

Supplementary Material for:

The Medicinal Chemist's Toolbox: An Analysis of Reactions Used in the
Pursuit of Drug Candidates.

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Table S1 Breakdown of references in dataset by target class

Area	AZ	GSK	Pfizer	Total
Kinase	14	14	5	33
GPCR - Peptidic	2	14	7	23
GPCR - Amine	1	9	8	18
Other	2	5	9	16
Protease	1	9	2	12
Anti-infective	3	2	3	8
Nuclear Hormone Receptors	0	6	2	8
Transporter	0	0	8	8
GPCR - lipid	1	4	1	6
Ion Channel	0	1	4	5
PDE	0	1	1	2
Total	24	65	50	139

Table S2 Breakdown of reactions in the dataset by target class

Area	AZ	GSK	Pfizer	Total
Kinase	614	1012	326	1952
GPCR - Peptidic	66	886	157	1109
Other	64	318	537	919
GPCR - Amine	23	580	305	908
Protease	54	497	134	685
Transporter	0	0	503	503
Anti-infective	138	100	155	393
GPCR - lipid	158	198	14	370
NHR	0	223	67	290
Ion Channel	0	25	86	111
PDE	0	58	17	75
Total	1117	3897	2301	7315

Table S3 Breakdown of compounds in the dataset by target class

Area	AZ	GSK	Pfizer	Total
Kinase	368	338	129	835
GPCR - Peptidic	70	398	121	589
GPCR - Amine	15	336	161	512
Other	26	94	254	374
Protease	22	216	50	288
GPCR - lipid	50	167	29	246
Transporter	0	0	232	232
Anti-infective	51	81	46	178
NHR	0	118	23	141
Ion Channel	0	23	107	130
PDE	0	30	11	41
Total	602	1801	1163	3566

Table S4 Known sources of enantiopure chiral centres

Source of chirality	% of Total Enantiopure Centres	% of Subclass
Chiral Pool – i.e. purchased enantiopure material	86.5	
Asymmetric synthesis	6.3	
Organocatalysis		57.4
Diastereoselective reduction of enantiopure ketone		22.7
Jacobsen Epoxidation		11.9
Enantioselective hydrogenation		5.9
Resolution	7.2	
Chromatographic separation of diastereomers following reaction with enantiopure precursor		62.1
Lipase resolution		22.4
Chiral HPLC/SFC		12.1
Unknown/unspecified		3.4