

# SUPPORTING INFORMATION

## Screening of Big Pharma's library against various *in-house* biological targets

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**Table S1.** *In vitro* inhibitory potencies of Merck's Mini Library against MurA, MurC, DdlB, mAChE, hBChE, hMAO-A/B.

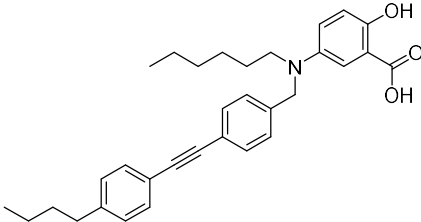
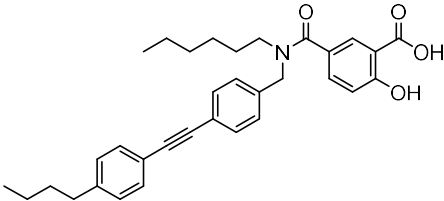
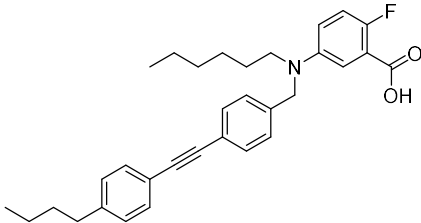
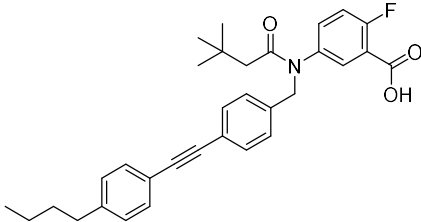
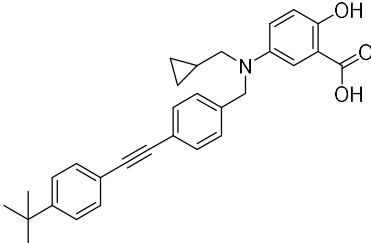
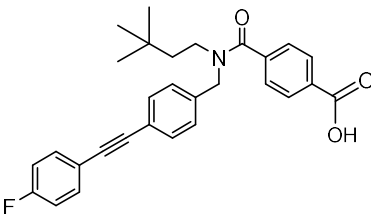
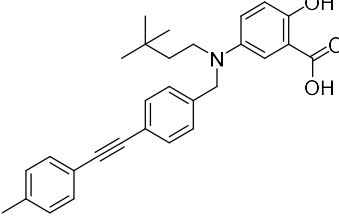
Compound	hBChE (RA [%] <sup>3</sup> /IC <sub>50</sub> )	mAChE (RA [%] <sup>3</sup> /IC <sub>50</sub> )	hMAO-A (RA <sup>a</sup> [%])	hMAO-B (RA <sup>a</sup> [%])	MurC (RA <sup>b</sup> [%])	MurA (RA <sup>b</sup> [%])	DdlB (RA <sup>b</sup> [%])
MS-ML10	35.6 ± 0.3 nM	64	75	82	74	110	96
MS-ML11	78.8 ± 10.3 nM	82	31	45	89	100	95
MS-ML12	4654 ± 712 nM	108	75	81	88	100	96
MS-ML13	100	114	79	82	100	96	96
MS-ML14	93	110	84	87	105	100	97
MS-ML60	92	114	85	89	92	100	96
MS-ML61	81	109	96	96	101	105	105
MS-ML62	99	99	99	94	105	111	107
MS-ML35	105	102	92	89	104	101	103
MS-ML36	98	97	89	88	103	121	101
MS-ML38	96	88	84	89	102	100	101
MS-ML37	104	102	82	87	108	100	102
MS-ML39	101	93	84	88	101	100	103
MS-ML40	96	106	87	88	99	98	104
MS-ML63	92	99	86	92	86	100	105
MS-ML64	96	99	92	92	86	112	106
MS-ML46	104	99	100	93	102	104	103
MS-ML47	102	96	95	90	101	104	100
MS-ML48	103	98	87	89	102	66	104
MS-ML53	56	100	78	86	101	105	109
MS-ML50	92	98	61	87	104	79	104
MS-ML49	101	101	65	87	96	105	105
MS-ML51	1594 ± 99 nM	95	93	89	92	104	105
MS-ML52	90	94	100	87	93	99	112
MS-ML57	100	101	99	95	100	102	100
MS-ML58	101	88	96	89	98	98	98
MS-ML59	88	91	95	89	98	92	103

MS-ML54	103	111	86	90	99	102	99
MS-ML55	100	107	81	89	100	102	101
MS-ML56	97	106	42	85	99	85	100
MS-ML22	73	103	77	71	97	72	100
MS-ML23	73	99	90	90	103	103	113
MS-ML06	95	106	92	100	104	96	98
MS-ML07	91	98	91	95	99	96	100
MS-ML08	76	90	60	76	108	83	100
MS-ML09	92	88	86	92	89	94	91
MS-ML41	74	96	80	91	103	96	95
MS-ML42	102	105	85	92	100	100	96
MS-ML43	86	103	93	93	92	102	98
MS-ML44	101	97	94	98	95	109	110
MS-ML01	83	106	84	105	45	86	84
MS-ML05	91	96	79	93	55	90	91
MS-ML03	87	92	83	97	61	100	81
MS-ML02	103	110	73	94	74	106	90
MS-ML04	94	103	88	97	85	97	91
MS-ML66	101	102	67	100	72	79	81
MS-ML65	91	91	74	91	64	86	69
MS-ML67	103	98	77	94	76	98	106
MS-ML16	100	103	81	75	90	99	97
MS-ML17	99	112	72	85	100	94	103
MS-ML18	90	97	74	80	98	98	107
MS-ML19	97	107	49	72	100	98	102
MS-ML69	97	76	83	73	87	90	95
MS-ML68	28	66	96	86	94	85	90
MS-ML72	94	99	92	96	92	92	98
MS-ML71	102	99	74	89	92	92	102
MS-ML70	110	117	94	52	88	99	100

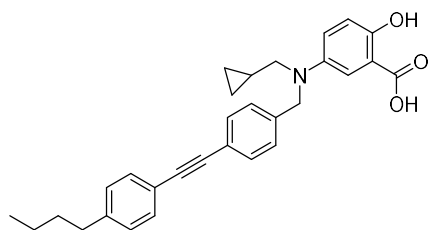
MS-ML20	100	117	94	91	92	99	101
MS-ML21	100	105	86	85	93	102	106
MS-ML24	60	<b>414 ± 40 nM</b>	57	64	83	<b>15</b>	116
MS-ML25	108	<b>369 ± 55 nM</b>	73	77	98	<b>0</b>	114
MS-ML26	68	<b>359 ± 39 nM</b>	60	92	73	<b>7</b>	114
MS-ML33	100	110	68	91	82	95	111
MS-ML34	106	102	78	79	96	130	99
MS-ML27	97	106	102	91	101	98	96
MS-ML28	102	103	99	89	92	89	100
MS-ML29	94	81	92	86	98	88	95
MS-ML30	85	104	79	80	90	89	94
MS-ML45	100	92	76	87	97	102	110
MS-ML31	84	89	78	<b>13</b>	94	94	98
MS-ML32	93	87	90	93	101	97	101
MS-ML15	103	108	94	96	89	110	97
MS-ML73	60	105	88	74	89	106	90
MS-ML74	84	103	86	83	103	101	93
MS-ML75	76	90	94	68	87	101	90
MS-ML76	61	107	78	81	86	105	98
MS-ML77	94	116	81	82	80	94	96
MS-ML78	97	104	82	81	98	98	99
MS-ML79	103	98	86	94	97	99	93
MS-ML80	73	95	82	<b>11</b>	96	93	94

<sup>a</sup> RA was determined at 10 μM; <sup>b</sup> RA was determined at 50 μM, the active compounds are bolded.

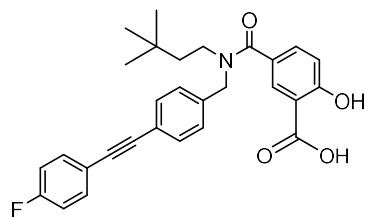
**Table S2.** Structures of salicylic acid analogues.

Compounds	Structure
MS-ML24	
MS-ML25	
MS-ML26	
1	
2	
3	
4	

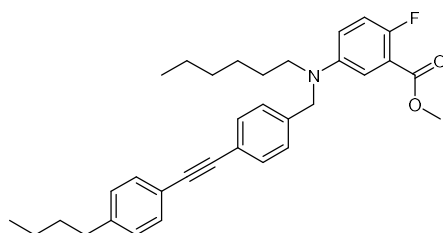
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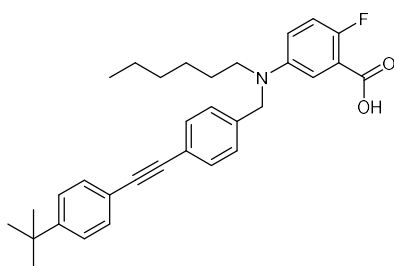
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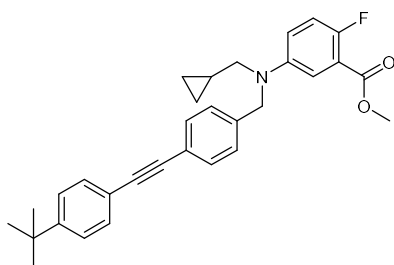
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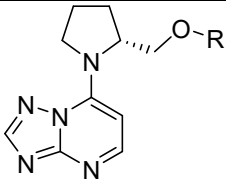
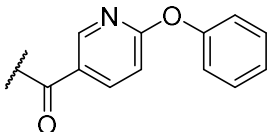
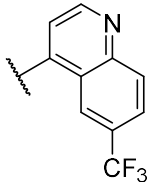
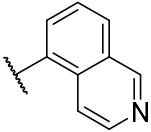
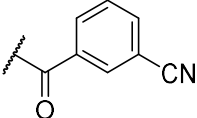
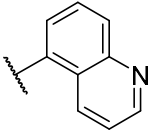
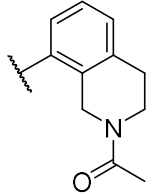
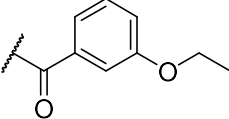
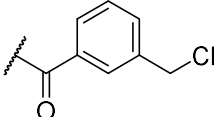
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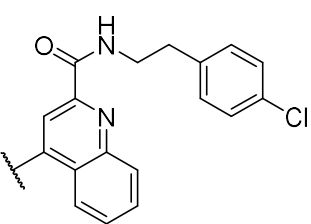
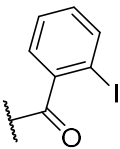
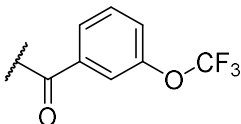


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**Table S3.** *In vitro* inhibitory potencies of triazaindolizines derivatives against hMAO-B and hMAO-A.

				
Compounds (Rack Barcode: DTBR00058180)	R	hMAO-B		hMAO-A
		RA <sup>a</sup> [%]	IC <sub>50</sub> [nM]	RA <sup>a</sup> [%]
MS-ML31		17	900 ± 100	98
S1		75	/	70
S2		88	/	87
S3		91	/	96
S4		99	/	80
S5		98	/	94
S6		88	/	96
S7		93	/	70

<b>S8</b>		104	/	86
<b>S9</b>		93	/	90
<b>S10</b>		81	/	92

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<sup>a</sup> RA was determined at 10  $\mu$ M.



