Supporting Information

Index of Ideality of Correlation and Correlation Contradiction Index: A Confluent Perusal on Acetylcholinesterase Inhibitors.

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Table S1 Percentage of Identity of the Three Splits.

	Set	Split 1	Split 2	Split 3
Split 1	Training	100	35.82	46.8
	Calibration	100	12.9	5.88
	Validation	100	9.09	9.09
Split 2	Training		100	41.26
	Calibration		100	16.21
	Validation		100	10.81
Split 3	Training			100
	Calibration			100
	Validation			100

To measure (%) of non-identity of splits into the training, calibration, and validation sets, examined in this work (33).

$$\text{Identity (\%)} = N_{i.j}/0.5\ (N_i+N_j) \times 100$$

Where, Ni,j is the number of substances which are distributed into the same set for both i-th split and j-th split (training calibration and validation), Ni is the number of substances which are distributed into the set for i-th split and Nj is the number of substances which are distributed into the set for j-th split.

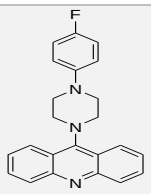
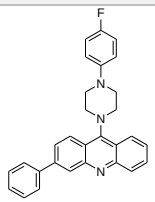
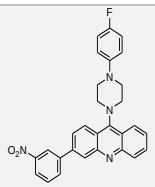
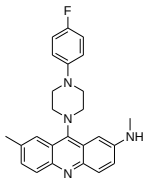
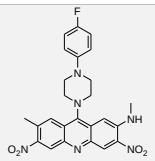
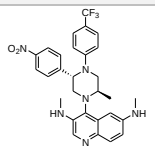
Table S2 The distribution of collected data into the training (+), calibration (#) and validation (*) sets; experimental and calculated pIC_{50} values; and domain of applicability for suggested models.

SPLITS			Inhibitors		pIC50				Domain of Applicability		
1	2	3	Comp.	SMILES	Exp.	Calc.			1	2	3
						Eq.	Eq.	Eq.			
#	+	+	A1	c1(OCC(=O)N2CCN(CC)CC2)ccc(NC(=O)C)cc1	1.242	1.4471	1.0373	1.242	Y	N	Y
+	+	+	A2	c1(OCC(=O)N2CCN(c3ccccc3)CC2)ccc(NC(=O)C)cc1	2.78	1.903	2.1009	2.78	Y	N	Y
+	+	+	A3	c1(OCC(=O)N2CCN(c3c(F)cccc3)CC2)ccc(NC(=O)C)cc1	1.519	2.0642	2.1798	1.519	Y	N	N
+	+	+	A4	c1(OCC(=O)N2CCN(c3ccc(F)cc3)CC2)ccc(NC(=O)C)cc1	1.36	1.9191	2.0652	1.36	Y	N	N
+	+	#	A5	c1(OCC(=O)N2CCN(c3ncccc3)CC2)ccc(NC(=O)C)cc1	1.291	1.5923	1.7977	1.291	Y	N	Y
+	+	#	A6	c1(OCC(=O)N2CCN(c3ncccn3)CC2)ccc(NC(=O)C)cc1	1.807	1.4638	1.4821	1.807	N	N	Y
*	*	+	A7	c1(O[C@@H](C(=O)N2CCN(C(=O)c3ccco3)CC2)C)ccc(NC(=O)C)cc1	1.9722	1.4965	1.7555	1.972	Y	N	Y
+	+	#	B1	c1(OCCCN2CCN(CC)CC2)ccc(NC(=O)C)cc1	1.098	1.731	1.4296	1.098	Y	Y	Y

+	#	+	B2	c1(OCCCN2CCN(c3ccccc3)CC2)ccc(NC(=O)C)cc1	2.857	2.1869	2.4932	2.857	Y	Y	Y
#	+	+	B3	c1(OCCCN2CCN(c3c(F)cccc3)CC2)ccc(NC(=O)C)cc1	2.866	2.3482	2.5721	2.866	Y	N	N
+	+	+	B4	c1(OCCCN2CCN(c3ccc(F)cc3)CC2)ccc(NC(=O)C)cc1	3.31	2.2031	2.4575	3.31	Y	N	N
+	#	+	B5	c1(OCCCN2CCN(c3cccc(Cl)c3)CC2)ccc(NC(=O)C)cc1	1.988	2.3421	2.3184	1.988	Y	Y	N
+	#	+	B6	c1(OCCCN2CCN(c3ccccn3)CC2)ccc(NC(=O)C)cc1	1.778	2.0584	2.1776	1.778	Y	Y	Y
+	*	+	B7	c1(OCCCN2CCN(c3ncccn3)CC2)ccc(NC(=O)C)cc1	1.561	1.7477	1.8744	1.561	N	Y	Y
#	+	+	C1	s1c(c2ccccc2)nnc1NC(=O)c1cc(Cl)ccc1	2.388	2.073	2.1575	2.388	Y	Y	N
+	*	+	C2	s1c(c2ccccc2)nnc1NC(=O)c1cc(OC(=O)C)ccc1	2.423	2.3214	2.4115	2.423	Y	Y	Y
*	+	#	C3	s1c(c2ccccc2)nnc1NC(=O)C[C@H](C)CC(C)(C)C	1.626	1.4557	1.7779	1.626	Y	Y	Y
+	#	+	C4	s1c(Cc2ccccc2)nnc1NC(=O)c1cccc(CCl)c1	1.693	2.0119	1.8109	1.693	Y	Y	N
+	*	*	C5	s1c(Cc2ccccc2)nnc1NC(=O)c1cccc(OC(=O)C)c1	1.936	2.2603	2.0649	1.9937	Y	Y	Y
#	+	#	C6	s1c(Cc2ccccc2)nnc1NC(=O)C[C@H](C)CC(C)(C)C	1.567	1.5208	1.5138	1.567	Y	Y	Y
#	#	+	D1	s1c(c2ccccc2Cl)nnc1NC(=O)c1cc(CCl)ccc1	2.523	2.1563	2.2598	2.523	Y	Y	N
*	+	+	D2	s1c(c2ccccc2Cl)nnc1NC(=O)c1cc(OC(=O)C)ccc1	2.5186	2.306	2.4302	2.519	Y	Y	N
+	#	#	D3	s1c(c2ccccc2Cl)nnc1NC(=O)C[C@H](C)CC(C)(C)C	1.862	1.4692	1.7687	1.862	Y	Y	Y
#	+	+	D4	s1c(c2ccccc2Cl)nnc1NC(=O)c1cc(C(F)(F)F)cc(C(F)(F)F)c1	2.562	2.1891	2.3815	2.4398	Y	Y	Y
+	#	+	D5	s1c(c2ccc(C)cc2)nnc1NC(=O)c1ccc(CCl)c1	1.901	1.9073	1.9785	2.0178	Y	Y	N
*	+	+	D6	s1c(c2ccc(C)cc2)nnc1NC(=O)c1ccc(OC(=O)C)c1	1.9666	2.1557	2.2325	2.1363	Y	Y	Y
#	+	*	D7	s1c(c2ccc(C)cc2)nnc1NC(=O)C[C@H](C)CC(C)(C)C	1.626	1.4162	1.6814	1.8103	Y	Y	Y
#	+	+	D8	s1c(c2ccc(C)cc2)nnc1NC(=O)c1cc(C(F)(F)F)cc(C(F)(F)F)c1	2.149	2.1094	2.3053	2.4134	Y	N	N
*	#	+	E1	c1(OC[C@@H](CN2CCCC2)O)ccc(NC(=O)c2cc(OC)c(OC)c(OC)c2)cc1	2.1249	1.9254	2.0345	2.0048	Y	Y	Y
#	+	#	E2	c1(OC[C@H](CN2CCCCC2)O)ccc(NC(=O)c2cc(OC)c(OC)c(OC)c2)cc1	2.125	1.932	2.1276	2.1504	Y	Y	Y
*	+	#	E3	c1(OC[C@H](CN2CCOCC2)O)ccc(NC(=O)c2cc(OC)c(OC)c(OC)c2)cc1	2.1871	2.115	2.1152	1.9881	Y	Y	Y
#	#	+	E4	c1(OC[C@@H](CN(C)C)O)ccc(NC(=O)c2cc(OC)c(OC)c(OC)c2)cc1	2.187	2.0328	2.0119	2.3667	Y	Y	Y
#	+	+	E5	c1(OCCN2CCCC2)ccc(NC(=O)c2cc(OC)c(OC)c(OC)c2)cc1	2.347	2.1068	2.1196	2.0797	Y	Y	Y
*	+	*	E6	c1(OCCN2CCOCC2)ccc(NC(=O)c2cc(OC)c(OC)c(OC)c2)cc1	2.0223	2.2964	2.091	2.063	Y	Y	Y
+	#	+	E7	c1(OCCN2CCCCC2)ccc(NC(=O)c2cc(OC)c(OC)c(OC)c2)cc1	1.783	2.1133	2.1697	2.2253	Y	Y	Y
+	#	+	E8	c1(OCCN(C)C)ccc(NC(=O)c2cc(OC)c(OC)c(OC)c2)cc1	2.398	2.0276	2.1327	2.3394	Y	Y	Y
#	*	+	G1	c1c2c(N3CCN(c4ccc(F)cc4)CC3)c3ccccc3nc2ccc1	2.664	2.6614	2.9161	2.7065	Y	Y	Y
*	+	+	G2	c1c2c(N3CCN(c4ccccc4)CC3)c3ccc(Cl)c3nc2ccc1	2.6459	2.9099	3.0249	2.8123	Y	Y	Y
+	+	#	G3	c1c2c(N3CCN(c4ccc(F)cc4)CC3)c3cccc(Cl)c3nc2ccc1	3.481	2.9212	2.8505	2.8511	Y	Y	Y
+	+	#	G4	c1c2c(N3CCN(c4c(F)cccc4)CC3)c3cccc(Cl)c3nc2ccc1	3.398	2.9813	3.0455	2.8484	Y	Y	Y
+	*	+	G5	c1c2c(N3CCN(CC)CC3)c3cccc(Cl)c3nc2ccc1	2.824	2.4677	2.3965	2.8814	Y	Y	Y
#	+	*	G6	c1c2c(N3CCN(C)CC3)c3cccc(Cl)c3nc2ccc1	2.44	2.2864	2.3989	2.7455	Y	Y	Y

+	+	#	G7	c1c2c(N3CCN(c4cc(Cl)ccc4)CC3)c3cccc(F)c3nc2ccc1	2.268	2.9212	2.8505	2.8511	Y	Y	Y
+	+	#	G8	c1c2c(N3CCN(c4cc(Cl)ccc4)CC3)c3cc(F)ccc3nc2ccc1	2.166	2.7761	2.7359	2.7489	Y	Y	Y
+	#	#	G9	c1c2c(N3CCN(c4ccc(F)cc4)CC3)c3cc(Cl)ccc3nc2ccc1	2.532	2.7761	2.7359	2.7489	Y	Y	Y
+	#	#	G10	c1c2c(N3CCN(c4ccc(F)cc4)CC3)c3cccc(C)c3nc2ccc1	2.932	2.7669	2.9342	2.7899	Y	Y	Y
+	*	*	G11	c1c2c(N3CCN(c4ccc(F)cc4)CC3)c3cc(C)cc(C)c3nc2ccc1	2.775	2.7274	2.8376	2.7712	Y	Y	Y
+	#	#	G12	c1c2c(N3CCN(c4c(F)cccc4)CC3)c3cc(C)cc(C)c3nc2ccc1	2.706	2.7875	3.0327	2.7685	Y	Y	Y
*	+	#	G13	c1c2c(N3CCN(CC)CC3)c3cc(C)cc(C)c3nc2ccc1	2.4776	2.271	2.4989	2.9847	Y	Y	Y
+	+	#	H1	c1c2C(=O)/C(=C\c3ccc(OC(=O)c4ccccc4F)cc3)/Cc2ccc1	1.852	1.594	1.7858	1.3866	Y	Y	Y
*	+	#	H2	c1c2C(=O)/C(=C\c3ccc(OC(=O)c4cccc(CCl)c4)cc3)/Cc2ccc1	1.5675	1.38	1.5148	1.2936	Y	Y	Y
+	#	*	H3	c1c2C(=O)/C(=C\c3ccc(OC(=O)c4cccc(OC(F)(F)F)c4)cc3)/Cc2ccc1	1.91	1.8249	1.6745	1.6185	N	Y	Y
+	*	*	H4	c1c2C(=O)/C(=C\c3ccc(OC(=O)c4ccc(CCl)cc4)cc3)/Cc2ccc1	1.098	1.3199	1.3197	1.2963	Y	Y	Y
+	*	+	H5	c1c2C(=O)/C(=C\c3ccc(OC(=O)c4ccc([N+](=O)[O-])cc4)cc3)/Cc2ccc1	1.311	1.646	1.3882	1.542	Y	Y	Y
#	+	*	H6	c1c2C(=O)/C(=C\c3ccc(OC(=O)c4cc(OC)c(OC)c(OC)c4)cc3)/Cc2ccc1	1.852	1.7991	1.7958	1.5835	Y	Y	Y
+	*	*	H7	c1c2C(=O)/C(=C\c3ccc(OC(=O)c4ccc(F)cc4)cc3)/Cc2ccc1	1.392	1.4611	1.3882	1.2908	Y	Y	Y
*	+	+	H8	c1c2C(=O)/C(=C\c3ccc(OC(=O)c4cc(Cl)cc(Cl)c4)cc3)/Cc2ccc1	1.3638	1.5455	1.3306	1.1576	Y	Y	Y
+	#	#	H9	c1c2C(=O)/C(=C\c3ccc(OC(=O)c4ccccc4)cc3)/Cc2ccc1	1.464	1.4194	1.5338	1.3842	Y	Y	Y
*	+	#	H10	c1c2C(=O)/C(=C\c3ccc(OC(=O)c4ccc(OC)cc4)cc3)/Cc2ccc1	1.4101	1.5472	1.393	1.5275	Y	Y	Y
+	#	*	H11	c1c2C(=O)/C(=C\c3ccc(OC(=O)c4cc(C(F)(F)F)cc(C(F)(F)F)c4)cc3)/Cc2ccc1~	1.92	1.6607	1.7052	1.6365	N	Y	Y

Table S3 Designed Compounds with Structure and Calculated pIC50.

SR. no.	SMILES	PIC_{50}	Structure
G1	c1c2c(N3CCN(c4ccc(F)cc4)CC3)c3ccccc3nc2ccc1	2.663 (exp.) 2.92 (calc.)	
DD1	c1(c2c(nc3c1ccc(c3)c1ccccc1)cccc2)N1CCN(CC1)c1ccc(cc1)F	3.45	
DD2	c1(N2CCN(c3ccc(F)cc3)CC2)c2c(cc(c3cc([N+](=O)[O-])ccc3)cc2)nc2ccccc12	4.33	
DD3	c1(N2CCN(c3ccc(F)cc3)CC2)c2c(ccc(C)c2)nc2ccc(NC)cc12	3.33	
DD4	c1(N2CCN(c3ccc(F)cc3)CC2)c2c(cc([N+](=O)[O-])c(C)c2)nc2cc([N+](=O)[O-])c(NC)cc12	3.52	
DD5	c1(C(F)(F)F)ccc(N2C[C@@H](C)N(c3c4cc(NC)ccc4ncc3NC)C[C@@H]2c2ccc([N+](=O)[O-])cc2)cc1	3.36	

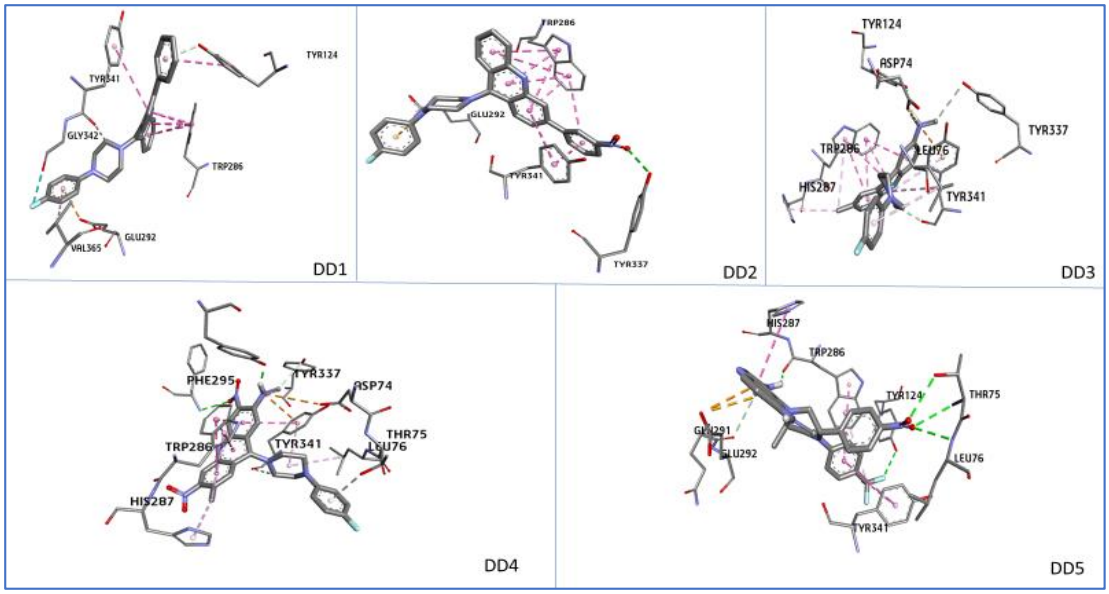


Figure S1 Binding Interactions of Designed Compounds.