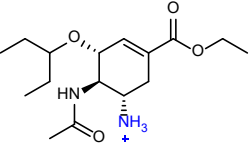
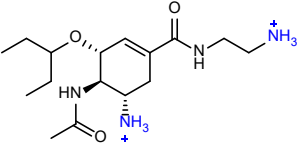
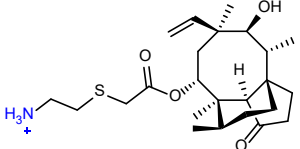
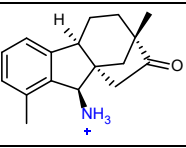
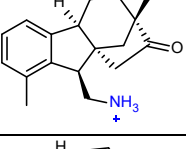
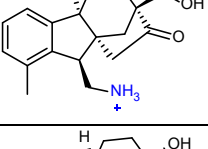
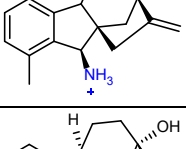
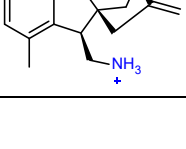
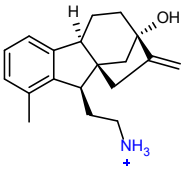
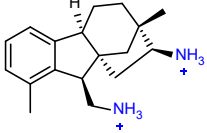
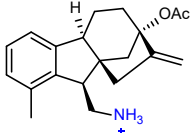
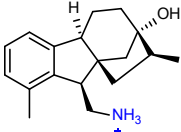
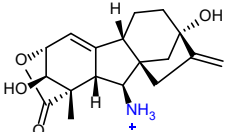
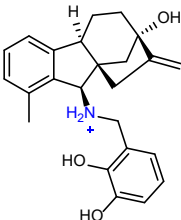
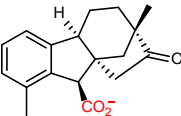
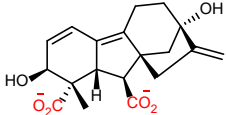
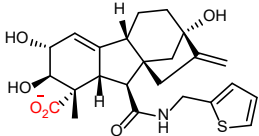
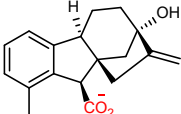
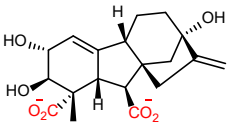
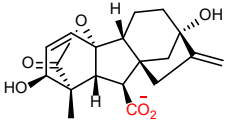
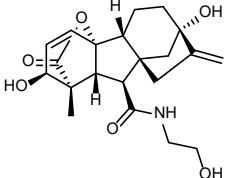
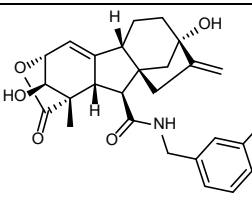
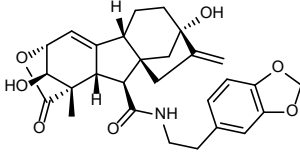
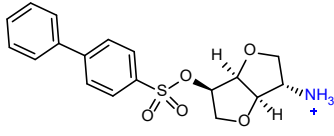
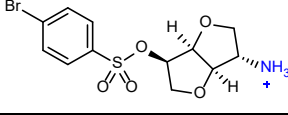
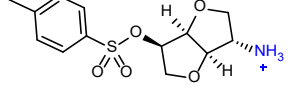
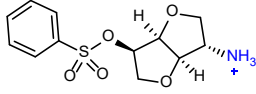
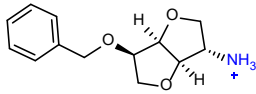
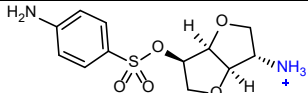
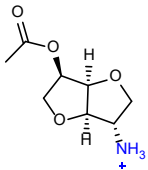
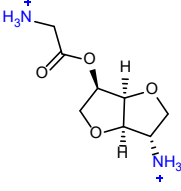
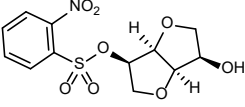
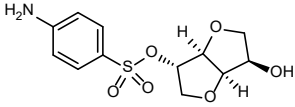
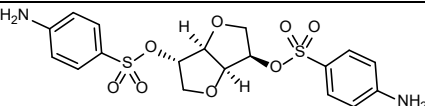
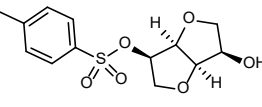
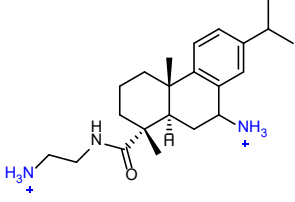
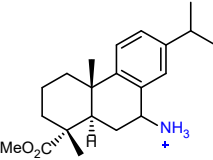
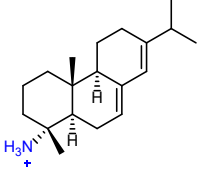
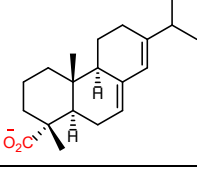


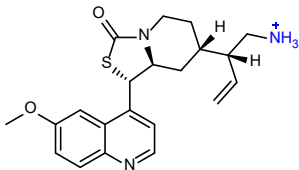
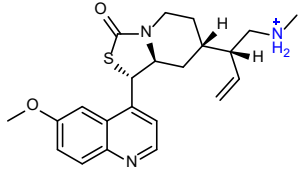
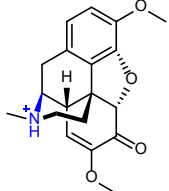
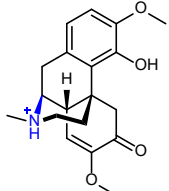
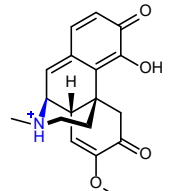
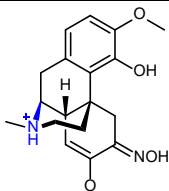
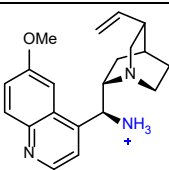
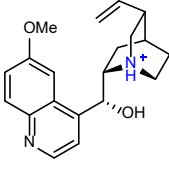
**Table S1.** Accumulation of 67 compounds used to develop the eNTRY rules in *E. coli*.<sup>5</sup> Names from the original publication are written in parenthesis, along with main text compound reference numbers. Accumulation measured in nmol/10<sup>12</sup> CFUs in *E. coli* MG1655 (*E. coli* data in this table is taken from Richter, et. al.<sup>5</sup>) and *P. aeruginosa* PAO1. All experiments were performed in biological triplicate. The s.e.m. is reported for accumulation values. Properties were calculated as described above. An asterisk (\*) is used to indicate compounds that accumulate to a statistically significant level.

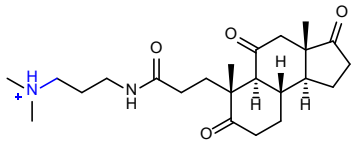
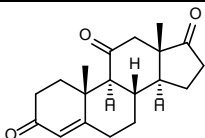
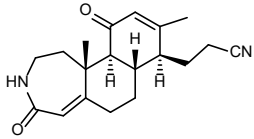
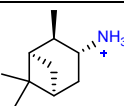
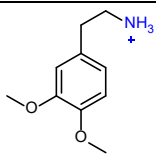
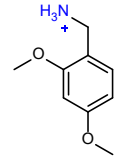
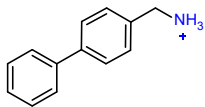
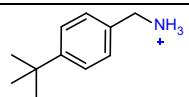
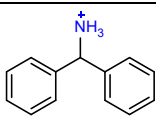
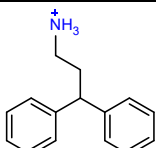
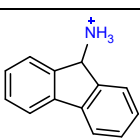
Structure	Cmpd	Functional Group	MW	ClogD <sub>7.4</sub>	# RB	Glob	PA Accum.	EC Accum.
	<b>1.1</b> (4-47, 67)	Primary amine	312	-0.72	8	0.17	218 ± 3	83 ± 11
	<b>1.2</b> (4-28-a, 68)	Primary amine (Diamine)	327	-3.91	8	0.15	505 ± 17*	895 ± 2*
	<b>1.3</b> (4-57)	Primary amine	438	0.74	7	0.36	88 ± 4	20 ± 5
	<b>1.4</b> (4-23)	Primary amine	255	1.44	0	0.19	61 ± 8	515 ± 50*
	<b>1.5</b> (4-3-a, 65)	Primary amine	270	0.95	1	0.20	629 ± 32*	1696 ± 203*
	<b>1.6</b> (4-6, 21)	Primary amine	285	-0.33	2	0.20	818 ± 51*	1487 ± 59*
	<b>1.7</b> (4-13, 6)	Primary amine	255	0.46	0	0.18	320 ± 37	756 ± 94*
	<b>1.8</b> (4-7, 58)	Primary amine	269	-0.09	1	0.19	943 ± 77*	1335 ± 8*

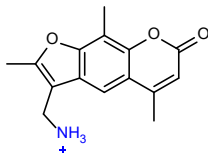
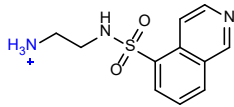
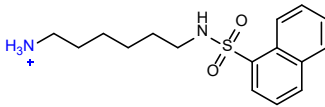
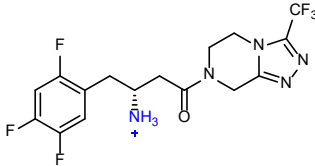
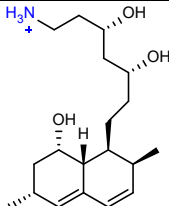
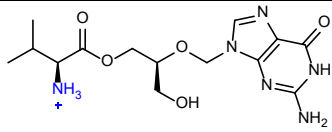
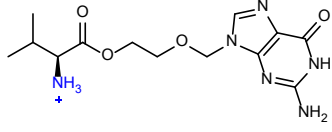
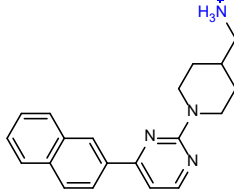
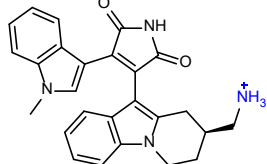
Structure	Cmpd	Functional Group	MW	ClogD <sub>7.4</sub>	# RB	Glob	PA Accum.	EC Accum.
	<b>1.9</b> <b>(4-3)</b>	Primary amine	283	0.09	2	0.20	780 ± 18*	1887 ± 179*
	<b>1.10</b> <b>(4-8, 66, 70)</b>	Primary amine (Diamine)	270	-2.49	1	0.21	2490 ± 62*	946 ± 138*
	<b>1.11</b> <b>(4-9, 57)</b>	Primary amine	311	0.36	2	0.14	317 ± 43	922 ± 46*
	<b>1.12</b> <b>(4-4)</b>	Primary amine	271	0	3	0.19	1157 ± 69*	1650 ± 69*
	<b>1.13</b> <b>(4-30)</b>	Primary amine	317	-2.32	0	0.19	242 ± 5	330 ± 78*
	<b>1.14</b> <b>(2-17)</b>	Secondary amine	377	1.93	3	0.18	192 ± 31	493 ± 161*
	<b>1.15</b> <b>(2-42)</b>	Carboxylic acid	284	0.57	1	0.20	66 ± 1	138 ± 7
	<b>1.16</b> <b>(2-43)</b>	Carboxylic acid	346	-5.79	2	0.21	51 ± 7	104 ± 20
	<b>1.17</b> <b>(2-51)</b>	Carboxylic acid	460	-2.09	4	0.17	22 ± 2	61 ± 13
	<b>1.18</b> <b>(2-52)</b>	Carboxylic acid	284	-0.23	1	0.18	58 ± 5	64 ± 5

Structure	Cmpd	Functional Group	MW	ClogD <sub>7.4</sub>	# RB	Glob	PA Accum.	EC Accum.
	<b>1.19</b> <b>(2-54)</b>	Carboxylic acid	364	-6.53	2	0.24	78 ± 5	59 ± 4
	<b>1.20</b> <b>(2-61)</b>	Carboxylic acid	346	-2.71	1	0.22	69 ± 25	15 ± 10
	<b>1.21</b> <b>(2-72)</b>	Neutral	389	-2.21	3	0.22	104 ± 3	80 ± 4
	<b>1.22</b> <b>(2-74)</b>	Neutral	470	1.98	3	0.18	37 ± 1	74 ± 6
	<b>1.23</b> <b>(2-79)</b>	Neutral	494	1.29	4	0.24	29 ± 1	56 ± 2
	<b>1.24</b> <b>(4-1, 48)</b>	Primary amine	361	0.6	4	0.06	282 ± 37	1965 ± 108*
	<b>1.25</b> <b>(4-5, 49)</b>	Primary amine	364	-0.28	3	0.11	217 ± 3	1647 ± 108*
	<b>1.26</b> <b>(4-10, 50)</b>	Primary amine	299	-0.53	3	0.10	163 ± 39	877 ± 29*
	<b>1.27</b> <b>(4-19)</b>	Primary amine	285	-1.05	3	0.13	278 ± 31	616 ± 30*
	<b>1.28</b> <b>(4-21, 24)</b>	Primary amine	235	-0.73	3	0.19	240 ± 18	552 ± 12*
	<b>1.29</b> <b>(4-34)</b>	Primary amine	300	-1.87	3	0.13	235 ± 17	331 ± 68*

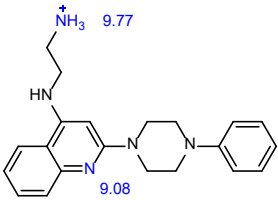
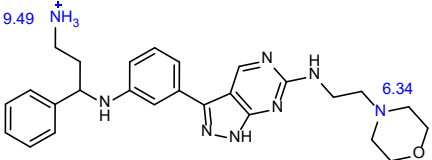
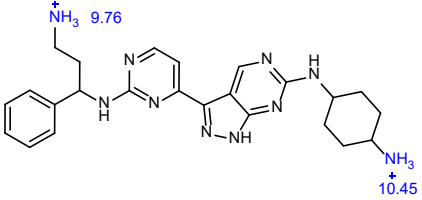
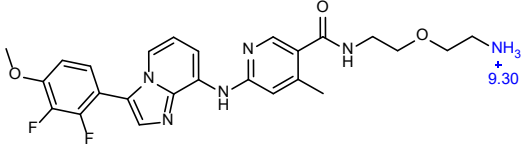
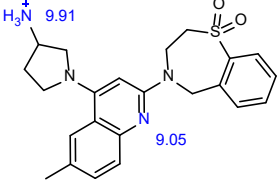
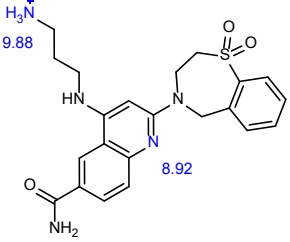
Structure	Cmpd	Functional Group	MW	ClogD <sub>7.4</sub>	# RB	Glob	PA Accum.	EC Accum.
	<b>1.30</b> <b>(4-37-a)</b>	Primary amine	188	-2.66	2	0.16	0 ± 0	372 ± 3*
	<b>1.31</b> <b>(4-55-a)</b>	Primary amine	270	-3.75	3	0.16	0 ± 0	23 ± 0
	<b>1.32</b> <b>(2-94)</b>	Neutral (Nitro)	331	0.58	4	0.15	6 ± 2	0 ± 0
	<b>1.33</b> <b>(2-95)</b>	Neutral (Aniline)	301	-0.18	3	0.12	52 ± 6	193 ± 15
	<b>1.34</b> <b>(2-97)</b>	Neutral (Aniline)	456	1.04	6	0.20	92 ± 3	113 ± 2
	<b>1.35</b> <b>(3-37)</b>	Neutral	300	1.16	3	0.11	39 ± 1	152 ± 29
	<b>1.36</b> <b>(4-6-a, 22, 71)</b>	Primary amine (Diamine)	360	-0.70	4	0.11	1380 ± 60*	1344 ± 43*
	<b>1.37</b> <b>(4-25, 8)</b>	Primary amine	329	2.31	3	0.17	596 ± 70*	477 ± 75*
	<b>1.38</b> <b>(4-55)</b>	Primary amine	273	1.19	1	0.12	569 ± 54*	28 ± 6
	<b>1.39</b> <b>(2-57)</b>	Carboxylic acid	302	2.22	2	0.12	211 ± 28	34 ± 5

Structure	Cmpd	Functional Group	MW	ClogD <sub>7.4</sub>	# RB	Glob	PA Accum.	EC Accum.
	<b>1.40</b> <b>(4-26, 62)</b>	Primary amine	384	0.14	5	0.33	399 ± 79*	458 ± 58*
	<b>1.41</b> <b>(2-18, 61)</b>	Secondary amine	398	0.24	6	0.35	128 ± 1	413 ± 8*
	<b>1.42</b> <b>(2-29)</b>	Tertiary amine	327	0.58	2	0.32	45 ± 5	407 ± 6*
	<b>1.43</b> <b>(2-32)</b>	Tertiary amine	329	0.65	2	0.34	99 ± 3	218 ± 10
	<b>1.44</b> <b>(2-33)</b>	Tertiary amine	313	0.84	1	0.44	90 ± 4	213 ± 48
	<b>1.45</b> <b>(2-35)</b>	Tertiary amine	344	-0.09	2	0.38	159 ± 23	204 ± 26
	<b>1.46</b> <b>(4-42)</b>	Primary amine	323	0.33	4	0.24	224 ± 11	167 ± 12
	<b>1.47</b> <b>(2-30)</b>	Tertiary amine	324	0.86	4	0.20	259 ± 15	261 ± 16

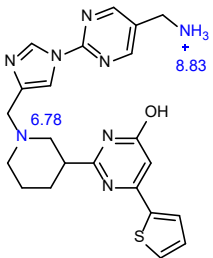
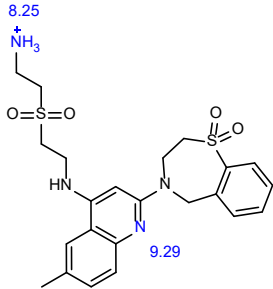
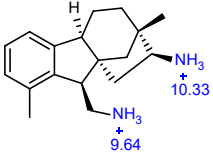
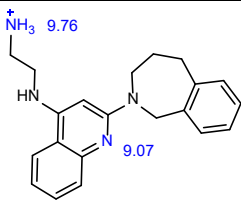
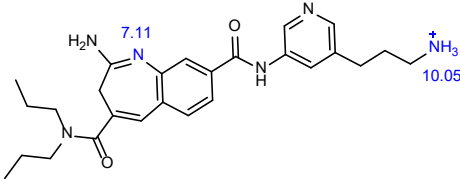
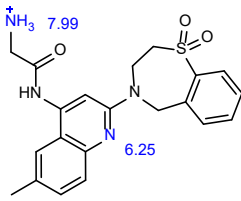
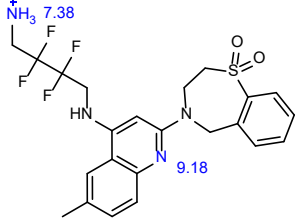
Structure	Cmpd	Functional Group	MW	ClogD <sub>7.4</sub>	# RB	Glob	PA Accum.	EC Accum.
	<b>1.48</b> <b>(2-39)</b>	Tertiary amine	405	0.69	7	0.14	0 ± 0	72 ± 5
	<b>1.49</b> <b>(2-67)</b>	Neutral	300	3.01	0	0.18	17 ± 2	91 ± 21
	<b>1.50</b> <b>(2-73)</b>	Neutral	312	1.79	3	0.16	63 ± 0	36 ± 1
	<b>1.51</b> <b>(4-12, 77A)</b>	Primary amine	153	-0.97	0	0.36	1050 ± 20*	761 ± 65*
	<b>1.52</b> <b>(4-37)</b>	Primary amine	181	-1.24	4	0.12	233 ± 17	255 ± 19
	<b>1.53</b> <b>(4-39)</b>	Primary amine	167	-0.77	3	0.07	279 ± 7	206 ± 22
	<b>1.54</b> <b>(4-18, 23)</b>	Primary amine	183	0.71	1	0.06	1817 ± 102*	617 ± 1*
	<b>1.55</b> <b>(4-15)</b>	Primary amine	163	0.56	2	0.12	498 ± 54*	726 ± 19*
	<b>1.56</b> <b>(4-27)</b>	Primary amine	183	1.24	2	0.17	346 ± 18*	415 ± 20*
	<b>1.57</b> <b>(4-49)</b>	Primary amine	211	0.77	4	0.20	364 ± 45*	61 ± 3
	<b>1.58</b> <b>(4-17)</b>	Primary amine	181	0.63	0	0.05	1327 ± 81*	617 ± 10*

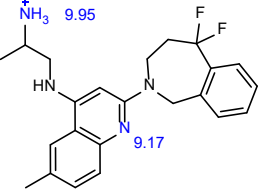
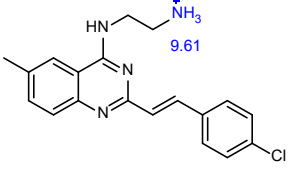
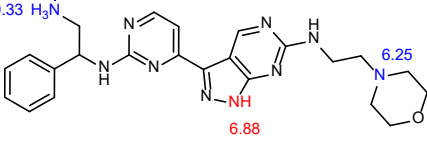
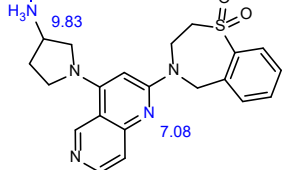
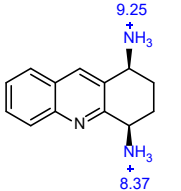
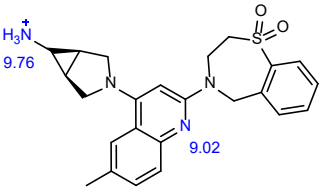
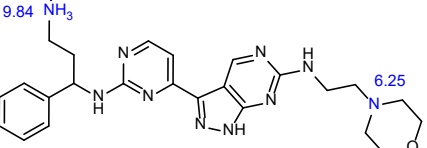
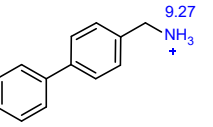
Structure	Cmpd	Functional Group	MW	ClogD <sub>7.4</sub>	# RB	Glob	PA Accum.	EC Accum.
	<b>1.59</b> <b>(4-11)</b>	Primary amine	257	0.24	1	0.05	476 ± 36*	817 ± 203*
	<b>1.60</b> <b>(4-31)</b>	Primary amine	251	-1.94	4	0.08	235 ± 38	316 ± 12*
	<b>1.61</b> <b>(4-46, 54)</b>	Primary amine	306	-0.13	8	0.15	399 ± 63*	108 ± 16
	<b>1.62</b> <b>(4-36, 25)</b>	Primary amine	407	-0.14	5	0.16	514 ± 28*	275 ± 9
	<b>1.63</b> <b>(4-35)</b>	Primary amine	323	-1.68	7	0.21	231 ± 13	323 ± 60
	<b>1.64</b> <b>(4-43)</b>	Primary amine	354	-1.55	9	0.21	70 ± 7	165 ± 9
	<b>1.65</b> <b>(4-45)</b>	Primary amine	324	-0.92	8	0.21	44 ± 5	141 ± 6
	<b>1.66</b> <b>(4-53)</b>	Primary amine	318	0.92	3	0.08	1303 ± 61*	40 ± 3
	<b>1.67</b> <b>(4-58, 26, 55)</b>	Primary amine	425	0.35	3	0.30	1193 ± 27*	17 ± 7

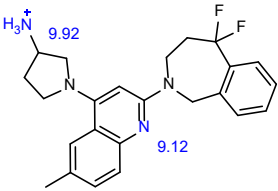
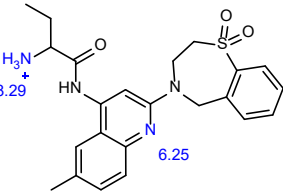
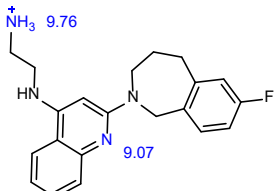
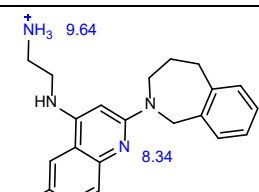
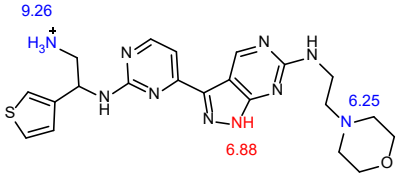
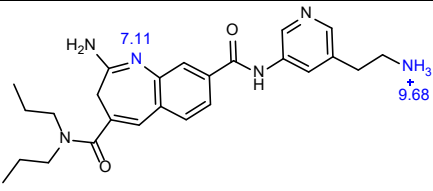
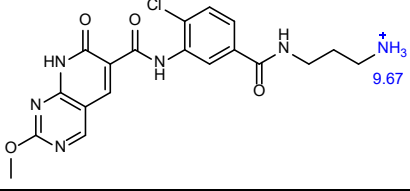
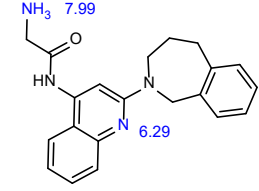
**Table S2.** Accumulation of all primary amines. Accumulation is measured in nmol/10<sup>12</sup> CFUs in *P. aeruginosa* PAO1 and *E. coli* MG1655. For compound source please refer to the **Compound Master Table**. Compound reference numbers for main text figures are listed in parenthesis. All experiments were performed in biological triplicate. The s.e.m. is reported for accumulation values. Acidic pK<sub>a</sub>s are in red and basic pK<sub>a</sub>s are in blue. Properties were calculated as described above. An asterisk (\*) is used to indicate compounds that accumulate to a statistically significant level. n.d. = not determined.

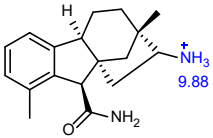
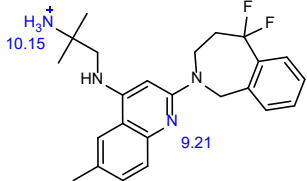
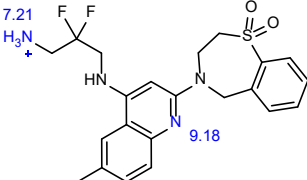
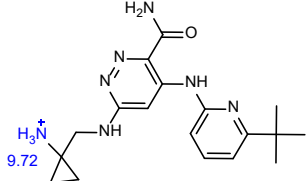
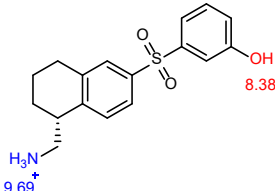
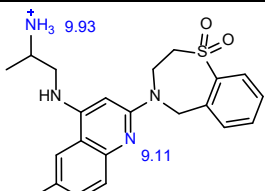
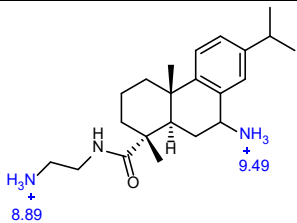
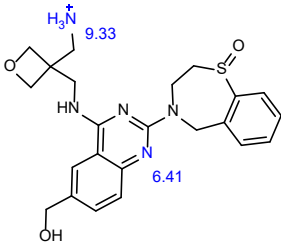
Structure	Cmpd	ClogD <sub>7.4</sub>	Formal charge	Q_vsa_Ppos	vsa_don	PA Accum.	EC Accum.
	<b>2.1 (60)</b>	-0.45	1.243	140	29.1	4540 ± 6*	6851 ± 73*
	<b>2.2</b>	-0.03	1.593	156	29.1	4367 ± 12*	7457 ± 348*
	<b>2.3 (72)</b>	-3.21	1.997	149	46.9	3433 ± 12*	5600 ± 134*
	<b>2.4 (39)</b>	-0.01	1.429	80	29.1	2757 ± 277*	6846 ± 157*
	<b>2.5 (41)</b>	-0.68	1.821	115	23.4	2667 ± 64*	3360 ± 17*
	<b>2.6</b>	-2.76	1.470	150	46.9	2650 ± 180*	5446 ± 50*

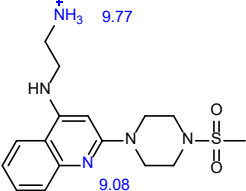
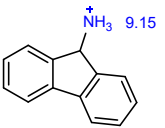
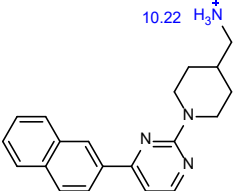
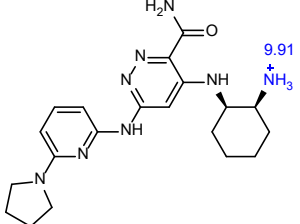
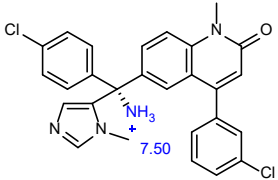
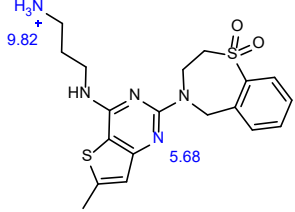
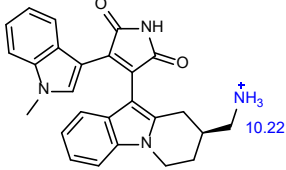
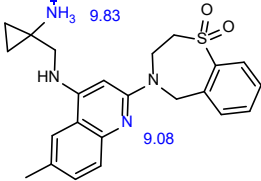


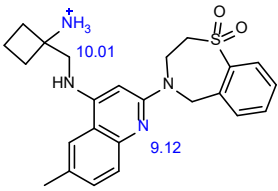
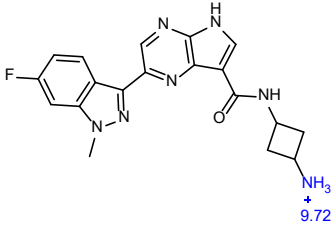
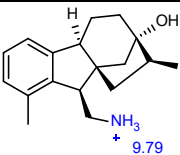
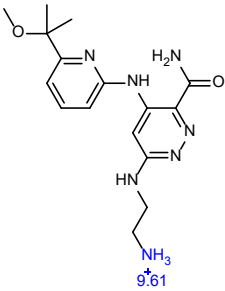
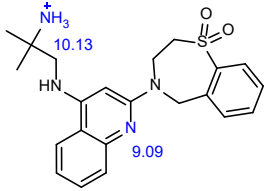
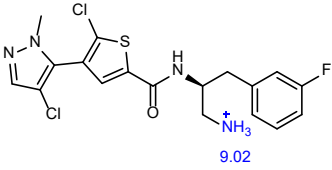
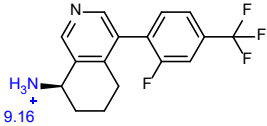
Structure	Cmpd	ClogD <sub>7.4</sub>	Formal charge	Q_vsa_Ppos	vsa_don	PA Accum.	EC Accum.
	<b>2.7</b>	0.03	1.810	142	23.4	2630 ± 370*	2109 ± 178*
	<b>2.8 (40)</b>	-1.09	0.610	127	29.1	2500 ± 32*	3215 ± 81*
	<b>2.9 (66, 70)</b>	-2.49	1.997	68	35.5	2490 ± 62*	946 ± 139*
	<b>2.10</b>	0.02	1.259	114	29.1	2487 ± 156*	3150 ± 21*
	<b>2.11</b>	-0.55	1.221	102	41.2	2333 ± 224*	6314 ± 516*
	<b>2.12</b>	1.50	1.100	111	23.4	2207 ± 223*	2310 ± 166*
	<b>2.13</b>	2.16	0.401	103	11.4	2113 ± 398*	1535 ± 61*

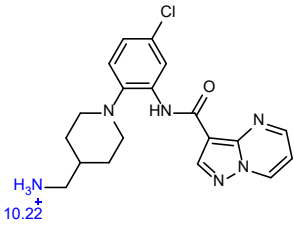
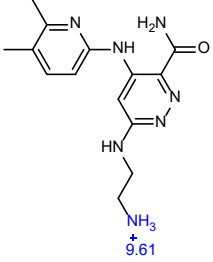
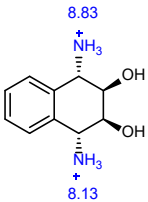
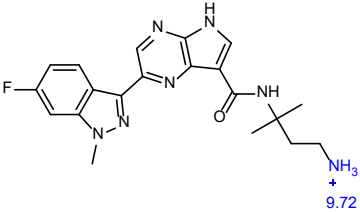
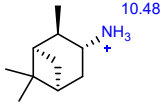
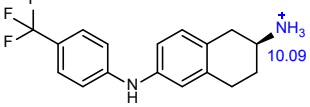
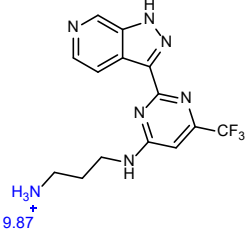
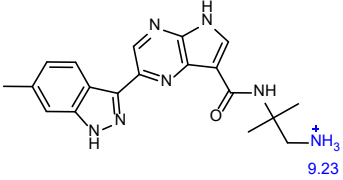
Structure	Cmpd	ClogD <sub>7.4</sub>	Formal charge	Q_vsa_Ppos	vsa_don	PA Accum.	EC Accum.
	<b>2.14</b>	0.97	1.245	106	29.1	2017 ± 33*	2898 ± 8*
	<b>2.15 (4)</b>	2.81	1.491	90	23.4	1943 ± 41*	2926 ± 184*
	<b>2.16</b>	-0.76	1.509	178	29.1	1923 ± 65*	9021 ± 17*
	<b>2.17</b>	-1.84	2.177	148	23.4	1880 ± 6*	5143 ± 47*
	<b>2.18 (69)</b>	-2.08	1.780	65	35.5	1860 ± 45*	2161 ± 66*
	<b>2.19</b>	-0.86	2.022	106	17.7	1853 ± 18*	4769 ± 9*
	<b>2.20 (76)</b>	-0.98	1.585	178	29.1	1823 ± 98*	6127 ± 151*
	<b>2.21 (23)</b>	0.71	0.996	39	17.7	1817 ± 102*	616 ± 10*

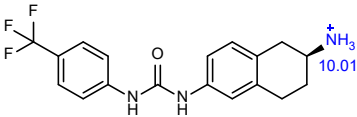
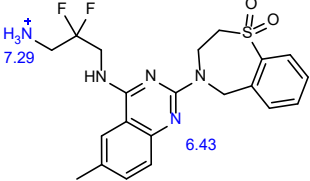
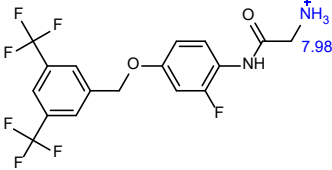
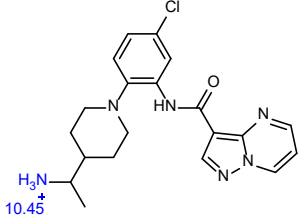
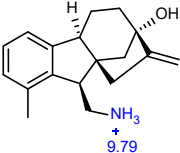
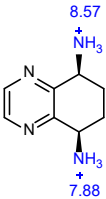
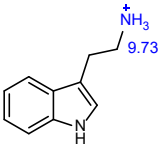
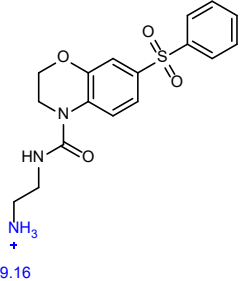
Structure	Cmpd	ClogD <sub>7.4</sub>	Formal charge	Q_vsa_Ppos	vsa_don	PA Accum.	EC Accum.
	<b>2.22</b>	1.18	1.813	111	23.4	1783 ± 89*	2674 ± 12*
	<b>2.23 (64)</b>	2.33	1.260	101	23.4	1757 ± 64*	909 ± 70*
	<b>2.24</b>	0.17	1.253	114	29.1	1757 ± 206*	3593 ± 45*
	<b>2.25</b>	0.74	1.202	114	29.1	1749 ± 396*	3757 ± 20*
	<b>2.26</b>	-0.91	1.538	178	29.1	1743 ± 7*	6389 ± 192*
	<b>2.27</b>	-0.71	1.214	102	41.2	1740 ± 65*	4004 ± 147*
	<b>2.28</b>	-2.18	0.753	132	34.8	1737 ± 63*	2366 ± 283*
	<b>2.29</b>	2.64	1.141	105	23.4	1727 ± 224*	2847 ± 5*

Structure	Cmpd	ClogD <sub>7.4</sub>	Formal charge	Q_vsa_Ppos	vsa_don	PA Accum.	EC Accum.
	<b>2.30 (12)</b>	-0.38	0.999	59	35.5	1623 ± 47*	851 ± 76*
	<b>2.31</b>	1.07	1.268	103	29.1	1587 ± 182*	2114 ± 33*
	<b>2.32</b>	1.54	0.641	123	29.1	1583 ± 42*	2492 ± 115*
	<b>2.33</b>	0.47	1.042	116	46.9	1577 ± 88*	1181 ± 73*
	<b>2.34 (20)</b>	0.96	0.981	56	17.7	1573 ± 41*	1254 ± 115*
	<b>2.35</b>	-0.89	1.228	110	29.1	1420 ± 35*	4186 ± 35*
	<b>2.36 (22, 71)</b>	-0.70	1.979	90	41.2	1380 ± 60*	1344 ± 25*
	<b>2.37</b>	-1.20	1.667	198	29.1	1370 ± 25*	3747 ± 383*

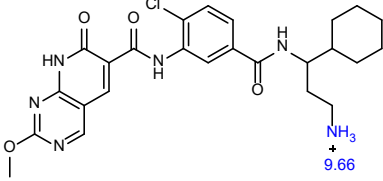
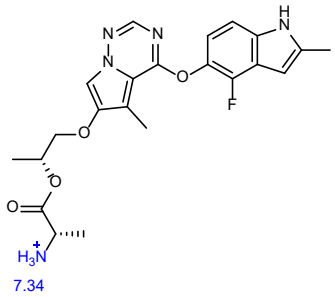
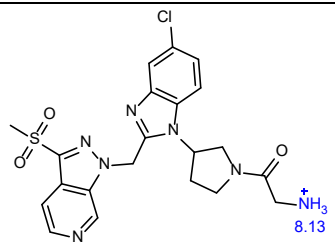
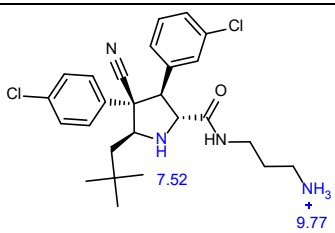
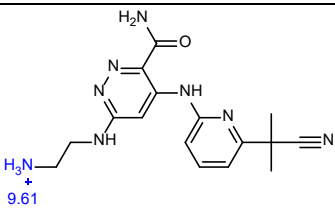
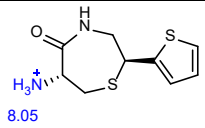
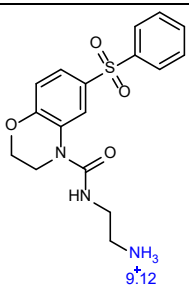
Structure	Cmpd	ClogD <sub>7.4</sub>	Formal charge	Q_vsa_Ppos	vsa_don	PA Accum.	EC Accum.
	<b>2.38 (59)</b>	-3.62	1.222	124	29.1	1360 ± 61*	1450 ± 37*
	<b>2.39</b>	0.63	0.973	29	17.7	1327 ± 81*	617 ± 1*
	<b>2.40</b>	0.92	1.002	88	17.7	1303 ± 61*	40 ± 3
	<b>2.41</b>	-0.18	1.063	146	46.9	1280 ± 32*	3887 ± 92*
	<b>2.42</b>	4.19	0.882	83	5.7	1253 ± 73*	629 ± 48*
	<b>2.43</b>	0.29	1.935	127	23.4	1213 ± 61*	3491 ± 81*
	<b>2.44 (26, 55)</b>	0.35	0.997	74	23.4	1193 ± 27*	17 ± 7
	<b>2.45 (43)</b>	-0.81	1.220	107	29.1	1183 ± 52*	1708 ± 37*

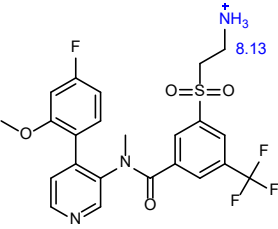
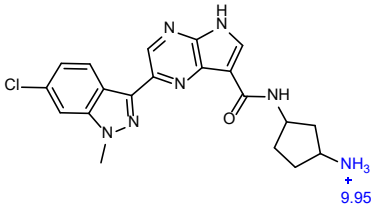
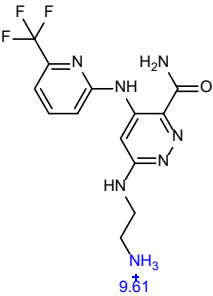
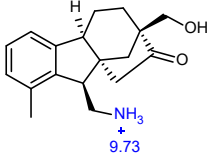
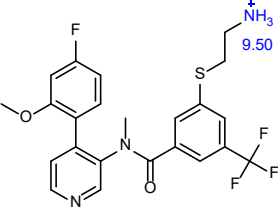
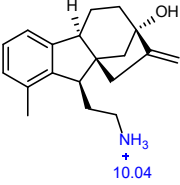
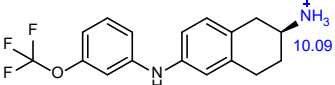
Structure	Cmpd	ClogD <sub>7.4</sub>	Formal charge	Q_vsa_Ppos	vsa_don	PA Accum.	EC Accum.
	2.46	-0.54	1.240	107	29.1	1173 ± 23*	2455 ± 95*
	2.47	-1.53	1.002	82	23.4	1157 ± 46*	2805 ± 38*
	2.48	0	0.998	49	17.7	1157 ± 69*	1650 ± 69*
	2.49	-0.80	0.996	129	46.9	1150 ± 12*	1155 ± 39*
	2.50	-1.27	1.248	107	29.1	1113 ± 18*	3794 ± 86*
	2.51	2.13	0.989	64	23.4	1113 ± 88*	393 ± 7*
	2.52	1.60	0.979	38	17.7	1111 ± 84*	1278 ± 39*

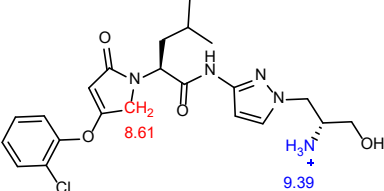
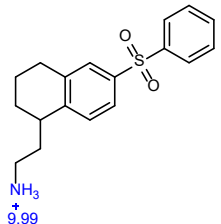
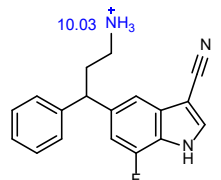
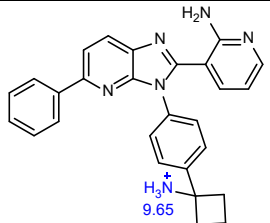
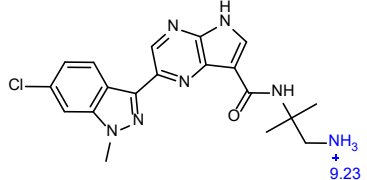
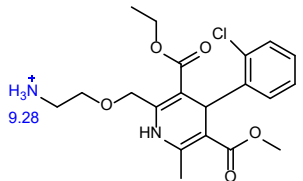
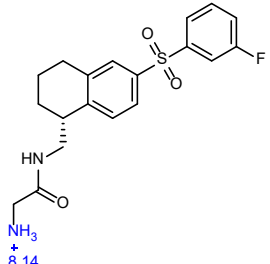
Structure	Cmpd	ClogD <sub>7.4</sub>	Formal charge	Q_vsa_Ppos	vsa_don	PA Accum.	EC Accum.
	<b>2.53</b>	-0.48	0.999	104	23.4	1110 ± 45*	926 ± 28*
	<b>2.54</b>	-1.15	1.057	129	46.9	1080 ± 35*	2287 ± 5*
	<b>2.55</b>	-3.70	1.759	70	17.7	1062 ± 53*	1181 ± 86*
	<b>2.56</b>	-0.84	1.005	89	23.4	1054 ± 36*	2315 ± 9*
	<b>2.57</b> <b>(77A)</b>	-0.97	0.999	29	17.7	1050 ± 20*	762 ± 65*
	<b>2.58</b>	1.72	0.998	47	23.4	1046 ± 154*	1290 ± 92*
	<b>2.59</b> <b>(78A)</b>	-0.69	1.029	111	23.4	1027 ± 49*	1731 ± 82*
	<b>2.60</b>	-0.20	1.000	102	23.4	1025 ± 68*	2557 ± 145*

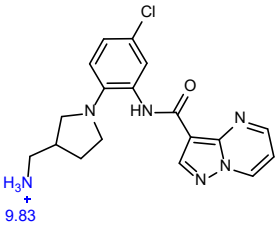
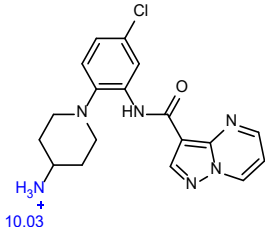
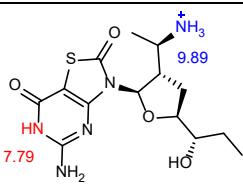
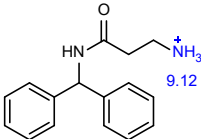
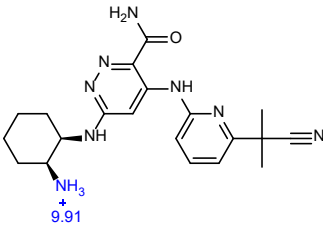
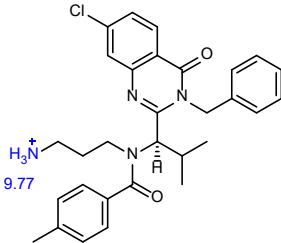
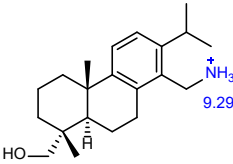
Structure	Cmpd	ClogD <sub>7.4</sub>	Formal charge	Q_vsa_Ppos	vsa_don	PA Accum.	EC Accum.
	<b>2.61</b>	1.47	0.998	73	29.1	986 ± 150*	1372 ± 182*
	<b>2.62</b>	2.97	0.769	138	29.1	985 ± 105*	1022 ± 129*
	<b>2.63 (46)</b>	2.42	0.415	94	23.4	970 ± 79*	1039 ± 26*
	<b>2.64</b>	-0.19	0.999	94	23.4	946 ± 67*	737 ± 41*
	<b>2.65 (58)</b>	-0.09	0.998	49	17.7	943 ± 77*	1335 ± 8*
	<b>2.66</b>	-3.36	1.699	49	17.7	921 ± 73*	1461 ± 25*
	<b>2.67</b>	-0.77	0.999	48	23.4	905 ± 18*	792 ± 14*
	<b>2.68</b>	-0.95	0.984	72	23.4	904 ± 67*	706 ± 52*

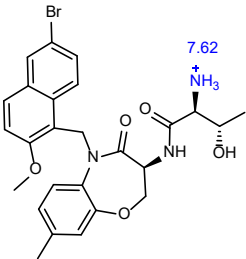
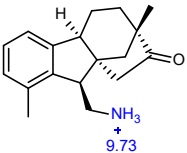
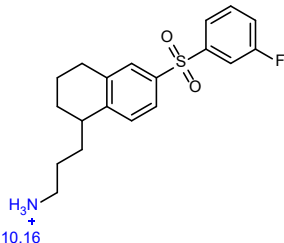
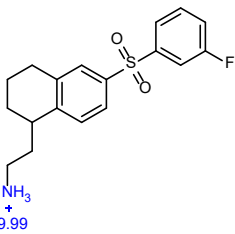
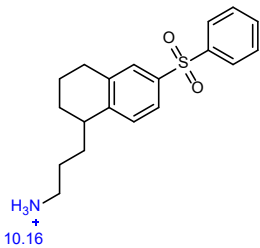
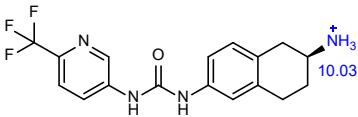
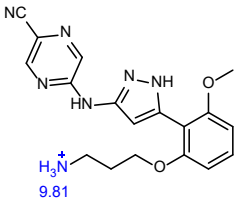


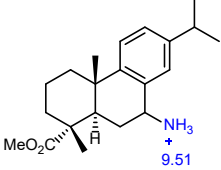
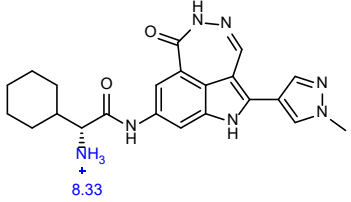
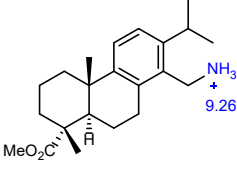
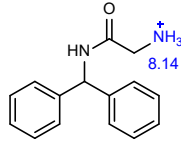
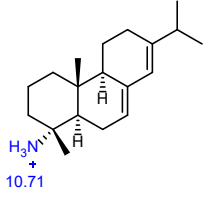
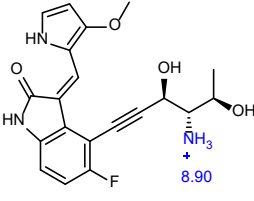
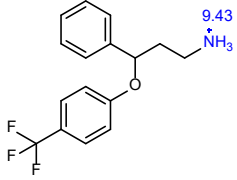
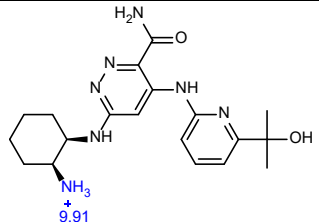
Structure	Cmpd	ClogD <sub>7.4</sub>	Formal charge	Q_vsa_Ppos	vsa_don	PA Accum.	EC Accum.
	2.69	0	0.752	136	34.8	861 ± 26*	668 ± 54*
	2.70	3.23	0.296	78	5.7	851 ± 67*	29 ± 5
	2.71 (47)	-0.99	0.863	87	17.7	850 ± 8*	690 ± 46*
	2.72	1.73	1.012	93	23.4	847 ± 30*	717 ± 23*
	2.73 (14)	-0.58	0.993	149	46.9	838 ± 47*	1745 ± 76*
	2.74 (38)	0.74	0.380	45	5.7	838 ± 50*	1295 ± 3*
	2.75	-0.58	0.984	72	23.4	828 ± 81*	762 ± 52*

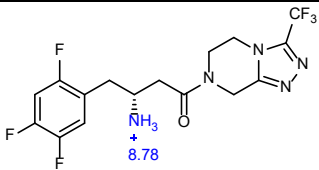
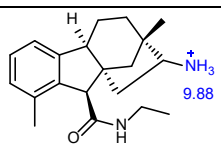
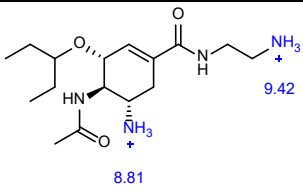
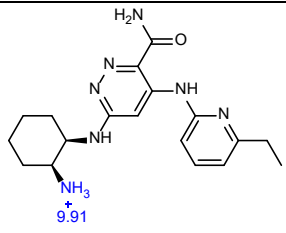
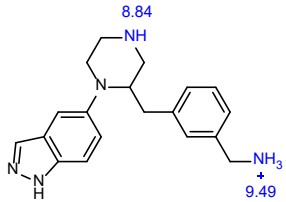
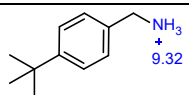
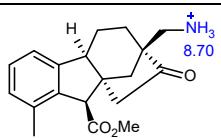
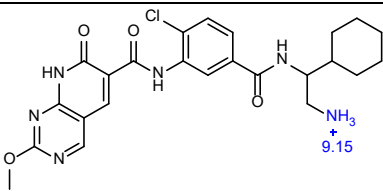
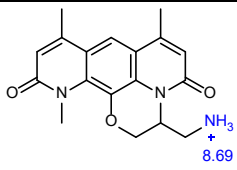
Structure	Cmpd	ClogD <sub>7.4</sub>	Formal charge	Q_vsa_Ppos	vsa_don	PA Accum.	EC Accum.
	<b>2.76</b>	1.61	0.093	68	17.7	824 ± 60*	213 ± 4
	<b>2.77</b>	-0.75	1.007	82	23.4	823 ± 7*	2455 ± 167*
	<b>2.78</b>	-0.49	0.990	138	46.9	821 ± 34*	2189 ± 73*
	<b>2.79 (21)</b>	-0.33	0.997	58	17.7	818 ± 51*	1487 ± 58*
	<b>2.80 (42)</b>	1.74	1.039	61	17.7	787 ± 29*	312 ± 31*
	<b>2.81</b>	0.09	0.999	49	17.7	780 ± 18*	1867 ± 179*
	<b>2.82 (16)</b>	2.28	0.998	53	23.4	766 ± 33*	1076 ± 37*

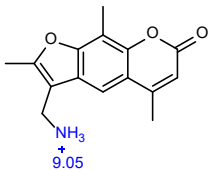
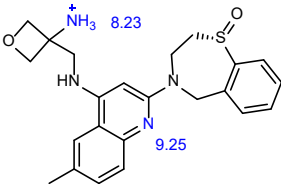
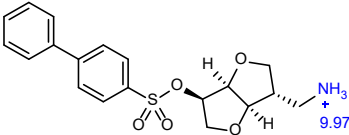
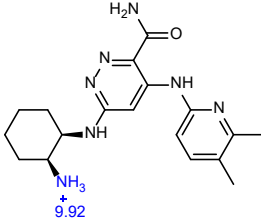
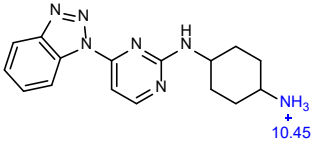
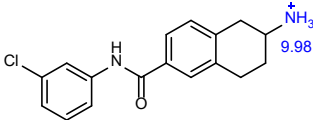
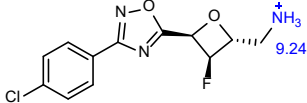
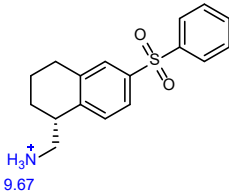
Structure	Cmpd	ClogD <sub>7.4</sub>	Formal charge	Q_vsa_Ppos	vsa_don	PA Accum.	EC Accum.
	<b>2.83 (44)</b>	-0.03	0.738	101	23.4	765 ± 104*	302 ± 25
	<b>2.84</b>	1.39	0.999	46	17.7	759 ± 25*	851 ± 68*
	<b>2.85 (10)</b>	0.87	0.999	68	23.4	757 ± 35*	1281 ± 74*
	<b>2.86</b>	1.95	1.026	68	35.5	757 ± 90*	330 ± 30*
	<b>2.87</b>	0.02	1.003	89	23.4	743 ± 106*	1568 ± 80*
	<b>2.88 (31)</b>	-0.37	0.993	92	23.4	741 ± 45*	426 ± 7*
	<b>2.89 (45)</b>	1.43	0.711	67	23.4	730 ± 47*	447 ± 44*

Structure	Cmpd	ClogD <sub>7.4</sub>	Formal charge	Q_vsa_Ppos	vsa_don	PA Accum.	EC Accum.
	<b>2.90</b>	-0.61	0.998	104	23.4	724 ± 41*	1013 ± 8*
	<b>2.91</b>	-0.81	0.997	94	23.4	700 ± 14*	836 ± 44*
	<b>2.92</b>	-2.48	0.987	129	41.2	690 ± 49*	521 ± 13*
	<b>2.93</b>	0.30	0.980	64	23.4	670 ± 66*	840 ± 37*
	<b>2.94 (13)</b>	0.59	0.996	129	46.9	666 ± 22*	450 ± 24*
	<b>2.95 (34, 56)</b>	3.25	0.999	92	17.7	658 ± 113*	244 ± 31
	<b>2.96</b>	2.34	0.996	49	17.7	649 ± 26*	467 ± 44*

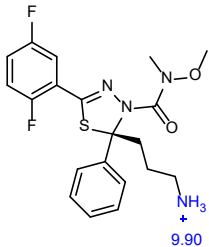
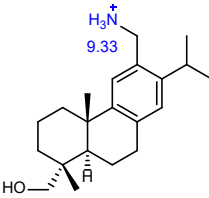
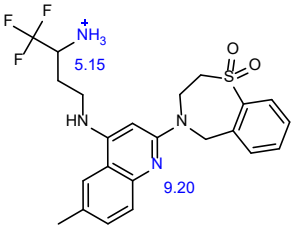
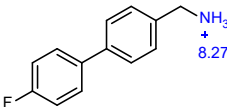
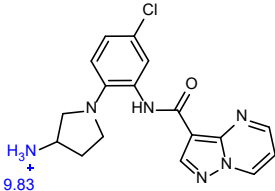
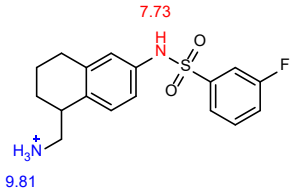
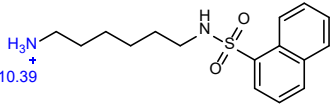
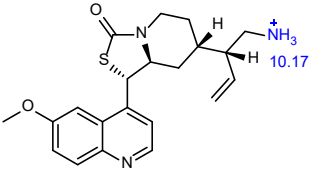
Structure	Cmpd	ClogD <sub>7.4</sub>	Formal charge	Q_vsa_Ppos	vsa_don	PA Accum.	EC Accum.
	<b>2.97</b>	2.28	0.399	90	23.4	638 ± 29*	107 ± 12
	<b>2.98 (65)</b>	0.95	0.998	48	17.7	629 ± 32*	1696 ± 117*
	<b>2.99</b>	1.84	0.999	46	17.7	622 ± 31*	790 ± 38*
	<b>2.100</b>	1.54	0.999	46	17.7	616 ± 47*	854 ± 61*
	<b>2.101</b>	1.70	0.999	46	17.7	610 ± 20*	560 ± 7*
	<b>2.102</b>	0.64	0.998	73	29.1	607 ± 51*	1685 ± 72*
	<b>2.103</b>	-1.19	0.998	110	23.4	599 ± 26*	1131 ± 146*

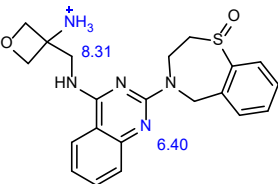
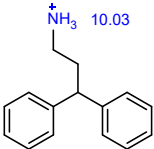
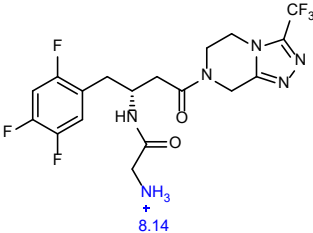
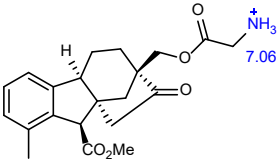
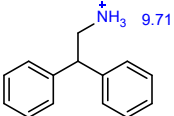
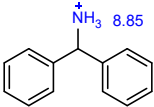
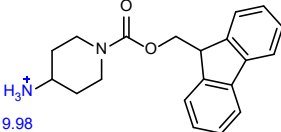
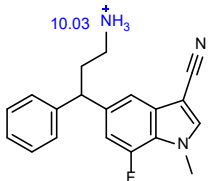
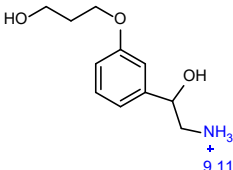
Structure	Cmpd	ClogD <sub>7.4</sub>	Formal charge	Q_vsa_Ppos	vsa_don	PA Accum.	EC Accum.
	<b>2.104 (8)</b>	2.31	0.994	44	17.7	596 ± 70*	477 ± 75*
	<b>2.105</b>	0.74	0.658	98	38.5	594 ± 50*	1283 ± 54*
	<b>2.106</b>	2.99	0.996	54	17.7	591 ± 28*	710 ± 56*
	<b>2.107</b>	0.97	0.676	64	23.4	572 ± 30*	931 ± 90*
	<b>2.108</b>	1.19	0.999	26	17.7	569 ± 54*	28 ± 6
	<b>2.109</b>	-0.50	0.863	85	29.1	563 ± 48*	1264 ± 58*
	<b>2.110 (18)</b>	1.46	0.996	53	17.7	547 ± 12*	936 ± 203*
	<b>2.111</b>	-0.27	0.999	119	46.9	529 ± 37*	812 ± 94*

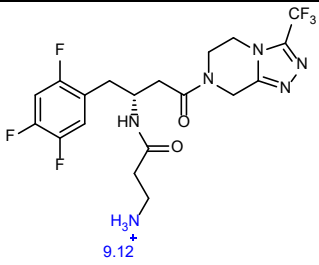
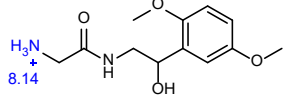
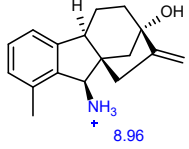
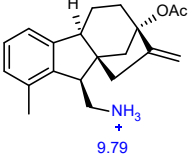
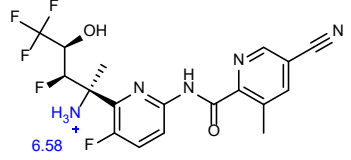
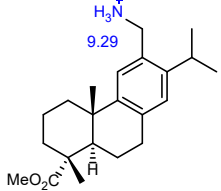
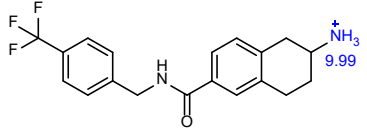
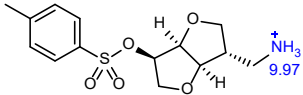
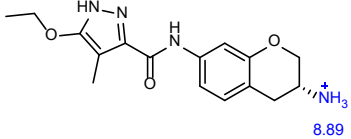
Structure	Cmpd	ClogD <sub>7.4</sub>	Formal charge	Q_vsa_Ppos	vsa_don	PA Accum.	EC Accum.
	<b>2.112 (25)</b>	-0.14	0.910	64	17.7	514 ± 28*	275 ± 9
	<b>2.113 (11)</b>	0.20	0.999	51	23.4	508 ± 10*	127 ± 10
	<b>2.114 (68)</b>	-3.91	1.849	119	46.9	505 ± 17*	895 ± 2*
	<b>2.115</b>	0.23	1.052	109	46.9	500 ± 20*	724 ± 58*
	<b>2.116 (75)</b>	-1.62	1.968	112	23.4	500 ± 112*	621 ± 55*
	<b>2.117</b>	0.56	0.996	39	17.7	498 ± 54*	726 ± 19*
	<b>2.118</b>	0	0.987	62	17.7	496 ± 12*	320 ± 29*
	<b>2.119</b>	0.46	0.744	136	34.8	491 ± 10*	317 ± 4*
	<b>2.120</b>	-0.87	0.885	68	17.7	484 ± 91*	1114 ± 135*

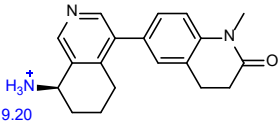
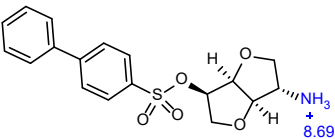
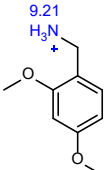
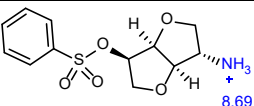
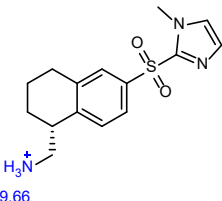
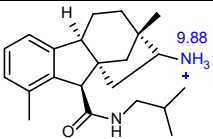
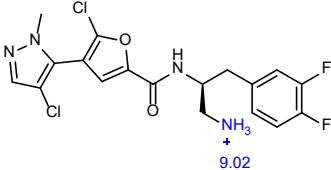
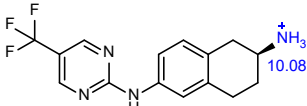
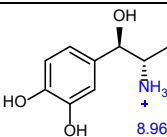
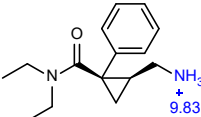
Structure	Cmpd	ClogD <sub>7.4</sub>	Formal charge	Q_vsa_Ppos	vsa_don	PA Accum.	EC Accum.
	2.121	0.24	0.990	54	17.7	476 ± 36*	817 ± 203*
	2.122	-0.37	1.157	144	29.1	467 ± 25*	826 ± 117*
	2.123 (30)	-0.34	0.989	51	17.7	453 ± 39*	1290 ± 76*
	2.124	0.02	1.060	109	46.9	451 ± 34*	840 ± 76*
	2.125	-0.54	1.000	74	23.4	439 ± 7*	540 ± 27*
	2.126	1.18	0.998	51	23.4	438 ± 15*	1871 ± 75*
	2.127	0.23	0.920	78	17.7	429 ± 13*	2161 ± 133*
	2.128	1.30	0.998	46	17.7	425 ± 25*	539 ± 10*

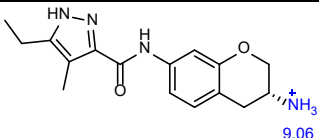
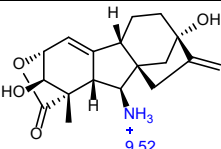
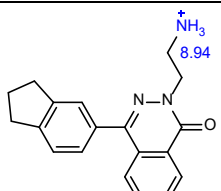
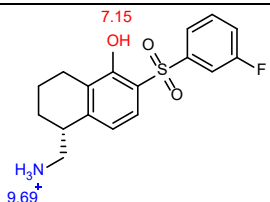
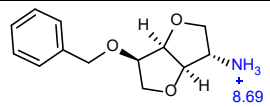
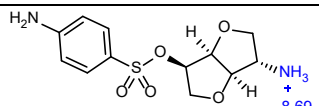
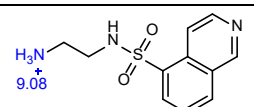
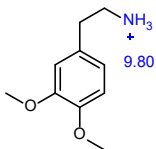
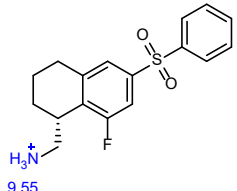


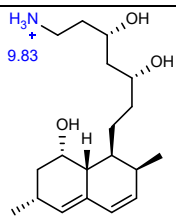
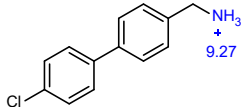
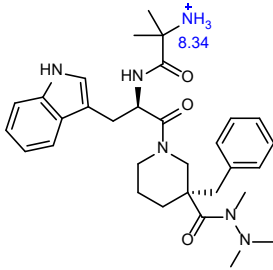
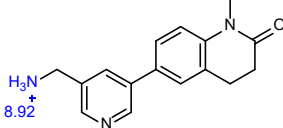
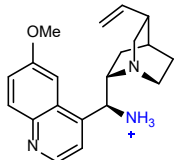
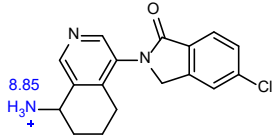
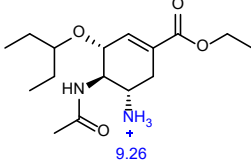
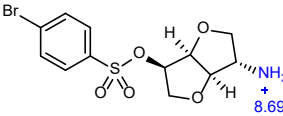
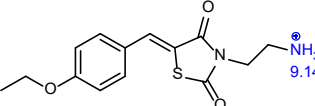
Structure	Cmpd	ClogD <sub>7.4</sub>	Formal charge	Q_vsa_Ppos	vsa_don	PA Accum.	EC Accum.
	<b>2.129 (32)</b>	1.69	0.999	65	17.7	422 ± 22*	99 ± 3
	<b>2.130</b>	2.31	0.996	49	17.7	414 ± 20*	196 ± 29
	<b>2.131</b>	2.11	0.619	108	11.4	413 ± 40*	154 ± 4
	<b>2.132</b>	0.85	0.996	39	17.7	408 ± 3*	894 ± 43*
	<b>2.133</b>	-0.72	0.992	94	23.4	406 ± 8*	796 ± 59*
	<b>2.134</b>	0.90	0.222	58	25.8	403 ± 13*	494 ± 2*
	<b>2.135 (54)</b>	-0.13	0.999	58	25.8	399 ± 63*	108 ± 16
	<b>2.136 (62)</b>	0.14	1.044	64	17.7	399 ± 79*	458 ± 58*

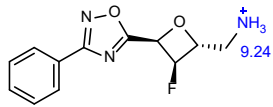
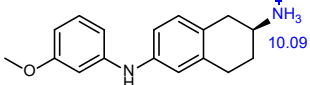
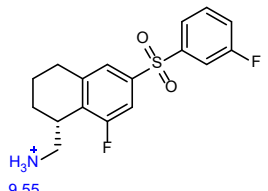
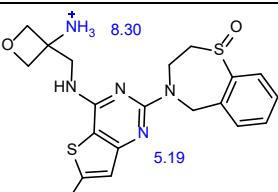
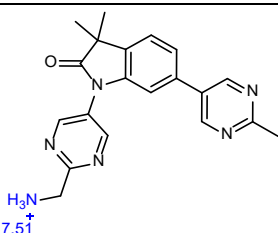
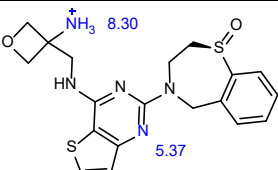
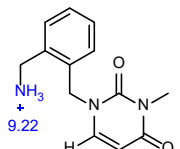
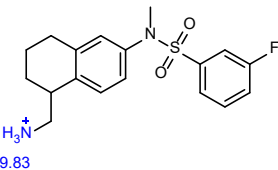
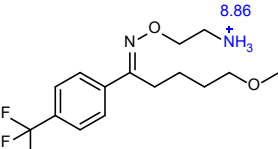
Structure	Cmpd	ClogD <sub>7.4</sub>	Formal charge	Q_vsa_Ppos	vsa_don	PA Accum.	EC Accum.
	2.137	0.56	1.196	159	29.1	388 ± 6*	3066 ± 366*
	2.138	0.77	0.999	17	0	364 ± 45*	61 ± 3
	2.139	-0.66	0.682	99	23.4	359 ± 40*	42 ± 5
	2.140	1.74	0.163	55	0	353 ± 83*	328 ± 56
	2.141	0.65	0.997	39	17.7	351 ± 28*	1155 ± 85*
	2.142	1.24	0.987	29	17.7	346 ± 18*	415 ± 21*
	2.143 (37)	-0.02	0.994	48	17.7	337 ± 23*	1181 ± 33*
	2.144 (9)	1.09	0.999	59	17.7	332 ± 10*	911 ± 60*
	2.145	-2.01	0.991	65	17.7	330 ± 12*	1731 ± 82*

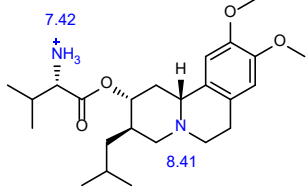
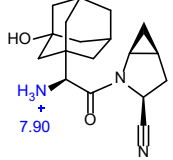
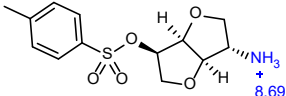
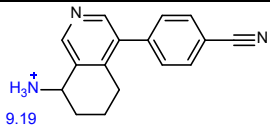
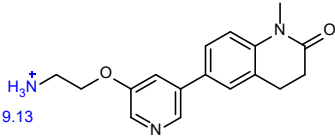
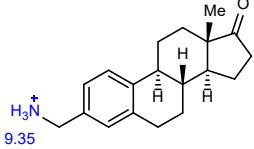
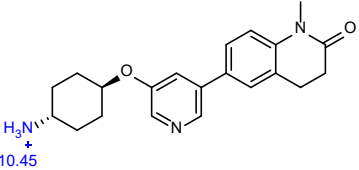
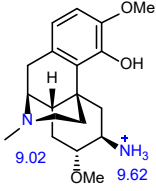
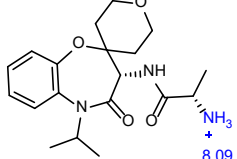
Structure	Cmpd	ClogD <sub>7.4</sub>	Formal charge	Q_vsa_Ppos	vsa_don	PA Accum.	EC Accum.
	<b>2.146</b>	-1.32	0.980	99	23.4	323 ± 6*	268 ± 22
	<b>2.147 (35)</b>	-1.76	0.683	76	23.4	322 ± 4*	244 ± 15
	<b>2.148 (6)</b>	0.46	0.992	39	17.7	320 ± 37	756 ± 94*
	<b>2.149 (57)</b>	0.36	0.998	54	17.7	317 ± 43	922 ± 46*
	<b>2.150</b>	2.46	0.063	102	5.7	307 ± 129	132 ± 23
	<b>2.151</b>	2.96	0.996	54	17.7	305 ± 3*	749 ± 23*
	<b>2.152</b>	1.15	0.998	73	23.4	304 ± 20*	944 ± 56*
	<b>2.153</b>	-1.47	0.989	51	17.7	301 ± 31*	632 ± 33*
	<b>2.154</b>	-0.10	0.965	76	23.4	287 ± 2	899 ± 55*

Structure	Cmpd	ClogD <sub>7.4</sub>	Formal charge	Q_vsa_Ppos	vsa_don	PA Accum.	EC Accum.
	<b>2.155 (53)</b>	-0.05	0.983	42	17.7	287 ± 17	437 ± 28*
	<b>2.156 (48)</b>	0.60	0.836	41	17.7	282 ± 37	1965 ± 108*
	<b>2.157</b>	-0.77	0.990	39	17.7	279 ± 7	206 ± 22
	<b>2.158</b>	-1.05	0.837	41	17.7	278 ± 31	616 ± 30*
	<b>2.159</b>	1.55	0.997	46	17.7	274 ± 55	276 ± 34
	<b>2.160</b>	1.09	0.999	51	23.4	270 ± 5	67 ± 1
	<b>2.161</b>	0.97	0.984	75	23.4	259 ± 22	104 ± 9
	<b>2.162</b>	0.49	0.998	62	23.4	257 ± 26	1092 ± 62*
	<b>2.163</b>	-1.67	0.961	65	17.7	253 ± 4	462 ± 11*
	<b>2.164 (36)</b>	-0.91	0.997	52	17.7	251 ± 5	445 ± 29

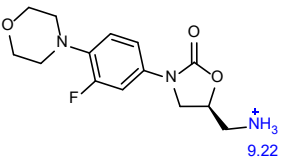
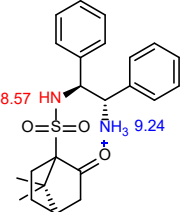
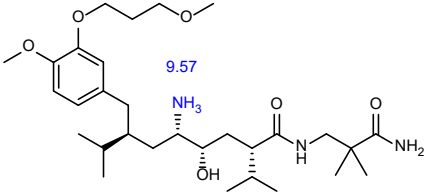
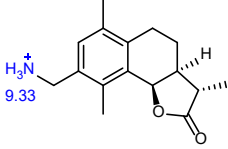
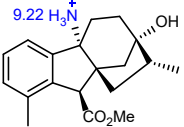
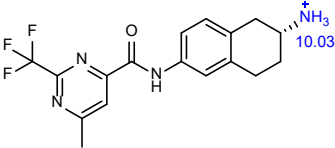
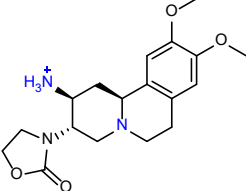
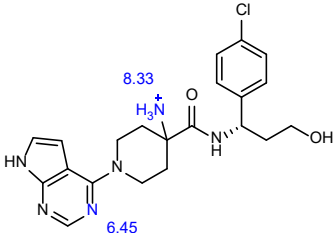
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	2.165	0.34	0.974	70	23.4	245 ± 7	555 ± 38*
	2.166	-2.32	0.987	69	17.7	242 ± 5	330 ± 78*
	2.167	1.63	0.882	59	17.7	242 ± 19	282 ± 4*
	2.168 (19)	1.84	0.747	46	17.7	241 ± 25	402 ± 113*
	2.169 (24)	-0.73	0.889	44	17.7	240 ± 18	552 ± 12*
	2.170	-1.87	0.837	58	35.5	235 ± 17	331 ± 68
	2.171	-1.94	0.990	58	25.8	235 ± 38	316 ± 12*
	2.172	-1.24	0.998	39	17.7	233 ± 17	255 ± 19
	2.173	0.10	0.998	46	17.7	232 ± 4	245 ± 4

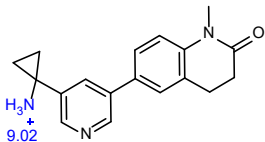
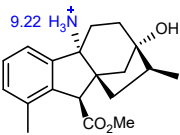
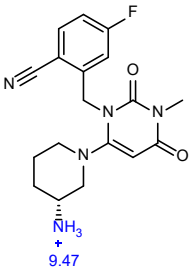
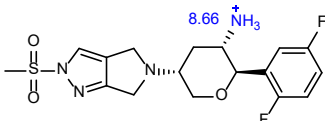
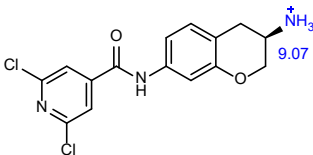
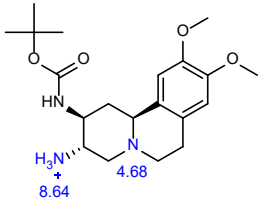
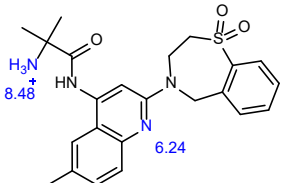
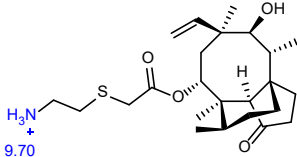
Structure	Cmpd	ClogD <sub>7.4</sub>	Formal charge	Q_vsa_Ppos	vsa_don	PA Accum.	EC Accum.
	2.174	-1.68	0.998	70	17.7	231 ± 13	323 ± 60
	2.175	1.31	0.996	39	17.7	231 ± 24	525 ± 115*
	2.176	1.38	0.852	85	29.1	226 ± 12	426 ± 7*
	2.177	-0.48	0.979	30	0	225 ± 7	301 ± 11
	2.178	0.33	1.132	65	0	224 ± 11	167 ± 12
	2.179 (51)	0.53	0.984	55	17.7	222 ± 11	500 ± 10*
	2.180 (67)	-0.72	0.820	73	23.4	218 ± 3	83 ± 11
	2.181 (49)	-0.28	0.836	41	17.7	217 ± 3	1647 ± 108*
	2.182	-0.25	0.915	67	17.7	217 ± 29	140 ± 18

Structure	Cmpd	ClogD <sub>7.4</sub>	Formal charge	Q_vsa_Ppos	vsa_don	PA Accum.	EC Accum.
	<b>2.183</b>	-0.33	0.920	78	17.7	213 ± 1	1867 ± 127*
	<b>2.184 (15)</b>	0.69	0.998	38	23.4	213 ± 39	1040 ± 77*
	<b>2.185</b>	1.70	0.997	46	17.7	212 ± 3	541 ± 136*
	<b>2.186</b>	1.13	1.406	151	23.4	212 ± 16	549 ± 6*
	<b>2.187</b>	1.19	0.908	74	17.7	193 ± 3	130 ± 1
	<b>2.188</b>	0.48	1.403	151	23.4	191 ± 5	275 ± 51
	<b>2.189</b>	-1.55	0.994	83	17.7	185 ± 14	294 ± 0
	<b>2.190</b>	0.76	0.999	49	17.7	182 ± 20	231 ± 30
	<b>2.191 (17, 33)</b>	1.05	0.952	55	17.7	168 ± 5	n.d.

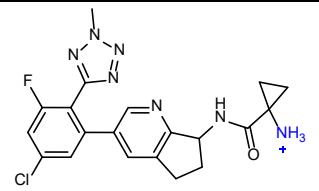
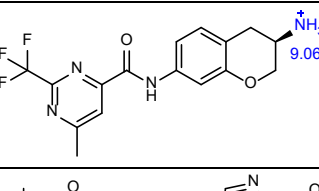
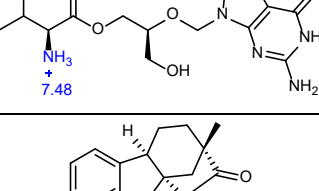
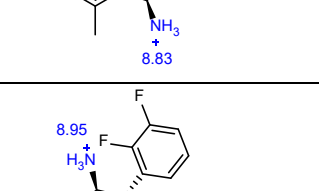
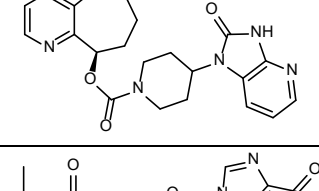
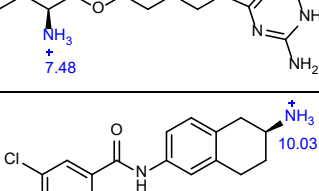
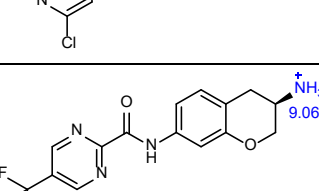
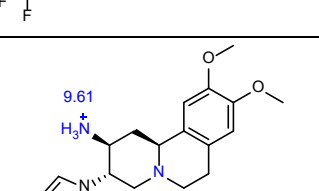
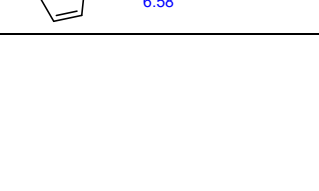
Structure	Cmpd	ClogD <sub>7.4</sub>	Formal charge	Q_vsa_Ppos	vsa_don	PA Accum.	EC Accum.
	<b>2.192</b>	2.74	1.257	73	0	167 ± 20	119 ± 21
	<b>2.193</b>	-0.70	0.704	76	17.7	163 ± 18	205 ± 12
	<b>2.194 (50)</b>	-0.53	0.837	41	17.7	163 ± 39	877 ± 29*
	<b>2.195 (52)</b>	0.40	0.980	49	17.7	161 ± 12	929 ± 39*
	<b>2.196</b>	-1.00	0.986	52	17.7	158 ± 14	370 ± 21*
	<b>2.197</b>	1.63	0.996	48	17.7	148 ± 11	208 ± 28
	<b>2.198</b>	-0.78	1.003	42	17.7	146 ± 2	222 ± 7
	<b>2.199 (73)</b>	-2.74	1.966	88	17.7	141 ± 4	256 ± 11
	<b>2.200</b>	-0.61	0.734	70	23.4	137 ± 11	17 ± 0

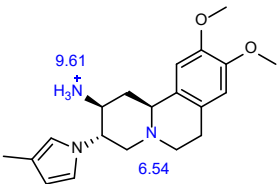
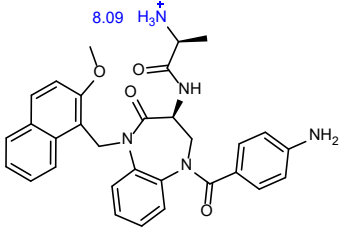
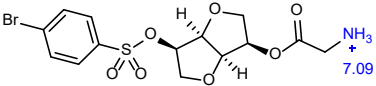
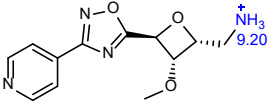
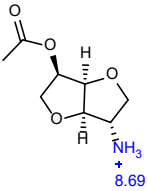
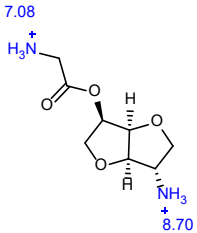


Structure	Cmpd	ClogD <sub>7.4</sub>	Formal charge	Q_vsa_Ppos	vsa_don	PA Accum.	EC Accum.
	2.201	-0.70	0.883	85	17.7	136 ± 2	658 ± 42*
	2.202	2.08	0.988	59	25.8	135 ± 3	53 ± 4
	2.203	2.54	0.995	91	41.2	132 ± 15	43 ± 1
	2.204	0.95	0.995	59	17.7	131 ± 67	272 ± 18
	2.205	-0.07	0.978	51	17.7	130 ± 6	221 ± 26
	2.206	0.66	0.998	78	23.4	119 ± 27	142 ± 11
	2.207	-1.21	1.175	54	17.7	118 ± 7	125 ± 2
	2.208	0.15	0.613	120	5.7	114 ± 2	135 ± 9

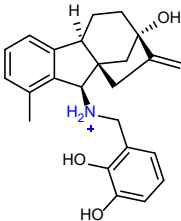
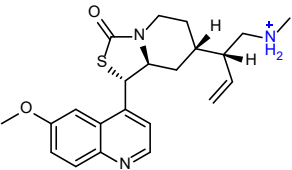
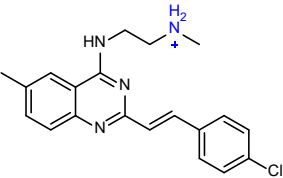
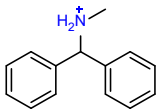
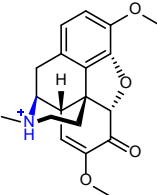
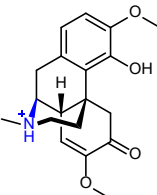
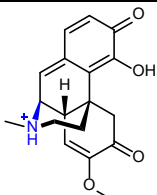
Structure	Cmpd	ClogD <sub>7.4</sub>	Formal charge	Q_vsa_Ppos	vsa_don	PA Accum.	EC Accum.
	2.209	-0.78	0.979	52	17.7	113 ± 1	495 ± 96
	2.210	-0.07	0.978	51	17.7	113 ± 18	215 ± 53
	2.211	-0.73	1.890	130	17.7	105 ± 3	189 ± 7
	2.212	-3.06	1.229	82	17.7	99 ± 7	223 ± 6
	2.213	0.84	0.973	69	23.4	97 ± 26	1369 ± 164*
	2.214	0.33	0.992	63	23.4	92 ± 1	267 ± 7
	2.215 (63)	2.07	1.362	98	23.4	92 ± 6	273 ± 4
	2.216	0.74	0.998	73	17.7	88 ± 4	20 ± 5

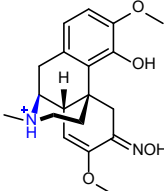
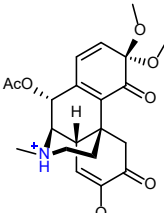
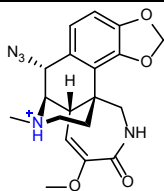
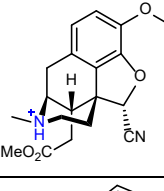
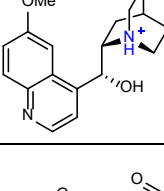
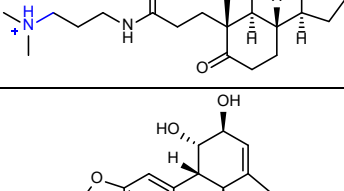
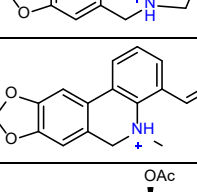
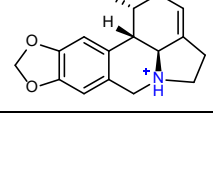
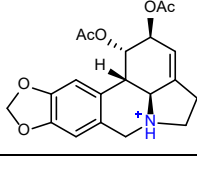
Structure	Cmpd	ClogD <sub>7.4</sub>	Formal charge	Q_vsa_Ppos	vsa_don	PA Accum.	EC Accum.
	2.217	0.56	0.973	78	23.4	87 ± 3	208 ± 4
	2.218 (74)	-0.87	1.890	130	17.7	86 ± 10	141 ± 9
	2.219	-0.64	0.963	78	17.7	83 ± 0	907 ± 142*
	2.220	-1.10	1.250	57	23.4	81 ± 3	99 ± 2
	2.221	2.71	0.183	91	23.4	79 ± 8	63 ± 6
	2.222	0.41	0.991	157	17.7	74 ± 4	110 ± 5
	2.223	0.07	0.448	80	0	74 ± 4	97 ± 2
	2.224	2.37	0.177	51	0	74 ± 7	154 ± 18
	2.225	-0.58	0.985	42	17.7	72 ± 1	258 ± 28

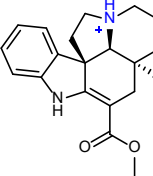
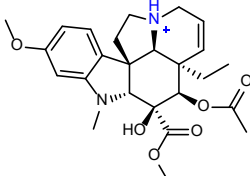
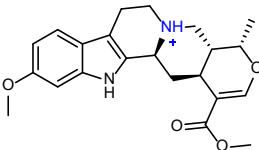
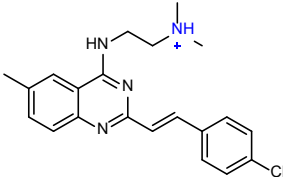
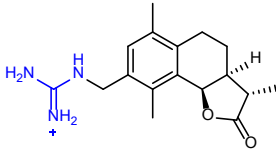
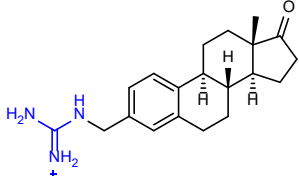
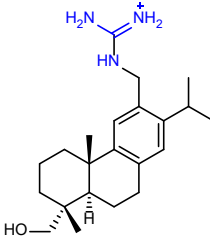
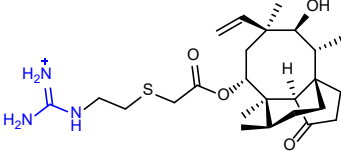
Structure	Cmpd	ClogD <sub>7.4</sub>	Formal charge	Q_vsa_Ppos	vsa_don	PA Accum.	EC Accum.
	2.226	1.75	0.772	63	23.4	72 ± 8	87 ± 5
	2.227	0.56	0.973	78	23.4	71 ± 6	127 ± 8
	2.228	-1.55	0.352	119	23.4	70 ± 7	165 ± 9
	2.229	1.44	0.989	37	17.7	61 ± 8	515 ± 50*
	2.230	1.31	0.888	94	23.4	50 ± 2	86 ± 16
	2.231	-0.92	0.360	109	23.4	44 ± 5	141 ± 6
	2.232	0.97	0.998	69	23.4	42 ± 13	768 ± 24*
	2.233	-0.03	0.973	71	23.4	39 ± 7	418 ± 24*
	2.234	-0.41	1.158	32	17.7	33 ± 4	20 ± 2

Structure	Cmpd	ClogD <sub>7.4</sub>	Formal charge	Q_vsa_Ppos	vsa_don	PA Accum.	EC Accum.
	2.235	0.11	1.156	32	17.7	23 ± 3	17 ± 1
	2.236	1.57	0.737	110	41.2	14 ± 0	11 ± 0
	2.237	0.76	0.135	43	0	2 ± 1	10 ± 1
	2.238	-1.88	0.996	78	17.7	0 ± 0	14 ± 5
	2.239	-2.66	0.859	44	17.7	0 ± 0	372 ± 3*
	2.240	-3.75	0.993	61	17.7	0 ± 0	23 ± 0

**Table S3.** Accumulation of all non-primary amines. Accumulation measured in nmol/10<sup>12</sup> CFUs in *P. aeruginosa* PAO1 and *E. coli* MG1655. For compound source please refer to the **Compound Master Table**. Compound reference numbers for main text figures are listed in parenthesis. All experiments were performed in biological triplicate. The s.e.m. is reported for accumulation values. Properties were calculated as described above. An asterisk (\*) is used to indicate compounds that accumulate to a statistically significant level. n.d. = not determined.

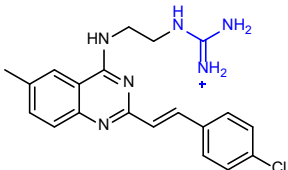
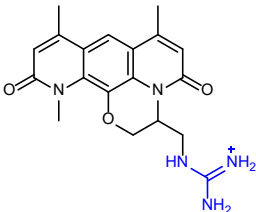
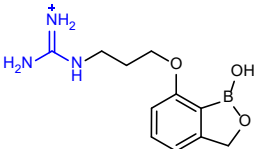
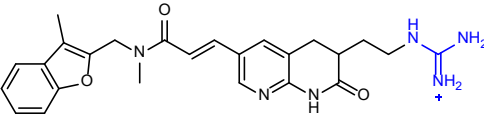
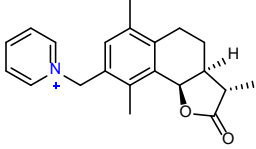
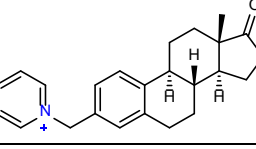
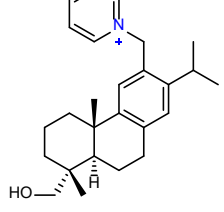
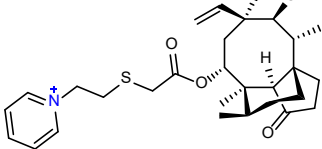
Structure	Cmpd	Functional Group	MW	ClogD <sub>7.4</sub>	PA Accum.	EC Accum.
	<b>3.1</b>	Secondary amine	377	1.93	192 ± 31	493 ± 161*
	<b>3.2 (61)</b>	Secondary amine	398	0.24	128 ± 1	413 ± 8*
	<b>3.3 (3)</b>	Secondary amine	367	3.28	1323 ± 33	4228 ± 90
	<b>3.4</b>	Secondary amine	197	1.63	56 ± 6	n.d.
	<b>3.5</b>	Tertiary amine	327	0.58	45 ± 5	407 ± 6*
	<b>3.6</b>	Tertiary amine	329	0.65	99 ± 3	218 ± 10
	<b>3.7</b>	Tertiary amine	313	0.84	90 ± 4	213 ± 48

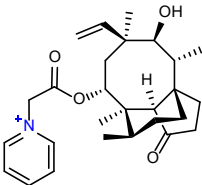
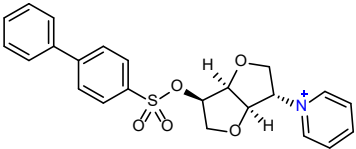
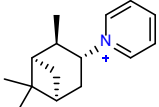
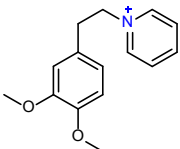
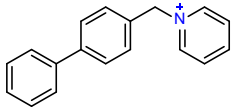
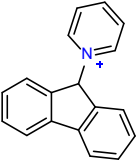
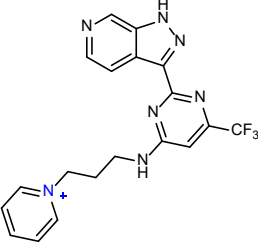
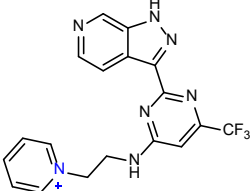
Structure	Cmpd	Functional Group	MW	ClogD <sub>7.4</sub>	PA Accum.	EC Accum.
	3.8	Tertiary amine	344	-0.09	159 ± 23	204 ± 26
	3.9	Tertiary amine	417	0.48	7 ± 3	n.d.
	3.10	Tertiary amine	383	-0.38	24 ± 6	n.d.
	3.11	Tertiary amine	342	0.28	75 ± 1	n.d.
	3.12	Tertiary amine	324	0.86	259 ± 15	261 ± 16
	3.13	Tertiary amine	405	0.69	0 ± 0	72 ± 5
	3.14	Tertiary amine	287	-0.46	182 ± 3	n.d.
	3.15	Tertiary amine	265	3.84	13 ± 0	n.d.
	3.16	Tertiary amine	371	0.06	25 ± 2	n.d.

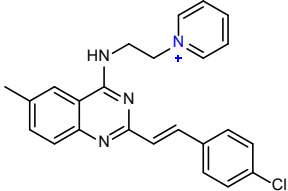
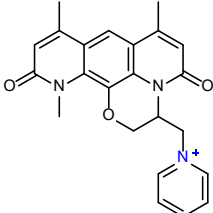
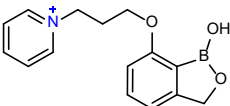
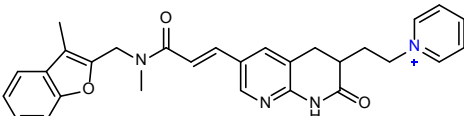
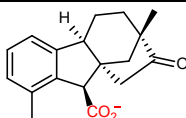
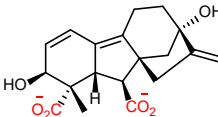
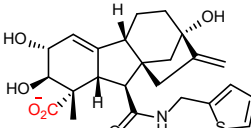
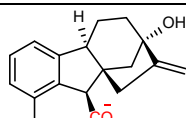
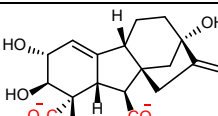
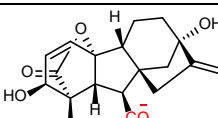
Structure	Cmpd	Functional Group	MW	ClogD <sub>7.4</sub>	PA Accum.	EC Accum.
	3.17	Tertiary amine	336	0.90	63 ± 9	n.d.
	3.18	Tertiary amine	457	0.59	49 ± 1	n.d.
	3.19	Tertiary amine	382	2.05	56 ± 2	n.d.
	3.20 (2)	Tertiary amine	353	4.41	517 ± 28*	1923 ± 294*
	3.21	Guanidinium	301	0.30	95 ± 1	156 ± 49
	3.22	Guanidinium	325	0.99	409 ± 29*	1202 ± 268*
	3.23	Guanidinium	358	1.66	493 ± 117*	824 ± 167*
	3.24	Guanidinium	480	0.23	123 ± 9	46 ± 15

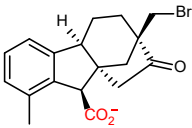
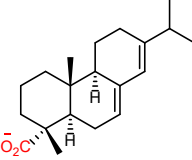
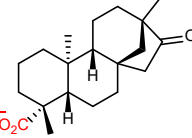
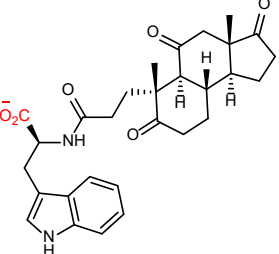
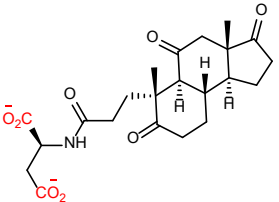
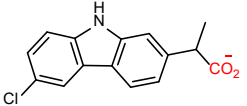
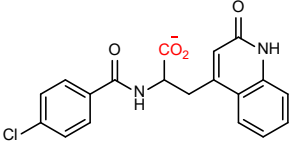
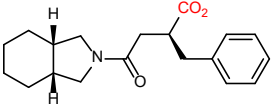
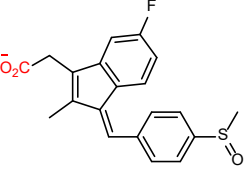


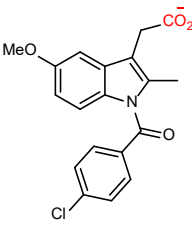
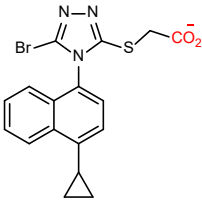
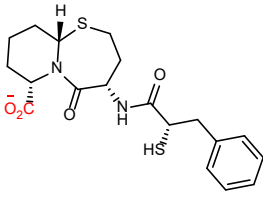
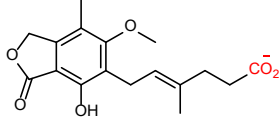
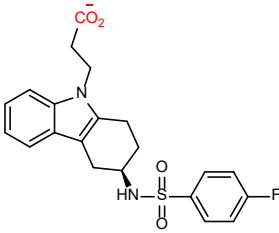
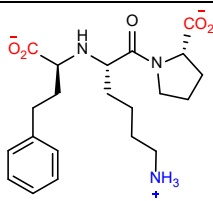
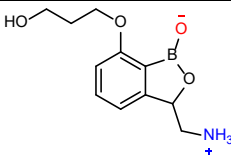
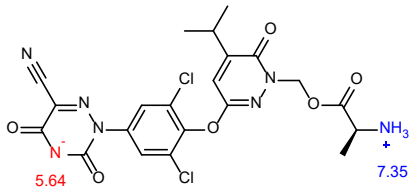
Structure	Cmpd	Functional Group	MW	ClogD <sub>7.4</sub>	PA Accum.	EC Accum.
	3.25	Guanidinium	420	-0.22	222 ± 21	105 ± 23
	3.26	Guanidinium	403	-0.55	744 ± 56*	1741 ± 89*
	3.27 (29, 77G)	Guanidinium	195	-0.96	915 ± 68*	1483 ± 135*
	3.28	Guanidinium	223	-1.67	209 ± 7	319 ± 12*
	3.29	Guanidinium	225	0	1295 ± 191*	4736 ± 300*
	3.30 (28)	Guanidinium	223	-0.19	1055 ± 55*	1848 ± 284*
	3.31 (78G)	Guanidinium	379	-0.76	1050 ± 65*	2324 ± 106*
	3.32	Guanidinium	365	-0.82	1737 ± 124*	3267 ± 249*

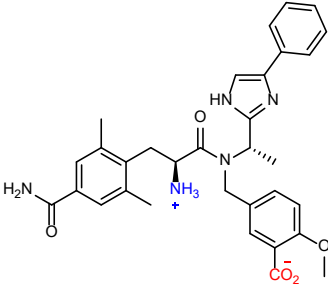
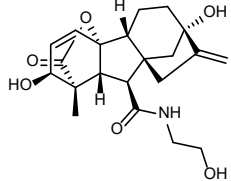
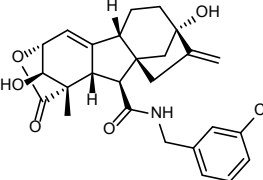
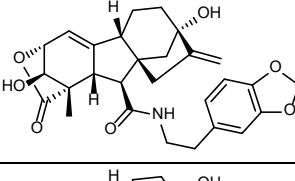
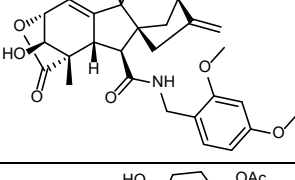
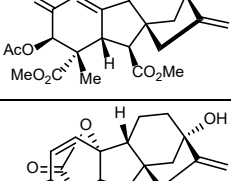
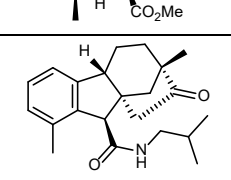
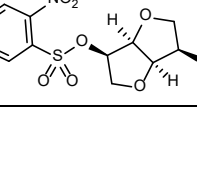

Structure	Cmpd	Functional Group	MW	ClogD <sub>7.4</sub>	PA Accum.	EC Accum.
	<b>3.33 (27)</b>	Guanidinium	381	2.57	2693 ± 232*	1932 ± 28*
	<b>3.34</b>	Guanidinium	367	-2.26	44 ± 1	434 ± 22*
	<b>3.35</b>	Guanidinium	249	-1.20	325 ± 26*	874 ± 93*
	<b>3.36 (79G)</b>	Guanidinium	461	-0.29	929 ± 39*	2259 ± 196*
	<b>3.37</b>	Pyridinium	322	0.48	64 ± 10	62 ± 9
	<b>3.38</b>	Pyridinium	346	1.18	97 ± 9	69 ± 19
	<b>3.39</b>	Pyridinium	379	1.84	86 ± 13	116 ± 27
	<b>3.40</b>	Pyridinium	501	0.41	118 ± 19	64 ± 7

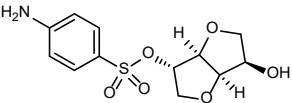
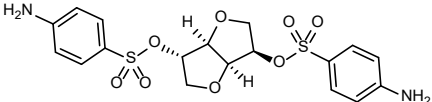
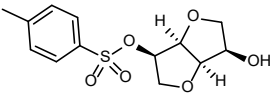
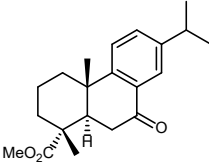
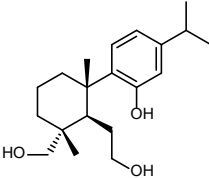
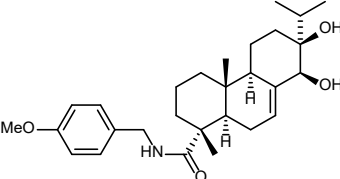
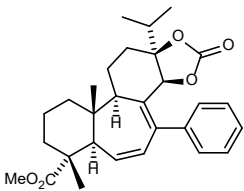
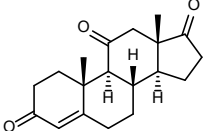
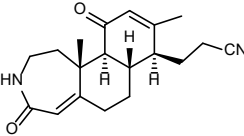
Structure	Cmpd	Functional Group	MW	ClogD <sub>7.4</sub>	PA Accum.	EC Accum.
	3.41	Pyridinium	441	-0.07	85 ± 13	88 ± 11
	3.42	Pyridinium	424	-0.38	179 ± 14	345 ± 48*
	3.43 (77P)	Pyridinium	202	-1.07	245 ± 9	124 ± 10
	3.44	Pyridinium	244	-1.49	83 ± 1	138 ± 15
	3.45	Pyridinium	246	0.18	385 ± 18*	576 ± 78*
	3.46	Pyridinium	244	0	353 ± 69*	137 ± 29
	3.47 (78P)	Pyridinium	400	-0.93	187 ± 17	732 ± 9*
	3.48	Pyridinium	386	-1.01	488 ± 10*	562 ± 31*

Structure	Cmpd	Functional Group	MW	ClogD <sub>7.4</sub>	PA Accum.	EC Accum.
	3.49	Pyridinium	402	2.39	313 ± 10*	518 ± 35*
	3.50	Pyridinium	388	-2.08	13 ± 1	198 ± 11
	3.51	Pyridinium	270	-1.19	143 ± 6	233 ± 19
	3.52 (79P)	Pyridinium	482	-0.10	120 ± 17	762 ± 37*
	3.53	Carboxylic acid	284	0.57	66 ± 1	138 ± 7
	3.54	Carboxylic acid	346	-5.79	51 ± 7	104 ± 20
	3.55	Carboxylic acid	460	-2.09	22 ± 2	61 ± 13
	3.56 (5)	Carboxylic acid	284	-0.23	58 ± 5	64 ± 5
	3.57	Carboxylic acid (di-acid)	364	-6.53	78 ± 5	59 ± 4
	3.58	Carboxylic acid	346	-2.71	69 ± 14	63 ± 12

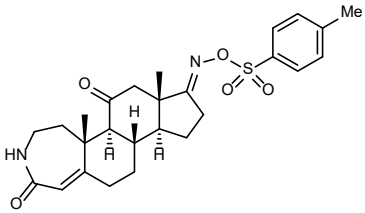
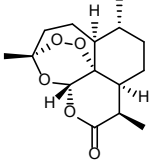
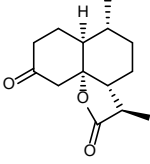
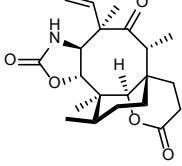
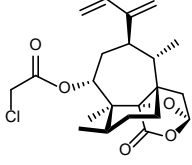
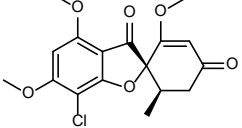
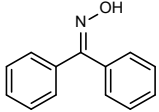
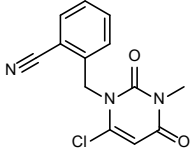
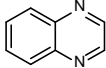
Structure	Cmpd	Functional Group	MW	ClogD <sub>7.4</sub>	PA Accum.	EC Accum.
	3.59	Carboxylic acid	363	0.47	68 ± 3	n.d.
	3.60	Carboxylic acid	302	2.22	211 ± 28	34 ± 5
	3.61	Carboxylic acid	318	1.46	86 ± 7	n.d.
	3.62	Carboxylic acid	507	0.37	51 ± 2	n.d.
	3.63	Carboxylic acid (di-acid)	435	-4.28	51 ± 2	n.d.
	3.64	Carboxylic acid	274	0.30	176 ± 2	n.d.
	3.65	Carboxylic acid	371	-0.61	63 ± 9	n.d.
	3.66	Carboxylic acid	315	0.22	70 ± 4	n.d.
	3.67	Carboxylic acid	341	-0.18	0 ± 0	n.d.

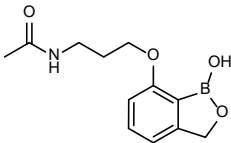
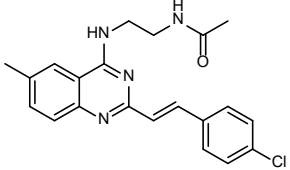
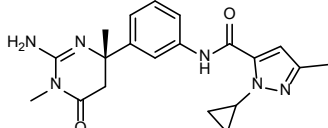
Structure	Cmpd	Functional Group	MW	ClogD <sub>7.4</sub>	PA Accum.	EC Accum.
	3.68	Carboxylic acid	358	0.27	78 ± 1	n.d.
	3.69	Carboxylic acid	404	0.24	118 ± 10	n.d.
	3.70	Carboxylic acid	409	-1.22	13 ± 3	n.d.
	3.71	Carboxylic acid	320	0.17	53 ± 1	n.d.
	3.72	Carboxylic acid	418	0.28	88 ± 4	n.d.
	3.73	Zwitterionic	405	-3.50	55 ± 0	496 ± 84*
	3.74	Zwitterionic	237	-0.78	953 ± 59	2161 ± 211
	3.75	Zwitterionic	535	0.49	3 ± 0	0 ± 0

Structure	Cmpd	Functional Group	MW	ClogD <sub>7.4</sub>	PA Accum.	EC Accum.
	3.76	Zwitterionic	570	0.35	50 ± 1	94 ± 12
	3.77	Neutral	389	-2.21	104 ± 3	80 ± 4
	3.78	Neutral	470	1.98	37 ± 1	74 ± 6
	3.79	Neutral	494	1.29	29 ± 1	56 ± 2
	3.80	Neutral	496	1.06	60 ± 10	n.d.
	3.81	Neutral	491	0.34	36 ± 3	n.d.
	3.82	Neutral	359	1.26	0 ± 0	n.d.
	3.83	Neutral	339	4.13	26 ± 0	n.d.
	3.84	Neutral (Nitro)	331	0.58	6 ± 2	0 ± 0

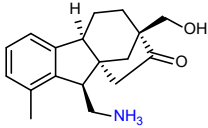
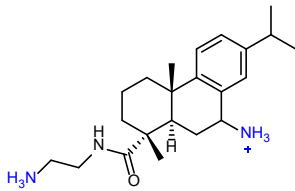
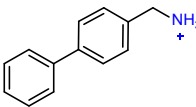
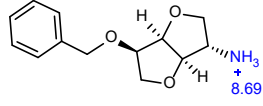
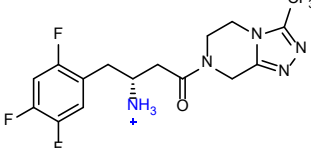
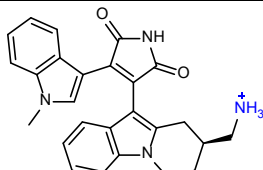
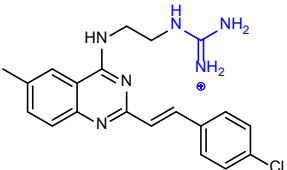
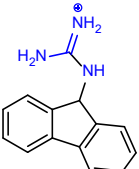
Structure	Cmpd	Functional Group	MW	ClogD <sub>7.4</sub>	PA Accum.	EC Accum.
	<b>3.85</b>	Neutral (Aniline)	301	-0.18	52 ± 6	193 ± 15
	<b>3.86</b>	Neutral (Aniline)	456	1.04	92 ± 3	113 ± 2
	<b>3.87</b>	Neutral	300	1.16	39 ± 1	152 ± 29
	<b>3.88</b> (7)	Neutral	328	4.75	232 ± 18	n.d.
	<b>3.89</b>	Neutral	320	3.93	263 ± 29	n.d.
	<b>3.90</b>	Neutral	456	4.19	274 ± 14	n.d.
	<b>3.91</b>	Neutral	465	6.53	109 ± 15	n.d.
	<b>3.92</b>	Neutral	300	3.01	17 ± 2	91 ± 21
	<b>3.93</b>	Neutral	312	1.79	63 ± 0	36 ± 1

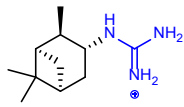
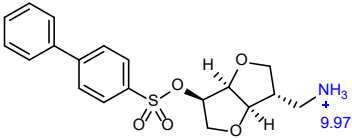
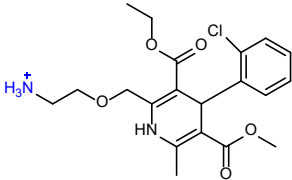
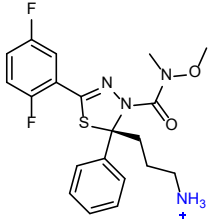
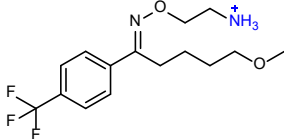
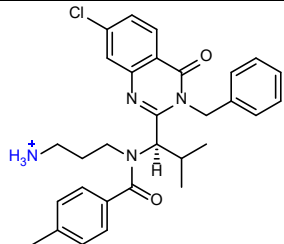
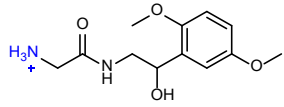
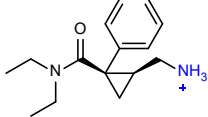
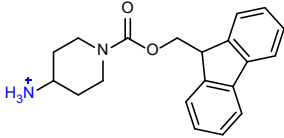
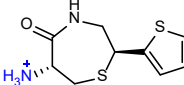


Structure	Cmpd	Functional Group	MW	ClogD <sub>7.4</sub>	PA Accum.	EC Accum.
	3.94	Neutral	485	4.10	232 ± 26	n.d.
	3.95	Neutral	282	3.11	0 ± 0	n.d.
	3.96	Neutral	236	2.83	36 ± 3	n.d.
	3.97	Neutral	375	3.46	42 ± 0	n.d.
	3.98	Neutral	409	4.27	0 ± 0	n.d.
	3.99	Neutral	353	2.17	39 ± 6	31 ± 1
	3.100	Neutral	197	3.44	40 ± 0	n.d.
	3.101	Neutral	276	1.84	28 ± 3	36 ± 4
	3.102	Neutral	130	1.30	29 ± 0	86 ± 9

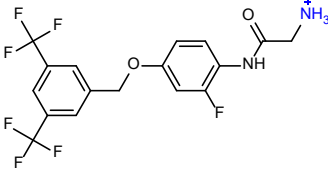
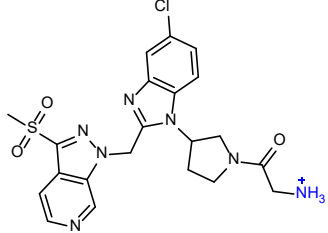
Structure	Cmpd	Functional Group	MW	ClogD <sub>7.4</sub>	PA Accum.	EC Accum.
	<b>3.103</b>	Neutral	249	0.90	96 ± 15	1347 ± 189*
	<b>3.104 (1)</b>	Neutral	367	4.87	288 ± 5	295 ± 18
	<b>3.105</b>	Neutral	380	1.14	157 ± 1	195 ± 7

**Table S4a.** Assessment of mode of uptake for monoamines, diamines, and guanidiniums. Accumulation measured in nmol/10<sup>12</sup> CFUs in *P. aeruginosa* PA14 and *P. aeruginosa* PA14  $\Delta$ 40. For compound source please refer to the **Compound Master Table**. All experiments were performed in biological triplicate. The s.e.m. is reported for accumulation values. Compound numbers in parenthesis refer to **Fig. 3a** and **3b**. An asterisk (\*) is used to indicate compounds that accumulate to a statistically significant level.

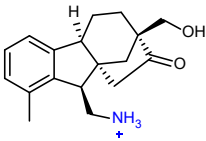
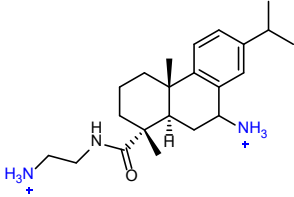
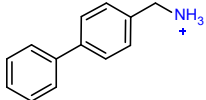
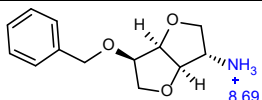
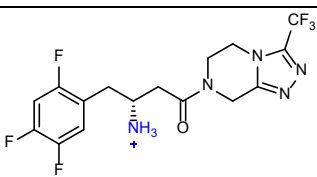
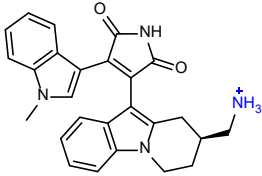
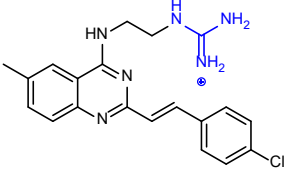
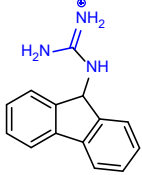
Structure	Cmpd	PA14 Accum.	PA14 $\Delta$ 40 Accum.	PA14 Accum. w/MgCl <sub>2</sub>
	<b>4.1</b> (21)	1957 $\pm$ 30*	1864 $\pm$ 129*	55 $\pm$ 5
	<b>4.2</b> (22, 71)	978 $\pm$ 83*	1476 $\pm$ 28*	175 $\pm$ 13
	<b>4.3</b> (23)	2243 $\pm$ 369*	2211 $\pm$ 96*	375 $\pm$ 95*
	<b>4.4</b> (24)	405 $\pm$ 35*	411 $\pm$ 78*	22 $\pm$ 3
	<b>4.5</b> (25)	440 $\pm$ 59*	385 $\pm$ 109*	34 $\pm$ 7
	<b>4.6</b> (26, 55)	936 $\pm$ 117*	1119 $\pm$ 171*	585 $\pm$ 88*
	<b>4.7</b> (27)	584 $\pm$ 34*	605 $\pm$ 7*	23 $\pm$ 6
	<b>4.8</b> (28)	2396 $\pm$ 140*	2406 $\pm$ 254*	124 $\pm$ 30

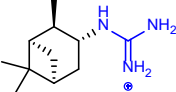
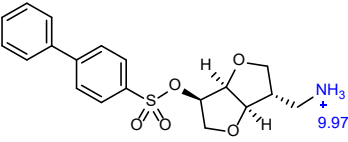
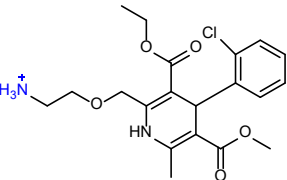
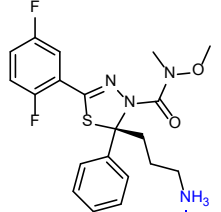
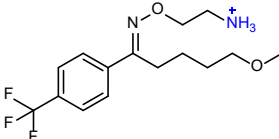
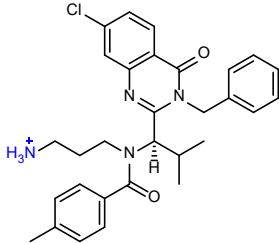
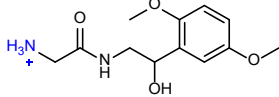
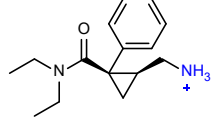
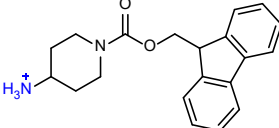
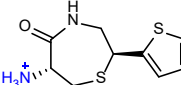
Structure	Cmpd	PA14 Accum.	PA14 $\Delta$ 40 Accum.	PA14 Accum. w/MgCl <sub>2</sub>
	<b>4.9</b> <b>(29, 77G)</b>	1913 $\pm$ 70*	2280 $\pm$ 75*	573 $\pm$ 107*
	<b>4.10</b> <b>(30)</b>	1086 $\pm$ 179*	1161 $\pm$ 51*	96 $\pm$ 41
	<b>4.11</b> <b>(31)</b>	936 $\pm$ 79*	724 $\pm$ 42*	459 $\pm$ 22*
	<b>4.12</b> <b>(32)</b>	443 $\pm$ 28*	418 $\pm$ 32*	163 $\pm$ 14
	<b>4.13</b> <b>(17, 33)</b>	611 $\pm$ 48*	614 $\pm$ 110*	306 $\pm$ 42
	<b>4.14</b> <b>(34, 56)</b>	421 $\pm$ 176*	436 $\pm$ 71*	499 $\pm$ 235*
	<b>4.15</b> <b>(35)</b>	244 $\pm$ 27	330 $\pm$ 10*	146 $\pm$ 26
	<b>4.16</b> <b>(36)</b>	329 $\pm$ 22*	369 $\pm$ 36*	157 $\pm$ 17
	<b>4.17</b> <b>(37)</b>	962 $\pm$ 84*	733 $\pm$ 262*	541 $\pm$ 18*
	<b>4.18</b> <b>(38)</b>	1164 $\pm$ 35*	1045 $\pm$ 37*	949 $\pm$ 100*

Structure	Cmpd	PA14 Accum.	PA14 $\Delta$ 40 Accum.	PA14 Accum. w/MgCl <sub>2</sub>
	<b>4.19</b> <b>(39)</b>	2053 $\pm$ 306*	1580 $\pm$ 168*	1003 $\pm$ 192*
	<b>4.20</b> <b>(40)</b>	2403 $\pm$ 100*	2303 $\pm$ 180*	1297 $\pm$ 76*
	<b>4.21</b> <b>(41)</b>	3453 $\pm$ 201*	3411 $\pm$ 35*	2662 $\pm$ 116*
	<b>4.22</b> <b>(42)</b>	435 $\pm$ 80*	536 $\pm$ 90*	189 $\pm$ 42
	<b>4.23</b> <b>(43)</b>	1965 $\pm$ 89*	1895 $\pm$ 15*	901 $\pm$ 11*
	<b>4.24</b> <b>(44)</b>	453 $\pm$ 62*	389 $\pm$ 72*	241 $\pm$ 69
	<b>4.25</b> <b>(45)</b>	879 $\pm$ 356*	1188 $\pm$ 171*	394 $\pm$ 38*

Structure	Cmpd	PA14 Accum.	PA14 $\Delta$ 40 Accum.	PA14 Accum. w/MgCl <sub>2</sub>
	<b>4.26 (46)</b>	1141 $\pm$ 50*	1419 $\pm$ 123*	1092 $\pm$ 133*
	<b>4.27 (47)</b>	737 $\pm$ 43*	791 $\pm$ 25*	220 $\pm$ 17

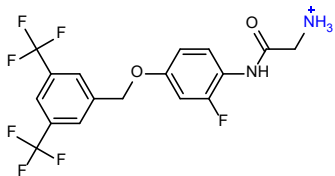
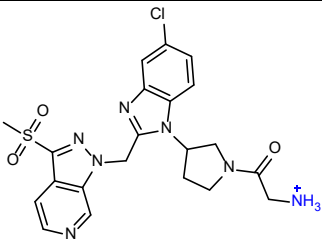
**Table S4b.** Assessment of mode of uptake for monoamines, diamines, and guanidiniums. Accumulation measured in nmol/10<sup>12</sup> CFUs in *P. aeruginosa* PAO1 and *E. coli* MG1655. For compound source please refer to the **Compound Master Table**. All experiments were performed in biological triplicate. The s.e.m. is reported for accumulation values. Compound numbers in parenthesis refer to **Extended Data Fig. 5b and 5d**. An asterisk (\*) is used to indicate compounds that accumulate to a statistically significant level.

Structure	Cmpd	PAO1 Accum.	PAO1 Accum. w/PMBN	EC MG1655 Accum.	EC MG1655 Accum. w/MgCl <sub>2</sub>
	<b>4.1 (21)</b>	818 ± 51*	838 ± 47*	1487 ± 58*	201 ± 1
	<b>4.2 (22, 71)</b>	1380 ± 60*	1781 ± 77*	1344 ± 25*	310 ± 89*
	<b>4.3 (23)</b>	1817 ± 102*	n.d.	616 ± 10*	n.d.
	<b>4.4 (24)</b>	240 ± 10	92 ± 1	552 ± 12*	517 ± 26*
	<b>4.5 (25)</b>	514 ± 28*	636 ± 12*	275 ± 9	514 ± 9*
	<b>4.6 (26, 55)</b>	1193 ± 27*	1961 ± 48*	17 ± 7	101 ± 18
	<b>4.7 (27)</b>	2693 ± 232*	1180 ± 175*	1932 ± 16*	1584 ± 472*
	<b>4.8 (28)</b>	1055 ± 55*	124 ± 30	1848 ± 164*	1274 ± 121*

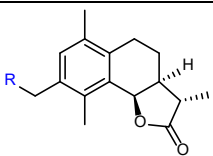
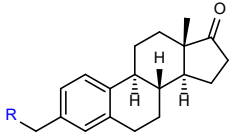
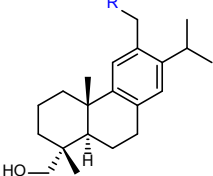
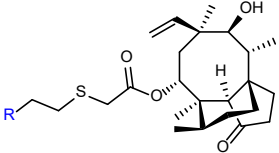
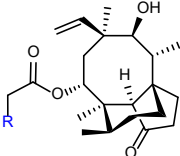
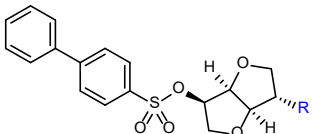
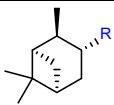
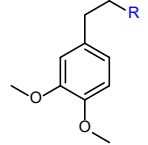
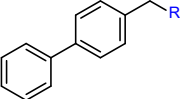
Structure	Cmpd	PAO1 Accum.	PAO1 Accum. w/PMBN	EC MG1655 Accum.	EC MG1655 Accum. w/MgCl <sub>2</sub>
	<b>4.9 (29, 77G)</b>	915 ± 68*	573 ± 107*	1483 ± 78*	820 ± 36*
	<b>4.10 (30)</b>	453 ± 39*	1032 ± 43*	1290 ± 76*	326 ± 3*
	<b>4.11 (31)</b>	741 ± 45*	2215 ± 130*	426 ± 7*	226 ± 22
	<b>4.12 (32)</b>	422 ± 22*	1717 ± 46*	99 ± 3	54 ± 9
	<b>4.13 (17, 33)</b>	168 ± 5	990 ± 105*	1422 ± 103*	136 ± 1
	<b>4.14 (34, 56)</b>	658 ± 113*	1445 ± 69*	244 ± 31	101 ± 25
	<b>4.15 (35)</b>	322 ± 4*	n.d.	244 ± 15	n.d.
	<b>4.16 (36)</b>	251 ± 5	322 ± 22*	445 ± 29*	160 ± 25
	<b>4.17 (37)</b>	327 ± 23*	1820 ± 127*	1181 ± 33*	360 ± 73*
	<b>4.18 (38)</b>	838 ± 50*	1081 ± 55*	1295 ± 3*	776 ± 22*

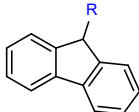
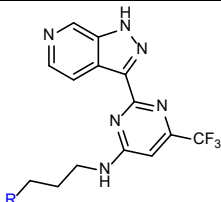
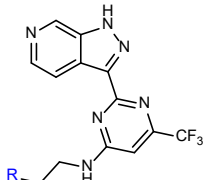
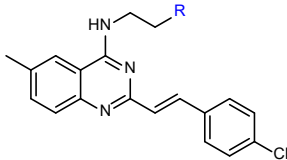
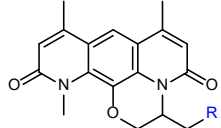
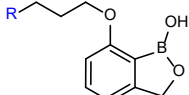
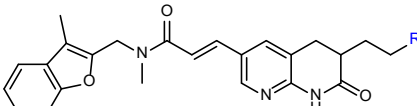




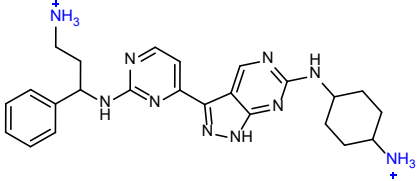
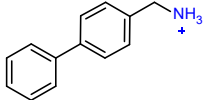
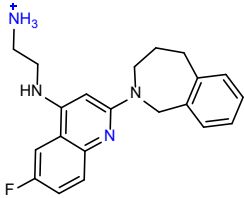
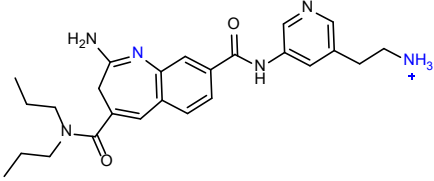
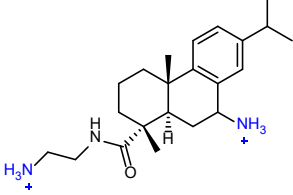
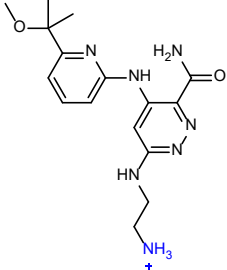
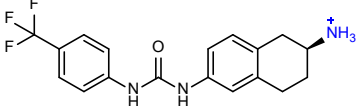
Structure	Cmpd	PAO1 Accum.	PAO1 Accum. w/PMBN	EC MG1655 Accum.	EC MG1655 Accum. w/MgCl <sub>2</sub>
	<b>4.26 (46)</b>	970 ± 79*	1850 ± 91*	1039 ± 24*	934 ± 170*
	<b>4.27 (47)</b>	850 ± 8*	1195 ± 20	690 ± 46*	226 ± 19

**Table S5.** Accumulation of amine, guanidinium, and pyridinium comparators. Accumulation measured in nmol/10<sup>12</sup> CFUs in *P. aeruginosa* PAO1. For compound source please refer to the **Compound Master Table**. Compounds are notated where R= amine (A), guanidinium (G), and pyridinium (P), as previously described.<sup>6</sup> All experiments were performed in biological triplicate. The s.e.m. is reported for accumulation values. An asterisk (\*) is used to indicate compounds that accumulate to a statistically significant level.

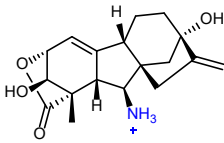
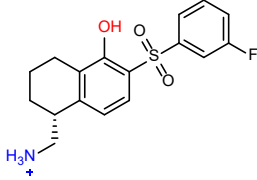
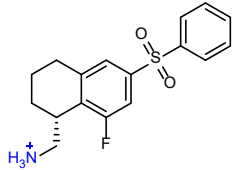
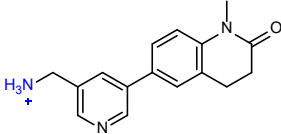
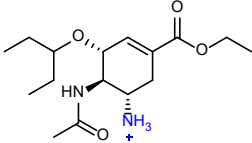
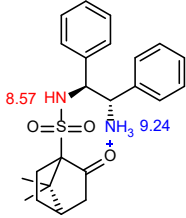
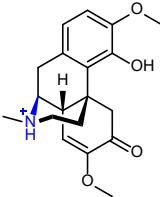
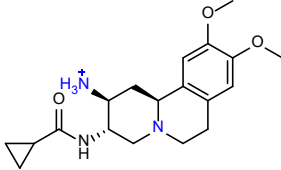
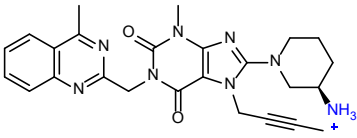
Structure	Cmpd	PA Accum. Amine	PA Accum. Guanidinium	PA Accum. Pyridinium
	5.1	131 ± 67	95 ± 1	64 ± 10
	5.2	148 ± 11	409 ± 29*	97 ± 9
	5.3	414 ± 20*	493 ± 117*	86 ± 13
	5.4	88 ± 4	123 ± 9	118 ± 19
	5.5	74 ± 7	222 ± 21	85 ± 13
	5.6	282 ± 37	744 ± 56*	179 ± 14
	5.7 (77)	1050 ± 20*	915 ± 68*	245 ± 9
	5.8	233 ± 17	209 ± 7	83 ± 1
	5.9	1817 ± 102*	1295 ± 191*	385 ± 18*

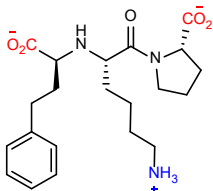
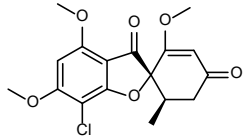
Structure	Cmpd	PA Accum. Amine	PA Accum. Guandinium	PA Accum. Pyridinium
	<b>5.10</b>	927 ± 81*	1055 ± 55*	353 ± 69*
	<b>5.11 (78)</b>	1027 ± 49*	1050 ± 65*	187 ± 17
	<b>5.12</b>	1213 ± 113*	1737 ± 124*	488 ± 10*
	<b>5.13</b>	1943 ± 41*	2693 ± 232*	313 ± 10*
	<b>5.14</b>	484 ± 91*	44 ± 1	13 ± 1
	<b>5.15</b>	491 ± 64*	325 ± 26*	143 ± 6
	<b>5.16 (79)</b>	650 ± 42*	929 ± 39*	120 ± 17

**Table S6.** Accumulation of all compounds tested in multiple PA strains. Accumulation measured in nmol/10<sup>12</sup> CFUs in *P. aeruginosa* PAO1, PA14, and PA1280. For compound source please refer to the **Compound Master Table**. Compound reference numbers for main text figures are listed in parenthesis. All experiments were performed in biological triplicate. The s.e.m. is reported for accumulation values.

Structure	Cmpd	PAO1 Accum.	PA14 Accum.	PA1280 Accum.
	<b>6.1</b> <b>(72)</b>	3433 ± 12*	1853 ± 162*	1370 ± 159*
	<b>6.2</b> <b>(23)</b>	1817 ± 102*	1277 ± 119*	1190 ± 25*
	<b>6.3</b>	1749 ± 396*	1720 ± 12*	1340 ± 51*
	<b>6.4</b>	1740 ± 65*	2157 ± 134*	883 ± 9*
	<b>6.5</b> <b>(22, 71)</b>	1380 ± 60*	498 ± 55*	508 ± 2*
	<b>6.6</b>	1150 ± 12*	1123 ± 58*	547 ± 1*
	<b>6.7</b>	986 ± 150*	1106 ± 166*	790 ± 11*

Structure	Cmpd	PAO1 Accum.	PA14 Accum.	PA1280 Accum.
	<b>6.8 (31)</b>	741 ± 45*	595 ± 16*	642 ± 52*
	<b>6.9</b>	724 ± 41*	1507 ± 113*	627 ± 45*
	<b>6.10</b>	616 ± 47*	1643 ± 39*	753 ± 35*
	<b>6.11</b>	529 ± 37*	401 ± 10*	180 ± 20
	<b>6.12</b>	406 ± 8*	1067 ± 7*	402 ± 31*
	<b>6.13</b>	388 ± 6*	538 ± 12*	234 ± 25
	<b>6.14 (9)</b>	332 ± 10*	1243 ± 82*	573 ± 37*
	<b>6.15</b>	287 ± 2	767 ± 51*	425 ± 14*
	<b>6.16 (53)</b>	287 ± 17	176 ± 2	166 ± 2

Structure	Cmpd	PAO1 Accum.	PA14 Accum.	PA1280 Accum.
	6.17	242 ± 5	79 ± 2	123 ± 3
	6.18	241 ± 25	708 ± 46*	235 ± 16
	6.19	232 ± 4	267 ± 26	177 ± 2
	6.20	225 ± 7	67 ± 2	71 ± 2
	6.21 (67)	218 ± 3	133 ± 7	117 ± 11
	6.22	135 ± 3	86 ± 2	98 ± 10
	6.23	99 ± 3	39 ± 1	66 ± 3
	6.24	81 ± 3	53 ± 1	38 ± 1
	6.25	74 ± 4	33 ± 1	70 ± 9

Structure	Cmpd	PAO1 Accum.	PA14 Accum.	PA1280 Accum.
	6.26	55 ± 0	51 ± 1	25 ± 0
	6.27	39 ± 6	18 ± 0	36 ± 2

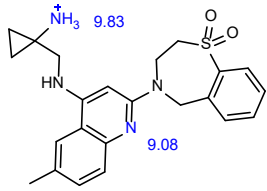
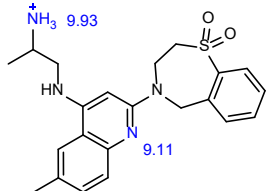
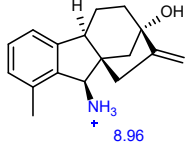
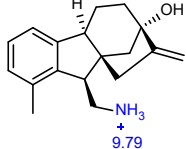
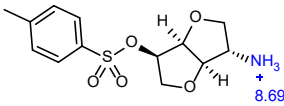
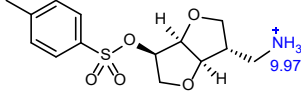
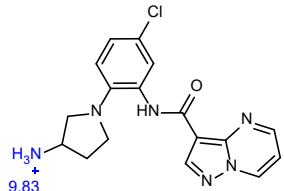


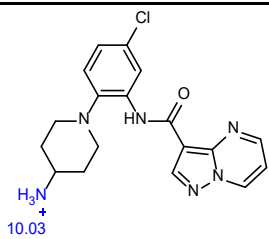
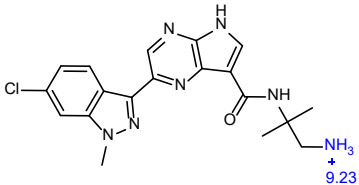
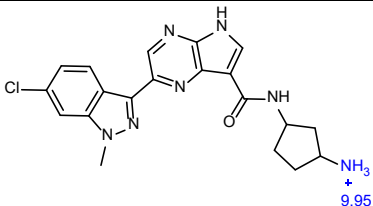
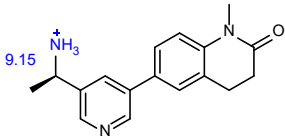
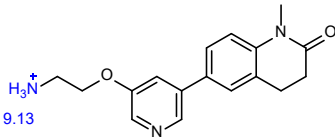
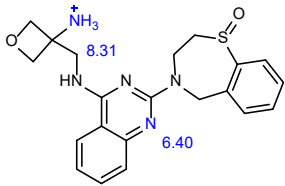
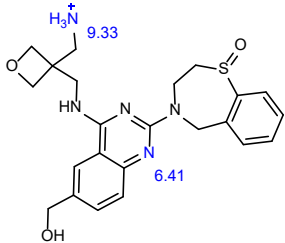
**Table S7:** MICs of fusidic acid and FA prodrug against 75 clinical isolates of *P. aeruginosa*. MICs were performed according to CLSI guidelines. All compounds were tested in biological triplicate.

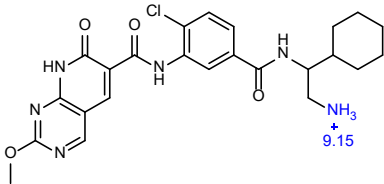
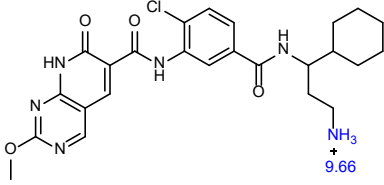
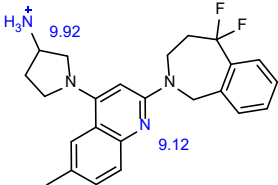
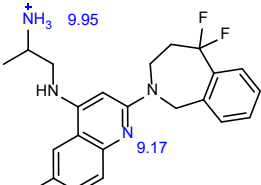
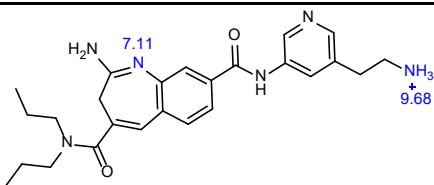
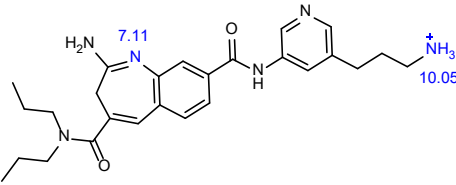
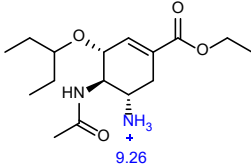
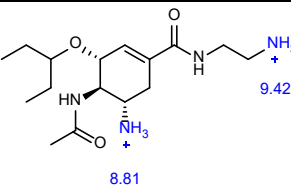
Bacterial strain	MIC (µg/mL)	
	Fusidic acid	FA prodrug
<b>Reference strains</b>		
PAO1	1024	4
PA14	>1024	8
<b>AR Bank Isolate #</b>		
0054	>1024	16
0064	>1024	16
0090	>1024	16
0092	>1024	16
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0229	>1024	16
0230	>1024	16
0231	>1024	8
0232	>1024	16
0233	>1024	16
0234	1024	8
0235	>1024	8
0236	>1024	16
0237	>1024	16
0239	>1024	8
0240	>1024	16
0241	>1024	16
0242	>1024	8
0243	>1024	16
0244	>1024	16
0245	>1024	16
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0252	>1024	16
0254	>1024	32
0265	>1024	16
0763	>1024	16
0767	>1024	16
0769	>1024	16
0772	>1024	8
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1001	>1024	16
1174	>1024	16
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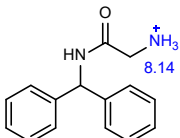
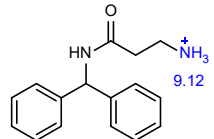
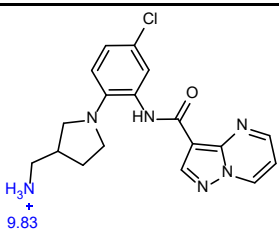
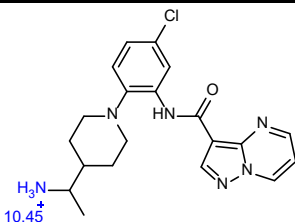
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2243	>1024	16
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CI-03	1024	8
CI-04	>1024	16
CI-05	>1024	8
CI-06	>1024	8
CI-07	>1024	8
CI-08	>1024	8
CI-09	>1024	8
CI-10	>1024	16
CI-11	>1024	8
CI-12	>1024	8
CI-13	>1024	16
CI-14	>1024	8
CI-15	>1024	8
CI-19	>1024	8
<b>Other strains (ref.)</b>		
1113	>1024	16
1727	>1024	8

**Table S8.** Structures, accumulation values, pKa values, and MMP series numbers for data presented in **Extended Data Fig. 3d**. Matched molecular pairs show a correlation between amine pK<sub>a</sub> and accumulation in *P. aeruginosa* PAO1. The pKa estimation was calculated using the software MoKa (v3.2.2) from Molecular Discovery suite. Accumulation units are reported in nmol/10<sup>12</sup> CFUs. All compounds were tested in biological triplicate. The average and s.e.m. are reported for accumulation values.

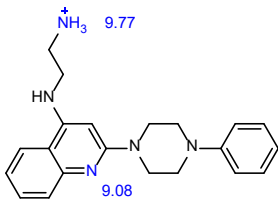
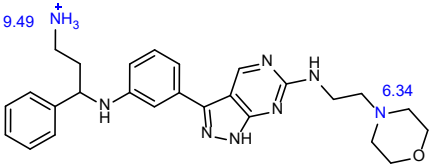
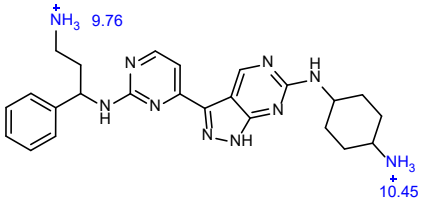
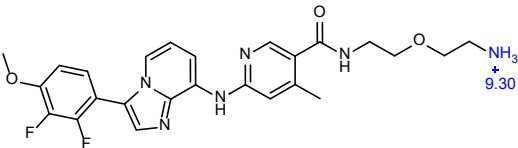
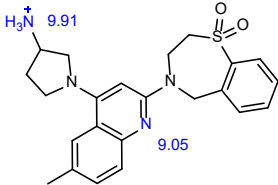
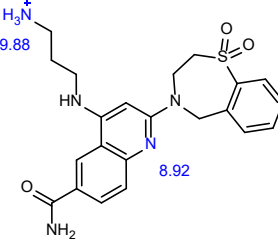
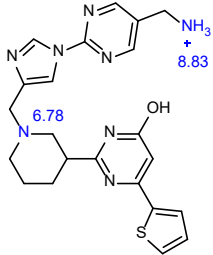
Compound Name	Structure	Accumulation (nmol/10 <sup>12</sup> CFUs)	Basic pKa	MMP series
2.45		1183	8.21	1
2.35		1420	9.03	1
2.148		320	9.34	2
2.65		943	10.16	2
2.194		163	7.53	3
2.153		301	9.33	3
2.133		406	8.91	4

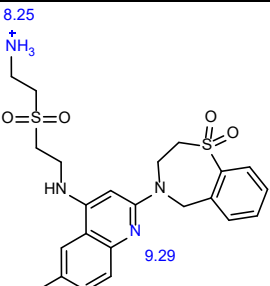
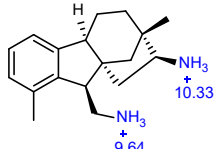
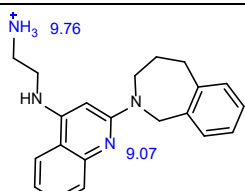
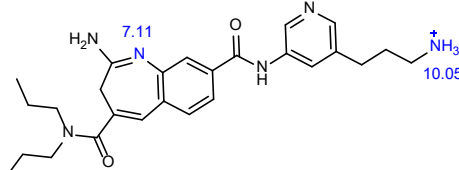
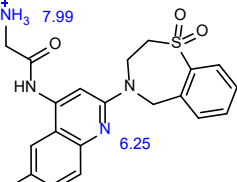
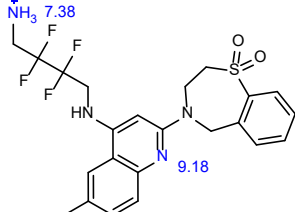
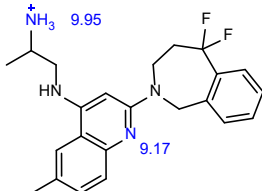
2.91		700	9.77	4
2.87		743	8.73	5
2.77		823	9.84	5
2.225		72	8.75	6
2.196		158	9.16	6
2.137		388	6.88	7
2.37		1370	8.86	7

2.119		491	9	8
2.69		861	10.01	8
2.22		1783	8.74	9
2.14		2017	9.03	9
2.27		1740	9.34	10
2.11		2333	9.81	10
2.180		218	7.28	11
2.114		505	8.45	11

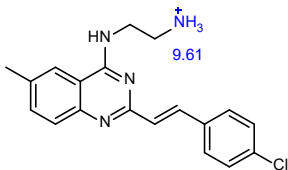
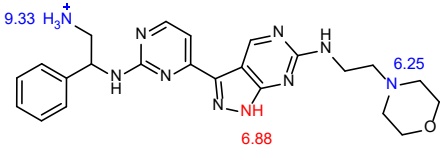
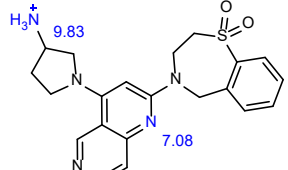
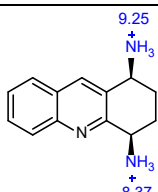
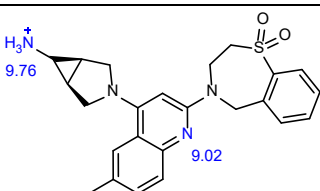
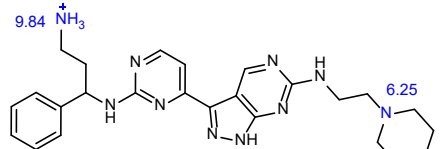
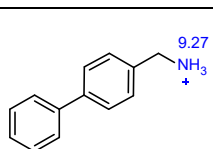
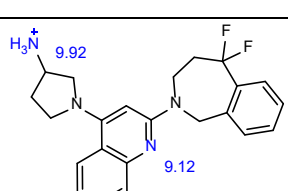
<b>2.107</b>		<b>572</b>	<b>7.45</b>	<b>12</b>
<b>2.93</b>		<b>670</b>	<b>8.91</b>	<b>12</b>
<b>2.90</b>		<b>724</b>	<b>9.84</b>	<b>13</b>
<b>2.64</b>		<b>946</b>	<b>10.25</b>	<b>13</b>

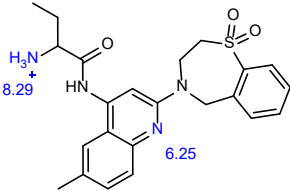
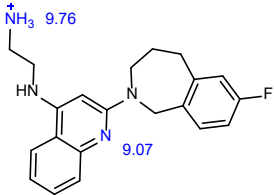
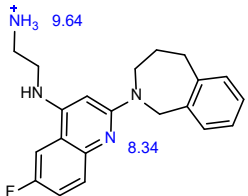
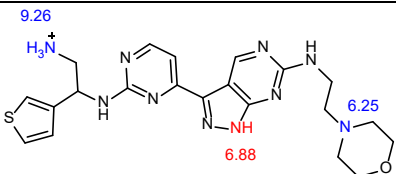
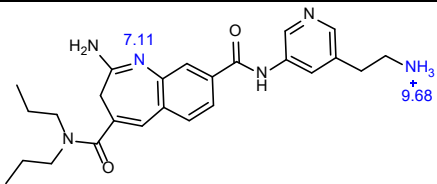
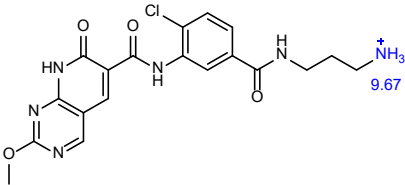
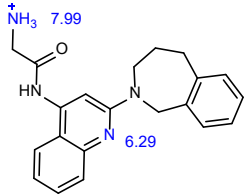
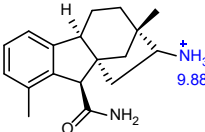
## Compound Master Table

Structure	SI table numbers	Figures the compound appears in	Prior ID, references, and characterization	Commercial source
	<b>2.1</b> <b>(60)</b>	Figs. 2a, 2b ED Fig. 3a, 3e	Roche compound (ID: <b>EC-06678</b> )	n/a
	<b>2.2</b>	Figs. 2a, 2b ED Fig. 3e	Roche compound (ID: <b>EC-15031</b> )	n/a
	<b>2.3, 6.1</b> <b>(72)</b>	Figs. 2a, 2b ED Figs. 3e, 6b, 6g	Roche compound (ID: <b>EC-03603</b> )	n/a
	<b>2.4, 4.19</b> <b>(39)</b>	Figs. 2a, 2b, 3 ED Fig. 3e, 5b, 5d	Roche compound (ID: <b>EC-14093</b> )	n/a
	<b>2.5, 4.21</b> <b>(41)</b>	Figs. 2a, 2b, 3 ED Fig. 3e, 5b, 5d	Roche compound (ID: <b>EC-11907</b> )	n/a
	<b>2.6</b>	Figs. 2a, 2b ED Fig. 3e	Roche compound (ID: <b>EC-14290</b> )	n/a
	<b>2.7</b>	Figs. 2a, 2b ED Fig. 3e	<b>11a<sup>7</sup></b>	n/a

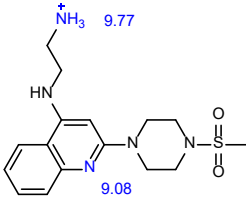
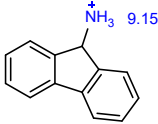
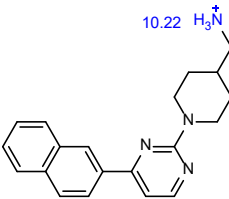
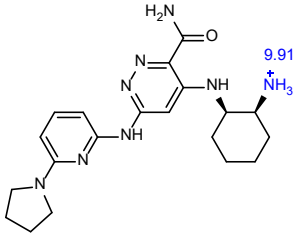
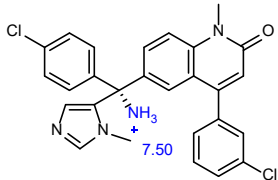
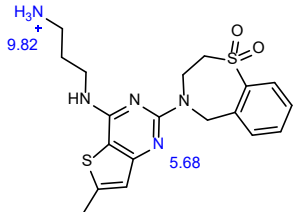
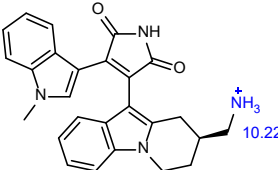
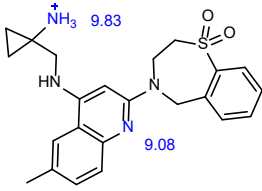
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	2.8, 4.20 (40)	Figs. 2a, 2b, 3 ED Figs. 2a, 3e, 5b, 5d	Roche compound (ID: <b>EC-13033</b> )	n/a
	1.10, 2.9 (66, 70)	Figs. 1e, 2b, 2b ED Fig. 3e, 6a, 6b	<b>4-8</b> (2-4, 3-14) <sup>5</sup>	n/a
	2.10	Figs. 2a, 2b ED Fig. 3e	Roche compound (ID: <b>EC-05140</b> )	n/a
	2.11	Figs. 2a, 2b ED Figs. 3d, 3e	Roche compound (ID: <b>EC-02332</b> )	n/a
	2.12	Figs. 2a, 2b ED Fig. 3e	Roche compound (ID: <b>EC-17520</b> )	n/a
	2.13	Figs. 2a, 2b ED Figs. 2a, 3e	Roche compound (ID: <b>EC-10214</b> )	n/a
	2.14	Figs. 2a, 2b ED Figs. 3d, 3e	Roche compound (ID: <b>EC-19785</b> )	n/a

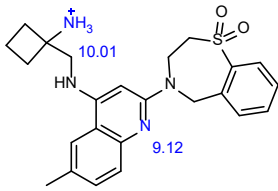
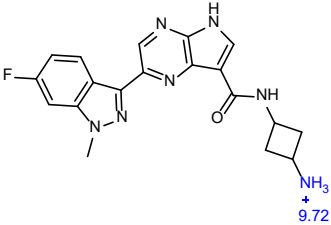
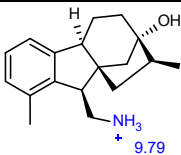
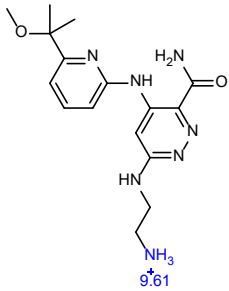
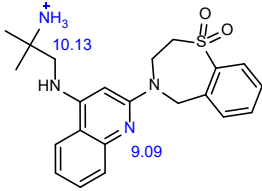
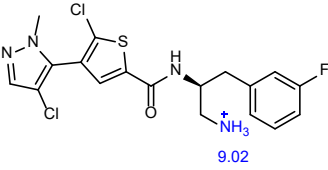
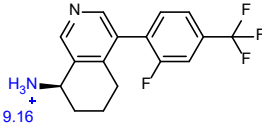


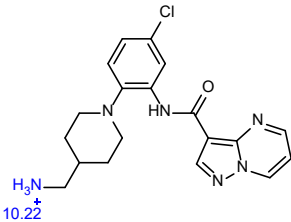
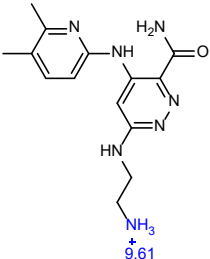
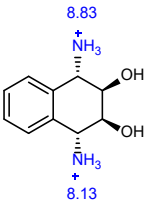
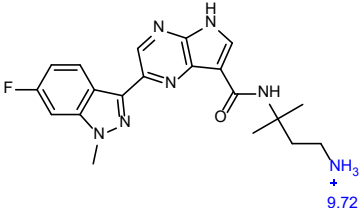
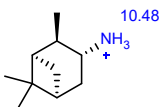
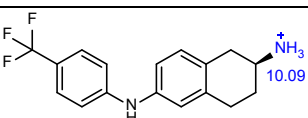
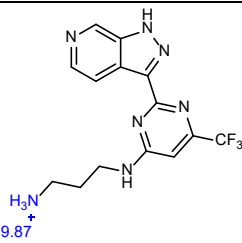
Structure	SI table numbers	Figures the compound appears in	Prior ID, references, and characterization	Commercial source
	<b>2.15, 5.13A (4)</b>	Figs. 1d, 2a, 2b ED Figs. 3e, 6d	<b>31<sup>6</sup></b>	n/a
	<b>2.16</b>	Figs. 2a, 2b ED Fig. 3e	Roche compound (ID: <b>EC-13448</b> )	n/a
	<b>2.17</b>	Figs. 2a, 2b ED Fig. 3e	Roche compound (ID: <b>EC-14206</b> )	n/a
	<b>2.18 (69)</b>	Figs. 2a, 2b ED Figs. 3e, 6b	<b>8g<sup>8</sup></b>	n/a
	<b>2.19</b>	Figs. 2a, 2b ED Fig. 3e	Roche compound (ID: <b>EC-05482</b> )	n/a
	<b>2.20 (76)</b>	Figs. 2a, 2b ED Figs. 3e, 6c	Roche compound (ID: <b>EC-11340</b> )	n/a
	<b>1.54, 2.21, 4.3, 5.9A, 6.2 (23)</b>	Figs. 1e, 2a, 2b, 3 ED Figs. 2a, 3e, 5b, 5d, 6d, 6g	<b>4-18<sup>5</sup></b>	4-Phenylbenzylamine; Sigma Aldrich (552313)
	<b>2.22</b>	Figs. 2a, 2b ED Figs. 3d, 3e	Roche compound (ID: <b>EC-11344</b> )	n/a

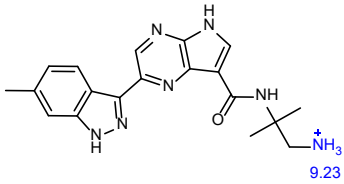
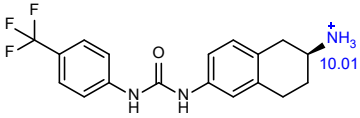
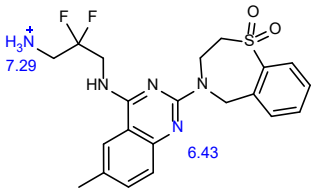
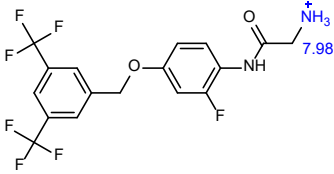
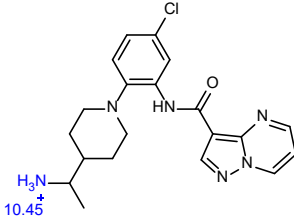
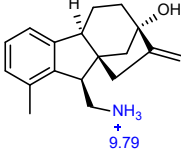
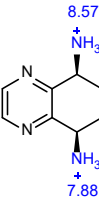
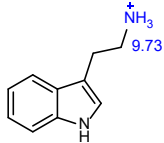
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	2.24	Figs. 2a, 2b ED Fig. 3e	Roche compound (ID: <b>EC-17799</b> )	n/a
	2.25, 6.3	Figs. 2a, 2b ED Figs. 3e, 6g	Roche compound (ID: <b>EC-19772</b> )	n/a
	2.26	Figs. 2a, 2b ED Fig. 3e	Roche compound (ID: <b>EC-18820</b> )	n/a
	2.27, 6.4	Figs. 2a, 2b ED Figs. 3d, 3e, 6g	Roche compound (ID: <b>EC-06151</b> )	n/a
	2.28	Figs. 2a, 2b ED Figs. 2a, 3e	Roche compound (ID: <b>EC-08777</b> )	n/a
	2.29	Figs. 2a, 2b ED Fig. 3e	Roche compound (ID: <b>EC-16593</b> )	n/a
	2.30 (12)	Figs. 2a, 2b, 2c ED Figs. 2a, 3e	Reported here	n/a

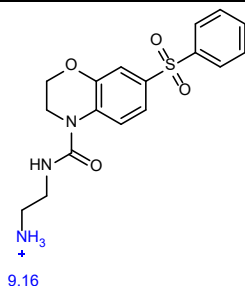
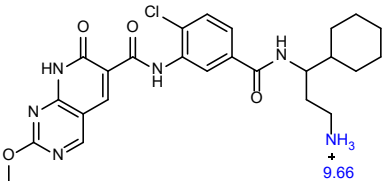
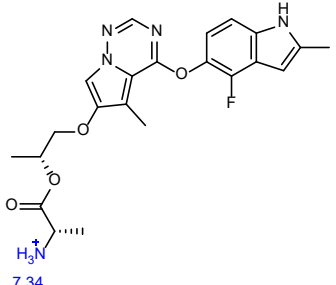
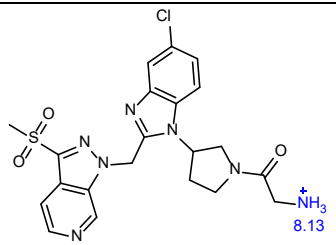
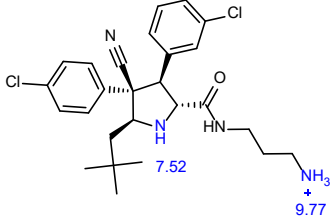
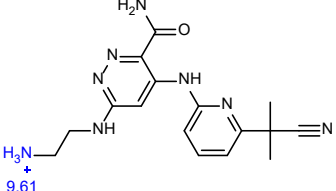
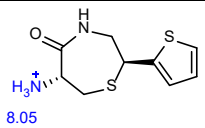
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	2.31	Figs. 2a, 2b ED Fig. 3e	Roche compound (ID: <b>EC-15438</b> )	n/a
	2.32	Figs. 2a, 2b ED Figs. 2a, 3e	Roche compound (ID: <b>EC-03002</b> )	n/a
	2.33	Figs. 2a, 2b ED Fig. 3e	Roche compound (ID: <b>EC-20291</b> )	n/a
	2.34 (20)	Figs. 2a, 2b, 2e ED Figs. 2a, 3e	Roche compound (ID: <b>EC-04375</b> )	n/a
	2.35	Figs. 2a, 2b ED Figs. 3d, 3e	Roche compound (ID: <b>EC-19376</b> )	n/a
	1.36, 2.36, 4.2, 6.5 (22, 71)	Figs. 1e, 2a, 2b, 3 ED Figs. 3e, 5b, 5d, 6b, 6g	<b>4-6-a<sup>5</sup></b>	n/a
	2.37	Figs. 2a, 2b ED Figs. 3d, 3e	Roche compound (ID: <b>EC-10271</b> )	n/a

Structure	SI table numbers	Figures the compound appears in	Prior ID, references, and characterization	Commercial source
	<b>2.38 (59)</b>	Figs. 2a, 2b ED Figs. 3a, 3e	Roche compound (ID: <b>EC-14123</b> )	n/a
	<b>1.58, 2.39, 5.10A</b>	Figs. 1e, 2a, 2b ED Figs. 2a, 3e, 6d	<b>4-17<sup>5</sup></b>	9-Aminofluorene; Sigma Aldrich (A55608)
	<b>1.66, 2.40</b>	Figs. 1e, 2a, 2b ED Fig. 2a	<b>4-53<sup>5</sup></b>	WAY-262611; Cayman Chemicals (17704)
	<b>2.41</b>	Figs. 2a, 2b ED Fig. 3e	Roche compound (ID: <b>EC-19141</b> )	n/a
	<b>2.42</b>	Figs. 2a, 2b ED Fig. 3e	n/a	Tipifarnib; Sigma Aldrich (SML1668)
	<b>2.43</b>	Figs. 2a, 2b ED Fig. 3e	Roche compound (ID: <b>EC-12609</b> )	n/a
	<b>1.67, 2.44, 4.6 (26, 55)</b>	Figs. 1e, 2a, 2b, 3 ED Figs. 1, 2a, 2c, 5a, 5b, 5d	<b>4-58<sup>5</sup></b>	Bisindolylmaleimide X; Cayman Chemicals (17511)
	<b>2.45, 4.23 (43)</b>	Figs. 2a, 2b, 3 ED Figs. 3d, 3e, 5b, 5d	Roche compound (ID: <b>EC-19264</b> )	n/a

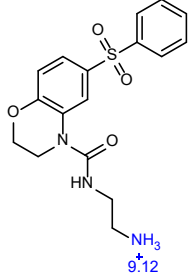
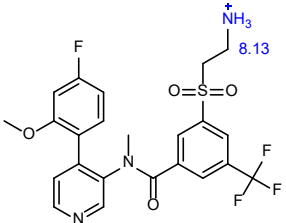
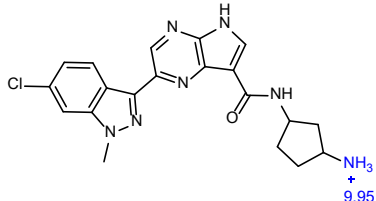
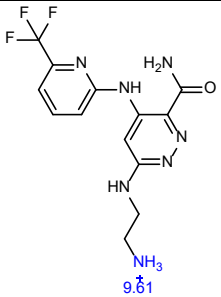
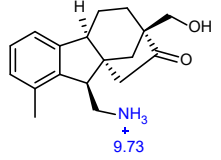
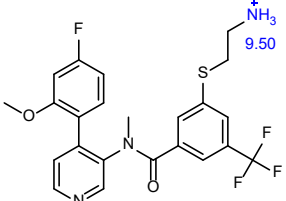
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	2.46	Figs. 2a, 2b ED Fig. 3e	Roche compound (ID: <b>EC-19228</b> )	n/a
	2.47	Figs. 2a, 2b ED Figs. 2a, 3e	Roche compound (ID: <b>EC-09780</b> )	n/a
	1.12, 2.48	Figs. 1e, 2a, 2b ED Figs. 2a, 3e	4-4 <sup>5</sup>	n/a
	2.49, 6.6	Figs. 2a, 2b ED Figs. 2a, 3e, 6g	Roche compound (ID: <b>EC-03341</b> )	n/a
	2.50	Figs. 2a, 2b ED Fig. 3e	Roche compound (ID: <b>EC-20264</b> )	n/a
	2.51	Figs. 2a, 2b ED Figs. 2a, 3e	n/a	Afuresertib; MedChemExpress (HY-15727)
	2.52	Figs. 2a, 2b ED Figs. 2a, 3e	Roche compound (ID: <b>EC-01414</b> )	n/a

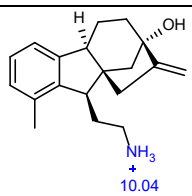
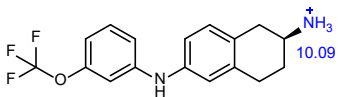
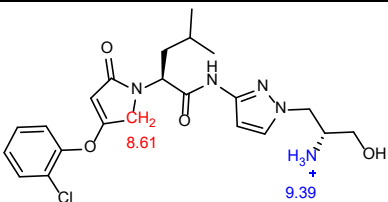
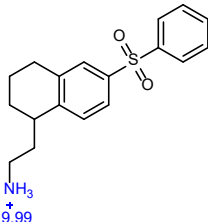
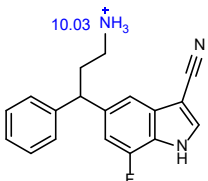
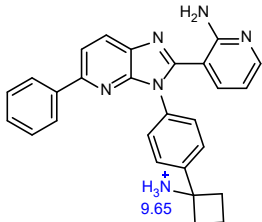
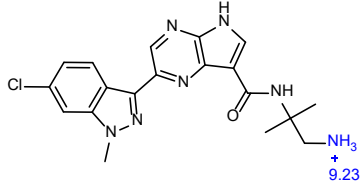
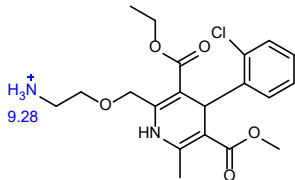
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	2.54	Figs. 2a, 2b ED Fig. 3e	Roche compound (ID: <b>EC-07576</b> )	n/a
	2.55	Figs. 2a, 2b ED Fig. 3e	<b>9a<sup>9</sup></b>	n/a
	2.56	Figs. 2a, 2b ED Figs. 2a, 3e	Roche compound (ID: <b>EC-17614</b> )	n/a
	1.51, 2.57, 5.7A (77A)	Figs. 1e, 2a, 2b ED Figs. 2a, 3e, 6d, 6e	<b>4-12<sup>5</sup></b>	(1R, 2R, 3R, 5S)-(-)- isopinocampheylamine; Sigma Aldrich (391654)
	2.58	Figs. 2a, 2b ED Figs. 2a, 3e	Roche compound (ID: <b>EC-19529</b> )	n/a
	2.59, 5.11A (78A)	Figs. 2a, 2b ED Figs. 3e, 6d, 6e	<b>S4<sup>6</sup></b>	n/a

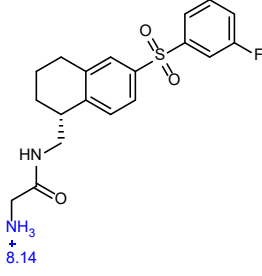
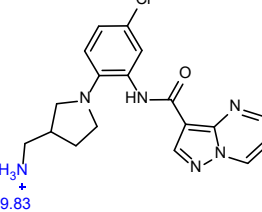
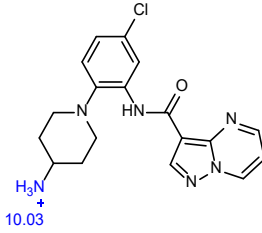
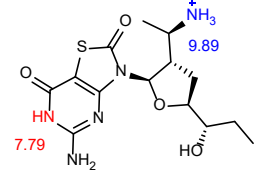
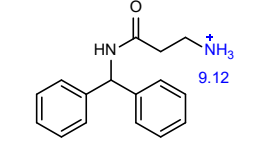
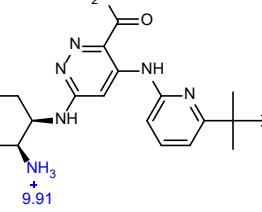
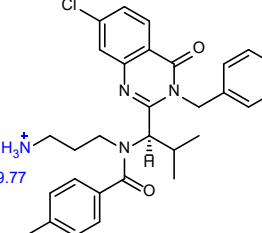
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	2.61, 6.7	Figs. 2a, 2b ED Figs. 2a, 3e, 6g	Roche compound (ID: <b>EC-08219</b> )	n/a
	2.62	Figs. 2a, 2b ED Figs. 2a, 3e	Roche compound (ID: <b>EC-09507</b> )	n/a
	2.63, 4.26 (46)	Figs. 2a, 2b, 3 ED Figs. 2a, 3e, 5b, 5d	Roche compound (ID: <b>EC-09549</b> )	n/a
	2.64	Figs. 2a, 2b ED Figs. 2a, 3d, 3e	Roche compound (ID: <b>EC-07247</b> )	n/a
	1.8, 2.65 (58)	Figs. 1e, 2a, 2b ED Figs. 2a, 3a, 3d, 3e	<b>4-7</b> <sup>5</sup>	n/a
	2.66	Figs. 2a, 2b ED Fig. 3e	<b>8f</b> <sup>8</sup>	n/a
	2.67	Figs. 2a, 2b ED Figs. 2a, 3e	<b>19A</b> <sup>6</sup>	n/a

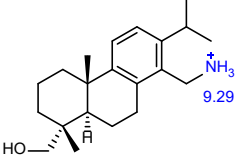
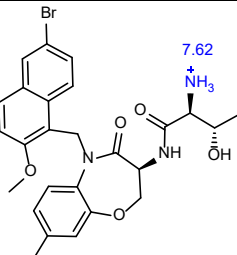
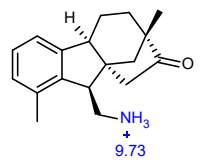
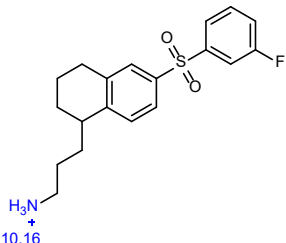
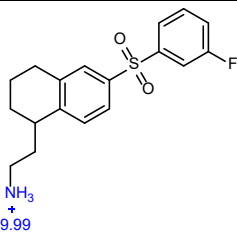
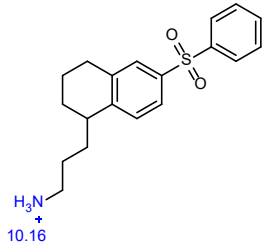
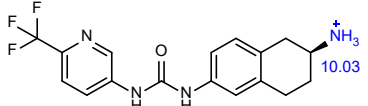
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	2.69	Figs. 2a, 2b ED Figs. 2a, 3d, 3e	Roche compound (ID: <b>EC-20792</b> )	n/a
	2.70	Figs. 2a, 2b ED Fig. 2a	n/a	Brivanib alaninate; Cayman Chemicals (23690)
	2.71, 4.27 (47)	Figs. 2a, 2b, 3 ED Figs. 2a, 3e, 5b, 5d	Roche compound (ID: <b>EC-12371</b> )	n/a
	2.72	Figs. 2a, 2b ED Fig. 3e	Roche compound (ID: <b>EC-01187</b> )	n/a
	2.73 (14)	Figs. 2a, 2b, 2d ED Figs. 2a, 3e	Roche compound (ID: <b>EC-12921</b> )	n/a
	2.74, 4.18 (38)	Figs. 2a, 2b, 3 ED Figs. 2a, 3e, 5b, 5d	n/a	(2S,6R)-6-Amino-2-(2-thienyl)-1,4-thiazepan-5-one; AK Scientific (R766)

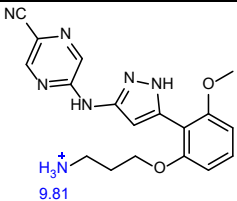
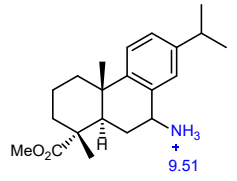
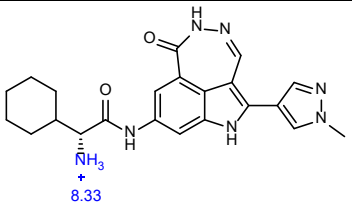
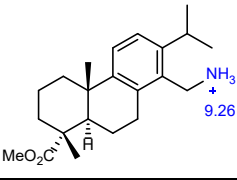
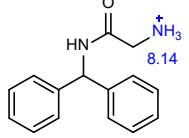
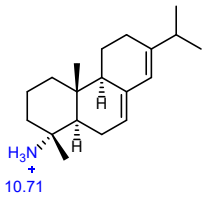
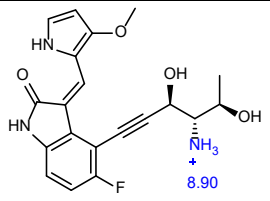
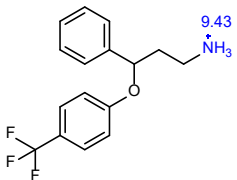


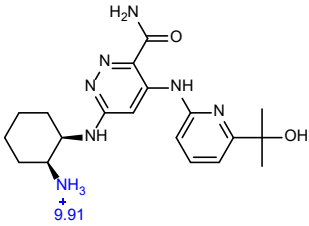
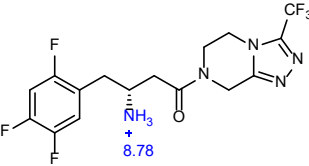
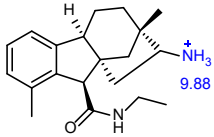
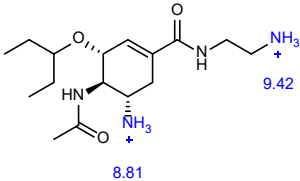
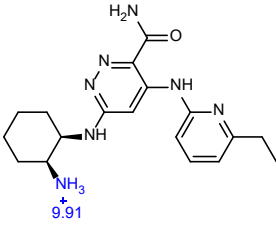
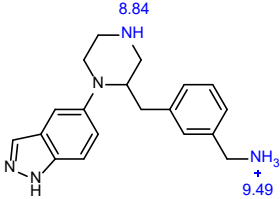
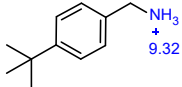
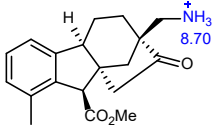
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	2.76	Figs. 2a, 2b ED Fig. 2a	Roche compound (ID: <b>EC-19776</b> )	n/a
	2.77	Figs. 2a, 2b ED Figs. 2a, 3d, 3e	Roche compound (ID: <b>EC-18790</b> )	n/a
	2.78	Figs. 2a, 2b ED Figs. 2a, 3e	Roche compound (ID: <b>EC-13937</b> )	n/a
	1.6, 2.79, 4.1 (21)	Figs. 1e, 2a, 2b, 3 ED Figs. 2a, 3e, 5b, 5d	<b>4-6<sup>5</sup></b>	n/a
	2.80, 4.22 (42)	Figs. 2a, 2b, 3 ED Figs. 3e, 5b, 5d	Roche compound (ID: <b>EC-03534</b> )	n/a

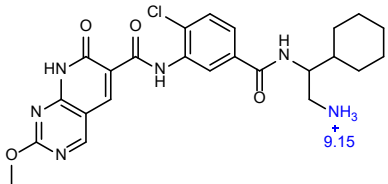
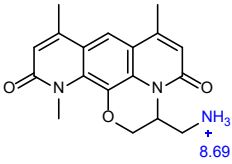
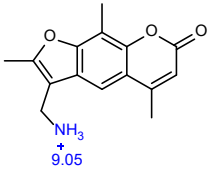
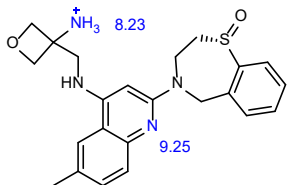
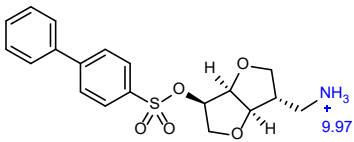
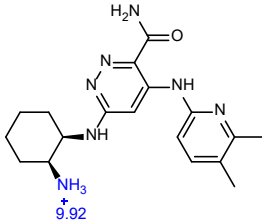
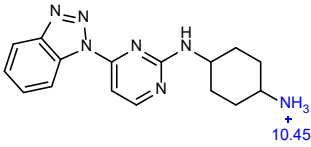
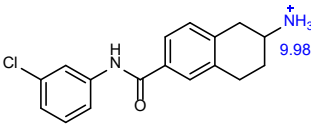
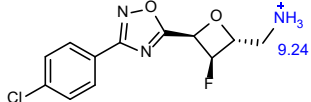
Structure	SI table numbers	Figures the compound appears in	Prior ID, references, and characterization	Commercial source
	1.9, 2.81	Figs. 1e, 2a, 2b ED Figs. 2a, 3e	4-3 <sup>5</sup>	n/a
	2.82 (16)	Figs. 2a, 2b, 2d ED Figs. 2a, 3e	Roche compound (ID: EC-10749)	n/a
	2.83, 4.24 (44)	Figs. 2a, 2b, 3 ED Fig. 2a, 5b, 5d	Roche compound (ID: EC-03757)	n/a
	2.84	Figs. 2a, 2b ED Figs. 2a, 3e	Roche compound (ID: EC-02818)	n/a
	2.85 (10)	Figs. 2a, 2b, 2c ED Fig. 3e	Roche compound (ID: EC-01328)	n/a
	2.86	Figs. 2a, 2b ED Fig. 3e	n/a	ARQ-092; Cayman Chemicals (21388)
	2.87	Figs. 2a, 2b ED Figs. 2a, 3d, 3e	Roche compound (ID: EC-19380)	n/a
	2.88, 4.11, 6.8 (31)	Figs. 2a, 2b, 3 ED Figs. 2a, 3e, 5b, 5d, 6g	n/a	Amlodipine; Sigma Aldrich (AMBH2D6FD9FC)

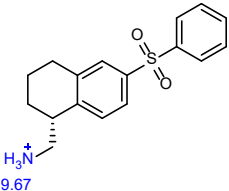
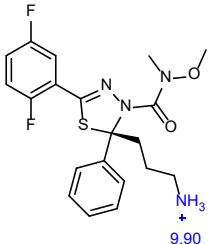
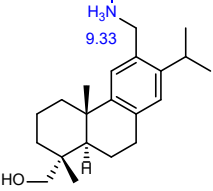
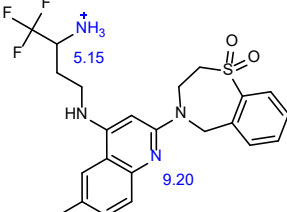
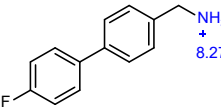
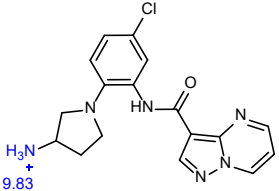
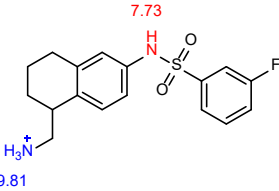
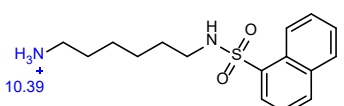
Structure	SI table numbers	Figures the compound appears in	Prior ID, references, and characterization	Commercial source
	2.89, 4.25 (45)	Figs. 2a, 2b, 3 ED Figs. 2a, 3e, 5b, 5d	Roche compound (ID: <b>EC-05491</b> )	n/a
	2.90, 6.9	Figs. 2a, 2b ED Figs. 2a, 3d, 3e, 6g	Roche compound (ID: <b>EC-20297</b> )	n/a
	2.91	Figs. 2a, 2b ED Figs. 2a, 3d, 3e	Roche compound (ID: <b>EC-04155</b> )	n/a
	2.92	Figs. 2a, 2b ED Figs. 2a, 3e	Roche compound (ID: <b>EC-15674</b> )	n/a
	2.93	Figs. 2a, 2b ED Figs. 2a, 3d, 3e	<b>6A</b> <sup>6</sup>	n/a
	2.94 (13)	Figs. 2a, 2b, 2d ED Figs. 2a, 3e	Roche compound (ID: <b>EC-18814</b> )	n/a
	2.95, 4.14 (34, 56)	Figs. 2a, 2b, 3 ED Figs. 2a, 2c, 5b, 5d	n/a	Ispinesib; Cayman Chemicals (18014)

Structure	SI table numbers	Figures the compound appears in	Prior ID, references, and characterization	Commercial source
	2.96	Figs. 2a, 2b ED Figs. 2a, 3e	1A <sup>6</sup>	n/a
	2.97	Figs. 2a, 2b ED Fig. 2a	Roche compound (ID: EC-02669)	n/a
	1.5, 2.98 (65)	Figs. 1e, 2a, 2b ED Figs. 2a, 3e, 5b, 5d, 6a	4-3-a <sup>5</sup>	n/a
	2.99	Figs. 2a, 2b ED Figs. 2a, 3e	Roche compound (ID: EC-03312)	n/a
	2.100, 6.10	Figs. 2a, 2b ED Figs. 2a, 3e, 6g	Roche compound (ID: EC-06713)	n/a
	2.101	Figs. 2a, 2b ED Figs. 2a, 3e	Roche compound (ID: EC-03922)	n/a
	2.102	Figs. 2a, 2b ED Figs. 2a, 3e	Roche compound (ID: EC-20408)	n/a

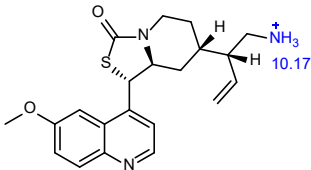
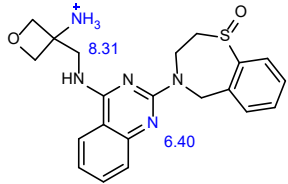
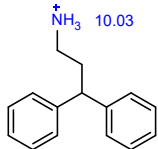
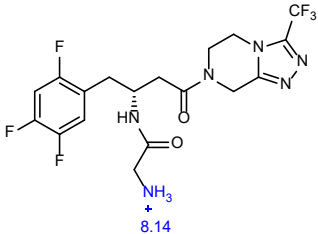
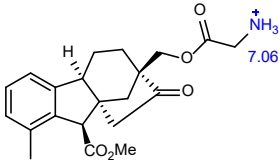
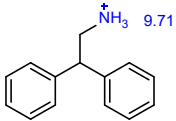
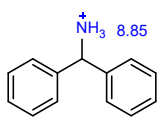
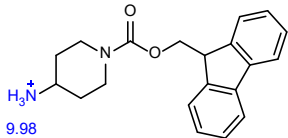
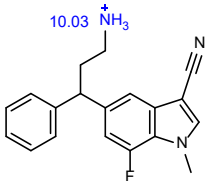
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	2.103	Figs. 2a, 2b ED Figs. 2a, 3e	n/a	LY2606368; Cayman Chemicals (21490)
	1.37, 2.104 (8)	Figs. 1d, 1e, 2a, 2b ED Figs. 2a, 3e	4-25 <sup>5</sup>	n/a
	2.105	Figs. 2a, 2b ED Fig. 3e	n/a	PF-477736; Cayman Chemicals (17859)
	2.106	Figs. 2a, 2b ED Figs. 2a, 3e	Reported here	n/a
	2.107	Figs. 2a, 2b ED Figs. 2a, 3d, 3e	12A <sup>6</sup>	n/a
	1.38, 2.108	Figs. 2a, 2b	4-55 <sup>5</sup>	n/a
	2.109	Figs. 2a, 2b ED Fig. 3e	Roche compound (ID: EC-12183)	n/a
	2.110 (18)	Figs. 2a, 2b, 2e ED Figs. 2a, 3e	n/a	Norfluoxetine; Cayman Chemicals (15900)

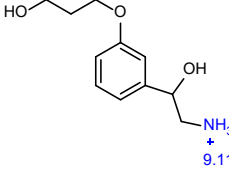
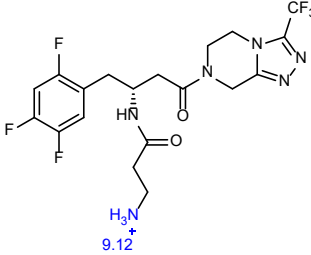
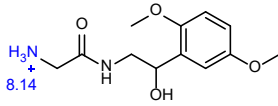
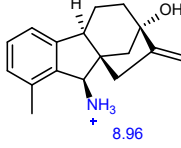
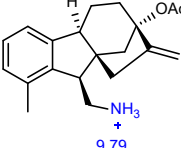
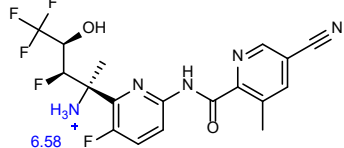
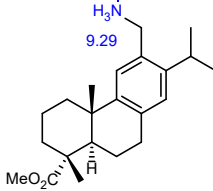
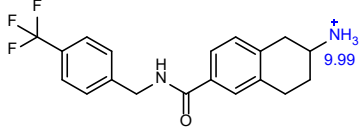
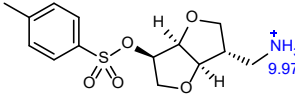
Structure	SI table numbers	Figures the compound appears in	Prior ID, references, and characterization	Commercial source
	2.111, 6.11	Figs. 2a, 2b ED Figs. 2a, 3e, 6g	Roche compound (ID: <b>EC-06640</b> )	n/a
	1.62, 2.112, 4.5 (25)	Figs. 1e, 2a, 2b, 3 ED Figs. 2a, 3e, 5b, 5d	<b>4-36</b> <sup>5</sup>	Sitagliptin; AK Scientific (J96214)
	2.113 (11)	Figs. 2a, 2b, 2c ED Fig. 2a	Reported here	n/a
	1.2, 2.114 (68)	Figs. 1e, 2a, 2b ED Figs. 3d, 3e, 6a	<b>4-28-a</b> <sup>5</sup>	n/a
	2.115	Figs. 2a, 2b ED Fig. 3e	Roche compound (ID: <b>EC-12745</b> )	n/a
	2.116 (75)	Figs. 2a, 2b ED Figs. 3e, 6c	Roche compound (ID: <b>EC-10065</b> )	n/a
	1.55, 2.117	Figs. 1e, 2a, 2b ED Figs. 2a, 3e	<b>4-15</b> <sup>5</sup>	4- <i>tert</i> -butylbenzylamine; AK Scientific (J52905)
	2.118	Figs. 2a, 2b ED Figs. 2a, 3e	Reported here	n/a

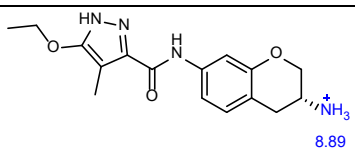
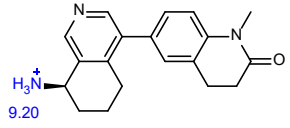
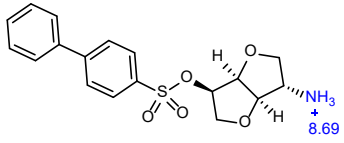
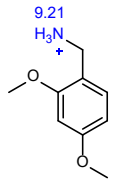
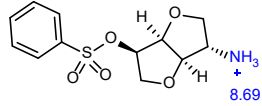
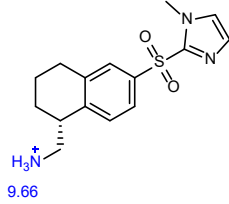
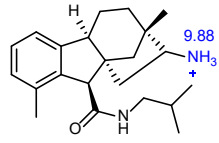
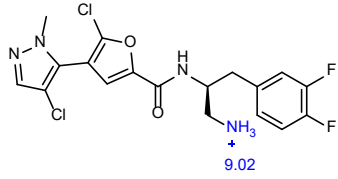
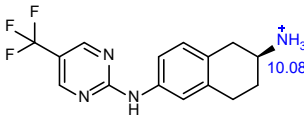
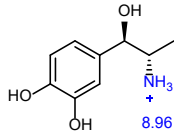
Structure	SI table numbers	Figures the compound appears in	Prior ID, references, and characterization	Commercial source
	2.119	Figs. 2a, 2b ED Figs. 2a, 3d, 3e	Roche compound (ID: <b>EC-15047</b> )	n/a
	2.120	Figs. 2a, 2b ED Figs. 2a, 3e	<b>6-DNM-NH3<sup>5</sup></b>	n/a
	1.59, 2.121	Figs. 1e, 2a, 2b ED Figs. 2a, 3e	<b>4-11<sup>5</sup></b>	4'-Aminomethyl-4,5',8-trimethylpsoralen; Cayman Chemicals (17162)
	2.122	Figs. 2a, 2b ED Fig. 3e	Roche compound (ID: <b>EC-01813</b> )	n/a
	2.123, 4.10 (30)	Figs. 2a, 2b, 3 ED Figs. 2a, 3e, 5b, 5d	Reported here	n/a
	2.124	Figs. 2a, 2b ED Fig. 3e	Roche compound (ID: <b>EC-17219</b> )	n/a
	2.125	Figs. 2a, 2b ED Figs. 2a, 3e	Roche compound (ID: <b>EC-20452</b> )	n/a
	2.126	Figs. 2a, 2b ED Figs. 2a, 3e	Roche compound (ID: <b>EC-17621</b> )	n/a
	2.127	Figs. 2a, 2b ED Figs. 2a, 3e	Roche compound (ID: <b>EC-10018</b> )	n/a

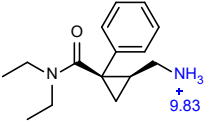
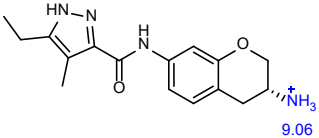
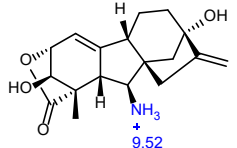
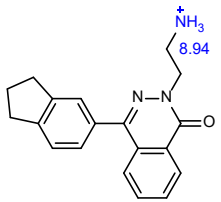
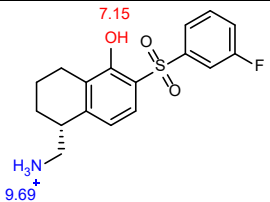
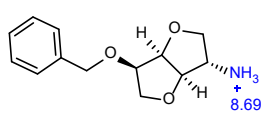
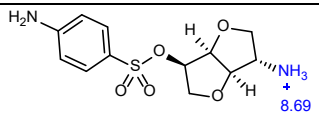
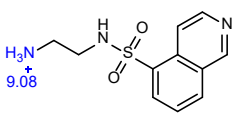
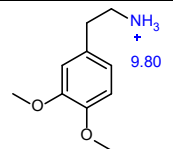
Structure	SI table numbers	Figures the compound appears in	Prior ID, references, and characterization	Commercial source
	2.128	Figs. 2a, 2b ED Figs. 2a, 3e	Roche compound (ID: <b>EC-10000</b> )	n/a
	2.129, 4.12 (32)	Figs. 2a, 2b, 3 ED Fig. 2a, 5b, 5d	n/a	ARRY-520; Cayman Chemicals (21883)
	2.130	Figs. 2a, 2b ED Fig. 2a	<b>7A</b> <sup>6</sup>	n/a
	2.131	Figs. 2a, 2b ED Fig. 2a	Roche compound (ID: <b>EC-14350</b> )	n/a
	2.132	Figs. 2a, 2b ED Figs. 2a, 3e	n/a	4'-fluoro-biphenyl-4- methanamine; Carbosynth (FF157939)
	2.133, 6.12	Figs. 2a, 2b ED Figs. 2a, 3d, 3e	Roche compound (ID: <b>EC-18826</b> )	n/a
	2.134	Figs. 2a, 2b ED Figs. 2a, 3e	Roche compound (ID: <b>EC-03822</b> )	n/a
	1.61, 2.135 (54)	Figs. 1e, 2a, 2b ED Fig. 2a, 2c	<b>4-46</b> <sup>5</sup>	W-5; Cayman Chemicals (14271)

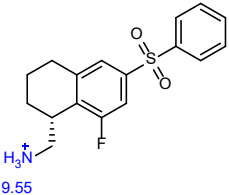
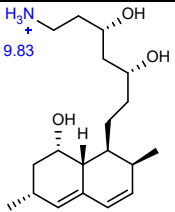
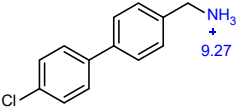
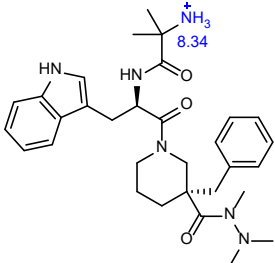
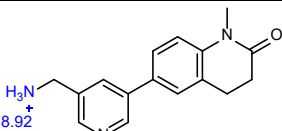
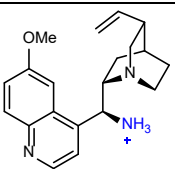
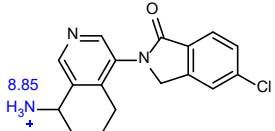
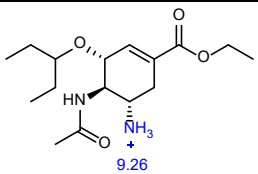
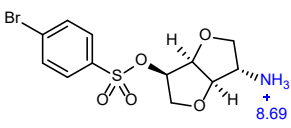


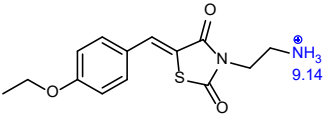
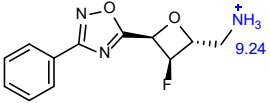
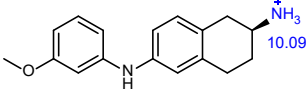
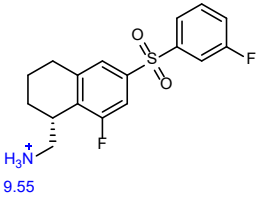
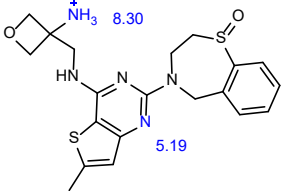
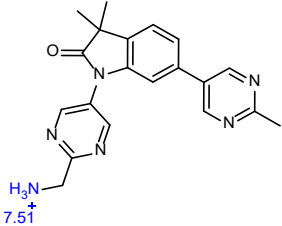
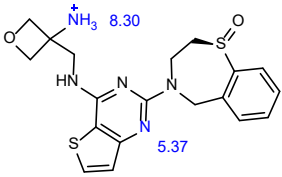
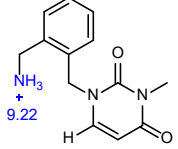
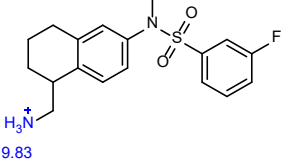
Structure	SI table numbers	Figures the compound appears in	Prior ID, references, and characterization	Commercial source
	<b>1.40, 2.136 (62)</b>	Figs. 1e, 2a, 2b ED Figs. 3b, 3e	<b>4-26<sup>5</sup></b>	n/a
	<b>2.137, 6.13</b>	Figs. 2a, 2b ED Figs. 3d, 3e, 6g	Roche compound (ID: <b>EC-08631</b> )	n/a
	<b>1.57, 2.138</b>	Figs. 2a, 2b ED Fig. 2a	<b>4-49<sup>5</sup></b>	3,3-Diphenylpropylamine; Sigma Aldrich (136298)
	<b>2.139</b>	Figs. 2a, 2b ED Fig. 2a	Made as previously reported <sup>10</sup>	n/a
	<b>2.140</b>	Figs. 2a, 2b ED Fig. 2a	Reported here	n/a
	<b>2.141</b>	Figs. 2a, 2b ED Fig. 2a	n/a	2,2-Diphenylethylamine; Sigma Aldrich (D206709)
	<b>1.56, 2.142</b>	Figs. 1e, 2a, 2b ED Figs. 2a, 3e	<b>4-27<sup>5</sup></b>	Aminodiphenylmethane; Sigma Aldrich (176885)
	<b>2.143, 4.17 (37)</b>	Figs. 2a, 2b, 3 ED Figs. 2a, 3e, 5b, 5d	n/a	1-Fmoc-4-aminopiperidine hydrochloride; AK Scientific (0040AF)
	<b>2.144, 6.14 (9)</b>	Figs. 2a, 2b, 2c ED Figs. 2a, 3e, 6g	Roche compound (ID: <b>EC-04901</b> )	n/a

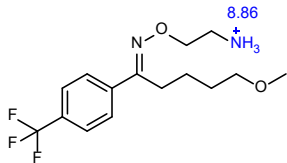
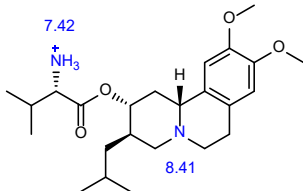
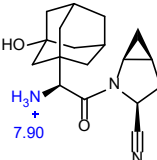
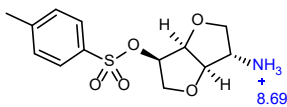
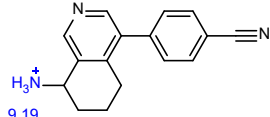
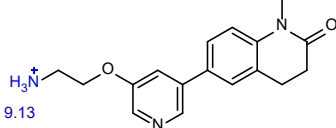
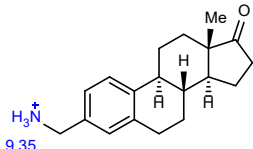
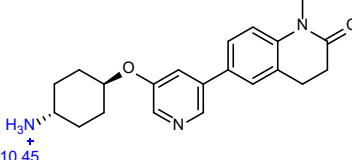
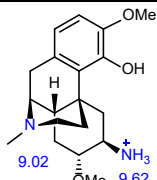
Structure	SI table numbers	Figures the compound appears in	Prior ID, references, and characterization	Commercial source
	2.145	Figs. 2a, 2b ED Figs. 2a, 3e	Reported here	n/a
	2.146	Figs. 2a, 2b ED Fig. 2a	Made as previously reported <sup>10</sup>	n/a
	2.147, 4.15 (35)	Figs. 2a, 2b, 3 ED Fig. 2a, 5b, 5d	n/a	Midodrine; Cayman Chemicals (17349)
	1.7, 2.148 (6)	Figs. 1d, 1e, 2a, 2b ED Figs. 2a, 3d	4-13 <sup>5</sup>	n/a
	1.11, 2.149 (57)	Figs. 1e, 2a, 2b ED Figs. 2a, 3a	4-9 <sup>5</sup>	n/a
	2.150	Figs. 2a, 2b	Roche compound (ID: EC-16088)	n/a
	2.151	Figs. 2a, 2b ED Figs. 2a, 3e	9A <sup>6</sup>	n/a
	2.152	Figs. 2a, 2b ED Figs. 2a, 3e	Roche compound (ID: EC-14298)	n/a
	2.153	Figs. 2a, 2b ED Figs. 2a, 3d, 3e	Reported here	n/a

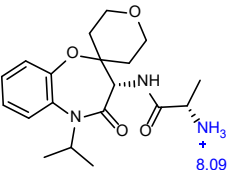
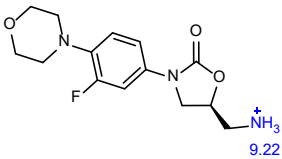
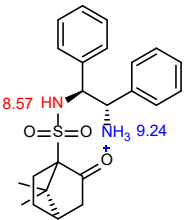
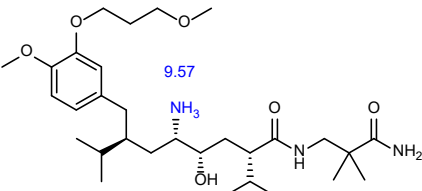
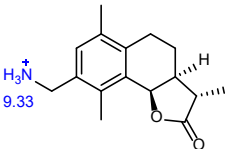
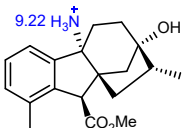
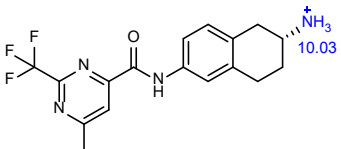
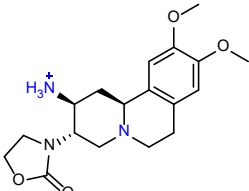
Structure	SI table numbers	Figures the compound appears in	Prior ID, references, and characterization	Commercial source
	<b>2.154, 6.15</b>	Figs. 2a, 2b ED Figs. 2a, 6g	Roche compound (ID: <b>EC-17492</b> )	n/a
	<b>2.155, 6.16 (53)</b>	Figs. 2a, 2b ED Figs. 2a, 2b, 6g	Roche compound (ID: <b>EC-03493</b> )	n/a
	<b>1.24, 2.156, 5.6A (48)</b>	Figs. 1e, 2a, 2b ED Figs. 2a, 2b, 6d	<b>4-1<sup>5</sup>; 13A<sup>6</sup></b>	n/a
	<b>1.53, 2.157</b>	Figs. 2a, 2b	<b>4-39<sup>5</sup></b>	3,4-Dimethoxybenzylamine; AK Scientific (P724)
	<b>1.27, 2.158</b>	Figs. 1e, 2a, 2b ED Fig. 2a	<b>4-19<sup>5</sup></b>	n/a
	<b>2.159</b>	Figs. 2a, 2b ED Fig. 2a	Roche compound (ID: <b>EC-00566</b> )	n/a
	<b>2.160</b>	Figs. 2a, 2b ED Fig. 2a	Reported here	n/a
	<b>2.161</b>	Figs. 2a, 2b ED Fig. 2a	n/a	Uprosertib; Cayman Chemicals (19904)
	<b>2.162</b>	Figs. 2a, 2b ED Fig. 2a	Roche compound (ID: <b>EC-04644</b> )	n/a
	<b>2.163</b>	Figs. 2a, 2b ED Fig. 2a	n/a	Levonordefrin; Cayman Chemicals (23993)

Structure	SI table numbers	Figures the compound appears in	Prior ID, references, and characterization	Commercial source
	<b>2.164, 4.16 (36)</b>	Figs. 2a, 2b, 3 ED Fig. 2a, 5b, 5d	n/a	Milnacipran; AK Scientific (G420)
	<b>2.165</b>	Figs. 2a, 2b ED Fig. 2a	Roche compound (ID: <b>EC-13961</b> )	n/a
	<b>1.13, 2.166, 6.17</b>	Figs. 1e, 2a, 2b ED Figs. 2a, 6g	<b>4-30<sup>5</sup></b>	n/a
	<b>2.167</b>	Figs. 2a, 2b ED Fig. 2a	n/a	2-(2-aminoethyl)-4-(2,3-dihydro-1H-inden-5-yl)-1,2-dihydrophthalazin-1-one; Sigma Aldrich (CAS #: 866133-39-3)
	<b>2.168, 6.18 (19)</b>	Figs. 2a, 2b, 2e ED Figs. 2a, 6g	Roche compound (ID: <b>EC-03683</b> )	n/a
	<b>1.28, 2.169, 4.4 (24)</b>	Figs. 1e, 2a, 2b, 3 ED Fig. 2a, 5b, 5d	<b>4-21<sup>5</sup></b>	n/a
	<b>1.29, 2.170</b>	Figs. 1e, 2a, 2b ED Fig. 2a	<b>4-34<sup>5</sup></b>	n/a
	<b>1.60, 2.171</b>	Figs. 1e, 2a, 2b	<b>4-31<sup>5</sup></b>	N-(2-aminoethyl)-5-isoquinolinesulfonamide; Cayman Chemicals (13312)
	<b>1.52, 2.172, 5.8A</b>	Figs. 1e, 2a, 2b ED Figs. 2a, 6d	<b>4-37<sup>5</sup></b>	3,4-Dimethoxyphenethylamine; Sigma Aldrich (D136204)

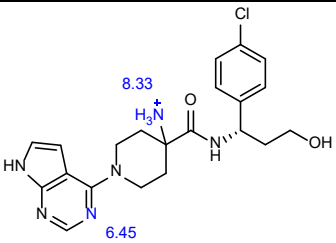
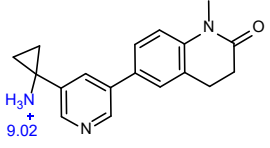
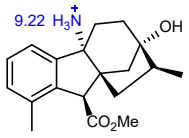
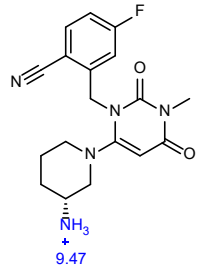
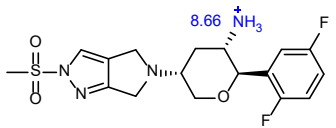
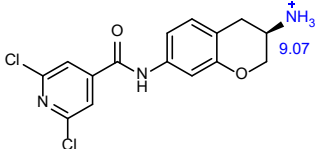
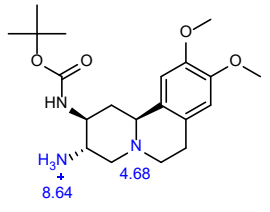
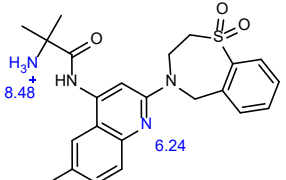
Structure	SI table numbers	Figures the compound appears in	Prior ID, references, and characterization	Commercial source
	<b>2.173, 6.19</b>	Figs. 2a, 2b, ED Figs. 2a, 6g	Roche compound (ID: <b>EC-14621</b> )	n/a
	<b>1.63, 2.174</b>	Figs. 1e, 2a, 2b ED Fig. 2a	<b>4-35<sup>5</sup></b>	n/a
	<b>2.175</b>	Figs. 2a, 2b ED Fig. 2a	n/a	(4'-Chloro[1,1'-biphenyl]-4-yl)methanamine; Sigma Aldrich (PH014524)
	<b>2.176</b>	Figs. 2a, 2b	n/a	Anamorelin; Sigma Aldrich (SML2519)
	<b>2.177, 6.20</b>	Figs. 2a, 2b ED Fig. 6g	Roche compound (ID: <b>EC-02030</b> )	n/a
	<b>1.46, 2.178</b>	Figs. 1e, 2a, 2b	<b>4-42<sup>5</sup></b>	n/a
	<b>2.179 (51)</b>	Figs. 2a, 2b ED Figs. 2a, 2b	Roche compound (ID: <b>EC-20121</b> )	n/a
	<b>1.1, 2.180, 6.21 (67)</b>	Figs. 1e, 2a, 2b ED Figs. 2a, 3d, 6a, 6g	<b>4-47<sup>5</sup></b>	n/a
	<b>1.25, 2.181 (49)</b>	Figs. 1e, 2a, 2b ED Figs. 2a, 2b	<b>4-5<sup>5</sup></b>	n/a

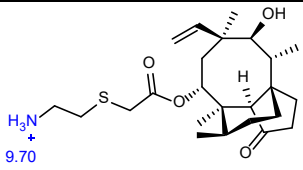
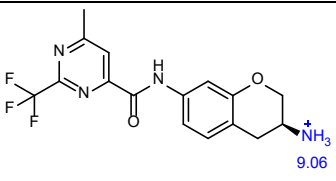
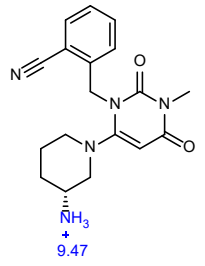
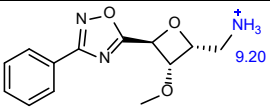
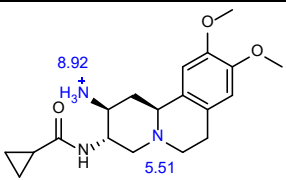
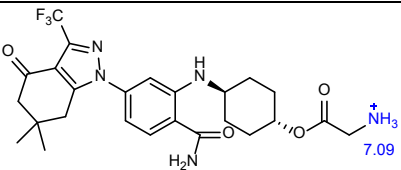
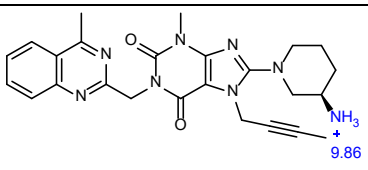
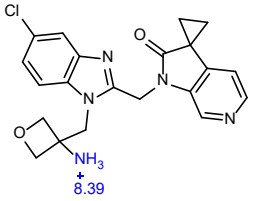
Structure	SI table numbers	Figures the compound appears in	Prior ID, references, and characterization	Commercial source
	2.182	Figs. 2a, 2b ED Fig. 2a	n/a	3-(2-Aminoethyl)-5-((4-ethoxyphenyl)methylene)-2,4-thiazolidinedione; Alfa Chemistry Product List (ACM294675799)
	2.183	Figs. 2a, 2b ED Fig. 2a	Roche compound (ID: <b>EC-11816</b> )	n/a
	2.184 (15)	Figs. 2a, 2b, 2d ED Fig. 2a	Roche compound (ID: <b>EC-18386</b> )	n/a
	2.185	Figs. 2a, 2b ED Fig. 2a	Roche compound (ID: <b>EC-02499</b> )	n/a
	2.186	Figs. 2a, 2b ED Fig. 2a	Roche compound (ID: <b>EC-12003</b> )	n/a
	2.187	Figs. 2a, 2b ED Fig. 2a	Roche compound (ID: <b>EC-19484</b> )	n/a
	2.188	Figs. 2a, 2b ED Fig. 2a	Roche compound (ID: <b>EC-18619</b> )	n/a
	2.189	Figs. 2a, 2b ED Fig. 2a	Reported here	n/a
	2.190	Figs. 2a, 2b ED Fig. 2a	Roche compound (ID: <b>EC-12068</b> )	n/a

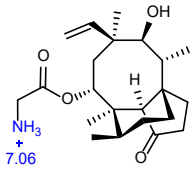
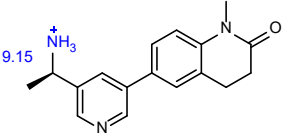
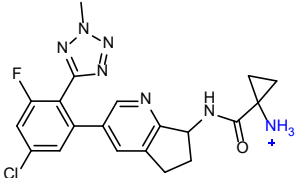
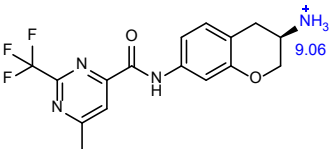
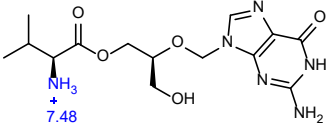
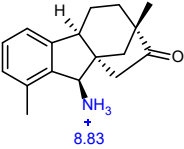
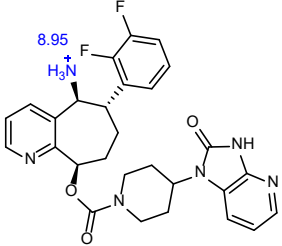
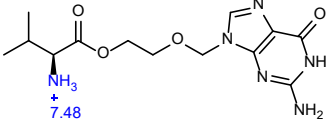
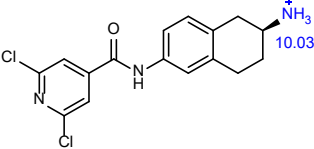
Structure	SI table numbers	Figures the compound appears in	Prior ID, references, and characterization	Commercial source
	<b>2.191, 4.13 (17, 33)</b>	Figs. 2a, 2b, 2e, 3 ED Figs. 5b, 5d	n/a	Fluvoxamine; AK Scientific (C924)
	<b>2.192</b>	Figs. 2a, 2b	n/a	Valbenazine; Cayman Chemicals (26809)
	<b>2.193</b>	Figs. 2a, 2b ED Fig. 2a	n/a	Saxagliptin; Sigma Aldrich (SML3046)
	<b>1.26, 2.194 (50)</b>	Figs. 1e, 2a, 2b ED Figs. 2a, 2b, 3d	<b>4-10<sup>5</sup>; 14A<sup>6</sup></b>	n/a
	<b>2.195 (52)</b>	Figs. 2a, 2b ED Figs. 2a, 2b	Roche compound (ID: <b>EC-07579</b> )	n/a
	<b>2.196</b>	Figs. 2a, 2b ED Fig. 3d	Roche compound (ID: <b>EC-06538</b> )	n/a
	<b>2.197, 5.2A</b>	Figs. 2a, 2b ED Figs. 2a, 6d	<b>3A<sup>6</sup></b>	n/a
	<b>2.198</b>	Figs. 2a, 2b ED Fig. 2a	Roche compound (ID: <b>EC-11860</b> )	n/a
	<b>2.199 (73)</b>	Figs. 2a, 2b ED Fig. 6c	<b>50<sup>11</sup></b>	n/a

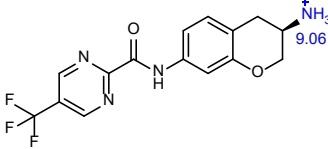
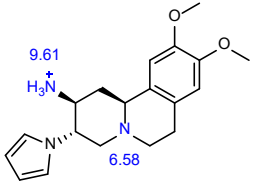
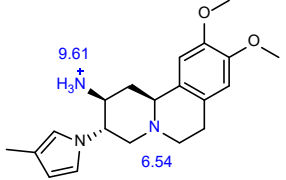
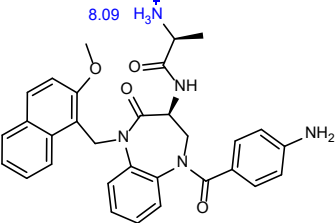
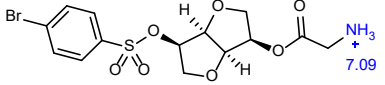
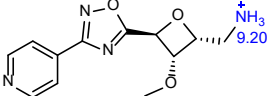
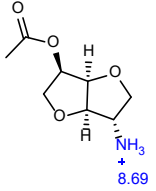
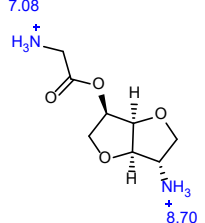
Structure	SI table numbers	Figures the compound appears in	Prior ID, references, and characterization	Commercial source
	2.200	Figs. 2a, 2b ED Fig. 2a	Roche compound (ID: <b>EC-11433</b> )	n/a
	2.201	Figs. 2a, 2b ED Fig. 2a	n/a	(5S)-5-(Aminomethyl)-3-[3-fluoro-4-(4-morpholinyl)phenyl]-1,3-oxazolidin-2-one; Carbosynth (IA58038)
	2.202, 6.22	Figs. 2a, 2b ED Fig. 6g	n/a	N-[(1S,2S)-2-amino-1,2-diphenylethyl]-7,7-dimethyl-2-oxobicyclo[2.2.1]heptane-1-sulfonamide; Aurora Fine Chemicals (160.482.367)
	2.203	Figs. 2a, 2b ED Fig. 2a	n/a	Aliskiren; MedChemExpress (HY-12176)
	2.204, 5.1A	Figs. 2a, 2b ED Figs. 2a, 6d	<b>2A<sup>6</sup></b>	n/a
	2.205	Figs. 2a, 2b ED Fig. 2a	Reported here	n/a
	2.206	Figs. 2a, 2b ED Fig. 2a	Roche compound (ID: <b>EC-07715</b> )	n/a
	2.207	Figs. 2a, 2b	Roche compound (ID: <b>EC-15985</b> )	n/a

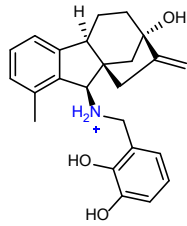
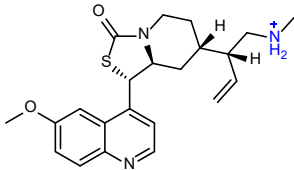
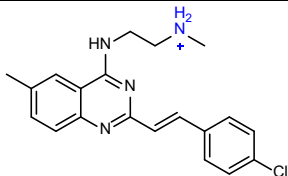
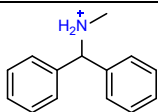
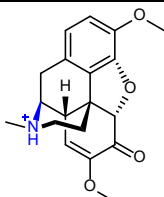
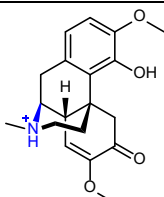
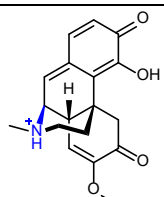
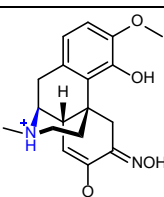


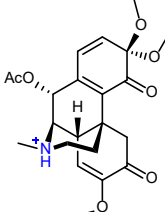
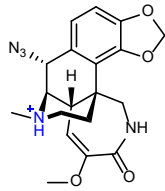
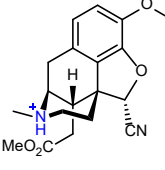
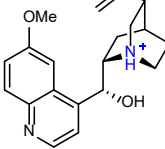
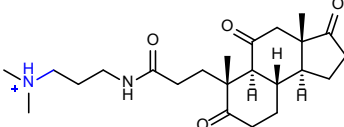
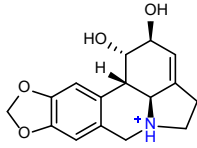
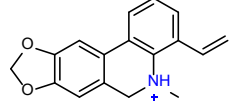
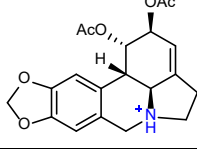
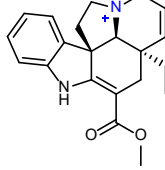
Structure	SI table numbers	Figures the compound appears in	Prior ID, references, and characterization	Commercial source
	2.208	Figs. 2a, 2b ED Fig. 2a	n/a	AZD5363; Cayman Chemicals (15406)
	2.209	Figs. 2a, 2b	Roche compound (ID: <b>EC-00837</b> )	n/a
	2.210	Figs. 2a, 2b	Reported here	n/a
	2.211	Figs. 2a, 2b	n/a	Trelagliptin; AK Scientific (2763AH)
	2.212	Figs. 2a, 2b	n/a	MK-3102; Cayman Chemicals (21454)
	2.213	Figs. 2a, 2b ED Fig. 2a	Roche compound (ID: <b>EC-15867</b> )	n/a
	2.214	Figs. 2a, 2b ED Fig. 2a	Roche compound (ID: <b>EC-11553</b> )	n/a
	2.215 (63)	Figs. 2a, 2b ED Fig. 3b	Roche compound (ID: <b>EC-15221</b> )	n/a

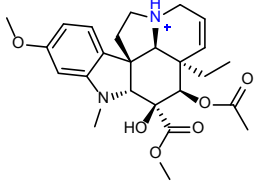
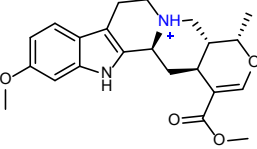
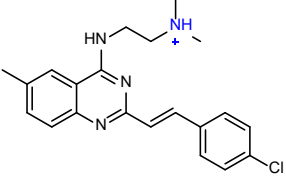
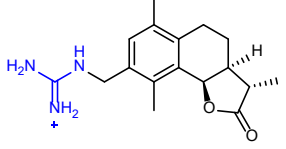
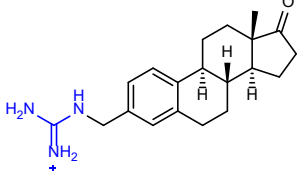
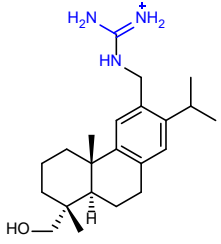
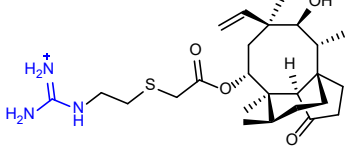
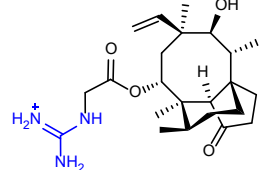
Structure	SI table numbers	Figures the compound appears in	Prior ID, references, and characterization	Commercial source
	<b>1.3, 2.216, 5.4A</b>	Figs. 1e, 2a, 2b ED Figs. 2a, 6d	<b>4-57<sup>5</sup>; 10A<sup>6</sup></b>	n/a
	<b>2.217</b>	Figs. 2a, 2b ED Fig. 2a	Roche compound (ID: <b>EC-04619</b> )	n/a
	<b>2.218 (74)</b>	Figs. 2a, 2b ED Fig. 6c	n/a	Alogliptin; AK Scientific (J99093)
	<b>2.219</b>	Figs. 2a, 2b ED Fig. 2a	Roche compound (ID: <b>EC-14894</b> )	n/a
	<b>2.220, 6.24</b>	Figs. 2a, 2b ED Fig. 6g	Roche compound (ID: <b>EC-12850</b> )	n/a
	<b>2.221</b>	Figs. 2a, 2b ED Fig. 2a	n/a	PF-04929113; Cayman Chemicals (18270)
	<b>2.222, 6.25</b>	Figs. 2a, 2b ED Figs. 2a, 6g	n/a	Linagliptin; AK Scientific (X1062)
	<b>2.223</b>	Figs. 2a, 2b	Roche compound (ID: <b>EC-03501</b> )	n/a

Structure	SI table numbers	Figures the compound appears in	Prior ID, references, and characterization	Commercial source
	<b>2.224, 5.5A</b>	Figs. 2a, 2b ED Figs. 2a, 6d	<b>11A<sup>6</sup></b>	n/a
	<b>2.225</b>	Figs. 2a, 2b ED Fig. 3d	Roche compound (ID: <b>EC-10518</b> )	n/a
	<b>2.226</b>	Figs. 2a, 2b	Roche compound (ID: <b>EC-08600</b> )	n/a
	<b>2.227</b>	Figs. 2a, 2b ED Fig. 2a	Roche compound (ID: <b>EC-18413</b> )	n/a
	<b>1.64, 2.228</b>	Figs. 1e, 2a, 2b	<b>4-43<sup>5</sup></b>	Valganciclovir; AA Blocks (AA00215S)
	<b>1.4, 2.229</b>	Figs. 1e, 2a, 2b ED Fig. 2a	<b>4-23<sup>5</sup></b>	n/a
	<b>2.230</b>	Figs. 2a, 2b	n/a	Rimegepant; Cayman Chemicals (26338)
	<b>1.65, 2.231</b>	Figs. 1e, 2a, 2b	<b>4-45<sup>5</sup></b>	Valacyclovir; AA Blocks (AA000MPL)
	<b>2.232</b>	Figs. 2a, 2b ED Fig. 2a	Roche compound (ID: <b>EC-16363</b> )	n/a

Structure	SI table numbers	Figures the compound appears in	Prior ID, references, and characterization	Commercial source
	<b>2.233</b>	Figs. 2a, 2b ED Fig. 2a	Roche compound (ID: <b>EC-15751</b> )	n/a
	<b>2.234</b>	Figs. 2a, 2b	Roche compound (ID: <b>EC-09273</b> )	n/a
	<b>2.235</b>	Figs. 2a, 2b	Roche compound (ID: <b>EC-17867</b> )	n/a
	<b>2.236</b>	Figs. 2a, 2b ED Fig. 2a	Roche compound (ID: <b>EC-09961</b> )	n/a
	<b>2.237</b>	Figs. 2a, 2b ED Fig. 2a	Reported here	n/a
	<b>2.238</b>	Figs. 2a, 2b	Roche compound (ID: <b>EC-10962</b> )	n/a
	<b>1.30, 2.239</b>	Figs. 1e, 2a, 2b	<b>4-37-a<sup>5</sup></b>	n/a
	<b>1.31, 2.240</b>	Figs. 1e, 2a, 2b	<b>4-55-a<sup>5</sup></b>	n/a

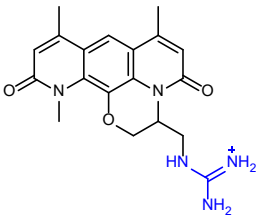
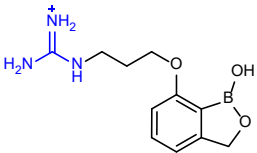
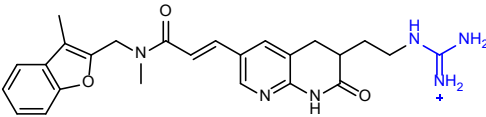
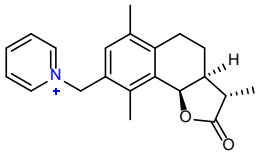
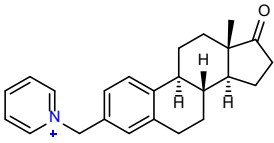
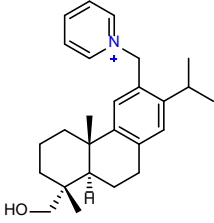
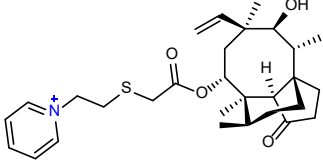
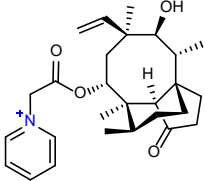
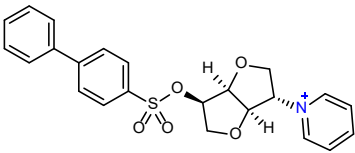
Structure	SI table numbers	Figures the compound appears in	Prior ID, references, and characterization	Commercial source
	1.14, 3.1	Fig. 2a	2-17 <sup>5</sup>	n/a
	1.41, 3.2 (61)	Fig. 2a ED Fig. 3b	2-18 <sup>5</sup>	n/a
	3.3 (3)	Figs. 1d, 2a	Z15 <sup>12</sup>	n/a
	3.4	Fig. 2a	n/a	N-Methyl-1,1-diphenylmethanamine; AK Scientific (4477AD)
	1.42, 3.5	Fig. 2a	2-29 <sup>5</sup> , 15 <sup>11</sup>	n/a
	1.43, 3.6, 6.23	Fig. 2a ED Fig. 6g	2-32 <sup>5</sup> , 1 <sup>11</sup>	Sinomenine; Avachem Scientific (1214)
	1.44, 3.7	Fig. 2a	2-33 <sup>5</sup> , 3 <sup>11</sup>	n/a
	1.45, 3.8	Fig. 2a	2-35 <sup>5</sup> , 49 <sup>11</sup>	n/a

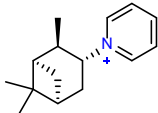
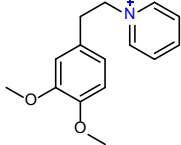
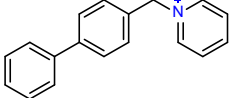
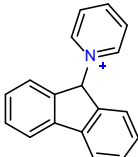
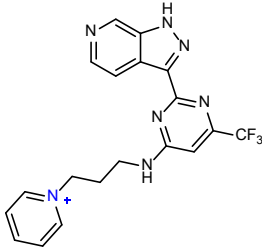
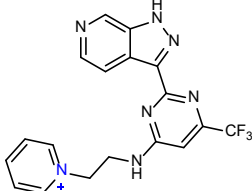
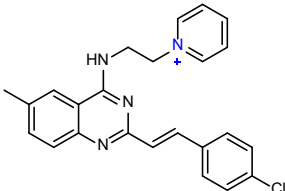
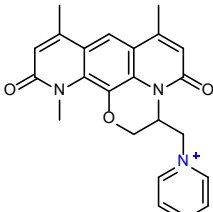
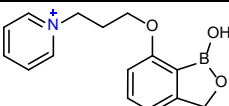
Structure	SI table numbers	Figures the compound appears in	Prior ID, references, and characterization	Commercial source
	3.9	Fig. 2a	32 <sup>11</sup>	n/a
	3.10	Fig. 2a	13 <sup>11</sup>	n/a
	3.11	Fig. 2a	6 <sup>11</sup>	n/a
	1.47, 3.12	Fig. 2a	2-30 <sup>5</sup>	n/a
	1.48, 3.13	Fig. 2a	2-39 <sup>5</sup>	n/a
	3.14	Fig. 2a	1 <sup>13</sup>	Lycorine; Vesino Industrial Co. Ltd. (VN10052)
	3.15	Fig. 2a	2 <sup>13</sup>	n/a
	3.16	Fig. 2a	15 <sup>13</sup>	n/a
	3.17	Fig. 2a	n/a	Tabersonine; AK Scientific (J51610)

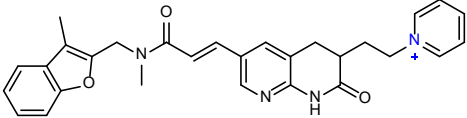
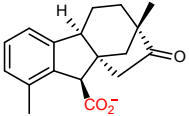
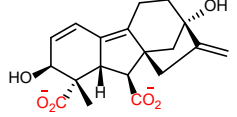
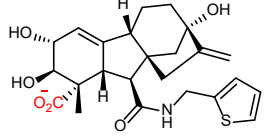
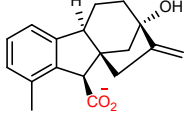
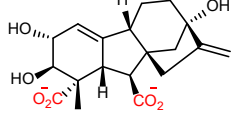
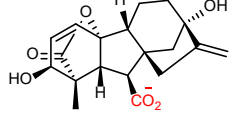
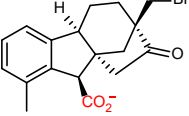
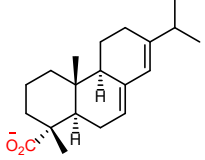
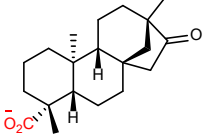
Structure	SI table numbers	Figures the compound appears in	Prior ID, references, and characterization	Commercial source
	3.18	Fig. 2a	n/a	Vindoline; AK Scientific (O453)
	3.19	Fig. 2a	n/a	Tetraphylline was a generous gift from Prof. Kuehne
	3.20 (2)	Figs. 1d, 2a	Z11 <sup>12</sup>	n/a
	3.21, 5.1G	Fig. 2a ED Fig. 6d	2G <sup>6</sup>	n/a
	3.22, 5.2G	Fig. 2a ED Fig. 6d	3G <sup>6</sup>	n/a
	3.23, 5.3G	Fig. 2a ED Fig. 6d	7G <sup>6</sup>	n/a
	3.24, 5.4G	Fig. 2a ED Fig. 6d	10G <sup>6</sup>	n/a
	3.25, 5.5G	Fig. 2a ED Fig. 6d	11G <sup>6</sup>	n/a

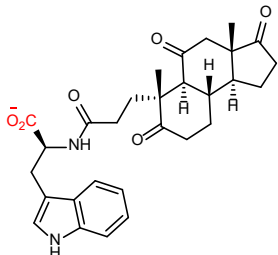
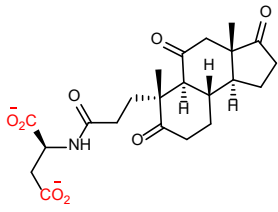
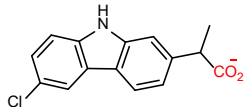
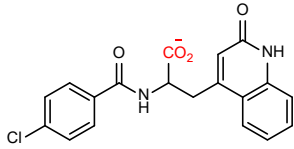
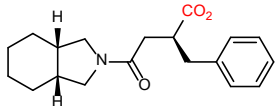
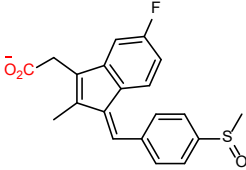
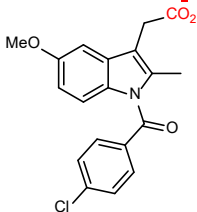
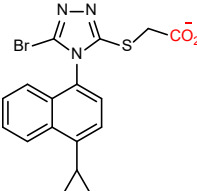
Structure	SI table numbers	Figures the compound appears in	Prior ID, references, and characterization	Commercial source
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	3.27, 4.9, 5.7G (29, 77G)	Figs. 2a, 3 ED Fig. 6d	16G <sup>6</sup>	n/a
	3.28, 5.8G	Fig. 2a ED Fig. 6d	17G <sup>6</sup>	n/a
	3.29, 5.9G	Fig. 2a ED Fig. 6d	18G <sup>6</sup>	n/a
	3.30, 4.8, 5.10G (28)	Figs. 2a, 3 ED Fig. 6d	20G <sup>6</sup>	n/a
	3.31, 5.11G (78G)	Fig. 2a ED Fig. 6d	S5 <sup>6</sup>	n/a
	3.32, 5.12G	Fig. 2a ED Fig. 6d	36 <sup>6</sup>	n/a
	3.33, 4.7, 5.13G (27)	Figs. 2a, 3 ED Fig. 6d	32 <sup>6</sup>	n/a

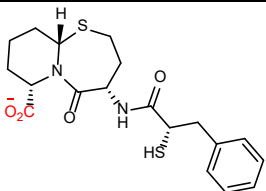
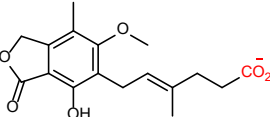
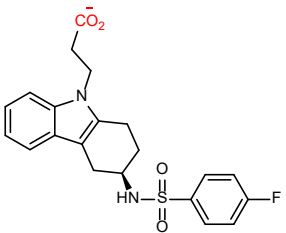
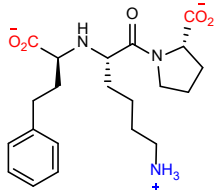
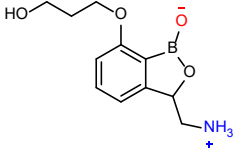
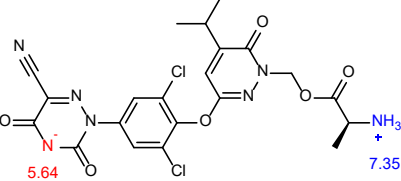
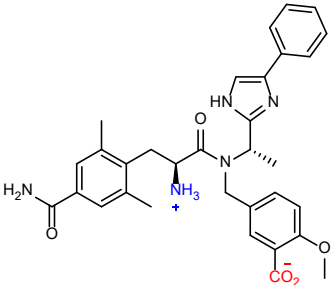


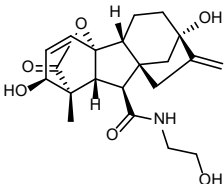
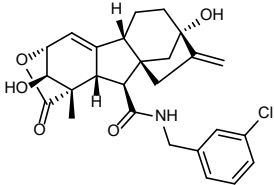
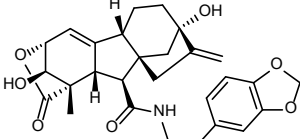
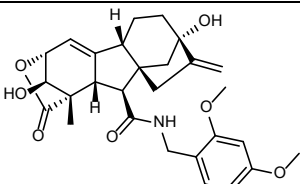
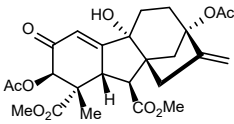
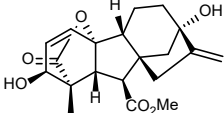
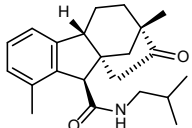
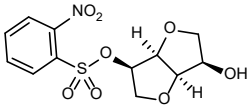
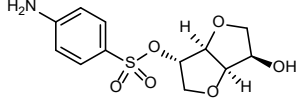
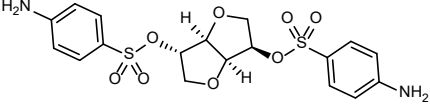
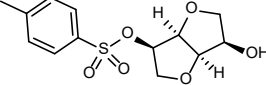
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	3.35, 5.15G	Fig. 2a ED Fig. 6d	45 <sup>6</sup>	n/a
	3.36, 5.16G (79G)	Fig. 2a ED Fig. 6d	23 <sup>6</sup>	n/a
	3.37, 5.1P	Fig. 2a ED Fig. 6d	2P <sup>6</sup>	n/a
	3.38, 5.2P	Fig. 2a ED Fig. 6d	3P <sup>6</sup>	n/a
	3.39, 5.3P	Fig. 2a ED Fig. 6d	7P <sup>6</sup>	n/a
	3.40, 5.4P	Fig. 2a ED Fig. 6d	10P <sup>6</sup>	n/a
	3.41, 5.5P	Fig. 2a ED Fig. 6d	11P <sup>6</sup>	n/a
	3.42, 5.6P	Fig. 2a ED Fig. 6d	13P <sup>6</sup>	n/a

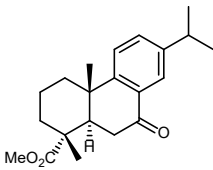
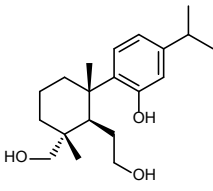
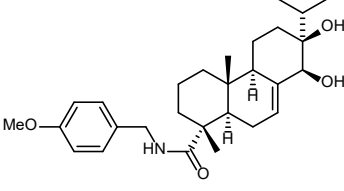
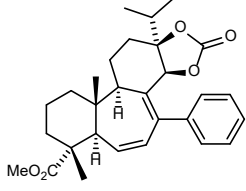
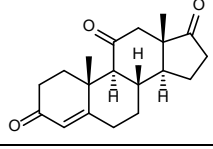
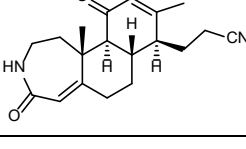
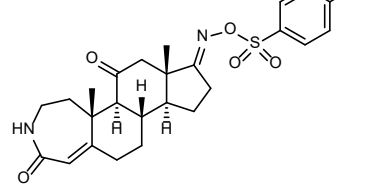
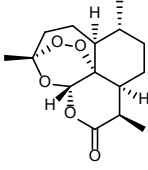
Structure	SI table numbers	Figures the compound appears in	Prior ID, references, and characterization	Commercial source
	<b>3.43, 5.7P (77P)</b>	Fig. 2a ED Fig. 6d	<b>16P<sup>6</sup></b>	n/a
	<b>3.44, 5.8P</b>	Fig. 2a ED Fig. 6d	<b>17P<sup>6</sup></b>	n/a
	<b>3.45, 5.9P</b>	Fig. 2a ED Fig. 6d	<b>18P<sup>6</sup></b>	n/a
	<b>3.46, 5.10P</b>	Fig. 2a ED Fig. 6d	<b>20P<sup>6</sup></b>	n/a
	<b>3.47, 5.11P (78P)</b>	Fig. 2a ED Fig. 6d	<b>S6<sup>6</sup></b>	n/a
	<b>3.48, 5.12P</b>	Fig. 2a ED Fig. 6d	<b>37<sup>6</sup></b>	n/a
	<b>3.49, 5.13P</b>	Fig. 2a ED Fig. 6d	<b>33<sup>6</sup></b>	n/a
	<b>3.50, 5.14P</b>	Fig. 2a ED Fig. 6d	<b>28<sup>6</sup></b>	n/a
	<b>3.51, 5.15P</b>	Fig. 2a ED Fig. 6d	<b>46<sup>6</sup></b>	n/a

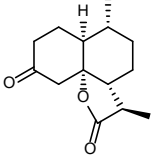
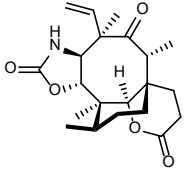
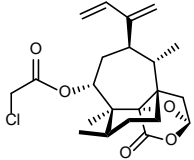
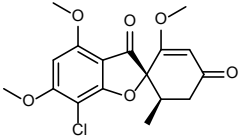
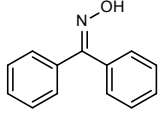
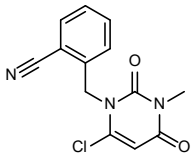
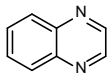
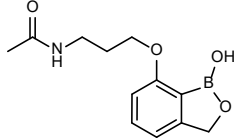
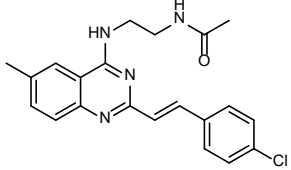
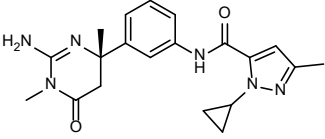
Structure	SI table numbers	Figures the compound appears in	Prior ID, references, and characterization	Commercial source
	<b>3.52, 5.16P (79P)</b>	Fig. 2a ED Fig. 6d	<b>24<sup>6</sup></b>	n/a
	<b>1.15, 3.53</b>	Fig. 2a	<b>2-42<sup>5</sup></b>	n/a
	<b>1.16, 3.54</b>	Fig. 2a	<b>2-43<sup>5</sup></b>	n/a
	<b>1.17, 3.55</b>	Fig. 2a	<b>2-51<sup>5</sup></b>	n/a
	<b>1.18, 3.56 (5)</b>	Figs. 1d, 2a	<b>2-52<sup>5</sup></b>	n/a
	<b>1.19, 3.57</b>	Fig. 2a	<b>2-54<sup>5</sup></b>	n/a
	<b>1.20, 3.58</b>	Fig. 2a	<b>2-61<sup>5</sup></b>	Gibberellic acid; AK Scientific (K339)
	<b>3.59</b>	Fig. 2a	<b>a-47<sup>14</sup></b>	n/a
	<b>1.39, 3.60</b>	Fig. 2a	<b>2-57<sup>5</sup></b>	Abietic acid; Cayman Chemical (24927)
	<b>3.61</b>	Fig. 2a	n/a	Isosteviol; AA Blocks (AA00BE2Z)

Structure	SI table numbers	Figures the compound appears in	Prior ID, references, and characterization	Commercial source
	3.62	Fig. 2a	A12o <sup>15</sup>	n/a
	3.63	Fig. 2a	A12l <sup>15</sup>	n/a
	3.64	Fig. 2a	n/a	Carprofen; AK Scientific (H092)
	3.65	Fig. 2a	n/a	Rebamipide; Cayman Chemical (17186)
	3.66	Fig. 2a	n/a	Mitiglinide; Cayman Chemical (30693)
	3.67	Fig. 2a	n/a	Sulindac; Cayman Chemical (10004386)
	3.68	Fig. 2a	n/a	Indomethacin; Cayman Chemical (70270)
	3.69	Fig. 2a	n/a	Lesinurad; Cayman Chemical (23688)

Structure	SI table numbers	Figures the compound appears in	Prior ID, references, and characterization	Commercial source
	3.70	Fig. 2a	n/a	Omapatrilat; Cayman Chemical (31738)
	3.71	Fig. 2a	n/a	Mycophenolic acid; Ambeed Inc. Product List (A399663)
	3.72	Fig. 2a	n/a	Ramatroban; Ambeed Inc. Product List (A436709)
	3.73, 6.26	Fig. 2a ED Fig. 6g	n/a	Lisinopril; Cayman Chemical (16833)
	3.74	Fig. 2a	42 <sup>6</sup>	n/a
	3.75	Fig. 2a	Roche compound (ID: EC-17602)	n/a
	3.76	Fig. 2a	n/a	Eluxadoline; Toronto Research Chemicals (E508195)

Structure	SI table numbers	Figures the compound appears in	Prior ID, references, and characterization	Commercial source
	1.21, 3.77	Fig. 2a	2-72 <sup>5</sup>	n/a
	1.22, 3.78	Fig. 2a	2-74 <sup>5</sup>	n/a
	1.23, 3.79	Fig. 2a	2-79 <sup>5</sup>	n/a
	3.80	Fig. 2a	G16e <sup>15</sup>	n/a
	3.81	Fig. 2a	G15 <sup>15</sup>	n/a
	3.82	Fig. 2a	GA-4 <sup>16</sup>	n/a
	3.83	Fig. 2a	G19 <sup>15</sup>	n/a
	1.32, 3.84	Fig. 2a	2-94 <sup>5</sup>	n/a
	1.33, 3.85	Fig. 2a	2-95 <sup>5</sup>	n/a
	1.34, 3.86	Fig. 2a	2-97 <sup>5</sup>	n/a
	1.35, 3.87	Fig. 2a	3-37 <sup>5</sup>	n/a

Structure	SI table numbers	Figures the compound appears in	Prior ID, references, and characterization	Commercial source
	3.88 (7)	Figs. 1d, 2a	AA4 <sup>17</sup>	n/a
	3.89	Fig. 2a	AA7 <sup>17</sup>	n/a
	3.90	Fig. 2a	AA31f <sup>17</sup>	n/a
	3.91	Fig. 2a	AA23 <sup>17</sup>	n/a
	1.49, 3.92	Fig. 2a	2-67 <sup>5</sup>	Adrenosterone; TCI (A1397)
	1.50, 3.93	Fig. 2a	2-73 <sup>5</sup> ; A6 <sup>15</sup>	n/a
	3.94	Fig. 2a	A16 <sup>15</sup>	n/a
	3.95	Fig. 2a	n/a	Artemisinin; AK Scientific (F947)

Structure	SI table numbers	Figures the compound appears in	Prior ID, references, and characterization	Commercial source
	3.96	Fig. 2a	8 <sup>18</sup>	n/a
	3.97	Fig. 2a	P15 <sup>19</sup>	n/a
	3.98	Fig. 2a	P5 <sup>19</sup>	n/a
	3.99, 6.27	Fig. 2a ED Fig. 6g	n/a	Griseofulvin; AK Scientific (M542)
	3.100	Fig. 2a	n/a	Benzophenone oxime; Ambeed Inc. Product List (A292313)
	3.101	Fig. 2a	n/a	2-[(6-Chloro-3,4-dihydro-3-methyl-2,4-dioxo-1(2H)-pyrimidinyl)methyl]benz onitrile; AK Scientific (Z1750)
	3.102	Fig. 2a	n/a	Quinoxaline; AK Scientific (X0038)
	3.103	Fig. 2a	A12 <sup>20</sup>	n/a
	3.104 (1)	Figs. 1d, 2a	30 <sup>6</sup>	n/a
	3.105	Fig. 2a	Roche compound (ID: EC-01597)	n/a





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