Application of the Goldilocks Effect to the Design of Potent and Selective Inhibitors of Phenylethanolamine *N*-Methyltransferase: Balancing pK_a and Steric Effects in the Optimization of 3-Methyl-1,2,3,4-tetrahydroisoquinoline Inhibitors by β-Fluorination.

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Content:

Compound	Formula	Calculated			Found		
		C	H	N	C	H	N
11b·HCl	$C_{10}H_{10}BrF_2N$·HCl	40.23	3.71	4.69	40.07	3.58	4.62
12b·HCl	$C_{11}H_{10}F_5NO_2$·HCl	45.93	3.85	4.87	45.67	3.60	4.72
13b·HCl	$C_{10}H_{10}F_2IN$·HCl	34.76	3.21	4.05	34.76	2.97	3.96
14b·HCl	$C_{12}H_{13}F_5N_2O_2S$·HCl	37.85	3.71	7.36	37.69	3.58	7.15
15b·HCl	$C_{10}H_{10}F_2N_2O_2$·HCl	45.38	4.19	10.58	45.38	4.04	10.54
16b·HCl	$C_{10}H_{12}F_2N_2O_2S$·HCl	40.20	4.39	9.38	40.40	4.23	9.24
17b·HCl	$C_{16}H_{15}ClF_2N_2O_2S$·HCl·¼H_2O	46.44	4.02	6.77	46.30	3.83	6.65
18b·HCl	$C_{11}H_{10}F_2N_2$·HBr	45.70	3.83	9.69	45.65	3.75	9.55
19b·HCl	$C_{10}H_{11}F_2N$·HBr	45.48	4.58	5.30	45.64	4.57	5.22
20b·HCl	$C_{11}H_{13}F_2NO_2S$·HCl	44.37	4.74	4.70	44.46	4.67	4.58
21b·HCl	$C_{12}H_{16}F_2N_2O_2S$·HCl	44.10	5.24	8.57	44.11	5.03	8.38
22b·HCl	$C_{13}H_{18}F_2N_2O_2S$·HCl	45.81	5.62	8.22	45.86	5.47	8.04
23b·HCl	$C_{14}H_{21}F_2N_2O_3S$·HCl	45.34	5.71	7.55	45.34	5.68	7.48
24b·HCl	$C_{14}H_{20}F_2N_2O_2S$·HCl	47.39	5.97	7.89	47.42	5.77	7.79
25b·HCl	$C_{16}H_{15}F_2N_3O_4S$·HCl·¼H_2O	45.29	3.92	9.90	45.35	3.79	9.78
14c·HCl	$C_{12}H_{12}F_6N_2O_2S$·HCl	36.14	3.29	7.03	36.30	3.17	6.91
17c·HCl	$C_{16}H_{14}ClF_3N_2O_2S$·HCl	44.98	3.54	6.56	45.07	3.47	6.46
23c·HCl	$C_{14}H_{20}F_3N_2O_3S$·HCl	47.72	5.43	7.95	47.76	5.14	7.85
25c·HCl	$C_{16}H_{14}F_3N_3O_4S$·HCl	44.68	4.37	8.68	44.44	4.32	8.48