

Positio	Site	Compound Info	CMPD-ID	donor	acceptor	occupancy
T1_9	Primary	Hit	7256141	SegC2-UNK900-Main	SegC2-GLU556-Side	171.7%
T1_4	Primary	Hit	3186499	SegC2-ARG521-Side	SegC2-UNK900-Main	84.5%
T1_1	Primary	Hit	15944862	SegC2-ARG521-Side	SegC2-UNK900-Main	73.5%
T1_6	Primary	Hit	3185712	SegC2-ARG538-Main	SegC2-UNK900-Main	50.9%
T1_1	Primary	Hit	15944862	SegC2-LEU536-Main	SegC2-UNK900-Main	50.3%
T1_5	Primary	Hit	5826369	SegC2-LEU536-Main	SegC2-UNK900-Main	48.5%
T1_5	Primary	Hit	5826369	SegC2-UNK900-Main	SegC2-LYS467-Main	42.0%
T1_7	Primary	Hit	1432744	SegC2-UNK900-Main	SegC2-HIS468-Main	32.1%
T1_3	Primary	Hit	5973599	SegC2-GLY472-Main	SegC2-UNK900-Main	31.6%
T1_7	Primary	Hit	1432744	SegC2-ARG521-Side	SegC2-UNK900-Main	30.7%
T1_8	Primary	Hit	1919699	SegC2-LEU536-Main	SegC2-UNK900-Main	29.8%
T1_3	Primary	Hit	5973599	SegC2-GLY470-Main	SegC2-UNK900-Main	29.5%
T1_7	Primary	Hit	1432744	SegC2-TYR518-Side	SegC2-UNK900-Main	27.1%
T1_1	Primary	Hit	15944862	SegC2-TYR518-Side	SegC2-UNK900-Main	24.1%
T1_6	Primary	Hit	3185712	SegC2-UNK900-Main	SegC2-GLU556-Side	21.7%
T1_3	Primary	Hit	5973599	SegC2-GLN471-Main	SegC2-UNK900-Main	20.8%
T1_5	Primary	Hit	5826369	SegC2-PHE465-Main	SegC2-UNK900-Main	20.2%
T1_5	Primary	Hit	5826369	SegC2-ARG521-Side	SegC2-UNK900-Main	19.4%
T1_1	Primary	Hit	15944862	SegC2-UNK900-Main	SegC2-HIS468-Main	18.8%
T1_4	Primary	Hit	3186499	SegC2-UNK900-Main	SegC2-LYS467-Main	17.3%
T1_3	Primary	Hit	5973599	SegC2-UNK900-Main	SegC2-HIS468-Main	16.4%
T1_9	Primary	Hit	7256141	SegC2-GLY470-Main	SegC2-UNK900-Main	15.8%
T1_10	Primary	Hit	3185717	SegC2-UNK900-Main	SegC2-GLN471-Main	14.9%
T1_3	Primary	Hit	5973599	SegC2-ARG522-Side	SegC2-UNK900-Main	13.4%
T1_3	Primary	Hit	5973599	SegC2-LYS467-Side	SegC2-UNK900-Main	13.1%
T1_6	Primary	Hit	3185712	SegC2-LEU536-Main	SegC2-UNK900-Main	13.1%
T1_11	Primary	Hit	1452563	SegC2-UNK900-Main	SegC2-PHE465-Main	13.1%
T1_9	Primary	Hit	7256141	SegC2-UNK900-Main	SegC2-LYS467-Main	12.5%
T1_6	Primary	Hit	3185712	SegC2-UNK900-Main	SegC2-LEU536-Main	11.6%
T1_9	Primary	Hit	7256141	SegC2-UNK900-Main	SegC2-ARG522-Side	11.6%
T1_12	Primary	Hit	1107365	SegC2-LEU536-Main	SegC2-UNK900-Side	10.1%
T1_3	Primary	Hit	5973599	SegC2-UNK900-Main	SegC2-GLY472-Main	9.8%
T1_7	Primary	Hit	1432744	SegC2-GLY470-Main	SegC2-UNK900-Main	9.8%
T1_12	Primary	Hit	1107365	SegC2-ARG521-Side	SegC2-UNK900-Main	9.5%
T1_11	Primary	Hit	1452563	SegC2-UNK900-Main	SegC2-ARG469-Main	8.0%
T1_3	Primary	Hit	5973599	SegC2-UNK900-Main	SegC2-UNK900-Main	7.7%
T1_1	Primary	Hit	15944862	SegC2-UNK900-Main	SegC2-ARG469-Side	7.4%
T1_4	Primary	Hit	3186499	SegC2-ARG522-Side	SegC2-UNK900-Main	7.1%
T1_4	Primary	Hit	3186499	SegC2-TYR518-Side	SegC2-UNK900-Main	6.9%
T1_2	Primary	Hit	3167530	SegC2-TYR518-Side	SegC2-UNK900-Main	6.6%
T1_3	Primary	Hit	5973599	SegC2-UNK900-Main	SegC2-ARG469-Side	6.6%
T1_10	Primary	Hit	3185717	SegC2-LEU536-Main	SegC2-UNK900-Main	6.6%
T1_12	Primary	Hit	1107365	SegC2-UNK900-Main	SegC2-LEU536-Main	6.6%
T1_12	Primary	Hit	1107365	SegC2-UNK900-Main	SegC2-TRP464-Side	6.0%
T1_5	Primary	Hit	5826369	SegC2-UNK900-Main	SegC2-HIS468-Main	5.7%
T1_2	Primary	Hit	3167530	SegC2-ARG521-Side	SegC2-UNK900-Main	5.4%

Positio	Site	Compound Info	CMPD-ID	donor	acceptor	occupancy
T1_8	Primary	Hit	1919699	SegC2-ARG521-Side	SegC2-UNK900-Main	5.4%
T1_9	Primary	Hit	7256141	SegC2-TYR518-Side	SegC2-UNK900-Main	5.4%
T1_10	Primary	Hit	3185717	SegC2-UNK900-Main	SegC2-UNK900-Main	5.4%
T1_2	Primary	Hit	3167530	SegC2-LEU536-Main	SegC2-UNK900-Main	4.8%
T1_2	Primary	Hit	3167530	SegC2-UNK900-Main	SegC2-ARG469-Side	4.2%
T1_3	Primary	Hit	5973599	SegC2-ARG521-Side	SegC2-UNK900-Main	4.2%
T1_5	Primary	Hit	5826369	SegC2-LYS467-Main	SegC2-UNK900-Main	4.2%
T1_6	Primary	Hit	3185712	SegC2-UNK900-Main	SegC2-PRO535-Side	4.2%
T1_8	Primary	Hit	1919699	SegC2-UNK900-Main	SegC2-ARG469-Side	4.2%
T1_10	Primary	Hit	3185717	SegC2-UNK900-Main	SegC2-LEU536-Main	4.2%
T1_1	Primary	Hit	15944862	SegC2-UNK900-Main	SegC2-GLU556-Side	3.9%
T1_12	Primary	Hit	1107365	SegC2-PHE465-Main	SegC2-UNK900-Main	3.9%
T1_5	Primary	Hit	5826369	SegC2-LYS514-Side	SegC2-UNK900-Main	3.6%
T1_7	Primary	Hit	1432744	SegC2-UNK900-Main	SegC2-ARG469-Side	3.6%
T1_8	Primary	Hit	1919699	SegC2-LEU536-Side	SegC2-UNK900-Main	3.6%
T1_5	Primary	Hit	5826369	SegC2-TYR518-Side	SegC2-UNK900-Main	3.3%
T1_10	Primary	Hit	3185717	SegC2-UNK900-Main	SegC2-ARG538-Side	3.3%
T1_11	Primary	Hit	1452563	SegC2-UNK900-Main	SegC2-GLN471-Main	3.3%
T1_12	Primary	Hit	1107365	SegC2-LEU536-Main	SegC2-UNK900-Main	3.3%
T1_1	Primary	Hit	15944862	SegC2-LEU536-Side	SegC2-UNK900-Main	3.0%
T1_5	Primary	Hit	5826369	SegC2-UNK900-Main	SegC2-GLN471-Main	3.0%
T1_9	Primary	Hit	7256141	SegC2-UNK900-Main	SegC2-PHE465-Side	3.0%
T1_11	Primary	Hit	1452563	SegC2-UNK900-Main	SegC2-HIS468-Main	3.0%
T1_11	Primary	Hit	1452563	SegC2-LYS467-Side	SegC2-UNK900-Main	3.0%
T1_11	Primary	Hit	1452563	SegC2-LYS461-Main	SegC2-UNK900-Main	3.0%
T1_12	Primary	Hit	1107365	SegC2-TYR518-Side	SegC2-UNK900-Main	3.0%
T1_1	Primary	Hit	15944862	SegC2-GLY470-Main	SegC2-UNK900-Main	2.7%
T1_1	Primary	Hit	15944862	SegC2-LYS514-Side	SegC2-UNK900-Main	2.7%
T1_3	Primary	Hit	5973599	SegC2-GLY473-Main	SegC2-UNK900-Main	2.7%
T1_5	Primary	Hit	5826369	SegC2-PHE465-Side	SegC2-UNK900-Main	2.7%
T1_5	Primary	Hit	5826369	SegC2-LEU536-Side	SegC2-UNK900-Main	2.7%
T1_6	Primary	Hit	3185712	SegC2-UNK900-Main	SegC2-ARG469-Side	2.7%
T1_11	Primary	Hit	1452563	SegC2-GLY462-Main	SegC2-UNK900-Main	2.7%
T1_1	Primary	Hit	15944862	SegC2-UNK900-Main	SegC2-LYS467-Main	2.4%
T1_1	Primary	Hit	15944862	SegC2-ARG469-Side	SegC2-UNK900-Main	2.4%
T1_6	Primary	Hit	3185712	SegC2-UNK900-Main	SegC2-SER537-Side	2.4%
T1_9	Primary	Hit	7256141	SegC2-UNK900-Main	SegC2-HIS468-Main	2.4%
T1_11	Primary	Hit	1452563	SegC2-UNK900-Main	SegC2-UNK900-Main	2.4%
T1_2	Primary	Hit	3167530	SegC2-LEU536-Side	SegC2-UNK900-Main	2.1%
T1_2	Primary	Hit	3167530	SegC2-LYS514-Side	SegC2-UNK900-Main	2.1%
T1_4	Primary	Hit	3186499	SegC2-UNK900-Main	SegC2-ARG469-Side	2.1%
T1_5	Primary	Hit	5826369	SegC2-UNK900-Main	SegC2-TRP464-Side	2.1%
T1_5	Primary	Hit	5826369	SegC2-TRP464-Main	SegC2-UNK900-Main	2.1%
T1_6	Primary	Hit	3185712	SegC2-UNK900-Main	SegC2-LYS514-Main	2.1%
T1_9	Primary	Hit	7256141	SegC2-UNK900-Main	SegC2-GLY463-Main	2.1%
T1_10	Primary	Hit	3185717	SegC2-ARG538-Side	SegC2-UNK900-Main	2.1%

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T1_1	Primary	Hit	15944862	SegC2-UNK900-Main	SegC2-ARG521-Side	1.8%
T1_2	Primary	Hit	3167530	SegC2-UNK900-Main	SegC2-UNK900-Main	1.8%
T1_3	Primary	Hit	5973599	SegC2-TYR518-Side	SegC2-UNK900-Main	1.8%
T1_5	Primary	Hit	5826369	SegC2-UNK900-Main	SegC2-LEU536-Main	1.8%
T1_6	Primary	Hit	3185712	SegC2-LEU536-Side	SegC2-UNK900-Main	1.8%
T1_6	Primary	Hit	3185712	SegC2-PRO535-Side	SegC2-UNK900-Main	1.8%
T1_7	Primary	Hit	1432744	SegC2-GLN471-Main	SegC2-UNK900-Main	1.8%
T1_8	Primary	Hit	1919699	SegC2-UNK900-Main	SegC2-GLN471-Main	1.8%
T1_9	Primary	Hit	7256141	SegC2-UNK900-Main	SegC2-GLN471-Main	1.8%
T1_9	Primary	Hit	7256141	SegC2-ARG522-Side	SegC2-UNK900-Main	1.8%
T1_10	Primary	Hit	3185717	SegC2-UNK900-Main	SegC2-ILE558-Main	1.8%
T1_11	Primary	Hit	1452563	SegC2-LYS467-Main	SegC2-UNK900-Main	1.8%
T1_2	Primary	Hit	3167530	SegC2-UNK900-Main	SegC2-LEU536-Side	1.5%
T1_4	Primary	Hit	3186499	SegC2-GLY470-Main	SegC2-UNK900-Main	1.5%
T1_4	Primary	Hit	3186499	SegC2-UNK900-Main	SegC2-GLU556-Side	1.5%
T1_7	Primary	Hit	1432744	SegC2-ARG469-Side	SegC2-UNK900-Main	1.5%
T1_7	Primary	Hit	1432744	SegC2-ARG538-Side	SegC2-UNK900-Main	1.5%
T1_11	Primary	Hit	1452563	SegC2-ARG522-Side	SegC2-UNK900-Main	1.5%
T1_1	Primary	Hit	15944862	SegC2-ARG522-Side	SegC2-UNK900-Main	1.2%
T1_1	Primary	Hit	15944862	SegC2-UNK900-Main	SegC2-ARG522-Side	1.2%
T1_2	Primary	Hit	3167530	SegC2-UNK900-Main	SegC2-TYR518-Side	1.2%
T1_3	Primary	Hit	5973599	SegC2-UNK900-Main	SegC2-GLY463-Main	1.2%
T1_4	Primary	Hit	3186499	SegC2-UNK900-Main	SegC2-GLN471-Main	1.2%
T1_4	Primary	Hit	3186499	SegC2-UNK900-Main	SegC2-GLY463-Main	1.2%
T1_6	Primary	Hit	3185712	SegC2-ARG538-Side	SegC2-UNK900-Main	1.2%
T1_7	Primary	Hit	1432744	SegC2-UNK900-Main	SegC2-TYR518-Side	1.2%
T1_7	Primary	Hit	1432744	SegC2-UNK900-Main	SegC2-GLY470-Main	1.2%
T1_8	Primary	Hit	1919699	SegC2-TYR518-Side	SegC2-UNK900-Main	1.2%
T1_8	Primary	Hit	1919699	SegC2-UNK900-Main	SegC2-ARG469-Main	1.2%
T1_8	Primary	Hit	1919699	SegC2-UNK900-Main	SegC2-ARG538-Side	1.2%
T1_10	Primary	Hit	3185717	SegC2-GLY470-Main	SegC2-UNK900-Main	1.2%
T1_10	Primary	Hit	3185717	SegC2-UNK900-Main	SegC2-LYS514-Main	1.2%
T1_11	Primary	Hit	1452563	SegC2-TYR518-Side	SegC2-UNK900-Main	1.2%
T1_11	Primary	Hit	1452563	SegC2-UNK900-Main	SegC2-LYS467-Main	1.2%
T1_11	Primary	Hit	1452563	SegC2-ARG469-Side	SegC2-UNK900-Main	1.2%
T1_11	Primary	Hit	1452563	SegC2-HIS468-Side	SegC2-UNK900-Main	1.2%
T1_12	Primary	Hit	1107365	SegC2-UNK900-Main	SegC2-GLN471-Main	1.2%