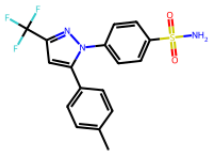
Astinova AI Platform — De Novo / Generative Design Report

Target: COX-2 (public) · goal-directed analogues of a public pyrazole-sulfonamide chemotype

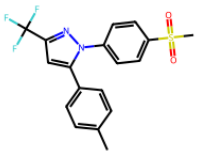
Illustrative sample on a public target/compound — for format demonstration.

Generated analogues

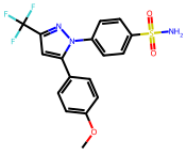
ID	Computed profile
DGN-1	MW 381 | cLogP 3.51 | TPSA 78 | QED 0.75
DGN-2	MW 380 | cLogP 4.27 | TPSA 52 | QED 0.68
DGN-3	MW 397 | cLogP 3.21 | TPSA 87 | QED 0.73
DGN-4	MW 385 | cLogP 3.34 | TPSA 78 | QED 0.70



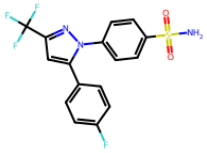
DGN-1



DGN-2



DGN-3



DGN-4

Designs are goal-directed variations of a public COX-2 pyrazole-sulfonamide chemotype, generated to explore substituent effects on lipophilicity and polarity. Computational proposals for prioritisation; require synthesis and assay.