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Structure-based design and computational screening of fyn kinase inhibitors targeting neurodegenerative pathways in alzheimer's disease

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Supplementary data

Suppl. Table 1 — Energy minimisation protocol for the molecular dynamics simulation performed through Amber 2022

Stage	Maximum number of steps (steepest descent)*	Maximum number of steps (conjugate gradient)*	Total number of steps*	Weight for the positional restraints. (in kcal/mol-Å^2)	Restrained elements
1	2000	3000	5000	500	Protein and ligand
2	1000	4000	5000	500	Protein and ligand, except for their hydrogen
3	1000	4000	5000	500	The backbone of protein and ligand
4	1000	4000	5000	50	Protein and ligand, except for their hydrogen
5	1000	4000	5000	50	The backbone of protein and ligand
6	1000	4000	5000	5	Protein and ligand, except for their hydrogen
7	1000	4000	5000	5	The backbone of protein and ligand
8	1000	4000	5000	0.2	The backbone of protein and ligand

Suppl. Table 2 — LGA parameters for virtual screening and precision docking

Docking	Number of GA run	Population size	Maximum number of generations	Maximum number of evaluations	Rate of Gene mutation	Rate of crossing over
Virtual screening	10	150	27000	250000	0.02	0.8
Precision docking	100	150	27000	2500000	0.02	0.8

Suppl Table 3: Molecular and pharmacokinetic properties of virtual hits obtained from SWISS ADME and DeepPK.

id	MOL_WEIGHT	Log (P)	#ACCEPTORS	#DONORS	Lipinski Violation	#ROTATABLE BONDS	pKa Acid	Human Intestinal Absorption	P-Glycoprotein Inhibitor	P-Glycoprotein Substrate	Blood-Brain Barrie	CYP 1A2 Inhibitor	CYP 2C19 Inhibitor	CYP 2C9 Inhibitor	CYP 2D6 Inhibitor	CYP 3A4 Inhibitor	Number of CYP enzyme inhibited	AMES Mutagenesis	Carcinogenesis	hERG Blockers
MolPort-047-153-863	556.622	4.75	6	2	1	2	8.77	Absorbed	Non-Inhibitor	Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	1	Safe	Safe	Toxic
MolPort-003-983-855	453.454	2.69	6	3	0	1	5.31	Absorbed	Non-Inhibitor	Substrate	Penetrable	Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	1	Safe	Safe	Toxic
MolPort-046-426-293	480.524	3.77	7	2	0	2	9.16	Absorbed	Non-Inhibitor	Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	1	Safe	Safe	Toxic
MolPort-047-152-878	586.648	4.44	7	2	1	3	8.32	Absorbed	Non-Inhibitor	Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	1	Safe	Safe	Toxic
MolPort-044-561-474	482.54	3.14	7	3	0	2	9.09	Absorbed	Non-Inhibitor	Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	1	Safe	Safe	Toxic
MolPort-023-276-484	393.402	4.15	5	1	0	0	9.96	Absorbed	Non-Inhibitor	Substrate	Non-Penetrable	Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	1	Safe	Safe	Safe
MolPort-004-963-441	467.481	3.59	7	2	0	1	9.75	Absorbed	Non-Inhibitor	Substrate	Penetrable	Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	2	Safe	Safe	Toxic
MolPort-006-168-050	482.54	3.28	7	3	0	2	9.14	Absorbed	Non-Inhibitor	Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	1	Safe	Safe	Toxic
MolPort-046-196-907	453.454	2.72	6	3	0	1	5.35	Absorbed	Non-Inhibitor	Substrate	Penetrable	Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	1	Safe	Safe	Toxic
MolPort-019-939-264	584.632	5.01	7	1	2	3	8.64	Absorbed	Non-Inhibitor	Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	1	Safe	Safe	Toxic

MolPort-004-963-434	466.541	3.73	6	2	0	2	9.83	Absorbed	Non-Inhibitor	Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	1	Safe	Safe	Toxic
MolPort-003-848-372	439.471	3.22	6	3	0	1	9.64	Absorbed	Non-Inhibitor	Substrate	Penetrable	Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	1	Safe	Safe	Toxic
Molport-047-152-765	570.649	5.04	6	1	2	3	9.12	Absorbed	Non-Inhibitor	Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	1	Safe	Safe	Toxic
MolPort-023-276-626	570.649	4.97	6	1	1	3	9.12	Absorbed	Non-Inhibitor	Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	1	Safe	Safe	Toxic
MolPort-044-724-239	466.541	3.94	6	2	0	2	9.93	Absorbed	Non-Inhibitor	Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	1	Safe	Safe	Toxic
MolPort-003-848-298	467.481	3.58	7	2	0	1	9.74	Absorbed	Non-Inhibitor	Substrate	Non-Penetrable	Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	2	Safe	Safe	Toxic
MolPort-046-857-188	457.486	2.97	6	5	0	1	7.24	Absorbed	Non-Inhibitor	Substrate	Penetrable	Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	1	Safe	Safe	Toxic
MolPort-035-765-887	615.777	5.41	9	2	2	7	8.69	Absorbed	Non-Inhibitor	Substrate	Non-Penetrable	Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	2	Safe	Toxic	Toxic
MolPort-006-827-844	370.364	3.56	5	3	0	2	8.64	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	3	Safe	Safe	Safe
MolPort-039-057-764	525.944	5.16	7	1	2	5	8.58	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	3	Safe	Safe	Toxic
MolPort-003-959-454	570.385	3.06	8	5	1	3	8.84	Absorbed	Non-Inhibitor	Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	0	Safe	Safe	Safe
Molport-051-907-006	901.821	3.53	11	3	2	17	-17621	Absorbed	Inhibitor	Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	1	Safe	Safe	Toxic
MolPort-002-747-121	391.404	4.3	5	2	0	2	6.69	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	4	Safe	Safe	Safe
MolPort-005-944-489	338.315	3.4	6	3	0	0	6.91	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	2	Toxic	Safe	Safe
MolPort-002-818-255	461.415	4.55	9	2	0	4	8.28	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	4	Toxic	Safe	Safe
MolPort-044-726-375	422.342	0.54	11	8	2	2	4.16	Non-Absorbed	Non-Inhibitor	Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	0	Toxic	Safe	Safe
MolPort-028-	474.421	3.38	8	3	0	5	8.98	Absorbed	Non-	Non-	Non-	Non-	Non-	Inhibitor	Non-	Non-	1	Safe	Safe	Safe

855-625									Inhibitor	Substrate	Penetrable	Inhibitor	Inhibitor		Inhibitor	Inhibitor			
MolPort-003-006-399	382.206	3.61	3	2	0	1	10.92	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	Inhibitor	3	Toxic	Safe	Safe
MolPort-047-919-625	422.342	0.55	11	8	2	2	4.17	Non-Absorbed	Non-Inhibitor	Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	0	Toxic	Safe	Safe
MolPort-002-627-625	440.502	5.81	3	1	1	4	7.44	Absorbed	Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	3	Safe	Toxic	Safe
MolPort-019-931-827	468.458	1.88	8	5	0	6	4.51	Non-Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	0	Toxic	Safe	Safe
MolPort-044-726-322	406.343	0.83	10	7	1	2	4.07	Non-Absorbed	Non-Inhibitor	Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	0	Toxic	Safe	Safe
MolPort-027-717-169	417.425	3.66	7	5	0	3	10.72	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	3	Safe	Safe	Safe
MolPort-046-594-248	406.343	0.99	10	7	1	2	4.09	Non-Absorbed	Non-Inhibitor	Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	0	Toxic	Safe	Safe
MolPort-001-950-661	477.389	3.19	9	2	0	6	6.4	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	4	Toxic	Safe	Toxic
Molport-051-887-909	298.258	-1.44	8	4	0	0	7.77	Absorbed	Non-Inhibitor	Substrate	Non-Penetrable	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	2	Safe	Safe	Safe
MolPort-028-855-220	488.448	3.4	9	2	0	5	9.12	Absorbed	Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	2	Safe	Safe	Safe
MolPort-001-928-000	651.679	5.32	10	3	2	8	6.5	Absorbed	Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Inhibitor	Inhibitor	4	Safe	Safe	Safe
MolPort-002-215-929	306.365	3.17	3	1	0	1	9.26	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	4	Safe	Safe	Safe
MolPort-000-687-716	623.625	4.62	10	3	1	10	6.99	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Inhibitor	Inhibitor	Inhibitor	Inhibitor	Inhibitor	5	Safe	Safe	Safe
MolPort-003-006-436	348.274	1.4	6	2	0	2	9.47	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	3	Toxic	Toxic	Safe
MolPort-003-006-403	345.314	1.73	5	4	0	1	10.98	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Inhibitor	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	4	Toxic	Safe	Safe
MolPort-003-	427.826	5.27	6	1	1	2	6.26	Absorbed	Inhibitor	Non-	Non-	Non-	Inhibitor	Inhibitor	Non-	Inhibitor	3	Toxic	Toxic	Safe

820-841										Substrate	Penetrable	Inhibitor				Inhibitor				
MolPort-046-426-269	654.624	8.56	10	6	3	5	5.95	Non-Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	1	Safe	Safe	Safe
MolPort-045-901-648	442.196	-0.15	12	4	1	2	3.49	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	0	Toxic	Safe	Safe
MolPort-002-818-270	393.24	4.6	3	2	0	2	9.73	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Inhibitor	Inhibitor	5	Toxic	Toxic	Safe
MolPort-000-701-102	329.224	2.45	7	2	0	3	2.33	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	2	Toxic	Safe	Safe
MolPort-002-705-119	451.49	5.15	8	1	1	3	6.95	Absorbed	Inhibitor	Substrate	Non-Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	2	Toxic	Safe	Safe
MolPort-035-717-384	357.369	4.63	6	3	0	3	6.69	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	1	Safe	Safe	Safe
MolPort-045-901-649	490.396	0.42	16	6	2	4	5.56	Non-Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	2	Safe	Toxic	Safe
MolPort-051-701-210	413.437	1.22	7	1	0	2	9.41	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Safe	Safe
MolPort-046-424-270	397.774	1.74	8	2	0	2	8.52	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	1	Safe	Safe	Safe
MolPort-002-354-089	499.483	1.58	10	1	0	6	4.44	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	1	Safe	Safe	Safe
MolPort-047-940-715	414.469	2.06	7	1	0	4	9.67	Absorbed	Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	0	Safe	Safe	Toxic
MolPort-000-687-712	655.623	4.08	12	3	2	10	6.66	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Inhibitor	Inhibitor	4	Safe	Safe	Safe
MolPort-046-423-501	393.355	1.11	9	2	0	3	9.07	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	0	Safe	Safe	Safe
MolPort-002-832-823	526.046	5.89	7	1	2	4	7.77	Absorbed	Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Safe	Safe
MolPort-002-013-820	426.436	2.67	8	1	0	3	6.28	Absorbed	Non-Inhibitor	Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	1	Toxic	Safe	Safe
MolPort-000-655-063	375.209	1.99	10	1	0	4	3.96	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	4	Toxic	Toxic	Safe
MolPort-027-715-758	473.533	4.86	8	4	0	5	9.58	Absorbed	Non-Inhibitor	Substrate	Non-Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	3	Safe	Safe	Safe
MolPort-003-	440.257	3.47	6	3	0	3	8.67	Absorbed	Non-	Non-	Penetrabl	Inhibitor	Inhibitor	Non-	Non-	Non-	2	Safe	Safe	Safe

049-585									Inhibitor	Substrate	e			Inhibitor	Inhibitor	Inhibitor				
MolPort-019-894-385	367.456	3.04	5	1	0	2	9.59	Absorbed	Inhibitor	Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	0	Toxic	Safe	Toxic
MolPort-002-320-665	472.862	3.39	7	4	0	4	7.79	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	2	Safe	Toxic	Safe
MolPort-003-049-556	405.414	2.54	7	2	0	5	10.45	Absorbed	Inhibitor	Non-Substrate	Non-Penetrable	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	2	Safe	Safe	Safe
MolPort-039-339-101	406.343	0.93	10	7	1	2	4.1	Non-Absorbed	Non-Inhibitor	Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	0	Toxic	Safe	Safe
MolPort-002-324-337	488.32	1.59	14	2	1	4	4.74	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	2	Toxic	Toxic	Safe
MolPort-016-585-919	374.783	4.16	5	1	0	2	6.96	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Non-Inhibitor	Inhibitor	Inhibitor	Inhibitor	4	Safe	Safe	Safe
MolPort-002-707-756	447.454	5.14	8	1	1	4	8.04	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	1	Toxic	Toxic	Safe
MolPort-019-891-799	330.391	2.79	5	1	0	1	9.36	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	1	Toxic	Safe	Toxic
MolPort-003-049-539	460.675	3.71	6	3	0	3	8.04	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	2	Safe	Safe	Safe
MolPort-051-707-281	391.381	2.23	5	1	0	2	6.6	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Safe	Safe
MolPort-020-213-942	353.429	2.55	5	2	0	2	10.06	Absorbed	Inhibitor	Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	1	Toxic	Safe	Toxic
MolPort-019-892-216	330.391	2.92	5	1	0	1	9.13	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	2	Toxic	Safe	Toxic
MolPort-019-897-723	322.387	2.89	4	1	0	1	7.73	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	1	Toxic	Safe	Toxic
MolPort-002-898-410	334.726	3.17	7	2	0	0	5.68	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	3	Toxic	Safe	Safe
MolPort-003-820-852	439.862	5.13	7	1	1	3	8.7	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Toxic	Safe
MolPort-051-747-507	413.485	0.7	7	2	0	2	7.34	Absorbed	Inhibitor	Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	Inhibitor	2	Toxic	Safe	Safe
MolPort-001-910-143	401.422	4.12	6	1	0	5	10.64	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	4	Safe	Safe	Safe
MolPort-051-	416.437	2.5	7	2	0	5	9.5	Absorbed	Non-	Non-	Penetrabl	Inhibitor	Inhibitor	Inhibitor	Non-	Inhibitor	4	Toxic	Toxic	Safe

714-950									Inhibitor	Substrate	e				Inhibitor					
MolPort-020-285-215	438.557	2.98	6	3	0	6	9.29	Absorbed	Non-Inhibitor	Substrate	Non-Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	3	Safe	Safe	Toxic
MolPort-020-185-105	383.455	2.75	5	1	0	2	8.55	Absorbed	Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Safe	Safe	Safe
MolPort-003-049-518	460.675	3.58	6	3	0	3	8.02	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	3	Safe	Safe	Safe
MolPort-002-579-380	300.383	4.16	5	2	0	2	10.23	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	3	Toxic	Toxic	Safe
MolPort-019-891-687	364.405	2.39	7	1	0	2	8.33	Absorbed	Non-Inhibitor	Substrate	Penetrable	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	Inhibitor	3	Toxic	Safe	Toxic
MolPort-051-713-269	320.396	3.08	5	1	0	1	10.56	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	2	Toxic	Safe	Safe
MolPort-003-049-565	454.284	3.29	6	2	0	4	10.29	Absorbed	Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	3	Safe	Safe	Safe
MolPort-019-882-833	342.805	3.12	4	1	0	1	7.28	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	Inhibitor	2	Toxic	Safe	Toxic
MolPort-002-702-237	448.28	3.83	7	1	0	3	8.26	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Safe	Safe
MolPort-023-312-760	382.379	4.14	6	2	0	3	5.04	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	1	Safe	Safe	Safe
MolPort-019-881-294	322.387	2.94	4	1	0	1	8.06	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	2	Toxic	Safe	Toxic
MolPort-001-946-431	388.228	4.06	5	1	0	1	7.14	Absorbed	Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Inhibitor	Inhibitor	4	Toxic	Toxic	Safe
MolPort-035-791-859	349.346	2.75	7	1	0	3	9.82	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Safe	Safe
MolPort-000-564-777	488.32	1.66	14	2	1	4	4.52	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	1	Safe	Toxic	Safe
MolPort-003-049-546	454.284	3.24	6	2	0	4	10.17	Absorbed	Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	4	Safe	Safe	Safe
MolPort-020-226-643	316.364	2.56	5	2	0	1	9.25	Absorbed	Inhibitor	Non-Substrate	Non-Penetrable	Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	2	Toxic	Safe	Toxic
MolPort-003-136-336	435.396	1.9	9	2	0	5	8.78	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	3	Safe	Safe	Safe
MolPort-019-884-150	316.408	3.11	4	1	0	2	9.5	Absorbed	Inhibitor	Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	1	Toxic	Safe	Toxic
MolPort-000-	499.483	2.06	10	3	0	8	5.61	Absorbed	Non-	Non-	Non-	Inhibitor	Non-	Inhibitor	Non-	Non-	2	Safe	Safe	Safe

687-714									Inhibitor	Substrate	Penetrable		Inhibitor		Inhibitor	Inhibitor				
MolPort-000-687-721	579.613	3.23	10	1	1	6	4.67	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	4	Toxic	Safe	Safe
MolPort-046-423-621	393.355	1.05	9	2	0	3	8.76	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	1	Safe	Safe	Safe
MolPort-003-872-830	254.245	1.75	4	3	0	1	9.19	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	3	Toxic	Safe	Safe
MolPort-003-049-485	426.23	2.94	6	3	0	3	8.21	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	3	Safe	Safe	Safe
MolPort-001-932-894	385.332	4.04	8	1	0	6	7.55	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	4	Toxic	Safe	Toxic
MolPort-000-687-718	609.643	1.82	12	1	2	6	3.11	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	1	Toxic	Safe	Safe
MolPort-020-005-868	422.342	0.66	11	8	2	2	4.14	Non-Absorbed	Non-Inhibitor	Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	0	Toxic	Safe	Safe
MolPort-007-573-074	443.872	3.92	7	3	0	4	11.05	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	4	Safe	Safe	Safe
MolPort-051-709-291	375.384	4.35	7	1	0	4	9.59	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Inhibitor	Inhibitor	5	Toxic	Safe	Safe
MolPort-003-049-550	405.414	2.85	7	3	0	5	8.61	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	2	Safe	Safe	Safe
MolPort-023-294-935	367.365	1.04	6	3	0	3	11.19	Absorbed	Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	0	Safe	Safe	Safe
MolPort-019-882-198	356.433	2.29	6	1	0	2	9.06	Absorbed	Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	0	Toxic	Safe	Toxic
MolPort-035-717-093	342.358	3.43	5	2	0	4	6.47	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	1	Safe	Safe	Safe
MolPort-001-901-710	343.777	4.01	5	1	0	1	7.27	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Inhibitor	Inhibitor	4	Toxic	Toxic	Safe
MolPort-019-902-148	356.433	2.55	6	1	0	2	9.67	Absorbed	Inhibitor	Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	1	Toxic	Toxic	Toxic
MolPort-003-006-406	356.385	2.58	4	2	0	2	11.31	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	3	Toxic	Safe	Safe
MolPort-020-	368.462	1.09	6	1	0	2	6.93	Absorbed	Non-	Non-	Penetrabl	Non-	Non-	Non-	Non-	Non-	0	Toxic	Safe	Toxic

219-143									Inhibitor	Substrate	e	Inhibitor	Inhibitor	Inhibitor	Inhibitor	Inhibitor				
MolPort-020-206-802	363.465	1.63	6	2	0	3	6.18	Absorbed	Non-Inhibitor	Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	0	Toxic	Safe	Toxic
MolPort-002-676-352	443.872	3.81	7	3	0	4	11.05	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	3	Safe	Safe	Safe
MolPort-003-006-400	358.313	2.31	5	2	0	2	10.44	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	3	Toxic	Safe	Safe
MolPort-002-702-550	445.482	4.4	7	1	0	5	8.88	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Safe	Safe
MolPort-019-883-508	362.433	2.28	6	1	0	1	8.93	Absorbed	Non-Inhibitor	Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	0	Toxic	Safe	Toxic
MolPort-046-423-784	381.319	1.25	8	2	0	2	8.61	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	0	Safe	Safe	Safe
MolPort-000-762-916	572.485	2.85	9	1	1	6	5.12	Absorbed	Inhibitor	Substrate	Penetrable	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	Inhibitor	3	Safe	Toxic	Toxic
MolPort-002-143-477	371.404	3.44	8	2	0	3	7.22	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	2	Toxic	Safe	Safe
MolPort-020-212-234	327.391	2.37	5	2	0	2	8.85	Absorbed	Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	2	Toxic	Safe	Safe
MolPort-047-945-626	278.172	-0.42	8	4	0	0	4.36	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	2	Safe	Safe	Safe
MolPort-002-621-739	347.374	2.53	4	2	0	4	8.75	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	3	Safe	Toxic	Safe
MolPort-051-750-750	304.353	2.61	5	1	0	1	9.72	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Safe	Safe
MolPort-047-116-039	482.485	2.33	9	4	0	3	7.28	Non-Absorbed	Non-Inhibitor	Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	0	Toxic	Safe	Safe
MolPort-019-891-038	363.421	0.72	6	2	0	4	7.59	Absorbed	Non-Inhibitor	Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	0	Toxic	Safe	Toxic
MolPort-051-715-534	352.401	2.8	6	1	0	4	9.91	Absorbed	Inhibitor	Non-Substrate	Non-Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	4	Toxic	Toxic	Toxic
MolPort-002-613-761	346.386	3.39	4	1	0	4	7.63	Absorbed	Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	4	Safe	Toxic	Safe
MolPort-002-205-898	484.346	6.09	6	1	1	4	7.87	Absorbed	Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Toxic	Safe

MolPort-020-226-391	367.456	3.19	5	1	0	4	8.19	Absorbed	Inhibitor	Substrate	Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Inhibitor	Inhibitor	4	Toxic	Safe	Safe
MolPort-000-186-321	414.874	2.93	7	1	0	3	6.98	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	Inhibitor	4	Safe	Safe	Toxic
MolPort-000-643-886	524.576	3.63	7	2	1	7	7.46	Absorbed	Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Safe	Safe	Safe
MolPort-002-192-090	384.355	3.01	8	1	0	3	7.14	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	2	Toxic	Toxic	Safe
MolPort-002-604-011	451.359	2.43	13	4	1	6	6.53	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Safe	Safe
MolPort-000-186-937	472.954	3.05	8	1	0	6	6.77	Absorbed	Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Inhibitor	Inhibitor	5	Safe	Safe	Toxic
MolPort-019-911-431	328.24	2.36	7	2	0	4	5.2	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Inhibitor	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	3	Toxic	Safe	Safe
MolPort-002-902-036	410.433	4.15	7	1	0	4	7.19	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	2	Safe	Safe	Safe
MolPort-002-708-473	396.41	3.06	7	1	0	2	6.8	Absorbed	Non-Inhibitor	Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	1	Toxic	Safe	Safe
MolPort-002-674-545	409.427	3.14	7	3	0	4	11.71	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	3	Safe	Safe	Safe
MolPort-002-834-001	433.446	4.96	6	1	0	4	7.42	Absorbed	Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Toxic	Safe
MolPort-051-706-801	334.423	3.69	5	1	0	2	9.87	Absorbed	Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Safe	Safe
MolPort-000-186-464	422.51	3.66	7	1	0	5	7.36	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Inhibitor	Inhibitor	5	Safe	Safe	Toxic
MolPort-023-295-946	381.392	2.09	7	2	0	3	12.65	Non-Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Safe	Safe	Safe
MolPort-001-962-958	532.581	5.11	9	1	2	7	7.15	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	2	Safe	Safe	Safe
MolPort-019-899-400	315.38	2.02	5	1	0	1	7.48	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	1	Toxic	Safe	Toxic
MolPort-003-049-553	389.415	3.24	6	2	0	5	10.35	Absorbed	Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	2	Safe	Safe	Safe
MolPort-044-	344.394	0.75	6	3	0	3	7.21	Absorbed	Non-	Substrate	Non-	Inhibitor	Non-	Non-	Non-	Non-	1	Toxic	Safe	Safe

830-678									Inhibitor		Penetrable		Inhibitor	Inhibitor	Inhibitor	Inhibitor			
MolPort-000-698-315	382.405	1.17	8	2	0	4	6.55	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Safe	Safe	Safe
MolPort-002-980-289	340.43	3.67	4	1	0	3	8.09	Absorbed	Inhibitor	Substrate	Penetrable	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	Inhibitor	3	Safe	Safe	Safe
MolPort-002-542-027	454.467	3.38	9	2	0	5	5.53	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Inhibitor	Inhibitor	3	Safe	Safe	Safe
MolPort-001-894-169	531.481	0.72	12	5	2	10	6.5	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	1	Safe	Safe	Safe
MolPort-003-007-815	392.212	3.37	3	2	0	1	10.53	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	3	Safe	Safe	Safe
MolPort-003-049-492	395.806	2.88	6	2	0	4	10.15	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	2	Safe	Safe	Safe
MolPort-003-049-507	409.833	3.52	6	2	0	5	10.1	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	2	Safe	Safe	Safe
MolPort-044-725-931	327.38	1.99	5	2	0	2	9.5	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	3	Safe	Safe	Toxic
MolPort-003-079-345	409.377	2.28	7	2	0	5	9.69	Absorbed	Inhibitor	Non-Substrate	Penetrable	Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	1	Safe	Safe	Safe
MolPort-003-899-968	420.202	2.01	12	2	1	4	-0.77	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Inhibitor	Inhibitor	4	Toxic	Safe	Safe
MolPort-000-793-958	424.371	3.84	9	2	0	5	7.17	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Safe	Toxic	Safe
MolPort-000-765-961	435.36	0.1	11	2	1	6	6.42	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	0	Toxic	Safe	Safe
MolPort-020-229-604	278.359	2.72	4	2	0	1	8.69	Absorbed	Inhibitor	Substrate	Penetrable	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	2	Toxic	Safe	Safe
MolPort-019-899-423	347.374	3.93	6	2	0	4	8.95	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	4	Toxic	Safe	Safe
MolPort-002-987-633	308.341	2.33	6	1	0	1	6.45	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	Inhibitor	3	Toxic	Safe	Safe
MolPort-001-894-048	353.341	3.4	7	1	0	1	6.75	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Inhibitor	Inhibitor	4	Toxic	Toxic	Safe
MolPort-023-296-727	357.801	3	5	2	0	2	12.11	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Safe	Safe

MolPort-001-995-820	355.357	2.55	7	2	0	2	6.94	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	2	Toxic	Toxic	Safe
MolPort-051-710-091	344.374	2.83	5	2	0	5	8.36	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	3	Toxic	Toxic	Safe
MolPort-003-049-574	389.415	3.28	6	2	0	5	10.43	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	2	Safe	Safe	Safe
MolPort-051-701-253	423.398	2.65	5	1	0	2	7.02	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Inhibitor	Inhibitor	4	Safe	Safe	Safe
MolPort-020-230-701	367.412	2.46	6	2	0	2	7.98	Absorbed	Inhibitor	Non-Substrate	Non-Penetrable	Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	1	Toxic	Safe	Toxic
MolPort-019-881-663	375.48	2.29	7	1	0	2	8.09	Absorbed	Non-Inhibitor	Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	0	Toxic	Safe	Toxic
MolPort-020-204-996	334.379	2.1	6	2	0	2	8.03	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	1	Toxic	Safe	Toxic
MolPort-000-687-720	555.591	3.23	10	3	1	6	5.71	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	2	Safe	Safe	Safe
MolPort-019-890-966	350.422	2.7	6	1	0	3	9.25	Absorbed	Non-Inhibitor	Substrate	Penetrable	Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	1	Toxic	Safe	Toxic
MolPort-003-006-442	355.397	3.68	3	2	0	2	11.22	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	3	Toxic	Safe	Safe
MolPort-051-714-445	389.846	2.51	5	1	0	2	8.3	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Inhibitor	Inhibitor	4	Safe	Safe	Safe
MolPort-019-891-339	348.406	2.41	6	1	0	2	7.69	Absorbed	Non-Inhibitor	Substrate	Penetrable	Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	1	Toxic	Safe	Toxic
MolPort-003-006-439	359.41	2.95	4	2	0	2	10.81	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	4	Toxic	Safe	Safe
MolPort-003-363-804	405.414	2.4	7	2	0	5	10.02	Absorbed	Inhibitor	Non-Substrate	Non-Penetrable	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	2	Safe	Safe	Safe
MolPort-019-901-650	364.449	2.05	6	1	0	4	9.28	Absorbed	Non-Inhibitor	Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	1	Toxic	Safe	Toxic
MolPort-051-752-399	346.39	3.11	5	2	0	4	5.8	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Inhibitor	Inhibitor	5	Safe	Safe	Safe
MolPort-002-181-677	463.472	4.41	7	1	0	5	8.39	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Safe	Safe
MolPort-035-881-696	397.391	2.11	8	2	0	3	11.62	Non-Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	4	Safe	Safe	Safe
MolPort-020-	370.412	3.6	5	2	0	6	9.18	Absorbed	Non-	Non-	Penetrabl	Inhibitor	Inhibitor	Inhibitor	Non-	Inhibitor	4	Toxic	Toxic	Toxic

200-832									Inhibitor	Substrate	e				Inhibitor					
MolPort-019-718-522	362.307	3.9	4	1	0	3	9.13	Absorbed	Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	2	Toxic	Safe	Safe
MolPort-007-686-452	345.742	2.32	6	1	0	2	7.5	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	1	Safe	Safe	Safe
MolPort-019-889-309	308.385	2.33	5	1	0	1	7.92	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	2	Toxic	Safe	Toxic
MolPort-020-217-476	344.34	2.83	4	2	0	1	7.18	Absorbed	Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	Inhibitor	2	Toxic	Safe	Toxic
MolPort-051-709-211	360.421	1.95	7	2	0	3	9.49	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	2	Toxic	Safe	Toxic
MolPort-046-424-758	311.257	0.11	9	2	0	1	6.77	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	1	Safe	Toxic	Safe
209769	339.358	3.52	6	1	0	2	8.56	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Safe	Safe
MolPort-007-565-121	267.284	3.26	4	1	0	2	9.99	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	3	Toxic	Safe	Safe
MolPort-003-162-025	421.413	2.07	8	2	0	6	10.15	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Safe	Safe
MolPort-019-894-202	348.406	2.34	6	1	0	2	7.74	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	0	Toxic	Safe	Toxic
MolPort-051-706-566	349.442	-0.01	7	2	0	1	9.22	Absorbed	Non-Inhibitor	Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	0	Toxic	Safe	Toxic
MolPort-001-962-992	438.487	5.27	6	1	1	5	5.77	Absorbed	Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	1	Toxic	Safe	Safe
MolPort-019-900-421	361.401	3.85	6	1	0	5	9.57	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Safe	Toxic
MolPort-020-232-770	359.433	2.7	6	2	0	2	7.88	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	1	Toxic	Safe	Safe
MolPort-000-774-030	455.341	2.93	11	2	1	6	6.97	Absorbed	Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Safe	Safe
MolPort-002-974-989	415.471	2.9	6	3	0	3	6.95	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	3	Safe	Safe	Safe
MolPort-051-700-967	388.475	2.93	7	2	0	3	8.83	Absorbed	Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	2	Toxic	Toxic	Toxic
MolPort-002-549-400	496.504	3.36	10	1	0	6	5.5	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	1	Safe	Safe	Safe

MolPort-002-709-867	420.497	5.12	6	1	1	5	6.1	Absorbed	Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	1	Safe	Safe	Safe
MolPort-028-960-099	380.245	4.94	4	1	0	3	10.3	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	4	Toxic	Safe	Safe
MolPort-020-192-827	379.464	1.84	6	3	0	4	6.31	Absorbed	Non-Inhibitor	Substrate	Penetrable	Non-Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	1	Safe	Safe	Toxic
MolPort-002-696-141	343.228	3.28	4	1	0	1	6.49	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	2	Safe	Safe	Safe
MolPort-051-751-750	335.342	2.49	6	1	0	2	7.78	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	2	Toxic	Safe	Safe
MolPort-039-138-765	278.172	0.17	8	4	0	0	4.67	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	2	Safe	Safe	Safe
MolPort-001-917-885	369.384	2.94	7	1	0	3	8.49	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Safe	Safe
MolPort-051-711-243	281.315	2.08	5	2	0	1	7.51	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	2	Toxic	Safe	Safe
MolPort-051-746-168	370.46	2.25	6	1	0	3	8.96	Absorbed	Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	1	Toxic	Safe	Toxic
MolPort-003-049-577	405.414	2.46	7	2	0	5	10.09	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	2	Safe	Safe	Safe
MolPort-009-765-630	283.243	1.19	4	3	0	2	6.89	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	0	Safe	Safe	Safe
MolPort-002-810-877	441.512	5.43	6	1	1	4	10.4	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Safe	Safe
MolPort-020-191-152	335.411	2.04	5	2	0	3	6.8	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	1	Toxic	Safe	Safe
MolPort-001-982-700	411.465	4.13	7	1	0	5	8.17	Absorbed	Non-Inhibitor	Substrate	Non-Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	2	Toxic	Safe	Safe
MolPort-051-705-300	392.503	3.42	6	1	0	5	8.26	Absorbed	Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	1	Toxic	Safe	Toxic
MolPort-002-579-250	446.328	2.09	11	1	1	8	6.06	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	4	Toxic	Safe	Safe
MolPort-046-423-862	355.31	0	10	2	0	3	6.8	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	1	Safe	Toxic	Safe
MolPort-051-715-424	392.459	1.9	6	1	0	4	6.98	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	1	Toxic	Safe	Safe

MolPort-020-230-229	336.395	1.63	6	2	0	3	9.84	Absorbed	Non-Inhibitor	Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	0	Toxic	Safe	Toxic
MolPort-000-187-256	454.508	1.52	9	2	0	7	6.73	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	Inhibitor	4	Safe	Toxic	Toxic
MolPort-051-706-661	404.426	2.46	7	2	0	7	9.54	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Safe	Toxic
MolPort-001-837-962	238.246	1.68	3	2	0	1	10.18	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	3	Toxic	Toxic	Safe
MolPort-020-220-856	343.412	0.84	6	3	0	3	6.38	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	1	Safe	Safe	Safe
MolPort-001-934-016	597.539	4.19	12	1	2	8	5.47	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Inhibitor	Inhibitor	5	Toxic	Safe	Safe
MolPort-000-773-043	451.359	0.1	12	3	1	6	6.14	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	0	Toxic	Safe	Safe
MolPort-020-201-123	331.423	3.37	4	2	0	3	9.3	Absorbed	Inhibitor	Non-Substrate	Penetrable	Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	Inhibitor	3	Toxic	Safe	Toxic
MolPort-051-710-820	390.447	2.18	8	2	0	4	9.74	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	2	Toxic	Safe	Toxic
MolPort-002-716-525	418.482	3.97	8	2	0	6	5.71	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Inhibitor	Inhibitor	3	Safe	Safe	Safe
MolPort-000-907-432	357.442	3.92	6	2	0	3	7.58	Absorbed	Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Inhibitor	Inhibitor	4	Toxic	Safe	Safe
MolPort-044-724-431	371.462	2.8	3	2	0	3	8.06	Absorbed	Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	4	Safe	Safe	Safe
MolPort-001-962-956	498.52	3.89	10	2	0	7	5.78	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	1	Safe	Safe	Safe
MolPort-000-516-174	264.332	2.27	4	1	0	1	6.88	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	0	Toxic	Safe	Safe
MolPort-020-194-144	310.788	2.73	4	2	0	1	9.01	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	2	Toxic	Safe	Toxic
MolPort-002-716-733	451.953	4.23	5	2	0	5	6.72	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Safe	Safe	Safe
MolPort-000-185-485	456.527	3.76	7	1	0	4	8.56	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Inhibitor	Inhibitor	5	Safe	Safe	Toxic
MolPort-002-709-416	397.438	3.73	7	1	0	5	8.44	Absorbed	Non-Inhibitor	Substrate	Non-Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Safe	Safe

MolPort-020-232-406	318.384	1.32	6	1	0	1	7.22	Absorbed	Non-Inhibitor	Non-Substrate	e Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	0	Toxic	Safe	Toxic
MolPort-051-709-459	417.425	3.17	8	2	0	6	9.37	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Toxic	Toxic
Molport-051-866-696	339.351	1.91	6	2	0	4	5.32	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	0	Safe	Toxic	Safe
MolPort-007-563-352	527.506	5.5	7	1	2	6	7.56	Absorbed	Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	2	Toxic	Safe	Safe
MolPort-002-980-292	333.222	3.55	4	1	0	1	5.99	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	Inhibitor	3	Toxic	Safe	Toxic
MolPort-020-185-537	330.391	3.66	5	1	0	4	9.7	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	4	Safe	Safe	Safe
MolPort-001-946-423	383.411	3.26	7	1	0	4	8.46	Absorbed	Non-Inhibitor	Substrate	Non-Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	2	Toxic	Safe	Safe
MolPort-001-890-573	325.331	3.14	6	2	0	1	6.99	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Inhibitor	Inhibitor	4	Toxic	Toxic	Safe
MolPort-001-675-116	370.408	4.67	4	1	0	4	10.74	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	2	Safe	Safe	Safe
MolPort-002-819-920	396.752	4.3	4	1	0	3	8.86	Absorbed	Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	2	Toxic	Safe	Safe
MolPort-008-336-200	255.233	1.33	3	3	0	2	5.82	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	0	Safe	Safe	Safe
MolPort-051-713-178	390.447	2.04	8	2	0	4	9.51	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	2	Toxic	Safe	Toxic
MolPort-000-424-555	356.33	3.86	7	2	0	4	8.91	Absorbed	Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Inhibitor	Inhibitor	5	Safe	Safe	Safe
MolPort-051-709-827	292.302	0.88	7	1	0	1	9.82	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	0	Toxic	Safe	Safe
MolPort-002-136-113	453.483	4.76	8	1	0	6	5.61	Absorbed	Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Toxic	Safe
MolPort-001-946-425	383.411	3.18	7	1	0	4	8.43	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	2	Toxic	Safe	Safe
MolPort-051-714-040	319.364	2.09	5	2	0	2	9.5	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	2	Toxic	Safe	Safe
MolPort-002-173-697	394.394	2.53	8	1	0	4	8.02	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrabl	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	1	Toxic	Safe	Safe

MolPort-000-414-107	345.387	4.01	7	2	0	3	8.59	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	2	Safe	Safe	Safe
MolPort-003-079-340	393.378	3.1	6	2	0	5	10.01	Absorbed	Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	2	Safe	Safe	Safe
MolPort-023-298-059	323.356	2.36	5	2	0	2	12.6	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	2	Toxic	Safe	Safe
MolPort-019-890-020	303.325	2.99	5	2	0	1	9.74	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Inhibitor	Inhibitor	Inhibitor	Inhibitor	Inhibitor	5	Toxic	Toxic	Safe
MolPort-019-915-631	338.319	2.94	6	1	0	3	10.11	Absorbed	Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Inhibitor	Inhibitor	5	Toxic	Safe	Safe
MolPort-001-949-351	494.551	5.42	7	1	1	8	6.45	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	2	Safe	Safe	Safe
MolPort-019-890-870	334.427	2.04	6	1	0	2	8.66	Absorbed	Non-Inhibitor	Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	0	Toxic	Safe	Toxic
MolPort-051-712-243	317.352	2.4	6	1	0	3	9.64	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Safe	Safe
MolPort-020-191-312	308.389	1.98	6	1	0	2	7.13	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	0	Toxic	Safe	Safe
MolPort-000-683-901	345.402	4.98	5	1	0	4	10.64	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	4	Toxic	Safe	Safe
MolPort-020-221-948	338.411	2.65	6	2	0	4	7.28	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	Inhibitor	2	Safe	Safe	Toxic
MolPort-020-196-180	334.423	3.42	5	2	0	3	9.18	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	Inhibitor	4	Toxic	Safe	Toxic
MolPort-028-960-568	428.261	4.88	5	1	0	5	8.6	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	4	Toxic	Safe	Safe
MolPort-000-781-376	406.381	3.78	9	2	0	5	7.95	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Safe	Toxic	Safe
MolPort-051-711-816	317.295	2.56	5	1	0	3	6.42	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	2	Toxic	Safe	Safe
MolPort-051-702-804	358.401	2.49	6	1	0	4	10.12	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Safe	Safe	Safe
MolPort-019-718-525	326.327	3.81	4	1	0	3	10.02	Absorbed	Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Safe	Safe
MolPort-007-686-455	356.294	1.3	8	1	0	3	6.28	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	0	Toxic	Safe	Safe

MolPort-000-683-902	345.402	4.84	5	1	0	4	10.57	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	4	Toxic	Safe	Safe
MolPort-002-795-814	384.435	4.92	4	1	0	5	10.41	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	2	Safe	Safe	Safe
MolPort-019-718-524	326.327	3.6	4	1	0	3	9.9	Absorbed	Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	4	Toxic	Safe	Safe
MolPort-002-743-126	459.918	4.01	8	1	0	4	7.41	Absorbed	Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	2	Toxic	Toxic	Safe
MolPort-020-198-282	366.371	3.32	5	1	0	3	5.38	Absorbed	Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	Inhibitor	3	Toxic	Safe	Toxic
MolPort-003-162-015	405.414	2.85	7	2	0	6	10.29	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	2	Safe	Safe	Safe
MolPort-019-718-520	346.745	3.85	4	1	0	3	9.19	Absorbed	Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	4	Toxic	Safe	Safe
MolPort-001-960-314	555.457	6.2	7	1	2	8	7.08	Absorbed	Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	1	Safe	Safe	Safe
MolPort-001-962-997	378.457	3.31	7	1	0	4	6.34	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	1	Toxic	Safe	Safe
MolPort-002-136-108	455.326	4.81	7	2	0	5	5.29	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Inhibitor	Inhibitor	3	Toxic	Safe	Safe
MolPort-019-718-530	326.327	3.67	4	1	0	3	10.04	Absorbed	Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Safe	Safe
MolPort-039-053-544	285.259	1.45	4	3	0	3	8.9	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	0	Safe	Safe	Safe
MolPort-051-751-324	390.447	3.58	8	2	0	6	8.96	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	3	Safe	Safe	Toxic
MolPort-019-718-532	342.782	4.31	4	1	0	3	10.6	Absorbed	Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Safe	Safe
MolPort-002-543-666	476.561	5.66	7	1	1	7	7.21	Absorbed	Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	1	Toxic	Safe	Safe
MolPort-019-880-958	362.389	2.4	7	1	0	5	9.41	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	2	Safe	Safe	Toxic
MolPort-051-703-822	276.299	1.88	5	1	0	1	7.94	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	1	Toxic	Safe	Safe
MolPort-051-	299.761	3.41	4	1	0	1	8.9	Absorbed	Non-	Non-	Penetrabl	Inhibitor	Inhibitor	Inhibitor	Non-	Inhibitor	4	Toxic	Safe	Safe

706-546									Inhibitor	Substrate	e				Inhibitor					
MolPort-035-717-166	405.255	3.72	5	1	0	2	4.46	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	1	Toxic	Safe	Safe
MolPort-020-224-643	368.444	1.96	6	2	0	2	9	Absorbed	Inhibitor	Substrate	Non-Penetrable	Non-Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	2	Toxic	Safe	Toxic
MolPort-019-894-153	346.434	3.04	5	1	0	4	8.61	Absorbed	Inhibitor	Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	1	Toxic	Safe	Toxic
MolPort-007-549-977	362.307	4.03	4	1	0	3	9.47	Absorbed	Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	2	Toxic	Safe	Safe
MolPort-007-563-331	446.488	3.61	9	3	0	7	5.62	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	2	Safe	Safe	Safe
MolPort-020-221-031	347.466	2.17	5	1	0	3	7.25	Absorbed	Non-Inhibitor	Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	0	Toxic	Safe	Toxic
MolPort-019-718-499	322.364	4	4	1	0	3	10.7	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	4	Safe	Safe	Safe
MolPort-002-697-644	409.322	2.38	12	2	1	6	6.72	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	4	Toxic	Toxic	Safe
MolPort-019-718-511	330.29	3.39	4	1	0	3	8.91	Absorbed	Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Safe	Safe
MolPort-019-718-529	342.782	4.32	4	1	0	3	10.51	Absorbed	Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	4	Toxic	Safe	Safe
MolPort-020-198-856	354.435	2.22	7	1	0	2	6.7	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	0	Toxic	Safe	Toxic
5486762	482.558	4.25	8	2	0	8	6.04	Absorbed	Inhibitor	Substrate	Penetrable	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	Inhibitor	4	Toxic	Safe	Toxic
MolPort-020-216-800	335.455	3.58	5	1	0	4	7.92	Absorbed	Non-Inhibitor	Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	Inhibitor	2	Toxic	Safe	Safe
MolPort-019-915-629	336.391	4.28	4	1	0	4	10.35	Absorbed	Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	4	Toxic	Safe	Safe
MolPort-047-920-097	344.394	0.75	6	3	0	3	7.21	Absorbed	Non-Inhibitor	Substrate	Non-Penetrable	Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	1	Toxic	Safe	Safe
MolPort-000-643-948	481.507	4.1	7	1	0	6	7.13	Absorbed	Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	4	Safe	Safe	Safe
MolPort-020-203-117	335.411	2.3	6	1	0	3	8.4	Absorbed	Non-Inhibitor	Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	0	Toxic	Safe	Toxic
MolPort-019-718-537	342.782	4.25	4	1	0	3	10.63	Absorbed	Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Safe	Safe
MolPort-051-711-701	380.448	2.36	6	2	0	4	7.33	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	1	Safe	Safe	Safe
MolPort-007-	338.319	2.63	5	2	0	4	7.32	Absorbed	Non-	Non-	Non-	Non-	Non-	Non-	Non-	Non-	0	Safe	Safe	Safe

902-862									Inhibitor	Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Inhibitor	Inhibitor			
MolPort-020-230-030	361.405	3.49	7	1	0	5	7.7	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	3	Safe	Safe	Safe
MolPort-020-217-311	360.82	3.25	5	1	0	3	5.67	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	Inhibitor	2	Toxic	Safe	Toxic
MolPort-019-915-635	342.782	4.32	4	1	0	3	10.49	Absorbed	Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Safe	Safe
MolPort-005-914-353	415.409	1.96	7	3	0	3	8.77	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	3	Safe	Safe	Safe
MolPort-000-516-180	294.358	2.53	5	1	0	2	7.63	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	0	Toxic	Safe	Safe
MolPort-019-718-526	326.327	3.78	4	1	0	3	9.86	Absorbed	Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	4	Toxic	Safe	Safe
MolPort-000-516-177	324.384	1.92	6	1	0	3	7.63	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	0	Toxic	Safe	Safe
MolPort-019-718-512	330.29	3.29	4	1	0	3	8.61	Absorbed	Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Safe	Safe
MolPort-020-194-954	300.749	1.86	5	3	0	1	6.02	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	2	Toxic	Safe	Safe
MolPort-051-710-656	319.286	3.1	4	1	0	1	6.65	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	2	Safe	Safe	Safe
MolPort-009-753-850	342.358	2.16	6	1	0	3	4.69	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	1	Toxic	Safe	Safe
MolPort-051-716-861	348.366	0.94	7	2	0	5	7.6	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	2	Toxic	Toxic	Safe
MolPort-019-718-494	322.364	3.87	4	1	0	3	10.95	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	3	Safe	Safe	Safe
MolPort-002-699-190	394.42	3.28	10	2	0	5	7.43	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	4	Safe	Safe	Safe
MolPort-000-252-466	333.269	2.37	3	2	0	2	8.72	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	2	Safe	Safe	Safe
MolPort-051-705-481	378.476	3.09	6	1	0	5	7.8	Absorbed	Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	1	Safe	Safe	Toxic
MolPort-051-714-989	394.475	2.02	7	1	0	6	5.23	Absorbed	Non-Inhibitor	Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	1	Safe	Safe	Safe
MolPort-020-221-440	364.474	1.97	6	3	0	1	7.59	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	2	Toxic	Safe	Safe
MolPort-007-550-711	397.456	2.92	6	2	0	4	9.79	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	4	Toxic	Safe	Safe
MolPort-000-	437.887	4.61	6	2	0	5	5.33	Absorbed	Non-	Non-	Penetrabl	Non-	Non-	Inhibitor	Inhibitor	Non-	2	Safe	Safe	Safe

919-038									Inhibitor	Substrate	e	Inhibitor	Inhibitor			Inhibitor			
MolPort-019-718-531	342.782	3.96	4	1	0	3	10.41	Absorbed	Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	4	Toxic	Safe	Safe
MolPort-019-718-513	330.29	3.53	4	1	0	3	8.93	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Safe	Safe
MolPort-001-900-105	455.768	5.72	5	1	1	4	6.82	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Safe	Safe
MolPort-000-516-179	308.385	2.85	5	1	0	3	7.29	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	0	Toxic	Safe	Safe
MolPort-051-740-607	392.415	3.32	8	1	0	6	9.29	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	2	Safe	Safe	Toxic
MolPort-051-749-485	418.453	3.31	7	2	0	7	9.36	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	4	Toxic	Safe	Toxic
MolPort-003-910-837	330.208	2.85	8	2	0	2	2.88	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Inhibitor	Non-Inhibitor	Inhibitor	Inhibitor	Inhibitor	4	Toxic	Toxic	Safe
MolPort-002-253-629	356.454	4.77	5	1	0	4	7.15	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Safe	Safe
MolPort-001-674-842	376.334	4.28	4	1	0	4	9.11	Absorbed	Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	2	Safe	Safe	Safe
MolPort-019-898-122	361.401	3.37	6	2	0	6	10.18	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	4	Toxic	Safe	Safe
MolPort-019-718-519	346.745	3.85	4	1	0	3	9.76	Absorbed	Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Safe	Safe
MolPort-000-919-039	463.006	5.68	6	1	1	5	5.97	Absorbed	Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	2	Safe	Safe	Safe
MolPort-007-551-397	337.335	1.98	5	2	0	4	10.75	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	2	Toxic	Toxic	Safe
MolPort-019-718-518	346.745	3.78	4	1	0	3	9.31	Absorbed	Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Safe	Safe
MolPort-019-718-523	362.307	3.91	4	1	0	3	9.49	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	2	Toxic	Safe	Safe
MolPort-020-219-464	294.362	0.65	6	1	0	1	9.09	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	0	Toxic	Safe	Safe
MolPort-051-707-825	307.313	1.66	6	2	0	2	9.64	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	3	Toxic	Toxic	Safe
MolPort-007-550-707	363.2	4.29	4	1	0	3	10.38	Absorbed	Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Safe	Safe
MolPort-020-228-653	333.395	3.38	6	1	0	4	8.49	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	4	Safe	Safe	Safe

MolPort-002-549-717	420.881	4.19	7	2	0	5	5.29	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Inhibitor	Non-Inhibitor	Inhibitor	Inhibitor	Inhibitor	4	Safe	Safe	Safe
MolPort-051-710-375	355.401	1.78	5	1	0	2	7.9	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Safe	Safe	Safe
MolPort-005-914-045	413.393	2.46	7	2	0	2	10.04	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	4	Safe	Safe	Safe
MolPort-020-224-371	360.421	1.72	7	2	0	3	8.72	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	Inhibitor	2	Toxic	Safe	Toxic
MolPort-000-768-222	347.374	2.32	5	2	0	4	8.08	Absorbed	Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	4	Safe	Toxic	Safe
MolPort-002-551-254	365.254	2.65	4	2	0	2	4.4	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Safe	Safe	Safe
MolPort-001-949-347	570.472	6.14	7	2	2	8	7.23	Absorbed	Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	1	Safe	Safe	Safe
MolPort-044-830-674	539.705	4.83	5	3	1	9	8.81	Absorbed	Inhibitor	Substrate	Non-Penetrable	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Safe	Toxic
MolPort-003-717-048	411.483	3.19	6	2	0	5	9.59	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	3	Toxic	Toxic	Safe
MolPort-051-703-908	404.426	2.92	7	2	0	7	9.72	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	4	Toxic	Safe	Toxic
MolPort-019-718-497	336.391	4.35	4	1	0	4	10.39	Absorbed	Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Safe	Safe
MolPort-020-213-922	361.43	1.58	6	1	0	2	7.66	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Safe	Safe
MolPort-001-895-542	367.368	3.21	7	1	0	2	7.86	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	1	Toxic	Safe	Safe
MolPort-002-799-624	326.359	2.65	5	1	0	2	4.1	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	1	Toxic	Safe	Safe
MolPort-002-987-635	322.412	3.34	5	1	0	4	8.59	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	Inhibitor	2	Toxic	Safe	Toxic
MolPort-000-706-303	452.495	4.31	8	1	0	5	4.8	Absorbed	Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	1	Safe	Safe	Safe
100641419	310.309	2.45	5	2	0	3	9.06	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Safe	Safe
MolPort-020-	331.379	1.99	6	1	0	3	9.28	Absorbed	Non-	Non-	Penetrabl	Non-	Inhibitor	Inhibitor	Non-	Inhibitor	3	Toxic	Safe	Safe

202-716									Inhibitor	Substrate	e	Inhibitor			Inhibitor						
Molport-051-890-546	326.469	3.66	5	1	0	1	5.77	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	1	Safe	Safe	Safe
MolPort-019-880-584	330.844	2.47	5	1	0	1	7.27	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	2	Toxic	Safe	Toxic
MolPort-002-943-075	308.337	3.46	4	1	0	3	10.84	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	3	Safe	Toxic	Safe
MolPort-001-662-632	351.413	4.58	5	1	0	2	8.58	Absorbed	Non-Inhibitor	Substrate	Non-Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	2	Toxic	Safe	Safe
MolPort-029-941-996	351.362	1.82	5	2	0	4	10.81	Absorbed	Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Safe	Safe
MolPort-000-773-164	425.39	2.53	12	2	1	6	7.34	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Safe	Safe
MolPort-000-683-903	359.429	5.38	5	1	1	5	10.33	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	4	Toxic	Safe	Safe
MolPort-001-029-034	319.368	3.65	6	1	0	3	7.66	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Safe	Safe
MolPort-020-216-294	334.335	2.03	6	2	0	5	8.21	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	3	Toxic	Toxic	Safe
MolPort-002-716-041	433.507	3.71	6	2	0	6	7.65	Absorbed	Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Safe	Safe	Safe
MolPort-003-717-200	379.441	4	6	1	0	3	7.84	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	4	Toxic	Safe	Safe
MolPort-020-246-946	310.309	2.45	5	2	0	3	9.06	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Safe	Safe
MolPort-002-742-435	443.463	3.51	8	1	0	4	7.16	Absorbed	Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	2	Toxic	Toxic	Safe
MolPort-027-836-659	328.368	2.9	6	3	0	5	6.76	Absorbed	Non-Inhibitor	Substrate	Non-Penetrable	Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	2	Toxic	Toxic	Toxic
MolPort-000-755-699	437.351	2.96	11	2	1	6	7.56	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Safe	Safe
MolPort-019-718-495	322.364	3.85	4	1	0	4	10.8	Absorbed	Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	4	Safe	Toxic	Safe
MolPort-051-706-455	350.403	2.42	6	2	0	5	7.86	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	4	Toxic	Toxic	Safe
MolPort-000-727-234	442.544	5.46	7	1	1	7	6.46	Absorbed	Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	2	Safe	Safe	Safe

MolPort-051-716-066	335.367	2.54	7	1	0	4	9.38	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Safe	Safe
MolPort-002-980-294	384.483	4.31	5	1	0	5	8.4	Absorbed	Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	Inhibitor	3	Safe	Safe	Safe
MolPort-006-249-105	362.845	4.92	5	1	0	3	6.98	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	4	Toxic	Safe	Safe
MolPort-019-718-538	342.326	2.95	5	1	0	4	9.59	Absorbed	Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Safe	Safe
MolPort-001-963-002	418.434	2.77	9	4	0	5	5.96	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	2	Safe	Safe	Safe
MolPort-019-718-510	330.29	3.34	4	1	0	3	8.83	Absorbed	Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Safe	Safe
MolPort-019-718-507	366.373	3.62	6	1	0	5	10.22	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	4	Safe	Safe	Safe
MolPort-002-624-357	487.263	4.28	11	2	1	5	7.86	Absorbed	Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	4	Toxic	Safe	Safe
MolPort-019-718-521	346.745	3.9	4	1	0	3	9.6	Absorbed	Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Safe	Safe
MolPort-002-573-601	378.352	2.89	10	2	0	5	7.48	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	4	Safe	Safe	Safe
MolPort-000-769-329	409.322	1.98	12	2	1	6	6.87	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Toxic	Safe
MolPort-051-708-566	305.341	2.6	6	1	0	3	9.36	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Safe	Safe
MolPort-002-795-672	336.347	2.6	5	1	0	4	10.27	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	2	Safe	Toxic	Safe
MolPort-051-710-009	352.438	2.6	6	1	0	5	7.89	Absorbed	Non-Inhibitor	Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	1	Safe	Safe	Toxic
MolPort-051-714-074	344.374	2.18	5	1	0	2	7.85	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Safe	Toxic	Safe
MolPort-019-896-288	305.341	2.53	6	1	0	3	9.15	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Safe	Safe
MolPort-020-206-505	308.389	1.17	6	1	0	1	8.62	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	0	Toxic	Safe	Toxic
MolPort-051-713-459	354.479	2.94	6	1	0	3	6.33	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	Inhibitor	3	Toxic	Safe	Safe
MolPort-019-718-514	328.755	3.6	4	1	0	3	10.3	Absorbed	Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	4	Toxic	Safe	Safe
MolPort-001-889-450	325.331	3.09	6	2	0	1	6.82	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	3	Toxic	Toxic	Safe

MolPort-051-701-693	349.394	3.01	7	1	0	4	9.07	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Safe	Safe
MolPort-019-718-515	328.755	3.71	4	1	0	3	10.81	Absorbed	Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Safe	Safe
MolPort-003-079-385	407.386	2.24	8	3	0	5	9.18	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	1	Toxic	Safe	Safe
MolPort-051-711-774	325.368	2.34	6	1	0	2	8.41	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	1	Toxic	Safe	Safe
MolPort-051-707-783	309.325	2.39	6	1	0	2	8.17	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	1	Toxic	Safe	Safe
MolPort-007-550-922	322.364	3.7	4	1	0	4	10.56	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	3	Safe	Toxic	Safe
MolPort-003-715-600	377.227	4.55	4	1	0	4	10.06	Absorbed	Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	2	Safe	Safe	Safe
MolPort-007-554-472	326.327	3.48	4	1	0	4	9.69	Absorbed	Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	2	Safe	Safe	Safe
MolPort-003-717-671	337.335	1.57	5	2	0	4	11.3	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	2	Toxic	Toxic	Safe
MolPort-007-553-491	350.374	2.86	5	1	0	5	10	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	2	Safe	Toxic	Safe
MolPort-002-272-806	456.571	5.62	7	1	1	7	6.2	Absorbed	Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Safe	Safe	Safe
MolPort-006-249-222	450.365	4.84	6	1	0	4	7.02	Absorbed	Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Safe	Safe
MolPort-002-819-904	342.782	3.95	4	1	0	4	10.36	Absorbed	Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	2	Safe	Safe	Safe
MolPort-003-013-116	322.364	3.73	4	1	0	4	10.49	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	3	Safe	Toxic	Safe
MolPort-051-713-217	339.395	2.29	6	2	0	5	9.45	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	2	Safe	Safe	Safe
MolPort-006-249-218	454.353	4.27	7	1	0	5	6.19	Absorbed	Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Toxic	Safe
MolPort-000-760-018	437.351	2.88	11	2	1	6	7.55	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Safe	Safe
MolPort-019-890-080	308.385	2.41	5	1	0	2	8.64	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	1	Toxic	Safe	Toxic
MolPort-051-711-337	351.391	1.43	7	2	0	5	8.13	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Toxic	Safe
MolPort-020-220-858	344.418	3.31	5	1	0	3	7.51	Absorbed	Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Inhibitor	Inhibitor	3	Safe	Safe	Toxic

MolPort-002-677-694	374.875	4.42	4	1	0	3	7.99	Absorbed	Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	Inhibitor	4	Toxic	Safe	Safe
MolPort-000-671-077	340.342	3.27	6	1	0	2	4.92	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	1	Toxic	Safe	Safe
MolPort-051-703-673	321.34	2.67	6	2	0	4	9.32	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	4	Toxic	Safe	Safe
MolPort-005-978-788	391.431	3.06	4	3	0	4	10.73	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Inhibitor	Inhibitor	Inhibitor	Inhibitor	Inhibitor	5	Toxic	Safe	Toxic
MolPort-002-686-287	399.479	4.03	6	2	0	5	6.23	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Inhibitor	Inhibitor	3	Safe	Safe	Safe
MolPort-020-200-504	310.426	2.58	5	1	0	1	7.99	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	1	Toxic	Safe	Toxic
MolPort-003-136-338	435.396	1.92	9	2	0	5	8.79	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	3	Safe	Safe	Safe
MolPort-001-946-433	359.392	4.66	5	1	0	1	7.83	Absorbed	Inhibitor	Substrate	Non-Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Inhibitor	Inhibitor	4	Toxic	Toxic	Safe
MolPort-002-819-891	326.327	3.41	4	1	0	4	9.6	Absorbed	Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	2	Safe	Safe	Safe
MolPort-001-962-960	342.427	4.09	5	1	0	4	6.65	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	4	Toxic	Safe	Safe
MolPort-003-722-255	393.468	4.26	6	1	0	4	7.67	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	4	Toxic	Safe	Safe
MolPort-002-734-386	337.339	2.24	7	1	0	1	6.57	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Toxic	Safe
MolPort-019-890-943	376.46	2.25	6	2	0	4	7.4	Absorbed	Non-Inhibitor	Substrate	Penetrable	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	2	Toxic	Safe	Toxic
MolPort-051-707-539	323.381	2.02	6	2	0	2	8.51	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	4	Toxic	Safe	Safe
MolPort-002-711-247	422.448	2.68	8	1	0	6	8.15	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	2	Toxic	Safe	Safe
MolPort-002-739-656	371.349	1.3	8	1	0	4	8.19	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	0	Toxic	Safe	Safe
MolPort-020-227-148	320.396	2.83	5	2	0	4	8.87	Absorbed	Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	Inhibitor	3	Toxic	Safe	Safe
MolPort-004-256-436	364.43	2.84	7	2	0	3	5.33	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	Inhibitor	2	Safe	Safe	Safe
MolPort-020-	380.354	2.78	5	2	0	5	6.73	Absorbed	Non-	Non-	Penetrabl	Inhibitor	Inhibitor	Inhibitor	Non-	Inhibitor	4	Toxic	Safe	Toxic

192-337									Inhibitor	Substrate	e				Inhibitor					
MolPort-051-703-344	299.305	2.45	5	1	0	2	7.94	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Safe	Safe
MolPort-035-705-708	327.38	1.77	5	2	0	2	9.23	Absorbed	Inhibitor	Substrate	Non-Penetrable	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	3	Safe	Safe	Toxic
MolPort-019-718-506	352.346	3.15	6	1	0	4	10.26	Absorbed	Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	4	Toxic	Safe	Safe
MolPort-005-914-867	426.436	1.77	6	3	0	3	10.15	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	2	Safe	Safe	Safe
MolPort-000-758-115	434.416	0.96	10	2	0	7	7.5	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	0	Safe	Safe	Safe
MolPort-002-326-584	327.322	3.04	5	1	0	1	6.07	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Inhibitor	Inhibitor	4	Toxic	Toxic	Safe
MolPort-019-915-633	378.306	4.11	5	1	0	4	8.66	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	2	Toxic	Safe	Safe
MolPort-002-597-120	406.381	3.67	9	2	0	5	7.79	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	4	Safe	Toxic	Safe
MolPort-019-718-508	352.346	3.12	6	1	0	4	10.36	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Safe	Safe
MolPort-000-736-219	315.829	3.26	4	1	0	1	3.23	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	2	Safe	Safe	Safe
MolPort-051-709-023	310.361	0	7	2	0	1	8.25	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	0	Toxic	Safe	Safe
MolPort-000-670-193	339.358	3.39	6	1	0	2	8.56	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	1	Toxic	Safe	Safe
MolPort-051-749-814	408.502	2.75	6	2	0	8	3.56	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	0	Safe	Safe	Toxic
MolPort-019-884-172	367.43	3.5	7	1	0	5	9.06	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	4	Toxic	Toxic	Toxic
MolPort-019-897-241	351.362	2.99	7	1	0	5	8.12	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	4	Toxic	Toxic	Toxic
MolPort-000-517-301	294.31	3	4	1	0	3	10.59	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	2	Toxic	Safe	Safe
MolPort-019-882-238	365.393	2.15	8	1	0	5	8.59	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	2	Toxic	Safe	Safe
MolPort-001-762-445	269.212	3.19	5	1	0	1	4.46	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	Inhibitor	4	Toxic	Toxic	Safe
MolPort-002-987-638	352.438	2.83	6	1	0	5	8.38	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	Inhibitor	2	Toxic	Safe	Toxic
MolPort-019-	340.404	3.54	5	1	0	4	10.2	Absorbed	Non-	Non-	Penetrabl	Inhibitor	Inhibitor	Inhibitor	Non-	Inhibitor	4	Safe	Toxic	Safe

718-535									Inhibitor	Substrate	e				Inhibitor					
MolPort-051-715-927	345.362	1.15	6	1	0	2	9.04	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Safe	Toxic	Safe
MolPort-002-353-133	433.924	4.14	6	2	0	6	5.27	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	Inhibitor	2	Safe	Safe	Safe
MolPort-002-569-125	428.517	5.02	7	1	1	7	6.28	Absorbed	Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	2	Safe	Safe	Safe
MolPort-051-744-153	359.389	2.32	7	1	0	3	9.09	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	2	Toxic	Safe	Safe
MolPort-019-707-233	354.362	3.04	6	1	0	5	11.01	Absorbed	Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Safe	Safe
MolPort-020-220-769	335.411	2.63	6	1	0	2	8.76	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	2	Safe	Safe	Safe
MolPort-019-718-501	324.336	2.97	5	1	0	4	10.93	Absorbed	Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Safe	Safe
MolPort-019-899-881	361.405	3.26	7	1	0	6	9.27	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Toxic	Safe
MolPort-001-946-428	355.426	3.93	6	1	0	2	7.53	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	3	Toxic	Toxic	Safe
MolPort-051-701-691	365.393	2.18	8	1	0	5	8.65	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	2	Toxic	Safe	Safe
MolPort-007-550-708	308.337	3.27	4	1	0	4	10.26	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	2	Safe	Safe	Safe
MolPort-044-375-962	408.849	3.85	7	2	0	4	9.35	Absorbed	Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	2	Safe	Safe	Safe
MolPort-002-832-242	268.341	2.39	4	1	0	1	4.29	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	3	Safe	Safe	Safe
MolPort-051-743-976	361.405	2.31	7	1	0	4	9.93	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Safe	Safe
MolPort-002-597-806	435.36	2.25	12	3	1	6	7.35	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Safe	Safe
MolPort-020-221-226	379.372	3.4	7	2	0	6	5.3	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	1	Toxic	Safe	Safe
MolPort-002-639-764	462.47	3.94	11	2	1	9	9.31	Absorbed	Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Safe	Safe	Safe
MolPort-019-915-630	354.362	2.46	6	1	0	5	10.67	Absorbed	Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	3	Safe	Safe	Safe
MolPort-019-	326.327	3.68	4	1	0	3	9.99	Absorbed	Inhibitor	Non-	Penetrabl	Inhibitor	Inhibitor	Non-	Non-	Inhibitor	3	Toxic	Safe	Safe

718-536										Substrate	e			Inhibitor	Inhibitor					
MolPort-002-987-636	366.465	3.14	6	1	0	6	8.28	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	Inhibitor	2	Safe	Safe	Toxic
MolPort-001-960-305	448.979	6.26	6	1	1	8	7.5	Absorbed	Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Safe	Safe	Safe
MolPort-002-703-992	384.356	1.99	10	1	0	4	6.09	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Safe	Safe
MolPort-019-888-328	367.43	3.44	7	1	0	5	8.8	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Safe	Toxic
MolPort-003-704-241	437.351	2.75	11	2	1	6	7.4	Absorbed	Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Safe	Safe
MolPort-007-684-206	389.502	3.86	5	2	0	6	9.67	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Safe	Safe	Safe
Molport-049-227-714	353.403	1.9	4	2	0	2	7.4	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	1	Safe	Safe	Safe
MolPort-051-708-068	348.454	1.9	6	1	0	2	9.92	Absorbed	Non-Inhibitor	Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	0	Toxic	Safe	Toxic
MolPort-039-033-335	361.365	3.47	8	2	0	5	7.22	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	3	Safe	Safe	Toxic
MolPort-002-729-181	449.923	4.36	7	2	0	6	7.07	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	Inhibitor	2	Safe	Safe	Safe
MolPort-019-898-779	336.443	2.5	5	2	0	3	8.22	Absorbed	Non-Inhibitor	Substrate	Penetrable	Non-Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	1	Toxic	Safe	Toxic
MolPort-001-760-066	432.384	1.58	11	2	1	6	8.71	Non-Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	0	Safe	Safe	Safe
MolPort-003-820-190	338.363	3.33	5	1	0	5	10.74	Absorbed	Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Safe	Safe
MolPort-002-351-865	306.394	4.23	5	1	0	4	5.14	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Inhibitor	Inhibitor	4	Toxic	Safe	Safe
MolPort-000-837-473	430.489	4.35	8	1	0	7	7.02	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	1	Safe	Safe	Safe
MolPort-051-752-687	348.366	0.79	7	2	0	5	7.56	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	4	Toxic	Toxic	Toxic
MolPort-019-718-502	354.362	3	6	1	0	5	10.75	Absorbed	Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	4	Safe	Safe	Safe
MolPort-051-743-525	366.465	2.82	6	1	0	6	8.28	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	1	Toxic	Safe	Toxic

MolPort-051-703-182	408.502	2.14	7	1	0	7	5.45	Absorbed	Non-Inhibitor	Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	1	Safe	Safe	Safe
MolPort-019-886-214	322.372	0.92	7	1	0	2	7.77	Absorbed	Non-Inhibitor	Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	0	Toxic	Safe	Toxic
MolPort-002-542-203	345.376	3.96	7	1	0	3	7.58	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	4	Safe	Safe	Safe
MolPort-001-888-028	324.336	2.99	5	1	0	4	11.09	Absorbed	Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Safe	Safe
MolPort-019-902-572	363.421	3.6	6	2	0	5	9.54	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	4	Toxic	Safe	Toxic
MolPort-019-718-505	340.404	3.59	5	1	0	4	10.17	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	4	Safe	Toxic	Safe
MolPort-004-895-249	267.244	2.18	4	1	0	2	6.01	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	1	Toxic	Safe	Toxic
MolPort-019-915-634	378.306	4.13	5	1	0	4	8.83	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	2	Toxic	Safe	Safe
MolPort-020-186-493	336.42	1.09	6	3	0	1	8.18	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	Inhibitor	2	Toxic	Safe	Toxic
MolPort-002-136-105	521.44	6.28	7	1	2	9	6.4	Absorbed	Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	1	Safe	Safe	Safe
MolPort-003-049-573	405.414	2.51	7	2	0	5	10.12	Absorbed	Inhibitor	Non-Substrate	Penetrable	Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	1	Safe	Safe	Safe
MolPort-051-710-670	347.378	1.96	7	1	0	3	9.85	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	2	Toxic	Safe	Safe
Molport-051-864-639	383.404	2.36	7	2	0	6	4.49	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	0	Toxic	Safe	Safe
MolPort-023-297-504	359.336	2.37	5	2	0	2	10.46	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	2	Toxic	Safe	Safe
MolPort-000-783-804	414.49	4.43	7	1	0	7	6.18	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	2	Safe	Safe	Safe
MolPort-051-707-699	351.479	2.59	6	1	0	2	10.1	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	Inhibitor	2	Toxic	Safe	Toxic
MolPort-051-751-390	367.522	2.74	6	2	0	3	6.09	Absorbed	Non-Inhibitor	Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	1	Toxic	Safe	Toxic
MolPort-019-718-539	346.745	3.93	4	1	0	3	9.69	Absorbed	Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Safe	Safe

MolPort-019-718-509	366.373	3.6	6	1	0	5	10.29	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	2	Safe	Safe	Safe
MolPort-020-227-865	362.481	2.52	6	1	0	3	10.53	Absorbed	Non-Inhibitor	Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	1	Toxic	Safe	Toxic
MolPort-051-710-240	282.303	1.92	6	1	0	2	8.46	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	2	Toxic	Safe	Safe
MolPort-001-733-967	521.524	6.03	6	2	2	4	8.78	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	2	Toxic	Safe	Safe
Molport-003-807-796	491.601	5.12	7	1	1	4	7.29	Absorbed	Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	2	Toxic	Safe	Safe
MolPort-001-960-306	442.544	5.57	7	2	1	8	5.54	Absorbed	Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	2	Safe	Safe	Safe
MolPort-019-897-234	370.46	2.14	6	1	0	3	9.03	Absorbed	Inhibitor	Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	Inhibitor	2	Toxic	Safe	Toxic
MolPort-019-718-504	338.363	3.39	5	1	0	5	10.63	Absorbed	Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	3	Safe	Safe	Safe
MolPort-002-804-537	364.325	2.14	10	2	0	5	7.3	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	4	Safe	Safe	Safe
MolPort-000-516-181	338.411	2.26	6	1	0	4	7.47	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	0	Toxic	Safe	Safe
MolPort-019-886-658	332.363	3.09	6	1	0	4	10.32	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	4	Toxic	Safe	Safe
MolPort-001-944-862	539.411	4.47	9	1	1	8	6.06	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	1	Safe	Safe	Safe
MolPort-002-171-820	343.777	3.2	5	1	0	1	6.88	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Inhibitor	Inhibitor	4	Toxic	Toxic	Safe
MolPort-002-627-243	394.351	2.81	11	2	1	6	8.36	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	4	Safe	Toxic	Safe
MolPort-019-891-844	366.377	2.21	8	1	0	5	8.75	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	2	Safe	Safe	Safe
MolPort-019-888-490	349.394	3.24	7	1	0	5	9.73	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	4	Toxic	Safe	Safe
MolPort-003-820-454	454.342	3.89	6	2	0	5	5.66	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Inhibitor	Inhibitor	3	Toxic	Safe	Safe
MolPort-044-543-724	472.449	4.97	8	2	0	5	6.83	Absorbed	Inhibitor	Non-Substrate	Non-Penetrable	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	Inhibitor	4	Safe	Toxic	Safe

MolPort-002-678-767	330.391	3.06	5	1	0	3	7.25	Absorbed	Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Toxic	Safe
MolPort-020-197-366	372.856	2.63	6	2	0	5	7.98	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	1	Safe	Safe	Safe
MolPort-000-788-474	452.862	3.9	10	2	0	7	8.51	Absorbed	Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Safe	Safe	Safe
MolPort-000-632-015	330.208	2.77	8	2	0	2	3.97	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Inhibitor	Non-Inhibitor	Inhibitor	Inhibitor	Inhibitor	4	Toxic	Safe	Safe
MolPort-051-706-855	282.303	1.92	6	1	0	2	8.55	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	1	Toxic	Safe	Safe
MolPort-001-939-282	449.333	4.71	6	1	0	5	5.52	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	2	Safe	Safe	Safe
MolPort-051-707-625	331.379	3.4	5	2	0	2	10.06	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Inhibitor	Inhibitor	Inhibitor	Inhibitor	Inhibitor	5	Toxic	Safe	Safe
MolPort-002-643-287	438.492	4.63	10	2	0	8	8.84	Absorbed	Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Safe	Safe	Safe
MolPort-051-750-693	368.418	2.57	8	1	0	5	8.84	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Safe	Safe
MolPort-002-799-626	356.385	2.82	6	1	0	3	5.02	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	1	Toxic	Safe	Safe
MolPort-019-898-587	335.367	2.5	7	1	0	4	9.19	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	4	Toxic	Toxic	Safe
MolPort-002-545-566	404.882	4.48	6	1	0	5	5.62	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	2	Safe	Safe	Safe
MolPort-051-705-257	363.377	3.03	8	1	0	5	9.16	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	2	Toxic	Safe	Safe
16545576	464.426	4.74	6	1	0	2	4.95	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	2	Toxic	Safe	Safe
MolPort-020-193-063	271.276	0.86	6	2	0	2	8.45	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	0	Toxic	Toxic	Safe
MolPort-019-939-184	378.435	3.95	4	1	0	2	9.62	Absorbed	Non-Inhibitor	Substrate	Penetrable	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	3	Safe	Toxic	Safe
MolPort-016-582-777	570.649	5.04	6	1	2	3	9.12	Absorbed	Non-Inhibitor	Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	1	Safe	Safe	Toxic

MolPort-001-962-967	306.35	3.03	6	2	0	3	5.92	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Toxic	Safe
MolPort-020-199-122	356.451	2.8	7	1	0	3	5.81	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	0	Toxic	Safe	Safe
MolPort-001-962-959	462.578	6.57	6	1	1	6	6.48	Absorbed	Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	1	Safe	Safe	Safe
MolPort-035-765-768	348.391	2.34	7	3	0	4	6.79	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	2	Safe	Safe	Safe
MolPort-002-898-445	322.324	3.53	7	1	0	3	5.47	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	4	Toxic	Safe	Safe
MolPort-019-707-232	312.3	3.15	4	1	0	3	9.78	Absorbed	Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Safe	Safe
MolPort-006-249-140	329.388	3.2	6	1	0	3	6.76	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	2	Toxic	Safe	Safe
MolPort-002-636-066	452.862	4.26	10	2	0	7	8.48	Absorbed	Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	4	Safe	Safe	Safe
MolPort-051-708-742	362.418	0.77	7	1	0	2	8.65	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Inhibitor	Inhibitor	4	Safe	Safe	Safe
MolPort-051-706-886	379.42	2.38	8	2	0	6	10.01	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	2	Toxic	Safe	Safe
MolPort-035-717-163	376.803	3.02	6	1	0	3	5.13	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	1	Toxic	Safe	Safe
MolPort-051-702-401	393.447	2.64	8	1	0	6	9.07	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	2	Safe	Safe	Safe
MolPort-019-884-142	280.331	1.55	5	1	0	1	8.8	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	0	Toxic	Safe	Toxic
MolPort-003-049-532	425.832	2.76	7	2	0	5	9.89	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	2	Safe	Safe	Safe
MolPort-002-677-705	400.482	3.38	6	1	0	5	8.81	Absorbed	Inhibitor	Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	1	Safe	Safe	Safe
MolPort-002-709-868	385.452	3.65	6	2	0	5	5.47	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	2	Safe	Safe	Safe
MolPort-006-249-197	310.382	2.78	6	2	0	4	6.3	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	1	Toxic	Safe	Safe
MolPort-003-079-339	409.377	2.32	7	2	0	5	9.66	Absorbed	Inhibitor	Non-Substrate	Penetrable	Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	1	Safe	Safe	Safe
MolPort-001-	448.551	5.53	6	1	1	7	8.22	Absorbed	Non-	Non-	Non-	Non-	Non-	Non-	Non-	Non-	0	Safe	Safe	Safe

949-349									Inhibitor	Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Inhibitor	Inhibitor			
MolPort-002-795-751	380.4	3.86	6	1	0	6	10.12	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	2	Safe	Safe	Safe
MolPort-051-750-464	347.378	2.19	7	2	0	3	9.31	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	2	Toxic	Safe	Safe
MolPort-002-743-757	443.463	3.62	8	1	0	4	7.15	Absorbed	Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	2	Toxic	Toxic	Safe
MolPort-007-663-980	390.508	4.85	3	1	0	3	6.76	Absorbed	Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Toxic	Safe
MolPort-002-625-871	470.808	3.23	11	2	1	5	7.22	Absorbed	Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	4	Toxic	Safe	Safe
MolPort-002-606-492	422.836	4.36	9	2	0	5	8.06	Absorbed	Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Inhibitor	Inhibitor	5	Safe	Toxic	Safe
MolPort-004-949-192	349.213	1.59	4	3	0	2	6.09	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	4	Safe	Safe	Safe
MolPort-002-191-980	380.455	4.29	6	1	0	4	8.44	Absorbed	Inhibitor	Substrate	Non-Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	3	Toxic	Toxic	Safe
MolPort-035-717-165	402.41	1.92	8	1	0	5	5.82	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	1	Toxic	Safe	Safe
MolPort-001-962-969	324.796	4	5	1	0	3	5.96	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Non-Inhibitor	Inhibitor	Inhibitor	Inhibitor	4	Toxic	Toxic	Safe
MolPort-000-803-642	424.446	3.38	11	2	1	7	8.48	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Safe	Toxic	Safe
MolPort-020-210-228	320.4	1.33	6	1	0	3	8.42	Absorbed	Non-Inhibitor	Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	0	Toxic	Safe	Safe
MolPort-051-749-036	339.395	2.39	6	1	0	5	9.73	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	2	Toxic	Safe	Safe
MolPort-003-049-469	361.361	2.17	6	2	0	4	10.39	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	2	Toxic	Safe	Safe
MolPort-004-418-238	393.697	4.29	5	1	0	4	6.08	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	4	Toxic	Safe	Safe
MolPort-020-213-642	354.479	2.98	6	1	0	3	6.37	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	Inhibitor	3	Toxic	Safe	Safe
MolPort-002-254-192	320.421	4.67	5	1	0	4	5.28	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	2	Toxic	Safe	Safe
MolPort-005-281-107	396.443	4.46	6	2	0	4	8.64	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	4	Safe	Safe	Safe
MolPort-001-946-426	378.222	3.93	5	1	0	1	6.49	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Inhibitor	Inhibitor	4	Toxic	Toxic	Safe
MolPort-023-	411.465	3.85	5	2	0	3	10.1	Absorbed	Non-	Non-	Penetrabl	Non-	Inhibitor	Inhibitor	Non-	Non-	2	Safe	Safe	Safe

306-537							1		Inhibitor	Substrate	e	Inhibitor			Inhibitor	Inhibitor				
MolPort-020-191-873	352.467	1.78	7	2	0	4	8.39	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	0	Toxic	Safe	Safe
MolPort-000-516-178	294.358	2.4	5	1	0	2	7.72	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	0	Toxic	Safe	Safe
MolPort-046-954-381	386.452	1.18	5	2	0	7	10.98	Absorbed	Non-Inhibitor	Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	0	Safe	Safe	Safe
MolPort-051-748-891	319.368	3.53	5	2	0	3	9.91	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Inhibitor	Inhibitor	Inhibitor	Inhibitor	Inhibitor	5	Toxic	Toxic	Safe
MolPort-035-717-164	386.411	2.74	7	1	0	5	5.67	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	0	Safe	Safe	Safe
MolPort-001-949-352	372.453	4.77	6	1	0	5	7.3	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	2	Safe	Safe	Safe
MolPort-023-306-532	414.381	2.32	7	2	0	3	10.18	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	2	Toxic	Safe	Safe
MolPort-002-898-479	318.258	3.69	5	1	0	2	3.63	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	3	Safe	Safe	Safe
MolPort-002-734-791	333.376	2.41	7	1	0	1	6.87	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Toxic	Safe
MolPort-035-669-648	488.882	4.53	7	2	0	5	4.26	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	2	Safe	Safe	Safe
MolPort-002-353-131	413.506	3.99	6	2	0	6	5.87	Absorbed	Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	1	Safe	Safe	Safe
MolPort-020-189-489	347.447	2.9	6	2	0	2	8.23	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Safe	Safe
MolPort-005-912-438	427.42	2.61	7	2	0	3	10.3	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	2	Safe	Safe	Safe
MolPort-051-742-799	405.845	2.15	6	2	0	2	6.78	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Inhibitor	Inhibitor	4	Safe	Safe	Safe
MolPort-002-716-039	491.587	4.4	7	2	0	8	7.81	Absorbed	Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Safe	Safe	Safe
MolPort-003-049-479	391.387	1.98	7	2	0	5	10.06	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	2	Toxic	Safe	Safe
MolPort-035-717-385	281.271	1.2	3	3	0	2	9.83	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	1	Safe	Safe	Safe
MolPort-020-194-994	334.427	2.43	6	1	0	3	7.29	Absorbed	Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	0	Toxic	Safe	Safe
MolPort-019-718-500	322.364	4.04	4	1	0	3	10.85	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	3	Safe	Safe	Safe

MolPort-020-212-852	363.446	2.19	7	2	0	3	8.72	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Safe	Safe
MolPort-001-766-597	296.246	0.29	8	2	0	2	2.7	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	1	Toxic	Safe	Safe
MolPort-001-900-106	358.426	3.82	6	2	0	4	6.13	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Inhibitor	Inhibitor	3	Toxic	Safe	Safe
MolPort-003-049-476	391.387	2.03	7	2	0	5	10.1	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	1	Toxic	Safe	Safe
MolPort-000-768-008	453.806	3.47	11	2	1	6	7.76	Absorbed	Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Safe	Safe
MolPort-000-683-899	361.401	4.58	6	1	0	5	10.49	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	4	Toxic	Safe	Safe
MolPort-006-249-153	332.388	3.98	6	1	0	3	5.8	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	4	Toxic	Toxic	Safe
MolPort-020-228-352	312.442	3.27	5	2	0	3	7.11	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	2	Toxic	Safe	Safe
MolPort-019-718-540	326.327	3.74	4	1	0	3	9.46	Absorbed	Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	4	Toxic	Safe	Safe
MolPort-002-744-844	392.422	3.03	7	1	0	5	8.27	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	1	Toxic	Safe	Safe
MolPort-035-669-150	478.581	5.01	7	2	1	6	6.5	Absorbed	Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	1	Safe	Safe	Safe
MolPort-002-136-117	340.364	2.33	8	2	0	4	5.51	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	1	Safe	Safe	Safe
MolPort-005-916-947	448.28	3.38	5	2	0	2	9.97	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	2	Safe	Safe	Safe
MolPort-002-544-404	510.575	5.26	9	1	2	9	5.36	Absorbed	Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	1	Safe	Safe	Safe
MolPort-006-822-593	314.389	1.94	6	2	0	5	9.88	Absorbed	Non-Inhibitor	Substrate	Non-Penetrable	Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	1	Toxic	Toxic	Safe
MolPort-051-716-836	301.375	1.72	7	1	0	2	7.77	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	1	Toxic	Safe	Safe
MolPort-000-718-398	442.497	3.25	10	1	0	8	5.96	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	2	Safe	Safe	Safe
MolPort-000-	400.438	4.57	7	1	0	6	7.92	Absorbed	Non-	Non-	Non-	Non-	Non-	Inhibitor	Non-	Inhibitor	2	Safe	Safe	Safe

674-577									Inhibitor	Substrate	Penetrable	Inhibitor	Inhibitor		Inhibitor					
MolPort-001-894-047	369.384	3.28	7	1	0	3	8.56	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Safe	Safe
MolPort-051-747-057	399.458	2.17	7	1	0	3	7.11	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	0	Safe	Safe	Safe
MolPort-016-583-874	360.342	-1.9	12	4	1	4	11.12	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	0	Toxic	Toxic	Safe
MolPort-020-186-382	284.388	2.26	5	1	0	1	6.05	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	1	Toxic	Safe	Safe
MolPort-000-726-150	378.407	4.49	5	1	0	4	6.01	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	2	Toxic	Safe	Safe
MolPort-035-669-181	442.529	3.2	8	2	0	5	5.88	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	1	Toxic	Safe	Safe
MolPort-019-718-527	326.327	3.85	4	1	0	3	9.81	Absorbed	Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Safe	Safe
MolPort-051-706-441	375.457	1.94	6	1	0	2	8.06	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Toxic	Safe
MolPort-020-197-257	364.449	2.63	6	2	0	6	8.45	Absorbed	Non-Inhibitor	Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	Inhibitor	2	Safe	Safe	Safe
MolPort-023-306-545	448.826	3.03	7	2	0	3	10.36	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	2	Toxic	Safe	Safe
MolPort-002-544-846	467.323	4.86	6	1	0	5	5.06	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	1	Safe	Safe	Safe
MolPort-051-703-259	398.47	2	6	1	0	4	7.3	Absorbed	Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Safe	Safe	Safe
MolPort-019-718-528	342.782	4.35	4	1	0	3	10.17	Absorbed	Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Safe	Safe
MolPort-000-779-699	543.244	5.66	6	2	2	5	5.73	Absorbed	Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	1	Safe	Safe	Safe
MolPort-001-831-999	360.211	3.49	5	1	0	3	6.78	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	4	Safe	Safe	Safe
MolPort-000-921-613	416.453	4.68	6	1	0	4	4.11	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	2	Toxic	Safe	Safe
MolPort-000-185-815	464.547	2.76	8	1	0	4	6.68	Absorbed	Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	Inhibitor	3	Safe	Safe	Toxic
MolPort-000-699-710	349.415	2.94	5	2	0	3	6.02	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Safe	Safe	Safe
MolPort-019-718-498	322.364	3.93	4	1	0	3	10.55	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Safe	Safe

MolPort-020-191-670	324.384	1.94	6	2	0	2	7.93	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	1	Toxic	Toxic	Safe
MolPort-000-674-580	414.465	4.86	7	1	0	7	7.51	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	1	Safe	Safe	Safe
MolPort-002-323-387	357.373	1.87	7	2	0	4	4.98	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	0	Toxic	Safe	Safe
MolPort-019-718-534	358.781	3.88	5	1	0	4	10.98	Absorbed	Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Safe	Safe
MolPort-019-718-517	346.745	3.76	4	1	0	3	9.53	Absorbed	Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Safe	Safe
MolPort-051-750-124	413.437	2.07	7	1	0	3	8.23	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Safe	Safe	Safe
MolPort-008-435-359	256.265	1.55	5	1	0	3	7.99	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	1	Safe	Safe	Safe
MolPort-003-711-615	404.882	4.63	6	1	0	5	5.59	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	2	Safe	Safe	Safe
MolPort-020-215-831	310.405	2.5	5	2	0	3	5.74	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	1	Safe	Safe	Safe
Molport-051-839-879	390.44	-0.36	8	1	0	7	5.19	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	0	Safe	Safe	Safe
MolPort-020-191-027	365.481	2.38	6	2	0	6	7.13	Absorbed	Non-Inhibitor	Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	1	Toxic	Safe	Toxic
MolPort-002-021-285	425.51	2.38	5	2	0	9	9.48	Absorbed	Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Inhibitor	Inhibitor	5	Safe	Safe	Toxic
MolPort-020-200-850	323.4	2.84	5	2	0	3	9.93	Absorbed	Non-Inhibitor	Substrate	Non-Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Inhibitor	Inhibitor	4	Toxic	Safe	Safe
MolPort-023-312-869	346.777	4.67	5	1	0	2	6.64	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	3	Toxic	Safe	Safe
MolPort-001-960-307	465.332	4.42	7	2	0	5	5.23	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	2	Safe	Safe	Safe
MolPort-002-543-183	405.508	2.99	7	2	0	6	4.33	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	1	Safe	Safe	Safe
MolPort-023-298-726	327.348	0.74	7	2	0	2	10.21	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	0	Safe	Safe	Safe
MolPort-002-551-707	390.424	3.54	8	1	0	6	4.52	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	1	Safe	Safe	Safe

MolPort-001-962-957	561.417	5.11	9	1	2	7	5.35	Absorbed	Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	1	Safe	Safe	Safe
MolPort-002-544-544	420.881	4.19	7	2	0	5	5.4	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Inhibitor	Inhibitor	3	Safe	Safe	Safe
MolPort-002-731-900	316.281	0.49	10	3	0	4	7.33	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	4	Toxic	Toxic	Safe
MolPort-023-306-533	394.394	2.09	6	2	0	2	10.01	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	1	Safe	Safe	Safe
MolPort-016-613-796	414.443	2.51	8	1	0	5	7.99	Absorbed	Inhibitor	Non-Substrate	Penetrable	Inhibitor	Non-Inhibitor	Inhibitor	Inhibitor	Inhibitor	4	Safe	Safe	Safe
MolPort-002-584-207	343.799	2.26	6	2	0	4	4.22	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	Inhibitor	2	Toxic	Safe	Safe
MolPort-000-923-185	474.398	4.33	7	2	0	6	4.36	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Safe	Safe
MolPort-019-894-098	342.805	2.38	4	1	0	1	7.27	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	Inhibitor	2	Toxic	Safe	Toxic
MolPort-038-387-899	368.418	3.23	8	1	0	5	6.34	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	1	Toxic	Safe	Safe
MolPort-003-013-052	308.337	3.54	4	1	0	3	10.52	Absorbed	Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Safe	Safe
MolPort-002-735-759	387.346	2.75	7	1	0	1	6	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	0	Toxic	Toxic	Safe
MolPort-002-542-096	483.778	5.47	6	1	1	5	5.74	Absorbed	Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	1	Safe	Safe	Safe
MolPort-020-219-107	282.372	1.71	5	2	0	1	9.07	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	Inhibitor	3	Toxic	Safe	Toxic
MolPort-001-962-952	339.38	1.59	7	2	0	5	5.5	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	1	Toxic	Safe	Safe
MolPort-002-549-763	325.353	1.18	7	3	0	4	4.38	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	1	Safe	Safe	Safe
MolPort-000-923-176	449.517	2.74	9	2	0	5	5.92	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	1	Toxic	Safe	Safe
MolPort-002-560-012	436.127	2.45	5	2	0	4	2.62	Non-Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	0	Safe	Safe	Safe
MolPort-002-	331.349	3.85	7	1	0	3	7.74	Absorbed	Non-	Non-	Penetrabl	Inhibitor	Inhibitor	Inhibitor	Non-	Inhibitor	4	Safe	Safe	Safe

509-320									Inhibitor	Substrate	e				Inhibitor					
MolPort-001-960-313	426.545	5.88	6	1	1	8	5.62	Absorbed	Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	2	Safe	Safe	Safe
MolPort-002-683-626	220.152	-0.45	8	4	0	0	6.7	Non-Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	0	Toxic	Safe	Safe
MolPort-005-912-729	415.478	3.05	6	2	0	3	8.59	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	3	Safe	Safe	Safe
MolPort-002-011-487	445.928	2.37	5	2	0	9	9.01	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Inhibitor	Inhibitor	5	Safe	Safe	Toxic
MolPort-002-570-219	386.436	3.57	7	2	0	5	5.27	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Inhibitor	Inhibitor	3	Safe	Safe	Safe
MolPort-005-913-631	369.384	2.46	5	2	0	2	10.23	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	3	Safe	Safe	Safe
MolPort-051-709-491	391.381	1.71	5	1	0	2	6.55	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Safe	Safe
MolPort-051-745-264	403.873	2.24	5	1	0	2	7.94	Absorbed	Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Safe	Safe	Safe
MolPort-006-758-419	392.433	3.11	6	2	0	6	8.62	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Inhibitor	Non-Inhibitor	Inhibitor	Inhibitor	Inhibitor	4	Safe	Safe	Safe
MolPort-020-221-692	352.463	2.48	6	2	0	3	6.42	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	Inhibitor	2	Safe	Safe	Toxic
MolPort-015-162-689	299.677	2.2	6	1	0	2	3.1	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Safe	Safe
MolPort-002-743-756	439.5	3.73	8	1	0	4	7.29	Absorbed	Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Toxic	Safe
MolPort-051-717-049	283.291	0.94	7	1	0	2	7.93	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	1	Toxic	Safe	Safe
MolPort-001-962-993	432.461	3.19	9	3	0	6	5.62	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	2	Safe	Safe	Safe
MolPort-000-924-983	377.86	3.55	6	1	0	4	5.84	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Inhibitor	Inhibitor	4	Safe	Safe	Safe
MolPort-006-249-144	348.456	4.08	6	1	0	3	6.13	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Safe	Safe
MolPort-002-744-223	309.354	1.48	6	2	0	4	3.98	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	0	Toxic	Safe	Safe
MolPort-051-711-529	408.458	1.51	7	2	0	6	6.83	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	1	Toxic	Safe	Toxic
MolPort-006-	345.387	2.78	7	2	0	3	6.47	Absorbed	Non-	Non-	Non-	Inhibitor	Inhibitor	Inhibitor	Inhibitor	Inhibitor	5	Safe	Safe	Safe

249-223									Inhibitor	Substrate	Penetrable								
MolPort-002-575-850	386.436	3.94	7	1	0	5	5.68	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	1	Safe	Safe	Safe
MolPort-002-629-331	406.431	2.76	10	2	0	4	8.28	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	4	Toxic	Safe	Safe
MolPort-051-701-098	282.303	1.62	6	1	0	2	9.11	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	2	Toxic	Safe	Safe
MolPort-039-139-587	520.039	4.65	9	2	1	8	8	Absorbed	Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	2	Safe	Safe	Safe
MolPort-002-621-152	451.918	3.75	8	2	0	6	9.14	Absorbed	Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Safe	Safe	Toxic
MolPort-002-546-866	530.694	5.92	8	1	2	10	6.45	Absorbed	Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	2	Safe	Safe	Safe
MolPort-023-294-073	408.281	2.65	6	2	0	2	10.02	Non-Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Safe	Safe
MolPort-002-595-097	476.612	3.98	9	2	0	5	4.61	Non-Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	2	Toxic	Safe	Safe
MolPort-002-814-003	364.423	2.86	5	2	0	8	10.72	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	2	Safe	Safe	Toxic
MolPort-000-920-127	501.395	5.17	8	1	2	7	7.43	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	2	Toxic	Safe	Safe
MolPort-000-919-894	417.469	4.29	6	2	0	5	5.67	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	2	Safe	Safe	Safe
MolPort-007-564-575	362.433	2.93	3	2	0	2	9.88	Absorbed	Inhibitor	Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	4	Safe	Safe	Toxic
MolPort-051-701-133	382.464	1.89	7	1	0	7	7.63	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	0	Safe	Safe	Toxic
MolPort-000-816-302	415.434	3.69	8	1	0	6	4.9	Absorbed	Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Safe	Safe
MolPort-006-828-068	302.315	1.32	7	2	0	2	6.73	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	2	Safe	Safe	Safe
MolPort-002-275-903	412.536	3.15	4	2	0	6	8.14	Absorbed	Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Inhibitor	Inhibitor	5	Safe	Safe	Safe
MolPort-051-	399.454	2.31	6	1	0	4	8.61	Absorbed	Non-	Non-	Penetrabl	Non-	Inhibitor	Inhibitor	Non-	Inhibitor	3	Safe	Safe	Safe

705-317									Inhibitor	Substrate	e	Inhibitor				Inhibitor					
MolPort-002-710-498	428.517	4.68	7	1	0	7	6.9	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	1	Safe	Safe	Safe
MolPort-001-016-792	311.301	0.08	8	2	0	3	4.23	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	1	Toxic	Safe	Safe
MolPort-000-805-020	476.409	3.4	13	2	1	6	8.02	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Safe	Safe
MolPort-004-479-026	468.582	6.18	7	2	1	6	5.72	Absorbed	Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	2	Safe	Safe	Safe
MolPort-000-921-121	460.371	4.28	7	2	0	5	4.77	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Safe	Safe
MolPort-001-897-102	294.27	2.88	7	1	0	2	5.14	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Safe	Safe
MolPort-051-710-278	391.381	1.43	5	1	0	2	6.46	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Safe	Safe
MolPort-001-766-591	295.258	0.5	8	2	0	1	3.78	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	1	Toxic	Safe	Safe
MolPort-000-774-267	435.36	0.28	11	2	1	6	6.31	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	0	Toxic	Safe	Safe
MolPort-003-049-580	405.414	2.59	7	2	0	5	10.5	Absorbed	Inhibitor	Non-Substrate	Non-Penetrable	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	2	Safe	Safe	Safe
MolPort-002-544-340	404.564	5.58	6	1	1	4	6.28	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Safe	Safe
MolPort-002-709-740	390.512	4.61	6	1	0	4	6.08	Absorbed	Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Safe	Safe
MolPort-020-205-294	269.308	1.63	5	2	0	2	8.67	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	1	Toxic	Safe	Safe
MolPort-020-211-078	362.393	1.57	6	3	0	5	8.15	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	2	Safe	Safe	Safe
MolPort-051-712-892	363.465	2.59	6	1	0	2	9.06	Absorbed	Non-Inhibitor	Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	0	Toxic	Safe	Toxic
MolPort-002-205-473	408.248	4.46	6	1	0	2	7.99	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Safe	Safe
MolPort-000-475-906	426.91	4.62	8	1	0	4	6.11	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	4	Toxic	Safe	Safe

MolPort-051-716-926	405.845	1.68	6	2	0	2	7.07	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Inhibitor	Inhibitor	4	Safe	Safe	Safe
MolPort-001-949-424	294.383	4.19	5	1	0	4	5.4	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Inhibitor	Inhibitor	4	Safe	Safe	Safe
MolPort-002-541-460	418.457	3.37	8	2	0	6	10.15	Absorbed	Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Safe	Safe	Toxic
MolPort-005-079-014	401.47	2.48	7	1	0	6	7.33	Absorbed	Inhibitor	Non-Substrate	Non-Penetrable	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	3	Safe	Safe	Safe
MolPort-002-039-080	312.369	2.71	4	2	0	5	8.37	Absorbed	Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	Inhibitor	4	Safe	Safe	Safe
MolPort-019-881-344	334.423	2.58	5	1	0	2	9.33	Absorbed	Non-Inhibitor	Substrate	Penetrable	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	2	Toxic	Safe	Toxic
MolPort-002-136-118	416.462	3.92	8	2	0	6	5.61	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Inhibitor	Inhibitor	3	Safe	Safe	Safe
MolPort-003-705-863	331.252	-0.1	11	3	1	4	6.94	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	4	Toxic	Toxic	Safe
MolPort-002-549-810	442.544	5.42	7	1	1	9	6.23	Absorbed	Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	2	Safe	Safe	Safe
MolPort-051-482-100	388.401	1.69	6	2	0	5	7.86	Absorbed	Inhibitor	Non-Substrate	Penetrable	Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	1	Safe	Safe	Safe
MolPort-000-923-174	435.534	3.44	8	2	0	6	6.01	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	1	Toxic	Safe	Safe
MolPort-002-735-556	337.339	2.15	7	1	0	1	6.65	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Toxic	Safe
MolPort-019-884-811	322.387	2.67	4	1	0	1	7.92	Absorbed	Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	1	Toxic	Safe	Toxic
MolPort-051-752-812	421.407	1.85	6	1	0	3	6.26	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Safe	Safe
MolPort-002-144-252	297.299	1.8	6	2	0	2	2.45	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	2	Toxic	Safe	Safe
MolPort-002-743-127	443.463	3.64	8	1	0	4	7.05	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	2	Toxic	Toxic	Safe
MolPort-000-921-437	433.493	2.62	9	1	0	7	7.21	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Inhibitor	Inhibitor	4	Safe	Safe	Safe
MolPort-002-821-216	427.352	4.57	6	1	0	4	5.82	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	4	Toxic	Safe	Safe
MolPort-002-	322.353	1.55	7	1	0	3	3.13	Absorbed	Non-	Non-	Penetrabl	Non-	Non-	Inhibitor	Non-	Non-	1	Toxic	Toxic	Safe

842-978									Inhibitor	Substrate	e	Inhibitor	Inhibitor		Inhibitor	Inhibitor					
MolPort-001-900-103	332.388	3.51	6	1	0	4	5.66	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	4	Toxic	Toxic	Safe
MolPort-001-941-213	396.472	4.14	8	1	0	8	6.09	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	1	Safe	Safe	Safe
MolPort-038-935-278	271.081	2.25	4	3	0	4	8.71	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	1	Safe	Safe	Toxic
MolPort-000-921-059	366.446	3.87	6	1	0	4	5.17	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	2	Toxic	Safe	Safe
MolPort-051-714-288	392.459	1.83	6	1	0	4	6.83	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Safe	Safe
MolPort-051-704-802	412.449	3.21	6	1	0	2	8.2	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Safe	Safe
MolPort-000-804-072	316.321	-1.08	9	4	0	4	5.5	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	0	Safe	Safe	Safe
MolPort-020-195-642	326.36	0.05	8	2	0	4	7.76	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	0	Toxic	Toxic	Safe
MolPort-002-842-977	310.342	1.58	7	1	0	2	3.46	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	0	Toxic	Toxic	Safe
MolPort-020-221-356	341.44	2.41	7	1	0	4	8.16	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	2	Toxic	Safe	Safe
MolPort-002-687-776	405.508	3.08	7	2	0	5	5.28	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	1	Toxic	Safe	Safe
MolPort-002-261-108	419.554	4.49	6	1	0	5	5.03	Absorbed	Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	2	Toxic	Safe	Safe
MolPort-023-312-870	362.845	4.83	5	1	0	2	7.4	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Inhibitor	Inhibitor	4	Toxic	Safe	Safe
MolPort-002-742-432	469.526	3.51	9	1	0	5	7.54	Absorbed	Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	2	Toxic	Toxic	Safe
MolPort-002-742-310	398.245	2.91	7	1	0	1	6.97	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Toxic	Safe
MolPort-002-136-116	338.436	4.79	6	1	0	6	6.75	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Safe	Safe
MolPort-000-779-533	419.535	3.69	7	2	0	5	5.33	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	2	Toxic	Safe	Safe
MolPort-020-217-675	338.386	1.92	5	1	0	2	7.41	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	0	Toxic	Safe	Toxic

MolPort-002-709-935	300.282	0.72	9	3	0	3	7.03	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	3	Safe	Toxic	Safe
MolPort-001-904-827	309.329	2.66	6	1	0	3	4.15	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Non-Inhibitor	Inhibitor	Inhibitor	Inhibitor	4	Toxic	Safe	Safe
MolPort-051-704-568	303.325	2.24	6	1	0	1	8.52	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	4	Toxic	Safe	Safe
MolPort-003-182-660	319.151	4.1	5	1	0	2	4.55	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Non-Inhibitor	Inhibitor	Inhibitor	Inhibitor	4	Toxic	Safe	Safe
MolPort-002-542-146	439.294	4.07	7	1	0	5	4.31	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	2	Safe	Safe	Safe
MolPort-001-957-398	394.843	3.83	7	1	0	5	4.42	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	2	Safe	Safe	Safe
MolPort-003-049-513	425.832	2.82	7	2	0	5	10.12	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	2	Safe	Safe	Safe
MolPort-000-921-060	382.901	4.35	6	1	0	4	5.86	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	4	Toxic	Safe	Safe
MolPort-020-230-516	348.406	1.65	6	2	0	1	10.13	Absorbed	Non-Inhibitor	Substrate	Non-Penetrable	Non-Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	1	Toxic	Safe	Toxic
MolPort-000-810-149	435.534	3.21	8	2	0	6	6.01	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	1	Toxic	Safe	Safe
MolPort-001-949-410	348.456	3.73	6	1	0	4	5.86	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	4	Toxic	Safe	Safe
MolPort-002-138-242	390.493	4.06	7	1	0	5	4.73	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	2	Safe	Safe	Safe
MolPort-001-664-861	494.96	4.23	9	1	0	8	6.22	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	1	Safe	Safe	Safe
MolPort-002-551-106	441.736	2.99	6	1	0	5	3.48	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Safe	Safe	Safe
MolPort-020-196-778	296.334	0.91	7	1	0	2	5.58	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	0	Toxic	Safe	Safe
MolPort-000-791-540	433.432	2.55	11	2	1	7	8.59	Absorbed	Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Safe	Toxic	Safe
MolPort-000-921-134	449.517	2.97	9	2	0	6	4.9	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	1	Toxic	Safe	Safe
MolPort-002-742-302	319.349	1.92	7	1	0	1	7.05	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Toxic	Safe
MolPort-002-	330.145	1.49	6	2	0	1	3.44	Absorbed	Non-	Non-	Penetrabl	Non-	Non-	Non-	Inhibitor	Non-	1	Toxic	Safe	Safe

138-542									Inhibitor	Substrate	e	Inhibitor	Inhibitor	Inhibitor		Inhibitor				
MolPort-019-899-929	349.394	2.84	7	1	0	4	8.7	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Safe	Safe
MolPort-047-913-138	312.417	3.23	5	2	0	5	9.93	Absorbed	Non-Inhibitor	Substrate	Non-Penetrable	Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	1	Toxic	Toxic	Safe
MolPort-000-727-645	351.456	3.65	5	2	0	3	5.71	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Inhibitor	Inhibitor	5	Toxic	Safe	Safe
MolPort-051-701-043	399.454	2.55	6	1	0	4	8.69	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Safe	Safe	Safe
MolPort-019-991-071	374.374	1.84	6	2	0	6	7.91	Absorbed	Inhibitor	Non-Substrate	Penetrable	Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	2	Safe	Safe	Safe
MolPort-035-924-399	291.694	1	4	3	0	3	5.29	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	0	Safe	Safe	Safe
MolPort-001-015-518	285.694	1.25	6	2	0	1	3.32	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	1	Toxic	Safe	Safe
MolPort-002-463-611	338.345	1.98	7	3	0	6	8.5	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Inhibitor	Inhibitor	5	Safe	Safe	Safe
MolPort-002-596-376	462.47	4.12	11	2	1	9	9.15	Absorbed	Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Safe	Safe	Safe
MolPort-009-752-916	296.286	1.25	7	2	0	3	4.26	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	1	Safe	Safe	Safe
MolPort-039-058-631	347.327	0.04	8	2	0	7	5.43	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	0	Safe	Toxic	Safe
MolPort-000-921-122	427.352	4.56	6	1	0	4	5.8	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Safe	Safe
MolPort-000-933-109	366.446	3.82	6	1	0	4	5.26	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Safe	Safe
MolPort-000-680-396	373.21	3.82	6	1	0	4	5.9	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Safe	Safe	Safe
MolPort-000-921-058	362.483	4.37	6	1	0	4	6.39	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	4	Toxic	Safe	Safe
MolPort-019-628-293	380.414	2.02	9	1	0	4	3.67	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Toxic	Safe
MolPort-000-814-253	296.291	1.74	7	1	0	2	3.11	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	1	Toxic	Safe	Safe
MolPort-016-605-355	268.341	2.71	3	1	0	3	9.79	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	4	Safe	Safe	Safe
MolPort-016-625-925	250.301	2.61	2	2	0	3	12.08	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrabl	Inhibitor	Inhibitor	Inhibitor	Inhibitor	Inhibitor	5	Toxic	Safe	Safe

MolPort-051-708-880	399.41	1.72	7	1	0	2	8.26	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Safe	Safe
MolPort-000-919-789	394.456	3.55	7	1	0	5	4.45	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	2	Toxic	Safe	Safe
MolPort-004-955-790	320.139	1.74	6	2	0	1	3.16	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	Inhibitor	2	Toxic	Safe	Safe
MolPort-000-704-245	308.41	4.76	5	1	0	3	5.96	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Inhibitor	Inhibitor	4	Safe	Safe	Safe
MolPort-002-898-431	332.285	3.96	5	1	0	3	3.45	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	1	Safe	Safe	Safe
MolPort-038-942-603	303.274	2.16	5	2	0	5	8.94	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	2	Toxic	Safe	Toxic
MolPort-002-543-042	434.59	4.55	7	1	0	5	5.31	Absorbed	Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	2	Toxic	Safe	Safe
MolPort-002-629-358	386.422	2.46	11	2	1	5	7.2	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	4	Toxic	Toxic	Safe
MolPort-000-838-750	453.98	3.84	7	2	0	7	4.73	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Safe	Safe	Safe
MolPort-001-962-970	349.375	2.08	8	1	0	4	5.22	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	1	Toxic	Safe	Safe
MolPort-001-733-987	383.355	2.5	7	2	0	4	8.32	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Toxic	Safe
MolPort-002-701-075	316.237	0.65	10	2	0	4	6.26	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	4	Toxic	Safe	Safe
MolPort-000-919-534	379.51	3.96	5	2	0	3	5.82	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Safe	Safe	Safe
MolPort-001-981-812	354.391	2.81	8	1	0	5	5.73	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	0	Toxic	Safe	Safe
MolPort-002-842-979	338.421	1.94	7	1	0	3	3.37	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	2	Toxic	Toxic	Safe
MolPort-001-949-350	398.491	5.1	6	1	1	7	7.02	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	1	Safe	Safe	Safe
MolPort-002-548-305	360.398	3.24	7	1	0	5	4.47	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	2	Safe	Safe	Safe
MolPort-002-569-909	444.516	4.78	8	1	0	8	6.81	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	1	Safe	Safe	Safe
MolPort-023-293-778	340.343	0.57	6	3	0	2	9.99	Non-Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	0	Safe	Safe	Safe

MolPort-002-987-634	282.322	1.95	4	1	0	1	5.07	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	0	Toxic	Safe	Safe
MolPort-002-574-421	338.392	3.04	7	1	0	5	4.75	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	1	Safe	Safe	Safe
MolPort-002-544-570	410.911	4.08	7	1	0	5	4.77	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	2	Toxic	Safe	Safe
MolPort-001-960-309	388.25	2.49	6	2	0	4	4.26	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	0	Safe	Safe	Safe
MolPort-002-734-790	365.443	2.59	8	1	0	2	6.94	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Toxic	Safe
MolPort-002-987-639	409.32	4.29	4	1	0	3	7.35	Absorbed	Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	Inhibitor	3	Toxic	Safe	Toxic
MolPort-001-766-590	251.249	0.45	6	2	0	1	2.87	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	0	Toxic	Safe	Safe
MolPort-002-559-631	368.418	3.2	8	1	0	6	5.82	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	0	Safe	Safe	Safe
MolPort-000-781-118	493.386	5.28	7	1	1	7	6.33	Absorbed	Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	1	Safe	Safe	Safe
MolPort-001-941-157	404.52	4.37	7	1	0	5	4.68	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	2	Toxic	Safe	Safe
MolPort-001-900-102	354.391	2.73	8	2	0	5	5.48	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	2	Safe	Safe	Safe
MolPort-020-214-296	330.823	2.34	5	3	0	4	9.33	Absorbed	Non-Inhibitor	Substrate	Non-Penetrable	Non-Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	2	Toxic	Safe	Safe
MolPort-001-960-312	324.365	2.64	7	1	0	4	4.73	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	0	Safe	Safe	Safe
MolPort-007-663-967	406.507	4.43	4	1	0	5	7.08	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Toxic	Safe
MolPort-051-741-054	352.398	1.34	8	2	0	4	7.91	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	0	Toxic	Safe	Toxic
MolPort-000-927-033	412.518	5.3	6	1	1	6	5.9	Absorbed	Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	2	Safe	Safe	Safe
MolPort-002-905-187	362.845	4.83	5	1	0	3	6.94	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Inhibitor	Inhibitor	5	Toxic	Safe	Safe
MolPort-020-	344.418	3.41	5	1	0	4	7.17	Absorbed	Inhibitor	Non-	Penetrabl	Non-	Inhibitor	Non-	Inhibitor	Inhibitor	3	Toxic	Toxic	Toxic

198-879										Substrate	e	Inhibitor		Inhibitor						
MolPort-002-345-222	339.8	2.37	5	1	0	4	8.81	Absorbed	Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	4	Safe	Safe	Toxic
MolPort-000-906-922	310.313	2.57	7	1	0	4	6.39	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	1	Toxic	Safe	Safe
MolPort-002-318-907	371.136	3.98	6	2	0	5	9.25	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Safe	Toxic
MolPort-004-479-035	405.395	3.02	9	1	0	6	3.25	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Toxic	Safe
MolPort-001-886-881	291.339	2.56	6	1	0	3	4.88	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Safe	Safe
MolPort-020-207-754	340.456	1.98	7	1	0	4	6.46	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	0	Toxic	Safe	Safe
MolPort-000-923-173	349.444	2.47	7	1	0	4	5.34	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	4	Toxic	Safe	Safe
MolPort-002-555-304	496.226	3.55	5	1	0	5	4.02	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	2	Safe	Safe	Safe
MolPort-000-791-519	469.292	4.2	9	2	0	4	8.01	Absorbed	Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	4	Safe	Safe	Safe
MolPort-000-680-387	357.211	4.75	5	1	0	4	4.71	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	2	Safe	Safe	Safe
MolPort-000-921-718	436.478	3.41	9	2	0	6	3.81	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	2	Toxic	Safe	Safe
MolPort-051-703-860	293.33	1.64	6	1	0	1	6.51	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	1	Toxic	Safe	Safe
MolPort-002-463-612	342.764	2.82	6	3	0	5	8.45	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	4	Safe	Toxic	Safe
MolPort-002-938-295	455.362	4.31	7	1	0	5	4.63	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	2	Safe	Safe	Safe
MolPort-002-905-189	392.871	5.03	6	1	1	4	7.99	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	2	Toxic	Safe	Safe
MolPort-001-024-401	303.369	4.13	5	1	0	2	6.9	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Safe	Safe
MolPort-002-143-743	286.255	0.06	9	3	0	3	7.65	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	4	Toxic	Toxic	Safe
MolPort-002-585-734	487.894	4.67	6	2	0	5	4.32	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	3	Safe	Safe	Safe
MolPort-002-550-382	407.291	2.36	6	1	0	5	3.66	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	2	Toxic	Safe	Safe
MolPort-002-	428.478	1.59	11	1	1	6	6.24	Absorbed	Non-	Non-	Penetrabl	Non-	Non-	Non-	Non-	Inhibitor	1	Toxic	Toxic	Safe

759-267									Inhibitor	Substrate	e	Inhibitor	Inhibitor	Inhibitor	Inhibitor						
MolPort-006-125-552	338.297	2.38	6	2	0	5	3.98	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	0	Safe	Safe	Safe
MolPort-051-707-847	407.836	1.59	5	1	0	2	6.66	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Inhibitor	Inhibitor	4	Safe	Safe	Safe
MolPort-003-024-485	463.468	2.46	11	1	1	8	6.78	Absorbed	Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	2	Safe	Safe	Safe
MolPort-020-209-866	282.322	2.14	4	2	0	1	6.85	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	Inhibitor	2	Toxic	Safe	Safe
MolPort-051-714-315	402.414	1.36	7	2	0	3	8.12	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	2	Safe	Safe	Safe
MolPort-051-714-008	320.377	3.38	6	1	0	1	8.55	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	4	Toxic	Safe	Safe
MolPort-030-044-062	332.407	2.08	3	1	0	3	10.11	Absorbed	Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Inhibitor	Inhibitor	5	Safe	Safe	Toxic
MolPort-002-867-195	315.72	0.84	7	2	0	2	3.33	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	Inhibitor	2	Toxic	Safe	Safe
MolPort-002-742-314	416.235	2.55	7	1	0	1	6.19	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Toxic	Safe
MolPort-003-015-060	382.445	3.61	8	1	0	7	5.88	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	0	Safe	Safe	Safe
MolPort-000-919-790	349.444	2.68	7	1	0	4	5.82	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	4	Toxic	Safe	Safe
MolPort-047-659-610	538.549	3.49	10	3	1	4	7.72	Absorbed	Non-Inhibitor	Substrate	Non-Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	3	Toxic	Safe	Safe
MolPort-000-687-696	513.47	0.91	10	4	1	7	6.88	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	2	Safe	Safe	Safe
MolPort-002-550-051	314.326	1.94	8	1	0	4	3.82	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	0	Safe	Safe	Safe
MolPort-000-788-864	444.516	4.59	8	1	0	8	6.78	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	1	Safe	Safe	Safe
MolPort-004-949-034	400.416	2.09	9	2	0	7	3.67	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	0	Safe	Safe	Safe
MolPort-020-206-341	308.36	2.38	4	2	0	1	7.84	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	1	Toxic	Safe	Toxic
MolPort-002-319-207	316.273	3.1	6	2	0	5	9.3	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	4	Toxic	Toxic	Safe

MolPort-021-805-184	297.274	-0.13	8	3	0	2	3.74	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	1	Toxic	Safe	Safe
MolPort-002-703-186	622.946	3.66	16	2	2	10	6.55	Absorbed	Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Safe	Safe
MolPort-002-319-220	317.257	2.48	6	1	0	5	8.07	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Safe	Toxic
MolPort-002-819-232	265.272	2.99	5	1	0	3	2.38	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	1	Safe	Safe	Safe
MolPort-000-745-754	295.322	2.17	5	1	0	3	5.46	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Safe	Safe
MolPort-002-742-312	375.413	2.68	8	1	0	4	7.13	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	2	Toxic	Toxic	Safe
MolPort-002-319-208	332.272	2.55	7	2	0	6	9.5	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	4	Toxic	Toxic	Safe
MolPort-002-832-134	321.365	2.66	7	1	0	4	6.28	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Inhibitor	Non-Inhibitor	Inhibitor	Inhibitor	Inhibitor	4	Toxic	Safe	Safe
MolPort-000-763-279	448.443	1.12	10	2	0	7	7.35	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	2	Safe	Safe	Safe
MolPort-002-809-592	309.329	1.41	7	2	0	4	3.56	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	0	Toxic	Safe	Safe
MolPort-000-792-947	405.508	3.71	7	2	0	5	5.56	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	2	Safe	Safe	Safe
MolPort-047-116-030	450.487	4.01	7	2	0	3	8.02	Absorbed	Non-Inhibitor	Substrate	Non-Penetrable	Non-Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	1	Toxic	Safe	Safe
MolPort-002-136-107	400.463	4.13	7	2	0	5	5.56	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	2	Safe	Safe	Safe
MolPort-002-319-218	303.23	2.24	6	1	0	5	9	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	4	Toxic	Safe	Toxic
MolPort-000-780-839	459.487	4.27	9	1	0	8	5.52	Absorbed	Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	2	Toxic	Safe	Safe
MolPort-051-751-385	372.432	1.86	6	1	0	3	8.22	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Safe	Safe	Safe
MolPort-002-318-913	336.691	3.53	6	2	0	5	9.78	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	4	Toxic	Safe	Toxic
MolPort-028-752-543	252.237	-0.77	7	2	0	1	2.69	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	0	Toxic	Safe	Safe

MolPort-002-352-051	356.454	4.42	5	1	0	4	7.12	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Safe	Safe
MolPort-051-710-337	320.179	2.9	4	1	0	1	7.73	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Inhibitor	Inhibitor	4	Toxic	Safe	Safe
MolPort-002-319-206	302.246	2.88	6	2	0	5	10.23	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	4	Toxic	Toxic	Toxic
MolPort-001-572-788	241.21	-0.26	7	2	0	1	1.53	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	0	Toxic	Safe	Safe
MolPort-002-701-930	323.787	4.25	5	1	0	2	6.19	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Inhibitor	Inhibitor	5	Toxic	Safe	Safe
MolPort-023-277-195	379.445	2.78	7	2	0	7	5.05	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	1	Toxic	Safe	Safe
MolPort-002-724-493	436.436	1.14	11	2	1	6	7.48	Absorbed	Inhibitor	Non-Substrate	Penetrable	Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	2	Safe	Toxic	Safe
MolPort-002-023-621	312.329	0.99	6	1	0	3	6.58	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	0	Safe	Toxic	Safe
MolPort-009-752-970	315.13	2.24	5	2	0	1	1.84	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	2	Safe	Safe	Safe
MolPort-051-488-607	442.564	0.84	8	3	0	10	9.39	Absorbed	Non-Inhibitor	Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	1	Toxic	Toxic	Toxic
MolPort-002-319-219	337.675	2.82	6	1	0	5	8.73	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	4	Toxic	Safe	Toxic
MolPort-000-732-626	396.472	4.19	8	1	0	8	5.92	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	2	Safe	Safe	Safe
MolPort-051-707-148	315.76	2.43	5	1	0	2	9.07	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Safe	Safe
MolPort-051-753-707	373.416	1.76	6	1	0	2	7.08	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Safe	Safe
MolPort-000-921-116	419.535	3.17	7	2	0	7	4.55	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	1	Safe	Safe	Safe
MolPort-002-550-237	299.315	0.76	7	2	0	4	3.49	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	0	Toxic	Toxic	Safe
MolPort-003-006-408	403.394	1.87	6	2	0	4	11.4	Absorbed	Inhibitor	Non-Substrate	Penetrable	Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	1	Toxic	Safe	Safe
MolPort-009-767-298	353.427	3.01	7	1	0	6	5.96	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	2	Toxic	Safe	Safe
MolPort-000-698-755	354.435	3.56	7	2	0	6	5.28	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Safe	Safe

MolPort-000-920-538	293.33	3.2	6	1	0	3	5.22	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Safe	Safe
MolPort-002-914-517	264.288	3.19	5	1	0	3	4.42	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	2	Safe	Safe	Safe
MolPort-002-136-110	268.301	1.73	5	3	0	1	4.35	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Safe	Safe
MolPort-002-542-454	411.317	5.39	5	1	1	4	6.75	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Inhibitor	Inhibitor	4	Toxic	Safe	Safe
MolPort-004-955-020	287.239	0.53	9	3	0	3	5.98	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	3	Toxic	Safe	Safe
MolPort-002-544-336	342.38	2.74	8	1	0	5	4.13	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	2	Safe	Toxic	Safe
MolPort-000-923-183	549.273	4.45	7	2	1	5	4.82	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	2	Safe	Safe	Safe
MolPort-002-912-173	332.367	2.79	7	1	0	5	5.61	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	1	Toxic	Safe	Safe
MolPort-051-717-110	400.486	2.06	6	1	0	3	8.1	Absorbed	Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	2	Toxic	Safe	Safe
MolPort-000-921-132	435.534	3	8	2	0	7	5.45	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	1	Toxic	Safe	Safe
MolPort-002-734-788	353.794	2.59	7	1	0	1	7.04	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Toxic	Safe
MolPort-002-832-120	376.466	3.46	7	1	0	5	4.53	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	2	Toxic	Safe	Safe
MolPort-002-570-787	270.292	2.1	4	2	0	1	2.32	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Safe	Safe
MolPort-051-741-275	344.85	2.56	5	3	0	4	8.9	Absorbed	Non-Inhibitor	Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	1	Toxic	Safe	Toxic
MolPort-001-904-828	416.462	3.72	8	2	0	6	6.15	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	1	Safe	Safe	Safe
MolPort-044-561-533	313.405	1.51	6	3	0	5	9.97	Absorbed	Non-Inhibitor	Substrate	Non-Penetrable	Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	1	Toxic	Toxic	Safe
MolPort-000-926-962	322.437	5.07	5	1	1	4	5.99	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Inhibitor	Inhibitor	4	Safe	Safe	Safe

MolPort-000-923-187	395.469	2.26	8	2	0	6	3.58	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	1	Toxic	Toxic	Safe
MolPort-001-923-375	321.384	3.95	6	1	0	5	6.61	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Safe	Safe
MolPort-002-980-293	333.222	2.9	4	1	0	1	5.96	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	Inhibitor	2	Toxic	Safe	Safe
MolPort-000-795-756	335.232	1.86	9	3	0	5	5.85	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	4	Toxic	Toxic	Safe
MolPort-007-663-993	394.471	4.77	3	1	0	4	6.1	Absorbed	Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	4	Toxic	Toxic	Safe
MolPort-002-625-742	446.471	4.21	10	2	0	6	8.41	Absorbed	Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Safe	Toxic	Safe
MolPort-010-698-298	495.576	3.41	4	2	0	7	8.9	Absorbed	Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Inhibitor	Inhibitor	3	Safe	Safe	Toxic
MolPort-000-165-619	237.218	1.1	4	2	0	1	0.93	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	0	Safe	Safe	Safe
MolPort-009-752-969	236.234	1.5	5	2	0	1	1.76	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	2	Safe	Safe	Safe
MolPort-000-680-395	359.183	3.48	6	1	0	3	6.32	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Non-Inhibitor	Inhibitor	Inhibitor	Inhibitor	4	Toxic	Safe	Safe
MolPort-002-550-179	364.474	5.19	6	1	1	8	5.82	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Safe	Safe	Safe
MolPort-002-144-248	345.225	4.3	5	1	0	2	5.13	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Non-Inhibitor	Inhibitor	Inhibitor	Inhibitor	4	Safe	Safe	Safe
MolPort-002-686-298	366.446	3.96	6	1	0	4	5.25	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Safe	Safe
MolPort-035-395-281	286.287	1.48	4	3	0	4	9.09	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	3	Toxic	Safe	Safe
MolPort-002-318-912	371.136	4	6	2	0	5	9.25	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Safe	Toxic
MolPort-047-945-573	314.389	1.94	6	2	0	5	9.88	Absorbed	Non-Inhibitor	Substrate	Non-Penetrable	Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	1	Toxic	Toxic	Safe
MolPort-019-784-439	268.301	2.25	6	3	0	1	5.07	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	2	Toxic	Safe	Safe
MolPort-009-752-915	266.26	1.69	6	2	0	2	3.33	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	1	Toxic	Safe	Safe
MolPort-002-	268.301	1.71	5	3	0	1	4.46	Absorbed	Non-	Non-	Non-	Non-	Non-	Inhibitor	Non-	Inhibitor	2	Toxic	Safe	Safe

551-700									Inhibitor	Substrate	Penetrable	Inhibitor	Inhibitor		Inhibitor				
MolPort-000-923-172	314.439	4.22	6	1	0	5	4.8	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	4	Toxic	Safe	Safe
MolPort-002-542-571	269.284	2.17	5	1	0	1	3.22	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	1	Toxic	Safe	Safe
MolPort-051-745-035	421.407	1.83	6	1	0	3	6.22	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Safe	Safe
MolPort-022-808-352	290.235	-0.24	7	2	0	4	4.73	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	0	Toxic	Safe	Safe
MolPort-000-922-323	357.464	2.09	7	2	0	5	3.97	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	1	Safe	Safe	Safe
MolPort-008-326-447	270.292	2.28	4	2	0	1	2.58	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Safe	Safe
MolPort-002-351-817	366.446	4.15	7	1	0	6	4.91	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	0	Safe	Safe	Safe
MolPort-000-777-472	331.198	3.02	4	2	0	1	3.36	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Safe	Safe
MolPort-000-933-319	286.747	2.77	4	2	0	1	3.56	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Non-Inhibitor	Inhibitor	Inhibitor	Inhibitor	4	Toxic	Safe	Safe
MolPort-002-700-911	484.353	0.51	17	2	1	8	3.79	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	2	Safe	Safe	Safe
MolPort-000-712-569	393.899	4.43	4	2	0	3	6.5	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Safe	Safe	Safe
MolPort-006-249-106	330.8	2.95	6	2	0	4	5.52	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Inhibitor	Inhibitor	3	Safe	Safe	Safe
MolPort-002-274-533	299.355	2.99	6	2	0	3	5.61	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	3	Safe	Safe	Safe
MolPort-002-626-794	456.825	3.59	10	2	0	6	7.6	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	4	Safe	Safe	Safe
MolPort-002-138-241	315.383	1.11	7	2	0	4	3.51	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	1	Toxic	Safe	Safe
MolPort-002-907-633	283.291	0.43	6	1	0	3	9.21	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	1	Safe	Safe	Safe
MolPort-047-154-049	313.405	1.84	6	2	0	5	10.43	Absorbed	Non-Inhibitor	Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	0	Toxic	Toxic	Toxic
MolPort-051-714-355	331.807	2.72	5	2	0	4	8.97	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Safe	Safe

MolPort-000-919-071	420.475	3.44	9	1	0	5	4.84	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	2	Toxic	Safe	Safe
MolPort-000-933-927	266.329	3.26	5	1	0	2	5.19	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	4	Toxic	Safe	Safe
MolPort-002-632-274	316.321	-0.18	8	4	0	4	8.29	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	0	Toxic	Safe	Safe
MolPort-002-319-209	330.3	3.54	6	2	0	5	9.19	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Toxic	Safe
MolPort-002-980-034	298.777	2.09	4	1	0	1	6.01	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	1	Toxic	Safe	Safe
MolPort-002-911-531	276.259	0.03	7	2	0	1	2.26	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	0	Toxic	Safe	Safe
MolPort-000-776-985	492.452	0.65	12	2	1	10	6.75	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	0	Safe	Safe	Safe
MolPort-000-921-125	314.439	4.15	6	1	0	4	4.43	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Safe	Safe	Safe
MolPort-000-680-388	264.288	3.4	5	1	0	2	5.05	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Safe	Safe	Safe
MolPort-002-136-112	403.261	3.64	7	1	0	4	4.63	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	0	Safe	Safe	Safe
MolPort-002-543-357	324.409	4.08	6	2	0	5	4.96	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Safe	Safe
MolPort-001-897-103	294.314	3.46	6	1	0	4	6.2	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	2	Toxic	Safe	Safe
MolPort-000-921-115	314.395	2.02	7	1	0	4	3.79	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	1	Toxic	Safe	Safe
MolPort-001-960-310	432.574	5.5	7	1	1	8	5.13	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	2	Safe	Safe	Safe
MolPort-051-708-049	331.379	2.14	6	1	0	2	10.42	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Safe	Safe
MolPort-002-724-424	292.284	-0.19	10	3	0	3	7	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	4	Toxic	Toxic	Safe
MolPort-002-551-562	338.392	3.22	7	1	0	4	5.13	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	1	Safe	Safe	Safe
MolPort-051-712-012	290.326	2.47	4	2	0	1	8.74	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Inhibitor	Inhibitor	4	Toxic	Safe	Safe
MolPort-000-778-971	497.859	3.72	12	2	1	8	8.1	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Toxic	Safe
MolPort-000-925-287	252.302	1.92	4	2	0	1	3.06	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Safe	Safe
MolPort-002-851-441	426.86	2.18	8	2	0	5	6.03	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	2	Safe	Safe	Safe

MolPort-002-980-291	324.384	2.26	6	1	0	3	7.85	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	0	Toxic	Safe	Safe
MolPort-020-204-901	346.768	1.92	4	2	0	1	5.74	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	Inhibitor	2	Toxic	Safe	Toxic
MolPort-002-821-298	400.485	2.85	9	1	0	7	4.22	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	1	Safe	Safe	Safe
MolPort-000-677-150	266.26	2.54	6	2	0	2	5.17	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	2	Safe	Safe	Safe
MolPort-002-572-701	434.908	4.46	7	1	0	6	6.31	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	2	Toxic	Safe	Safe
MolPort-001-663-913	268.251	3.06	5	1	0	2	3.82	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Safe	Safe	Safe
MolPort-000-680-392	296.305	3.48	5	1	0	4	3.54	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	2	Safe	Safe	Safe
MolPort-019-716-315	335.436	4.01	6	1	0	5	5.23	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Inhibitor	Inhibitor	4	Toxic	Safe	Safe
MolPort-016-627-790	317.334	-0.16	8	2	0	6	5.65	Non-Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	0	Safe	Safe	Safe
MolPort-000-921-377	298.396	3.24	6	1	0	4	4.22	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Safe	Safe
MolPort-009-752-968	264.288	2.55	5	2	0	2	3.43	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Safe	Safe	Safe
MolPort-051-715-879	317.295	2.2	5	1	0	2	5.57	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Safe	Safe
MolPort-000-921-114	371.491	2.41	7	1	0	6	4.12	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	1	Safe	Safe	Safe
MolPort-002-589-405	426.914	2.77	8	2	0	5	5.6	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Inhibitor	Inhibitor	3	Safe	Safe	Safe
MolPort-000-690-826	280.287	3.02	6	1	0	3	6.16	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	2	Toxic	Safe	Safe
MolPort-002-987-632	308.385	2.58	5	1	0	3	7.25	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	1	Toxic	Safe	Safe
MolPort-000-780-159	459.514	4.6	10	2	0	8	8.43	Absorbed	Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Safe	Safe	Safe
MolPort-001-917-890	591.15	5.33	6	1	2	2	8.09	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	1	Toxic	Safe	Safe
MolPort-005-915-880	442.504	2.78	6	3	0	3	9.95	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	2	Safe	Safe	Safe

MolPort-002-142-623	295.371	2.35	5	2	0	2	4.56	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Safe	Safe
MolPort-002-905-188	368.874	4.47	6	1	0	3	5.78	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	4	Toxic	Safe	Safe
MolPort-002-632-602	480.916	4.72	10	2	0	8	8.44	Absorbed	Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Safe	Safe	Safe
MolPort-002-630-793	473.453	2.89	11	3	1	7	8.22	Absorbed	Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Safe	Safe	Safe
MolPort-002-579-047	308.41	4.79	5	1	0	4	5.51	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Inhibitor	Inhibitor	4	Safe	Safe	Safe
MolPort-002-626-363	423.462	3.01	11	2	1	6	7.7	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Safe	Safe
MolPort-002-739-075	268.28	1.79	7	1	0	3	5.83	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	2	Toxic	Safe	Safe
MolPort-003-712-812	324.409	3.5	5	2	0	5	5.27	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Safe	Safe
MolPort-051-750-434	271.345	2.47	5	1	0	1	8.05	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	4	Toxic	Safe	Safe
MolPort-000-919-869	250.261	2.79	5	1	0	2	4.12	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Safe	Safe	Safe
MolPort-002-136-111	326.337	2.08	7	3	0	4	3.49	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	0	Safe	Safe	Safe
MolPort-002-585-431	473.558	3.34	8	2	0	8	7.09	Absorbed	Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	Inhibitor	2	Safe	Safe	Safe
MolPort-002-678-996	391.225	1.44	6	1	0	3	6.17	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	1	Safe	Safe	Safe
MolPort-003-716-111	426.494	4.28	7	1	0	5	9.24	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	4	Toxic	Safe	Safe
MolPort-002-583-584	300.774	4.07	5	1	0	2	5.31	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Inhibitor	Inhibitor	5	Toxic	Safe	Safe
MolPort-002-323-386	311.301	0.75	8	2	0	3	4.02	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	1	Toxic	Safe	Safe
MolPort-003-179-988	344.421	2.66	8	1	0	5	3.96	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	2	Safe	Safe	Safe
MolPort-000-923-175	437.525	3.38	7	2	0	7	4.39	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	1	Safe	Safe	Safe
MolPort-000-680-391	268.251	2.53	5	1	0	2	3.27	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Safe	Safe

MolPort-001-740-121	521.566	3.76	9	3	1	5	7.33	Non-Absorbed	Non-Inhibitor	Substrate	Non-Penetrable	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	3	Toxic	Safe	Safe
MolPort-002-544-912	394.5	5.32	7	1	1	8	5.89	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	1	Safe	Safe	Safe
MolPort-002-144-288	358.448	3.08	8	1	0	5	4.1	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	1	Safe	Safe	Safe
MolPort-002-583-103	343.799	1.36	6	2	0	4	3.84	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	Inhibitor	2	Toxic	Safe	Safe
MolPort-002-905-185	352.806	4.2	6	1	0	3	5.58	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	4	Toxic	Safe	Safe
MolPort-004-479-034	282.328	2.97	6	2	0	2	5.61	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Safe	Safe	Safe
MolPort-001-941-214	270.317	2.85	6	1	0	3	4.64	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Safe	Safe
MolPort-023-263-758	314.301	0.68	7	1	0	5	7.22	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	1	Toxic	Toxic	Safe
MolPort-002-907-195	316.748	2.33	5	1	0	3	8.05	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	1	Safe	Safe	Safe
MolPort-002-138-239	256.29	2.51	6	1	0	2	4.66	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	4	Toxic	Safe	Safe
MolPort-020-196-944	336.424	1.7	7	1	0	2	8.62	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	1	Toxic	Safe	Safe
MolPort-001-981-823	372.837	2.88	7	1	0	5	4.46	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	1	Safe	Safe	Safe
MolPort-002-714-540	346.208	0.39	6	2	0	4	3.17	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	1	Toxic	Safe	Safe
MolPort-002-098-645	334.397	2.74	4	2	0	6	9.83	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	2	Safe	Safe	Safe
MolPort-051-710-622	309.373	1.61	6	1	0	3	7.97	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	2	Toxic	Safe	Safe
MolPort-000-919-244	356.476	3.32	7	1	0	4	4.21	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	2	Safe	Safe	Safe
MolPort-000-922-217	400.485	2.68	9	1	0	7	4.01	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	1	Safe	Safe	Safe
MolPort-002-569-107	410.499	4.62	8	1	0	9	6.04	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	1	Safe	Safe	Safe
MolPort-002-987-642	400.482	3.75	6	1	0	5	8.99	Absorbed	Inhibitor	Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	1	Toxic	Safe	Toxic
MolPort-002-738-620	283.295	-0.63	8	2	0	2	4.07	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	0	Toxic	Toxic	Safe

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MolPort-000-921-113	371.491	2.78	7	2	0	4	3.95	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	2	Safe	Safe	Safe
MolPort-001-922-916	603.547	3.48	12	3	2	10	6.11	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Safe	Safe	Safe
MolPort-002-543-400	381.461	2.98	7	2	0	8	5.62	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	2	Toxic	Safe	Safe
MolPort-020-220-509	347.334	2.45	7	2	0	2	8.78	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Safe	Safe	Safe
MolPort-003-056-982	335.392	3.09	7	1	0	5	6.2	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	2	Toxic	Safe	Safe
MolPort-002-016-473	356.43	1.26	7	2	0	6	7.11	Absorbed	Non-Inhibitor	Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	0	Safe	Safe	Toxic
MolPort-002-629-832	466.889	3.82	10	2	0	7	8.46	Absorbed	Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	4	Safe	Toxic	Safe
MolPort-000-680-398	294.314	3.2	6	1	0	4	5.32	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	2	Safe	Safe	Safe
MolPort-002-138-240	297.368	2.2	7	1	0	3	4.24	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Safe	Safe
MolPort-002-142-488	280.356	3.59	5	1	0	3	5.24	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Safe	Safe	Safe
MolPort-019-938-939	281.34	3.72	5	1	0	3	3.16	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	3	Safe	Safe	Safe
MolPort-000-782-002	363.242	2.49	9	3	0	6	3.73	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	1	Toxic	Toxic	Safe
MolPort-006-249-219	422.466	3.11	9	1	0	7	6.66	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	Inhibitor	3	Toxic	Safe	Safe
MolPort-001-985-531	282.328	2.87	6	1	0	4	4.35	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	2	Toxic	Toxic	Safe
MolPort-006-707-457	251.249	1.6	6	1	0	2	4.42	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	2	Safe	Safe	Safe
MolPort-000-655-068	723.915	8.58	10	1	2	18	5.08	Absorbed	Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Safe	Safe	Safe
MolPort-000-680-390	298.733	3.1	5	1	0	3	4.23	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Safe	Safe	Safe
MolPort-001-	310.313	3.17	7	1	0	4	6.51	Absorbed	Non-	Non-	Penetrabl	Non-	Non-	Non-	Non-	Inhibitor	1	Toxic	Safe	Safe

928-183									Inhibitor	Substrate	e	Inhibitor	Inhibitor	Inhibitor	Inhibitor					
MolPort-023-282-498	318.289	0.74	8	1	0	5	7.16	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	2	Toxic	Safe	Safe
MolPort-000-920-031	378.482	3.94	7	1	0	5	6.42	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	2	Toxic	Safe	Safe
MolPort-001-768-764	248.072	1.61	5	3	0	3	8.46	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	1	Safe	Safe	Toxic
MolPort-000-909-319	310.313	2.95	7	1	0	4	6.57	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	1	Toxic	Safe	Safe
MolPort-001-903-907	386.458	2.25	9	1	0	7	3.8	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	1	Safe	Safe	Safe
MolPort-002-734-792	404.274	2.33	8	1	0	1	6.07	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Toxic	Safe
MolPort-002-629-802	448.443	3.82	11	3	1	7	8.18	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	4	Safe	Toxic	Safe
MolPort-020-190-663	372.831	2.16	5	1	0	2	6.9	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	0	Toxic	Safe	Toxic
MolPort-045-902-031	257.278	0.28	7	2	0	1	2.68	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	1	Toxic	Safe	Safe
MolPort-000-921-870	386.458	2.41	9	1	0	7	4	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	1	Safe	Safe	Safe
MolPort-002-023-624	381.219	1.79	6	1	0	3	6.55	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	1	Safe	Safe	Safe
MolPort-002-625-376	438.473	3.17	11	2	1	7	8.09	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	4	Toxic	Safe	Safe
MolPort-000-769-956	478.469	0.55	11	2	1	8	7.59	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	1	Safe	Safe	Safe
MolPort-002-926-575	274.37	1.96	5	1	0	2	3.81	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	4	Safe	Safe	Safe
MolPort-020-199-944	352.438	2.97	6	2	0	4	7.23	Absorbed	Non-Inhibitor	Substrate	Non-Penetrable	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	Inhibitor	3	Safe	Safe	Toxic
MolPort-044-809-211	276.281	0.7	7	2	0	2	6.48	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	0	Safe	Safe	Safe
MolPort-002-631-427	497.313	4.45	10	2	0	7	8.38	Absorbed	Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	4	Safe	Toxic	Safe
MolPort-002-987-637	382.464	2.8	7	1	0	6	7.8	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	1	Safe	Safe	Toxic
MolPort-020-232-437	361.232	1.72	5	3	0	1	6.1	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	Inhibitor	2	Toxic	Safe	Toxic
MolPort-002-	282.307	1.81	7	1	0	3	5.86	Absorbed	Non-	Non-	Penetrabl	Non-	Inhibitor	Inhibitor	Non-	Inhibitor	3	Toxic	Safe	Safe

735-739									Inhibitor	Substrate	e	Inhibitor			Inhibitor						
MolPort-047-637-467	393.421	3.84	6	2	0	9	4.62	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	1	Safe	Safe	Safe
MolPort-002-627-831	440.445	2.75	12	2	1	7	8.19	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Safe	Safe
MolPort-000-774-203	507.854	-0.81	11	2	2	6	5.78	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	0	Safe	Safe	Safe
MolPort-000-680-394	333.178	3.86	5	1	0	3	4.46	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Non-Inhibitor	Inhibitor	Inhibitor	Inhibitor	4	Safe	Safe	Safe
MolPort-006-249-199	407.296	4.26	5	1	0	3	6.71	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Safe	Safe
MolPort-000-680-397	280.287	2.85	6	1	0	3	5.98	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	3	Toxic	Safe	Safe
MolPort-005-913-453	464.348	4.36	5	2	0	2	9.2	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	3	Safe	Safe	Safe
MolPort-002-352-050	376.872	3.97	5	1	0	4	6.64	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Inhibitor	Inhibitor	4	Toxic	Safe	Safe
MolPort-001-992-665	360.393	1.15	7	2	0	6	7.27	Absorbed	Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	0	Safe	Safe	Toxic
MolPort-002-802-435	286.385	3.18	6	1	0	3	4.38	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	4	Toxic	Safe	Safe
MolPort-020-228-072	336.395	2.05	6	2	0	3	9.81	Absorbed	Non-Inhibitor	Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	1	Toxic	Safe	Toxic
MolPort-002-324-258	308.341	3.49	6	1	0	4	5.18	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Safe	Safe	Safe
MolPort-051-716-294	385.427	1.56	6	1	0	3	9.16	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	3	Safe	Safe	Safe
MolPort-051-542-028	576.698	3.51	9	3	1	13	8.72	Absorbed	Inhibitor	Substrate	Penetrable	Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	Inhibitor	3	Toxic	Toxic	Toxic
MolPort-000-933-244	272.358	2.84	6	1	0	2	4.38	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	4	Toxic	Safe	Safe
MolPort-035-946-101	419.441	1.87	7	3	0	7	7.14	Absorbed	Inhibitor	Non-Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	0	Safe	Safe	Safe
MolPort-019-893-809	364.405	2.19	7	1	0	2	8.76	Absorbed	Non-Inhibitor	Substrate	Penetrable	Non-Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	Inhibitor	3	Toxic	Safe	Toxic
MolPort-000-687-719	623.625	5.12	10	3	2	8	6.32	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Inhibitor	Inhibitor	Inhibitor	Inhibitor	Inhibitor	5	Safe	Safe	Safe
MolPort-002-028-518	364.492	3.1	4	1	0	5	7.37	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	2	Safe	Safe	Safe

MolPort-023-252-669	338.367	1.5	6	1	0	5	7.84	Absorbed	Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	1	Toxic	Safe	Safe
MolPort-001-766-592	257.278	0.17	7	2	0	1	2.67	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	0	Toxic	Safe	Safe
MolPort-023-256-333	354.366	0.88	7	1	0	6	7.81	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	2	Safe	Safe	Safe
MolPort-020-185-314	364.405	1.36	7	2	0	2	10.25	Absorbed	Non-Inhibitor	Substrate	Non-Penetrable	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	1	Toxic	Safe	Toxic
MolPort-051-752-650	410.865	2.24	7	2	0	6	7.4	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	4	Toxic	Toxic	Safe
MolPort-002-624-804	440.445	2.32	12	3	1	6	7.63	Absorbed	Non-Inhibitor	Non-Substrate	Non-Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	4	Toxic	Safe	Safe
MolPort-002-905-732	313.404	-0.04	6	2	0	4	8.33	Absorbed	Non-Inhibitor	Non-Substrate	Penetrable	Inhibitor	Inhibitor	Inhibitor	Non-Inhibitor	Inhibitor	4	Safe	Toxic	Safe
MolPort-002-286-918	378.45	3.03	5	2	0	8	9.62	Absorbed	Inhibitor	Non-Substrate	Non-Penetrable	Inhibitor	Inhibitor	Non-Inhibitor	Non-Inhibitor	Inhibitor	3	Safe	Safe	Safe

Suppl. Table 4 — Binding energy of compounds obtained from virtual screening

S. No.	Compound id	Binding Energy (kcal/mol)
1	staurosporine	-9.72
2	MolPort-023-306-537	-9.43
3	MolPort-005-915-880	-9.32
4	MolPort-005-914-867	-9.25
5	MolPort-003-049-539	-9.18
6	MolPort-003-049-585	-9.15
7	MolPort-000-414-107	-9.13
8	MolPort-005-916-947	-9.1
9	MolPort-003-049-507	-9.09
10	MolPort-023-306-533	-9.03
11	MolPort-005-912-438	-8.99
12	MolPort-046-423-501	-8.91
13	Molport-049-227-714	-8.77
14	MolPort-046-423-784	-8.75
15	MolPort-003-049-513	-8.66
16	MolPort-003-049-492	-8.65
17	MolPort-003-162-015	-8.61

18	MolPort-046-424-270	-8.57
19	Molport-051-890-546	-8.49
20	MolPort-002-555-304	-8.31
21	MolPort-035-717-384	-8.29
22	MolPort-000-758-115	-8.28
23	MolPort-002-902-036	-8.11
24	MolPort-000-919-038	-8.1
25	MolPort-002-700-911	-8.07
26	MolPort-000-763-279	-8.07
27	MolPort-003-049-574	-8.07
28	MolPort-035-717-385	-8.04
29	MolPort-002-678-996	-8.02
30	MolPort-051-747-057	-8
31	MolPort-001-960-309	-8
32	MolPort-044-809-211	-7.98
33	MolPort-046-423-621	-7.96
34	MolPort-002-696-141	-7.95
35	MolPort-007-550-708	-7.94
36	MolPort-003-049-532	-7.94
37	MolPort-020-220-769	-7.92
38	MolPort-002-795-814	-7.86
39	MolPort-000-252-466	-7.85
40	MolPort-000-736-219	-7.84
41	MolPort-001-675-116	-7.82
42	MolPort-035-669-648	-7.81
43	MolPort-002-938-295	-7.78
44	MolPort-007-686-452	-7.62
45	MolPort-051-713-217	-7.58
46	MolPort-002-544-846	-7.58
47	MolPort-023-256-333	-7.57
48	MolPort-001-949-350	-7.49
49	MolPort-020-197-366	-7.44
50	MolPort-051-714-315	-7.43
51	MolPort-002-353-133	-7.43
52	MolPort-002-354-089	-7.41
53	MolPort-000-919-244	-7.39
54	MolPort-051-711-701	-7.39
55	MolPort-002-023-624	-7.38
56	MolPort-000-769-956	-7.37

57	MolPort-006-828-068	-7.34
58	MolPort-002-028-518	-7.25
59	MolPort-020-215-831	-7.23
60	MolPort-002-907-195	-7.22
61	MolPort-051-702-401	-7.21
62	MolPort-002-098-645	-7.2
63	MolPort-002-136-112	-7.2
64	MolPort-002-795-751	-7.19
65	MolPort-000-680-387	-7.18
66	MolPort-019-718-509	-7.15
67	MolPort-002-710-498	-7.14
68	MolPort-000-923-175	-7.09
69	MolPort-020-211-078	-7.09
70	MolPort-002-551-707	-6.93
71	MolPort-003-015-060	-6.93
72	MolPort-002-575-850	-6.89
73	MolPort-002-551-562	-6.89
74	MolPort-035-717-164	-6.89
75	MolPort-002-569-909	-6.86
76	MolPort-002-543-183	-6.82
77	MolPort-051-710-656	-6.81
78	MolPort-000-921-114	-6.79
79	MolPort-002-144-288	-6.71
80	MolPort-009-752-970	-6.67
81	MolPort-000-165-619	-6.65
82	Molport-051-839-879	-6.61
83	MolPort-001-981-823	-6.6
84	MolPort-008-435-359	-6.53
85	MolPort-000-680-398	-6.51
86	MolPort-002-550-051	-6.51
87	MolPort-001-941-213	-6.51
88	MolPort-002-544-912	-6.5
89	MolPort-002-914-517	-6.49
90	MolPort-001-903-907	-6.48
91	MolPort-009-752-969	-6.4
92	MolPort-003-179-988	-6.4
93	MolPort-000-680-392	-6.38
94	MolPort-002-907-633	-6.37
95	MolPort-002-819-232	-6.27
96	MolPort-002-574-421	-6.24

97	MolPort-001-960-312	-6.23
98	MolPort-008-336-200	-6.21
99	MolPort-009-765-630	-6.1
100	MolPort-002-898-431	-6.06
101	MolPort-000-922-217	-6
102	MolPort-006-707-457	-5.95
103	MolPort-000-921-870	-5.88
104	MolPort-002-821-298	-5.71
105	MolPort-000-804-072	-5.35