Supporting Information

Investigation of quinoline-4-carboxylic acid as a highly potent scaffold for the development of alkaline phosphatase inhibitors: Synthesis, SAR analysis and molecular modelling studies

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\textsuperscript{1}H and \textsuperscript{13}C NMR spectra of synthesized compounds
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Ramachandran Plot for IAP model

Number of residues in favoured region (~98.0% expected) : 462  (96.9%)
Number of residues in allowed region (~2.0% expected) : 12  (2.5%)
Number of residues in outlier region : 3  (0.6%)

RAMPAGE by Paul de Bakker and Simon Lovell available at http://www.cns.ucsf.edu/RAMPAGE/
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FAMPA by Paul de Bakker and Simon Level available at http://www.crys.bioc.cam.ac.uk/rampage/
Structure validation by Cx geometry, i-j and Cx deviation, Proline Structure. Function & Genetica. 60: 437-469
Ramachandran plot for TNAP model

- General/Pre-Pro/Proline Favoured
- General/Pre-Pro/Proline Allowed
- Glycine Favoured
- Glycine Allowed

Number of residues in favoured region (~98.0% expected) : 455  (95.2%)
Number of residues in allowed region (~2.0% expected) : 15  (3.1%)
Number of residues in outlier region : 8  (1.7%)
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![Graph](image)

- **General Favoured**
- **Glycine Favoured**
- **Pre-Pro Favoured**
- **Proline Favoured**

**Legend**

- **General Allowed**
- **Glycine Allowed**
- **Pre-Pro Allowed**
- **Proline Allowed**

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Structure validation by Cα geometry: ϕα and Cα deviation. RAMPAGE: Structure, Function & Genetics, 60:437-460.