| H(41C) | H1c[1o1h1h] | methanol |
| H(42A) | H1o[1h] | water |
| H(42B) | H1o[1h] | water |

Table 15: Aspherical atomic scattering factors for nadifloxacin 0.5 $H_2O$. Invariom names and corresponding model compounds from the invariom database are listed for all atoms.

| Atom | Invariom Name | Model Compound |
|---|---|---|
| F(15) | F@6c | 1-fluorobenzene |
| F(65) | F@6c | 1-fluorobenzene |
| O(14) | O@6c | pyran-4-one ($\gamma$-pyrone) |
| O(13) | O2c | formaldehyde |
| O(12) | O1c1h | methanol |
| O(23) | O1c1h | methanol |
| O(63) | O2c | formaldehyde |
| O(62) | O1c1h | methanol |
| O(73) | O1c1h | methanol |
| O(64) | O@6c | pyran-4-one ($\gamma$-pyrone) |

| Atom | Invariom Name | Model Compound |
|---|---|---|
| O(4) | O1h1h | water |
| N(1) | 6-N#66c[#66c#6c]#6c[#6c1h]1c | 1,3-dimethylquinolin-4-one |
| N(20) | N@6c1c1c | *N,N*-dimethylbenzenamine |
| N(70) | N@6c1c1c | *N,N*-dimethylbenzenamine |
| N(51) | 6-N#66c[#66c#6c]#6c[#6c1h]1c | 1,3-dimethylquinolin-4-one |
| C(9) | 66-C#6n[#6c1c]#66c[#6c#6c]#6c[#6c1c] | 2,3-dihydro-5-oxo-(1H,5H)-benzo[ij]quinolizine |
| C(8) | 6-C#66c[#6n#66c]#6c[#6c1n]1c | 8-methylquinolin-7-amine |
| C(3) | 6-C#6c[2o#66c]#6c[#6n1h]1c | 3-methylquinolin-4-one |
| C(10) | 66-C#66c[#6n#6c]#6c[2o#6c]#6c[#6c1h] | quinolin-4-one |
| C(5) | 6-C#66c[#66c#6c]#6c[#6c1f]1h | 2-fluoronaphthalen |
| C(7) | 6-C#6c[#6c1f]#6c[#66c1c]1n | 3-fluoro-1-methylnaphthalen-2-amine |
| C(4) | 6-C2o#66c[#66c#6c]#6c[#6c1c] | 3-methyl-chromen-4-one |
| C(6) | 6-C#6c[#6c1n]#6c[#66c1h]1f | 3-fluoronaphthalen-2-amine |
| C(11) | C2o1o@6c | benzoic acid |
| C(16) | C@6c1c1h1h | isochroman |
| C(21) | C1n1c1h1h | ethylamine |
| C(25) | C1n1c1h1h | ethylamine |
| C(22) | C1c1c1h1h | propane |
| C(19) | C1c1h1h1h | ethane |
| C(2) | 6-C#6n[#66c1c]#6c[#6c1c]1h | 1,3-dimethylquinolin-4-one |
| C(17) | C1c1c1h1h | propane |
| C(18) | C@6n1c1c1h | 1-isopropylpyridin-2-one |
| C(24) | C1c1c1h1h | propane |
| C(23) | C1o1c1c1h | 2-propanol |
| C(59) | 66-C#6n[#6c1c]#66c[#6c#6c]#6c[#6c1c] | 2,3-dihydro-5-oxo-(1H,5H)-benzo[ij]quinolizine |
| C(54) | 6-C2o#66c[#66c#6c]#6c[#6c1c] | 3-methyl-chromen-4-one |
| C(57) | 6-C#6c[#6c1f]#6c[#66c1c]1n | 3-fluoro-1-methylnaphthalen-2-amine |
| C(55) | 6-C#66c[#66c#6c]#6c[#6c1f]1h | 2-fluoronaphthalen |
| C(53) | 6-C#6c[2o#66c]#6c[#6n1h]1c | 3-methylquinolin-4-one |
| C(56) | 6-C#6c[#6c1n]#6c[#66c1h]1f | 3-fluoronaphthalen-2-amine |
| C(58) | 6-C#66c[#6n#66c]#6c[#6c1n]1c | 8-methylquinolin-7-amine |
| C(60) | 66-C#66c[#6n#6c]#6c[2o#6c]#6c[#6c1h] | quinolin-4-one |
| C(68) | C@6n1c1c1h | 1-isopropylpyridin-2-one |
| C(66) | C@6c1c1h1h | isochroman |
| C(67) | C1c1c1h1h | propane |
| C(52) | 6-C#6n[#66c1c]#6c[#6c1c]1h | 1,3-dimethylquinolin-4-one |
| C(71) | C1n1c1h1h | ethylamine |
| C(61) | C2o1o@6c | benzoic acid |
| C(74) | C1c1c1h1h | propane |
| C(75) | C1n1c1h1h | ethylamine |
| C(72) | C1c1c1h1h | propane |
| C(69) | C1c1h1h1h | ethane |
| C(73) | C1o1c1c1h | 2-propanol |
| H(12) | H1o[1c] | methanol |
| H(23) | H1o[1c] | methanol |
| H(5) | H@6c | benzene |
| H(161) | H1c[@6c1c1h] | isochroman |
| H(162) | H1c[@6c1c1h] | isochroman |
| H(211) | H1c[1n1c1h] | ethylamine |
| H(212) | H1c[1n1c1h] | ethylamine |
| H(251) | H1c[1n1c1h] | ethylamine |

| Atom | Invariom Name | Model Compound |
|---|---|---|
| H(252) | H1c[1n1c1h] | ethylamine |
| H(221) | H1c[1c1c1h] | propane |
| H(222) | H1c[1c1c1h] | propane |
| H(191) | H1c[1c1h1h] | ethane |
| H(192) | H1c[1c1h1h] | ethane |
| H(193) | H1c[1c1h1h] | ethane |
| H(2) | H@6c | benzene |
| H(171) | H1c[1c1c1h] | propane |
| H(172) | H1c[1c1c1h] | propane |
| H(18) | H1c[@6n1c1c] | 1-isopropylpyridin-2-one |
| H(241) | H1c[1c1c1h] | propane |
| H(242) | H1c[1c1c1h] | propane |
| H(231) | H1c[1o1c1c] | 2-propanol |
| H(62) | H1o[1c] | methanol |
| H(73) | H1o[1c] | methanol |
| H(55) | H@6c | benzene |
| H(68) | H1c[@6n1c1c] | 1-isopropylpyridin-2-one |
| H(661) | H1c[@6c1c1h] | isochroman |
| H(662) | H1c[@6c1c1h] | isochroman |
| H(671) | H1c[1c1c1h] | propane |
| H(672) | H1c[1c1c1h] | propane |
| H(52) | H@6c | benzene |
| H(711) | H1c[1n1c1h] | ethylamine |
| H(712) | H1c[1n1c1h] | ethylamine |
| H(741) | H1c[1c1c1h] | propane |
| H(742) | H1c[1c1c1h] | propane |
| H(751) | H1c[1n1c1h] | ethylamine |
| H(752) | H1c[1n1c1h] | ethylamine |
| H(721) | H1c[1c1c1h] | propane |
| H(722) | H1c[1c1c1h] | propane |
| H(691) | H1c[1c1h1h] | ethane |
| H(692) | H1c[1c1h1h] | ethane |
| H(693) | H1c[1c1h1h] | ethane |
| H(731) | H1c[1o1c1c] | 2-propanol |
| H(41) | H1o[1h] | water |
| H(42) | H1o[1h] | water |

Table 16: Aspherical atomic scattering factors for norfloxacin anhydrate. Invariom names and corresponding model compounds from the invariom database are listed for all atoms.

| Atom | Invariom Name | Model Compound |
|---|---|---|
| F(15) | F@6c | 1-fluorobenzene |
| O(12) | O2c | formaldehyde |
| O(13) | O1c1h | methanol |
| O(14) | O@6c | pyran-4-one ($\gamma$-pyrone) |
| N(1) | 6-N#66c[#66c#6c]#6c[#6c1h]1c | 1,3-dimethylquinolin-4-one |
| N(20) | N@6c1c1c | *N*,*N*-dimethylbenzenamine |
| N(23) | N1c1c1h | dimethylamine |
| C(2) | 6-C#6n[#66c1c]#6c[#6c1c]1h | 1,3-dimethylquinolin-4-one |
| C(3) | 6-C#6c[2o#66c]#6c[#6n1h]1c | 3-methylquinolin-4-one |

| Atom | Invariom Name | Model Compound |
|---|---|---|
| C(11) | C2o1o@6c | benzoic acid |
| C(4) | 6-C2o#66c[#66c#6c]#6c[#6c1c] | 3-methyl-chromen-4-one |
| C(10) | 66-C#66c[#6n#6c]#6c[2o#6c]#6c[#6c1h] | quinolin-4-one |
| C(5) | 6-C#66c[#66c#6c]#6c[#6c1f]1h | 2-fluoronaphthalen |
| C(6) | 6-C#6c[#6c1n]#6c[#66c1h]1f | 3-fluoronaphthalen-2-amine |
| C(7) | 6-C#6c[#6c1f]#6c[#66c1h]1n | 3-fluoronaphthalen-2-amine |
| C(8) | 6-C#66c[#6n#66c]#6c[#6c1n]1h | 7-aminoquinolin-2-one |
| C(9) | 66-C#6n[#6c1c]#66c[#6c#6c]#6c[#6c1h] | 1,3-dimethylquinolin-4-one |
| C(25) | C1n1c1h1h | ethylamine |
| C(24) | C1n1c1h1h | ethylamine |
| C(22) | C1n1c1h1h | ethylamine |
| C(21) | C1n1c1h1h | ethylamine |
| C(16) | C@6n1c1h1h | 1-ethylpylpyridine-2-one |
| C(17) | C1c1h1h1h | ethane |
| H(13) | H1o[1c] | methanol |
| H(23A) | H1n[1c1c] | dimethylamine |
| H(2) | H@6c | benzene |
| H(5) | H@6c | benzene |
| H(8) | H@6c | benzene |
| H(25A) | H1c[1n1c1h] | ethylamine |
| H(25B) | H1c[1n1c1h] | ethylamine |
| H(24A) | H1c[1n1c1h] | ethylamine |
| H(24B) | H1c[1n1c1h] | ethylamine |
| H(22A) | H1c[1n1c1h] | ethylamine |
| H(22B) | H1c[1n1c1h] | ethylamine |
| H(21A) | H1c[1n1c1h] | ethylamine |
| H(21B) | H1c[1n1c1h] | ethylamine |
| H(16A) | H1c[@6n1c1h] | 1-ethylpylpyridine-2-one |
| H(16B) | H1c[@6n1c1h] | 1-ethylpylpyridine-2-one |
| H(17A) | H1c[1c1h1h] | ethane |
| H(17B) | H1c[1c1h1h] | ethane |
| H(17C) | H1c[1c1h1h] | ethane |

Table 17: Aspherical atomic scattering factors for norfloxacin 2 $H_2O$. Invariom names and corresponding model compounds from the invariom database are listed for all atoms.

| Atom | Invariom Name | Model Compound |
|---|---|---|
| F(15) | F@6c | 1-fluorobenzene |
| O(13) | O1.5c[1.5o@6c] | benzoic acid anion |
| O(12) | O1.5c[1.5o@6c] | benzoic acid anion |
| O(14) | O@6c | pyran-4-one ($\gamma$-pyrone) |
| O(2) | O1h1h | water |
| O(3) | O1h1h | water |
| N(23) | N1c1c1h1h | dimethylammonium |
| N(1) | 6-N#66c[#66c#6c]#6c[#6c1h]1c | 1,3-dimethylquinolin-4-one |
| N(20) | N@6c1c1c | *N,N*-dimethylbenzenamine |
| C(6) | 6-C#6c[#6c1n]#6c[#66c1h]1f | 3-fluoronaphthalen-2-amine |
| C(11) | C1.5o1.5o@6c | benzoic acid anion |
| C(4) | 6-C2o#66c[#66c#6c]#6c[#6c1c] | 3-methyl-chromen-4-one |

| Atom | Invariom Name | Model Compound |
|---|---|---|
| C(3) | 6-C#6c[2o#66c]#6c[#6n1h]1c | 3-methylquinolin-4-one |
| C(10) | 66-C#66c[#6n#6c]#6c[2o#6c]#6c[#6c1h] | quinolin-4-one |
| C(5) | 6-C#66c[#66c#6c]#6c[#6c1f]1h | 2-fluoronaphthalen |
| C(2) | 6-C#6n[#66c1c]#6c[#6c1c]1h | 1,3-dimethylquinolin-4-one |
| C(9) | 66-C#6n[#6c1c]#66c[#6c#6c]#6c[#6c1h] | 1,3-dimethylquinolin-4-one |
| C(8) | 6-C#66c[#6n#66c]#6c[#6c1n]1h | 7-aminoquinolin-2-one |
| C(7) | 6-C#6c[#6c1f]#6c[#66c1h]1n | 3-fluoronaphthalen-2-amine |
| C(16) | C@6n1c1h1h | 1-ethylpylpyridine-2-one |
| C(25) | C1n1c1h1h | ethylamine |
| C(21) | C1n1c1h1h | ethylamine |
| C(24) | C1n1c1h1h | ethylamine |
| C(22) | C1n1c1h1h | ethylamine |
| C(17) | C1c1h1h1h | ethane |
| H(23A) | H1n[1c1c1h] | dimethylammonium |
| H(23B) | H1n[1c1c1h] | dimethylammonium |
| H(5) | H@6c | benzene |
| H(2) | H@6c | benzene |
| H(8) | H@6c | benzene |
| H(16A) | H1c[@6n1c1h] | 1-ethylpylpyridine-2-one |
| H(16B) | H1c[@6n1c1h] | 1-ethylpylpyridine-2-one |
| H(25A) | H1c[1n1c1h] | ethylamine |
| H(25B) | H1c[1n1c1h] | ethylamine |
| H(21A) | H1c[1n1c1h] | ethylamine |
| H(21B) | H1c[1n1c1h] | ethylamine |
| H(24A) | H1c[1n1c1h] | ethylamine |
| H(24B) | H1c[1n1c1h] | ethylamine |
| H(22A) | H1c[1n1c1h] | ethylamine |
| H(22B) | H1c[1n1c1h] | ethylamine |
| H(17A) | H1c[1c1h1h] | ethane |
| H(17B) | H1c[1c1h1h] | ethane |
| H(17C) | H1c[1c1h1h] | ethane |
| H(021) | H1o[1h] | water |
| H(022) | H1o[1h] | water |
| H(031) | H1o[1h] | water |
| H(032) | H1o[1h] | water |

Table 18: Aspherical atomic scattering factors for ofloxacin. Invariom names and corresponding model compounds from the invariom database are listed for all atoms.

| Atom | Invariom Name | Model Compound |
|---|---|---|
| F(15) | F@6c | 1-fluorobenzene |
| O(13) | O2c | formaldehyde |
| O(14) | O@6c | pyran-4-one ($\gamma$-pyrone) |
| O(12) | O1c1h | methanol |
| O(16) | O@6c1c | anisole |
| N(1) | 6-N#66c[#66c#6c]#6c[#6c1h]1c | 1,3-dimethylquinolin-4-one |
| N(20) | N@6c1c1c | *N*,*N*-dimethylbenzenamine |
| N(23) | N1c1c1c | trimethylamine |
| C(2) | 6-C#6n[#66c1c]#6c[#6c1c]1h | 1,3-dimethylquinolin-4-one |
| C(9) | 66-C#6n[#6c1c]#66c[#6c#6c]#6c[#6c1o] | 8-hydroxy-1-methylquinolin-2-one |

| Atom | Invariom Name | Model Compound |
|---|---|---|
| C(10) | 66-C#66c[#6n#6c]#6c[2o#6c]#6c[#6c1h] | quinolin-4-one |
| C(11) | C2o1o@6c | benzoic acid |
| C(3) | 6-C#6c[2o#66c]#6c[#6n1h]1c | 3-methylquinolin-4-one |
| C(6) | 6-C#6c[#6c1n]#6c[#66c1h]1f | 3-fluoronaphthalen-2-amine |
| C(5) | 6-C#66c[#66c#6c]#6c[#6c1f]1h | 2-fluoronaphthalen |
| C(7) | 6-C#6c[#6c1f]#6c[#66c1o]1n | 2-amino-3-fluoronaphthalen-1-ol |
| C(8) | 6-C#66c[#6n#66c]#6c[#6c1n]1o | 7-amino-8-hydroxyquinolin-2-one |
| C(4) | 6-C2o#66c[#66c#6c]#6c[#6c1c] | 3-methyl-chromen-4-one |
| C(24) | C1n1c1h1h | ethylamine |
| C(21) | C1n1c1h1h | ethylamine |
| C(22) | C1n1c1h1h | ethylamine |
| C(18) | C@6n1c1c1h | 1-isopropylpyridin-2-one |
| C(17) | C1o1c1h1h | ethanol |
| C(19) | C1c1h1h1h | ethane |
| C(26) | C1n1h1h1h | methylamine |
| C(25) | C1n1c1h1h | ethylamine |
| H(2) | H@6c | benzene |
| H(12) | H1o[1c] | methanol |
| H(5) | H@6c | benzene |
| H(24A) | H1c[1n1c1h] | ethylamine |
| H(24B) | H1c[1n1c1h] | ethylamine |
| H(21A) | H1c[1n1c1h] | ethylamine |
| H(21B) | H1c[1n1c1h] | ethylamine |
| H(22A) | H1c[1n1c1h] | ethylamine |
| H(22B) | H1c[1n1c1h] | ethylamine |
| H(18) | H1c[@6n1c1c] | 1-isopropylpyridin-2-one |
| H(17A) | H1c[1o1c1h] | ethanol |
| H(17B) | H1c[1o1c1h] | ethanol |
| H(19A) | H1c[1c1h1h] | ethane |
| H(19B) | H1c[1c1h1h] | ethane |
| H(19C) | H1c[1c1h1h] | ethane |
| H(26A) | H1c[1n1h1h] | methylamine |
| H(26B) | H1c[1n1h1h] | methylamine |
| H(26C) | H1c[1n1h1h] | methylamine |
| H(25A) | H1c[1n1c1h] | ethylamine |
| H(25B) | H1c[1n1c1h] | ethylamine |

Table 19: Aspherical atomic scattering factors for sparfloxacin 3 $H_2O$. Invariom names and corresponding model compounds from the invariom database are listed for all atoms.

| Atom | Invariom Name | Model Compound |
|---|---|---|
| F(8) | F@6c | 1-fluorobenzene |
| F(15) | F@6c | 1-fluorobenzene |
| O(12) | O1.5c[1.5o@6c] | benzoic acid anion |
| O(13) | O1.5c[1.5o@6c] | benzoic acid anion |
| O(14) | O@6c | pyran-4-one ($\gamma$-pyrone) |
| O(2) | O1h1h | water |
| O(3) | O1h1h | water |
| O(4) | O1h1h | water |
| N(1) | 6-N#66c[#66c#6c]#6c[#6c1h]@3c | 1-cyclopropylquinolin-4-one |
| N(5) | =-N@6c1h1h | 4-aminopyrimidin-2-one |
| N(20) | N@6c1c1c | *N,N*-dimethylbenzenamine |

| Atom | Invariom Name | Model Compound |
|---|---|---|
| N(23) | N1c1c1h1h | dimethylammonium |
| C(2) | 6-C#6n[#66c@3c]#6c[#6c1c]1h | 1-cyclopropyl-3-methylquinolin-4-one |
| C(3) | 6-C#6c[2o#66c]#6c[#6n1h]1c | 3-methylquinolin-4-one |
| C(4) | 6-C2o#66c[#66c#6c]#6c[#6c1c] | 3-methyl-chromen-4-one |
| C(10) | 66-C#66c[#6n#6c]#6c[2o#6c]#6c[#6c1n] | 5-aminoquinolin-4-one |
| C(9) | 66-C#6n[#6c@3c]#66c[#6c#6c]#6c[#6c1f] | 1-cyclopropyl-8-fluoroquinolin-2-one |
| C(8) | 6-C#66c[#6n#66c]#6c[#6c1n]1f | 7-amino-8-fluoroquinolin-2-one |
| C(7) | 6-C#6c[#66c1f]#6c[#6c1f]1n | 1,3-difluoronaphthalen-2-amine |
| C(6) | 6-C#6c[#66c1n]#6c[#6c1n]1f | 2-fluoronaphthalene-1,3-diamine |
| C(5) | 6-C#66c[#66c#6c]#6c[#6c1f]1n | 2-fluoronaphthalen-1-amine |
| C(21) | C1n1c1h1h | ethylamine |
| C(22) | C1n1c1c1h | 2-aminopropane |
| C(24) | C1n1c1c1h | 2-aminopropane |
| C(25) | C1n1c1h1h | ethylamine |
| C(27) | C1c1h1h1h | ethane |
| C(26) | C1c1h1h1h | ethane |
| C(16) | 3-C#3c[#3c1h1h]#3c[#3c1h1h]@6n1h | 1-cyclopropylpyridine-2-one |
| C(17) | 3-C#3c[#3c@6n1h]#3c[#3c1h1h]1h1h | 1-cyclopropylpyridine-2-one |
| C(18) | 3-C#3c[#3c@6n1h]#3c[#3c1h1h]1h1h | 1-cyclopropylpyridine-2-one |
| C(11) | C1.5o1.5o@6c | benzoic acid anion |
| H(52) | H1n[@6c1h] | aniline |
| H(51) | H1n[@6c1h] | aniline |
| H(23A) | H1n[1c1c1h] | dimethylammonium |
| H(23B) | H1n[1c1c1h] | dimethylammonium |
| H(2) | H@6c | benzene |
| H(21A) | H1c[1n1c1h] | ethylamine |
| H(21B) | H1c[1n1c1h] | ethylamine |
| H(22A) | H1c[1n1c1c] | 2-aminopropane |
| H(24A) | H1c[1n1c1c] | 2-aminopropane |
| H(251) | H1c[1n1c1h] | ethylamine |
| H(252) | H1c[1n1c1h] | ethylamine |
| H(27A) | H1c[1c1h1h] | ethane |
| H(27B) | H1c[1c1h1h] | ethane |
| H(27C) | H1c[1c1h1h] | ethane |
| H(26A) | H1c[1c1h1h] | ethane |
| H(26B) | H1c[1c1h1h] | ethane |
| H(26C) | H1c[1c1h1h] | ethane |
| H(16) | H@3c | cyclopropane |
| H(17A) | H@3c | cyclopropane |
| H(17B) | H@3c | cyclopropane |
| H(18A) | H@3c | cyclopropane |
| H(18B) | H@3c | cyclopropane |
| H(021) | H1o[1h] | water |
| H(022) | H1o[1h] | water |
| H(031) | H1o[1h] | water |
| H(032) | H1o[1h] | water |
| H(041) | H1o[1h] | water |
| H(042) | H1o[1h] | water |