

Supplementary material

The efficiency of C-4 substituents in activating the β -lactam scaffold towards serine proteases and hydroxide ion

Jalmira Mulchande^a, Luísa Martins^a, Rui Moreira^a, Margarida Archer^b, Tania F. Oliveira^b, Jim Iley^c

a) i-Med-UL, Faculdade de Farmácia, Universidade de Lisboa, Av. Forças Armadas, 1600-083 Lisboa, Portugal; b) Instituto de Tecnologia Química e Biológica, Universidade Nova de Lisboa, ITQB-UNL, Av. República, Apt. 127, 2781-901 Oeiras, Portugal; c) Department of Chemistry, The Open University, Milton Keynes, MK7 6AA, UK

Table S1

X-ray data-collection statistics

Wavelength (Å)	0.82
Resolution range (Å)	37.95 - 1.66
Space group	P2 ₁ 2 ₁ 2 ₁
Unit cell parameters (Å)	a = 50.25, b = 57.94, c = 74.69
Total reflections	177649
Unique reflections	26474
Completeness (%)	96.9 (79.8)
Redundancy	4.3 (4.1)
R _{merge} * (%)	3.0 (9.3)
I/σ (I)	27.4 (14.7)

Values in parenthesis show the statistics of the highest resolution shell (1.75 - 1.66 Å).

$$* R_{merge} = \frac{\sum_{hkl} \sum_i |I_i(hkl) - \overline{I(hkl)}|}{\sum_{hkl} \sum_i I_i(hkl)}, \text{ where } I_i(hkl) \text{ is the } i^{\text{th}} \text{ measurement.}$$