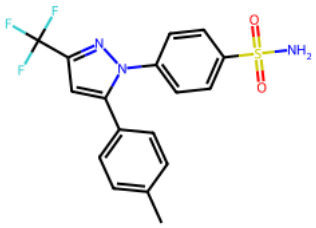
Astinova AI Platform — Metabolism & Reactivity Report

Example substrate: a public COX-2 inhibitor (celecoxib) · soft-spots & reactive-liability flags

Illustrative sample — synthetic data for format demonstration; not a specific client deliverable.



Formula	C17H14F3N3O2S
MW	381.4
cLogP	3.51
TPSA	78.0
HBD/HBA	1 / 4
Rotatable bonds	3
Aromatic rings	3

Predicted sites of metabolism (soft-spots)

Site	Likely reaction	Enzyme (predicted)	Confidence	Note
Aryl methyl (tolyl CH3)	Benzylic hydroxylation -> carboxylic acid	CYP2C9 (primary)	High	Dominant clearance route; forms hydroxymethyl then carboxylic-acid metabolite.
Pyrazole ring	Aromatic hydroxylation	CYP3A4 (minor)	Medium	Secondary oxidative pathway.
Sulfonamide N	Low turnover	—	Low	Largely metabolically stable; conjugation possible.

Reactive-liability flags

Alert	Assessment	Recommended follow-up
Sulfonamide moiety	Idiosyncratic hypersensitivity class-flag; not a bioactivation alert per se.	Note in risk profile; monitor if class-sensitised.
No epoxide/quinone precursor detected	No high-priority bioactivation motif in the core.	Standard reactive-metabolite screen sufficient.
Trifluoromethyl / pyrazole	Metabolically robust; no reactive-metabolite concern.	None.

Summary

Clearance is predicted to be oxidative and dominated by benzylic hydroxylation of the aryl-methyl group (CYP2C9), consistent with the known disposition of this substrate class. No high-priority bioactivation liability is flagged in the core scaffold. Predictions are model-based and should be confirmed with in vitro metabolite identification (microsomes/hepatocytes) and reactivity assays.