Electronic Supplementary Material (ESI) for Molecular BioSystems.

† Electronic Supplementary Information (ESI†)

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Table S1A Collected Mtb inhibitors of different assays from the ChEMBL database.

Parameter	Total compounds	Redundant data	Non-Redundant data
MIC $^{\$}$ *	15235	6238	8997
Activity	661	302	359
CC_{50}	3416	1062	2354
GI	847	211	636
IC_{50} $^{\$}$	11318	4502	6816
IC_{90}*	1229	13	1216
Inhibition	2921	635	2286
Ki	971	367	604
MIC_{50}*	216	77	139
MIC_{90}*	1644	873	771
MIC_{99}*	591	175	416
Ratio	597	175	416
Selectivity Index	785	75	710
$AvgIC_{90}$	319	249	70
$AvgCC_{50}$	157	92	65
CC_{25}	15	13	2
EC_{50}	143	21	122
EC_{90}	68	23	44
EC_{99}	28	2	26
CFU	62	35	27
GrowthIndex	206	177	29
IZ	82	8	74
Kd	180	21	159
Km	47	12	35
Log1/MMIC	296	246	50
log10CFU	304	206	98
log10CFU/ml	63	52	11
MBC	94	18	76
MIC_{95} *	139	36	103
$RatioIC_{50}$	153	56	97
Selectivity Ratio	58	20	38
Miscellaneous	1211	0	1211
Total	**44056**	**15992**	**26846**

$^{\$}$ Compounds used for model building, *Compounds used for model validation

The collected IC_{50} and MIC data values (reported in nanomolar concentration; nM) were converted to their negative logarithm values, i.e. pIC_{50} and pMIC. In some compounds, the cell-based inhibitory potency was reported in µg/ml and these values were first divided with their corresponding molecular weight, followed by the multiplication with 1000 and applied negative logarithm.

Table S1B List of molecular targets identified from the enzyme based assay results.

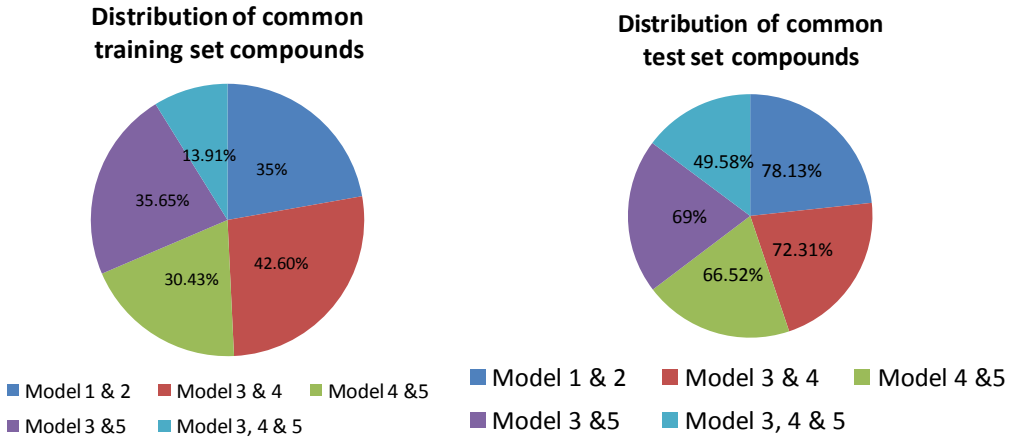
Target_CHEMBLID	Target_Name	Occurrence of Target
CHEMBL612545	acyl-CoA-synthesizing fatty acyl-CoA ligases (unchecked)	241
CHEMBL1849	Enoyl-[acyl-carrier-protein] reductase	149
CHEMBL3640	3-oxoacyl-[acyl-carrier-protein] synthase III	92
CHEMBL1744527	L-cysteine:1D-myo-inositol 2-amino-2-deoxy-alpha-D-glucopyranoside ligase	47
CHEMBL1908385	Serine/threonine-protein kinase pknB	36
CHEMBL4450	UDP-galactopyranose mutase	36
CHEMBL4542	Probable low molecular weight protein-tyrosine-phosphatase	36
CHEMBL4540	Phosphotyrosine-protein phosphatase PTPB	31
CHEMBL5091	1-deoxy-D-xylulose-5-phosphate synthase	29
CHEMBL4624	Fibonectin-binding protein C	25
CHEMBL3703	Mycothiol S-conjugate amidase	24
CHEMBL1744528	3 beta-hydroxysteroid dehydrogenase/Delta 5-->4-isomerase	20
CHEMBL4213	Cell division protein FtsZ	20
CHEMBL1275214	1,4-Dihydroxy-2-naphthoyl-CoA synthase	19
CHEMBL6069	Pantothenate synthetase	17
CHEMBL1795161	Thymidylate synthase thyX	14
CHEMBL5765	Peptide deformylase	14
CHEMBL1772929	HTH-type transcriptional regulator EthR	8
CHEMBL6086	ATP phosphoribosyltransferase	7
CHEMBL6176	Inorganic polyphosphate/ATP-NAD kinase	6
CHEMBL2006	DNA-directed RNA polymerase beta chain	5
CHEMBL2321612	O-acetylserine sulfhydrylase	5
CHEMBL5630	1-deoxy-D-xylulose 5-phosphate reductoisomerase	5
CHEMBL1667699	Isocitrate lyase	4
CHEMBL1795155	Epoxide hydrolase	4
CHEMBL1938225	dTDP-4-dehydrorhamnose reductase	4
CHEMBL6064	Transcriptional regulatory protein devR (dosR)	4
CHEMBL6067	LmbE-related protein	4
CHEMBL2069157	Intracellular chorismate mutase	3
CHEMBL1075096	UDP-galactofuranosyl transferase GlfT2	1
CHEMBL1287620	Fructose-bisphosphate aldolase	1
CHEMBL4165	DNA gyrase subunit A	1
CHEMBL4543	3-oxoacyl-[acyl-carrier-protein] synthase 2	1
CHEMBL4544	3-oxoacyl-[acyl-carrier-protein] synthase 1	1
CHEMBL5662	2,3-dihydroxybenzoate-AMP ligase	1
CHEMBL6066	Chorismate mutase-related protein	1

Table S2A Distribution of common training and test set compounds in different 2D-QSAR models.

S.NO	Training set	Test
Model 1	11, 86, 218, 246, 280, 281, 282, 283, 284, 285, 287, 289, 290, 291, 292, 293, 294, 295, 296, 298, 300, 301, 302, 304, 305, 306, 307, 308, 309, 310, 312, 313, 314, 316, 317, 319, 321, 322, 323, 324, 325, 326, 327, 331, 332, 333, 334, 336, 338, 339, 340, 342, 344, 345, 346, 347, 348, 349, 350, 351, 352, 354, 356, 357	255, 279, 286, 288, 297, 299, 303, 311, 315, 318, 320, 328, 329, 330, 335, 337, 341, 343, 353, 355,
Model 2	11, 86, 218, 255, 280, 282, 283, 285, 286, 287, 288, 290, 291, 292, 293, 295, 298, 299, 300, 301, 302, 303, 304, 305, 307, 308, 309, 310, 312, 313, 314, 315, 316, 317, 318, 320, 322, 323, 324, 326, 327, 328, 330, 331, 332, 334, 336, 337, 340, 342, 343, 344, 345, 346, 347, 348, 349, 350, 351, 352, 353, 354, 356, 357	246, 279, 281, 284, 289, 294, 296, 297, 306, 311, 319, 321, 325, 329, 333, 335, 338, 339, 341, 355,
Model 3	1, 2, 3, 4, 5, 6, 7, 8, 12, 14, 16, 20, 21, 25, 29, 31, 33, 34, 35, 36, 38, 39, 40, 41, 42, 43, 44, 45, 46, 51, 52, 53, 56, 57, 58, 59, 60, 61, 62, 63, 64, 66, 67, 70, 71, 72, 74, 76, 79, 81, 82, 83, 84, 85, 87, 93, 94, 95, 96, 97, 98, 99, 100, 101, 102, 103, 106, 107, 109, 111, 112, 113, 114, 116, 117, 118, 119, 120, 121, 122, 123, 125, 126, 127, 128, 130, 131, 132, 133, 134, 135, 136, 138, 139, 140, 141, 142, 143, 144, 146, 147, 148, 149, 154, 156, 157, 158, 159, 160, 161, 162, 163, 164, 165, 166, 167, 168, 169, 172, 173, 174, 175, 176, 177, 178, 179, 180, 181, 182, 183, 184, 186, 189, 190, 192, 193, 194, 195, 196, 197, 199, 200, 202, 203, 205, 206, 207, 209, 211, 213, 215, 216, 217, 218, 220, 221, 225, 226, 227, 228, 229, 231, 232, 233, 235, 236, 237, 238, 240, 242, 243, 244, 248, 249, 251, 253, 254, 255, 256, 258, 259, 261, 263, 264, 266, 268, 269, 270, 272, 275, 276, 277, 278, 279, 280, 281, 283, 284, 285, 286, 288, 293, 294, 295, 296, 298, 300, 303, 304, 305, 306, 307, 308, 309, 312, 313, 315, 316, 319, 321, 322, 324, 325, 327, 329, 331, 334, 336, 337, 338, 340, 341, 342, 344, 346, 347, 349, 352, 354, 355, 356, 357,	9, 10, 11, 13, 15, 17, 18, 19, 22, 23, 24, 26, 27, 28, 30, 32, 37, 47, 48, 49, 50, 54, 55, 65, 68, 69, 73, 75, 77, 78, 80, 86, 88, 89, 90, 91, 92, 104, 105, 108, 110, 115, 124, 129, 137, 145, 150, 151, 152, 153, 155, 170, 171, 185, 187, 188, 191, 198, 201, 204, 208, 210, 212, 214, 219, 222, 223, 224, 230, 234, 239, 241, 245, 246, 247, 250, 252, 257, 260, 262, 265, 267, 271, 273, 274, 282, 287, 289, 290, 291, 292, 297, 299, 301, 302, 310, 311, 314, 317, 318, 320, 323, 326, 328, 330, 332, 333, 335, 339, 343, 345, 348, 350, 351, 353
Model 4	1, 2, 3, 4, 5, 6, 8, 10, 12, 17, 19, 20, 21, 23, 25, 26, 28, 29, 31, 32, 34, 35, 36, 37, 40, 41, 43, 45, 46, 48, 50, 51, 52, 56, 58, 59, 60, 61, 63, 64, 67, 68, 69, 70, 71, 72, 73, 74, 75, 76, 78, 79, 80, 81, 82, 83, 84, 85, 86, 87, 88, 90, 91, 92, 95, 96, 97, 98, 101, 102, 103, 104, 106, 107, 109, 110, 111, 112, 114, 115, 116, 117, 118, 119, 120, 121, 122, 123, 125, 127, 129, 130, 133, 134, 135, 137, 138, 141, 142, 143, 144, 146, 147, 148, 149, 150, 151, 152, 156, 157, 158, 159, 161, 162, 163, 164, 165, 166, 169, 170, 171, 172, 176, 178, 179, 181, 182, 183, 184, 185, 187, 188, 192, 193, 194, 195, 197, 198, 199, 200, 201, 204, 205, 206, 207, 213, 214, 215, 216, 217, 218, 220, 221, 222, 224, 225, 226, 228, 229, 232, 234, 236, 237, 239, 240, 242, 243, 244, 245, 246, 248, 249, 251, 252, 253, 254, 255, 257, 258, 260, 262, 263, 267, 268, 269, 270, 272, 273, 275, 276, 277, 278, 279, 283, 285, 286, 288, 291, 292, 295, 296, 297, 298, 299, 300, 301, 302, 304, 305, 306, 307, 308, 309, 310, 311, 312, 313, 316, 317, 319, 322, 323, 326, 327, 329, 331, 333, 334, 335, 340, 342, 343, 344, 345, 347, 349, 352, 353, 354, 355, 356, 357,	7, 9, 11, 13, 14, 15, 16, 18, 22, 24, 27, 30, 33, 38, 39, 42, 44, 47, 49, 53, 54, 55, 57, 62, 65, 66, 77, 89, 93, 94, 99, 100, 105, 108, 113, 124, 126, 128, 131, 132, 136, 139, 140, 145, 153, 154, 155, 160, 167, 168, 173, 174, 175, 177, 180, 186, 189, 190, 191, 196, 202, 203, 208, 209, 210, 211, 212, 219, 223, 227, 230, 231, 233, 235, 238, 241, 247, 250, 256, 259, 261, 264, 265, 266, 271, 274, 280, 281, 282, 284, 287, 289, 290, 293, 294, 303, 314, 315, 318, 320, 321, 324, 325, 328, 330, 332, 336, 337, 338, 339, 341, 346, 348, 350, 351
Model 5	1, 2, 3, 4, 6, 7, 8, 9, 10, 13, 14, 15, 18, 20, 30, 33, 34, 35, 37, 38, 39, 42, 45, 47, 49, 50, 51, 52, 56, 57, 59, 62, 64, 65, 66, 67, 68, 69, 70, 71, 72, 76, 78, 79, 82, 83, 86, 88, 89, 90, 91, 92, 95, 98, 99, 101, 102, 103, 104, 105, 106, 107, 109, 110, 112, 114, 115, 116, 117, 119, 120, 124, 125, 126, 127, 128, 130, 131, 132, 133, 135, 136, 137, 138, 140, 141, 142, 144, 145, 146, 149, 151, 152, 153, 155, 156, 157, 158, 159, 160, 162, 163, 167, 168, 172, 173, 174, 175, 176, 180, 181, 183, 184, 185, 187, 188, 189, 190, 192, 193, 194, 195, 199, 200, 201, 202, 204, 205, 206, 207, 208, 211, 212, 213, 215, 216, 217, 218, 221, 222, 223, 227, 228, 230, 232, 233, 234, 235, 239, 241, 242, 243, 245, 246, 248, 249, 250, 251, 252, 254, 255, 256, 259, 262, 263, 265, 266, 268, 269, 270, 272, 273, 274, 275, 276, 277, 278, 279, 280, 281, 282, 283, 284, 285, 290, 291, 292, 293, 294, 295, 296, 298, 299, 301, 303, 304, 305, 307, 309, 310, 312, 313, 314, 315, 316, 317, 319, 320, 322, 323, 324, 325, 326, 327, 328, 329, 330, 331, 332, 333, 334, 336, 337, 338, 339, 340, 341, 342, 344, 345, 346, 347, 348, 349, 350, 351, 352, 353, 354, 355, 356, 357	5, 11, 12, 16, 17, 19, 21, 22, 23, 24, 25, 26, 27, 28, 29, 31, 32, 36, 40, 41, 43, 44, 46, 48, 53, 54, 55, 58, 60, 61, 63, 73, 74, 75, 77, 80, 81, 84, 85, 87, 93, 94, 96, 97, 100, 108, 111, 113, 118, 121, 122, 123, 129, 134, 139, 143, 147, 148, 150, 154, 161, 164, 165, 166, 169, 170, 171, 177, 178, 179, 182, 186, 191, 196, 197, 198, 203, 209, 210, 214, 219, 220, 224, 225, 226, 229, 231, 236, 237, 238, 240, 244, 247, 253, 257, 258, 260, 261, 264, 267, 271, 286, 287, 288, 289, 297, 300, 302, 306, 308, 311, 318, 321, 335, 343

Table S2B Co-incidence of descriptors in various training and test sets of the different 2D-QSAR models.

Distribution of common training set compounds in different 2D-QSAR models		
Model 1 & 2	50 (64): 78.13%	2,3,7,9,10,12,14,17,18,19,20,22,25,27,28,29,31,32,34,35,36,37,39,40,41,43,44,49,50,51,53,54,58,59,61,63,67,69,71,72,73,74,75,76,77,78,79,81,83,84
Model 3 & 4	175 (242): 72.31%	2,3,4,5,6,8,12,20,21,25,29,31,34,35,36,40,41,43,45,46,51,52,56,58,59,60,61,63,64,67,70,71,72,74,76,79,81,82,83,84,85,87,95,96,97,98,101,102,103,106,107,109,111,112,114,116,117,118,119,120,121,122,123,125,127,130,133,134,135,138,141,142,143,144,146,147,148,149,156,157,158,159,161,162,163,164,165,166169,172,176,178,179,181,182,183,184,192,193,194,195,197,199,200,205,206,207,213,215,216,217,218,220,221,225,226,228,229,232,236,237,240,242,243,244,248,249,251,253,254,255,258,263,268,269,270,272,275,276,277,278,279,283,285,286,288,295,296,298,300,304,305,306,307,308,309,312,313,316,319,322,327,329,331,334,340,342,344,347,349,352,354,355,356,357
Model 4 &5	161 (242) 66.52%	2,3,4,6,8,10,20,34,35,37,45,50,51,52,56,59,64,67,68,69,70,71,72,76,78,79,82,83,86,88,90,91,92,95,98,101,102,103,104,106,107,109,110,112,114,115,116,117,119,120,125,127,130,133,135,137,138,141,142,144,146,149,151,152,156,157,158,159,162,163,172,176,181,183,184,185,187,188,192,193,194,195,199,200,201,204,205,206,207,213,215,216,217,218,221,222,228,232,234,239,242,243,245,246,248,249,251,252,254,255,262,263,268,269,270,272,273,275,276,277,278,279,283,285,291,292,295,296,298,299,301,304,305,307,309,310,312,313,316,317,319,322,323,326,327,329,331,333,334,340,342,344,345,347,349,352,353,354,355,356,357
Model 3 &5	167 (242): 69%	2,3,4,6,7,8,14,20,33,34,35,38,39,42,45,51,52,56,57,59,62,64,66,67,70,71,72,76,79,82,83,95,98,99,101,102,103,106,107,109,112,114,116,117,119,120,125,126,127,128,130,131,132,133,135,136,138,140,141,142,144,146,149,156,157,158,159,160,162,163,167,168,172,173,174,175,176,180,181,183,184,189,190,192,193,194,195,199,200,202,205,206,207,211,213,215,216,217,218,221,227,228,232,233,235,242,243,248,249,251,254,255,256,259,263,266,268,269,270,272,275,276,277,278,279,280,281,283,284,285,293,294,295,296,298,303,304,305,307,309,312,313,315,316,319,322,324,325,327,329,331,334,336,337,338,340,341,342,344,346,347,349,352,354,355,356,357
Model 3, 4 & 5	120 (242): 49.58%	2,3,4,6,8,20,34,35,45,51,52,56,59,64,67,70,71,72,76,79,82,83,95,98,101,102,103,106,107,109,112,114,116,117,119,120,125,127,130,133,135,138,141,142,144,146,149,156,157,158,159,162,163,172,176,181,183,184,192,193,194,195,199,200,205,206,207,213,215,216,217,218,221,228,232,242,243,248,249,251,254,255,263,268,269,270,272,275,276,277,278,279,283,285,295,296,298,304,305,307,309,312,313,316,319,322,327,329,331,334,340,342,344,347,349,352,354,355,356,357
Distribution of common test set compounds in different 2D-QSAR models		
Model 1 & 2	7 (20): 35%	6,24,38,56,62,68,82
Model 3 & 4	49 (115): 42.6%	11,13,15,18,22,24,27,30,47,49,54,55,65,77,89,105,108,124,145,153,155,191,208,210,212,214,219,223,230,241,247,250,265,271,274,282,287,289,290,314,318,320,328,330,332,339,348,350,351
Model 4 &5	35 (115): 30.43%	11,16,22,24,27,44,53,54,55,77,93,94,100,108,113,139,154,177,186,191,196,203,209,210,219,231,238,247,261,264,271,287,289,318,321
Model 3 &5	41 (115): 35.65%	11,17,19,22,23,24,26,27,28,32,48,54,55,73,75,77,80,108,129,150,170,171,191,198,210,214,219,224,247,257,260,267,271,287,289,297,302,311,318,335,343
Model 3, 4 & 5	16 (115): 13.91%	11,22,24,27,54,55,77,108,191,210,219,247,271,287,289,318



Significance of identified descriptors

We have calculated 1444 PaDEL descriptors that are related to atom count descriptors (14), autocorrelation descriptors (346), Barysz matrix descriptors (91), BCUT descriptors (6), bond count descriptors (10), Burden modified eigenvalues descriptors (96), constitutional descriptors (12), electrotopological state atom type descriptors (489), extended topochemical atom descriptors (43), information content descriptors (42), MDE descriptors (19), ring count descriptors (68), topological charge descriptors (21), path count descriptors (22), Detour matrix descriptors (11), Chi descriptors (53), Topological distance matrix descriptors (11), Walk count descriptors (20), carbon types descriptors (9) and other descriptors (57).

Autocorrelation descriptors

These molecular descriptors were calculated from a molecular graph by summing the products of atom weights of the terminal atoms of all the paths of the considered path length (the lag). Autocorrelations are calculated by Moreau-Broto (ATS), Moran (MATS) and Geary (GATS) algorithms from lag 1 to lag 8 for four different weighting schemes.[36] The symbol for each of the autocorrelation descriptors is given by two indices such as lag (d) and weight (w). The 'lag' is defined as the topological distance between pairs of atoms. The topological distance between a pair of atoms (i, j) is given in the ijth entry in the topological level matrix. The lag can have any value from the set [0, 1, 2, 3, 4, 5, 6, 7, 8]. The weight can be m (relative atomic mass), p (polarizability), e (Sanderson electronegativity), i (ionization potential), c (charges) and v (Van der Waals volume). Relative mass is defined as the ratio of atomic mass of an atom to that of a carbon. Similarly, the other three weights p, e and v are scaled by the corresponding values for the carbon. For examples, MATS2e is the Moran autocorrelation descriptor of lag 2 that is weighted by Sanderson electronegativities. GATS6m is the Geary autocorrelation descriptor of lag 6 that is weighted by mass. ATSC3i is a centered Broto-Moreau autocorrelation descriptor of lag 3 that is weighted by first ionization potential.[36] The autocorrelation descriptors (ATS, MATS, and GATS) are calculated by the following equations.

$$ATSdw = \sum_{i=1}^{n} \sum_{j=1}^{n} \delta_{ij}(w_i w_j) \qquad (3)$$

where w_i and w_j are the weights of the atoms i and j and δ_{ij} is Kronecker delta, that is, $\delta_{ij} = 1$, if the ijth entry in the topological level matrix is d, and $\delta_{ij} = 0$ otherwise.

$$MATSdw = (n)(A)/(B)$$
$$A = (1/\Delta)\left(\sum_{i=1}^{n} \sum_{j=1}^{n} \delta_{ij}(w_i - \overline{w})(w_j - \overline{w})\right) \qquad (4)$$
$$B = \sum_{i=1}^{n} (w_i - \varpi)^2$$

where w_i and w_j are the weights of the atoms i and j, ω @ (m, p, e, v) ϖ is the mean of w_i over the entire molecule, and δ_{ij} is Kronecker delta, i.e. $\delta_{ij} = 1$ if the ijth entry in the topological level matrix is d, and $\delta_{ij} = 0$ otherwise.

$$GATSdw = ((n-1)/2)(A)/(B)$$
$$A = (1/\Delta)\left(\sum_{i=1}^{n} \sum_{j=1}^{n} \delta_{ij}(w_i - w_j)^2\right) \qquad (5)$$
$$B = \sum_{i=1}^{n} (w_i - \varpi)^2$$

where w_i and w_j are the weights of the atoms i and j, ω @ (m, p, e,
v), ϖ is the mean of w_i over the entire molecule, and δ_{ij} is Kronecker delta, i.e. $\delta_{ij} = 1$ if the ijth entry in the topological level matrix is d, and $\delta_{ij} = 0$ otherwise.

Barysz distance matrix based descriptors

The descriptor Barysz distance matrix D^z is a weighted distance matrix accounting for the presence of hetero atoms and multiple bonds.[36] The ijth entry in the matrix D^z is defined as follows

$$(D^Z)_{ij} = 1-(Z_C/Z_i), \quad if\ i=j$$
$$(D^Z)_{ij} = \sum_{b=1}^{d_{ij}} Z_C^{\,2}/(\pi_b^* Z_{b(1)} Z_{b(2)}), \quad if\ i\neq j \qquad (6)$$

where Z_C is the atomic number of carbon atom, Z_i is the atomic number of the ij[th] atom and the sum runs over all the bonds 'b' in the shortest path from the atom i to the atom j, d_{ij} is the topological distance (i.e. the number of bonds from the atom i to the atom j in the molecule) is the conventional bond order of the bond 'b', i.e. 1, 2, 3 and 1.5 for single, double, triple and aromatic bonds respectively, $Z_{b(1)}$ and $Z_{b(2)}$ are the atomic numbers of the atoms on the bond 'b'.

BCUT descriptors

BCUT (Burden - CAS - University of Texas eigen values) descriptors[37] are the eigen values of a connectivity matrix known as the Burden matrix.[37] These descriptors are based on a weighted version of the Burden matrix, which takes into account of both connectivity as well as atomic properties of a molecule. The weights are a variety of atom properties placed along with the diagonal of the Burden matrix. Currently, three weighting schemes are employed including atomic weight, partial charge (Gasteiger Marsilli) and polarizability. The descriptor works with the hydrogen depleted molecule. The descriptor returns the highest and lowest eigen values for these three classes of the descriptor in a single ArrayList. It is possible to specify an arbitrarily large number of eigen values to be returned. However, if the number (i.e. nhigh or nlow) is larger than the number of heavy atoms, the remaining eigen values will be NaN. The descriptor uses nhigh value, which indicates the number of highest eigen values (1) and nlow indicates the number of lowest eigen values (1).

Burden modified eigen values

Burden modified eigen values[36] are the eigen values of a modified connectivity matrix known as the Burden matrix. The Burden matrices 'M' are defined as the diagonal elements, M_{ww} are the weights w_i for atom A_i where the weights may be some property associated with the atoms such as m (relative atomic mass), p (polarizability), e (Sanderson electronegativity) and v (Van der Waals volume). The non-diagonal elements M_{wk} are 1 if $k = d_{ij}$ and 0 otherwise, where 'k' is the lag defined as the topological distance 'd' between the atom pair i-j and may have a value between 0 and 8. Thus for a given k, the non-diagonal element M_{ij} will be unity if the atoms i and j are apart by a topological distance k and zero otherwise. The highest and lowest eigen values of these matrices will discriminate descriptors.

Molecular path count

A path (or self-avoiding walk)[36] is a walk with no vertex repeated. Atomic path count is the number of paths of length m starting from the i[th] atom to any other atom in the molecule. Molecular path count P_m is the count of all paths in the molecule of length m

$$P^m = \sum_{i=1}^{n} P_i^{\,m} \qquad (10)$$

Molecular multiple path count of order m, piPCm: w_i, the weight of a path p_i as the sum of the bond orders of the bonds in the path p_i (the bond orders are respectively 1, 2, 3 and 1.5 for single, double, triple and aromatic bonds). piPCm is defined as the sum of the weights of the paths of length *m* in the molecule.

Atom type electrotopological descriptors

These are electrotopological intrinsic state (E-state Numbers) and E-state Indices (E-state contribution)[38] in which each skeletal atom or group is assigned an intrinsic state value, I_i, as follows:

$$I_i = [(2/N)^2 \delta^v + 1]/\delta \qquad (7)$$

The intrinsic state encodes the valence state electronegativity of the atom as well as its local topology through the use of the molecular connectivity simple and valence delta values, d and d^v Perturbation on atom *i*, arising from the presence of all other atoms *j*, is a function of the difference between the intrinsic atoms: I_i - I_j. The perturbation is diminished over distance; the functional dependence of the reduction is the square of the count of atoms in the shortest path between atoms *i* and *j* (r_{ij}). Perturbations are summed over the whole molecule:

$$\Delta I_i = \sum (I_i - I_j) / r_{ij}^2 \qquad (8)$$

The electrotopological state indices are computed for each atom in a molecule and encode information about both the topological environment of that atom and the electronic interactions due to all other atoms in the molecule. The topological relationship is based on the graph distance to each other atom. The electronic aspect is based on an intrinsic state plus perturbation due to intrinsic state differences between atoms in the molecule. The electrotopological state, called the E-State, of atom *i*, S_i, is given as the sum of the intrinsic state and the perturbations:

$$S_i = I_i + \Delta I_i \qquad (9)$$

Chi connectivity indices

Chi indices[39] represent the atomic connectivity of the molecular structure as graphs, atoms as vertices and covalent bonds as edges. According to Randic, Kier and Hall, these descriptors represent the additive value of the increments assigned to the specific structural fragments in terms of order and subgraph type such as path, cluster, path/cluster and chain. The general formula for the simple chi connectivity indices ($^m\chi_t$) is as follows

$$^m\chi_t = \sum_{i=1}^{A} {}^mC_i \qquad (11)$$

where m is bond order (0: atoms, 1: fragments of one bond, 2: fragment of two bonds etc), t is a type of calculation (p: path, c: cluster, pc: path/cluster, ch: chain or cycle) and A is a number of non-hydrogen atoms

Lipophilicity (logP)

Lipophilicity[40] is the tendency of a compound to partition between two phases such as an immiscible octanol and polar aqueous water phase. LogP follows a non-linear relationship with permeability. The permeability of a compound increases linearly with logP and decreases gradually after a particular threshold. AlogP calculates lipophilicity using generated model consisting of a regression equation based on the hydrophobicity contribution of 115 atom types.[40] AlogP estimates the number of atom types including C, H, O, N, S, Se, P, B, Si and halogens. Each atom in every structure is classified into one of the 115 atom types. Then, the estimated logP for any compound is given by

$$A\log P = \sum_i n_i a_i \qquad (12)$$

where n_i is the number of atoms of type i and a_i is the corresponding hydrophobicity constant.

Petitjean topological shape index

Petitjean developed the concept of the eccentricity of a graph vertex. According to the Petitjean definition, the eccentricity of a vertex corresponds to the distance from that vertex to the most remote vertex in the graph. The distance is obtained from the distance matrix as the count of edges between the two vertices. The graph radius 'R' is defined as the smallest vertex eccentricity in the graph. The graph diameter 'D' is defined as the largest vertex eccentricity in the graph. These eccentricities can be used as a vertex (atom) in topological indices. Petitjean also defined a graph shape index [I = (D - R)/ D], which characterizes the shape of various graphs. [36]

Extended Topochemical Atom (ETA) indices

ETA indices[41] were developed based on refinement of TAU descriptors. TAU descriptors are specifically useful for the contribution of molecular functionality, branching, shape and size factors towards biological activity or physicochemical parameters. Along with TAU descriptors, ETA determines the contribution of specific vertices or positions within the common substructures of molecular graph towards total functionality.[41]The detour matrix Delta is a symmetric matrix whose $(i,j)^{th}$ entry is the length of the longest path from vertex i to vertex j, or infinity if there is no such path. The most common convention is to take Δ_{ij}= 0. There is no efficient method for finding the entries of a detour matrix, but the detour matrix can be computed by finding the set of all spanning trees for a given graph, finding their distance matrices, and setting Δ_{ij}= $\max_{i,j}$ d_{ij}, where the maximum is taken over all spanning trees.

Table S3A Distribution of common descriptors across the models

Model 1	Model 2	Model 3	Model 4	Model 5
ALogp2	AATS2i	ATSC3i	AATSC6c	AATSC5e
ATSC1e	AATSC3e	AATSC5c	GATS7c	GATS8c
ATSC5i	AATSC3i	MATS1m	SpMAD_Dzs	**BCUTc-1l**
AATSC2c	GATS6e	MATS2e	**BCUTc-1l**	SpMin1_Bhp
AATSC3p	GATS1s	GATS6m	SpMin1_Bhs	**C3SP2**
MATS7i	GATS8s	BCUTp-1l	**C3SP2**	minHBint2
MATS1s	VR1_Dzp	SpMin1_Bhv	**SHBd**	minHsOH
GATS6s	**SM1_Dzs**	**SHBd**	minHdsCH	**mindsN**
VR2_Dzp	VCH-5	**mindsN**	**mindsN**	MDEN-22
SM1_Dzs	VE2_Dt	**maxHBint2**	**maxHBint2**	**R_TpiPCTPC**
SC-5	nHsOH	**R_TpiPCTPC**	sumI	**topoShape**
nHBint3	minHssNH	SRW9	piPC10	
mindsN	maxsssCH		**topoShape**	
ETA_Epsilon_3	maxssO			
MDEC-22	ETA_Psi_1			
	nHBAcc_Lipinski			
	nFRing			

Table S3B Important descriptors and its percentage contribution in 2D-QSAR model 1.

S.No	Name [Ref]	Type	Description	Coefficient	% Contribution
1	ALogp2 [1]	ALOGP	Ghose-Crippen LogKow	0.04	3.10
2	ATSC1e [2]	Autocorrelation	Centered Broto-Moreau autocorrelation - lag 1 / weighted by Sanderson electronegativities	0.80	4.61
3	ATSC5i [2]	Autocorrelation	Centered Broto-Moreau autocorrelation - lag 5 / weighted by first ionization potential	-0.01	-4.23
4	AATSC2c[2]	Autocorrelation	Average centered Broto-Moreau autocorrelation - lag 2 / weighted by charges	-252.24	-12.17
5	AATSC3p[2]	Autocorrelation	Average centered Broto-Moreau autocorrelation - lag 3 / weighted by polarizabilities	3.70	2.73
6	MATS7i [2]	Autocorrelation	Moran autocorrelation - lag 7 / weighted by first ionization potential	1.32	3.19
7	MATS1s [2]	Autocorrelation	Moran autocorrelation - lag 1 / weighted by I-state	-5.51	-11.72
8	GATS6s [2]	Autocorrelation	Geary autocorrelation - lag 6 / weighted by I-state	0.76	4.95
9	VR2_Dzp [2]	Barysz matrix	Normalized Randic-like eigenvector-based index from Barysz matrix / weighted by polarizabilities	0.02	2.46
10	SM1_Dzs [2]	Barysz matrix	Spectral moment of order 1 from Barysz matrix / weighted by I-state	0.47	16.75
11	SC-5 [3]	Chi cluster	Simple cluster, order 5	-0.72	-3.38
12	nHBint3[4]	Atom type electrotopological state	Count of E-State descriptors of strength for potential Hydrogen Bonds of path length 3	-0.39	-9.83
13	mindsN[4]	Atom type electrotopological state	Minimum atom-type E-State: : N-	0.33	13.47
14	ETA_Epsilon_3 [5]	Extended topochemical atom	A measure of electronegative atom count	-51.49	-4.62
15	MDEC-22[6]	Molecular distance edge	Molecular distance edge between all secondary carbons	0.02	2.80

'+' % Contribution: Favorable and '-' % Contribution: Unfavorable

Table S4 Important descriptors and its percentage contribution in 2D-QSAR model 2.

S. No	Name [Ref]	Type	Description	Coefficient	% Contribution
1	AATS2i [2]	Autocorrelation	Average Broto-Moreau autocorrelation - lag 2 / weighted by first ionization potential	-0.08	-6.46
2	AATSC3e [2]	Autocorrelation	Average centered Broto-Moreau autocorrelation - lag 3 / weighted by Sanderson electronegativities	48.30	7.09
3	AATSC3i[2]	Autocorrelation	Average centered Broto-Moreau autocorrelation - lag 3 / weighted by first ionization potential	1.97	6.22
4	GATS6e[2]	Autocorrelation	Geary autocorrelation - lag 6 / weighted by Sanderson electronegativities	0.47	2.16
5	GATS1s[2]	Autocorrelation	Geary autocorrelation - lag 1 / weighted by I-state	2.72	8.60
6	GATS8s[2]	Autocorrelation	Geary autocorrelation - lag 8 / weighted by I-state	-0.79	-4.40
7	VR1_Dzp[2]	Barysz matrix	Randic-like eigenvector-based index from Barysz matrix / weighted by polarizabilities	0.00	3.53
8	SM1_Dzs[2]	Barysz matrix	Spectral moment of order 1 from Barysz matrix / weighted by I-state	0.26	7.19
9	VCH-5[4]	Chi chain	Valence chain, order 5	3.76	2.69
10	VE2_Dt[2]	Detour matrix	Average coefficient sum of the last eigenvector from detour matrix	66.97	5.44
11	nHsOH[4]	Atom type electrotopological state	Count of atom-type H E-State: -OH	-1.17	-12.76
12	minHssNH[4]	Atom type electrotopological state	Minimum atom-type H E-State: -NH-	-1.42	-4.46
13	maxsssCH [4]	Atom type electrotopological state	Maximum atom-type E-State: > CH-	-1.10	-4.95
14	maxssO [4]	Atom type electrotopological state	Maximum atom-type E-State: -O-	-0.05	-2.01
15	ETA_Psi_1 [5]	Extended topochemical atom	A measure of hydrogen bonding propensity of the molecules and/or polar surface area	-18.97	-15.09
16	nHBAcc_Lipinski	Hbond acceptor count	Number of hydrogen bond acceptors (using Lipinski's definition: any nitrogen; any oxygen)	0.11	3.66
17	nFRing	Ring count	Number of fused rings	-0.14	-3.30

'+' % Contribution: Favorable and '-' % Contribution: Unfavorable

Table S5 Important descriptors and its percentage contribution in 2D-QSAR model 3.

S.No	Name [Ref]	Type	Description	Coefficient	% Contribution
1	ATSC3i[2]	Autocorrelation	Centered Broto-Moreau autocorrelation - lag 3 / weighted by first ionization potential	0.01	3.68
2	AATSC5c[2]	Autocorrelation	Average centered Broto-Moreau autocorrelation - lag 5 / weighted by charges	-92.33	-5.35
3	MATS1m[2]	Autocorrelation	Moran autocorrelation - lag 1 / weighted by mass	-8.16	-7.02
4	MATS2e[2]	Autocorrelation	Moran autocorrelation - lag 2 / weighted by Sanderson electronegativities	-0.99	-4.11
5	GATS6m[2]	Autocorrelation	Geary autocorrelation - lag 6 / weighted by mass	-0.36	-2.12
6	BCUTp-1l[7]	BCUT	nhigh lowest polarizability weighted BCUTS	-0.47	-11.37
7	SpMin1_Bhv[2]	Burden modified eigen values	Smallest absolute eigen value of Burden modified matrix - n 1 / weighted by relative van der Waals volumes	4.16	5.43
8	SHBd[4]	Atom type electrotopological state	Sum of E-States for (strong) hydrogen bond donors	-1.47	-16.94
9	mindsN[4]	Atom type electrotopological state	Minimum atom-type E-State: : N-	0.40	15.86
10	maxHBint2[4]	Atom type electrotopological state	Maximum E-State descriptors of strength for potential Hydrogen Bonds of path length 2	0.17	9.99
11	R_TpiPCTPC[2]	Path counts	Ratio of total conventional bond order (up to order 10) with total path count (up to order 10)	-0.33	-11.23
12	SRW9[2]	Walk counts	Self-returning walk count of order 9 (ln(1+x)	-0.08	-6.91

‘+‘ % Contribution: Favorable and ‘-’ % Contribution: Unfavorable

Table S6 Important descriptors and its percentage contribution in 2D-QSAR model 4.

S.No	Name [Ref]	Type	Description	Coefficient	% Contribution
1	AATSC6c [2]	Autocorrelation	Average centered Broto-Moreau autocorrelation - lag 6 / weighted by charges	99.95	5.95
2	GATS7c [2]	Autocorrelation	Geary autocorrelation - lag 7 / weighted by charges	-1.17	-5.57
3	SpMAD_Dzs [2]	Barysz matrix	Spectral mean absolute deviation from Barysz matrix / weighted by I-state	-0.16	-6.52
4	BCUTc-1l [7]	BCUT	nhigh lowest partial charge weighted BCUTS	-6.33	-4.98
5	SpMin1_Bhs [2]	Burden modified eigen values	Smallest absolute eigen value of Burden modified matrix - n 1 / weighted by relative I-state	4.86	7.60
6	C3SP2	Carbon types	Doubly bound carbon bound to three other carbons	-0.22	-6.45
7	SHBd[4]	Atom type electrotopological state	Sum of E-States for (strong) hydrogen bond donors	-1.46	-13.96
8	minHdsCH[4]	Atom type electrotopological state	Minimum atom-type H E-State: : CH-	-2.38	-4.75
9	mindsN[4]	Atom type electrotopological state	Minimum atom-type E-State: : N-	0.26	8.06
10	maxHBint2[4]	Atom type electrotopological state	Maximum E-State descriptors of strength for potential Hydrogen Bonds of path length 2	0.19	8.94
11	sumI[4]	Atom type electrotopological state	Sum of the intrinsic state values I	0.03	11.80
12	piPC10[4]	Path counts	Conventional bond order ID number of order 10 (ln(1+x)	-0.35	-9.92
13	topoShape	Topological	Petitjean topological shape index	3.58	5.51

'+' % Contribution: Favorable and '-' % Contribution: Unfavorable

Table S7 Important descriptors and its percentage contribution in 2D-QSAR model 5.

S.No	Name [Ref]	Type	Description	Coefficient	% Contribution
1	AATSC5e [2]	Autocorrelation	Average centered Broto-Moreau autocorrelation - lag 5 / weighted by Sanderson electronegativities	-10.66	-3.47
2	GATS8c [2]	Autocorrelation	Geary autocorrelation - lag 8 / weighted by charges	-0.75	-4.22
3	BCUTc-1l[7]	BCUT	nhigh lowest partial charge weighted BCUTS	-6.81	-6.85
4	SpMin1_Bhp[2]	Burden modified eigen values	Smallest absolute eigen value of Burden modified matrix - n 1 / weighted by relative polarizabilities	8.47	11.28
5	C3SP2	Carbon types	Doubly bound carbon bound to three other carbons	-0.26	-9.10
6	minHBint2[4]	Atom type electrotopological state	Minimum E-State descriptors of strength for potential Hydrogen Bonds of path length 2	0.10	5.25
7	MinHsOH[4]	Atom type electrotopological state	Minimum atom-type H E-State: -OH	-2.00	-9.60
8	MindsN[4]	Atom type electrotopological state	Minimum atom-type E-State: : N-	0.35	13.82
9	MDEN-22[6]	Molecular distance edge	Molecular distance edge between all secondary nitroqens	-0.73	-20.78
10	R_TpiPCTPC[2]	Path counts	Ratio of total conventional bond order (up to order 10) with total path count (up to order 10)	-0.28	-9.49
11	topoShape	Topological	Petitjean topological shape index	3.37	6.14

'+' % Contribution: Favorable and '-' % Contribution: Unfavorable

Significance of identified descriptors towards Mtb permeability

Petitjean topological shape index29 is the eccentricity of a vertex corresponds to the distance from that vertex to the most remote vertex in the graph. Toposhape29 is a topological descriptor that belongs to Petitjean topological shape index, which showed positive contribution to the model 4 (5.51%) and model 5 (6.14%).

Atomic path count [29] is the number of paths of length starting from one atom to any other atom in the molecule. R_TpiPCTPC is path count descriptor in model 3 (-11.23%) and in model 5 (-9.49%) contributing negatively to the Mtb inhibitory potency and it describes the ratio of the total conventional bond order (up to order 10) with total path count (up to order 10). piPC10 descriptor in model 4 (-9.92%) represents conventional bond order ID number of order 10 (ln(1+x)) and is negatively contributing to the cell permeability. SRW9 is a walk count descriptor (-9.61) that describes the self-returning walk count of order 9 (ln(1+x)) and it showed a negative contribution to the model 3. The next descriptor C3SP2 is contributing negatively in the model 4 (-6.45) and model 5 (-9.10) that indicates the doubly bound carbon bound to three other carbons. These descriptors characterize the carbon connectivity in terms of hybridization. From the analysis, R_TpiPCTPC, piPC10, SRW9 and C3SP2 descriptors showed negative contribution and these values in a given molecule should be minimal for governing cell permeability.

Barysz distance matrix descriptor is a weighted distance matrix accounting for the presence of hetero atoms and multiple bonds.[29] VR1_Dzp and VR2_Dzp descriptors represent Randic-like eigenvector-based index from Barysz matrix that is weighted

by polarizabilities. SM1_Dzs describes spectral moment of order 1 from Barysz matrix that is weighted by I-state and SpMAD_Dzs descriptor is indicated by the spectral mean absolute deviation from Barysz matrix that is weighted by I-state. [29] From the QSAR models, we have observed that the VR2_Dzp (2.46%), SM1_Dzs (16.75%) descriptors from model 1, VR1_Dzp (3.53%), SM1_Dzs (7.19%) descriptors from model 2 showed positive contribution, whereas SpMAD_Dzs descriptor in model 4 showed negative contribution towards the Mtb inhibitory potency.

BCUT descriptors[30] are the eigen values of a connectivity matrix which takes into account of both connectivity as well as atomic properties of a molecule such as atomic weight, partial charge and polarizability. BCUTp-1l (-11.37%) descriptor from model 3 indicates nhigh lowest polarizability weighted BCUTS and descriptor BCUTc-1l (-4.98%) from model 4, BCUTc-1l (-6.85%) from model 5 indicates nhigh lowest partial charge weighted BCUTS.[30] The descriptors BCUTp-1l, BCUTc-1l from model 3 to 5 showed negative contribution to the Mtb permeability.

Burden modified eigen values[29] are the eigen values of a modified connectivity matrix associated with the atomic properties such as relative atomic mass, polarizability, Sanderson electronegativity and Van der Waals volume. The descriptors SpMin1_Bhv (5.43%) from model 3, SpMin1_Bhs (7.60%) from model 4, SpMin1_Bhp (11.28%) from model 5 indicated that the smallest absolute eigen value of the Burden modified matrix - n 1, that is weighted by relative Van der Waals volumes, relative I-state and relative polarizabilities respectively and these properties showed positive contribution towards Mtb cell permeability. Hence, the increased optimal level of the descriptor values in a molecule could improve inhibitory potency against drug resistant Mtb strains.

Molecular Distance Edge (MDE)[34] descriptors are a set of 19 molecular graph-theoretical indices. The descriptors are designed to capture the structure and interaction between atoms in a molecular graph. The descriptor MDEC-22 (2.80%) in model 1 explains the molecular distance edge between all secondary carbons, which is directly proportional to the inhibitory potency, whereas the descriptor MDEN-22 (-20.78%) in model 5 describes the molecular distance edge between all secondary nitrogens, which is negatively contributing to the inhibitory potency.[34] Hence, the presence of molecular distance edge between all the secondary carbons in a molecule (model 1) could be favorable, whereas in model 5, the distance edge between all secondary nitrogens could be minimal for the better inhibitory potency.

Chi indices[31] represent the atomic connectivity of the molecular structure as graphs, atoms as vertices and covalent bonds as edges. SC-5 descriptor belongs to chi cluster category, which represents simple cluster, order 5. In model 1, SC-5 contributes negatively (-3.38%) to the Mtb cell permeability. Another descriptor, VCH-5 belongs to chi chain category, which indicates valence chain, order 5. VCH-5 descriptor is calculated using graph isomorphism to identify the various fragments and it showed positive contribution (2.69%) to the model 2.[31] Hence, the substitution of chi chain category, order 5 containing fragments in a molecule could provide better permeability.

Extended Topochemical Atom (ETA) indices[32] are developed based on refinement of TAU descriptors, which are specifically useful for the contribution of molecular functionality, branching, shape and size factors towards biological activity or physicochemical parameters. Along with TAU descriptors, ETA determines the contribution of specific vertices or positions within the common substructures of molecular graph towards total functionality. The descriptor ETA_Epsilon_3 belongs to ETA class of topological descriptors that gives a count of electronegative atom. It is contributing negatively (-4.62%) to the model.[32] Another ETA descriptor ETA_Psi_1 is also contributing negatively to the model (-15.09%) that represents a measure of hydrogen bonding propensity of the molecules and/or polar surface area. The detour matrix Delta[29] is another topological index used to understand structure-property relationships. The descriptor VE2_Dt belongs to Detour matrix, which showed positive contribution (5.44%) for cell permeability. SumI descriptor[30] represents a sum of the intrinsic state values I and showed positive contribution (11.80%) in model 4. SHBd descriptor in model 3 (-16.94%) and in model 4 (13.96%) represents the sum of E-States for strong hydrogen bond donors, which is negatively contributing to the Mtb inhibitory potency.[30] Hence, more number of strong hydrogen bond donors in a molecule may be unfavorable for gaining inhibitory potency.

Table S8 Confusion matrix parameters for model validation.

Parameter (%)	**Significance/Formula**
Accuracy (AC)	proportion of total number of correct predictions =[(A+D)/(A+B+C+D)]*100
True positive rate (TP) or Sensitivity	proportion of correctly identified active molecules = [D/(C+D)] *100
False positive rate (FP)	proportion of incorrectly identified inactive molecules = [B/(A+B)] *100
True negative rate (TN) or Specificity	proportion of correctly identified inactive molecules = [A/(A+B)] *100
False negative rate (FN)	proportion of incorrectly identified active molecules = [C/(C+D)] *100
Precision (PR)	proportion of correctly identified active molecules out of the total identified active molecules = [D/(B+D)] *100

A: true negatives, B: false positives, C: false negatives and D: true positives.

Table S9 Confusion matrix generated for the permeability 2D-QSAR models .

	Training set (Strategy I: 64, Strategy II: 242)									
Confusion matrix	Actual (Actives/ Inactives) in M1: 23/41, M2: 21/43, M3: 207/35, M4: 207/35 and M5: 194/48									
	Inactive (Predicted)					Active (Predicted)				
	Model 1	Model 2	Model 3	Model 4	Model 5	Model 1	Model 2	Model 3	Model 4	Model 5
Inactive (Actual)	A : 41	A : 42	A : 22	A : 27	A : 34	B : 0	B : 1	B : 13	B : 8	B : 14
Active (Actual)	C : 1	C : 1	C : 2	C : 6	C : 1	D : 22	D : 20	D : 205	D : 201	D : 193
	Test set (Strategy I: 20, Strategy II: 115)									
	Actual (Actives/ Inactives) in M1: 6/14, M2: 8/12, M3: 95/20, M4: 95/20 and M5: 108/7									
Confusion matrix	Inactive (Predicted)					Active (Predicted)				
	Model 1	Model 2	Model 3	Model 4	Model 5	Model 1	Model 2	Model 3	Model 4	Model 5
Inactive (Actual)	A : 13	A : 12	A :11	A : 13	A : 3	B : 1	B : 0	B : 9	B : 7	B : 4
Active (Actual)	C : 1	C : 1	C : 1	C : 5	C : 0	D : 5	D : 5	D : 94	D : 90	D : 108
	External Validation Set (9804 compounds with reported MIC values)									
Confusion matrix	Actual (Actives/ Inactives) in M1: 2341/3812, M2: 2746/4288, M3: 2665/4384, M4: 3453/6146 and M5: 3020/4999									
	Inactive (Predicted)					Active (Predicted)				
	Model 1	Model 2	Model 3	Model 4	Model 5	Model 1	Model 2	Model 3	Model 4	Model 5
Inactive (Actual)	A : 1744	A : 1724	A : 1361	A : 484	A : 1068	B : 2068	B : 2564	B : 3023	B : 5662	B : 3931
Active (Actual)	C : 708	C : 727	C : 683	C : 166	C : 513	D : 1633	D : 2019	D : 1982	D : 3287	D : 2507

Confusion matrix was generated to evaluate the performance of the classification models (M1: Model 1, M2: Model 2, M3: Model 3, M4: Model 4, M5: Model 5) containing training set, test set, and validation set. Each dataset was divided into two classes i.e. actives (pMIC ≥5) and inactives (pMIC <5). The predictive ability of the model was evaluated by comparing the experimental activity with predicted activity in terms of A: true negatives (predicting inactives as inactives), B: false positives (predicting inactives as actives), C: false negatives (predicting actives as inactives) and D: true positives (predicting actives as actives).

Table S10 Confusion matrix results for the obtained 2D-QSAR models.

Par	Model 1			Model 2			Model 3			Model 4			Model 5		
	Tr	Te	Val	Tr	Te	Val	Tr	Te	Val	Tr	Te	Val	Tr	Te	Val
AC	98.4	90.0	54.9	96.9	94.4	53.2	93.8	91.3	47.4	94.2	89.6	39.3	93.8	96.5	44.6
TP	95.7	83.3	70.0	95.2	83.3	73.5	99.0	98.9	74.4	97.1	94.7	95.2	99.5	100	83.0
FP	0.0	7.1	54.2	2.3	0.0	59.8	37.1	45.0	69.0	22.9	35.0	92.1	29.2	57.1	78.6
TN	100	92.9	45.8	97.7	100	40.2	62.9	55.0	31.0	77.1	65.0	7.9	70.8	42.9	21.4
FN	4.3	16.7	30.2	4.8	16.7	26.5	1.0	1.1	25.6	2.9	5.3	4.8	0.5	0.0	17.0
PR	100	83.3	44.1	95.2	100	44.1	94.0	91.3	39.6	96.2	92.8	36.7	93.2	96.4	38.9

The table shows the ranges of the true positive rate (95-100%, 83-100% & 70-95%), true negative rate (63-100%, 43-100% & 8-45%), accuracy (94-98%, 90-97% & 40-55%), precision (93-100%, 83-100% & 37-44%), false negative rate (0.5-5%, 0-17% & 5-30%), and false positive rate (0-37%, 0-57% & 54-92%) for the training set, test set and validation set in all five models respectively. Par: Parameters, AC: Accuracy, PR: Precision, TP: True positive rate, TN: True negative rate FN: False negative rate, FP: False positive rate, Tr: training set, Te: test set and Val: validation set.

Table S11 Validation of 2D-QSAR models with known Mtb drugs (27) and clinical candidates (5).

Mtb drugs/ clinical candidates	Model 1	Model 2	Model 3	Model 4	Model 5	OP	Consensus model
1-1-Pyrazinamide-DB00339	6.83	9.23	7.49	8.71	6.22	5	7.70
2-4-PAS-DB00233	4.75	5.60	8.02	10.29	7.65	4	7.26
III-Delamanid *	6.38	7.87	5.80	8.67	7.09	5	7.16
II-PA-824-CID-456199 *	5.93	8.78	5.95	8.12	6.69	5	7.10
2-4-Terizidone-CID-65720	8.46	7.43	6.63	5.87	6.57	5	6.99
1-1-Isoniazid-DB00951	5.73	6.99	5.81	8.62	7.09	5	6.85
2-3-Levofloxacin-DB01137	6.17	5.85	6.36	8.73	6.84	5	6.79
2-3-Ofloxacin-DB01165	6.17	5.85	6.36	8.73	6.84	5	6.79
2-4-Linezolid-DB00601	5.04	6.05	6.38	8.22	8.00	5	6.74
2-3-MoxifloxacinDB00218	4.93	6.01	5.54	8.32	6.85	4	6.33
2-3-Gatifloxacin-DB01044	5.64	6.43	5.30	7.91	6.09	5	6.27
2-4-Ethionamide-DB00609	5.43	6.60	4.89	7.62	6.16	4	6.14
3-5-Imipenem-DB01598	4.69	5.28	6.62	5.90	7.94	4	6.08
IIa-Sutezolid-CID-465951 *	3.60	4.87	6.10	7.82	7.40	3	5.96
2-3-Ciprofloxacin-DB00537	5.30	5.85	5.14	7.17	5.53	5	5.80
IIa-AZD5847 *	5.66	7.20	4.68	5.02	6.08	4	5.73
3-5-Clavulanate-DB00766	4.76	5.31	6.01	6.17	5.96	4	5.64
2-4-Cycloserine-DB00260	5.14	8.16	4.28	6.30	3.94	3	5.56
2-4-Thioacetazone	5.41	3.70	6.45	5.74	5.92	4	5.44
3-5-Clofazimine-DB00845	6.35	4.40	3.10	8.25	4.79	2	5.38
II-SQ109-CID-5274428 *	3.15	3.18	6.51	6.55	7.37	3	5.35
2-4-Prothionamide	4.65	4.64	5.19	7.34	4.58	2	5.28
1-1-Ethambutol-DB00330	4.50	4.24	5.67	6.20	5.38	3	5.20
2-2-Kanamycin-DB01172	3.35	7.76	1.70	3.01	7.93	2	4.75
3-5-Amoxicillin-DB01060	1.39	5.25	4.32	5.77	6.35	3	4.62
3-Calcitriol-DB00136	4.12	1.34	4.82	5.62	6.19	2	4.42
3-Thioridazine-DB00679	1.87	2.07	4.96	6.38	6.12	2	4.28
2-2-Amikacin-DB00479	2.54	5.05	1.64	3.05	8.12	2	4.08
3-5-Cilastatin-DB01597	1.32	5.02	3.77	4.11	5.39	2	3.92
2-2-Capreomycin-DB00314	3.35	10.69	1.15	0.50	3.20	1	3.78
2-2-Viomycin-CID-3037981	3.47	8.99	0.40	-0.25	3.14	1	3.15
2-2-Streptomycin-DB01082	0.62	6.47	-0.09	0.08	7.14	2	2.84

OP: occurrence of prediction, * represents clinical candidates.

Table S12 Identified level 1 scaffolds from the active dataset of compounds.

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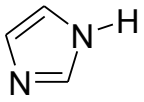
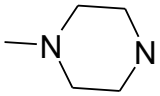
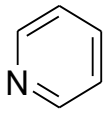
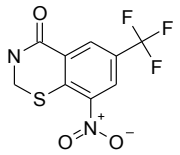
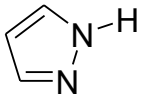
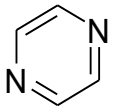
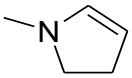
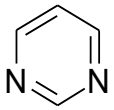
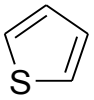
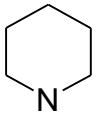
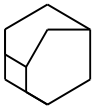
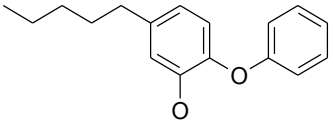
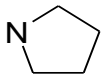
1 (170)		9 (13)	
2 (126)		10 (9)	
3 (50)		11 (7)	
4 (45)		12 (6)	
5 (20)		14 (5)	
6 (14)		13 (5)	
7 (13)		15 (3)	
8 (13)			

OS: occurrence of scaffold

Table S13 Identified level 3 scaffolds from the active dataset of compounds.

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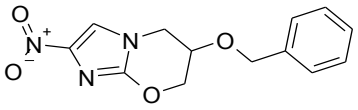
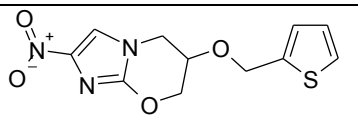
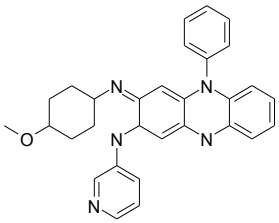
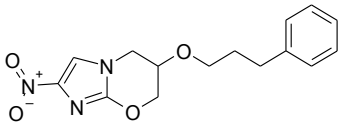
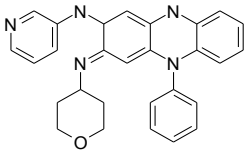
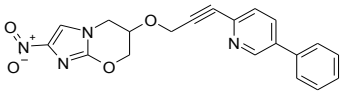
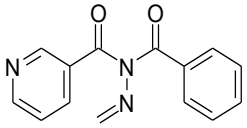
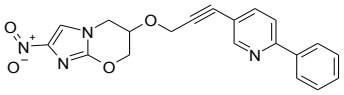
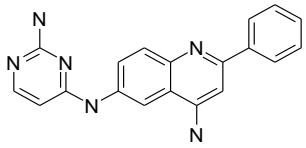
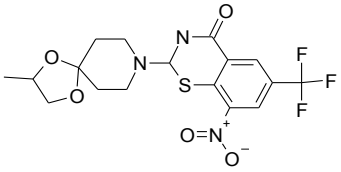
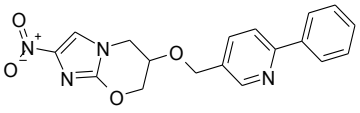
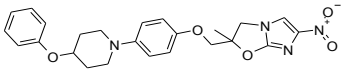
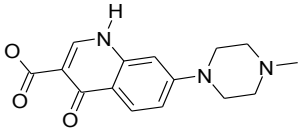
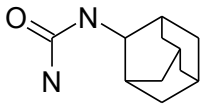
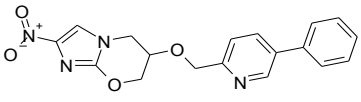
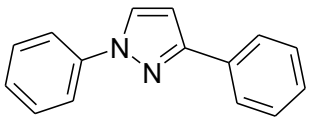
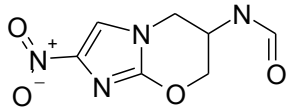
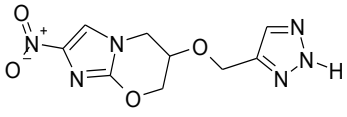
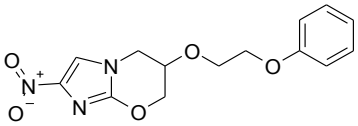
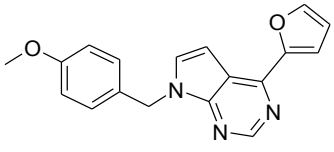
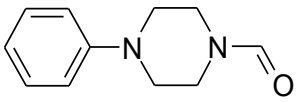
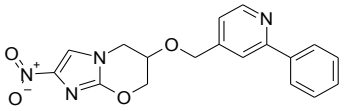
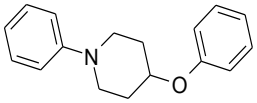
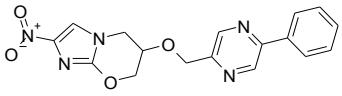
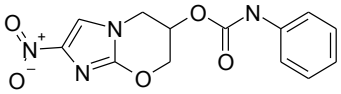
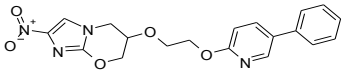
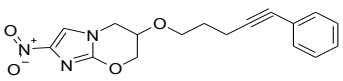
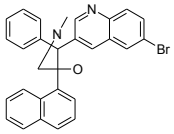
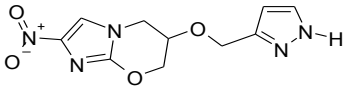
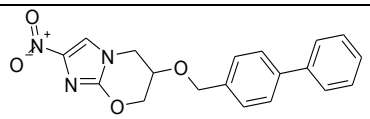
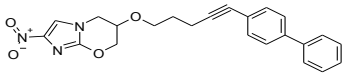
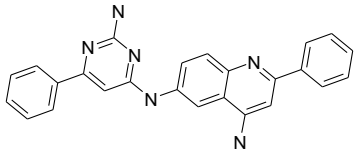
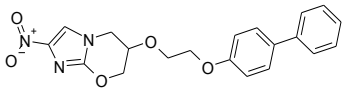
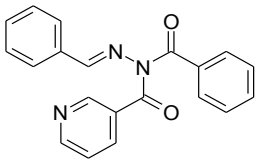
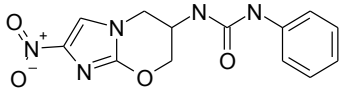
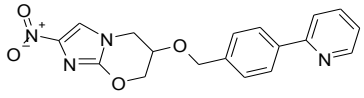
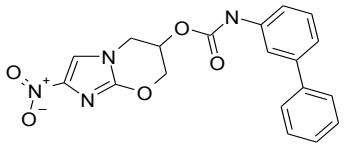
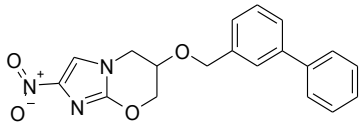
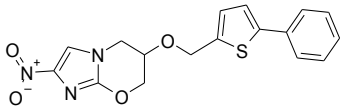
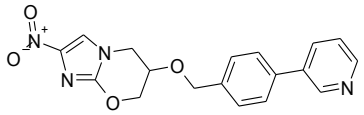
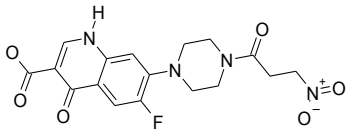
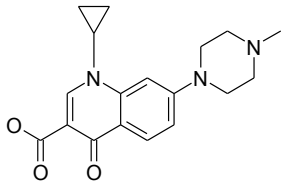
1_1_1 (65)		1_1_10 (4)	
2_1_1 (15)		1_1_8 (4)	
2_1_2 (13)		1_1_12 (4)	
2_5_1 (10)		1_1_11 (4)	
2_2_1 (10)		6_3_1 (4)	
1_1_2 (9)		1_2_1 (4)	
9_1_1 (7)		3_8_1 (3)	
1_1_3 (7)		11_1_1 (3)	
1_1_5 (6)		1_1_16 (3)	
1_1_4 (6)		5_2_1 (3)	

Scaffold_ID (OS)	Scaffold structure	Scaffold_ID (OS)	Scaffold structure
3_5_1 (5)		1_1_14 (3)	
6_1_1 (5)		1_1_15 (3)	
1_1_6 (5)		1_1_13 (3)	
1_1_7 (5)		2_4_2 (3)	
1_1_9 (4)			

OS: occurrence of scaffold

Table S14 Identified level 4 scaffolds from the active dataset of compounds.

Scaffold_ID (OS)	Scaffold structure	Scaffold_ID (OS)	Scaffold structure
1_1_1_1 (47)		1_1_7_1 (4)	
2_2_1_1 (9)		1_1_4_1 (3)	
2_5_1_1 (9)		1_1_5_1 (3)	
1_1_1_4 (5)		1_1_6_1 (3)	
1_1_1_3 (5)		1_1_10_1 (3)	
1_1_1_2 (5)		3_5_1_1 (3)	
9_1_1_1 (5)			

OS: occurrence of scaffold

S.No	Descriptors in Model	r2	Pred_r2	*Difference of Pred_r2
1	10	0.8762	0.7599	-0.0088
2	11	0.8912	0.7687	-0.0066
3	12	0.898	0.7753	-0.0265
4	13	0.9092	0.8018	-0.022
5	14	0.9196	0.8238	-0.0233
6	**15**	**0.9288**	**0.8471**	**0.0382**
7	16	0.9399	0.8089	0.017
8	17	0.9465	0.7919	-0.0159
9	18	0.9501	0.8078	0.0304
10	19	0.9571	0.7774	-0.0184
11	20	0.9615	0.7958	0.7958

S.No	Descriptors in Model	r2	Pred_r2	*Difference of Pred_r2
1	10	0.8382	0.5233	-0.0818
2	11	0.8644	0.6051	-0.101
3	12	0.8899	0.7061	-0.0064
4	13	0.9029	0.7125	-0.0371
5	14	0.9145	0.7496	-0.0407
6	15	0.925	0.7903	-0.0054
7	16	0.9375	0.7957	-0.0114
8	**17**	**0.9436**	**0.8071**	**-0.0026**
9	18	0.9486	0.8097	0.0128
10	19	0.9529	0.7969	0.0002
11	20	0.9566	0.7967	0.7967

* pred_r^2 values for (factor $_{n+1}$ – factor $_n$)

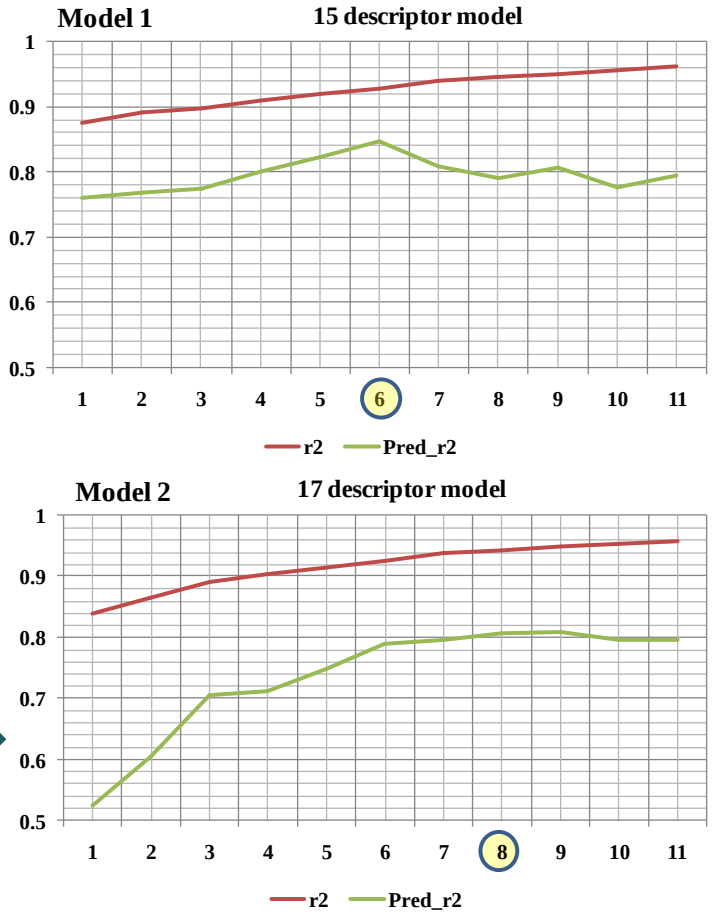
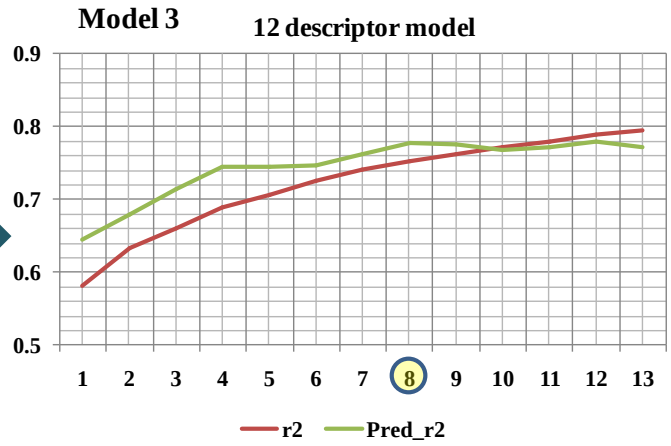
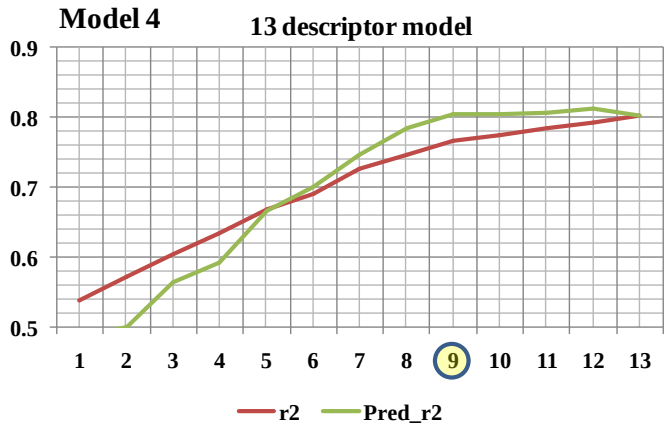


Fig. S1 The selection of optimal set of descriptors for Model 1 and Model 2.

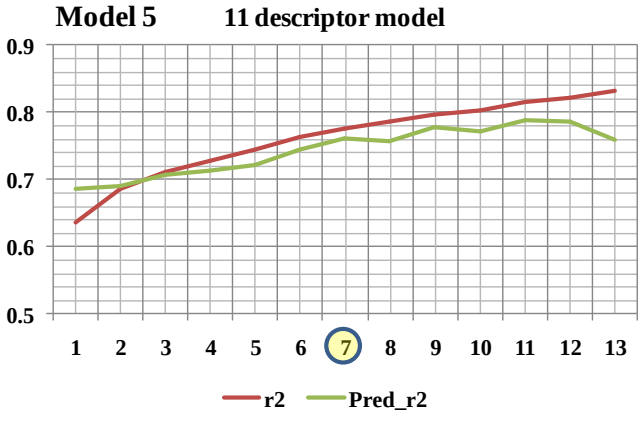
S.No	Descriptors in Model	r2	Pred_r2	*Difference of Pred_r2
1	5	0.5815	0.6454	0.035
2	6	0.6339	0.6803	0.034
3	7	0.6599	0.7147	0.030
4	8	0.6887	0.7443	0.001
5	9	0.7055	0.7451	0.002
6	10	0.7247	0.7471	0.016
7	11	0.7415	0.7629	0.015
8	**12**	**0.7524**	**0.778**	**-0.003**
9	13	0.763	0.7751	-0.007
10	14	0.7714	0.768	0.004
11	15	0.7795	0.7718	0.009
12	16	0.7884	0.7804	-0.008
13	17	0.7957	0.7722	-0.028
14	18	0.8023	0.7441	0.013



S.No	Descriptors in Model	r2	Pred_r2	*Difference of Pred_r2
1	5	0.5395	0.486	0.014
2	6	0.5731	0.5	0.065
3	7	0.6046	0.5646	0.028
4	8	0.6342	0.5927	0.074
5	9	0.6677	0.667	0.034
6	10	0.6913	0.701	0.047
7	11	0.7271	0.7475	0.037
8	12	0.7459	0.7849	0.019
9	**13**	**0.7662**	**0.8043**	**0.000**
10	14	0.7749	0.8041	0.003
11	15	0.7838	0.8076	0.004
12	16	0.7928	0.8118	-0.008
13	17	0.803	0.8035	0.006
14	18	0.8118	0.8091	0.004



S.No	Descriptors in Model	r2	Pred_r2	*Difference of Pred_r2
1	5	0.6359	0.6857	0.005
2	6	0.6868	0.6907	0.016
3	7	0.7112	0.7064	0.007
4	8	0.7269	0.7132	0.009
5	9	0.7441	0.7222	0.021
6	10	0.7623	0.7436	0.018
7	**11**	**0.7751**	**0.7615**	**-0.005**
8	12	0.7869	0.7569	0.020
9	13	0.7956	0.7768	-0.005
10	14	0.8029	0.7723	0.015
11	15	0.8153	0.7875	-0.001
12	16	0.8225	0.7866	-0.027
13	17	0.8329	0.7592	0.008
14	18	0.8382	0.7675	-0.006



* pred_r^2 values for (factor $_{n+1}$ – factor $_n$)

Fig. S2 The selection of optimal set of descriptors for Model 3, Model 4 and Model 5.

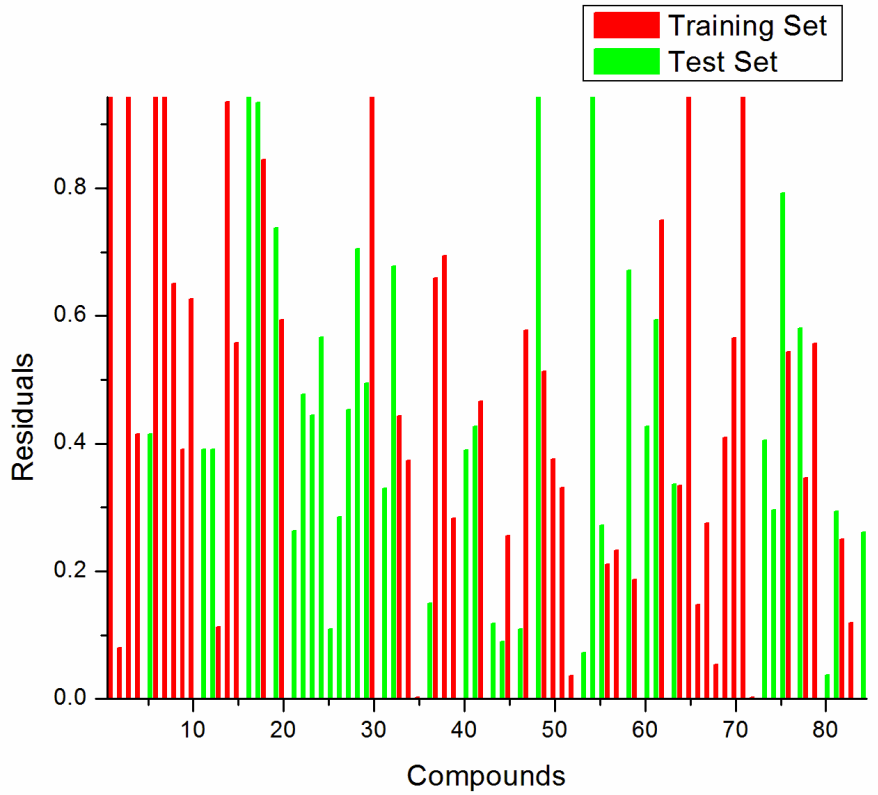


Fig. S3 Residual Bar graph for 2D-QSAR model 1.

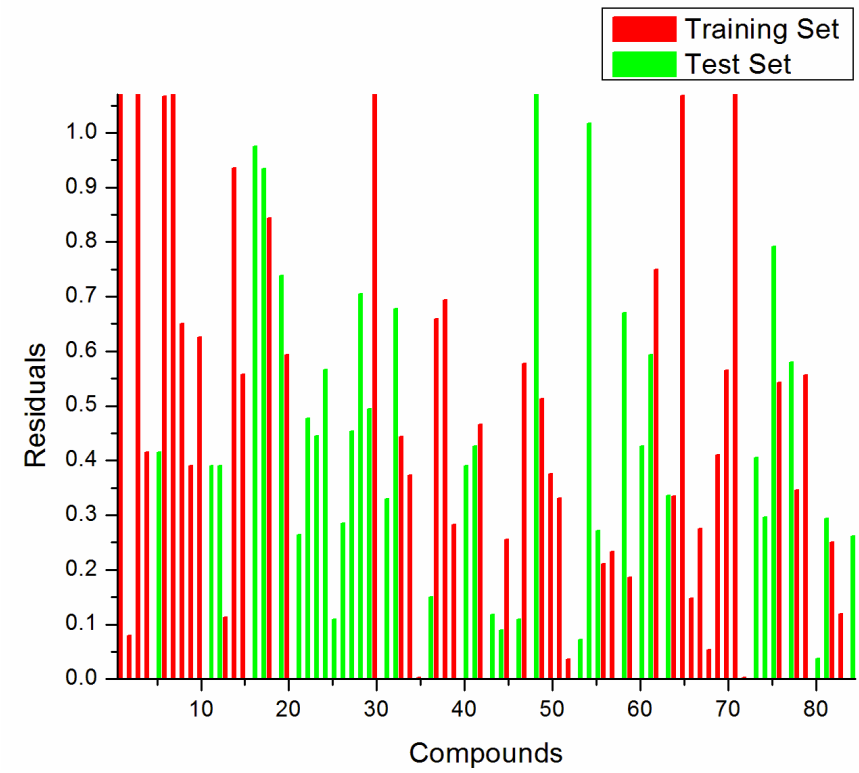


Fig. S4 Residual Bar graph for 2D-QSAR model 2.

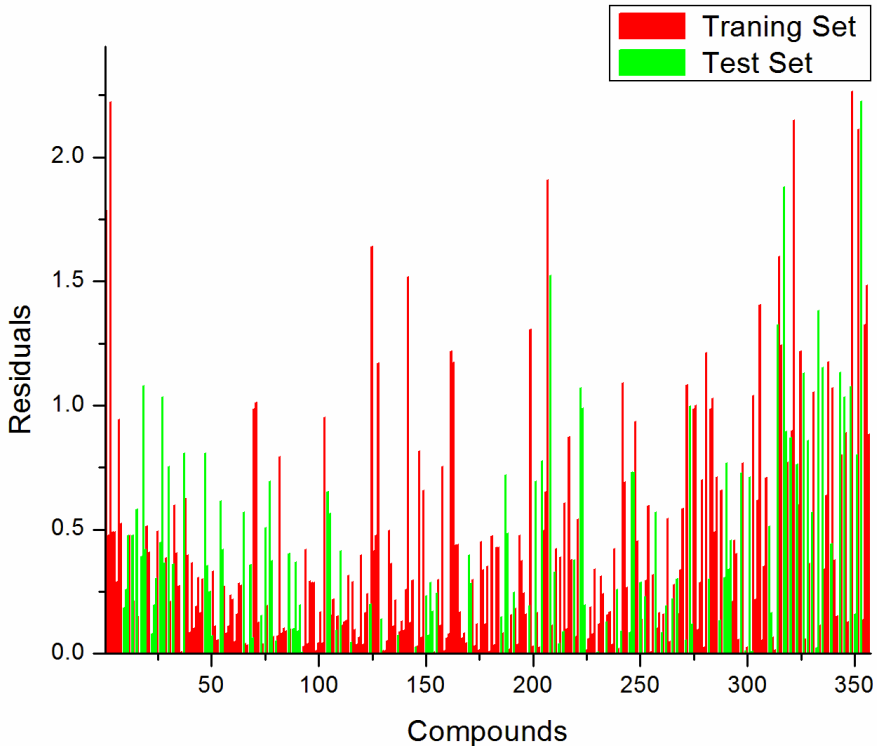


Fig. S5 Residual Bar graph for 2D-QSAR model 3.

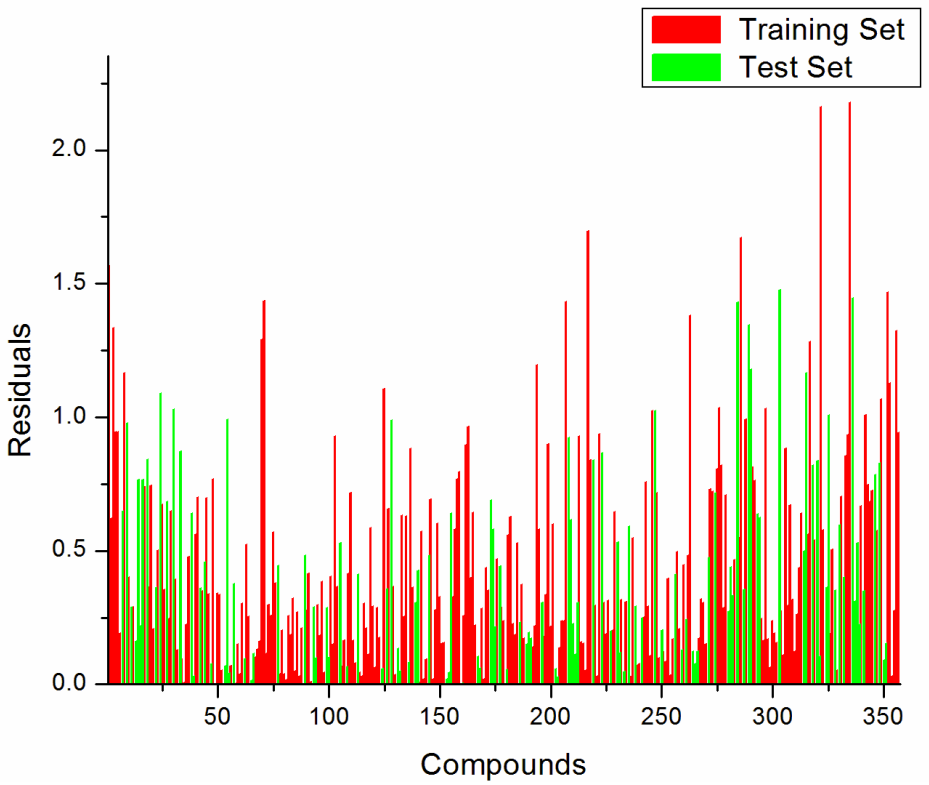


Fig. S6 Residual Bar graph for 2D-QSAR model 4.

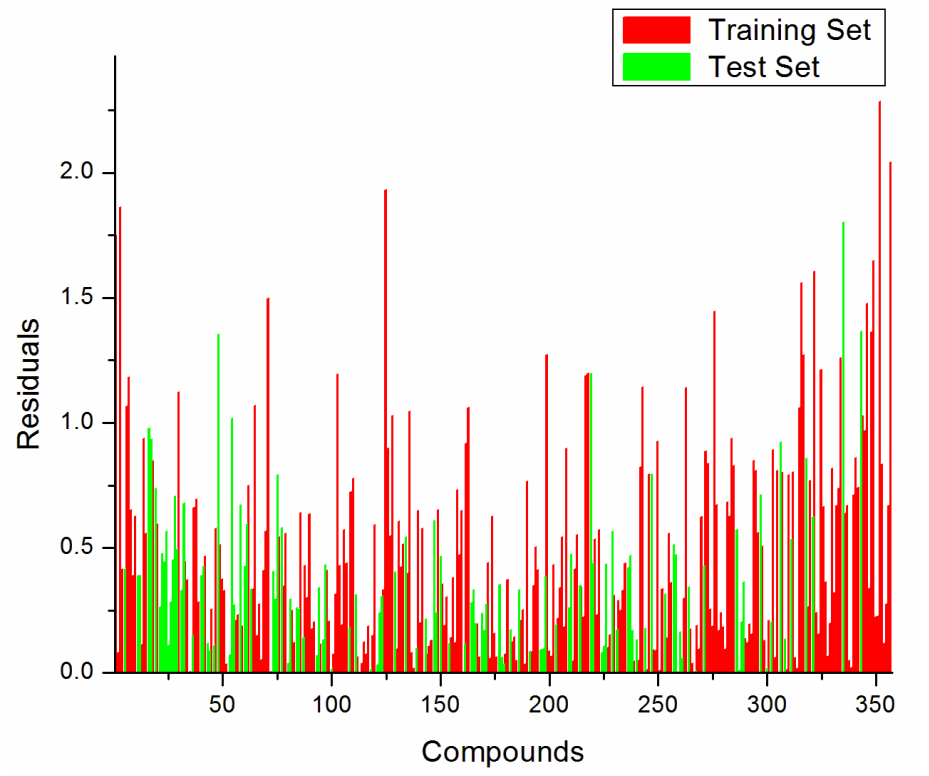


Fig. S7 Residual Bar graph for 2D-QSAR model 5.

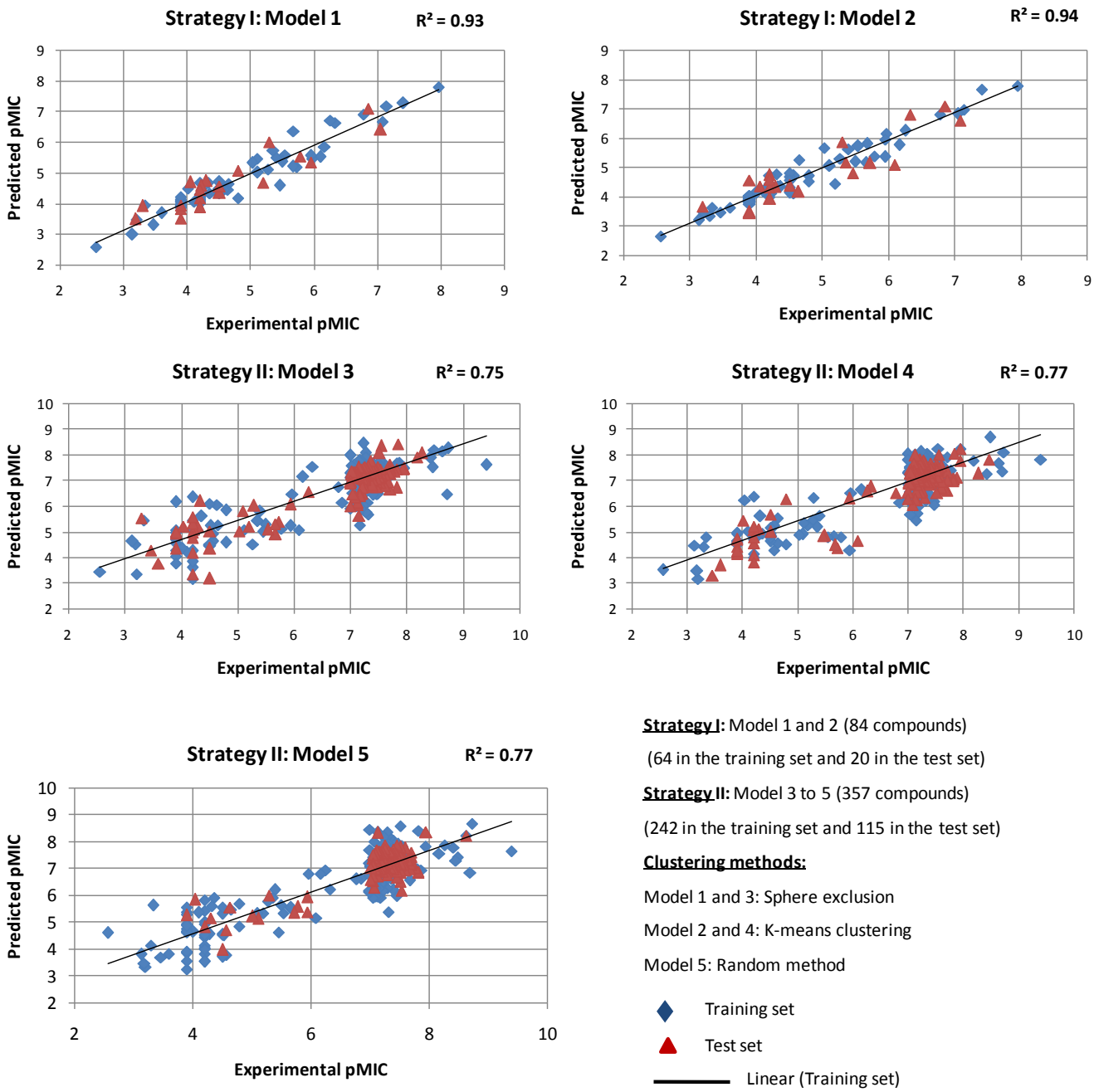


Fig. S8A Distribution of experimental and predicted pMIC values in different training and test sets. The data set compounds (strategy I: 84 compounds and strategy II: 357 compounds) were classified into five different training and test sets using sphere exclusion (model 1 & 3), k-means clustering (model 2 & 4) and random methods (model 5). In strategy I, 84 compounds were divided into 64, 20 as training set and test set respectively, whereas in strategy II, 357 compounds were divided into 242, 115 as training set and test set respectively.

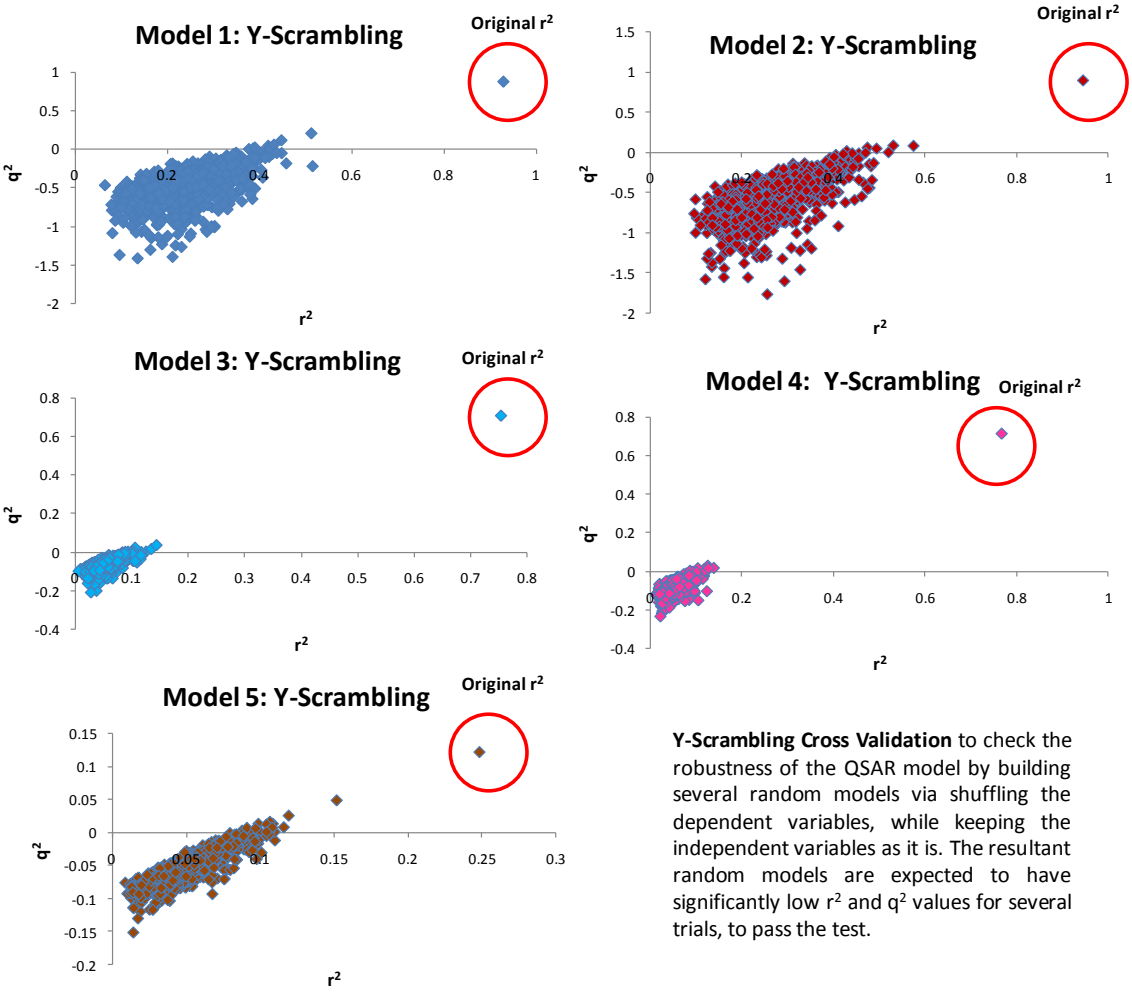


Fig. S8B Y-Scrambling cross validation analysis on the developed five QSAR models. From the models we observed that the original r^2 value is higher in all the models as compared to Y-scrambled 1000 models.

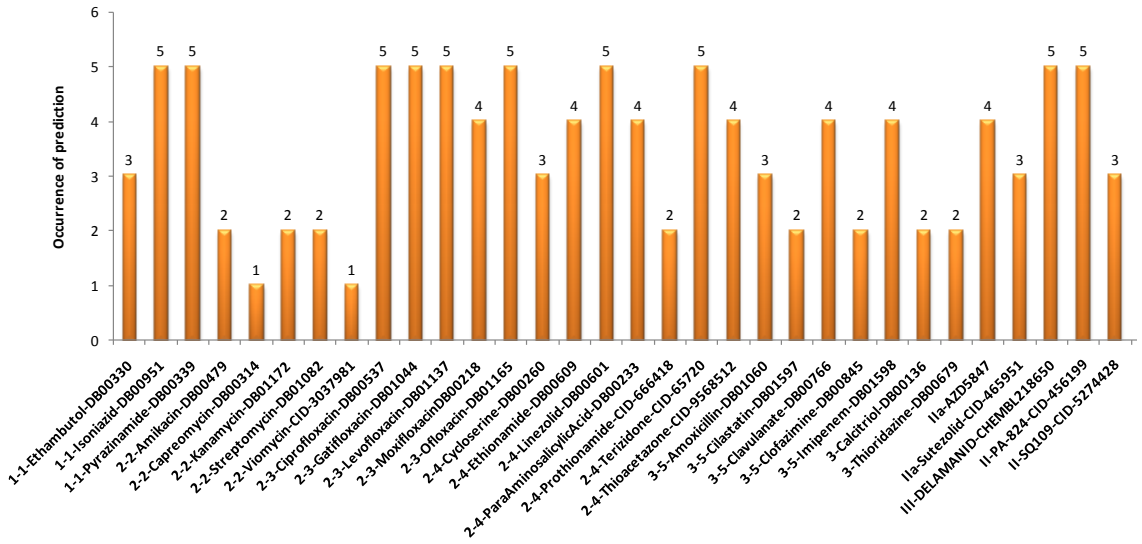


Fig. S9 Occurrence of prediction of Mtb drugs/clinical candidates using QSAR models. The predictive ability of QSAR models was tested with known Mtb drugs (27) and clinical candidates (5). The cut-off filter (pMIC ≤12 and pMIC ≥4) was applied for the best predicted compounds. The occurrence of prediction for each molecule among the QSAR models was displayed at the top of each bar. A total of 10, 7, 5, 8, 2 compounds were prioritized in all five, any four, any three, any two and any one of the models.

References

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2. R. Todeschini and V. Consonni, *Molecular Descriptors for Chemoinformatics*, Wiley-VCH Verlag GmbH & Co. kGaA, Second, Revised and Enlarged Edition edn., 2009.
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6. S. Liu, C. Cao and Z. Li, *J. Chem. Inf. Comput. Sci.*, 1998, **38**, 387-394.
7. R. S. Pearlman and K. M. Smith, *J. Chem. Inf. Comput. Sci.*, 1999, **39**, 28-35.

PRIVILEGED SCAFFOLDS

Identified Previledged Scaffolds				
Scaffold_ID	**Scaffolds_SMILE**	**Molset Size**	**Level**	mol_weight
1	c1c[nH]cn1	170	L1	68.0773
2	c1ccccn1	126	L1	79.0999
3	NC=O	50	L1	45.0406
4	c1cnccn1	45	L1	80.088
5	c1ccncn1	20	L1	80.088
6	C1CCCNC1	14	L1	85.1475
7	c1occc1	13	L1	68.074
8	N1CCCC1	13	L1	71.121
9	CN1CCNCC1	13	L1	100.162
10	c1nc(=O)c2cc(cc(c2s1)[N+](=O)[O-])C(F)(F)F	9	L1	278.208
11	c1c[nH]nc1	7	L1	68.0773
12	CN1C=CCC1	6	L1	83.1317
14	c1cccs1	5	L1	84.1396
13	C12CC3CC(CC(C3)C1)C2	5	L1	136.234
15	CCCCCc1ccc(Oc2ccccc2)c(O)c1	3	L1	256.339
1_1	[O-][N+](=O)c1cn2CCCOc2n1	159	L2	169.138
2_1	c1ncccc1Nc1cc2nc3ccccc3n(c2cc1=N)c1ccccc1	42	L2	365.43
2_2	c1ccc(nc1)c1ccccc1	32	L2	155.196
2_3	c1ccc(cn1)c1ccccc1	24	L2	155.196
2_4	c1nc2ccccc2cc1	14	L2	129.159
3_1	N(C=O)c1ccccc1	14	L2	121.137
2_5	C(=O)NCc1cccnc1	12	L2	136.151
3_3	C(=O)NCc1ccccc1	12	L2	135.163
3_4	c1ccc(cc1)C(=O)NC	11	L2	135.163
9_1	c1cc(N2CCN(CC2)C)ccc1	10	L2	176.258
3_5	N1CCN(CC1)C=O	6	L2	114.146
1_2	CC1(COc2ccccc2)Cn2cc(nc2O1)[N+](=O)[O-]	6	L2	275.26
6_2	N1CCC(CC1)Oc1ccccc1	6	L2	177.243
6_1	C1CCCN(C1)c1ccccc1	6	L2	161.243
3_7	C(=O)N1CCCC1	5	L2	99.1311
6_3	C1CCN(CC1)c1nc(=O)c2cc(cc(c2s1)[N+](=O)[O-])C(F)(F)F	5	L2	361.339
5_2	c1c(ncnc1)c1occc1	5	L2	146.146
11_1	c1cn(nc1)c1ccccc1	5	L2	144.173
12_1	COc1ccc(CN2C=CCC2)cc1	5	L2	189.254
3_8	O=C(N)NC1CCCCC1	4	L2	142.199

5_3	COc1ccc(Cn2ccc3cncnc23)cc1	4	L2	239.273
5_4	c1cnc(nc1)c1ccccc1	3	L2	156.184
9_3	N1CCN(Cc2ccccc2)CC1	3	L2	176.258
8_2	COc1c(N2CCCC2)c(F)cc2c(=O)ccn(C3CC3)c12	3	L2	302.343
1_1_1	[O-][N+](=O)c1cn2CC(COc2n1)OCc1ccccc1	65	L3	275.26
2_1_1	COC1CCC(CC1)/N=c1/cc2n(c3ccccc3)c3ccccc3nc2cc1Nc1cccnc1	15	L3	477.6
2_1_2	c1ncccc1Nc1cc2nc3ccccc3n(c2cc\1=N/C1CCOCC1)c1ccccc1	13	L3	449.547
2_5_1	C=NN(C(=O)c1ccccc1)C(=O)c1cccnc1	10	L3	253.256
2_2_1	c1cc(Nc2ccc3nc(cc(N)c3c2)c2ccccc2)nc(N)n1	10	L3	328.371
1_1_2	[O-][N+](=O)c1cn2CC(COc2n1)OCc1ccc(nc1)c1ccccc1	9	L3	352.344
9_1_1	OC(=O)c1c[nH]c2cc(N3CCN(CC3)C)ccc2c1=O	7	L3	287.314
1_1_3	[O-][N+](=O)c1cn2CC(COc2n1)OCc1ccc(cn1)c1ccccc1	7	L3	352.344
1_1_5	[O-][N+](=O)c1cn2CC(COc2n1)NC=O	6	L3	212.163
1_1_4	[O-][N+](=O)c1cn2CC(COc2n1)OCCOc1ccccc1	6	L3	305.286
3_5_1	c1cc(N2CCN(CC2)C=O)ccc1	5	L3	190.242
6_1_1	c1ccc(cc1)N1CCC(CC1)Oc1ccccc1	5	L3	253.339
1_1_6	[O-][N+](=O)c1cn2CC(COc2n1)OC(=O)Nc1ccccc1	5	L3	304.258
1_1_7	[O-][N+](=O)c1cn2CC(COc2n1)OCCCC#Cc1ccccc1	5	L3	327.335

1_1_9	[O-]\[N+](=O)c1cn2CC(COc2n1)OCc1cc[nH]n1	4	L3	265.225
1_1_10	[O-]\[N+](=O)c1cn2CC(COc2n1)OCc1cccs1	4	L3	281.288
1_1_8	[O-]\[N+](=O)c1cn2CC(COc2n1)OCCCc1ccccc1	4	L3	303.313
1_1_12	[O-]\[N+](=O)c1cn2CC(COc2n1)OCC#Cc1ccc(cn1)c1ccccc1	4	L3	376.365
1_1_11	[O-]\[N+](=O)c1cn2CC(COc2n1)OCC#Cc1ccc(nc1)c1ccccc1	4	L3	376.365
6_3_1	CC1COC2(CCN(CC2)c2nc(=O)c3cc(cc(c3s2)\[N+](=O)\[O-])C(F)(F)F)O1	4	L3	433.402
1_2_1	CC1(COc2ccc(cc2)N2CCC(CC2)Oc2ccccc2)Cn2cc(nc2O1)\[N+](=O)\[O-]	4	L3	450.487
3_8_1	O=C(N)NC1C2CC3CC(CC1C3)C2	3	L3	194.273
11_1_1	c1cn(nc1c1ccccc1)c1ccccc1	3	L3	220.269
1_1_16	[O-]\[N+](=O)c1cn2CC(COc2n1)OCc1cn[nH]n1	3	L3	266.214
5_2_1	COc1ccc(Cn2ccc3c(ncnc23)c2occc2)cc1	3	L3	305.331
1_1_14	[O-]\[N+](=O)c1cn2CC(COc2n1)OCc1ccnc(c1)c1ccccc1	3	L3	352.344
1_1_15	[O-]\[N+](=O)c1cn2CC(COc2n1)OCc1cnc(cn1)c1ccccc1	3	L3	353.332
1_1_13	[O-]\[N+](=O)c1cn2CC(COc2n1)OCCOc1ccc(cn1)c1ccccc1	3	L3	382.37
2_4_2	c1nc2ccc(Br)cc2cc1C(c1ccccc1)C(O)(CCN(C)C)c1cccc2ccccc12	3	L3	525.479

1_1_1_1	c1ccc(cc1)c1ccc(COC2COc3nc(cn3C2)[N+](=O)[O-])cc1	47	L4	351.356
2_2_1_1	c1ccccc1c1cc(Nc2ccc3nc(cc(N)c3c2)c2ccccc2)nc(N)n1	9	L4	404.467
2_5_1_1	c1ccc(/C=N/N(C(=O)c2ccccc2)C(=O)c2cccnc2)cc1	9	L4	329.352
1_1_1_4	[O-][N+](=O)c1cn2CC(COc2n1)OCc1ccc(cc1)c1ccccn1	5	L4	352.344
1_1_1_3	[O-][N+](=O)c1cn2CC(COc2n1)OCc1cccc(c1)c1ccccc1	5	L4	351.356
1_1_1_2	c1ccc(cn1)c1ccc(COC2COc3nc(cn3C2)[N+](=O)[O-])cc1	5	L4	352.344
9_1_1_1	OC(=O)c1cn(C2CC2)c2cc(N3CCN(CC3)C)ccc2c1=O	5	L4	327.378
1_1_7_1	[O-][N+](=O)c1cn2CC(COc2n1)OCCCC#Cc1ccc(cc1)c1ccccc1	4	L4	403.431
1_1_4_1	[O-][N+](=O)c1cn2CC(COc2n1)OCCOc1ccc(cc1)c1ccccc1	3	L4	381.382
1_1_5_1	[O-][N+](=O)c1cn2CC(COc2n1)NC(=O)Nc1ccccc1	3	L4	303.273
1_1_6_1	[O-][N+](=O)c1cn2CC(COc2n1)OC(=O)Nc1cccc(c1)c1ccccc1	3	L4	380.354
1_1_10_1	[O-][N+](=O)c1cn2CC(COc2n1)OCc1ccc(s1)c1ccccc1	3	L4	357.384
3_5_1_1	OC(=O)c1c[nH]c2cc(N3CCN(CC3)C(=O)CC[N+](=O)[O-])c(F)cc2c1=O	3	L4	392.338

COMPOUNDS USED FOR QSAR MODELS BUILDING

Compounds considered for models building

ID	CMPD_CHEMBLID	CANONICAL_SMILES	pMIC
1	CHEMBL575816	O=C(NN=C1CCCCC1)c2ccncc2	9.40
2	CHEMBL207938	CC(C)(C)OC(=O)N1CCN(CC1)c2ccc(CNC(=O)c3oc(cc3)[N+](=O)[O-])cn2	8.73
3	CHEMBL528999	[O-][N+](=O)c1oc(cc1)C(=O)N2CCC(CC2)Oc3ccc(OC(F)(F)F)cc3	8.70
4	CHEMBL1822872	C[C@H]1COC2(CCN(CC2)C3=NC(=O)c4cc(cc(c4S3)[N+](=O)[O-])C(F)(F)F)O1	8.63
5	CHEMBL1822873	C[C@@H]1COC2(CCN(CC2)C3=NC(=O)c4cc(cc(c4S3)[N+](=O)[O-])C(F)(F)F)O1	8.63
6	CHEMBL1169	Nc1ccc(C(=O)O)c(O)c1	8.49
7	CHEMBL1630259	COc1ccc(\C=N\N(C(=O)c2cccnc2)C(=O)c3cc(cc(c3)[N+](=O)[O-])[N+](=O)[O-])cc1	8.46
8	CHEMBL1631683	CN(C)CC[C@](O)([C@H](c1ccccc1)c2cnc3ccc(Br)cc3c2)c4cccc5ccccc45	8.42
9	CHEMBL376488	COc1nc2ccc(Br)cc2cc1[C@@H](c3ccccc3)[C@@](O)(CCN(C)C)c4ccccc5ccccc45	8.27
10	CHEMBL1630851	COc1ccc(\C=N\N(C(=O)c2cccnc2)C(=O)c3cc(ccc3Cl)[N+](=O)[O-])cc1OC	8.17
11	CHEMBL218650	C[C@]1(COc2ccc(cc2)N3CCC(CC3)Oc4ccc(OC(F)(F)F)cc4)Cn5cc(nc5O1)[N+](=O)[O-]	7.95
12	CHEMBL218650	C[C@]1(COc2ccc(cc2)N3CCC(CC3)Oc4ccc(OC(F)(F)F)cc4)Cn5cc(nc5O1)[N+](=O)[O-]	7.95
13	CHEMBL218973	C[C@]1(COc2ccc(cc2)N3CCC(CC3)Oc4ccc(cc4)C(F)(F)F)Cn5cc(nc5O1)[N+](=O)[O-]	7.94
14	CHEMBL1630848	COc1ccc(\C=N\N(C(=O)c2cccnc2)C(=O)c3ccccc3Br)cc1OC	7.87
15	CHEMBL381274	[O-][N+](=O)c1oc(cc1)C(=O)NCc2ccc(nc2)N3CCN(Cc4ccccc4)CC3	7.83
16	CHEMBL571531	[O-][N+](=O)c1cn2C[C@@H](COc2n1)OCc3ccc(cc3)c4ccc(Cl)cc4	7.82
17	CHEMBL572303	[O-][N+](=O)c1cn2C[C@@H](COc2n1)OCc3ccc(cc3)c4ccc(F)cc4	7.82
18	CHEMBL207968	CCOC(=O)N1CCN(CC1)c2ccc(CNC(=O)c3oc(cc3)[N+](=O)[O-])cc2	7.81
19	CHEMBL1630567	[O-][N+](=O)c1cn2C[C@@H](COc2n1)OCc3ccc(nc3)c4ccc(OC(F)(F)F)c(Cl)c4	7.77
20	CHEMBL441552	C[C@]1(COc2ccc(Cl)cc2)Cn3cc(nc3O1)[N+](=O)[O-]	7.71

21	CHEMBL2177972	COC1CCC(CC1)\N=C\2/C=C3N(c4ccc(cc4)C(F)(F)F)c5ccccc5N=C3C=C2Nc6cccnc6C	7.70
22	CHEMBL1629770	[O-][N+](=O)c1cn2C[C@@H](COc2n1)OCc3ccc(cn3)c4ccc(OC(F)F)cc4	7.70
23	CHEMBL1630564	[O-][N+](=O)c1cn2C[C@@H](COc2n1)OCc3ccc(nc3)c4ccc(OC(F)F)cc4	7.70
24	CHEMBL1836422	[O-][N+](=O)c1cn2C[C@@H](COc2n1)OCCOc3ccc(cn3)c4ccc(F)cc4	7.70
25	CHEMBL1836423	[O-][N+](=O)c1cn2C[C@@H](COc2n1)OCCOc3ccc(cn3)c4ccc(cc4)C(F)(F)F	7.70
26	CHEMBL1836432	[O-][N+](=O)c1cn2C[C@@H](COc2n1)OC\C=C\c3ccc(cc3)c4ccc(nc4)C(F)(F)F	7.70
27	CHEMBL1836445	[O-][N+](=O)c1cn2C[C@@H](COc2n1)OCC#Cc3ccc(cn3)c4ccc(cc4)C(F)(F)F	7.70
28	CHEMBL2177971	Cc1ncccc1NC2=CC3=Nc4ccccc4N(C3=C/C/2=N\C5CCOCC5)c6ccc(cc6)C(F)(F)F	7.68
29	CHEMBL2177952	COC1CCC(CC1)\N=C\2/C=C3N(c4ccc(Cl)cc4)c5ccccc5N=C3C=C2Nc6cccnc6C	7.68
30	CHEMBL206897	COc1c(N2CCN(Cn3c(O)c(N=NC(=O)N)c4ccccc34)C(C)C2)c(F)cc5C(=O)C(=CN(C6CC6)c15)C(=O)O	7.68
31	CHEMBL1630827	[O-][N+](=O)c1cn2C[C@@H](COc2n1)OCc3cnc(cn3)c4ccc(OC(F)(F)F)cc4	7.64
32	CHEMBL1630569	[O-][N+](=O)c1cn2C[C@@H](COc2n1)OCc3ccc(nc3)c4ccc(OC(F)(F)F)c(F)c4	7.60
33	CHEMBL1630835	[O-][N+](=O)c1cn2C[C@@H](COc2n1)OCc3cnc(nc3)c4ccc(cc4)C(F)(F)F	7.60
34	CHEMBL1632251	[O-][N+](=O)c1cn2C[C@@H](COc2n1)OCc3ccc(cc3)c4ncc(cc4Cl)C(F)(F)F	7.60
35	CHEMBL1836062	[O-][N+](=O)c1cn2C[C@@H](COc2n1)OCc3ccc(OCc4ccccc4)cc3	7.60
36	CHEMBL1836420	[O-][N+](=O)c1cn2C[C@@H](COc2n1)OCCOc3ccc(cc3)c4ccc(nc4)C(F)(F)F	7.60

37	CHEMBL1836443	[O-][N+](=O)c1cn2C[C@@H](COc2n1)OCC#Cc3ccc(cn3)c4ccc(OC(F)(F)F)cc4	7.60
38	CHEMBL1836447	[O-][N+](=O)c1cn2C[C@@H](COc2n1)OCC#Cc3ccc(cn3)c4ccc(OC(F)F)cc4	7.60
39	CHEMBL571403	[O-][N+](=O)c1cn2C[C@@H](COc2n1)OCc3ccc(cc3)c4ccc(cc4)C#N	7.60
40	CHEMBL2177927	COC1CCC(CC1)\N=C\2/C=C3N(c4ccc(Br)cc4)c5ccccc5N=C3C=C2Nc6cccnc6C	7.58
41	CHEMBL1630837	[O-][N+](=O)c1cn2C[C@@H](COc2n1)OCc3cnc(nc3)c4ccc(OC(F)(F)F)cc4	7.57
42	CHEMBL1945573	[O-][N+](=O)c1cn2C[C@@H](COc2n1)OC(=O)Nc3cccc(c3)c4ccc(F)cc4	7.57
43	CHEMBL2177933	COC1CCC(CC1)\N=C\2/C=C3N(c4ccc(OC(F)(F)F)cc4)c5ccccc5N=C3C=C2Nc6cccnc6OC	7.57
44	CHEMBL2177969	COC1CCC(CC1)\N=C\2/C=C3N(c4ccc(cc4)C(F)(F)F)c5ccccc5N=C3C=C2Nc6cccnc6OC	7.55
45	CHEMBL2177932	COc1ncccc1NC2=CC3=Nc4ccccc4N(C3=C/C/2=N\C5CCOCC5)c6ccc(OC(F)(F)F)cc6	7.55
46	CHEMBL2177922	COC1CCC(CC1)\N=C\2/C=C3N(c4ccc(cc4)C(F)(F)F)c5ccccc5N=C3C=C2Nc6ccc(C)nc6	7.54
47	CHEMBL2177272	[O-][N+](=O)c1cc(cc2C(=O)N=C(Sc12)N3CCC(CC3)c4ccccc4)C(F)(F)F	7.54
48	CHEMBL2177970	CC(C)\N=C\1/C=C2N(c3ccc(cc3)C(F)(F)F)c4ccccc4N=C2C=C1Nc5cccnc5C	7.54
49	CHEMBL2177968	COc1ncccc1NC2=CC3=Nc4ccccc4N(C3=C/C/2=N\C5CCOCC5)c6ccc(cc6)C(F)(F)F	7.53
50	CHEMBL1818386	Fc1ccc(NC(=O)NCC23CC4CC(CC(C4)C2)C3)c(F)c1F	7.53
51	CHEMBL2177949	COC1CCC(CC1)\N=C\2/C=C3N(c4ccc(Cl)cc4)c5ccccc5N=C3C=C2Nc6cccnc6OC	7.53
52	CHEMBL1630566	[O-][N+](=O)c1cn2C[C@@H](COc2n1)OCc3ccc(nc3)c4ccc(OC(F)(F)F)cc4Cl	7.52
53	CHEMBL1632257	[O-][N+](=O)c1cn2C[C@@H](COc2n1)OCc3ccc(cc3)c4ccc(nc4)C(F)(F)F	7.52
54	CHEMBL1945055	[O-][N+](=O)c1cn2C[C@@H](COc2n1)NC(=O)Nc3cccc(c3)c4ccc(F)cc4	7.52

55	CHEMBL565798	[O-][N+](=O)c1cn2C[C@@H](COc2n1)OCc3cnn(n3)c4ccc(OC(F)(F)F)cc4	7.52
56	CHEMBL571629	[O-][N+](=O)c1cn2C[C@@H](COc2n1)OCc3ccc(cc3)c4ccc(cc4)C(F)(F)F	7.52
57	CHEMBL571755	CCOc1ccccc1c2ccc(CO[C@@H]3COc4nc(cn4C3)[N+](=O)[O-])cc2	7.52
58	CHEMBL572264	[O-][N+](=O)c1cn2C[C@@H](COc2n1)OCc3ccc(cc3)c4ccc(OC(F)(F)F)c(Cl)c4	7.52
59	CHEMBL572325	[O-][N+](=O)c1cn2C[C@@H](COc2n1)OCc3ccc(cc3)c4ccc(Cl)c(OC(F)F)c4	7.52
60	CHEMBL583256	[O-][N+](=O)c1cn2C[C@@H](COc2n1)OCc3ccc(cc3)c4ccc(cc4Cl)C(F)(F)F	7.52
61	CHEMBL583460	[O-][N+](=O)c1cn2C[C@@H](COc2n1)OCc3ccc(cc3)c4ccc(F)c(F)c4	7.52
62	CHEMBL584961	[O-][N+](=O)c1cn2C[C@@H](COc2n1)OCc3ccc(cc3)c4ccc(OC(F)(F)F)c(F)c4	7.52
63	CHEMBL2177955	COC1CCC(CC1)\N=C\2/C=C3N(c4ccc(Cl)cc4)c5ccccc5N=C3C=C2Nc6ccc(C)nc6	7.52
64	CHEMBL2177960	COC1CCC(CC1)\N=C\2/C=C3N(c4ccc(F)cc4)c5ccccc5N=C3C=C2Nc6cccnc6OC	7.51
65	CHEMBL2177275	CCCOCC1COC2(CCN(CC2)C3=NC(=O)c4cc(cc(c4S3)[N+](=O)[O-])C(F)(F)F)O1	7.51
66	CHEMBL1818384	Fc1ccc(NC(=O)NC2C3CC4CC(CC2C4)C3)c(F)c1F	7.51
67	CHEMBL1630850	COc1ccc(\C=N\N(C(=O)c2cccnc2)C(=O)c3cccc(c3)[N+](=O)[O-])cc1	7.51
68	CHEMBL2177948	COc1ncccc1NC2=CC3=Nc4ccccc4N(C3=C/C/2=N\C5CCOCC5)c6ccc(Cl)cc6	7.51
69	CHEMBL1945829	[O-][N+](=O)c1cn2C[C@@H](COc2n1)OC(=O)N3CCN(CC3)c4ccc(OC(F)(F)F)cc4	7.48
70	CHEMBL1818394	O=C(NCCc1ccccc1)NC2C3CC4CC(CC2C4)C3	7.47
71	CHEMBL1818404	Cc1ccc(NC(=O)NC2CCCCCCC2)cc1Cl	7.47
72	CHEMBL1817983	CCOC(=O)C1=C(C)N(C(=C(C1c2cn(nc2c3ccccc3)c4ccccc4)C(=O)OCC)C)c5ccccc5Cl	7.46
73	CHEMBL1629747	[O-][N+](=O)c1cn2C[C@@H](COc2n1)OCc3ccnc(c3)c4ccc(OC(F)(F)F)cc4	7.46

74	CHEMBL1632254	[O-][N+](=O)c1cn2C[C@@H](COc2n1)OCc3ccc(cc3)c4ccc(F)cn4	7.46
75	CHEMBL1836435	[O-][N+](=O)c1cn2C[C@@H](COc2n1)OCC#Cc3ccc(cc3)c4ccc(F)cc4	7.46
76	CHEMBL1836457	[O-][N+](=O)c1cn2C[C@@H](COc2n1)OCCCC#Cc3ccc(cc3)c4ccc(OC(F)F)cc4	7.46
77	CHEMBL1945054	[O-][N+](=O)c1cn2C[C@@H](COc2n1)NC(=O)Nc3cccc(c3)c4ccc(cc4)C(F)(F)F	7.46
78	CHEMBL565592	[O-][N+](=O)c1cn2C[C@@H](COc2n1)OCc3nnn(n3)c4ccc(OC(F)(F)F)cc4	7.46
79	CHEMBL570989	[O-][N+](=O)c1cn2C[C@@H](COc2n1)OCc3ccc(cc3)c4ccc(Cl)c(c4)C(F)(F)F	7.46
80	CHEMBL572070	[O-][N+](=O)c1cn2C[C@@H](COc2n1)OCc3ccc(cc3)c4ccccc4OC(F)(F)F	7.46
81	CHEMBL572094	[O-][N+](=O)c1cn2C[C@@H](COc2n1)OCc3ccc(cc3)c4ccc(OC(F)(F)F)cc4	7.46
82	CHEMBL1818401	CCCCCCNC(=O)NC1C2CC3CC(CC1C3)C2	7.44
83	CHEMBL2177924	COc1ncccc1NC2=CC3=Nc4ccccc4N(C3=C/C/2=N\C5CCOCC5)c6ccc(Br)cc6	7.44
84	CHEMBL2177963	COC1CCC(CC1)\N=C\2/C=C3N(c4ccc(F)cc4)c5ccccc5N=C3C=C2Nc6ccccnc6C	7.43
85	CHEMBL508258	[O-][N+](=O)c1cn2C[C@@H](COc2n1)NCCCCc3ccc(OC(F)(F)F)cc3	7.41
86	CHEMBL1818383	COc1c2N(C=C(C(=O)O)C(=O)c2cc(F)c1N3C(C)CN(CC3C)C(=O)CC[N+](=O)[O-])C4CC4	7.40
87	CHEMBL1629766	[O-][N+](=O)c1cn2C[C@@H](COc2n1)OCc3ccc(cn3)c4ccc(cc4)C(F)(F)F	7.40
88	CHEMBL1629773	[O-][N+](=O)c1cn2C[C@@H](COc2n1)OCc3ccc(cn3)c4ccc(OC(F)(F)F)c(Cl)c4	7.40
89	CHEMBL1632264	[O-][N+](=O)c1cn2C[C@@H](COc2n1)OCc3ccc(cc3)c4ccc(OCc5ccccc5)nc4	7.40
90	CHEMBL1836069	[O-][N+](=O)c1cn2C[C@@H](COc2n1)OCCOc3ccc(OC(F)(F)F)cc3	7.40

91	CHEMBL1836418	[O-][N+](=O)c1cn2C[C@@H](COc2n1)OCCOc3ccc(cc3)c4ccc(F)cc4	7.40
92	CHEMBL1836419	[O-][N+](=O)c1cn2C[C@@H](COc2n1)OCCOc3ccc(cc3)c4ccc(cc4)C(F)(F)F	7.40
93	CHEMBL1836421	[O-][N+](=O)c1cn2C[C@@H](COc2n1)OCCOc3ccc(cn3)c4ccc(OC(F)(F)F)cc4	7.40
94	CHEMBL1836439	[O-][N+](=O)c1cn2C[C@@H](COc2n1)OCC#Cc3cccc(c3)c4ccc(F)cc4	7.40
95	CHEMBL1945572	[O-][N+](=O)c1cn2C[C@@H](COc2n1)OC(=O)Nc3cccc(c3)c4ccc(cc4)C(F)(F)F	7.40
96	CHEMBL569379	[O-][N+](=O)c1cn2C[C@@H](COc2n1)OCc3ccc(cc3)c4ccc(OC(F)(F)F)cc4Cl	7.40
97	CHEMBL570292	[O-][N+](=O)c1cn2C[C@@H](COc2n1)OCc3ccc(cc3)c4ccc(Oc5ccccc5)cc4	7.40
98	CHEMBL570990	[O-][N+](=O)c1cn2C[C@@H](COc2n1)OCc3ccc(cc3)c4cc(F)c(F)c(F)c4	7.40
99	CHEMBL571627	COc1c(F)cc(F)cc1c2ccc(CO[C@@H]3COc4nc(cn4C3)[N+](=O)[O-])cc2	7.40
100	CHEMBL571868	COc1ccc(cc1F)c2ccc(CO[C@@H]3COc4nc(cn4C3)[N+](=O)[O-])cc2	7.40
101	CHEMBL584098	[O-][N+](=O)c1cn2C[C@@H](COc2n1)OCc3ccc(cc3)c4ccc(Cl)c(OC(F)(F)F)c4	7.40
102	CHEMBL585349	CC(=O)c1ccc(cc1)c2ccc(CO[C@@H]3COc4nc(cn4C3)[N+](=O)[O-])cc2	7.40
103	CHEMBL1927214	ClCCSc1oc(Cc2ccc(Cl)cc2Cl)nn1	7.40
104	CHEMBL2177981	CC(C)\N=C\1/C=C2N(c3ccc(Br)cc3)c4ccccc4N=C2C=C1Nc5cccnc5	7.38
105	CHEMBL376416	Cc1ccc(OC[C@@]2(C)Cn3cc(nc3O2)[N+](=O)[O-])cc1	7.38
106	CHEMBL227875	[O-][N+](=O)c1cn2C[C@@H](COc2n1)OCc3ccc(OC(F)(F)F)cc3	7.38
107	CHEMBL1836075	[O-][N+](=O)c1cn2C[C@@H](COc2n1)OC\C=C\c3ccc(cn3)C(F)(F)F	7.37
108	CHEMBL1836414	[O-][N+](=O)c1cn2C[C@@H](COc2n1)OCCCc3ccc(cc3)c4ccc(cc4)C(F)(F)F	7.37

109	CHEMBL1257994	CCOC(=O)C1=C(C)NC(=O)NC1c2cn(nc2c3ccc(cc3)[N+](=O)[O-])c4ccccc4	7.35
110	CHEMBL219638	C[C@]1(COc2ccc(cc2)N3CCC(CC3)Oc4cccc(OC(F)(F)F)c4)Cn5cc(nc5O1)[N+](=O)[O-]	7.35
111	CHEMBL1632262	[O-][N+](=O)c1cn2C[C@@H](COc2n1)OCc3ccc(cc3)c4ccc(OC(F)F)nc4	7.35
112	CHEMBL1632263	COc1ccc(cn1)c2ccc(CO[C@@H]3COc4nc(cn4C3)[N+](=O)[O-])cc2	7.35
113	CHEMBL1836413	[O-][N+](=O)c1cn2C[C@@H](COc2n1)OCCCc3ccc(cc3)c4ccc(F)cc4	7.35
114	CHEMBL1836431	[O-][N+](=O)c1cn2C[C@@H](COc2n1)OC\C=C\c3ccc(cc3)c4ccc(cc4)C(F)(F)F	7.35
115	CHEMBL568332	[O-][N+](=O)c1cn2C[C@@H](COc2n1)OCc3ccn(n3)c4ccc(cc4)C(F)(F)F	7.35
116	CHEMBL569855	[O-][N+](=O)c1cn2C[C@@H](COc2n1)OCc3ccc(cc3)c4ccc(OC(F)(F)F)cc4F	7.35
117	CHEMBL570788	COc1cc(ccc1F)c2ccc(CO[C@@H]3COc4nc(cn4C3)[N+](=O)[O-])cc2	7.35
118	CHEMBL571315	[O-][N+](=O)c1cn2C[C@@H](COc2n1)OCc3ccc(cc3)c4cccc(F)c4	7.35
119	CHEMBL571405	[O-][N+](=O)c1cn2C[C@@H](COc2n1)OCc3ccc(cc3)c4ccc(OC(F)(F)F)c(c4)[N+](=O)[O-]	7.35
120	CHEMBL572310	[O-][N+](=O)c1cn2C[C@@H](COc2n1)OCc3ccc(cc3)c4ccc5ccccc5c4	7.35
121	CHEMBL576112	[O-][N+](=O)c1cn2C[C@@H](COc2n1)OCc3ccc(cc3)c4ccccc4	7.35
122	CHEMBL584540	COc1c(F)cc(cc1F)c2ccc(CO[C@@H]3COc4nc(cn4C3)[N+](=O)[O-])cc2	7.35
123	CHEMBL1630568	[O-][N+](=O)c1cn2C[C@@H](COc2n1)OCc3ccc(nc3)c4ccc(OC(F)(F)F)cc4F	7.33
124	CHEMBL1258342	CCOC(=O)C1=C(C)NC(=O)NC1c2cn(nc2c3ccc(F)cc3)c4ccccc4	7.32
125	CHEMBL44884	CC[C@@H](CO)NCCN[C@@H](CC)CO	7.31
126	CHEMBL219640	C[C@]1(COc2ccc(cc2)N3CCC(CC3)Oc4ccc(Cl)cc4)Cn5cc(nc5O1)[N+](=O)[O-]	7.31

127	CHEMBL519753	[O-][N+](=O)c1oc(cc1)C2=NOC(C2)c3ccc(cc3)N4CCC(CC4)Oc5ccc(cc5)C(F)(F)F	7.30
128	CHEMBL1254513	COc1ccc(Cn2ccc3c(nc(Cl)nc23)c4cccs4)cc1	7.30
129	CHEMBL1630551	[O-][N+](=O)c1cn2C[C@@H](COc2n1)OCc3ccc(cn3)c4ccc(OC(F)(F)F)c(F)c4	7.30
130	CHEMBL1630563	[O-][N+](=O)c1cn2C[C@@H](COc2n1)OCc3ccc(nc3)c4ccc(OC(F)(F)F)cc4	7.30
131	CHEMBL1836073	[O-][N+](=O)c1cn2C[C@@H](COc2n1)OC\C=C\c3ccc(OC(F)(F)F)cc3	7.30
132	CHEMBL1836081	[O-][N+](=O)c1cn2C[C@@H](COc2n1)OCCCC#Cc3ccc(OC(F)(F)F)cc3	7.30
133	CHEMBL1836444	[O-][N+](=O)c1cn2C[C@@H](COc2n1)OCC#Cc3ccc(cn3)c4ccc(F)cc4	7.30
134	CHEMBL1836449	[O-][N+](=O)c1cn2C[C@@H](COc2n1)OCC#Cc3ccc(nc3)c4ccc(F)cc4	7.30
135	CHEMBL1945579	[O-][N+](=O)c1cn2C[C@@H](COc2n1)OC(=O)Nc3ccc(cc3)c4ccc(OC(F)(F)F)cc4	7.30
136	CHEMBL489292	[O-][N+](=O)c1cn2C[C@@H](COc2n1)NC(=O)COc3ccc(OC(F)(F)F)cc3	7.30
137	CHEMBL565994	[O-][N+](=O)c1cn2C[C@@H](COc2n1)OCc3ccc(s3)c4ccc(nc4)C(F)(F)F	7.30
138	CHEMBL565997	[O-][N+](=O)c1cn2C[C@@H](COc2n1)OCc3ccc(s3)c4ccc(F)cc4	7.30
139	CHEMBL566195	[O-][N+](=O)c1cn2C[C@@H](COc2n1)OCc3cnn(n3)c4ccc(cc4)C(F)(F)F	7.30
140	CHEMBL566625	[O-][N+](=O)c1cn2C[C@@H](COc2n1)OCc3ccn(n3)c4ccc(OC(F)(F)F)cc4	7.30
141	CHEMBL570994	[O-][N+](=O)c1cn2C[C@@H](COc2n1)OCc3ccc(cc3)c4ccc(OC(F)F)cc4	7.30
142	CHEMBL273894	Cl.CNCc1cc(Cl)cc(Cl)c1	7.28
143	CHEMBL1630560	[O-][N+](=O)c1cn2C[C@@H](COc2n1)OCc3ccc(nc3)c4ccc(cc4)C(F)(F)F	7.28

144	CHEMBL2177925	COC1CCC(CC1)\N=C\2/C=C3N(c4ccc(Br)cc4)c5ccccc5N=C3C=C2Nc6cccnc6OC	7.28
145	CHEMBL2177936	COC1CCC(CC1)\N=C\2/C=C3N(c4ccc(OC(F)(F)F)cc4)c5ccccc5N=C3C=C2Nc6cccnc6	7.27
146	CHEMBL2177931	COc1ncccc1NC2=CC3=Nc4ccccc4N(C3=C/C/2=N\C(C)C)c5ccc(OC(F)(F)F)cc5	7.27
147	CHEMBL457781	COc1nc2ccc(Br)cc2cc1[C@@H](c3ccccc3)[C@](O)(CCN(C)C)c4cccc5ccccc45	7.27
148	CHEMBL2177962	Cc1ncccc1NC2=CC3=Nc4ccccc4N(C3=C/C/2=N\C5CCOCC5)c6ccc(F)cc6	7.27
149	CHEMBL2177274	COC(=O)[C@@H]1OC2(CCN(CC2)C3=NC(=O)c4cc(cc(c4S3)[N+](=O)[O-])C(F)(F)F)O[C@H]1c5ccccc5	7.26
150	CHEMBL1629750	[O-][N+](=O)c1cn2C[C@@H](COc2n1)OCc3ccnc(c3)c4ccc(OC(F)F)cc4	7.26
151	CHEMBL1836416	[O-][N+](=O)c1cn2C[C@@H](COc2n1)OCCCc3ccc(cc3)c4ccc(cn4)C(F)(F)F	7.26
152	CHEMBL1836417	[O-][N+](=O)c1cn2C[C@@H](COc2n1)OCCOc3ccc(cc3)c4ccc(OC(F)(F)F)cc4	7.26
153	CHEMBL1836453	[O-][N+](=O)c1cn2C[C@@H](COc2n1)OCCCC#Cc3ccc(cc3)c4ccc(OC(F)(F)F)cc4	7.26
154	CHEMBL1945577	[O-][N+](=O)c1cn2C[C@@H](COc2n1)OC(=O)Nc3ccc(cc3)c4ccc(cc4)C(F)(F)F	7.26
155	CHEMBL566203	[O-][N+](=O)c1cn2C[C@@H](COc2n1)OCc3ccc(s3)c4ccc(cc4)C#N	7.26
156	CHEMBL571849	COc1cccc(Cl)c1c2ccc(CO[C@@H]3COc4nc(cn4C3)[N+](=O)[O-])cc2	7.26
157	CHEMBL2177941	COC1CCC(CC1)\N=C\2/C=C3N(c4ccc(cc4)C(F)(F)F)c5ccccc5N=C3C=C2Nc6cccnc6	7.26
158	CHEMBL380835	[O-][N+](=O)c1oc(cc1)C(=O)N2CCc3cc(ccc3C2)N4CCN(Cc5ccccc5)CC4	7.25
159	CHEMBL2177935	FC(F)(F)Oc1ccc(cc1)N2C3=C\C(=N/C4CCOCC4)\C(=CC3=Nc5ccccc25)Nc6cccnc6	7.25
160	CHEMBL2177967	COc1ncccc1NC2=CC3=Nc4ccccc4N(C3=C/C/2=N\C(C)C)c5ccc(cc5)C(F)(F)F	7.24
161	CHEMBL2177983	COC1CCC(CC1)\N=C\2/C=C3N(c4ccc(Cl)cc4)c5ccccc5N=C3C=C2Nc6cccnc6	7.23
162	CHEMBL2177267	CN(C(=O)CN1CCN(CC1)C2=NC(=O)c3cc(cc(c3S2)[N+](=O)[O-])C(F)(F)F)c4ccccc4	7.23
163	CHEMBL1254512	COc1ccc(Cn2ccc3c(nc(Cl)nc23)c4occc4)cc1	7.22

164	CHEMBL1630550	[O-][N+](=O)c1cn2C[C@@H](COc2n1)OCc3ccc(cn3)c4ccc(OC(F)(F)F)cc4F	7.22
165	CHEMBL1630552	[O-][N+](=O)c1cn2C[C@@H](COc2n1)OCc3ccc(cn3)c4ccc(Cl)c(OC(F)(F)F)c4	7.22
166	CHEMBL1630562	[O-][N+](=O)c1cn2C[C@@H](COc2n1)OCc3ccc(nc3)c4ccc(F)cc4	7.22
167	CHEMBL1630574	[O-][N+](=O)c1cn2C[C@@H](COc2n1)OCc3ccc(nn3)c4ccc(cc4)C(F)(F)F	7.22
168	CHEMBL1630830	[O-][N+](=O)c1cn2C[C@@H](COc2n1)OCc3ncc(cn3)c4ccc(cc4)C(F)(F)F	7.22
169	CHEMBL1632250	[O-][N+](=O)c1cn2C[C@@H](COc2n1)OCc3ccc(cc3)c4ccc(cn4)C(F)(F)F	7.22
170	CHEMBL1945061	[O-][N+](=O)c1cn2C[C@@H](COc2n1)NC(=O)Nc3ccc(cc3)c4ccc(OC(F)(F)F)cc4	7.22
171	CHEMBL1945574	[O-][N+](=O)c1cn2C[C@@H](COc2n1)OC(=O)Nc3cccc(c3)c4ccc(OC(F)(F)F)cc4	7.22
172	CHEMBL1946007	[O-][N+](=O)c1cn2C[C@@H](COc2n1)OC(=O)N3CC[C@@H](C3)Oc4ccc(OC(F)(F)F)cc4	7.22
173	CHEMBL566644	COc1ccc(cc1F)c2ccc(CO[C@@H]3COc4nc(cn4C3)[N+](=O)[O-])s2	7.22
174	CHEMBL566846	Cn1nc(cc1CO[C@@H]2COc3nc(cn3C2)[N+](=O)[O-])c4ccc(OC(F)(F)F)cc4	7.22
175	CHEMBL567691	Cn1nc(cc1CO[C@@H]2COc3nc(cn3C2)[N+](=O)[O-])c4ccc(cc4)C(F)(F)F	7.22
176	CHEMBL571248	[O-][N+](=O)c1cn2C[C@@H](COc2n1)OCc3ccc(cc3)c4ccc(CNc5ccccc5)cc4	7.22
177	CHEMBL571867	[O-][N+](=O)c1cn2C[C@@H](COc2n1)OCc3cccc(c3)c4ccc(OC(F)F)cc4	7.22
178	CHEMBL572053	[O-][N+](=O)c1cn2C[C@@H](COc2n1)OCc3ccc(cc3)c4ccc(c(Cl)c4)C(F)(F)F	7.22
179	CHEMBL572285	[O-][N+](=O)c1cn2C[C@@H](COc2n1)OCc3ccc(cc3)c4cccc(Cl)c4	7.22

180	CHEMBL572298	[O-]][N+](=O)c1cn2C[C@@H](COc2n1)OCc3ccc(cc3)c4ccccc4Oc5ccccc5	7.22
181	CHEMBL1817677	Cc1ccc(NC(=O)NCC23CC4CC(CC(C4)C2)C3)cc1Cl	7.22
182	CHEMBL2177921	Cc1ccc(NC2=CC3=Nc4ccccc4N(C3=C/C/2=N\C5CCOCC5)c6ccc(cc6)C(F)(F)F)cn1	7.22
183	CHEMBL2177954	Cc1ccc(NC2=CC3=Nc4ccccc4N(C3=C/C/2=N\C5CCOCC5)c6ccc(Cl)cc6)cn1	7.22
184	CHEMBL1818388	CC1C(CC2CC1C2(C)C)NC(=O)Nc3ccc(F)c(F)c3F	7.21
185	CHEMBL2177980	CC(C)\N=C\1/C=C2N(c3ccc(OC(F)(F)F)cc3)c4ccccc4N=C2C=C1Nc5ccccnc5	7.21
186	CHEMBL2177973	CC(C)\N=C\1/C=C2N(c3ccc(cc3)C(F)(F)F)c4ccccc4N=C2C=C1Nc5ccc(C)nc5	7.21
187	CHEMBL1630854	COc1ccc(\C=N\N(C(=O)c2ccc(N)cc2)C(=O)c3cccnc3)cc1OC	7.21
188	CHEMBL2177982	Clc1ccc(cc1)N2C3=C\C(=N/C4CCOCC4)\C(=CC3=Nc5ccccc25)Nc6ccccnc6	7.21
189	CHEMBL1836429	[O-]][N+](=O)c1cn2C[C@@H](COc2n1)OC\C=C\c3ccc(cc3)c4ccc(OC(F)(F)F)cc4	7.20
190	CHEMBL2177979	CC(C)\N=C\1/C=C2N(c3ccc(cc3)C(F)(F)F)c4ccccc4N=C2C=C1Nc5cccnc5	7.20
191	CHEMBL1630855	COc1ccc(\C=N\N(C(=O)c2ccc(Cl)cc2)C(=O)c3cccnc3)cc1	7.20
192	CHEMBL2177947	COc1ncccc1NC2=CC3=Nc4ccccc4N(C3=C/C/2=N\C(C)C)c5ccc(Cl)cc5	7.19
193	CHEMBL2177956	Clc1ccc(cc1)N2C3=C\C(=N/C4CCOCC4)\C(=CC3=Nc5ccccc25)Nc6ccncc(Br)c6	7.19
194	CHEMBL1630853	Nc1ccc(cc1)C(=O)N(\N=C\c2cccc(c2)[N+](=O)[O-])C(=O)c3cccnc3	7.19
195	CHEMBL2177271	CN([C@H]1CCN(Cc2ccccc2)C1)C3=NC(=O)c4cc(cc(c4S3)[N+](=O)[O-])C(F)(F)F	7.19
196	CHEMBL1629769	[O-]][N+](=O)c1cn2C[C@@H](COc2n1)OCc3ccc(cn3)c4ccc(OC(F)(F)F)cc4	7.19
197	CHEMBL572106	COc1ccc(cc1)c2ccc(CO[C@@H]3COc4nc(cn4C3)[N+](=O)[O-])cc2	7.19
198	CHEMBL585577	COc1ccccc1c2ccc(CO[C@@H]3COc4nc(cn4C3)[N+](=O)[O-])cc2	7.19
199	CHEMBL1256651	CC1=C(N2C[C@@H]3NCCC=C3C2)C(=CN4C(=O)C(=CC(=C14)C5CC5)C(=O)O)F	7.19
200	CHEMBL2177958	COc1ncccc1NC2=CC3=Nc4ccccc4N(C3=C/C/2=N\C(C)C)c5ccc(F)cc5	7.18
201	CHEMBL1630852	COc1ccc(\C=N\N(C(=O)c2ccc(N)cc2)C(=O)c3cccnc3)cc1	7.18

202	CHEMBL1630849	COc1ccc(\C=N\N(C(=O)c2ccc(C)cc2)C(=O)c3cccnc3)cc1	7.17
203	CHEMBL570995	[O-][N+](=O)c1cn2C[C@@H](COc2n1)OCc3ccc(cc3)c4cccc(c4)C(F)(F)F	7.17
204	CHEMBL2177974	CC(C)\N=C\1/C=C2N(c3ccc(Cl)cc3)c4ccccc4N=C2C=C1Nc5cccnc5	7.17
205	CHEMBL2177265	[O-][N+](=O)c1cc(cc2C(=O)N=C(NCc3ccc4OCCOc4c3)Sc12)C(F)(F)F	7.17
206	CHEMBL2177269	CN(C)c1ccc(CN(C)C2=NC(=O)c3cc(cc(c3S2)[N+](=O)[O-])C(F)(F)F)cc1	7.16
207	CHEMBL1256993	COc1c(N2CC[C@H](C2)C(C)(C)N)c(F)cc3C(=O)C4=C(SNC4=O)N(C5CC5)c13	7.16
208	CHEMBL1254514	COc1ccc(Cn2ccc3c(nc(OC)nc23)c4occc4)cc1	7.15
209	CHEMBL1631954	[O-][N+](=O)c1cn2C[C@@H](COc2n1)OCc3cccc(c3)c4ccc(OCc5ccccc5)nc4	7.15
210	CHEMBL1836415	[O-][N+](=O)c1cn2C[C@@H](COc2n1)OCCCc3ccc(cc3)c4ccc(nc4)C(F)(F)F	7.15
211	CHEMBL1836450	[O-][N+](=O)c1cn2C[C@@H](COc2n1)OCC#Cc3ccc(nc3)c4ccc(cc4)C(F)(F)F	7.15
212	CHEMBL1836454	[O-][N+](=O)c1cn2C[C@@H](COc2n1)OCCCC#Cc3ccc(cc3)c4ccc(F)cc4	7.15
213	CHEMBL2037480	C[C@@H](N1C\C(=C/c2ccc(Cl)cc2Cl)\C3=C(C1)C(C(=C(N)O3)c4onc(n4)c5ccc(Cl)cc5)c6ccc(Cl)cc6Cl)c7ccccc7	7.15
214	CHEMBL569859	CSc1cccc(c1)c2cccc(CO[C@@H]3COc4nc(cn4C3)[N+](=O)[O-])c2	7.15
215	CHEMBL574867	CCc1ccc(cc1)C(=O)NCC2=C[C@@H]3Oc4ccccc4C(=O)C3=CN2c5nccc5C	7.15
216	CHEMBL2177978	CC(C)\N=C\1/C=C2N(c3ccc(F)cc3)c4ccccc4N=C2C=C1Nc5cccnc5	7.15
217	CHEMBL1197225	COc1c(N2C[C@@](C)(N)C3(CC3)C2)c(F)cc4C(=O)C(=CN([C@@H]5C[C@@H]5F)c14)C(=O)O	7.15
218	CHEMBL64	NNC(=O)c1ccncc1	7.14
219	CHEMBL64	NNC(=O)c1ccncc1	7.14
220	CHEMBL2177961	CC(C)\N=C\1/C=C2N(c3ccc(F)cc3)c4ccccc4N=C2C=C1Nc5cccnc5C	7.14
221	CHEMBL1652572	COc1c(N2CCN(CN3C(=O)C(=O)c4cc(F)ccc34)CC2)c(F)cc5C(=O)C(=CN(C6CC6)c15)C(=O)O	7.13
222	CHEMBL1630856	Nc1ccc(cc1)C(=O)N(\N=C\c2occc2)C(=O)c3cccnc3	7.13

223	CHEMBL32	COc1c(N2C[C@@H]3CCCN[C@@H]3C2)c(F)cc4C(=O)C(=CN(C5CC5)c14)C(=O)O	7.13
224	CHEMBL1630820	[O-][N+](=O)c1cn2C[C@@H](COc2n1)OCc3ccc(nn3)c4ccc(OC(F)(F)F)cc4	7.12
225	CHEMBL1632275	[O-][N+](=O)c1cn2C[C@@H](COc2n1)OCc3ccnc(c3)c4ccc(cc4)C(F)(F)F	7.12
226	CHEMBL566626	[O-][N+](=O)c1cn2C[C@@H](COc2n1)OCc3cn(nn3)c4ccc(OC(F)(F)F)cc4	7.12
227	CHEMBL578417	CSc1ccc(cc1)c2ccc(CO[C@@H]3COc4nc(cn4C3)[N+](=O)[O-])cc2	7.12
228	CHEMBL570993	CC(C)(C)OCc1ccc(cc1)c2ccc(CO[C@@H]3COc4nc(cn4C3)[N+](=O)[O-])cc2	7.11
229	CHEMBL571211	[O-][N+](=O)c1cn2C[C@@H](COc2n1)OCc3ccc(cc3)c4cccc(OC(F)(F)F)c4	7.11
230	CHEMBL571414	[O-][N+](=O)c1cn2C[C@@H](COc2n1)OCc3ccc(cc3)c4ccccc4C(F)(F)F	7.11
231	CHEMBL571461	CSc1cccc(c1)c2ccc(CO[C@@H]3COc4nc(cn4C3)[N+](=O)[O-])cc2	7.11
232	CHEMBL571854	[O-][N+](=O)c1cn2C[C@@H](COc2n1)OCc3cccc(c3)c4ccc(F)cc4	7.11
233	CHEMBL453102	[O-][N+](=O)c1cn2C[C@@H](COc2n1)NCCCCCc3ccc(OC(F)(F)F)cc3	7.11
234	CHEMBL455168	[O-][N+](=O)c1cn2C[C@@H](COc2n1)NCCCc3ccc(OC(F)(F)F)cc3	7.11
235	CHEMBL2177959	COc1ncccc1NC2=CC3=Nc4ccccc4N(C3=C/C/2=N\C5CCOCC5)c6ccc(F)cc6	7.10
236	CHEMBL1630825	[O-][N+](=O)c1cn2C[C@@H](COc2n1)OCc3cnc(cn3)c4ccc(cc4)C(F)(F)F	7.10
237	CHEMBL1632252	[O-][N+](=O)c1cn2C[C@@H](COc2n1)OCc3ccc(cc3)c4ccc(cn4)C#N	7.10
238	CHEMBL1632255	[O-][N+](=O)c1cn2C[C@@H](COc2n1)OCc3ccc(cc3)c4ccc(OC(F)F)cn4	7.10
239	CHEMBL1836433	[O-][N+](=O)c1cn2C[C@@H](COc2n1)OC\C=C\c3ccc(cc3)c4ccc(OC(F)F)cc4	7.10

240	CHEMBL1836452	[O-][N+](=O)c1cn2C[C@@H](COc2n1)OCC#Cc3ccc(nc3)c4ccc(OC(F)F) cc4	7.10
241	CHEMBL1946446	[O-][N+](=O)c1cn2C[C@@H](COc2n1)NC(=O)OCc3ccc(cc3)c4ccc(cc4) C(F)(F)F	7.10
242	CHEMBL262071	CCN(CC)C(=O)C1CCCN(C1)c2cc3N4C(=C(C(=O)O)C(=O)c3cc2F)Sc5c cccc45	7.10
243	CHEMBL463479	OC(=O)C1=CN(C2CC2)c3cc(N4CCN(Cc5ccc6OCOc6c5)CC4)c(cc3C1 =O)[N+](=O)[O-]	7.10
244	CHEMBL578202	[O-][N+](=O)c1cn2C[C@@H](COc2n1)OCc3ccc(cc3)c4ccccc4C=O	7.10
245	CHEMBL2177929	Cc1ccc(NC2=CC3=Nc4ccccc4N(C3=C/C/2=N\C5CCOCC5)c6ccc(Br)c c6)cn1	7.09
246	CHEMBL443904	CCCC[C@H](CN(O)C=O)C(=O)N1CCC[C@H]1c2nc3ccccc3[nH]2	7.08
247	CHEMBL443904	CCCC[C@H](CN(O)C=O)C(=O)N1CCC[C@H]1c2nc3ccccc3[nH]2	7.08
248	CHEMBL288149	CC(=O)NC[C@H]1CN(C(=O)O1)c2ccc(N3CCSCC3)c(F)c2	7.07
249	CHEMBL1630826	[O-][N+](=O)c1cn2C[C@@H](COc2n1)OCc3cnc(cn3)c4ccc(F)cc4	7.07
250	CHEMBL1836070	[O-][N+](=O)c1cn2C[C@@H](COc2n1)OCCOc3ccc(OCc4ccccc4)cc3	7.07
251	CHEMBL1836455	[O-][N+](=O)c1cn2C[C@@H](COc2n1)OCCCC#Cc3ccc(cc3)c4ccc(cc4)C (F)(F)F	7.07
252	CHEMBL1946445	[O-][N+](=O)c1cn2C[C@@H](COc2n1)NC(=O)OCc3ccc(cc3)c4ccc(F)cc 4	7.07
253	CHEMBL571193	CSc1ccccc1c2ccc(CO[C@@H]3COc4nc(cn4C3)[N+](=O)[O-])cc2	7.06
254	CHEMBL2177957	COC1CCC(CC1)\N=C\2/C=C3N(c4ccc(Cl)cc4)c5ccccc5N=C3C=C2Nc 6cncc(Br)c6	7.05
255	CHEMBL1818381	OC(=O)C1=CN(C2CC2)c3cc(N4CCN(CC4)C(=O)CC[N+](=O)[O-])c(F)cc3C1=O	7.05
256	CHEMBL1630565	COc1ccc(cc1F)c2ccc(CO[C@@H]3COc4nc(cn4C3)[N+](=O)[O-])cn2	7.05
257	CHEMBL1813821	COc1ccc(Cn2ccc3c(nc(Cl)cc23)c4occc4)cc1	7.05
258	CHEMBL1836078	[O-][N+](=O)c1cn2C[C@@H](COc2n1)OCC#Cc3ccc(OCc4ccccc4)cc3	7.05

259	CHEMBL1836430	[O-]][N+](=O)c1cn2C[C@@H](COc2n1)OC\C=C\c3ccc(cc3)c4ccc(F)cc4	7.05
260	CHEMBL1836442	[O-]][N+](=O)c1cn2C[C@@H](COc2n1)OCC#Cc3cccc(c3)c4ccc(OC(F)F)cc4	7.05
261	CHEMBL1836448	[O-]][N+](=O)c1cn2C[C@@H](COc2n1)OCC#Cc3ccc(nc3)c4ccc(OC(F)(F)F)cc4	7.05
262	CHEMBL1836581	[O-]][N+](=O)c1cn2C[C@@H](COc2n1)Oc3ccc(cc3)c4ccc(OC(F)(F)F)cc4	7.05
263	CHEMBL229121	CCCCCCCCCCCCCCCc1oc(nn1)c2ccncc2	7.05
264	CHEMBL585348	[O-]][N+](=O)c1cn2C[C@@H](COc2n1)OCc3ccc(cc3)c4ccc(cc4)c5ccccc5	7.05
265	CHEMBL1632259	[O-][N+](=O)c1cn2C[C@@H](COc2n1)OCc3ccc(cc3)c4ccc(F)nc4	7.02
266	CHEMBL571462	[O-][N+](=O)c1cn2C[C@@H](COc2n1)OCc3cccc(c3)c4ccccc4	7.02
267	CHEMBL584750	CSc1ccc(cc1)c2cccc(CO[C@@H]3COc4nc(cn4C3)[N+](=O)[O-])c2	7.02
268	CHEMBL585726	CC(C)(C)c1ccc(cc1)c2ccc(CO[C@@H]3COc4nc(cn4C3)[N+](=O)[O-])cc2	7.02
269	CHEMBL2177923	COc1ncccc1NC2=CC3=Nc4ccccc4N(C3=C/C/2=N\C(C)C)c5ccc(Br)cc5	7.02
270	CHEMBL584117	[O-]][N+](=O)c1cn2C[C@@H](COc2n1)OCc3ccc(cc3)c4ccc(OCCCN5CCOCC5)cc4	7.01
271	CHEMBL2177928	CC(C)\N=C\1/C=C2N(c3ccc(Br)cc3)c4ccccc4N=C2C=C1Nc5ccc(C)nc5	7.01
272	CHEMBL1078545	COc1cc2CC(C(=O)c3ccc(F)cc3)C(=O)c2cc1OC	7.00
273	CHEMBL1254435	COc1ccc(Cn2ccc3c(ncnc23)c4occc4)cc1	7.00
274	CHEMBL1836492	[O-]][N+](=O)c1cn2C[C@@H](COc2n1)Oc3ccc(cn3)c4ccc(cc4)C(F)(F)F	7.00
275	CHEMBL238454	OC(=O)C1=CN(c2ccc(F)cc2)c3nc(N4CCOC4)c(cc3C1=O)[N+](=O)[O-]	7.00
276	CHEMBL238455	CC(C)(C)N1C=C(C(=O)O)C(=O)c2cc(c(nc12)N3COCC3(C)C)[N+](=O)[O-]	7.00
277	CHEMBL474787	CCOC(=O)c1cc(COc2cc(nc3c(cccc23)C(F)(F)F)C(F)(F)F)on1	7.00
278	CHEMBL571835	CC(C)c1ccc(cc1)c2ccc(CO[C@@H]3COc4nc(cn4C3)[N+](=O)[O-])cc2	7.00

279	CHEMBL519613	ON(C[C@@H](CC1CC1)C(=O)N2CCC[C@H]2c3nc4ccccc4[nH]3)C=O	6.85
280	CHEMBL506649	CCCC[C@H](CN(O)C=O)C(=O)N1CCC[C@H]1c2oc3ccccc3n2	6.78
281	CHEMBL1818380	CCN1C=C(C(=O)O)C(=O)c2cc(F)c(cc12)N3CCN(CC3)C(=O)CC[N+](=O)[O-]	6.33
282	CHEMBL463859	ON(C[C@@H](CC1CC1)C(=O)N2CCC[C@H]2c3oc4ccccc4n3)C=O	6.25
283	CHEMBL33	C[C@H]1COc2c(N3CCN(C)CC3)c(F)cc4C(=O)C(=CN1c24)C(=O)O	6.16
284	CHEMBL2152073	Cc1cccc(c1)c2cc(Nc3ccc4nc(cc(N)c4c3)c5ccc(F)cc5)nc(N)n2	6.09
285	CHEMBL1090170	Cc1c(C(=O)NCc2ccccc2)[n+]([O-])c3cc(ccc3[n+]1[O-])C(F)(F)F	5.97
286	CHEMBL2152075	Nc1cc(nc2ccc(Nc3cc(nc(N)n3)c4ccc(F)cc4)cc12)c5ccc(F)cc5	5.94
287	CHEMBL364019	COc1ccc(Cn2cnc3c(nc(Cl)nc23)c4occc4)cc1	5.94
288	CHEMBL2152077	Nc1cc(nc2ccc(Nc3cc(nc(N)n3)c4ccccc4)cc12)c5ccc(F)cc5	5.78
289	CHEMBL2152072	Nc1cc(nc2ccc(Nc3cc(nc(N)n3)c4ccc(Cl)cc4)cc12)c5ccc(F)cc5	5.72
290	CHEMBL2152080	COc1cccc(c1)c2cc(N)c3cc(Nc4cc(nc(N)n4)c5ccc(Cl)cc5)ccc3n2	5.67
291	CHEMBL2152076	Nc1cc(nc2ccc(Nc3cc(nc(N)n3)c4cccc(Cl)c4)cc12)c5ccc(F)cc5	5.66
292	CHEMBL2152074	Nc1cc(nc2ccc(Nc3cc(nc(N)n3)c4ccc(cc4)C(F)(F)F)cc12)c5ccc(F)cc5	5.54
293	CHEMBL2152078	Nc1cc(nc2ccc(Nc3cc(nc(N)n3)c4ccccc4F)cc12)c5ccc(F)cc5	5.49
294	CHEMBL1224745	CCCCCc1ccc(Oc2ccccc2)c(O)c1	5.46
295	CHEMBL306946	O=C1N2C(=Nc3ccccc13)C(=O)c4ccccc24	5.39
296	CHEMBL2152079	COc1ccccc1c2cc(Nc3ccc4nc(cc(N)c4c3)c5ccc(F)cc5)nc(N)n2	5.35
297	CHEMBL192544	COc1ccc(Cn2cnc3c(ncnc23)c4occc4)cc1	5.29
298	CHEMBL2030513	COc1ccc2cc(ccc2c1)c3nc([nH]c3c4ccnc(N)c4)C(C)(C)C	5.27
299	CHEMBL505886	CCCCCCCCc1ccc(Oc2ccccc2)c(O)c1	5.19
300	CHEMBL264682	CCCCCCc1ccc(Oc2ccccc2)c(O)c1	5.11
301	CHEMBL2017870	CN(C)[C@@H]1CCN(C1)c2cc(Nc3cc(Cl)ccn3)nc(n2)c4ccccc4	5.10
302	CHEMBL2152081	Nc1cc(nc2ccc(Nc3cc(nc(N)n3)c4ccccn4)cc12)c5ccc(F)cc5	5.02
303	CHEMBL2017871	CN(C)[C@@H]1CCN(C1)c2cc(Nc3cc(ccn3)C(F)(F)F)nc(n2)c4cccc(c4)C#N	4.80
304	CHEMBL2017732	CN(C)[C@@H]1CCN(C1)c2cc(Nc3cc([nH]n3)C4CC4)nc(n2)c5ccccc5	4.80

305	CHEMBL2152084	Cc1cc(Nc2ccc3nc(cc(N)c3c2)c4ccc(F)cc4)nc(N)n1	4.65
306	CHEMBL592545	Cn1c2ccccc2c3nnc(SCCCN4C(=O)Nc5ccccc45)nc13	4.64
307	CHEMBL964	CCN(CC)C(=S)SSC(=S)N(CC)CC	4.57
308	CHEMBL405973	Oc1cc(Cc2ccccc2)ccc1Oc3ccc(Cl)cc3Cl	4.57
309	CHEMBL405402	CCCCc1ccc(Oc2ccc(Cl)cc2Cl)c(O)c1	4.52
310	CHEMBL2017736	CN1CCC(CNc2cc(Nc3cc([nH]n3)C4CC4)nc(n2)c5cccc(c5)C#N)CC1	4.51
311	CHEMBL2017730	CN1CCC(CNc2cc(Nc3cc([nH]n3)C4CC4)nc(n2)c5ccccc5)CC1	4.51
312	CHEMBL2017733	C(CN1CCCC1)Oc2cc(Nc3cc([nH]n3)C4CC4)nc(n2)c5ccccc5	4.51
313	CHEMBL2017731	CN1CCC(CC1)Nc2cc(Nc3cc([nH]n3)C4CC4)nc(n2)c5ccccc5	4.51
314	CHEMBL2017716	CS(=O)(=O)Nc1cccc(c1)c2nccc(Nc3cc([nH]n3)C4CC4)n2	4.51
315	CHEMBL592712	C=CCn1c2ccccc2c3nnc(SCCCN4C(=O)Nc5ccccc45)nc13	4.51
316	CHEMBL1738931	CO[C@H]([C@H](O)[C@@H](O)[C@H](O)\C=C\C(C)(C)C)C(=O)NCCOc1c(C)cc(C)cc1C	4.36
317	CHEMBL589101	CCn1c2ccccc2c3nnc(SCCCN4C(=O)Nc5ccccc45)nc13	4.33
318	CHEMBL259880	Oc1cc(CCCc2ccccc2)ccc1Oc3ccc(Cl)cc3Cl	4.30
319	CHEMBL260061	Oc1cc(CCc2ccccc2)ccc1Oc3ccc(Cl)cc3Cl	4.28
320	CHEMBL261521	CC(C)Cc1ccc(Oc2ccc(Cl)cc2Cl)c(O)c1	4.22
321	CHEMBL414086	CN(Cc1c2ccccc2cc3ccccc13)C(=O)C4CN(C5CCCCCCC5)C(=O)C4	4.20
322	CHEMBL386324	FC(F)(F)c1cc(Br)cc(NC(=O)C2CN(C3CCCCC3)C(=O)C2)c1	4.20
323	CHEMBL2017735	CN(C)CCNc1cc(Nc2cc([nH]n2)C3CC3)nc(n1)c4cccc(c4)C#N	4.20
324	CHEMBL2017737	CN1CCC(CNc2cc(Nc3cc([nH]n3)C4CC4)nc(n2)c5cccc(c5)S(=O)(=O)C)CC1	4.20
325	CHEMBL2017734	CN(C)[C@@H]1CCN(C1)c2cc(Nc3cc([nH]n3)C4CC4)nc(n2)c5cccc(c5)C#N	4.20
326	CHEMBL2017724	Fc1cccc(CCNc2nccc(Nc3cc([nH]n3)C4CC4)n2)c1	4.20
327	CHEMBL2017721	C1CCC(CC1)Nc2nccc(Nc3cc([nH]n3)C4CC4)n2	4.20
328	CHEMBL2017717	CS(=O)(=O)c1cccc(c1)c2nccc(Nc3cc([nH]n3)C4CC4)n2	4.20
329	CHEMBL2017727	C1CCC(C1)Nc2nccc(Nc3cc([nH]n3)C4CC4)n2	4.20
330	CHEMBL2017729	CN1CCN(CC1)c2cc(Nc3cc([nH]n3)C4CC4)nc(n2)c5ccccc5	4.20
331	CHEMBL2017718	CS(=O)(=O)NCc1ccc(cc1)c2nccc(Nc3cc([nH]n3)C4CC4)n2	4.20

332	CHEMBL2017722	CC(C)CCNc1nccc(Nc2cc([nH]n2)C3CC3)n1	4.20
333	CHEMBL2017715	NC(=O)c1cccc(c1)c2nccc(Nc3cc([nH]n3)C4CC4)n2	4.20
334	CHEMBL1989145	BrC1=C(Br)C(=O)c2ccccc2C1=O	4.10
335	CHEMBL2030500	COc1ccc2cc(ccc2c1)c3nc([nH]c3c4ccncc4)C(C)(C)C	4.05
336	CHEMBL2030517	CC(C)(C)c1nc(c2cnc3ccccc3c2)c([nH]1)c4ccncc4	4.01
337	CHEMBL2017725	Clc1ccccc1CCNc2nccc(Nc3cc([nH]n3)C4CC4)n2	3.90
338	CHEMBL2017719	N#Cc1cccc(c1)c2nccc(Nc3cc([nH]n3)C4CC4)n2	3.90
339	CHEMBL2017728	CN(C)CCNc1cc(Nc2cc([nH]n2)C3CC3)nc(n1)c4ccccc4	3.90
340	CHEMBL240533	O=C(N1CCN(CC1)C2c3ccccc3c4ccccc24)c5ccccc5	3.90
341	CHEMBL216579	O=C(N1CCN(CC1)C2c3ccccc3c4ccccc24)c5ccc6[nH]ccc6c5	3.90
342	CHEMBL2017720	C1CC1c2cc(Nc3ccnc(n3)c4cccnc4)n[nH]2	3.90
343	CHEMBL386329	CN(Cc1c2ccccc2cc3ccccc13)C(=O)C4CN(C5CCCCCC5)C(=O)C4	3.90
344	CHEMBL1224754	CN(C(=O)C1CN(C2CCCCCC2)C(=O)C1)c3cc(c(O)c(c3)c4ccccc4)c5ccccc5	3.90
345	CHEMBL392127	Cc1ccc(cc1)C(=O)N2CCN(CC2)C3c4ccccc4c5ccccc35	3.90
346	CHEMBL426702	CN(Cc1c2ccccc2cc3ccccc13)C(=O)C4CN(C5CC6CCC5C6)C(=O)C4	3.90
347	CHEMBL2017723	C(Nc1nccc(Nc2cc([nH]n2)C3CC3)n1)c4ccccc4	3.90
348	CHEMBL217594	CN(Cc1c2ccccc2cc3ccccc13)C(=O)C4CN(C5CCCCC5)C(=O)C4	3.90
349	CHEMBL239673	Cc1ccc(cc1C)C(=O)N2CCN(CC2)c3cccc(Cl)c3	3.90
350	CHEMBL2017726	C(Nc1nccc(Nc2cc([nH]n2)C3CC3)n1)C4CC4	3.60
351	CHEMBL2057353	O\N=C/Nc1nc2c(COc3cc4OCOc4cc23)s1	3.46
352	CHEMBL1224746	CCCCCCCCCCCCCCc1ccc(Oc2ccccc2)c(O)c1	3.34
353	CHEMBL2017714	Fc1ccc(cc1)c2nccc(Nc3cc([nH]n3)C4CC4)n2	3.30
354	CHEMBL375328	OC1=CC2=C(c3ccccc3)c4cc(O)c(O)cc4OC2=CC1=O	3.20
355	CHEMBL2057356	O\N=C/Nc1nc2c(CCOc3cc4OCOc4cc23)s1	3.18
356	CHEMBL2057348	COc1ccc2CCc3sc(N\C=N/O)nc3c2c1	3.14
357	CHEMBL203125	ON(CCCP(=O)(O)O)C=O	2.56

ChEMBL

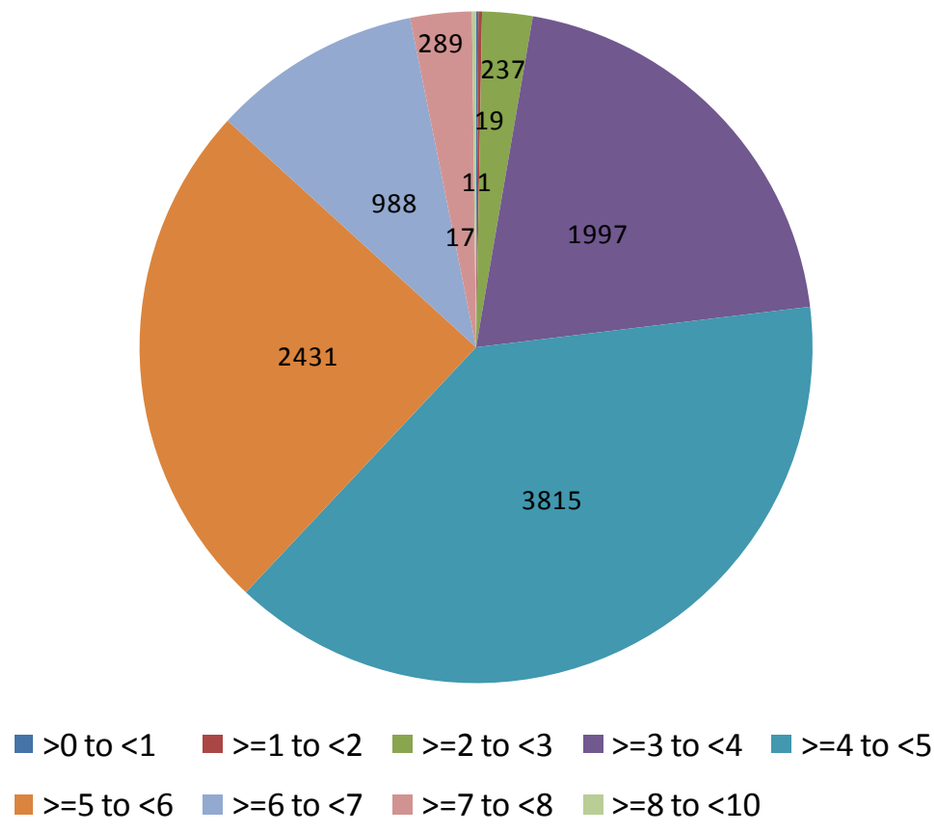
Independent Validation Set

(ChEMBL: 9804 compounds: **3727** actives and **6077** inactives)

Table: Distribution of "independent validation set" of 9804 compounds

Independent Validation Set: ChEMBL dataset containing **9804** cell based assay compounds (compounds were not considered neither in training set nor in test set)			
S. No	**pMIC Range**	**No.of compounds**	**DATA**
1	>0 to <1	11	Negative Data Set **(6077)**
2	>=1 to <2	17	
3	>=2 to <3	237	
4	>=3 to <4	1997	
5	>=4 to <5	3815	
6	>=5 to <6	2431	Positive Data Set **(3727)**
7	>=6 to <7	988	
8	>=7 to <8	289	
9	>=8 to <10	19	

Distribution of an independent validation set of 9804 compounds



ANTIMICROBIALS (ChEMBL)

Prioritized top 100 Antimicrobial Compounds								
CMPD_CHEMBLID	CANONICAL_SMILES	MIC	Unit	M1	M2	M3	M4	M5
CHEMBL1652634	CCO\N=C\1/C(=O)N(CCN2CCN(CC2)c3c(F)cc4C(=O)C(=CN(C5CC5)c4c3OC)C(=O)O)c6ccc(F)cc16	1310	nM	8.04	7.37	7.92	10.08	8.40
CHEMBL1652633	CCO\N=C\1/C(=O)N(CCN2CCN(CC2)c3c(F)cc4C(=O)C(=CN(C5CC5)c4c3OC)C(=O)O)c6ccccc16	5410	nM	8.17	7.38	7.85	9.85	8.46
CHEMBL1210953	COc1c(ccc2C(=O)C(=CN(C3CC3)c12)C(=O)O)N4CCCC(C4)N(C)CCN5C(=O)\C(=N/Nc6ccccc6)\c7cc(F)ccc57	3.12	ug.mL-1	7.96	8.17	7.14	9.32	7.73
CHEMBL1210944	CO\N=C/1\C(=O)N(CCN(C)C2CCCN(C2)c3ccc4C(=O)C(=CN(C5CC5)c4c3OC)C(=O)O)c6ccccc16	3.12	ug.mL-1	7.47	6.73	7.75	9.37	8.10
CHEMBL1210945	CO\N=C/1\C(=O)N(CCN(C)C2CCCN(C2)c3ccc4C(=O)C(=CN(C5CC5)c4c3OC)C(=O)O)c6ccc(F)cc16	3.12	ug.mL-1	7.26	6.65	7.83	9.60	8.04
CHEMBL1652584	COc1c(N2CCN(CCN3C(=O)\C(=N/O)\c4ccccc34)CC2)c(F)cc5C(=O)C(=CN(C6CC6)c15)C(=O)O	11380	nM	7.81	6.78	6.61	8.75	8.11
CHEMBL2048648	CCC1=CN([C@@H]2O[C@H](CO)[C@@H](N=[N+]=[N-])[C@@H]2F)C(=O)NC1=O	0	%	6.08	7.41	7.51	8.87	8.09
CHEMBL1652585	COc1c(N2CCN(CCN3C(=O)\C(=N/O)\c4cc(F)ccc34)CC2)c(F)cc5C(=O)C(=CN(C6CC6)c15)C(=O)O	22050	nM	7.79	7.06	6.67	8.61	7.74
CHEMBL483287	[O-][N+](=O)c1ccc(cc1)C(=O)CC(=O)C(F)(F)F	50	ug.mL-1	6.96	9.77	6.62	8.57	5.82
CHEMBL1915691	C[C@H]1COc2c(N3CCN(C)CC3)c(F)cc4C(=O)C(=CN1c24)C(=O)NCCCCCNC(=O)C5=CN6[C@@H](C)COc7c(N8CCN(C)CC8)c(F)cc(C5=O)c67	60	%	7.86	9.24	5.51	7.61	7.35
CHEMBL1791034	OC[C@H]1O[C@H](C[C@@H]1N=[N+]=[N-])N2C=C(F)C(=O)NC2=O			6.01	7.32	7.74	8.66	7.74
CHEMBL1652636	COc1c(N2CCN(CCN3C(=O)\C(=N/NC(=O)N)\c4cc(F)ccc34)CC2)c(F)cc5C(=O)C(=CN(C6CC6)c15)C(=O)O	5120	nM	7.92	7.24	6.40	8.56	7.04
CHEMBL1652635	COc1c(N2CCN(CCN3C(=O)\C(=N/NC(=O)N)\c4ccccc34)CC2)c(F)cc5C(=O)C(=CN(C6CC6)c15)C(=O)O	5280	nM	8.03	7.18	6.38	8.39	7.07
CHEMBL2048643	CCC1=CN([C@@H]2O[C@H](COC(=O)C)[C@@H](OC(=O)C)[C@@H]2F)C(=O)NC1=O	35	%	5.08	8.55	7.24	8.26	7.85
CHEMBL227446	Fc1c(F)c(F)c(\C=N\NC(=O)c2cc(c3ccccc3n2)C45CC6CC(CC(C6)C4)C5)c(F)c1F	16	%	5.83	7.53	8.72	7.75	6.83

CHEMBL387500	FC(F)(F)c1ccc(\C=N\NC(=O)c2cc(c3ccccc3n2)C45CC6CC(CC(C6)C4)C5)c(c1)C(F)(F)F	64	%	7.00	5.65	8.48	8.26	7.26
CHEMBL1210942	COc1c(ccc2C(=O)C(=CN(C3CC3)c12)C(=O)O)N4CCCC(C4)N(C)CCN5C(=O)\C(=N\O)\c6ccccc56	12.5	ug.mL-1	7.16	6.05	6.58	8.66	8.15
CHEMBL1210952	COc1c(ccc2C(=O)C(=CN(C3CC3)c12)C(=O)O)N4CCCC(C4)N(C)CCN5C(=O)\C(=N/Nc6ccccc6)\c7ccccc57	3.12	ug.mL-1	6.78	5.67	7.11	9.12	7.78
CHEMBL573100	COc1cc(\C=N\NC(=O)c2ccc(cc2)N3CCOCC3)cc(OC)c1OC	35.83	%	7.78	5.32	7.96	7.78	7.61
CHEMBL2048644	CCC1=CN([C@@H]2O[C@H](COC(=O)C)[C@@H](OC(=O)C)[C@@H]2F)C(=O)NC1=S	25	%	5.02	8.28	7.31	8.25	7.50
CHEMBL247443	FC(F)(F)C(N(CCCN1CCOCC1)C(=O)c2cccnc2)C(=O)NCC=C	72	%	7.01	7.83	7.24	6.96	7.26
CHEMBL1652582	COc1c(N2CCN(CCN3C(=O)C(=O)c4ccccc34)CC2)c(F)cc5C(=O)C(=CN(C6CC6)c15)C(=O)O	5840	nM	6.38	7.65	6.26	8.93	6.94
CHEMBL1652583	COc1c(N2CCN(CCN3C(=O)C(=O)c4cc(F)ccc34)CC2)c(F)cc5C(=O)C(=CN(C6CC6)c15)C(=O)O	2830	nM	6.42	7.90	6.39	8.80	6.58
CHEMBL247441	FC(F)(F)C(N(C1CCCCC1)C(=O)c2cccnc2)C(=O)NCC=C	60	%	6.38	8.38	6.97	7.12	6.90
CHEMBL607830	CC1=NNC(=O)C1CN2C(=O)C(=O)Nc3ccccc23	8.01	mm	5.59	6.20	6.22	9.01	8.65
CHEMBL575398	[O-][N+](=O)c1cccc(\C=N\NC(=O)c2ccc(cc2)N3CCOCC3)c1	9.12	%	7.65	4.54	8.25	7.74	7.34
CHEMBL1210950	COc1c(ccc2C(=O)C(=CN(C3CC3)c12)C(=O)O)N4CCCC(C4)N(C)CCN5C(=O)\C(=N/NC(=O)N)\c6ccccc56	12.5	ug.mL-1	7.42	6.28	6.36	8.32	7.13
CHEMBL1210542	COc1ccc(cc1)\C(=N\NC(=O)c2cnccn2)\C	100	ug.mL-1	7.67	4.92	7.65	8.97	6.16
CHEMBL1210940	COc1c(N2CCCC(C2)N(C)CCN3C(=O)C(=O)c4ccccc34)c(F)cc5C(=O)C(=CN(C6CC6)c15)C(=O)O	25	ug.mL-1	6.00	7.26	6.21	8.98	6.90
CHEMBL247254	FC(F)(F)C(N(CCCn1ccnc1)C(=O)c2cccnc2)C(=O)NCC=C	71	%	6.52	7.96	6.39	7.12	7.17
CHEMBL1938677	OC[C@H]1O[C@H](C[C@@H]1N=[N+]=[N-])N2C=C(Cl)C(=O)NC2=O	50	%	5.02	5.72	7.71	8.64	7.82
CHEMBL1289119	CCCCCC(=O)OCOC(=O)C1=CN2[C@@H](C)COc3c(N4CCN(C)CC4)c(F)cc(C1=O)c23	95	%	6.46	6.96	6.05	8.00	7.40
CHEMBL249881	COc1ccc2c(CCCC2(N(CCCN3CCOCC3)C(=O)c4cccnc4)C(=O)NCC=C)c1	64	%	5.86	6.43	6.93	7.75	7.81

CHEMBL1254874	Cc1c(C(=O)NCc2ccc(cc2)C(F)(F)F)[n+]([O-])c3ccccc3[n+]1[O-]	16.81	ug.mL-1	5.95	6.32	5.98	8.95	7.44
CHEMBL584126	CCCCCC(=O)OCC(=O)N1CCN(CC1)c2cc3N(C=C(C(=O)O)C(=O)c3cc2F)C4CC4	95	%	6.60	7.22	5.95	8.17	6.67
CHEMBL1829185	CCN1C=C(C(=O)O)C(=O)c2cc(F)c(cc12)N3CCN(CC3)\C=N\NC(=O)c4ccc(F)cc4	16000	nM	7.25	5.61	7.32	7.30	7.12
CHEMBL1289238	CCCCCCCCCC(=O)OCOC(=O)C1=CN2[C@@H](C)COc3c(N4CCN(C)CC4)c(F)cc(C1=O)c23	95	%	6.69	6.69	6.08	7.67	7.35
CHEMBL1777915	COc1ccc2c(c1)[n+]([O-])c(\C=N\NC(=O)c3ccncc3)c(C)[n+]2[O-]	590	nM	6.98	4.45	6.38	8.56	8.05
CHEMBL1917771	CCOC(=O)CN1C(C(OC)C1=O)C(S)(CC)CC			4.60	6.21	7.40	8.83	7.34
CHEMBL1255042	COc1ccc2c(c1)[n+]([O-])c(C(=O)NCc3ccc(cc3)C(F)(F)F)c(C)[n+]2[O-]	100	ug.mL-1	6.13	5.59	5.92	9.27	7.37
CHEMBL574972	CCCC(=O)OCC(=O)N1CCN(CC1)c2cc3N(C=C(C(=O)O)C(=O)c3cc2F)C4CC4			6.15	6.96	5.97	8.51	6.70
CHEMBL247444	FC(F)(F)C(N(C1CC1)C(=O)c2cccnc2)C(=O)NCC=C	74	%	6.37	8.84	6.11	6.22	6.65
CHEMBL573097	CC(=O)OCC(=O)N1CCN(CC1)c2cc3N(C=C(C(=O)O)C(=O)c3cc2F)C4CC4			5.91	6.82	6.14	8.69	6.63
CHEMBL247623	FC(F)(F)C(N(CC=C)C(=O)c1cccnc1)C(=O)NCC=C	6	%	5.85	8.26	6.78	6.55	6.71
CHEMBL1289355	CCCCNC(=O)C1=CN2[C@@H](C)COc3c(N4CCN(C)CC4)c(F)cc(C1=O)c23			6.36	5.68	5.88	8.26	7.93
CHEMBL1254959	Cc1c(C(=O)NCc2ccc(cc2)C(F)(F)F)[n+]([O-])c3cc(F)ccc3[n+]1[O-]	4.48	ug.mL-1	5.99	5.76	6.01	9.08	7.23
CHEMBL1915913	CCCCCCCCCCCCCCCCCCCC(=O)OCOC(=O)C1=CN2[C@@H](C)COc3c(N4CCN(C)CC4)c(F)cc(C1=O)c23			7.15	6.37	6.23	6.81	7.48
CHEMBL1777919	Cc1c(\C=N\NC(=O)c2ccncc2)[n+]([O-])c3cc(ccc3[n+]1[O-])C(F)(F)F	1500	nM	6.83	5.19	6.85	7.85	7.32
CHEMBL61673	C[C@H]1Cc2c(ccc(O)c2C(=O)O1)C(=O)O			4.53	5.49	7.46	9.07	7.48
CHEMBL574259	CCCCCCCC(=O)OCC(=O)N1CCN(CC1)c2cc3N(C=C(C(=O)O)C(=O)c3cc2F)C4CC4	95	%	6.66	6.70	5.99	8.00	6.61
CHEMBL336853	OCCOCN1C=C(C(CCl)N=[N+]=[N-])C(=O)NC1=O	50	%	5.75	5.16	7.86	8.41	6.77
CHEMBL247985	CC(C)(C)CN(C(C(=O)NCC=C)C(F)(F)F)C(=O)c1cccnc1	77	%	5.90	7.79	6.72	6.77	6.75
CHEMBL1289471	CCCCCCNC(=O)C1=CN2[C@@H](C)COc3c(N4CCN(C)CC4)c(F)cc(C1=O)c23			6.61	5.58	5.91	7.98	7.83

CHEMBL1288790	CCCCCCCCCCCCCCCC(=O)OCOC(=O)C1=CN2[C@@H](C)COc3c(N4CCN(C)CC4)c(F)cc(C1=O)c23			6.71	6.43	6.17	7.15	7.43
CHEMBL575170	CCCCCCCCCC(=O)OCC(=O)N1CCN(CC1)c2cc3N(C=C(C(=O)O)C(=O)c3cc2F)C4CC4	95	%	6.94	6.63	6.02	7.72	6.51
CHEMBL574280	Fc1ccc(\C=N\NC(=O)c2ccc(cc2)N3CCOCC3)cc1	83.22	%	6.92	3.28	8.43	7.85	7.33
CHEMBL1254960	Cc1c(C(=O)NCc2ccc(cc2)C(F)(F)F)[n+]([O-])c3cc(ccc3[n+]1[O-])C(F)(F)F	3.38	ug.mL-1	6.12	6.33	5.90	8.55	6.84
CHEMBL1791024	OC[C@H]1O[C@H](C[C@@H]1N=[N+]=[N-])N2C=C(Br)C(=O)NC2=O	30	%	5.11	4.39	7.66	8.67	7.83
CHEMBL570338	COc1ccc(\C=N\NC(=O)c2cnccn2)cc1	100	ug.mL-1	7.39	4.68	7.62	7.73	6.20
CHEMBL575381	CCCCCCCCC(=O)OCC(=O)N1CCN(CC1)c2cc3N(C=C(C(=O)O)C(=O)c3cc2F)C4CC4	95	%	6.83	6.74	6.01	7.62	6.34
CHEMBL1254875	Cc1c(C(=O)NCc2ccc(cc2)C(F)(F)F)[n+]([O-])c3cc(Cl)ccc3[n+]1[O-]	6.13	ug.mL-1	5.60	5.66	6.09	8.92	7.23
CHEMBL573544	CCCCCCCCCCCCCC(=O)OCC(=O)N1CCN(CC1)c2cc3N(C=C(C(=O)O)C(=O)c3cc2F)C4CC4	95	%	6.87	6.46	6.09	7.39	6.59
CHEMBL573526	CCCCCCCCCCCCCCCC(=O)OCC(=O)N1CCN(CC1)c2cc3N(C=C(C(=O)O)C(=O)c3cc2F)C4CC4			7.08	6.30	6.13	7.22	6.62
CHEMBL558008	O=C(N1N=C(CC1c2ccc(Oc3ccccc3)cc2)c4ccccn4)c5ccccc5	100	%	6.47	5.51	6.13	8.11	7.12
CHEMBL62462	OCCOCN1C=C(C(=C)N=[N+]=[N-])C(=O)NC1=O	25	%	5.47	4.60	7.70	9.01	6.56
CHEMBL1289580	CCCCCCCCNC(=O)C1=CN2[C@@H](C)COc3c(N4CCN(C)CC4)c(F)cc(C1=O)c23	95	%	6.55	5.22	5.95	7.82	7.80
CHEMBL1255041	Cc1ccc2c(c1)[n+]([O-])c(C(=O)NCc3ccc(cc3)C(F)(F)F)c(C)[n+]2[O-]	100	ug.mL-1	5.87	5.95	5.86	8.71	6.93
CHEMBL574277	CCCCCCCCCCCC(=O)OCC(=O)N1CCN(CC1)c2cc3N(C=C(C(=O)O)C(=O)c3cc2F)C4CC4	95	%	6.62	6.51	6.06	7.56	6.55
CHEMBL1254312	[O-][n+]1c(C(=O)Nc2ccccc2)c(c3ccccc3)[n+]([O-])c4ccc(cc14)C(F)(F)F	19.1	ug.mL-1	6.33	7.66	4.18	8.88	6.22
CHEMBL575387	CCCCCCCCCCC(=O)OCC(=O)N1CCN(CC1)c2cc3N(C=C(C(=O)O)C(=O)c3cc2F)C4CC4	95	%	7.05	6.51	6.04	7.37	6.27
CHEMBL1210543	C\C(=N/NC(=O)c1cnccn1)\c2ccc(Br)cc2	100	ug.mL-1	6.92	3.63	7.89	8.82	5.96

CHEMBL1289687	CCCCCCCCCCCCNC(=O)C1=CN2[C@@H](C)COc3c(N4CCN(C)CC4)c(F)cc(C1=O)c23	95	%	6.86	4.96	6.02	7.50	7.84
CHEMBL246602	COc1ccc2c(CCCC2(N(C3CCCCC3)C(=O)c4ccccnc4)C(=O)NCC=C)c1	72	%	4.69	5.82	6.70	7.92	8.00
CHEMBL389923	COc1ccccc1NC(=S)N2N=C(CC2c3cc(OC)c(OC)c(OC)c3)c4ccc(O)c(C)c4	92	%	6.62	6.09	6.15	7.74	6.44
CHEMBL1915678	OC(=O)C1=CN(C2CC2)c3cc(N4CCN(CC4)C(=O)COCc5ccccc5)c(F)cc3C1=O			6.18	6.37	6.06	8.07	6.31
CHEMBL134873	OCCOCN1C=C(C(CBr)N=[N+]=[N-])C(=O)NC1=O	50	%	5.59	4.19	7.91	8.43	6.82
CHEMBL1173140	COc1cc(\C=N\NC(=O)c2cnccn2)ccc1O	100	ug.mL-1	7.90	5.20	6.92	7.30	5.58
CHEMBL574275	O=C(N\N=C/1\OCC=C1)c2ccc(cc2)N3CCOCC3	15.04	%	6.16	4.19	7.41	7.69	7.41
CHEMBL247987	C=CCNC(=O)C1(CCCCC1)N(CCCN2CCOCC2)C(=O)c3cccnc3	49	%	5.33	5.81	6.75	7.39	7.54
CHEMBL399666	COc1ccc2c(CCCC2(N(CC=C)C(=O)c3cccnc3)C(=O)NCC=C)c1	80	%	4.50	5.85	6.59	8.05	7.79
CHEMBL223505	COc1ccc(cc1)\C(=N\NC(=S)N)\C	0.25	ug.mL-1	6.32	4.52	6.60	8.40	6.75
CHEMBL1254890	CCCCCCCCCCCCc1cccc(c1)C(=O)C2C=CN(CC(=O)OCC)C=C2C(=O)N	5300	nM	6.41	6.57	6.97	5.65	6.97
CHEMBL1287831	CCCCCCCCCCCCCCNC(=O)C1=CN2[C@@H](C)COc3c(N4CCN(C)CC4)c(F)cc(C1=O)c23	95	%	6.48	4.84	6.05	7.31	7.86
CHEMBL399770	COc1ccc2c(CCCC2(N(C3CC3)C(=O)c4ccccnc4)C(=O)NCC=C)c1	69	%	4.53	6.10	6.10	7.97	7.84
CHEMBL134162	OCCOCN1C=C(C(Cl)N=[N+]=[N-])C(=O)NC1=O	50	%	5.46	3.72	7.91	8.49	6.92
CHEMBL334434	OCC(CO)OCN1C=C(C(CCl)N=[N+]=[N-])C(=O)NC1=O	0	%	6.10	4.89	7.36	7.36	6.76
CHEMBL570123	Clc1ccc(\C=N\NC(=O)c2cnccn2)cc1	100	ug.mL-1	7.10	4.38	7.76	7.21	6.01
CHEMBL572618	OC(=O)C1=CN(C2CC2)c3cc(N4CCN(CC4)C(=O)CCl)c(F)cc3C1=O			5.42	6.09	6.02	8.32	6.51
CHEMBL64724	OCC(CO)OCN1C=C(C(=C)N=[N+]=[N-])C(=O)NC1=O	0	%	5.88	4.56	7.24	7.94	6.73
CHEMBL35179	OCCOCN1C=C(C(=O)NC1=O)[N+](=O)[O-]	0	%	4.67	5.79	7.02	8.27	6.59
CHEMBL1254622	Cc1c(C(=O)NCc2ccc3OCOc3c2)[n+]([O-])c4cc(Cl)c(Cl)cc4[n+]1[O-]	34.92	ug.mL-1	5.07	5.37	5.04	8.91	7.94
CHEMBL574272	CCCCCCCCC(=O)N1CCN(CC1)c2cc3N(C=C(C(=O)O)C(=O)c3cc2F)C4CC4	95	%	6.15	5.83	5.91	7.81	6.62
CHEMBL573315	CCCCC(=O)N1CCN(CC1)c2cc3N(C=C(C(=O)O)C(=O)c3cc2F)C4CC4			5.63	6.00	5.80	8.26	6.63

CHEMBL223287	[I-].CC[N+](C)(CC)CCOc1ccc(cc1)C(=O)N2C\C(=C/c3ccc(cc3)[N+](=O)[O-])\C(=O)\C(=C\c4ccc(cc4)[N+](=O)[O-])\C2	0	%	6.95	7.60	6.02	6.15	5.58
CHEMBL1210545	COc1ccc2nc(Cl)c(\C=N\NC(=O)c3cnccn3)cc2c1	100	ug.mL-1	6.97	5.08	6.36	7.63	6.27
CHEMBL457267	CCCCCCC[C@@H]1CC(=O)N[C@@H](CO)C(=O)O[C@H](CCCCCC)CC(=O)N[C@@H](CO)C(=O)O1	180000	nM	6.13	7.08	5.61	6.88	6.58
CHEMBL401252	CCCCC(N(CCCN1CCOCC1)C(=O)c2cccnc2)C(=O)NCC=C	69	%	5.83	5.90	6.67	6.65	7.20
CHEMBL1253781	Cc1c(C(=O)NCc2ccc(cc2)C(F)(F)F)[n+]([O-])c3cc(Cl)c(Cl)cc3[n+]1[O-]	6.58	ug.mL-1	5.50	5.50	6.11	8.38	6.76
CHEMBL1254469	Cc1c(C(=O)NCc2ccc3OCOc3c2)[n+]([O-])c4ccccc4[n+]1[O-]	22.75	ug.mL-1	5.67	5.59	4.71	8.51	7.76
CHEMBL1777918	Cc1c(\C=N\NC(=O)c2ccncc2)[n+]([O-])c3cc(F)ccc3[n+]1[O-]	580	nM	6.76	4.64	6.70	7.33	6.80

DrugBank

Prioritized top 100 DrugBank Compounds						
DrugBank	**Smile**	**M1**	**M2**	**M3**	**M4**	**M5**
DB05791	FC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)Br	10.61	11.59	8.28	8.61	6.02
DB02079	O=C(O)CON	7.68	7.50	11.16	10.47	7.37
DB02419	CCOC(=O)C(=O)N1CCCCC1	7.06	10.79	6.79	9.59	8.20
DB00778	COCCOCO\N=C(\[C@H](C)[C@H]1O)[C@H](C)C[C@@](C)(O)[C@H](O[C@H](O2)[C@H](O)[C@@H](N(C)C)C[C@H]2C)[C@@H](C)[C@@H]([C@@H](C)C(=O)O[C@H](CC)[C@@]1(C)O)O[C@@H](C3)O[C@@H](C)[C@H](O)[C@]3(C)OC	6.01	6.42	8.72	10.80	10.01
DB08089	FC(F)(F)CN(CC(F)(F)F)c(c1)ccc(c12)[nH]c(=O)cc2C(F)(F)F	8.55	9.84	6.87	9.68	7.00
DB01613	[O-][N+](=O)OC[C@H](O[N+]([O-])=O)[C@H](O[N+]([O-])=O)CO[N+]([O-])=O	9.67	11.87	6.06	8.31	6.03
DB02279	O=C(O)C(=O)c1ccccc1	6.95	11.37	6.95	9.80	6.40
DB04267	O=C(O)c1cccc(n1)C(=O)O	6.54	8.94	7.54	10.93	7.26
DB02838	[O-]C(=O)C1=[NH+]CCC1	5.22	10.08	7.30	9.79	8.79
DB01195	N1CCCCC1CNC(=O)c2c(OCC(F)(F)F)ccc(c2)OCC(F)(F)F	7.91	11.79	7.15	7.53	6.79
DB01361	C[C@@H]1C[C@H](N(C)C)[C@@H](OC(=O)C)[C@@H](O1)O[C@@H]([C@@H](C)C2)[C@@H](C)[C@H](O[C@H](O3)C[C@H](OC)[C@H]([C@@H]3C)OC(=O)C)[C@@H](C)C(=O)O[C@H](C)[C@H](C)[C@H](OC(=O)C)[C@@H](C)C(=O)[C@]24CO4	7.44	9.98	6.46	9.40	7.52
DB06781	CC(=O)OCC(=O)[C@@]1(OC(=O)CCC)CC[C@H]([C@@]12C)[C@H]3[C@](F)([C@H](C2)O)[C@]4(C)C([C@@H](F)C3)=CC(=O)C=C4	6.42	10.74	7.05	8.19	8.30
DB07177	CCCCCC(=O)/C=C/[C@H]([C@@H](C1)O)[C@@H](C1=O)C\C=C\CCCC(=O)O	9.58	11.18	6.58	6.69	6.63
DB04553	O=C(O)C(=O)CC	5.25	9.67	8.31	10.26	6.83
DB04488	[NH3+]CC(=O)N[C@@H](C([O-])=O)CCCCC(=O)N[C@@H]1C(=O)N([C@H]12)[C@@H](C([O-])=O)[C@@H](CS2)COC(=O)C	6.32	9.75	7.17	8.81	8.02

DB03759	[O-][N+](=O)c(c1)c([N+]([O-])=O)cc(c1=2)=NC(=O)C(N2)=O	8.35	9.17	6.91	7.23	8.00
DB07380	CC(=O)N[C@H](C(=O)C(F)(F)F)Cc1ccccc1	5.63	9.86	7.65	8.98	7.53
DB02660	NC(=O)O/N=C(\C)c1cc(c(cc1)OC)OC2CCCC2	6.60	8.43	7.50	8.81	8.03
DB01827	NC(=O)c1c(F)c(F)c(c(F)c1F)OC	7.46	7.98	6.28	10.21	7.36
DB00868	CCCCNc(cc1)ccc1C(=O)OCCOCCOCCOCCOCCOCCOCCOCCOC	7.41	9.13	7.26	7.80	7.28
DB01589	c1c(Cl)ccc(c12)N(CC(F)(F)F)C(=S)CN=C2c3c(F)cccc3	8.34	6.78	7.91	8.86	6.97
DB00801	c1c(Cl)ccc(c12)N(CC(F)(F)F)C(=O)CN=C2c3ccccc3	7.58	7.92	7.78	8.72	6.80
DB00176	c1cc(C(F)(F)F)ccc1C(=N\OCCN)\CCCCOC	7.05	6.51	7.64	8.83	8.59
DB01804	[O-]C(=O)[C@H]([NH3+])C=C	5.56	8.11	8.35	8.93	7.64
DB01874	C1C(=O)C[C@@H](N2C)CC[C@H]12	11.55	7.76	5.26	7.68	6.27
DB00339	NC(=O)c1cnccn1	6.83	9.23	7.49	8.71	6.22
DB02005	O=C(O)C(=O)/C=C/C	8.26	11.31	7.07	6.45	5.33
DB04629	CO[C@H]1CC[C@@H](C)[C@@H](O)[C@H](C)[C@H](OC(=O)[C@@H](N(C)C)COC)C\C=C\C=C\C(=O)O[C@@H](C\C=C\[C@H](OC)C[C@H](C)C/C=C1\C)[C@@H](C)[C@@H](O)[C@@H](C)CC[C@@H](OC(=O)[C@H](C)N(C)C)[C@H](C)[C@H](OC(=O)C)[C@H](C)/C=C/N(C=O)C	7.12	8.08	7.18	8.55	7.47
DB03811	O=C[C@H](N)CC1=CN=C[NH2+]1	6.81	8.37	7.60	7.98	7.63
DB03387	O=C(O)C(=O)N(O)C(C)C	8.19	10.24	6.65	7.26	5.95
DB01135	COc1c(OC)c(OC)cc(c12)CC[N+](C)(C2Cc3cc(OC)c(OC)c(c3)OC)CCCOC(=O)CCC(=O)OCCC[N+](C)(C4Cc5cc(OC)c(OC)c(c5)OC)CCc(c46)cc(OC)c(OC)c6OC	7.43	9.63	6.80	7.80	6.51
DB08642	COc1c(OC)cc(cc1OC)N(C)C[C@H](C2)CCC(=C23)N[C@@H](N)N=C3N	7.02	7.16	6.76	8.23	8.95
DB07072	n1nc(C(F)(F)F)n(c12)CCN(C2)[C@@H](CC3)C[C@H](N)[C@H]3c4c(F)cc(F)c(F)c4	7.20	10.48	6.78	7.80	5.85

DB01723	COc(c1)c(OC)c(OC)cc1[C@H](CC)C(=O)N2CCCC[C@@H]2C(=O)O[C@H](c3cc(ccc3)OCC(=O)O)CCc4cc(OC)c(cc4)OC	7.00	7.66	7.48	9.22	6.60
DB03096	NCCN1CCOCC1	6.79	8.49	6.67	7.98	7.83
DB03237	[O-]C(=O)C(=O)C[C@H](O)[C@H](C([O-])=O)O	9.22	10.54	6.14	5.79	6.04
DB01261	n1nc(C(F)(F)F)n(c12)CCN(C2)C(=O)C[C@H](N)Cc3c(F)cc(F)c(F)c3	7.43	11.01	6.22	7.19	5.85
DB01735	[O-]C(=O)[C@@H](CCl)[NH3+]	5.31	7.86	7.76	9.54	7.21
DB07081	FC(F)(F)c(n1)nn(c12)CCN([C@@H]2C)C(=O)C[C@H](N)Cc3c(F)cc(F)c(F)c3	7.29	10.56	6.32	7.35	6.09
DB02280	O=C(O)[C@@H](O)c1ccccc1	5.50	9.52	6.43	9.29	6.82
DB03357	O=C(O)[C@@H](O)c1ccccc1	5.50	9.52	6.43	9.29	6.82
DB04774	O=CN(C)\C=C\C[C@@H](OC)[C@@H](C)C(=O)CC[C@H](C)[C@H](OC)[C@H](C)[C@@H](OC(=O)/C=C/C=C(\C)C[C@H](C1)OC)[C@@H](C)/C=C/[C@H](OC)C[C@H](OC)[C@@H](C)/C=C/[C@@H](OC)C[C@H](OC)[C@@H](C)[C@@H](C2)OC(=O)C=C12	7.39	8.38	7.06	7.48	7.08
DB07553	FC(F)(F)C(=O)CCCCCCC(=O)Nc1ccccc1	5.88	8.40	7.37	8.46	7.28
DB08044	n1nc(C(F)(F)F)n(c12)CCN(C2)C(=O)C3=CC[C@@H]([C@H](C3)N)c4c(F)cc(F)c(F)c4	6.87	11.39	6.20	6.69	6.23
DB00732	COc(c1)c(OC)cc(c12)CC[N+](C)(C2Cc3cc(OC)c(cc3)OC)CCC(=O)OCCCCCOC(=O)CC[N+](C)(C4Cc5cc(OC)c(cc5)OC)CCc(c46)cc(OC)c(c6)OC	7.08	9.79	6.58	7.31	6.61
DB03820	[NH3+]CC(=O)N[C@@H](C([O-])=O)CCCCC(=O)N[C@@H]1C(=O)N([C@H]12)[C@H](C([O-])=O)C(S2)(C)C	5.26	9.87	5.97	8.23	7.99
DB04534	C1N=NC(C=12)=CC=C(C2)[N+]([O-])=O	7.17	7.27	6.73	9.19	6.96
DB03077	O=c1c(=O)c(N)c1NCCCOCCOCCOCCC	6.54	8.36	6.88	6.57	8.93
DB03774	O=C(O)[C@@H]([NH3+])CCC=O	6.05	8.52	8.32	7.39	6.97

DB02275	O=CCN1C(=O)[C@H](N=C1CN)CC(C=C2)C=CC2=O	6.88	8.42	7.28	6.64	8.01
DB02580	COCCOCCOCCOCCOCCOC	7.23	8.36	7.27	8.22	6.02
DB01206	ClCCN(N=O)C(=O)NC1CCCCC1	5.08	6.88	8.70	9.21	7.16
DB03229	O=C(O)C(=O)CC(C)C	7.37	8.99	6.92	7.85	5.73
DB07084	CC(=O)Nc(c1)ccc(c12)OCCOCCOc3c(cccc3)OCCOCCO2	6.96	7.09	7.48	8.30	7.03
DB00383	c1ccccc1C(O)(C2CCCCC2)C(=O)OCC3=NCCCN3C	5.87	5.80	7.87	8.98	8.24
DB04325	[NH3+]CCc1ccccc1	5.73	7.13	6.99	9.53	7.22
DB01892	CC(C)=CCCC1(C)C(CC=C(C)C)CC(CC=C(C)C)(C(=O)C12C(=O)C(C)C)C(=O)C(=C2O)CC=C(C)C	7.43	7.79	6.49	7.30	7.58
DB08987	CCCN(CC)C(CC)/C(O)=N/c(c1C)c(C)ccc1	7.33	6.41	7.13	8.00	7.66
DB06867	CCOCCOCCOCCOCCOCCOCC	7.43	8.44	7.04	7.69	5.90
DB04771	c1cc([N+]([O-])=O)ccc1C(=O)N[C@@H](CC(C)C)C(=O)N2CCC[C@H]2C(=O)NCCCCN=C(N)N	6.16	8.65	6.32	6.89	8.47
DB02888	COc(c1)c(OC)c(OC)cc1C(F)(F)C(=O)N2CCCC[C@H]2C(=O)O[C@@H](CCCc3ccccc3)CCCc4cccnc4	6.79	8.66	6.61	8.01	6.36
DB04212	CC(C([O-])=O)=[NH2+]	6.33	8.18	7.91	8.05	5.92
DB04528	[O-][N+](=O)c1c(O)ccc(c1)[N+]([O-])=O	6.65	6.94	5.99	9.56	7.24
DB01545	c1c(Cl)ccc(c12)NC(=O)C(C(=O)OCC)N=C2c3c(F)cccc3	7.02	5.40	7.29	8.73	7.92
DB06804	CCCCCCCCCc1ccc(cc1)OCCOCCOCCOCCOCCOCCOCCO	7.61	8.45	7.07	7.20	5.98
DB01413	Nc(n1)scc1C(=N\OC)\C(=O)N[C@@H]2C(=O)N([C@@H]23)C(C([O-])=O)=C(CS3)C[N+]4(C)CCCC4	5.32	7.71	7.08	8.67	7.52
DB05869	CC(=O)C(=O)OCC	7.06	8.97	6.79	7.66	5.74
DB02435	[NH3+]CC1CCCCC1	5.94	6.46	7.55	9.15	7.10
DB02068	O=C(O)CCCC[NH3+]	5.50	6.68	8.65	8.65	6.68
DB00348	C1CCC(=O)C(C1=O)C(=O)c2c([N+]([O-])=O)cc(C(F)(F)F)cc2	5.88	7.74	6.91	8.61	6.97

DB04775	CC[C@@H](OC)[C@@H](C)C(=O)CC[C@H](C)[C@H](OC)[C@H](C)[C@@H](OC(=O)\C=C/C=C(\C)C[C@H](C1)OC)[C@@H](C)/C=C/[C@H](OC)C[C@H](OC)[C@@H](C)/C=C/[C@@H](OC)C[C@H](OC)[C@@H](C)[C@@H](C2)OC(=O)C=C12	7.94	8.89	6.72	6.41	6.11
DB03705	[O-][N+](=O)c1c(NC)nc(N)[nH]c1=O	5.13	7.06	6.07	9.16	8.64
DB00122	OCC[N+](C)(C)C	5.55	5.01	7.76	10.55	7.14
DB01997	BrC1N=NC(C=12)C([N+]([O-])=O)=CC=C2	9.03	6.73	5.84	7.69	6.63
DB00996	O=C(O)CC1(CN)CCCCC1	6.01	7.48	7.10	8.64	6.69
DB02096	NC(=O)c1cn(cn1)[C@@H](CO)CCc2ccccc2	7.76	9.80	5.73	7.03	5.55
DB03556	OCCOCCOCCOCCOCCOCCOCCOCCOCC	8.16	8.88	6.71	7.08	5.03
DB04948	N1CCN=C1C(C)Oc2c(Cl)cccc2Cl	5.62	6.18	6.68	9.24	8.14
DB08721	O1CCN=C1c2cc(Cl)c(c(Cl)c2)OCCCCCc(on3)cc3COCOCCO	6.86	7.06	6.97	8.15	6.82
DB08266	CCC\C(C)=C\C=C(C)\C(=O)[C@@H](C(=O)O1)C(=O)C=C1[C@H](C)CCC/C=N/C(=O)OC	6.98	6.12	7.97	7.21	7.57
DB06892	OCCONC(=O)C1=CC=C(F)[C@@H](F)C\1=N/c2c(F)cc(I)cc2	8.22	5.75	8.06	7.01	6.79
DB01676	Cc1c([N+]([O-])=O)cc([N+]([O-])=O)cc1[N+]([O-])=O	6.62	7.81	5.95	9.34	6.06
DB00877	C1C[C@@H](O)[C@H](OC)C[C@@H]1C[C@H](C)[C@@H](OC(=O)[C@H]2N(C(=O)C3=O)CCCC2)CC(=O)[C@H](C)/C=C(\C)[C@@H](O)[C@@H](OC)C(=O)[C@H](C)C[C@H](C)/C=C/C=C/C=C(\C)[C@@H](OC)C[C@@H](O4)CC[C@@H](C)[C@]34O	7.43	10.09	6.18	6.33	5.75
DB04737	N#C[C@@H](O)c1ccccc1	7.73	7.48	6.04	8.45	5.96
DB08823	C[C@@H]1[C@@H](N(C)C)CC[C@@H](O1)O[C@H]([C@@H](C)C2=O)CCC[C@H](CC)OC(=O)C[C@H](C2=3)[C@H]4[C@@H](C3)[C@H]5[C@H](C=C4)C[C@H](C5)O[C@H](C6)[C@H](OC)[C@H](OC)[C@H]([C@@H]6C)OC	6.38	7.27	5.93	7.97	8.05

DB02227	O=C(O)[C@@H]1C[C@H](O)[C@H](CO1)O	5.93	7.97	6.20	7.80	7.68
DB03243	[NH3+]Cc1ccc(F)cc1	7.03	5.85	7.49	7.81	7.38
DB04783	O=CN(C)\C=C\C[C@@H](OC)[C@@H](C)C(=O)CC[C@H](C)[C@H](OC)[C@H](C)[C@@H](OC(=O)\C=C\C=C(\C)C[C@H](C1)OC)[C@@H](C)/C=C/[C@H](OC)C[C@H](O)[C@@H](C)/C=C/[C@@H](OC)C[C@H](OC)[C@@H](C)[C@@H]([C@H]2O)OC(=O)C=C12	7.43	7.02	6.76	7.34	6.97
DB02078	COCCOCCOCCOC	6.63	7.46	7.21	8.51	5.69
DB02130	[O-]C(=O)c1cc(OC)c(O)cc1	5.92	6.78	6.13	10.79	5.86
DB05154	FC(F)(F)Oc(cc1)ccc1CO[C@H](CO2)Cn(c23)cc(n3)[N+]([O-])=O	5.93	8.78	5.95	8.12	6.69
DB07548	n1cccc(F)c1CNC(=O)Cn2c(=O)c(ncc2C)NCC(F)(F)c3ccccn3	5.17	9.46	6.91	7.64	6.29
DB03286	[N-]=[N+]=N[C@]1([C@@H](N)O)[C@@H](O)[C@H](O)[C@@H](O)[C@@H](O1)CO	7.95	7.50	6.10	6.36	7.53
DB02080	CC(C)(C)CC(C)(C)c1ccc(cc1)OCCOCCOCCOC	6.24	6.32	7.15	8.36	7.36
DB03709	O=C(O)CN(CCO)CCO	6.42	6.60	7.05	7.73	7.60
DB00673	FC(F)(F)c1cc(C(F)(F)F)cc(c1)[C@@H](C)O[C@H]([C@@H]2c3ccc(F)cc3)OCCN2Cc4n[nH]c(=O)[nH]4	6.93	8.01	6.21	8.78	5.45
DB04504	C1N=CCC[C@@H]1N	6.07	6.19	8.29	8.06	6.72
DB01155	O=C(O)c(c1=O)cn(C2CC2)c(c13)nc(c(F)c3)N(C4)CC(CN)/C4=N/OC	7.15	6.34	6.53	8.16	7.15
DB06207	OCCCN(CC1)c(c12)c(C(=O)N)cc(c2)C[C@@H](C)NCCOc(c3OCC(F)(F)F)cccc3	7.50	7.30	6.48	7.82	6.16
DB06614	CC(=O)NC(C(CC)CC)[C@@H]([C@@H](C1)N=C(N)N)[C@H](O)[C@H]1C(=O)O	6.04	5.33	6.73	8.63	8.50

Asinex

Prioritized top 100 Asinex Compounds						
Asinex	**Structure**	**M1**	**M2**	**M3**	**M4**	**M5**
33	N1(C(=O)Cc2n[nH]c(=O)c3c2cccc3)[C@H](CN(Cc2cc(OC)ccc2)CC1)C	5.12	5.64	6.31	7.80	7.43
40	N1(C(=O)c2oncc2)[C@H](CN(Cc2cc(OC)ccc2)CC1)C	5.02	5.85	5.85	7.44	6.88
49	N1(C(=O)c2oc(cc2)Cn2nccc2)[C@H](CN(Cc2cc(OC)ccc2)CC1)C	5.04	5.77	5.58	7.35	6.60
56	N1(CC(=O)N2CCOCC2)[C@H](CN(Cc2cc(OC)ccc2)CC1)C	5.70	5.64	6.81	7.64	7.09
65	N1(C(=O)COc2ccccc2)[C@H](CN(Cc2cc(OC)ccc2)CC1)C	5.13	5.05	6.54	7.74	7.41
76	N1(C(=O)c2ncc(nc2)C)[C@H](CN(Cc2cc(OC)ccc2)CC1)C	5.01	5.20	6.48	7.21	6.77
80	N1([C@@H](C(=O)OC)CCc2c1cccc2)C(=O)COC	5.29	6.77	6.72	9.19	7.73
109	N1(C(=O)c2c(cc(o2)CN2CCOCC2)C)[C@H](CN(Cc2occc2)CC1)C(C)C	5.01	5.88	5.48	8.16	7.24
113	N1(C(=O)c2cn(nc2)CC)[C@H](CN(Cc2occc2)CC1)C(C)C	5.53	5.43	5.42	7.41	6.64
116	c1(C(=O)N2[C@H](CN(Cc3occc3)CC2)C(C)C)c(nn(c1)CC)C	5.11	5.22	5.39	7.54	6.68
117	N1(C(=O)c2oc(cc2)Cn2nccc2)[C@H](CN(Cc2occc2)CC1)C(C)C	5.17	6.38	5.14	7.72	6.61
118	c12n(c(cc(n2)C)C(F)F)ncc1C(=O)N1[C@H](CN(Cc2occc2)CC1)C(C)C	6.23	7.33	5.52	7.98	6.71
120	n12c(C(F)(F)F)cc(nc1cc(n2)C(=O)N1[C@H](CN(Cc2occc2)CC1)C(C)C)C	6.45	8.21	5.34	8.39	6.67
121	n1(nc(c2c(c1=O)cccc2)C)CC(=O)N1[C@H](CN(Cc2occc2)CC1)C(C)C	5.36	5.70	5.19	7.28	6.95
130	n1(c(=O)c2c(cn1)cccc2)CC(=O)N1[C@H](CN(Cc2occc2)CC1)C(C)C	5.10	5.85	5.23	7.27	6.95
138	N1(C(=O)c2nccnc2)[C@H](CN(Cc2c(F)cccc2)CC1)C(C)C	5.42	5.18	6.52	7.42	6.22
142	N1(C(=O)Cc2n[nH]c(=O)c3c2cccc3)[C@H](CN(Cc2c(F)cccc2)CC1)C(C)C	5.24	5.76	6.32	7.45	6.54
143	c1(c2n(nc1)cccn2)C(=O)N1[C@H](CN(Cc2c(F)cccc2)CC1)C(C)C	7.67	9.44	5.04	7.33	6.01
146	c1(C(=O)N2[C@H](CN(Cc3c(F)cccc3)CC2)C(C)C)c(n(nc1)CC)C	5.35	5.20	5.87	7.47	6.67
149	N1(C(=O)c2oc(cc2)Cn2nccc2)[C@H](CN(Cc2c(F)cccc2)CC1)C(C)C	5.50	5.88	5.61	8.00	6.95

151	n1(nc(c2c(c1=O)cccc2)C)CC(=O)N1[C@H](CN(Cc2c(F)cccc2)CC1)C(C)C	5.66	5.60	6.02	7.17	6.77
152	c1(C(=O)N2[C@H](CN(Cc3c(F)cccc3)CC2)C(C)C)n[nH]c(=O)c2c1cccc2	5.34	6.15	6.45	8.23	6.93
155	n1(c(=O)c2c(cn1)cccc2)CC(=O)N1[C@H](CN(Cc2c(F)cccc2)CC1)C(C)C	5.41	5.62	6.02	7.17	6.76
160	N1(C(=O)c2cc(=O)c3c(o2)ccc(c3)C)[C@H](CN(Cc2c(F)cccc2)CC1)C(C)C	5.34	5.74	5.64	7.48	6.93
197	n1(nc(ccc1=O)c1cc2c(OCCO2)cc1)C[C@H]1N(C(=O)Cc2ccc(F)cc2)CCC1	5.50	6.85	5.18	7.79	6.77
201	n1(nc(ccc1=O)c1ccc(cc1)F)C[C@H]1N(C(=O)Cc2c(OC)cccc2)CCC1	5.04	5.89	5.22	7.52	6.74
202	n1(nc(ccc1=O)c1ccc(cc1)F)C[C@H]1N(C(=O)Cc2ccc(cc2)OC)CCC1	5.02	6.02	5.32	7.94	6.93
206	n1(nc(ccc1=O)c1ccc(cc1)F)C[C@H]1N(C(=O)c2cc3c(OCCO3)cc2)CCC1	5.40	6.88	5.49	7.56	6.32
219	n1(nc(ccc1=O)c1ccc(cc1)F)C[C@H]1N(C(=O)CCC2CCCC2)CCC1	5.04	5.60	5.12	6.66	6.51
220	n1(nc(ccc1=O)c1ccc(cc1)F)C[C@H]1N(C(=O)COC)CCC1	5.28	6.62	5.08	8.18	6.97
265	n1(nc(ccc1=O)c1ccc(cc1)OC)C[C@H](NC(=O)c1ncc(nc1)C)CC	5.55	5.92	5.24	8.00	5.71
267	n1(nc(ccc1=O)c1ccc(cc1)OC)C[C@H](NC(=O)c1cc2c(OCCO2)cc1)CC	5.35	6.01	5.51	8.38	6.80
276	n1(nc(ccc1=O)c1cc(c(cc1)F)F)C[C@H](NC(=O)c1nccnc1)CC	5.67	7.45	5.68	7.81	5.05
277	n1(nc(ccc1=O)c1cc(c(cc1)F)F)C[C@H](NC(=O)c1ncccc1)CC	5.20	7.20	5.59	7.80	5.56
280	n1(nc(ccc1=O)c1cc(c(cc1)F)F)C[C@H](NC(=O)CCc1c(onc1C)C)CC	5.53	6.80	5.34	7.56	5.87
286	n1(nc(ccc1=O)c1cc(c(cc1)F)F)C[C@H](NC(=O)c1cc2c(OCCO2)cc1)CC	5.40	7.24	6.02	8.26	6.42
290	n1(nc(ccc1=O)c1cc(c(cc1)F)F)C[C@H](NC(=O)COC)CC	5.21	7.60	5.38	8.67	6.70
292	n1(nc(ccc1=O)c1cc(c(cc1)F)F)C[C@H](NC(=O)Cc1ccc(cc1)OC)CC	5.25	6.49	5.76	8.48	6.70
293	n1(nc(ccc1=O)c1cc(c(cc1)F)F)C[C@H](NC(=O)Cc1c(OC)cccc1)CC	5.26	6.31	5.63	8.23	6.58
297	n1(nc(ccc1=O)c1cc(c(cc1)F)F)C[C@H](NC(=O)CCn1nccc1)CC	5.41	6.82	5.04	7.77	5.89

298	n1(nc(ccc1=O)c1cc(c(cc1)F)F)C[C@H](NC(=O)CCn1nccc1C)CC	5.26	6.71	5.14	7.61	5.92
299	n1(nc(ccc1=O)c1cc(c(cc1)F)F)C[C@H](NC(=O)c1ncc(nc1)C)CC	5.61	7.38	5.73	8.12	5.50
300	n1(nc(ccc1=O)c1cc(c(cc1)F)F)C[C@H](NC(=O)c1cn(nc1)C(C)C)CC	5.33	6.71	5.12	7.56	5.75
343	n1(nnc2c(c1=O)cccc2)C[C@H](NC(=O)c1nccnc1)CC	5.51	7.17	5.18	7.39	5.30
357	n1(nnc2c(c1=O)cccc2)C[C@H](NC(=O)Cc1c(OC)cccc1)CC	5.02	5.68	5.24	7.92	6.81
358	n1(c(=O)c2c(cn1)cccc2)C[C@H](NC(=O)c1nccnc1)CC	5.51	7.15	5.51	7.42	5.67
359	n1(c(=O)c2c(cn1)cccc2)C[C@H](NC(=O)c1ncc(nc1)C)CC	5.82	7.65	5.54	7.73	6.16
376	n1(c(=O)c2c(cn1)cccc2)C[C@H](NC(=O)Cc1c(ccc(c1)OC)OC)CC	5.10	5.53	5.79	7.45	6.74
432	n1(nc(ccc1=O)c1ccc(cc1)OC)C[C@@H](NC(=O)c1nccnc1)C	5.50	5.64	5.16	8.66	5.98
433	n1(nc(ccc1=O)c1ccc(cc1)OC)C[C@@H](NC(=O)c1ncc(nc1)C)C	5.45	5.63	5.21	8.10	5.64
435	n1(nc(ccc1=O)c1ccc(cc1)OC)C[C@@H](NC(=O)c1n[nH]c(=O)cc1)C	5.49	6.23	5.10	8.08	5.47
444	n1(nc(ccc1=O)c1cc(c(cc1)F)F)C[C@@H](NC(=O)c1nccnc1)C(C)C	5.38	7.44	5.62	7.75	5.09
445	n1(nc(ccc1=O)c1cc(c(cc1)F)F)C[C@@H](NC(=O)c1ncc(nc1)C)C(C)C	5.37	7.36	5.68	8.07	5.54
447	n1(nc(ccc1=O)c1cc(c(cc1)F)F)C[C@@H](NC(=O)c1c2c(ccn1)cccc2)C(C)C	5.11	7.49	5.36	7.80	5.39
448	n1(nc(ccc1=O)c1cc(c(cc1)F)F)C[C@@H](NC(=O)CCn1nccc1C)C(C)C	5.06	6.75	5.08	7.63	5.98
449	n1(nc(ccc1=O)c1cc(c(cc1)F)F)C[C@@H](NC(=O)CCn1nc(cc1C)C)C(C)C	6.54	9.35	5.15	7.23	5.55
452	n1(nc(ccc1=O)c1cc(c(cc1)F)F)C[C@@H](NC(=O)CCc1c(onc1C)C)C(C)C	5.38	6.81	5.26	7.56	5.95
455	n1(nc(c(c1C)C)C)CC(=O)N[C@H](Cn1nc(ccc1=O)c1cc(c(cc1)F)F)C(C)C	5.25	7.18	5.23	7.44	5.87
456	n1(nc(ccc1=O)c1cc(c(cc1)F)F)C[C@@H](NC(=O)c1n[nH]c(=O)cc1)C(C)C	5.48	8.07	5.27	8.18	5.37
458	c1(C(=O)N[C@H](Cn2nc(ccc2=O)c2cc(c(cc2)F)F)C(C)C)c(nn(c1)CC)C	5.21	7.29	5.13	7.81	5.91
459	n1(nc(ccc1=O)c1cc(c(cc1)F)F)C[C@@H](NC(=O)c1cn(nc1)CC)C(C)C	5.20	7.02	5.01	7.71	5.77

652	n1(nc(C2CC2)ccc1=O)C[C@@H](NC(=O)c1nccnc1)C(C)C	5.11	5.78	5.82	7.77	6.86
691	c1(nnn(c1)C[C@H]1CN(C(=O)c2cnccc2)CCC1)C(=O)N1CCOCC1	6.11	5.61	5.35	8.07	6.93
692	c1(nnn(c1)C[C@@H]1CN(C(=O)c2cnccc2)CCC1)C(=O)N1CCOCC1	6.11	5.61	5.35	8.07	6.93
693	c1(nnn(c1)C[C@H]1CN(C(=O)c2nccnc2)CCC1)C(=O)N1CCOCC1	6.92	6.79	5.51	8.26	6.85
694	c1(nnn(c1)C[C@@H]1CN(C(=O)c2nccnc2)CCC1)C(=O)N1CCOCC1	6.92	6.79	5.51	8.26	6.85
697	c1(nnn(c1)C[C@H]1CN(C(=O)c2occc2)CCC1)C(=O)N1CCOCC1	6.22	6.54	5.39	7.84	6.46
698	c1(nnn(c1)C[C@@H]1CN(C(=O)c2occc2)CCC1)C(=O)N1CCOCC1	6.22	6.54	5.39	7.84	6.46
699	c1(n(nc(c1)C(C)(C)C)C)C(=O)N1C[C@@H](Cn2nnc(C(=O)N3CCOCC3)c2)CCC1	6.15	6.46	5.11	7.74	6.78
700	c1(nnn(c1)C[C@@H]1CN(C(=O)c2cn(nc2)CC)CCC1)C(=O)N1CCOCC1	6.72	6.09	5.21	7.39	6.35
701	c1(nnn(c1)C[C@H]1CN(C(=O)Cn2nc(cc2C)C)CCC1)C(=O)N1CCOCC1	7.37	6.99	5.43	7.68	6.77
702	c1(nnn(c1)C[C@@H]1CN(C(=O)Cn2nc(cc2C)C)CCC1)C(=O)N1CCOCC1	7.37	6.99	5.43	7.68	6.77
726	c1(nnn(c1)C[C@H]1CN(C(=O)c2ncc(nc2)C)CCC1)C(=O)NCCOC	6.17	5.88	6.32	8.84	7.15
727	c1(nnn(c1)C[C@@H]1CN(C(=O)c2ncc(nc2)C)CCC1)C(=O)NCCOC	6.17	5.88	6.32	8.84	7.15
728	c1(nnn(c1)C[C@@H]1CN(C(=O)c2nccc2)CCC1)C(=O)NCCOC	5.74	5.75	6.30	8.63	7.18
729	c1(nnn(c1)C[C@H]1CN(C(=O)c2ccncc2)CCC1)C(=O)NCCOC	5.11	5.17	6.17	8.41	6.85
730	c1(nnn(c1)C[C@H]1CN(C(=O)c2n[nH]cc2)CCC1)C(=O)NCCOC	6.03	6.02	5.43	8.10	6.82
732	c1(nnn(c1)C[C@@H]1CN(C(=O)c2occc2)CCC1)C(=O)NCCOC	5.67	6.15	6.22	9.00	7.41
735	c1(nnn(c1)C[C@H]1CN(C(=O)c2noc(c2)CCC)CCC1)C(=O)N1CCOCC1	7.08	6.61	5.24	7.93	6.90
736	c1(nnn(c1)C[C@H]1CN(C(=O)c2cc(no2)C(C)C)CCC1)C(=O)N1CCOCC1	7.02	6.98	5.16	7.53	6.77
738	c1(C(=O)N2C[C@H](Cn3nnc(c3)C(=O)NCCOC)CCC2)c(n(nc1)C)C	5.66	5.48	6.01	8.18	6.60
739	c1(C(=O)N2C[C@@H](Cn3nnc(c3)C(=O)NCCOC)CCC2)c(n(nc1)C)C	5.66	5.48	6.01	8.18	6.60
740	c1(C(=O)N2C[C@@H](Cn3nnc(c3)C(=O)NCCOC)CCC2)c(noc1)C	5.61	5.74	6.03	8.62	6.94

744	N1(C(=O)c2ncc(nc2)C)C[C@H](CNC(=O)c2occc2)CCC1	5.54	6.21	6.28	8.81	7.62
745	N1(C(=O)c2ncc(nc2)C)C[C@@H](CNC(=O)c2occc2)CCC1	5.54	6.21	6.28	8.81	7.62
747	N1(C(=O)c2n[nH]cc2)C[C@H](CNC(=O)c2occc2)CCC1	5.59	6.67	5.44	8.14	7.27
748	N1(C(=O)c2nccnc2)C[C@H](CNC(=O)c2occc2)CCC1	5.63	6.65	6.32	8.45	7.14
749	N1(C(=O)c2nccnc2)C[C@@H](CNC(=O)c2occc2)CCC1	5.63	6.65	6.32	8.45	7.14
754	c1(C(=O)N2C[C@H](Cn3nnc(C(=O)N4CCOCC4)c3)CCC2)c(n(nc1)CC)C	6.41	6.17	5.28	7.52	6.44
755	c1(C(=O)N2C[C@@H](Cn3nnc(C(=O)N4CCOCC4)c3)CCC2)c(n(nc1)CC)C	6.41	6.17	5.28	7.52	6.44
793	n1(nc(ccc1=O)c1cc(c(cc1)F)F)C[C@@H](NC(=O)c1nccnc1)CC	5.67	7.45	5.68	7.81	5.05
794	n1(nc(ccc1=O)c1cc(c(cc1)F)F)C[C@@H](NC(=O)c1ncccc1)CC	5.20	7.20	5.59	7.80	5.56
796	n1(nc(ccc1=O)c1cc(c(cc1)F)F)C[C@@H](NC(=O)CCc1c(onc1C)C)CC	5.53	6.80	5.34	7.56	5.87
801	n1(nc(ccc1=O)c1cc(c(cc1)F)F)C[C@@H](NC(=O)c1ncc(nc1)C)CC	5.61	7.38	5.73	8.12	5.50
812	n1(c(=O)c2c(cn1)cccc2)C[C@@H](NC(=O)c1nccnc1)CC	5.51	7.15	5.51	7.42	5.67
813	n1(c(=O)c2c(cn1)cccc2)C[C@@H](NC(=O)c1ncc(nc1)C)CC	5.82	7.65	5.54	7.73	6.16
824	n1(c(=O)c2c(cn1)cccc2)C[C@@H](NC(=O)Cc1c(ccc(c1)OC)OC)CC	5.10	5.53	5.79	7.45	6.74
840	c1(nnn(c1)C[C@@H]1CN(C(=O)c2onc(c2)C)CCC1)C(=O)N1CCOCC1	7.05	7.10	5.20	8.24	7.12
879	n1(nc(ccc1=O)c1ccc(cc1)OC)C[C@H](NC(=O)c1ncccc1)CC	5.12	5.62	5.08	8.55	6.55
885	n1(nnnc1)c1ccc(NC(=O)CN2C[C@H](N(C[C@H]2C)Cc2occc2)C)cc1	5.18	5.48	5.25	7.90	5.80

ZINC

Prioritized top 100 Zinc Compounds						
ZINC	**smile**	**M1**	**M2**	**M3**	**M4**	**M5**
ZINC70670154	C[C@]12CC[C@H]3[C@H]([C@]1(CC[C@@H]2C1=CC(=O)OC1)O)CC[C@]1([C@@]3(CC[C@@H](C1)O)/C=N/Cc1cccc(c1OC)OC)O	11.61	9.74	8.88	8.99	9.87
ZINC01532558	C(C(=O)C(=O)[O-])O	11.94	10.39	11.49	7.35	7.75
ZINC79210221	CCCCCCCCCCCC/N=C/[C@]12CC[C@@H](C[C@]1(CC[C@@H]1[C@@H]2CC[C@]2([C@@]1(CC[C@@H]2C1=CC(=O)OC1)O)C)O)O[C@H]1C[C@@H]([C@@H]([C@@H](O1)C)O)O	11.45	8.71	8.83	8.82	10.51
ZINC79210227	CCCCCCCCCCCC/N=C/[C@]12CC[C@@H](C[C@]1(CC[C@@H]1[C@@H]2CC[C@]2([C@@]1(CC[C@@H]2C1=CC(=O)OC1)O)C)O)O[C@@H]1C[C@H]([C@@H]([C@@H](O1)C)O)O	11.45	8.71	8.83	8.82	10.51
ZINC79210231	CCCCCCCCCCCC/N=C/[C@]12CC[C@@H](C[C@]1(CC[C@@H]1[C@@H]2CC[C@]2([C@@]1(CC[C@@H]2C1=CC(=O)OC1)O)C)O)O[C@H]1C[C@H]([C@@H]([C@@H](O1)C)O)O	11.45	8.71	8.83	8.82	10.51
ZINC79210370	CCCCCCCCCCCC/N=C/[C@]12CC[C@@H](C[C@]1(CC[C@@H]1[C@@H]2CC[C@]2([C@@]1(CC[C@@H]2C1=CC(=O)OC1)O)C)O)O[C@@H]1C[C@@H]([C@@H]([C@@H](O1)C)O)O	11.45	8.71	8.83	8.82	10.51
ZINC34785078	C([C@@H](C(F)(F)F)[O-])[NH3+]	9.50	7.56	9.58	9.19	11.92
ZINC36378398	C([C@H](C(F)(F)F)[O-])[NH3+]	9.50	7.56	9.58	9.19	11.92
ZINC20462978	CN(C)c1ccc(cc1)C(=O)N1CC[C@H]([C@H](C1)CC[N@@H+](C)CCc1ccccn1)CC(=O)[O-]	11.53	10.09	8.76	8.18	8.93
ZINC12482649	CN(Cc1cc(no1)C[C@H]1C[NH2+]CC[C@H]1CC(=O)NCc1ccc(cc1)F)c1ccccc1	11.07	9.95	8.24	8.23	8.92
ZINC20467021	C[C@@H]1[C@H](CC[C@]2([C@H]1[C@H]([C@@H](CC2)[C@H](C)C(=O)N(C)CCC#N)O)C)NC(=O)c1ccncc1	10.60	8.66	9.18	8.56	9.28
ZINC20467023	C[C@@H]1[C@H](CC[C@]2([C@H]1[C@H]([C@H](CC2)[C@H](C)C(=O)N(C)CCC#N)O)C)NC(=O)c1ccncc1	10.60	8.66	9.18	8.56	9.28
ZINC19364242	C(C[NH+](CC(=O)[O-])CC(=O)[O-])N(CC(=O)[O-])CC(=O)[O-]	8.89	9.55	9.24	11.78	6.55
ZINC08623789	c1ccc(cc1)CNC(=O)C[C@@H]1CC[NH2+]C[C@@H]1Cc1cc(on1)c1ccccn1	11.49	10.88	7.49	7.74	8.07
ZINC03869277	C(C(=O)C(=O)[O-])S	10.78	7.82	10.85	7.88	8.30
ZINC72109537	C1COCCC1(CC(=O)[O-])[NH3+]	8.64	8.41	7.92	11.57	8.86
ZINC79203940	C[C@@H](CCC(=O)[C@@H](C)[C@@H]1/C(=N\Nc2ccc(cc2[N+](=O)[O-])[N+](=O)[O-])/C[C@@H]2[C@@]1(CC[C@@H]1[C@@H]2CC=C2[C@@]1(CC[C@@H](C2)OC(=O)C)C)C)CNC(=O)C	9.18	9.18	8.17	9.50	9.26

ZINC79203945	C[C@H](CCC(=O)[C@@H](C)[C@@H]1/C(=N\Nc2ccc(cc2[N+](=O)[O-])[N+](=O)[O-])/C[C@@H]2[C@@]1(CC[C@@H]1[C@@H]2CC=C2[C@@]1(CC[C@@H](C2)OC(=O)C)C)C)CNC(=O)C	9.18	9.18	8.17	9.50	9.26
ZINC79203954	C[C@@H](CCC(=O)[C@H](C)[C@@H]1/C(=N\Nc2ccc(cc2[N+](=O)[O-])[N+](=O)[O-])/C[C@@H]2[C@@]1(CC[C@@H]1[C@@H]2CC=C2[C@@]1(CC[C@@H](C2)OC(=O)C)C)C)CNC(=O)C	9.18	9.18	8.17	9.50	9.26
ZINC79203955	C[C@H](CCC(=O)[C@H](C)[C@@H]1/C(=N\Nc2ccc(cc2[N+](=O)[O-])[N+](=O)[O-])/C[C@@H]2[C@@]1(CC[C@@H]1[C@@H]2CC=C2[C@@]1(CC[C@@H](C2)OC(=O)C)C)C)CNC(=O)C	9.18	9.18	8.17	9.50	9.26
ZINC20467248	C[C@@H]1[C@H](CC[C@]2([C@H]1[C@H]([C@@H](CC2)[C@H](C)C(=O)NCCOC)O)C)NC(=O)c1cncnc1	10.91	9.27	8.62	7.87	8.57
ZINC20467250	C[C@@H]1[C@H](CC[C@]2([C@H]1[C@H]([C@H](CC2)[C@H](C)C(=O)NCCOC)O)C)NC(=O)c1cncnc1	10.91	9.27	8.62	7.87	8.57
ZINC04273375	CC(=O)OC[C@@H]1[C@H]([C@@H]([C@H]([C@H](O1)N=C=S)OC(=O)C)OC(=O)C)O[C@@H]1[C@@H]([C@H]([C@@H](CO1)OC(=O)C)OC(=O)C)OC(=O)C	9.01	8.07	8.94	10.15	8.74
ZINC03999671	CCOC(=O)[C@@H]1[C@@H]([C@@H]([C@@](CC1=O)(C)O)C(=O)OCC)c1cccnc1	9.12	8.19	8.86	9.49	9.23
ZINC03999672	CCOC(=O)[C@H]1[C@@H]([C@@H]([C@@](CC1=O)(C)O)C(=O)OCC)c1cccnc1	9.12	8.19	8.86	9.49	9.23
ZINC03999673	CCOC(=O)[C@@H]1[C@H]([C@@H]([C@@](CC1=O)(C)O)C(=O)OCC)c1cccnc1	9.12	8.19	8.86	9.49	9.23
ZINC03999674	CCOC(=O)[C@H]1[C@H]([C@@H]([C@@](CC1=O)(C)O)C(=O)OCC)c1cccnc1	9.12	8.19	8.86	9.49	9.23
ZINC85542252	CC(=O)O[C@@H]1C[C@@]2(C=C[C@H]([C@]3([C@@H]1[C@](CC[C@@H]3O)(C)C1CCCCC1)[C@]2(CCC1=CC(=O)OC1)O)O)C	11.67	8.13	7.69	8.45	8.69
ZINC70708251	C[C@@H]1[C@@H]([C@@H](C[C@@H](O1)O[C@@H]1CC[C@@]2([C@H]3CC[C@@]4([C@@H](CC[C@@]4([C@@H]3CC[C@@]2(C1)O)O)C1=CC(=O)OC1)C)/C=N/NC(=S)N)OC)O	9.72	7.94	8.21	8.72	9.99
ZINC70708256	C[C@H]1[C@@H]([C@@H](C[C@@H](O1)O[C@@H]1CC[C@@]2([C@H]3CC[C@@]4([C@@H](CC[C@@]4([C@@H]3CC[C@@]2(C1)O)O)C1=CC(=O)OC1)C)/C=N/NC(=S)N)OC)O	9.72	7.94	8.21	8.72	9.99

ZINC70708259	C[C@@H]1[C@H]([C@@H](C[C@@H](O1)O[C@@H]1CC[C@@]2([C@H]3CC[C@@]4([C@@H](CC[C@@]4([C@@H]3CC[C@@]2(C1)O)O)C1=CC(=O)OC1)C)/C=N/NC(=S)N)OC)O	9.72	7.94	8.21	8.72	9.99
ZINC70708261	C[C@H]1[C@H]([C@@H](C[C@@H](O1)O[C@@H]1CC[C@@]2([C@H]3CC[C@@]4([C@@H](CC[C@@]4([C@@H]3CC[C@@]2(C1)O)O)C1=CC(=O)OC1)C)/C=N/NC(=S)N)OC)O	9.72	7.94	8.21	8.72	9.99
ZINC04151567	Cn1cc(nc1)S(=O)(=O)N[C@H]1CCN([C@@H](C1)C(=O)N1CCC[C@@H]1C(=O)OC)C(=O)COCC(=O)[O-]	10.39	8.61	8.16	8.18	9.10
ZINC00039905	c1ccnc(c1)C(=O)[O-]	11.93	10.39	7.36	6.82	7.80
ZINC70670043	CC(=O)OC[C@@H]1[C@H]([C@@H]([C@H]([C@@H](O1)n1c(=O)n(c(=O)cn1)Cc1ccc(c(c1)[N+](=O)[O-])OC)OC(=O)C)OC(=O)C)OC(=O)C	10.04	9.02	8.41	8.20	8.62
ZINC70670044	CC(=O)OC[C@@H]1[C@H]([C@@H]([C@H]([C@H](O1)n1c(=O)n(c(=O)cn1)Cc1ccc(c(c1)[N+](=O)[O-])OC)OC(=O)C)OC(=O)C)OC(=O)C	10.04	9.02	8.41	8.20	8.62
ZINC85902136	C[C@H]1CCC(=NC1)[C@@H](C)[C@H]1[C@@H](C[C@@H]2[C@@]1(CC[C@@H]1[C@H]2CC=C2[C@@]1(CC[C@@H](C2)O[C@@H]1[C@@H]([C@H]([C@@H]([C@H](O1)COC(=O)C)OC(=O)C)OC(=O)C)OC(=O)C)C)C)OC(=O)C	7.81	7.61	9.11	9.85	9.76
ZINC85902147	C[C@H]1CCC(=NC1)[C@@H](C)[C@H]1[C@H](C[C@@H]2[C@@]1(CC[C@@H]1[C@H]2CC=C2[C@@]1(CC[C@@H](C2)O[C@@H]1[C@@H]([C@H]([C@@H]([C@H](O1)COC(=O)C)OC(=O)C)OC(=O)C)OC(=O)C)C)C)OC(=O)C	7.81	7.61	9.11	9.85	9.76
ZINC85902149	C[C@H]1CCC(=NC1)[C@@H](C)[C@H]1[C@@H](C[C@@H]2[C@@]1(CC[C@@H]1[C@H]2CC=C2[C@@]1(CC[C@@H](C2)O[C@@H]1[C@@H]([C@H]([C@@H]([C@H](O1)COC(=O)C)OC(=O)C)OC(=O)C)OC(=O)C)C)C)OC(=O)C	7.81	7.61	9.11	9.85	9.76
ZINC85902151	C[C@H]1CCC(=NC1)[C@@H](C)[C@H]1[C@H](C[C@H]2[C@@]1(CC[C@@H]1[C@H]2CC=C2[C@@]1(CC[C@@H](C2)O[C@@H]1[C@@H]([C@H]([C@@H]([C@H](O1)COC(=O)C)OC(=O)C)OC(=O)C)OC(=O)C)C)C)OC(=O)C	7.81	7.61	9.11	9.85	9.76
ZINC13353964	C([C@@H]([C@H](C(=O)[O-])O)[NH3+])C(=O)[O-]	9.46	6.94	8.42	11.64	7.59
ZINC85875377	CC(C)(C)OC(=O)NC1CCN(CC1)C(=O)COc1ccc2c(c1)c(=O)n1c(n2)CCC1	11.77	7.96	7.49	7.58	9.23
ZINC33831450	C([C@H](C(=O)N)C(=O)[O-])[C@@H](C(=O)[O-])[NH3+]	9.27	6.11	8.56	11.09	8.90

ZINC85493074	CC1=C2[C@H]([C@H]([C@@H]3CC[C@H]([C@]4([C@H]3[C@H]([C@@H](C2(C)C)C[C@@H]1OC(=O)C)OC(=O)C)CO4)OC(=O)C[C@@H](c1ccccc1)[NH2+]C)OC(=O)c1cccnc1)OC(=O)C	10.50	7.61	8.20	8.84	8.69
ZINC01532540	CCC(=O)C(=O)[O-]	11.20	6.97	7.83	9.19	8.57
ZINC00173747	CC(=O)N1C[C@@]2(CN(C[C@](C1)([C@H]2O)C)C(=O)C)C	9.11	10.50	6.51	9.59	7.92
ZINC04221675	c1cc(sc1)C[C@@H](C(=O)N)NC(=O)[C@@H]1C[C@H](CCN1C(=O)COCC(=O)[O-])NC(=O)c1cnccn1	11.09	8.09	8.11	8.09	8.24
ZINC01481961	C1[C@@H](ON=C1Cl)[C@@H](C(=O)[O-])[NH3+]	9.47	7.60	6.63	11.22	8.69
ZINC03871381	C1[C@H](ON=C1Cl)[C@@H](C(=O)[O-])[NH3+]	9.47	7.60	6.63	11.22	8.69
ZINC03871382	C1[C@@H](ON=C1Cl)[C@H](C(=O)[O-])[NH3+]	9.47	7.60	6.63	11.22	8.69
ZINC03871383	C1[C@H](ON=C1Cl)[C@H](C(=O)[O-])[NH3+]	9.47	7.60	6.63	11.22	8.69
ZINC85888651	CC(=O)OC[C@@H]1[C@@H]([C@@H]([C@H]([C@@H](O1)O[C@@H]1[C@H](O[C@H]([C@@H]([C@H]1OC(=O)C)OC(=O)C)Sc1cccc2c1nccc2)COC(=O)C)OC(=O)C)OC(=O)C)OC(=O)C	10.01	8.18	9.01	8.28	8.11
ZINC85893767	CC(=O)OC[C@@H]1[C@H]([C@@H]([C@H]([C@H](O1)O[C@@H]1[C@H](O[C@H]([C@@H]([C@H]1OC(=O)C)OC(=O)C)Sc1cccc2c1nccc2)COC(=O)C)OC(=O)C)OC(=O)C)OC(=O)C	10.01	8.18	9.01	8.28	8.11
ZINC05415150	CC[C@H]1CN(CC[C@H]1CC(=O)NCC=C)C(=O)C(C)(C)C	10.93	9.65	7.00	7.87	8.08
ZINC01482113	C(CC(=O)[O-])[C@@H](C(=O)[O-])[NH3+]	9.69	6.71	8.08	11.17	7.86
ZINC20463899	c1ccnc(c1)C[NH2+][C@@H]1[C@H]2CO[C@H](O2)[C@@H]([C@H]1[O-])[N@@H+]1CC[C@H](CC1)C(=O)N	7.61	7.88	8.89	8.65	10.38
ZINC12655870	CC(=O)N[C@@H]1[C@H]([C@@H]([C@H](O[C@H]1OCCCCN=[N+]=[N-])COC(=O)C)OC(=O)C)OC(=O)C	8.44	7.61	8.88	9.88	8.56
ZINC67910953	CCCC[C@@H](C)[C@@H]([C@@H](C[C@@H](C)CCCCC[C@@H](C[C@@H]([C@@H](C)NC(=O)C)O)O)OC(=O)C[C@@H](CC(=O)[O-])C(=O)[O-])OC(=O)C[C@@H](CC(=O)[O-])C(=O)[O-]	11.00	9.41	6.72	9.27	6.95
ZINC67910954	CCCC[C@H](C)[C@@H]([C@@H](C[C@@H](C)CCCCCC[C@@H](C[C@@H]([C@@H](C)NC(=O)C)O)O)OC(=O)C[C@@H](CC(=O)[O-])C(=O)[O-])OC(=O)C[C@@H](CC(=O)[O-])C(=O)[O-]	11.00	9.41	6.72	9.27	6.95
ZINC67910957	CCCC[C@@H](C)[C@H]([C@@H](C[C@@H](C)CCCCCC[C@@H](C[C@@H]([C@@H](C)NC(=O)C)O)O)OC(=O)C[C@@H](CC(=O)[O-])C(=O)[O-])OC(=O)C[C@@H](CC(=O)[O-])C(=O)[O-]	11.00	9.41	6.72	9.27	6.95

ZINC67910959	CCCC[C@H](C)[C@H]([C@@H](C[C@@H](C)CCCCCC[C@@H](C[C@@H]([C@@H](C)NC(=O)C)O)O)OC(=O)C[C@@H](CC(=O)[O-])C(=O)[O-])OC(=O)C[C@@H](CC(=O)[O-])C(=O)[O-]	11.00	9.41	6.72	9.27	6.95
ZINC04221755	COCC(=O)N1CC[C@@H](C[C@H]1C(=O)N1CCC[C@@H]1C(=O)OC)n1c(c(nn1)C(=O)N)C(=O)N	10.36	7.97	7.19	9.04	8.68
ZINC04029942	CC1(C[C@@]2(CCO1)N1[C@@H](CC(=N1)c1ccccc1Cl)c1cccc(c1O2)OC)C	10.75	8.82	7.83	7.36	8.44
ZINC04029943	CC1(C[C@]2(CCO1)N1[C@@H](CC(=N1)c1ccccc1Cl)c1ccc(c1O2)OC)C	10.75	8.82	7.83	7.36	8.44
ZINC20465065	c1cnc(nc1)N1CCN(CC1)[C@H]1[C@H](O[C@H]([C@H]1O)CO)CNC(=O)N1CCOCC1	11.48	9.11	7.25	7.07	8.28
ZINC04237032	CCCCCC(=O)Nc1nc2c(s1)C[C@H]1[C@]([C@@H]2CC(=O)NCc2ccco2)(CC[C@H]([C@@]1(C)CO)O)C	10.74	8.65	7.12	7.58	8.93
ZINC00157015	C1CC[NH2+][C@@H](C1)C(=O)[O-]	10.48	8.88	7.11	8.85	7.65
ZINC12481707	C[NH+](C)Cc1cc(no1)C[C@H]1C[NH2+]CC[C@H]1CC(=O)NC1CCCCC1	7.67	10.54	7.85	7.88	9.01
ZINC12660323	c1ccc2c(c1)CN1CC[C@H](C1=N2)OC(=O)Nc1cccc(c1)Oc1c(c(c(c(c1F)F)F)F)F	11.08	6.60	8.43	9.08	7.75
ZINC12660325	c1ccc2c(c1)CN1CC[C@@H](C1=N2)OC(=O)Nc1cccc(c1)Oc1c(c(c(c(c1F)F)F)F)F	11.08	6.60	8.43	9.08	7.75
ZINC04277868	CC(=O)N1CCN([C@@H](C1)C(=O)N[C@@H](CC1CCCCC1)C(=O)N)C(=O)C1CC[NH2+]CC1	11.51	7.51	7.05	8.61	8.23
ZINC15672799	CN(CC(=O)N)C(=O)C[C@@H]1CC[NH2+]C[C@@H]1Cc1cc(on1)C(=O)[O-]	9.09	8.12	8.55	8.22	8.93
ZINC13464821	C[C@@H]1[C@@H]2[C@@H](N(C(=O)N([C@H]2N(C(=O)N1C)C)C)C)C	10.80	10.10	6.34	8.42	7.20
ZINC19795995	C1C[NH2+]Cc2c1c(no2)[O-]	9.25	11.50	6.54	7.49	8.03
ZINC04221718	CC(C)C[C@H](C(=O)N)NC(=O)[C@@H]1C[C@H](CCN1C(=O)COCC(=O)[O-])NC(=O)c1cnccn1	9.94	8.34	8.67	7.53	8.30
ZINC00625932	CC(C)OC(=O)[C@H]1[C@H]([C@@H]([C@@](CC1=O)(C)O)C(=O)OC(C)C)c1cccc(c1)OC	11.84	7.88	7.15	8.01	7.89
ZINC04039771	CC(C)OC(=O)[C@@H]1[C@@H]([C@@H]([C@@](CC1=O)(C)O)C(=O)OC(C)C)c1cccc(c1)OC	11.84	7.88	7.15	8.01	7.89
ZINC04039772	CC(C)OC(=O)[C@H]1[C@@H]([C@@H]([C@@](CC1=O)(C)O)C(=O)OC(C)C)c1cccc(c1)OC	11.84	7.88	7.15	8.01	7.89
ZINC04039776	CC(C)OC(=O)[C@@H]1[C@H]([C@@H]([C@@](CC1=O)(C)O)C(=O)OC(C)C)c1cccc(c1)OC	11.84	7.88	7.15	8.01	7.89
ZINC85542564	C[C@@H]1C[C@H]([C@H]2[C@](CCC[C@@]2([C@]1(CCC1=CC(=O)OC1)O)CCCC(C)C)(C)C1CCCCC1)OC(=O)C	11.39	7.37	7.52	7.85	8.61
ZINC04097510	C1[C@H](ONC1=O)[C@@H](C(=O)[O-])[NH3+]	9.26	7.34	7.15	10.64	8.28
ZINC13459143	CCC/C(=N/CC(=O)[O-])/C1=C(CC([C@@H](C1=O)C(=O)OC)(C)C)[O-]	6.84	7.31	9.15	10.29	9.06

ZINC09033302	CC(=O)OC[C@@H]1[C@@H]([C@@H]([C@@H]([C@@H](O1)n1c(=O)[nH]c(=O)c(n1)N(C)C)OC(=O)C)OC(=O)C)OC(=O)C	8.21	7.01	9.20	10.02	8.22
ZINC34716119	CC(=O)OC[C@H]1[C@@H]([C@@H]([C@@H]([C@@H](O1)n1c(=O)[nH]c(=O)c(n1)N(C)C)OC(=O)C)OC(=O)C)OC(=O)C	8.21	7.01	9.20	10.02	8.22
ZINC34716121	CC(=O)OC[C@@H]1[C@H]([C@@H]([C@@H]([C@@H](O1)n1c(=O)[nH]c(=O)c(n1)N(C)C)OC(=O)C)OC(=O)C)OC(=O)C	8.21	7.01	9.20	10.02	8.22
ZINC34716123	CC(=O)OC[C@H]1[C@H]([C@@H]([C@@H]([C@@H](O1)n1c(=O)[nH]c(=O)c(n1)N(C)C)OC(=O)C)OC(=O)C)OC(=O)C	8.21	7.01	9.20	10.02	8.22
ZINC20463891	c1ccc2c(c1)cc(cn2)C[NH2+][C@@H]1[C@H]2CO[C@H](O2)[C@@H]([C@H]1[O-])[N@H+]1CC[C@@H](CC1)C(=O)N	8.67	7.87	8.41	7.96	9.70
ZINC35446978	c1cc(ccc1CO[C@@H]1CCN2[C@@H](C1)C(=O)N1C[C@H](C[C@H]1C2=O)n1c(c(nn1)C(=O)N)C(=O)N)F	10.76	7.95	7.37	7.55	8.94
ZINC04742652	COc1cc(cc(c1OC)OC)[C@@H]1c2cc3c(cc2C2=NN(C[C@H]2[C@@H]1C(=O)[O-])c1ccccc1)OCO3	10.79	8.64	7.23	7.66	8.25
ZINC15673448	COC(=O)c1cc(no1)C[C@H]1C[NH2+]CC[C@H]1CC(=O)NC1CCCCC1	8.49	9.38	8.19	7.64	8.87
ZINC04221750	c1ccc(cc1)C[C@H](C(=O)N)NC(=O)[C@@H]1C[C@H](CCN1C(=O)COCC(=O)[O-])NC(=O)c1cnccn1	9.37	7.96	8.68	8.20	8.35
ZINC15672803	COc1ccc(cc1OC)CNC(=O)C[C@@H]1CC[NH2+]C[C@@H]1Cc1cc(on1)C(=O)[O-]	8.55	9.04	8.34	8.20	8.43
ZINC05260695	C[C@@H](C(=O)[O-])[NH2+][C@@H](CCC[NH3+])C(=O)[O-]	8.70	7.41	8.37	10.26	7.81
ZINC85543355	C[C@]1([C@@H]2CC[C@](O1)(C[C@H]2[NH3+])C1CCCCC1)C1CCCCC1	9.74	8.59	6.18	8.87	9.13
ZINC20463064	C1CC[NH+](CC1)CC[C@H]1CN(CC[C@H]1CC(=O)[O-])C(=O)C1CCC1	10.05	8.44	7.38	8.46	8.13
ZINC01531039	C(CNC(=O)C(=O)[O-])[C@@H](C(=O)[O-])[NH3+]	10.11	8.17	7.81	8.10	8.21
ZINC04222469	C[C@@]12CC[C@H]([C@@]([C@H]1Cc1c(nc(s1)NC(=O)COC)[C@H]2CC(=O)NCCOC)(C)CO)O	9.05	7.75	7.68	9.08	8.81
ZINC13779018	C([C@@H](C(=O)[O-])[NH3+])n1c([O-])nc(=O)o1	11.02	6.45	7.88	9.12	7.87
ZINC22066252	C([C@H](C(=O)[O-])[NH3+])n1c([O-])nc(=O)o1	11.02	6.45	7.88	9.12	7.87
ZINC85541365	CC(=O)OC[C@@]12[C@H](CC[C@]([C@]31[C@@H]([C@@H]([C@@H]([C@H]2OC(=O)c1ccccc1)OC(=O)c1cccnc1)C(O3)(C)C)OC(=O)C)(C)O)OC(=O)/C=C\c1ccccc1	8.98	7.14	8.22	9.22	8.72