**Table S13.**

Data collection and refinement statistics for drug-NQO2 co-crystals (molecular replacement). Data analysis and structure validation was carried out with MOLPROBITY(*119*) and PHENIX(*120*).

| | *NQO2 Crenolanib (5LBY)* | *NQO2 Pacritinib (5LBZ)* | *NQO2 Volitinib (5LBW)* |
|---|---|---|---|
| ***Data collection*** | | | |
| *Space group* | P212121 | P212121 | P212121 |
| *Cell dimensions* | | | |
| *a, b, c (Å)* | 61.6, 79.4, 106.6 | 61.4, 79.2, 106.2 | 57.4, 81.4, 106.4 |
| *α, β, γ (°)* | 90, 90, 90 | 90, 90, 90 | 90, 90, 90 |
| *Resolution (Å)* | 44.3 - 1.4 (1.45 - 1.4)a | 48.6 - 1.4 (1.45 - 1.4)a | 44.5 - 1.9 (1.97-1.9)a |
| $R_{merge}$ | 0.039 (0.276)a | 0.045 (0.329)a | 0.110 (0.976)a |
| *I/s(I)* | 22.6 (5.1)a | 21.1 (5.3)a | 7.5 (1.3)a |
| *CC1/2* | 0.999 (0.95)a | 0.999 (0.93)a | 0.996 (0.56)a |
| *Completeness (%)* | 0.93 (0.90)a | 0.95 (0.91)a | 0.90 (0.93)a |
| *Redundancy* | 4.6 (64.4)a | 4.5 (4.4)a | 4.7 (4.0)a |
| ***Refinement*** | | | |
| *Resolution (Å)* | 44.3 - 1.4 | 48.6 - 1.4 | 44.5 - 1.90 |
| *No. reflections* | 96,392 | 97,697 | 36,195 |
| *Rwork / Rfree* | 0.124 / 0.142 | 0.126 / 0.145 | 0.238/ 0.247 |
| *No. atoms* | | | |
| *Protein* | 3711 | 3697 | 3643 |
| *Ligands* | 174 | 198 | 160 |
| *Water* | 436 | 428 | 39 |
| *B factors* | | | |
| *Protein* | 14.6 | 13.1 | 42.1 |
| *Ligands* | 12.1 | 14.6 | 46.6 |
| *Water* | 26.9 | 25.1 | 37.7 |
| *R.m.s. deviations* | | | |
| *Bond lengths (Å)* | 0.96 | 0.96 | 0.97 |
| *Bond angles (°)* | 6.7 | 6.6 | 6.6 |

[a] Values in parentheses are for highest-resolution shell.