

Fallen Angel Drugs - Optimization Summary

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Total Drugs: 23 Successful: 23 Errors: 0

Successfully Processed

#	Drug	Task	Output File
1	Tarenflurbil (Flurizan)	BBBP	01 TarenflurbilFlurizan.md
2	Gavestinel (GV-150,526)	BBBP	02 GavestinelGV-150526.md
3	NXY-059 (Cerovive)	BBBP	03 NXY-059Cerovive.md
4	PF-03758309 (PF-3758309)	HIA	04 PF-03758309PF-3758309.md
5	Olcegepant (BIBN-4096BS)	HIA	05 OlcegepantBIBN-4096BS.md
6	EPI-506 (ralaniten acetate / prodrug of EPI-002)	HIA	06 EPI-506ralanitenacetateprodrugof_EPI-002.md
7	KPT-9274	HIA	07 KPT-9274.md
8	Valeresol	HIA	08 Valeresol.md
9	Fialuridine (FIAU)	DILI	09 FialuridineFIAU.md
10	Ximelagatran (Exanta / oral direct thrombin inhibitor)	DILI	10 XimelagatranExanta_oraldirectthrombininhibitor.md
11	Fasiglifam (TAK-875)	DILI	11 FasiglifamTAK-875.md
12	Lapaquinstat acetate (TAK-475)	DILI	12 Lapaquinstatacetate_TAK-475.md
13	Danuglipron (Pfizer)	DILI	13 DanuglipronPfizer.md
14	Rosiglitazone	BBBP	14 Rosiglitazone.md
15	Paclitaxel / other taxanes	BBBP	15 Paclitaxelothertaxanes.md
16	Mibepradil (Posicor)	CYP3A4	16 MibepradilPosicor.md
17	Nefazodone (Serzone)	CYP3A4	17 NefazodoneSerzone.md
18	GSK1059615	HIA	18 GSK1059615.md
19	Neflamapimod (VX-745)	HIA	19 NeflamapimodVX-745.md
20	SAR260301	CYP3A4	20 SAR260301.md
21	Taranabant (MK-0364)	DILI	21 TaranabantMK-0364.md
22	NYX-059	BBBP	22 NYX-059.md
23	AZD-3514	HIA	23 AZD-3514.md

Errors

None

Configuration

- **Number of beams:** 12
- **Depth:** 3
- **CSV source:** /shared/nas2/knguye71/mCLM_nov/fallenangel.csv

Features Included

Each slide includes: - ADMET score predictions (6 tasks: ames, bbbp, cyp3a4, dili, hia, pgp) - QED (drug-likeness) analysis with change tracking - **Molecular block count and changes** (shows structural modifications) - Step-by-step optimization path with before/after comparisons - Safety threshold analysis - Overall improvement statistics