

POSTER PRESENTATIONS

CRYSTAL AND MOLECULAR STRUCTURES OF 1-ALKYL-QUINAZOLIN-4(3H)-ONES WITH *p*-CHLOROPHENYL FRAGMENT

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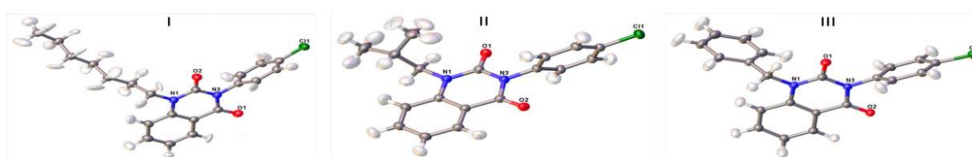
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Quinazolin-4(3H)-one and quinazoline-2,4-dione cores represent key pharmacophores widely encountered in medicinal chemistry and materials science [1,2].

We present the crystal structures of three novel 4-chlorophenyl quinazolinones: 3-(4-chlorophenyl)-1-heptylquinazoline-2,4(1H,3H)-dione (**I**), 3-(4-chlorophenyl)-1-isobutylquinazoline-2,4(1H,3H)-dione (**II**), and 1-benzyl-3-(4-chlorophenyl)quinazoline-2,4(1H,3H)-dione (**III**). Refinement against single-crystal X-ray data using *NoSpherA2* [3] with non-spherical atomic scattering factors overcame standard independent atom model (*IAM*) limitations. Tailor-made quantum chemical wavefunctions improved refinement statistics (R_1 , wR_2 ; see Table), produced physically meaningful bond lengths, minimized residual electron density, and enabled precise characterization of hydrogen-bonding networks and crystal packing.



Data refinement	I	II	III
IAM/SHELXL			
R_1 ($[I \geq 2\sigma(I)]$ / all)	0.0325 / 0.0333	0.0337 / 0.0348	0.0409 / 0.0447
wR_2 ($[I \geq 2\sigma(I)]$ / all)	0.0870 / 0.0875	0.0945 / 0.0952	0.1017 / 0.1041
HAR/NoSpherA2			
R_1 ($[I \geq 2\sigma(I)]$ / all)	0.0278 / 0.0286	0.0195 / 0.0203	0.0335 / 0.0370
wR_2 ($[I \geq 2\sigma(I)]$ / all)	0.0758 / 0.0762	0.0574 / 0.0580	0.0829 / 0.0848

Crystallographic data for **I–III** (CCDC 2579374, 2579373, 2579371) are available free from the CCDC: www.ccdc.cam.ac.uk/data_request/cif.

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References:

1. Singh *et al.*, *Mini reviews in medicinal chemistry*. 2013, 3 (8): 1177–1194.
2. Auti *et al.*, *RSC Adv.* 2020, 10 (68): 41353–41392.
3. Kleemiss *et al.*, *Chemical Science*. 2021, 12(5), 1675–1692.