

Ensemble-Based Virtual Screening Led to the Discovery of Novel Lead Molecules as Potential NMBA

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Table S1. The NMBA database collected from the literature and used in molecular property filters.

Compound	Formula	SMILES	DOI	M.W.	Charge	logP
Patel1996-7	C52H68N2O8	<chem>O=C(CC/C=C/CCC(OCCC[N+](C)CC(C=C(OC)C(OC)=C2)=C2C(CC3=CC=CC=C3)C1)=O)OCCC[N+](C)CC5=CC(OC)=C(OC)C=C5C(CC6=CC=CC=C6)C4</chem>	10.1016/0928-0987(95)00032-1	848	+2	4.036
Patel1996-8	C52H66F2N2O8	<chem>O=C(CC/C=C/CCC(OCCC[N+](C)CC(C=C(OC)C(OC)=C2)=C2C(CC3=CC(F)=CC=C3)C1)=O)OCCC[N+](C)CC5=CC(OC)=C(OC)C=C5C(CC6=CC(F)=CC=C6)C4</chem>	10.1016/0928-0987(95)00032-1	884	+2	4.322
Patel1996-9	C52H66Cl2N2O8	<chem>O=C(CC/C=C/CCC(OCCC[N+](C)CC(C=C(OC)C(OC)=C2)=C2C(CC3=CC=C(Cl)C=C3)C1)=O)OCCC[N+](C)CC5=CC(OC)=C(OC)C=C5C(CC6=CC=C(Cl)C=C6)C4</chem>	10.1016/0928-0987(95)00032-1	916	+2	5.462
Patel1996-10	C56H76N2O12	<chem>O=C(CC/C=C/CCC(OCCC[N+](C)CC(C=C(OC)C(OC)=C2)=C2C(CC3=CC(OC)=C(OC)C=C3)C1)=O)OCCC[N+](C)CC5=CC(OC)=C(OC)C=C5C(CC6=CC(OC)=C(OC)C=C6)C4</chem>	10.1016/0928-0987(95)00032-1	968	+2	3.352
Brittain1977-1a	C28H24N6	<chem>C[N+](C)C(N(N=N)N2C(C=CC=C3)=C3[N+](C)=C2C4=CC=CC=C4)C5=C1C=CC=C5)C6=CC=CC=C6</chem>	10.1111/j.1476-5381.1977.tb09738.x	444	+2	-2.696
Brittain1977-1b	C30H28N6	<chem>C[N+](C)C(N(N=N)N2C(C=CC=C3)=C3[N+](C)=C2C4=CC=C(C)C=C4)C5=C1C=CC=C5)C6=CC=C(C)C=C6</chem>	10.1111/j.1476-5381.1977.tb09738.x	472	+2	-1.698
Brittain1977-1c	C30H28N6O2	<chem>C[N+](C)C(N(N=N)N2C(C=CC=C3)=C3[N+](C)=C2C4=CC=C(OC)C=C4)C5=C1C=CC=C5)C6=CC=C(OC)C=C6</chem>	10.1111/j.1476-5381.1977.tb09738.x	504	+2	-2.598
Ginsburg1971-3	C27H30NO2	<chem>O=C(OCC[N+](C)C(C)C(C=CC=C2)=C2C3=C1C=CC=C3)CC4=CC=CC=C4</chem>	10.1111/j.1476-5381.1971.tb07161.x	400	+1	2.890
Ginsburg1971-5	C21H26N3O6	<chem>O=C(OCC[N+](C)C(C)C(C1=CC=C([N+](C)C([O-])=O)C=C1)CC2=CC=C([N+](C)C([O-])=O)C=C2</chem>	10.1111/j.1476-5381.1971.tb07161.x	416	+1	1.042
Ginsburg1971-9	C26H46N2O4	<chem>O=C(OCC[N+](C)C(C)C(C)CC1=C(C(C(OCC[N+](C)C(C)C(C)C)=O)C=CC=C1</chem>	10.1111/j.1476-5381.1971.tb07161.x	450	+2	-2.712
Ginsburg1971-11	C26H46N2O4	<chem>O=C(OCC[N+](C)C(C)C(C)CC1=CC(C(C(OCC[N+](C)C(C)C(C)C)=O)C=CC=C1</chem>	10.1111/j.1476-5381.1971.tb07161.x	450	+2	-2.662
Ginsburg1971-12	C20H34N2O4	<chem>O=C(OCC[N+](C)C(C)C(C)CC1=CC=C(C(C(OCC[N+](C)C(C)C(C)C)=O)C=C1</chem>	10.1111/j.1476-5381.1971.tb07161.x	366	+2	-5.836

Ginsburg1971-13	C26H46N2O4	<chem>O=C(OCC[N+](CC)(CC)CC)CC1=CC=C(CC(OCC[N+](CC)(CC)CC)=O)C=C1</chem>	10.1111/j.1476-5381.1971.tb07161.x	450	+2	-2.662
Ginsburg1971-15	C28H30NO2	<chem>O=C(OCC[N+](CC)(CC)C1C(C=CC=C2)=C2C3=C1C=CC=C3)/C=C/C/C4=CC=CC=C4</chem>	10.1111/j.1476-5381.1971.tb07161.x	412	+1	3.416
Ginsburg1971-17	C28H29ClNO2	<chem>O=C(OCC[N+](CC)(CC)C1C(C=CC=C2)=C2C3=C1C=CC=C3)/C=C/C/C4=CC=C(Cl)C=C4</chem>	10.1111/j.1476-5381.1971.tb07161.x	446	+1	4.139
Ginsburg1971-19	C28H29N2O4	<chem>O=C(OCC[N+](CC)(CC)C1C(C=CC=C2)=C2C3=C1C=CC=C3)/C=C/C/C4=C([N+])([O-])C=CC=C4</chem>	10.1111/j.1476-5381.1971.tb07161.x	457	+1	3.169
Ginsburg1971-21	C28H29N2O4	<chem>O=C(OCC[N+](CC)(CC)C1C(C=CC=C2)=C2C3=C1C=CC=C3)/C=C/C/C4=CC([N+])([O-])C=CC=C4</chem>	10.1111/j.1476-5381.1971.tb07161.x	457	+1	3.169
Ginsburg1971-23	C28H29N2O4	<chem>O=C(OCC[N+](C1C(C=CC=C2)=C2C3=C1C=CC=C3)(CC)CC)/C=C/C/C4=CC=C([N+])([O-])C=C4</chem>	10.1111/j.1476-5381.1971.tb07161.x	457	+1	3.169
Ginsburg1971-25	C28H32NO2	<chem>O=C(OCC[N+](CC)(C1C(C=CC=C2)=C2C3=C1C=CC=C3)CC)CC=C4=CC=CC=C4</chem>	10.1111/j.1476-5381.1971.tb07161.x	414	+1	3.367
Boros1999-1	C54H71ClN2O14	<chem>C[N@+](C@H)1CC2=CC(OC)=C(OC)C(OC)=C2)(CCCCOC/C=C(Cl)/C(OCCC[N@+])3(C)CCC(C=C(OC)C(OC)=C4)=C4[C@H]3CC5=CC(OC)=C(OC)C(OC)=C5)=O)OCCC6=C1C=C(OC)C(OC)=C6</chem>	10.1021/jm990060j	1006	+2	2.600
Boros1999-2	C52H67ClN2O14	<chem>C[N@+](CCCCOC/C=C(C(OCCC[N@+])1(C)CCC2=C(C=C(C(OC)=C2)OC)[C@H]1C3=CC(OC)=C(OC)C(OC)=C3)=O)Cl)=O)(CCC4=C5C=C(C(OC)=C4)OC)[C@H]5C6=CC(OC)=C(C(OC)=C6)OC</chem>	10.1021/jm990060j	978	+2	1.842
Boros1999-3	C52H68N2O14	<chem>C[N@+](CCCCOC/C=C/C(OCCC[N@+])1(C)CCC2=C(C=C(C(OC)=C2)OC)[C@H]1C3=CC(OC)=C(OC)C(OC)=C3)=O)O)(CCC4=C5C=C(C(OC)=C4)OC)[C@H]5C6=CC(OC)=C(C(OC)=C6)OC</chem>	10.1021/jm990060j	944	+2	1.189
Boros1999-6a	C53H69ClN2O14	<chem>C[N@+](C@H)1(C=C2OC)=CC(OC)=C2OC)C(C(C1)=C3)=CC(OC)=C3OC)CCCCOC/C=C(Cl)/C(OCCC[N@+])(CCC4=CC(OC)=C5OC)C)[C@H](C4=C5)CC(C=C6OC)=CC(OC)=C6OC)=O)=O</chem>	10.1021/jm990060j	992	+2	2.221
Boros1999-4	C52H67ClN2O14	<chem>C[N@+](C@H)1C2=CC(OC)=C(OC)C(OC)=C2)(CCCCOC/C=C(Cl)/C(OCCC[N@+])3(C)CCC(C=C(OC)C(OC)=C4)=C4[C@H]3C5=CC(OC)=C(OC)C(OC)=C5)=O)OCCC6=C1C=C(OC)C(OC)=C6</chem>	10.1021/jm990060j	978	+2	1.842
Laudexium	C52H74N2O8	<chem>C[N+](CCCCCCCCC[N+])2(C)C(CC3=CC=C(OC)C(OC)=C3)C(C=C(OC)C(OC)=C4)=C4CC2)C(CC5=CC(OC)=C(OC)C=C5)C6=C(C(OC)=C(OC)C=C6CC1</chem>	10.1002/med.20036	854	+2	3.578
Atracurium	C53H72N2O12	<chem>C[N+](CCC(OCCCCCOC(C[N+])2(C)C(CC3=CC=C(OC)C(OC)=C3)C(C=C(OC)C(OC)=C4)=C4CC2)=O)O)C(CC5=CC(OC)=C(OC)C=C5)C6=CC(OC)=C(OC)C=C6CC1</chem>	10.1002/med.20036	928	+2	3.497
Mivacurium	C58H80N2O14	<chem>COC(C(OC)=C1)=C(OC)C=C1CC2[N+](C)(CCCCOC(CC/C=C/CCC(OCCC[N+])3(C)C(CC4=CC(OC)=C(OC)C(OC)=C4)C5=CC(OC)=C(OC)C=C5CC3)=O)O)CCC6=C2C=C(OC)C(OC)=C6</chem>	10.1002/med.20036	1028	+2	2.636
Doxacurium	C56H78N2O16	<chem>COC1=CC(CC2C3=C(C(OC)=C(C=C3CC[N+])2(CCCOC(CCC(OCC[N+])4(CCC5=CC(OC)=C(C(OC)=C5C4CC6=CC(OC)=C(C(OC)=</chem>	10.1002/med.20036	1034	+2	1.042

		<chem>C6)OC)OC)C=O)=O)C)OC)OC)=CC(OC)=C1OC</chem>				
Oxalolaudonium	C48H62N2O10	<chem>COC1=C(OC)C=C(C[N+](C)(CCCOC(C(OCCC[N+])2(C)C(CC3=CC=C(OC)C(OC)=C3)C(C=CC=C4)=C4CC2)=O)=O)C(CC5=CC=C(O)C)C(OC)=C5)C6)C6=C1</chem>	10.1002/med.20036	826	+2	2.329
d-Tubocurarine	C37H42N2O6	<chem>OC1=C(OC2=CC=C3C=C2)C([C@@]([N+](C)(C)CC4)([H])CC5=C=C(O)C(OC(C(OC)=C6)=CC7=C6CC[N+](C)([H])[C@@]7([H])C3)=C5)=C4C=C1OC</chem>	10.1021/jm020574+	610	+2	4.412
Metocurine	C39H46N2O6	<chem>C[N+]1(C)[C@@](CC2=CC=C(O)C(OC(C(OC)=C3)=CC4=C3CC[N+](C)(C)[C@@]4([H])C5)=C2)([H])C6=C(CC1)C=C(OC)C(OC)=C6OC7=CC=C5C=C7</chem>	10.1021/jm020574+	638	+2	0.53
Boros2003-20a	C54H71ClN2O14	<chem>C[N+](CCC1=C2C=C(OC)C(OC)=C1)(CCCOC(/C(Cl)=C/C(OCCC[N+])3(C)C(CC4=CC(OC)=C(OC)C(OC)=C4)C(C=C(OC)C(OC)=C5)=C5CC3)=O)=O)C2CC6=CC(OC)=C(OC)C(OC)=C6</chem>	10.1021/jm020574+	1006	+2	2.600
Boros2003-20b	C52H63ClN2O14	<chem>C[N+](CCC1=C2C=C(OCO3)C3=C1)(CCCOC(/C(Cl)=C/C(OCCC[N+])4(C)C(CC5=CC(OC)=C(OC)C(OC)=C5)C(C=C(OCO6)C6=C7)=C7CC4)=O)=O)C2CC8=CC(OC)=C(OC)C(OC)=C8</chem>	10.1021/jm020574+	974	+2	3.214
Boros2003-20c	C52H67ClN2O14	<chem>C[N+]1(CCCOC(/C(Cl)=C/C(OCCC[N+])2(C)C(C3=CC(OC)=C(OC)C(OC)=C3)C(C=C(OC)C(OC)=C4)=C4CC2)=O)=O)C(C5=CC(OC)=C(OC)C(OC)=C5)C6=C(C=C(OC)C(OC)=C6)CC1</chem>	10.1021/jm020574+	978	+2	1.842
Boros2003-21	C52H68N2O14	<chem>C[N+]1(CCCOC(/C=C/C(OCCC[N+])2(C)C(C3=CC(OC)=C(OC)C(OC)=C3)C(C=C(OC)C(OC)=C4)=C4CC2)=O)=O)C(C5=CC(OC)=C(OC)C(OC)=C5)C6=C(C=C(OC)C(OC)=C6)CC1</chem>	10.1021/jm020574+	944	+2	1.189
Boros2003-24g	C54H71ClN2O15	<chem>COC1=C(OC)C([C@@H](CC2=CC(OC)=C(OC)C(OC)=C2)[N@@+](CCCOC(/C(Cl)=C/C(OCCC[N@@+])3(C)[C@@H](C4=CC(OC)=C(OC)C(OC)=C4)C(C=C(OC)C(OC)=C5)=C5CC3)=O)=O)(C)CC6)=C6C=C1OC</chem>	10.1021/jm020574+	1022	+2	1.863
Boros2003-24i	C52H67ClN2O14	<chem>COC1=CC([C@@H](CC2=CC(OC)=C(OC)C(OC)=C2)[N@@+](CCCOC(/C(Cl)=C/C(OCCC[N+])3([H])[C@@H](C4=CC(OC)=C(OC)C(OC)=C4)C(C=C(OC)C(OC)=C5)=C5CC3)=O)=O)(C)CC6)=C6C=C1OC</chem>	10.1021/jm020574+	978	+2	5.794
Boros2003-24j	C51H65ClN2O12	<chem>COC1=CC([C@@H](CC2=CC(OC)=C(OC)C(OC)=C2)[N@@+](CCCOC(/C(Cl)=C/C(OCCC[N@@+])3(C)[C@@H](C4=CC=C(OC)C=C4)C(C=C(OC)C(OC)=C5)=C5CC3)=O)=O)(C)CC6)=C6C=C1OC</chem>	10.1021/jm020574+	932	+2	2.840
Boros2003-24k	C50H61ClF2N2O11	<chem>COC1=CC([C@@H](CC2=CC(OC)=C(OC)C(OC)=C2)[N@@+](CCCOC(/C(Cl)=C/C(OCCC[N@@+])3(C)[C@@H](C4=CC=C(F)C(F)=C4)C(C=C(OC)C(OC)=C5)=C5CC3)=O)=O)(C)CC6)=C6C=C1OC</chem>	10.1021/jm020574+	938	+2	3.137
Boros2003-24l	C53H67ClN2O13	<chem>C[N+](CCC1=C2C=C(OC)C(OC)=C1)(CCCOC(/C(Cl)=C/C(OCCC[N+])34(C(C5=CC(OC)=C(OC)C=C5CC4)C(C=C(OC)C(OC)=C6)=C6CC3)=O)=O)C2CC7=CC(OC)=C(OC)C(OC)=C7</chem>	10.1021/jm020574+	974	+2	2.444
Boros2003-24m	C53H67ClN2O13	<chem>C[N+](CCC1=C2C=C(OC)C(OC)=C1)(CCCOC(/C=C(Cl)/C(OCCC[N+])34(C(C5=CC(OC)=C(OC)C=C5CC4)C(C=C(OC)C(OC)=C6)=C6CC3)=O)=O)C2CC7=CC(OC)=C(OC)C(OC)=C7</chem>	10.1021/jm020574+	974	+2	2.444

Boros2003-24n	C54H69CIN2O15	<chem>O=C(/C(Cl)=C/C(OCCCN[+])1(C)C(C2=CC(OC)=C(OC)C(OC)=C2)C(C=C(OC)C(OC)=C3)=C3CC1)=O)OCCCN[+])4(CCC5=C6C(OC)=C(OC)C(OC)=C5)C6CC7=C(C4)C(OC)=C(OC)C(OC)=C7</chem>	10.1021/jm020574+	1020	+2	1.519
Boros2003-25a	C57H80N2O14	<chem>C[N+](CCC1=C2C=C(OC)C(OC)=C1)(CCCOC(CCCCCC(OCCC[N+])3(C)[C@H](C4=CC(OC)=C(OC)C(OC)=C4)C(C=C(OC)C(OC)=C5)=C5CC3)=O)=O)C2CC6=CC(OC)=C(OC)C(OC)=C6</chem>	10.1021/jm020574+	1016	+2	2.741
Boros2003-25b	C55H76N2O14	<chem>C[N+](CCC1=C2C=C(OC)C(OC)=C1)(CCCOC(CCCCC(OCCC[N+])3(C)[C@@H](C4=CC(OC)=C(OC)C(OC)=C4)C(C=C(OC)C(OC)=C5)=C5CC3)=O)=O)C2CC6=CC(OC)=C(OC)C(OC)=C6</chem>	10.1021/jm020574+	988	+2	1.683
Boros2003-25c	C56H78N2O14	<chem>C[N+](CCC1=C2C=C(OC)C(OC)=C1)(CCCOC(CCCCC(OCCC[N+])3(C)[C@@H](C4=CC(OC)=C(OC)C(OC)=C4)C(C=C(OC)C(OC)=C5)=C5CC3)=O)=O)C2CC6=CC(OC)=C(OC)C(OC)=C6</chem>	10.1021/jm020574+	1002	+2	2.212
Boros2003-25e	C58H82N2O14	<chem>C[N+](CCC1=C2C=C(OC)C(OC)=C1)(CCCOC(CCCCCC(OCC[N+])3(C)[C@@H](C4=CC(OC)=C(OC)C(OC)=C4)C(C=C(OC)C(OC)=C5)=C5CC3)=O)=O)C2CC6=CC(OC)=C(OC)C(OC)=C6</chem>	10.1021/jm020574+	1030	+2	3.270
Boros2003-25f	C59H84N2O14	<chem>C[N+](CCC1=C2C=C(OC)C(OC)=C1)(CCCOC(CCCCCC(OC[N+])3(C)[C@@H](C4=CC(OC)=C(OC)C(OC)=C4)C(C=C(OC)C(OC)=C5)=C5CC3)=O)=O)C2CC6=CC(OC)=C(OC)C(OC)=C6</chem>	10.1021/jm020574+	1044	+2	3.799
Boros2003-27a	C53H71FN2O14	<chem>C[N+](CCC1=C2C=C(OC)C(OC)=C1)(CCCOC([C@@H](F)CC(OC[N+])3(C)[C@@H](C4=CC(OC)=C(OC)C(OC)=C4)C(C=C(OC)C(OC)=C5)=C5CC3)=O)=O)C2CC6=CC(OC)=C(OC)C(OC)=C6</chem>	10.1021/jm020574+	978	+2	1.502
Boros2003-27b	C54H72F2N2O14	<chem>C[N+](CCC1=C2C=C(OC)C(OC)=C1)(CCCOC(C(F)(CCC(OCCCN[+])3(C)[C@@H](C4=CC(OC)=C(OC)C(OC)=C4)C(C=C(OC)C(OC)=C5)=C5CC3)=O)F)=O)C2CC6=CC(OC)=C(OC)C(OC)=C6</chem>	10.1021/jm020574+	1010	+2	2.030
Boros2003-27c	C53H70F2N2O14	<chem>C[N+](CCC1=C2C=C(OC)C(OC)=C1)(CCCOC(C(C(OCCCN[+])3(C)[C@@H](C4=CC(OC)=C(OC)C(OC)=C4)C(C=C(OC)C(OC)=C5)=C5CC3)=O)(F)F)=O)C2CC6=CC(OC)=C(OC)C(OC)=C6</chem>	10.1021/jm020574+	996	+2	2.575
Boros2003-27d	C54H72F2N2O15	<chem>C[N+](CCC1=C2C(OC)=C(OC)C(OC)=C1)(CCCOC(C(C(OCCC[N+])3(C)[C@@H](C4=CC(OC)=C(OC)C(OC)=C4)C(C=C(OC)C(OC)=C5)=C5CC3)=O)(F)F)=O)C2CC6=CC(OC)=C(OC)C(OC)=C6</chem>	10.1021/jm020574+	1026	+2	2.217
Boros2003-27f	C53H70F2N2O14	<chem>C[N+](CCC1=C2C=C(OC)C(OC)=C1)(CCCOC(C(C(F)(C(OCCC[N+])3(C)[C@@H](C4=CC(OC)=C(OC)C(OC)=C4)C(C=C(OC)C(OC)=C5)=C5CC3)=O)=O)C2CC6=CC(OC)=C(OC)C(OC)=C6</chem>	10.1021/jm020574+	996	+2	2.575
Boros2003-28a	C53H69FN2O14	<chem>C[N+](CCC1=C2C=C(OC)C(OC)=C1)(CCCOC(/C(F)=C/C(OCCC[N+])3(C)[C@@H](C4=CC(OC)=C(OC)C(OC)=C4)C(C=C(OC)C(OC)=C5)=C5CC3)=O)=O)C2CC6=CC(OC)=C(OC)C(OC)=C6</chem>	10.1021/jm020574+	976	+2	1.621
Boros2003-28b	C54H71FN2O15	<chem>C[N+](CCC1=C2C(OC)=C(OC)C(OC)=C1)(CCCOC(/C(F)=C/C(OC[N+])3(C)[C@@H](C4=CC(OC)=C(OC)C(OC)=C4)C(C=C(OC)C(OC)=C5)=C5CC3)=O)=O)C2CC6=CC(OC)=C(OC)C(OC)=C6</chem>	10.1021/jm020574+	1006	+2	1.263
Gyermek2006-1	C43H56N2O12	<chem>C[N@@+])1(CC2=CC(OC(C)=O)=C(OC(C)=O)C=C2)[C@H]3CCC[C@@H]1C[C@@H](OC(CC(O[C@H]4C[C@H]5CCC[C@@H](C4)[N@@+])5(CC6=CC=C(OC(C)=O)C(OC(C)=O)=C6)C)=O)=O)C3</chem>	10.1016/j.lfs.2006.01.038	792	+2	-4.445

Gyermek2006-2	C44H58N2O12	C[N@@+](CC2=CC(OC(C)=O)=C(OC(C)=O)C=C2)[C@H]3CCC[C@@H]1C[C@@H](OC(CCC(O[C@H]4C[C@H]5CCC[C@@H](C4)[N@@+](CC6=CC=C(OC(C)=O)C(OC(C)=O)=C6)C)=O)C3	10.1016/j.lfs.2006.01.038	806	+2	-4.09
Gyermek2006-3	C45H60N2O12	C[N@@+](CC2=CC(OC(C)=O)=C(OC(C)=O)C=C2)[C@H]3CCC[C@@H]1C[C@@H](OC(CCCC(O[C@H]4C[C@H]5CCC[C@@H](C4)[N@@+](CC6=CC=C(OC(C)=O)C(OC(C)=O)=C6)C)=O)C3	10.1016/j.lfs.2006.01.038	820	+2	-3.735
Gyermek2006-4	C46H62N2O12	C[N@@+](CC2=CC(OC(C)=O)=C(OC(C)=O)C=C2)[C@H]3CCC[C@@H]1C[C@@H](OC(CCCCC(O[C@H]4C[C@H]5CCC[C@@H](C4)[N@@+](CC6=CC=C(OC(C)=O)C(OC(C)=O)=C6)C)=O)C3	10.1016/j.lfs.2006.01.038	834	+2	-3.786
Gyermek2006-5	C47H64N2O12	C[N@@+](CC2=CC(OC(C)=O)=C(OC(C)=O)C=C2)[C@H]3CCC[C@@H]1C[C@@H](OC(CCCCC(O[C@H]4C[C@H]5CCC[C@@H](C4)[N@@+](CC6=CC=C(OC(C)=O)C(OC(C)=O)=C6)C)=O)C3	10.1016/j.lfs.2006.01.038	848	+2	-3.257
Gyermek2006-6	C48H66N2O12	C[N@@+](CC2=CC(OC(C)=O)=C(OC(C)=O)C=C2)[C@H]3CCC[C@@H]1C[C@@H](OC(CCCCC(O[C@H]4C[C@H]5CCC[C@@H](C4)[N@@+](CC6=CC=C(OC(C)=O)C(OC(C)=O)=C6)C)=O)C3	10.1016/j.lfs.2006.01.038	862	+2	-2.728
Gyermek2006-7	C44H56N2O12	C[N@@+](CC2=CC(OC(C)=O)=C(OC(C)=O)C=C2)[C@H]3CCC[C@@H]1C[C@@H](OC(/C=C/C(O[C@H]4C[C@H]5CCC[C@@H](C4)[N@@+](CC6=CC=C(OC(C)=O)C(OC(C)=O)=C6)C)=O)C3	10.1016/j.lfs.2006.01.038	804	+2	-3.73
Gyermek2006-8	C44H55CIN2O12	C[N@@+](CC2=CC(OC(C)=O)=C(OC(C)=O)C=C2)[C@H]3CCC[C@@H]1C[C@@H](OC(/C(CI)=C/C(O[C@H]4C[C@H]5CCC[C@@H](C4)[N@@+](CC6=CC=C(OC(C)=O)C(OC(C)=O)=C6)C)=O)C3	10.1016/j.lfs.2006.01.038	838	+2	-3.08
Gyermek2006-9	C48H64N2O12	C[N@@+](CC2=CC(OC(C)=O)=C(OC(C)=O)C=C2)[C@H]3CCC[C@@H]1C[C@@H](OC(CC/C=C/CCC(O[C@H]4C[C@H]5CCC[C@@H](C4)[N@@+](CC6=CC=C(OC(C)=O)C(OC(C)=O)=C6)C)=O)C3	10.1016/j.lfs.2006.01.038	860	+2	-3.212
Gyermek2006-10	C44H58N2O12S	C[N@@+](CC2=CC(OC(C)=O)=C(OC(C)=O)C=C2)[C@H]3CCC[C@@H]1C[C@@H](OC(CSCC(O[C@H]4C[C@H]5CCC[C@@H](C4)[N@@+](CC6=CC=C(OC(C)=O)C(OC(C)=O)=C6)C)=O)C3	10.1016/j.lfs.2006.01.038	838	+2	-4.32
Gyermek2006-11	C46H60N2O12	C[N@@+](CC2=CC(OC(C)=O)=C(OC(C)=O)C=C2)[C@H]3CCC[C@@H]1C[C@@H](OC([C@@H]4[C@@H](CC4)C(O[C@H]5C[C@H]6CCC[C@@H](C5)[N@@+](CC7=CC=C(OC(C)=O)C(OC(C)=O)=C7)C)=O)C3	10.1016/j.lfs.2006.01.038	832	+2	-3.806
Gyermek2006-12	C47H62N2O12	C[N@@+](CC2=CC(OC(C)=O)=C(OC(C)=O)C=C2)[C@H]3CCC[C@@H]1C[C@@H](OC([C@@H]4[C@@H](CCC4)C(O[C@H]5C[C@H]6CCC[C@@H](C5)[N@@+](CC7=CC=C(OC(C)=O)C(OC(C)=O)=C7)C)=O)C3	10.1016/j.lfs.2006.01.038	846	+2	-3.247

		C)=O)=C7)C)=O)=O)C3					
Gyermek2006-13	C48H64N2O12	C[N@@+](CC2=CC(OC(C)=O)=C(OC(C)=O)C=C2)[C@H]3CCC[C@@H]1C[C@@H](OC([C@@H]4[C@@H](CCCC4)C(O[C@H]5C[C@H]6CCC[C@@H](C5)[N@@+](CC7=CC=C(OC(C)=O)C(O)C(C)=O)=C7)C)=O)=O)C3	10.1016/j.lfs.2006.01.0	860	+2	-2.688	38
Gyermek2006-14	C49H62N2O12	C[N@@+](CC2=CC(OC(C)=O)=C(OC(C)=O)C=C2)[C@H]3CCC[C@@H]1C[C@@H](OC(C4=C(C5CC[C@H]4C5)C(O[C@H]6C[C@H]7CCC[C@@H](C6)[N@@+](CC8=CC=C(OC(C)=O)C(OC(C)=O)=C8)C)=O)=O)C3	10.1016/j.lfs.2006.01.0	870	+2	-2.053	38
Gyermek2006-15	C48H66N2O12	C[N@@+](CC2=CC(OC(CC)=O)=C(OC(CC)=O)C=C2)[C@H]3CCC[C@@H]1C[C@@H](OC(CCC(O[C@H]4C[C@H]5CCC[C@@H](C4)[N@@+](CC6=CC=C(OC(CC)=O)C(OC(CC)=O)=C6)C)=O)=O)C3	10.1016/j.lfs.2006.01.0	862	+2	-1.974	38
Gyermek2006-16	C49H68N2O12	C[N@@+](CC2=CC(OC(CC)=O)=C(OC(CC)=O)C=C2)[C@H]3CCC[C@@H]1C[C@@H](OC(CCCC(O[C@H]4C[C@H]5CCC[C@@H](C4)[N@@+](CC6=CC=C(OC(CC)=O)C(OC(CC)=O)=C6)C)=O)=O)C3	10.1016/j.lfs.2006.01.0	876	+2	-1.619	38
Gyermek2006-17	C52H74N2O12	C[N@@+](CC2=CC(OC(CC)=O)=C(OC(CC)=O)C=C2)[C@H]3CCC[C@@H]1C[C@@H](OC(CCCCCC(O[C@H]4C[C@H]5CCC[C@@H](C4)[N@@+](CC6=CC=C(OC(CC)=O)C(OC(CC)=O)=C6)C)=O)=O)C3	10.1016/j.lfs.2006.01.0	918	+2	-0.612	38
Gyermek2006-18	C48H64N2O12	C[N@@+](CC2=CC(OC(CC)=O)=C(OC(CC)=O)C=C2)[C@H]3CCC[C@@H]1C[C@@H](OC(/C=C/C(O[C@H]4C[C@H]5CCC[C@@H](C4)[N@@+](CC6=CC=C(OC(CC)=O)C(OC(CC)=O)=C6)C)=O)=O)C3	10.1016/j.lfs.2006.01.0	860	+2	-1.614	38
Gyermek2006-19	C48H63ClN2O12	C[N@@+](CC2=CC(OC(CC)=O)=C(OC(CC)=O)C=C2)[C@H]3CCC[C@@H]1C[C@@H](OC(/C(Cl)=C/C(O[C@H]4C[C@H]5CCC[C@@H](C4)[N@@+](CC6=CC=C(OC(CC)=O)C(OC(CC)=O)=C6)C)=O)=O)C3	10.1016/j.lfs.2006.01.0	894	+2	-0.961	38
Gyermek2006-20	C51H70N2O12	C[N@@+](CC2=CC(OC(CC)=O)=C(OC(CC)=O)C=C2)[C@H]3CCC[C@@H]1C[C@@H](OC([C@@H](CCC4)C4C(O[C@H]5C[C@H]6CCC[C@@H](C5)[N@@+](CC7=CC=C(OC(CC)=O)C(OC(CC)=O)=C7)C)=O)=O)C3	10.1016/j.lfs.2006.01.0	902	+2	-1.131	38
Gyermek2006-21	C52H72N2O12	C[N@@+](CC2=CC(OC(CC)=O)=C(OC(CC)=O)C=C2)[C@H]3CCC[C@@H]1C[C@@H](OC([C@@H](CCCC4)[C@@H]4C(O[C@H]5C[C@H]6CCC[C@@H](C5)[N@@+](CC7=CC=C(OC(CC)=O)C(OC(CC)=O)=C7)C)=O)=O)C3	10.1016/j.lfs.2006.01.0	916	+2	-0.572	38
Gyermek2006-22	C41H56N2O10	C[N@@+](CC2=CC(OC)=C(OC(C)=O)C=C2)[C@H]3CCC[C@@H]1C[C@@H](OC(CC(O[C@H]4C[C@H]5CCC[C@@H](C4)[N@@+](CC6=CC=C(OC(C)=O)C(OC)=C6)C)=O)=O)C3	10.1016/j.lfs.2006.01.0	736	+2	-3.305	38
Gyermek2006-23	C43H60N2O10	C[N@@+](CC2=CC(OC)=C(OC(C)=O)C=C2)[C@H]3CCC[C@@H]1C[C@@H](OC(CCCC(O[C@H]4C[C@H]5CCC[C@@H](C4)[N@@+](CC6=CC=C(OC(C)=O)C(OC)=C6)C)=O)=O)C3	10.1016/j.lfs.2006.01.0	764	+2	-2.595	38

		@+][5(CC6=CC=C(OC(C)=O)C(OC)=C6C)=O)C3				
Gyermek2006-24	C45H64N2O10	C[N@+][1](CC2=CC(OC)=C(OC(C)=O)C=C2)[C@H]3CCC[C@@H]1C[C@@H](OC(CCCCC(O[C@H]4C[C@H]5CCC[C@@H](C4)[N@+][5(CC6=CC=C(OC(C)=O)C(OC)=C6C)=O)C3	10.1016/j.lfs.2006.01.0	792	+2	-2.117
Gyermek2006-25	C46H66N2O10	C[N@+][1](CC2=CC(OC)=C(OC(C)=O)C=C2)[C@H]3CCC[C@@H]1C[C@@H](OC(CCCCC(O[C@H]4C[C@H]5CCC[C@@H](C4)[N@+][5(CC6=CC=C(OC(C)=O)C(OC)=C6C)=O)C3	10.1016/j.lfs.2006.01.0	806	+2	-1.588
Gyermek2006-26	C42H56N2O10	C[N@+][1](CC2=CC(OC)=C(OC(C)=O)C=C2)[C@H]3CCC[C@@H]1C[C@@H](OC(/C=C/C(O[C@H]4C[C@H]5CCC[C@@H](C4)[N@+][5(CC6=CC=C(OC(C)=O)C(OC)=C6C)=O)C3	10.1016/j.lfs.2006.01.0	748	+2	-2.590
Gyermek2006-27	C42H55CIN2O10	C[N@+][1](CC2=CC(OC)=C(OC(C)=O)C=C2)[C@H]3CCC[C@@H]1C[C@@H](OC(/C(Cl)=C/C(O[C@H]4C[C@H]5CCC[C@@H](C4)[N@+][5(CC6=CC=C(OC(C)=O)C(OC)=C6C)=O)C3	10.1016/j.lfs.2006.01.0	782	+2	-1.937
Gyermek2006-28	C42H58N2O10S	C[N@+][1](CC2=CC(OC)=C(OC(C)=O)C=C2)[C@H]3CCC[C@@H]1C[C@@H](OC(CSCC(O[C@H]4C[C@H]5CCC[C@@H](C4)[N@+][5(CC6=CC=C(OC(C)=O)C(OC)=C6C)=O)C3	10.1016/j.lfs.2006.01.0	782	+2	-3.180
Gyermek2006-29	C46H64N2O10	C[N@+][1](CC2=CC(OC)=C(OC(C)=O)C=C2)[C@H]3CCC[C@@H]1C[C@@H](OC(C(CCCC4)[C@@H]4C(O[C@H]5C[C@H]6CC[C@@H](C5)[N@+][6(CC7=CC=C(OC(C)=O)C(OC)=C7C)=O)=O)C3	10.1016/j.lfs.2006.01.0	804	+2	-1.548
Gyermek2006-30	C47H62N2O10	C[N@+][1](CC2=CC(OC)=C(OC(C)=O)C=C2)[C@H]3CCC[C@@H]1C[C@@H](OC(C([C@H]4CC[C@H]5C4)=C5C(O[C@H]6C[C@H]7CCC[C@@H](C6)[N@+][7(CC8=CC=C(OC(C)=O)C(OC)=C8C)=O)C3	10.1016/j.lfs.2006.01.0	814	+2	-0.913
Gyermek2006-31	C41H54Cl2N2O8	C[N@+][1](CC2=CC(Cl)=C(OC(C)=O)C=C2)[C@H]3CCC[C@@H]1C[C@@H](OC(CCCC(O[C@H]4C[C@H]5CCC[C@@H](C4)[N@+][5(CC6=CC=C(OC(C)=O)C(Cl)=C6C)=O)C3	10.1016/j.lfs.2006.01.0	772	+2	-0.827
Gyermek2006-32	C42H56Cl2N2O8	C[N@+][1](CC2=CC(Cl)=C(OC(C)=O)C=C2)[C@H]3CCC[C@@H]1C[C@@H](OC(CCCC(O[C@H]4C[C@H]5CCC[C@@H](C4)[N@+][5(CC6=CC=C(OC(C)=O)C(Cl)=C6C)=O)C3	10.1016/j.lfs.2006.01.0	786	+2	-0.878
Gyermek2006-33	C41H54N4O12	C[N@+][1](CC2=CC([N+](O-))=O)C(OC(C)=O)C=C2)[C@H]3CCC[C@@H]1C[C@@H](OC(CCCC(O[C@H]4C[C@H]5CCC[C@@H](C4)[N@+][5(CC6=CC=C(OC(C)=O)C([N+](O-))=O)C6C)=O)C3	10.1016/j.lfs.2006.01.0	794	+2	-2.547
Gyermek2006-34	C45H62N2O8	C[N@+][1](CC2=C(OC)C=CC(OC)=C2)[C@H]3CCC[C@@H]1C[C@@H](OC(C([C@H]4CC[C@H]5C4)=C5C(O[C@H]6C[C@H]7CC[C@@H](C6)[N@+][7(CC8=CC(OC)=CC=C8OC)C)=O)C3	10.1016/j.lfs.2006.01.0	758	+2	0.927
Gyermek2006-35	C43H56N4O10	C[N@+][1](CC2=C(OC)C=CC([N+](O-))=O)C2)[C@H]3CCC[C@@H]1C[C@@H](OC(C([C@H]4CC[C@H]5C4)=C5C(O[C@H]6C[C@H]7CCC[C@@H](C6)[N@+][7(CC8=CC([N+](O-))=O)C=C8OC)C)=O)C3	10.1016/j.lfs.2006.01.0	788	+2	0.835
Gyermek2006-36	C45H64N2O12	C[N@+][1](CC2=CC(OC)=C(OC(C)=O)C(OC)=C2)[C@H]3CCC[C@@H]1C[C@@H](OC(C(CCCC(O[C@H]4C[C@H]5CCC[C@@H](C4)[N@+][5(CC6=CC=C(OC(C)=O)C(OC)=C6C)=O)C3	10.1016/j.lfs.2006.01.0	824	+2	-3.311

		@@H]1C[C@@H](OC(CCCC(O[C@H]4C[C@H]5CCC[C@@H](C 4)[N@@+]5(CC6=CC(OC)=C(OC(C)=O)C(OC)=C6C)=O)=O)C3	38				
Gyermek2006-37	C47H68N2O12	C[N@@+]1(CC2=CC(OC)=C(OC(C)=O)C(OC)=C2)[C@H]3CCC[C @@H]1C[C@@H](OC(CCCCC(O[C@H]4C[C@H]5CCC[C@@H (C4)[N@@+]5(CC6=CC(OC)=C(OC(C)=O)C(OC)=C6C)=O)=O)C 3	10.1016/j.lfs.2006.01.0	852	+2	-2.833	
Gyermek2006-38	C48H70N2O12	C[N@@+]1(CC2=CC(OC)=C(OC(C)=O)C(OC)=C2)[C@H]3CCC[C @@H]1C[C@@H](OC(CCCCC(O[C@H]4C[C@H]5CCC[C@@ H](C4)[N@@+]5(CC6=CC(OC)=C(OC(C)=O)C(OC)=C6C)=O)=O) C3	10.1016/j.lfs.2006.01.0	866	+2	-2.304	
Gyermek2006-39	C44H62N2O12S	C[N@@+]1(CC2=CC(OC)=C(OC(C)=O)C(OC)=C2)[C@H]3CCC[C @@H]1C[C@@H](OC(CSCC(O[C@H]4C[C@H]5CCC[C@@H](C 4)[N@@+]5(CC6=CC(OC)=C(OC(C)=O)C(OC)=C6C)=O)=O)C3	10.1016/j.lfs.2006.01.0	842	+2	-3.896	
Gyermek2006-40	C44H60N2O12	C[N@@+]1(CC2=CC(OC)=C(OC(C)=O)C(OC)=C2)[C@H]3CCC[C @@H]1C[C@@H](OC(/C=C/C(O[C@H]4C[C@H]5CCC[C@@H](C4)[N@@+]5(CC6=CC(OC)=C(OC(C)=O)C(OC)=C6C)=O)=O)C3	10.1016/j.lfs.2006.01.0	808	+2	-3.306	
Gyermek2006-41	C48H68N2O12	C[N@@+]1(CC2=CC(OC)=C(OC(C)=O)C(OC)=C2)[C@H]3CCC[C @@H]1C[C@@H](OC(C(CCCC4)[C@@H]4C(O[C@H]5C[C@H]6 CCC[C@@H](C5)[N@@+]6(CC7=CC(OC)=C(OC(C)=O)C(OC)=C 7C)=O)=O)C3	10.1016/j.lfs.2006.01.0	864	+2	-2.264	
Gyermek2006-42	C49H66N2O12	C[N@@+]1(CC2=CC(OC)=C(OC(C)=O)C(OC)=C2)[C@H]3CCC[C @@H]1C[C@@H](OC(C(C4CCC5C4)=C5C(O[C@H]6C[C@H]7C CC[C@@H](C6)[N@@+]7(CC8=CC(OC)=C(OC(C)=O)C(OC)=C8) C)=O)=O)C3	10.1016/j.lfs.2006.01.0	874	+2	-1.629	
Gyermek2006-43	C47H68N2O12	C[N@@+]1(CC2=CC(OC)=C(OC(CC)=O)C(OC)=C2)[C@H]3CCC[C@@H]1C[C@@H](OC(CCCC(O[C@H]4C[C@H]5CCC[C@@H](C4)[N@@+]5(CC6=CC(OC)=C(OC(CC)=O)C(OC)=C6C)=O)=O)C 3	10.1016/j.lfs.2006.01.0	852	+2	-2.253	
Gyermek2006-44	C49H64N2O16	C[N@@+]1(CC2=CC(OC(C)=O)=C(OC(C)=O)C(OC(C)=O)=C2)[C @H]3CCC[C@@H]1C[C@@H](OC(CCCC(O[C@H]4C[C@H]5CC C[C@@H](C4)[N@@+]5(CC6=CC(OC(C)=O)=C(OC(C)=O)C(OC(C)=O)=C6C)=O)=O)C3	10.1016/j.lfs.2006.01.0	936	+2	-5.591	
Gyermek2006-45	C49H62N2O16	C[N@@+]1(CC2=CC(OC(C)=O)=C(OC(C)=O)C(OC(C)=O)=C2)[C @H]3CCC[C@@H]1C[C@@H](OC(/C=C/C(C(O[C@H]4C[C@H]5 CCC[C@@H](C4)[N@@+]5(CC6=CC(OC(C)=O)=C(OC(C)=O)C(OC(C)=O)=C6C)=O)=O)C3	10.1016/j.lfs.2006.01.0	934	+2	-5.619	
Booij2000-9c	C14H30N4O2	C[N+](C)(C)CC(NCC(NCC[N+])1(CCCC1C)=O)=O	10.1021/jm0010062	286	+2	-7.494	
Booij2000-11c	C35H45N7O7	O=C(NCC(NCC(NCC[N+](CC1=CC=CC=C1)(CC2=CC=C([N+](O -))=O)C=C2)C)=O)C[N+](CC4=CC=C([N+](O-))=O)C=C4)C CCCC3	10.1021/jm0010062	675	+2	-1.234	
Booij2000-15a	C27H40N4O2	C[N+](CC1=CC=CC=C1)(CC2=CC=CC=C2)CC(NCC(NCC[N+])3(C)CCCC3)=O)=O	10.1021/jm0010062	452	+2	-2.749	

Booij2000-15c	C36H46N6O7	<chem>O=C(NC(CC1=CC=CC=C1)C(NCC[N+](CC3=CC=C([N+])([O-])=O)C=C3)CCOCC2)=O)C[N+](CC5=CC=C([N+])([O-])=O)C=C5)CCCC4</chem>	10.1021/jm0010062	674	+2	1.416
Booij2000-20a	C26H45N5O3	<chem>C[N+](CC(N(C)CC(N(CC(N(CC[N+](C)(CC2=CC=CC=C2)C)C)=O)C)=O)O)CCCCC1</chem>	10.1021/jm0010062	475	+2	-3.486
Booij2000-20c	C38H51N7O7	<chem>O=C(N(C)CC(N(CC(N(C)CC[N+](CC1=CC=C([N+])([O-])=O)C=C1)(C)CC2=CC=CC=C2)=O)C)=O)C[N+](CC4=CC=C([N+])([O-])=O)C=C4)CCCCC3</chem>	10.1021/jm0010062	717	+2	0.334
Booij2000-20e	C38H49N7O7	<chem>O=C(N(C)CC(N(CC(N1CC[N+](CC2=CC=CC=C2)(CC3=CC=C([N+])([O-])=O)C=C3)CC1)=O)C)=O)C[N+](CC5=CC=C([N+])([O-])=O)C=C5)CCCCC4</chem>	10.1021/jm0010062	715	+2	1.397
Gyermek1999-1	C43H54Br2N2O6	<chem>C[N@+](C@H)(CC1)([H])C[C@H]2OC(CCC(O[C@@H](C[C@@]3([H])CC4C[C@@]4([H])[N@+]3(C)C=C/CC5=CC(C=CC(OC)=C6)=C6C(OC)=C5)=O)([C@@]1([H])C2)CCC(C=C7)=CC(Br)=C7Br</chem>	WO9921854	852	+2	0.525
Gyermek1999-2	C42H58N2O12	<chem>C[N@+](C@H)(CC1)CC2OC(CCC(OC(C[C@@H]3CC4)C[C@@H]4[N@+]3(C)CC(C=C5OC)=CC(OC)=C5OC(C)=O)=O)([C@@H]1C2)CC(C=C6OC)=CC(OC)=C6OC(C)=O</chem>	WO9921854	782	+2	-4.784
Gyermek1999-3	C50H70N2O12	<chem>C[N@+](C@H)(CC1)CC2OC(CCC(OC(C[C@H]3CC4)C[C@H]4[N@+]3(C)CC(C=CC(OC(CCC)=O)=C5)=C5OC(CCC)=O)=O)([C@@H]1C2)CC(C=CC(OC(CCC)=O)=C6)=C6OC(CCC)=O</chem>	WO9921854	890	+2	-0.276
Gyermek1999-4	C46H62N2O12	<chem>C[N@+](C@H)(CC1)CC2OC(CCC(OC(C[C@H]3CC4)C[C@H]4[N@+]3(C)CC(C=C5)=CC(OC(CC)=O)=C5OC(CC)=O)=O)([C@@H]1C2)CC(C=C6)=CC(OC(CC)=O)=C6OC(CC)=O</chem>	WO9921854	834	+2	-3.092
Gyermek1999-5	C36H48N4O10	<chem>C[N@+](C@H)(CC1)CC2OC(CCC(OC(C[C@H]3CC4)C[C@H]4[N@+]3(C)CC(C=C5[N](=O)=O)=C(C=C5)OC)=O)([C@@H]1C2)CC(C=C6[N](=O)=O)=C(C=C6)OC</chem>	WO9921854	696	+2	-2.32
Gyermek1999-6	C42H58N2O12	<chem>C[N@+](C@H)(CC1)CC2OC(CCC(OC(C[C@@H]3CC4)C[C@@H]4[N@+]3(C)CC(C=C5OC)=CC(OC)=C5OC(C)=O)=O)([C@@H]1C2)CC(C=C6OC)=CC(OC)=C6OC(C)=O</chem>	WO9921854	782	+2	-4.784
Gyermek1999-7	C38H48Cl2N2O8	<chem>C[N@+](C@H)(CC1)CC2OC(CCC(OC(C[C@H]3CC4)C[C@H]4[N@+]3(C)CC(C=C5)=CC(Cl)=C5OC(C)=O)=O)([C@@H]1C2)CC(C=C6)=CC(Cl)=C6OC(C)=O</chem>	WO9921854	730	+2	-2.30
Gyermek1999-8	C44H58N2O12	<chem>C[N+](C(CC1)CC2OC(CCC(OC(CC3CC4)CC4[N+](C)CCC(C=C5)=CC(OC(C)=O)=C5OC(C)=O)=O)(C1C2)CCC(C=C6)=CC(OC(C)=O)=C6OC(C)=O</chem>	WO9921854	806	+2	-6.25
Gyermek1999-9	C42H54N2O12	<chem>C[N@+](C@H)(CC1)CC2OC(CCC(OC(C[C@H]3CC4)C[C@H]4[N@+]3(C)CC(C=C5OC(C)=O)=C(C=C5)OC(C)=O)=O)([C@H]1C2)CC(C=C6OC(C)=O)=C(C=C6)OC(C)=O</chem>	WO9921854	778	+2	-4.508
Gyermek1999-10	C40H54N2O10	<chem>C[N@+](C@H)(CC1)CC2OC(CCC(OC(C[C@@H]3CC4)C[C@@H]4[N@+]3(C)CC(C=C5)=CC(OC)=C5OC(C)=O)=O)([C@@H]1C2)CC(C=C6)=CC(OC)=C6OC(C)=O</chem>	WO9921854	722	+2	-4.068

Gyermek1999-11	C40H58N2O10	<chem>C[N@+](C[C@H](CC1)CC2OC(CCC(OC(C[C@H]3CC4)C[C@H]4[N@+]3(C)CC(C=C5OC)=CC(OC)=C5OC)=O)([C@H]1C2)CC(C=C6OC)=CC(OC)=C6OC</chem>	WO9921854	726	+2	-3.644
Gyermek1999-12	C42H62N2O8	<chem>C[N@+](C[C@H](CC1)CC2OC(CCC(OC(C[C@H]3CC4)C[C@H]4[N@+]3(C)CC(C=C5)=CC(OC)=C5OC)=O)([C@H]1C2)CC(C=C6)=CC(OC)=C6OC</chem>	WO9921854	722	+2	-0.812
Gyermek1999-13	C40H50N2O8	<chem>O=C(C1=CC(C(OC(C2)C(CC3)CC[N+]23CC(C=C4OC)=C(C=C4)OC)=O)=CC=C1)OC5C[N+]6(CCC5CC6)CC(C=C7OC)=C(C=C7)OC</chem>	WO9921854	686	+2	1.569
Gyermek1999-14	C57H86N2O12	<chem>O=C(OC(CC1C)CC([N+](C)1CCC(C=C2)=CC(OC(CC)=O)=C2OC(CC)=O)C)CCCC3(CCCC3)CCCC(OC(CC4C)CC([N+](C)4CCC(C=C5)=CC(OC(CC)=O)=C5OC(CC)=O)C)=O</chem>	WO9921854	990	+2	0.757
Gyermek1999-15	C50H70N2O12	<chem>C[N@@+](C[C@H](CC1)CC2OC(CCC(OC(C[C@H]3CC4)C[C@H]4[N@+]3(C)CCCC(C=C5)=CC(OC(CC)=O)=C5OC(CC)=O)=O)([C@@H]1C2)CCCC(C=C6)=CC(OC(CC)=O)=C6OC(CC)=O</chem>	WO9921854	890	+2	-3.376
Gyermek1999-16	C50H58N2O12	<chem>C[N@@+](C[C@H](CC1)CC2OC(CCC(OC(C[C@H]3CC4)C[C@H]4[N@+]3(C)CC5=CC(C=CC=C6OC(C)=O)=C6C=C5OC(C)=O)=O)([C@@H]1C2)CC7=CC(C=CC=C8OC(C)=O)=C8C=C7OC(C)=O</chem>	WO9921854	878	+2	-2.254
Gyermek1999-17	C46H58N2O16	<chem>C[N@+](C[C@H](CC1)CC2OC(CCC(OC(C[C@H]3CC4)C[C@H]4[N@+]3(C)CC(C=C5OC(C)=O)=CC(OC(C)=O)=C5OC(C)=O)=O)([C@H]1C2)CC(C=C6OC(C)=O)=CC(OC(C)=O)=C6OC(C)=O</chem>	WO9921854	894	+2	-7.064
Gyermek1999-18	C44H60N2O12	<chem>C[N@@+](C[C@@](CC1)([H])C[C@@H]2OC(/C=C/C(O[C@@H](C[C@@]3([H])CC4)C[C@@]4([H])[N@+]3(C)CC(C=C5OC)=CC(OC)=C5OC(CC)=O)=O)([C@]1([H])C2)CC(C=C6OC)=CC(OC)=C6OC(CC)=O</chem>	WO9921854	808	+2	-3.366
Gyermek1999-19	C48H64N2O12	<chem>C[N@@+](C[C@@](CC1)([H])C[C@@H]2OC(C(CC3)C3C(O[C@@H](C[C@@]4([H])CC5)C[C@@]5([H])[N@+]4(C)CC(C=C6)=CC(OC(CC)=O)=C6OC(CC)=O)=O)([C@]1([H])C2)CC(C=C7)=CC(OC(CC)=O)=C7OC(CC)=O</chem>	WO9921854	860	+2	-2.808
Gyermek1999-20	C48H66N2O12	<chem>C[N@@+](C[C@@](CC1)([H])C[C@@H]2OC(CCCCC(O[C@@H](C[C@@]3([H])CC4)C[C@@]4([H])[N@+]3(C)CC(C=C5)=CC(OC(CC)=O)=C5OC(CC)=O)=O)([C@]1([H])C2)CC(C=C6)=CC(OC(CC)=O)=C6OC(CC)=O</chem>	WO9921854	862	+2	-2.788
Gyermek1999-21	C47H64N2O12	<chem>C[N@@+](C[C@@](CC1)([H])C[C@@H]2OC(CCCC(O[C@@H](C[C@@]3([H])CC4)C[C@@]4([H])[N@+]3(C)CC(C=C5)=CC(OC(C)=O)=C5OC(CC)=O)=O)([C@]1([H])C2)CC(C=C6)=CC(OC(C)=O)=C6OC(CC)=O</chem>	WO9921854	848	+2	-2.737
Gyermek1999-22	C47H58N2O12	<chem>C[N@@+](C[C@@](CC1)([H])C[C@H]2OC([C@@H]([C@@]3([H])C[C@]4([H])C=C3)[C@H]4C(O[C@H](C[C@@]5([H])CC6)C[C@@]6([H])[N@+]5(C)CC(C=C7)=CC(OC(C)=O)=C7OC(C)=O)=O)([C@]1([H])C2)CC(C=C8)=CC(OC(C)=O)=C8OC(C)=O</chem>	WO9921854	842	+2	-4.015
Gyermek1999-23	C43H56N2O12	<chem>C[N@@+](C[C@@](CC1)([H])C[C@@H]2OC(CCCC(O[C@@H](C[C@@]3([H])C[C@H]4C(O[C@H](C[C@@]5([H])CC6)C[C@@]6([H])[N@+]5(C)CC(C=C7)=CC(OC(C)=O)=C7OC(C)=O)=O)([C@]1([H])C2)CC(C=C8)=CC(OC(C)=O)=C8OC(C)=O</chem>	WO9921854	792	+2	-4.853

		<chem>C@@]3([H])CC4C[C@@]4([H])[N@+]3(C)CC(C=C5)=CC(OC(C)=O)=C5OC(C=O)=O)O)([C@]1([H])C2CC(C=C6)=CC(OC(C)=O)=C6OC(C)=O</chem>				
Gyermek1999-24	C46H60N2O12	<chem>C[N@@+](C[C@@](CC1)([H])C[C@@H]2OC(C(CCC3)CC3C(O[C@@H](C[C@@]4([H])CC5C[C@@@]5([H])[N@+]4(C)CC(C=C6)=CC(OC(C)=O)=C6OC(C=O)=O)O)([C@]1([H])C2CC(C=C7)=CC(OC(C)=O)=C7OC(C)=O</chem>	WO9921854	832	+2	-3.980
Gyermek1999-25	C44H58N2O12	<chem>C[N@@+](C[C@@](CC1)([H])C[C@@H]2OC(C(CCC3)C3C(O[C@@H](C[C@@]4([H])[N@+](C)(C([H])CC4)CC(C=C5)=CC(OC(C)=O)=C5OC(C=O)C)=O)O)([C@]1([H])C2CC(C=C6)=CC(OC(C)=O)=C6OC(C)=O</chem>	WO9921854	806	+2	-3.17
Gyermek1999-26	C47H58N2O12	<chem>C[N@@+](C[C@@](CC1)([H])C[C@@H]2OC([C@@H]([C@@]3([H])C[C@@]4([H])C=C3)[C@H]4C(O[C@@H](C[C@@]5([H])CC6C[C@@]6([H])[N@+]5(C)CC(C=C7)=CC(OC(C)=O)=C7OC(C)=O)O)O)([C@]1([H])C2CC(C=C8)=CC(OC(C)=O)=C8OC(C)=O</chem>	WO9921854	842	+2	-4.015
Gyermek1999-27	C44H60N2O10	<chem>C[N@@+](C[C@@](CC1)([H])C[C@@H]2OC(C(CCC3)CC3C(O[C@@H](C[C@@]4([H])CC5C[C@@@]5([H])[N@+]4(C)CC(C=C6)=CC(OC)=C6OC(C=O)=O)O)([C@]1([H])C2CC(C=C7)=CC(OC)=C7OC(C)=O</chem>	WO9921854	776	+2	-2.84
Gyermek1999-28	C42H56N2O10	<chem>C[N@@+](C[C@@](CC1)([H])C[C@@H]2OC(C(CCC3)C3C(O[C@@H](C[C@@]4([H])CC5C[C@@@]5([H])[N@+]4(C)CC(C=C6)=CC(OC)=C6OC(C=O)=O)O)([C@]1([H])C2CC(C=C7)=CC(OC)=C7OC(C)=O</chem>	WO9921854	748	+2	-3.784
Gyermek1999-29	C45H58N2O10	<chem>O=C([C@@H]([C@@]1([H])C[C@]2([H])C=C1)[C@H]2C(O[C@@H](C[C@@]3([H])CC4C[C@@@]4([H])[N@+]3(C)CC(C=C5)=CC(OC)=C5OC(C=O)=O)O[C@H](C[C@]6([H])CC7C[C@]7([H])[N@+]6(C)CC(C=C8)=CC(OC)=C8OC(C)=O</chem>	WO9921854	786	+2	-2.875
Gyermek1999-30	C48H68N2O12	<chem>C[N@@+](C[C@@](CC1)([H])C[C@@H]2OC(C(CCC3)CC3C(O[C@@H](C[C@@]4([H])CC5C[C@@@]5([H])[N@+]4(C)CC(C=C6OC)=CC(OC)=C6OC(CC)=O)O)O)([C@]1([H])C2CC(C=C7OC)=CC(OC)=C7OC(CC)=O</chem>	WO9921854	864	+2	-2.498
Gyermek1999-31	C44H60N2O12	<chem>C[N@@+](C[C@@](CC1)([H])C[C@@H]2OC(C(CCC3)C3C(O[C@@H](C[C@@]4([H])CC5C[C@@@]5([H])[N@+]4(C)CC(C=C6OC)=C(C(OC)=C6OC(C=O)=O)O)([C@]1([H])C2CC(C=C7OC)=CC(OC)=C7OC(C)=O</chem>	WO9921854	808	+2	-4.50
Gyermek1999-32	C47H62N2O12	<chem>O=C([C@@H]([C@@]1([H])C[C@]2([H])C=C1)[C@H]2C(O[C@@H](C[C@@]3([H])CC4C[C@@@]4([H])[N@+]3(C)CC(C=C5OC)=CC(OC)=C5OC(C=O)=O)O[C@H](C[C@]6([H])CC7C[C@]7([H])[N@+]6(C)CC(C=C8OC)=CC(OC)=C8OC(C)=O</chem>	WO9921854	846	+2	-3.591
Gyermek1999-33	C47H68N2O12	<chem>C[N@@+](C[C@@](CC1)([H])C[C@@H]2OC(CCCCCC(O[C@@H](C[C@@]3([H])CC4C[C@@@]4([H])[N@+]3(C)CC(C=C5OC)=CC(OC)=C5OC(C=O)=O)O)([C@]1([H])C2CC(C=C6OC)=CC(O</chem>	WO9921854	852	+2	-2.893

		C)=C6OC(C)=O				
Gyermek1999-34	C45H68N2O10	C[N@@+](C@H)(CC1)[H]C[C@@H]2OC(CCCCCC(O[C@@H](C[C@@]3([H])CC4)C[C@@]4([H])[N@+](3(C)CC(C=C5OC)=CC(OC)=C5OC)=O)([C@]1([H])C2)CC(C=C6OC)=CC(OC)=C6OC	WO9921854	796	+2	-1.753
Gyermek1999-35	C43H58N2O8	C[N@@+](C@H)(CC1)[H]C[C@@H]2OC([C@@H]([C@@]3([H])C[C@@]4([H])C=C3)[C@H]4C(O[C@@H](C[C@@]5([H])CC6C[C@@]6([H])[N@+](5(C)CC(C=C7OC)=C(C=C7)OC)=O)([C@]1([H])C2)CC(C=C8OC)=C(C=C8)OC	WO9921854	730	+2	-1.035
Gyermek1999-36	C50H68N2O12	C[N@@+](C@H)(CCC1)CC2OC(C(C3)C3C(OC(C[C@@H]4CCCC5)C[C@@H]5[N@+](4(C)CC(C=C6)=CC(OC(CC)=O)=C6OC(CC)=O)=O)([C@@H]1C2)CC(C=C7)=CC(OC(CC)=O)=C7OC(CC)=O	WO9921854	888	+2	-1.69
Gyermek1999-37	C51H72N2O12	C[N@@+](C@H)(CCC1)CC2OC(CCCCC(OC(C[C@@H]3CCC4)C[C@@H]4[N@+](3(C)CC(C=C5)=CC(OC(CC)=O)=C5OC(CC)=O)=O)([C@@H]1C2)CC(C=C6)=CC(OC(CC)=O)=C6OC(CC)=O	WO9921854	904	+2	-1.141
Gyermek1999-38	C50H70N2O12	C[N@+](C@H)(CCC1)CC2OC(CCCCC(OC(C[C@@H]3CCC4)C[C@@H]4[N@@+](3(C)CC(C=C5)=CC(OC(CC)=O)=C5OC(CC)=O)=O)([C@H]1C2)CC(C=C6)=CC(OC(CC)=O)=C6OC(CC)=O	WO9921854	890	+2	-1.67
Gyermek1999-39	C49H68N2O12	C[N@@+](C@H)(CCC1)CC2OC(CCCC(OC(C[C@@H]3CCC4)C[C@@H]4[N@+](3(C)CC(C=C5)=CC(OC(CC)=O)=C5OC(CC)=O)=O)([C@@H]1C2)CC(C=C6)=CC(OC(CC)=O)=C6OC(CC)=O	WO9921854	876	+2	-1.619
Gyermek1999-40	C46H60N2O12	C[N@+](C@H)(CCC1)CC2OC(C(C3)C3C(OC(C[C@@H]4CC(C5)C[C@@H]5[N@@+](4(C)CC(C=C6)=CC(OC(C)=O)=C6OC(C)=O)=O)([C@H]1C2)CC(C=C7)=CC(OC(C)=O)=C7OC(C)=O	WO9921854	832	+2	-3.806
Gyermek1999-41	C48H66N2O12	C[N@+](C@H)(CCC1)CC2OC(CCCCC(OC(C[C@@H]3CCC4)C[C@@H]4[N@@+](3(C)CC(C=C5)=CC(OC(C)=O)=C5OC(C)=O)=O)([C@H]1C2)CC(C=C6)=CC(OC(C)=O)=C6OC(C)=O	WO9921854	862	+2	-2.728
Gyermek1999-42	C47H64N2O12	C[N@@+](C@H)(CCC1)CC2OC(CCCCC(OC(C[C@@H]3CCC4)C[C@@H]4[N@+](3(C)CC(C=C5)=CC(OC(C)=O)=C5OC(C)=O)=O)([C@@H]1C2)CC(C=C6)=CC(OC(C)=O)=C6OC(C)=O	WO9921854	848	+2	-3.257
Gyermek1999-43	C46H62N2O12	C[N@+](C@H)(CCC1)CC2OC(CCCCC(OC(C[C@@H]3CCC4)C[C@@H]4[N@@+](3(C)CC(C=C5)=CC(OC(C)=O)=C5OC(C)=O)=O)([C@H]1C2)CC(C=C6)=CC(OC(C)=O)=C6OC(C)=O	WO9921854	834	+2	-3.786
Gyermek1999-44	C45H60N2O12	C[N@@+](C@H)(CCC1)CC2OC(CCCC(OC(C[C@@H]3CCC4)C[C@@H]4[N@+](3(C)CC(C=C5)=CC(OC(C)=O)=C5OC(C)=O)=O)([C@@H]1C2)CC(C=C6)=CC(OC(C)=O)=C6OC(C)=O	WO9921854	820	+2	-3.735
Gyermek1999-45	C43H54N2O10	O=C([C@@H]([C@]1([H])C[C@@]2([H])C=C1)[C@H]2C(OC(C3)C(CC4)CC[N+](34CC(C=C5)=CC(OC)=C5OC(C)=O)=O)OC(C6)C(CC7)CC[N+](67CC(C=C8)=CC(OC)=C8OC(C)=O	WO9921854	758	+2	-0.325
Gyermek1999-46	C38H54N2O8	C[N@@+](C@H)(CC1)CC2OC(CCC(OC(C[C@@H]3CC4)C[C@@H]4[N@+](3(C)CC(C=C5OC)=C(C=C5)OC)=O)([C@@H]1C2)CC(C=C6OC)=C(C=C6)OC	WO9921854	666	+2	-2.228

Gyermek1999-47	C40H58N2O10	<chem>C[N+]([C@@H](CC1)CC2OC(CCC(OC(C[C@H]3CC4)C[C@H]4[N@+]3(C)CC(C=C5OC)=CC(OC=C5OC)=O)O)([C@H]1C2)CC(C=C6OC)=CC(OC)=C6OC</chem>	WO9921854	726	+2	-3.644
Gyermek1999-48	C42H54N2O12	<chem>C[N@@+](C@@)(CC1)([H])C[C@@H]2OC(CCC(O[C@H](C[C@]3([H])CC4)C[C@]4([H])[N@@+]3(C)CC(C=C5)=CC(OC(C)=O=C5OC(C)=O)=O)([C@]1([H])C2)CC(C=C6)=CC(OC(C)=O)=C6OC(C)=O</chem>	WO9921854	778	+2	-5.208
Gyermek2002-1	C41H60N2O6	<chem>C[N+]1(C)C2CCC1CC(OC(C(C3=CC=CC=C3)COC(CCCCOC(C(OC4C5CCC(C4)[N+]5(C)C)=O)C6=CC=CC=C6)=O)C2</chem>	10.1016/s0163-7258(02)00296-6	676	+2	-3.911
Gyermek2002-2	C39H56N2O6	<chem>C[N@+]1(C)CCCC[N@@+]2(C)C3CCC2C[C@@H](OC(C(C4=CC=CC=C4)CO)=O)C3)C5CCC1C[C@H](OC(C(C6=CC=CC=C6)CO)=O)C5</chem>	10.1016/s0163-7258(02)00296-6	648	+2	-5.156
Gyermek2002-3	C44H66N2O6	<chem>C[N@+]1(C)CCCCCCCC[N@@+]2(C)C3CCC2C[C@@H](OC(C(C4=CC=CC=C4)CO)=O)C3)C5CCC1C[C@H](OC(C(C6=CC=CC=C6)CO)=O)C5</chem>	10.1016/s0163-7258(02)00296-6	718	+2	-2.512
Gyermek2002-4	C38H46N2O4	<chem>C[N@+]1(C)C2=CC=C(C[N@@+]3(C)C4CCC3C[C@@H](OC(C5=CC=CC=C5)=O)C4)C=C2)C6CCC1C[C@H](OC(C7=CC=CC=C7)=O)C6</chem>	10.1016/s0163-7258(02)00296-6	594	+2	-0.588
Gyermek2002-5	C40H50N2O6	<chem>C[N@+]1(C)C2=CC=C(C[N@@+]3(C)C4CCC3C[C@@H](OC(C(C5=CC=CC=C5)O)=O)C4)C=C2)C6CCC1C[C@H](OC(C(C7=CC=C(C=C7)O)=O)C6</chem>	10.1016/s0163-7258(02)00296-6	654	+2	-2.699
Gyermek2002-6	C42H54N2O6	<chem>C[N@+]1(C)C2=CC=C(C[N@@+]3(C)C4CCC3C[C@@H](OC(C(C5=CC=CC=C5)CO)=O)C4)C=C2)C6CCC1C[C@H](OC(C(C7=CC=CC=C7)CO)=O)C6</chem>	10.1016/s0163-7258(02)00296-6	682	+2	-2.956
Gyermek2002-7	C22H36N2O4	<chem>C[N+]1(C)C2CCC1CC(OC(/C=C\OC3CC4CCC(C3)[N+]4(C)C)=O)O)C2</chem>	10.1016/s0163-7258(02)00296-6	392	+2	-7.12
Gyermek2002-8	C26H38N2O4	<chem>C[N+]1(C)C2CCC1CC(OC(C3=CC=C(C(OC4CC5CCC(C4)[N+]5(C)C)=O)C=C3)=O)C2</chem>	10.1016/s0163-7258(02)00296-6	442	+2	-5.824
Gyermek2002-9	C34H44N2O4	<chem>C[N@@+]1(C)C2=CC=CC=C2)C3CCC1C[C@H](OC(/C=C\O[C@H]4CC5CCC(C4)[N@+]5(C)CC6=CC=CC=C6)=O)O)C3</chem>	10.1016/s0163-7258(02)00296-6	544	+2	-1.884
Gyermek2002-10	C38H44BrN2O4	<chem>C[N@@+]1(C)C2=CC(Br)=CC=C2)C3CCC1C[C@H](OC(C4=CC=C(C(O[C@H]5CC6CCC(C5)[N@+]6(C)CC7=CC=CC(Br)=C7)O)=O)C4)=O)C3</chem>	10.1016/s0163-7258(02)00296-6	750	+2	1.138
Gyermek2002-11	C38H52N2O4	<chem>C[N@@+]1(C)C2CCC1C[C@H](OC([C@@H]3C(C=CC=C4)=C4[C@](CC3)(C5=CC=CC=C5)C(O[C@H]6CC7CCC(C6)[N@+]7(C)C)=O)O)C2</chem>	10.1016/s0163-7258(02)00296-6	600	+2	-3.416
Gyermek2002-12	C22H38N2O4	<chem>C[N+]1(C)C2CCC1CC(OC(CCC(OC3CC4CCC(C3)[N+]4(C)C)=O)=O)C2</chem>	10.1016/s0163-7258(02)00296-6	394	+2	-7.84
Gyermek2002-13	C23H40N2O4	<chem>C[N+]1(C)C2CCC1CC(OC(CCCC(OC3CC4CCC(C3)[N+]4(C)C)=O)=O)C2</chem>	10.1016/s0163-7258(02)00296-6	408	+2	-7.125
Gyermek2002-14	C24H42N2O4	<chem>C[N+]1(C)C2CCC1CC(OC(CCCC(OC3CC4CCC(C3)[N+]4(C)C)=O)=O)C2</chem>	10.1016/s0163-7258(02)00296-6	422	+2	-7.176

Gyermek2002-15	C25H44N2O4	C[N+](C)C2CCC1CC(OC(CCCCCC(OC3CC4CCC(C3)[N+](C)C)=O)=O)C2	10.1016/s0163-7258(02)00296-6	436	+2	-6.647
Gyermek2002-16	C26H46N2O4	C[N+](C)C2CCC1CC(OC(CCCCCC(OC3CC4CCC(C3)[N+](C)C)=O)=O)C2	10.1016/s0163-7258(02)00296-6	450	+2	-6.118
Gyermek2002-17	C27H48N2O4	C[N+](C)C2CCC1CC(OC(CCCCCC(OC3CC4CCC(C3)[N+](C)C)=O)=O)C2	10.1016/s0163-7258(02)00296-6	464	+2	-5.589
Gyermek2002-18	C28H50N2O4	C[N+](C)C2CCC1CC(OC(CCCCCC(OC3CC4CCC(C3)[N+](C)C)=O)=O)C2	10.1016/s0163-7258(02)00296-6	478	+2	-5.06
Gyermek2002-19	C29H52N2O4	C[N+](C)C2CCC1CC(OC(CCCCCC(OC3CC4CCC(C3)[N+](C)C)=O)=O)C2	10.1016/s0163-7258(02)00296-6	492	+2	-4.531
Gyermek2002-20	C30H54N2O4	C[N+](C)C2CCC1CC(OC(CCCCCC(OC3CC4CCC(C3)[N+](C)C)=O)=O)C2	10.1016/s0163-7258(02)00296-6	506	+2	-4.002
Gyermek2002-21	C31H56N2O4	C[N+](C)C2CCC1CC(OC(CCCCCC(OC3CC4CCC(C3)[N+](C)C)=O)=O)C2	10.1016/s0163-7258(02)00296-6	520	+2	-2.473
Gyermek2002-22	C32H58N2O4	C[N+](C)C2CCC1CC(OC(CCCCCC(OC3CC4CCC(C3)[N+](C)C)=O)=O)C2	10.1016/s0163-7258(02)00296-6	534	+2	-2.944
Gyermek2002-23	C35H44Cl4N2O4	C[N@@+](C)C2CCC1CC(OC(CCCCCC(OC3CC4CCC(C3)[N+](C)C)=O)=O)C2	10.1016/s0163-7258(02)00296-6	696	+2	0.963
Gyermek2002-24	C22H36NO8	O=C(CCCCC(O)=O)OCC[N@+](C@H)(CC1)CC2OC(CCCCC(O)=O)(C@H)1C2)C	10.1016/s0163-7258(02)00296-6	442	+2	-1.907
Gyermek2002-25	C22H42N2O4	O=C(CCCCC(OCC[N+](CCCC1)C)=O)OCC[N+](CCCC2)C	10.1016/s0163-7258(02)00296-6	398	+2	-2.475
Gyermek2002-26	C34H50N2O4	O=C(CCCCC(OCC[N+](CCCC1)CC2=CC=CC=C2)=O)OCC[N+](CCCC3)CC4=CC=CC=C4	10.1016/s0163-7258(02)00296-6	550	+2	2.278
Gyermek2002-27	C28H46N2O8	CC(OCC[N@+](C@H)(CC1)CC2OC(CCC(OC(C@H)3CC4)C[C@H]4[N@+](C)CCOC(C)=O)=O)(C@H)1C2)C=O	10.1016/s0163-7258(02)00296-6	538	+2	-4.433
Gyermek2002-28	C38H50N2O8	O=C(C(OCC[N@+](C@H)(CC1)CC2OC(CC3=CC=CC=C3)=O)(C@H)1C2)C=O)OCC[N@+](C@H)(CC4)CC5OC(CC6=CC=C(C6)=O)(C@H)4C5)C	10.1016/s0163-7258(02)00296-6	662	+2	-1.588
Gyermek2002-29	C44H62N2O8	O=C(CCCCCC(OCC[N@+](C@H)(CC1)CC2OC(CC3=CC=CC=C3)=O)(C@H)1C2)C=O)OCC[N@+](C@H)(CC4)CC5OC(CC6=CC=CC=C6)=O)(C@H)4C5)C	10.1016/s0163-7258(02)00296-6	746	+2	0.205
Gyermek2002-30	C44H62N2O8	O=C(CCCCCC(OCC[N@+](C@H)(CC1)CC2OC(CC3=CC=CC=C3)=O)(C@H)1C2)C=O)OCC[N@+](C@H)(CC4)CC5OC(CC6=CC=CC=C6)=O)(C@H)4C5)C	10.1016/s0163-7258(02)00296-6	746	+2	-1.211
Gyermek2002-31	C44H62N2O8	O=C(CCCCCC(OCC[N@+](C@H)(CC1)CC2OC(CC3=CC=CC=C3)=O)(C@H)1C2)C=O)OCC[N@+](C@H)(CC4)CC5OC(CC6=CC=CC=C6)=O)(C@H)4C5)C	10.1016/s0163-7258(02)00296-6	746	+2	0.065
Gyermek2002-32	C41H56N2O8	O=C(CCCCCC(OCC[N@+](C@H)(CC1)CC2OC(C3=CC=CC=C3)=O)(C@H)1C2)C=O)OCC[N@+](C@H)(CC4)CC5OC(CC6=CC=CC=C6)=O)(C@H)4C5)C	10.1016/s0163-7258(02)00296-6	704	+2	0.258

Gyermek2002-33	C32H54N2O8	O=C(CCCCCC(OCC[N@+](C@H)(CC1)CC2OC(C)=O)(C@@H]1C2)C)=O)OCC[N@+](C@H)(CC3)CC4OC(C)=O)(C@H]3C4)C	10.1016/s0163-7258(02)00296-6	594	+2	-3.071
Gyermek2002-34	C42H58N2O8	O=C(CCC(OCCC[N@+](C@H)(CC1)CC2OC(CC3=CC=CC=C3)=O)(C@@H]1C2)C)=O)OCCC[N@+](C@H)(CC[C@H]4CC5)[C@@H]5OC(CC6=CC=CC=C6)=O)C	10.1016/s0163-7258(02)00296-6	718	+2	0.504
Gyermek2002-35	C42H58N2O8	O=C(C(OCCCC[N@+](C@H)(CC1)CC2OC(CC3=CC=CC=C3)=O)(C@@H]1C2)C)=O)OCCCC[N@+](C@H)(CC4)CC5OC(CC6=CC=CC=C6)=O)(C@H]4C5)C	10.1016/s0163-7258(02)00296-6	718	+2	-3.704
Gyermek2002-36	C30H50N2O8	O=C(CCCCC(OCC[N@+](C@H)(CC1)CC2OC(C)=O)(C@@H]1C2)C)=O)OCC[N@+](C@H)(CC3)CC4OC(C)=O)(C@H]3C4)C	10.1016/s0163-7258(02)00296-6	566	+2	-4.129
Gyermek2002-37	C43H60N2O8	O=C(CCCC(OCCC[N@+](C@H)(CC1)CC2OC(CC3=CC=CC=C3)=O)(C@@H]1C2)C)=O)OCCC[N@+](C@H)(CC4)CC5OC(C6=CC=CC=C6)=O)(C@H]4C5)C	10.1016/s0163-7258(02)00296-6	732	+2	-1.16
Gyermek2002-38	C37H48N2O8	O=C(C1=CC=CC=C1)OCC[N@+](C@H)(CC2)CC3OC(CC(O)C(C[C@H]4CC5)C[C@H]5[N@+](4)C)CCOC(C6=CC=CC=C6)=O)=O)(C@H]2C3)C	10.1016/s0163-7258(02)00296-6	648	+2	-1.339
Gyermek2002-39	C46H66N2O8	O=C(CCCCCC(OCCC[N@+](C@H)(CC1)CC2OC(CC3=CC=CC=C3)=O)(C@H]1C2)C)=O)OCC[N@+](C@H)(CC4)CC5OC(CC6=CC=CC=C6)=O)(C@H]4C5)C	10.1016/s0163-7258(02)00296-6	774	+2	-0.153
Gyermek2002-40	C40H54N2O8	O=C(CCCCC(OCC[N@+](C@H)(CC1)CC2OC(C3=CC=CC=C3)=O)(C@@H]1C2)C)=O)OCC[N@+](C@H)(CC4)CC5OC(C6=CC=CC=C6)=O)(C@H]4C5)C	10.1016/s0163-7258(02)00296-6	690	+2	-0.271
Gyermek2002-41	C41H56N2O8	O=C(CC(OCCC[N@+](C@H)(CC1)CC2OC(CC3=CC=CC=C3)=O)(C@@H]1C2)C)=O)OCCC[N@+](C@H)(CC4)CC5OC(CC6=CC=CC=C6)=O)(C@H]4C5)C	10.1016/s0163-7258(02)00296-6	704	+2	-1.87
Gyermek2002-42	C41H56N2O8	O=C(CCCC(OCC[N@+](C@@)(CC1)([H])C[C@H]2OC(CC3=C=C=CC=C3)=O)(C@]1([H])C2)C)=O)OCC[N@+](C@@)(CC4)([H])C[C@H]5OC(CC6=CC=CC=C6)=O)(C@]4([H])C5)C	10.1016/s0163-7258(02)00296-6	704	+2	-0.802
Gyermek2002-43	C39H52N2O8	O=C(CC(OCC[N@+](C@@H)(CC1)CC2OC(CC3=CC=CC=C3)=O)(C@H]1C2)C)=O)OCC[N@+](C@H)(CC4)CC5OC(CC6=CC=CC=C6)=O)(C@H]4C5)C	10.1016/s0163-7258(02)00296-6	676	+2	-1.512
Gyermek2002-44	C43H60N2O8	O=C(CCCCC(OCC[N@+](C@H)(CC1)CC2OC(CC3=CC=CC=C3)=O)(C@@H]1C2)C)=O)OCC[N@+](C@H)(CC4)CC5OC(CC6=CC=CC=C6)=O)(C@H]4C5)C	10.1016/s0163-7258(02)00296-6	732	+2	-0.324
Gyermek2002-45	C38H50N2O8	O=C(CCC(OCC[N@+](C@H)(CC1)CC2OC(C3=CC=CC=C3)=O)(C@@H]1C2)C)=O)OCC[N@+](C@H)(CC4)CC5OC(C6=CC=CC=C6)=O)(C@H]4C5)C	10.1016/s0163-7258(02)00296-6	662	+2	-0.575
Gyermek2002-46	C42H58N2O8	O=C(CCCCC(OCC[N@+](C@H)(CC1)CC2OC(CC3=CC=CC=C3)=O)(C@@H]1C2)C)=O)OCC[N@+](C@H)(CC4)CC5OC(CC6=CC=CC=C6)=O)(C@H]4C5)C	10.1016/s0163-7258(02)00296-6	718	+2	-0.853
Gyermek2002-47	C40H54N2O8	O=C(CCC(OCC[N@+](C@H)(CC1)CC2OC(CC3=CC=CC=C3)=O)	10.1016/s0163-	690	+2	-1.157

		<chem>([C@@H]1C2C)=O)OCC[N@+](C@H)(CC4)CC5OC(CC6=C</chem>	7258(02)00296-6			
		<chem>C=CC=C6)=O)([C@H]4C5)C</chem>				
Gyermek2002-48	C42H58N2O8	<chem>O=C(CCCCCC(OCC[N@+](C@H)(CC1)CC2OC(C3=CC=CC=C3</chem>	10.1016/s0163-	718	+2	0.787
		<chem>)=O)([C@@H]1C2C)=O)OCC[N@+](C@H)(CC4)CC5OC(C6</chem>	7258(02)00296-6			
		<chem>=CC=CC=C6)=O)([C@H]4C5)C</chem>				
Gyermek2002-49	C22H42N2O4	<chem>O=C(CCCCC(OCC[N+](CCCCC1C)=O)OCC[N+](CCCCC2)C</chem>	10.1016/s0163-	398	+2	-2.475
			7258(02)00296-6			
Gyermek2002-50	C42H62N2O4	<chem>C[N@+](C@H)(CC1)CC2OC(CC3=CC=CC=C3)=O)([C@H]1C2</chem>	10.1016/s0163-	658	+2	-0.726
		<chem>)CCCCCCCC[N@+](C@H)(CC4)CC5OC(CC6=CC=CC=C6)=O</chem>	7258(02)00296-6			
		<chem>)([C@@H]4C5)C</chem>				
Gyermek2002-51	C28H54N2O2	<chem>C[N@+](C@H)(CC1)([H])C[C@@H]2O)([C@]1([H])C2)CCCC</chem>	10.1016/s0163-	450	+2	-4.836
		<chem>CCCCCC[N@+](C@H)(CC3)([H])C[C@H]4O)([C@@]3([H])C4)C</chem>	7258(02)00296-6			
Gyermek2002-52	C25H48N2O2	<chem>C[N@+](C@H)(CC1)([H])C[C@@H]2O)([C@]1([H])C2)CCCC</chem>	10.1016/s0163-	408	+2	-6.423
		<chem>CCCC[N@+](C@H)(CC3)([H])C[C@H]4O)([C@@]3([H])C4)C</chem>	7258(02)00296-6			
Gyermek2002-53	C24H46N2O2	<chem>C[N@+](C@H)(CC1)([H])C[C@@H]2O)([C@]1([H])C2)CCCC</chem>	10.1016/s0163-	394	+2	-6.952
		<chem>CCC[N@+](C@H)(CC3)([H])C[C@H]4O)([C@@]3([H])C4)C</chem>	7258(02)00296-6			
Gyermek2002-54	C23H44N2O2	<chem>C[N@+](C@H)(CC1)([H])C[C@@H]2O)([C@]1([H])C2)CCCC</chem>	10.1016/s0163-	380	+2	-7.481
		<chem>CC[N@+](C@H)(CC3)([H])C[C@H]4O)([C@@]3([H])C4)C</chem>	7258(02)00296-6			
Gyermek2002-55	C28H54N2	<chem>C[N@+](C@H)2CC[C@@H]1CCC2)CCCCCCCCCCCC[N@@</chem>	10.1016/s0163-	418	+2	-0.662
		<chem>+](C@H)4CC[C@H]3CCC4)C</chem>	7258(02)00296-6			
Gyermek2002-56	C27H52N2	<chem>C[N@+](C@H)2CC[C@@H]1CCC2)CCCCCCCCCCCC[N@@+</chem>	10.1016/s0163-	404	+2	-1.191
		<chem>](C@H)4CC[C@H]3CCC4)C</chem>	7258(02)00296-6			
Gyermek2002-57	C26H50N2	<chem>C[N@+](C@H)2CC[C@@H]1CCC2)CCCCCCCCCCCC[N@@+](C@</chem>	10.1016/s0163-	390	+2	-1.72
		<chem>)(C@H)4CC[C@H]3CCC4)C</chem>	7258(02)00296-6			
Gyermek2002-58	C25H48N2	<chem>C[N@+](C@H)2CC[C@@H]1CCC2)CCCCCCCCCCCC[N@@+](C@</chem>	10.1016/s0163-	376	+2	-2.249
		<chem>H)4CC[C@H]3CCC4)C</chem>	7258(02)00296-6			
Gyermek2002-59	C24H46N2	<chem>C[N@+](C@H)2CC[C@@H]1CCC2)CCCCCCCCCCCC[N@@+](C@</chem>	10.1016/s0163-	362	+2	-2.778
		<chem>@H)4CC[C@H]3CCC4)C</chem>	7258(02)00296-6			
Gyermek2002-60	C23H44N2	<chem>C[N@+](C@H)2CC[C@@H]1CCC2)CCCCCCCCCCCC[N@@+](C@</chem>	10.1016/s0163-	348	+2	-3.307
		<chem>@H)4CC[C@H]3CCC4)C</chem>	7258(02)00296-6			
Gyermek2002-61	C22H42N2	<chem>C[N@+](C@H)2CC[C@@H]1CCC2)CCCCCCCCCCCC[N@@+](C@</chem>	10.1016/s0163-	334	+2	-3.836
		<chem>@H)4CC[C@H]3CCC4)C</chem>	7258(02)00296-6			
Gyermek2002-62	C21H40N2	<chem>C[N@+](C@H)2CC[C@@H]1CCC2)CCCCCCCCCCCC[N@@+](C@H)4CC</chem>	10.1016/s0163-	320	+2	-4.365
		<chem>[C@@H]3CCC4)C</chem>	7258(02)00296-6			
Gyermek2002-63	C19H36N2	<chem>C[N@+](C@H)2CCC[C@@H]1CC2)CCCC[N@+](C@H)4CC</chem>	10.1016/s0163-	292	+2	-3.943
		<chem>C[C@H]3CC4)C</chem>	7258(02)00296-6			
Gyermek2002-64	C20H38N2	<chem>C[N@+](C@H)2CCC[C@@H]1CC2)CCCC[N@+](C@H)4C</chem>	10.1016/s0163-	306	+2	-4.894
		<chem>CC[C@H]3CC4)C</chem>	7258(02)00296-6			
Gyermek2002-65	C22H42N2O2	<chem>C[N@+](C@H)(CC1)([H])C[C@H]2O)([C@]1([H])C2)CCCCC[</chem>	10.1016/s0163-	366	+2	-8.01
		<chem>N@@+](C@H)(CC3)([H])C[C@H]4O)([C@@]3([H])C4)C</chem>	7258(02)00296-6			
Gyermek2002-66	C26H50N2O2	<chem>C[N@+](C@H)(CC1)CC2O)([C@H]1C2)CCCCCCCCCCCC[N@+]</chem>	10.1016/s0163-	422	+2	-5.894
		<chem>([C@H](CC3)CC4O)([C@@H]3C4)C</chem>	7258(02)00296-6			

Rocuronium	C32H53N2O4	O=C(C)O[C@@H]([C@H]1[N+](CCCC2)CC=C)[C@](CC3)(C)[C@](C1)([H])[C@@](CC4)([H])[C@@]3([H])[C@@]([C@]4([H])C[C@@H]5O)(C)C[C@@H]5N6CCOCC6	10.2174/138955705402 3215	529	+1	2.433
Vecuronium	C34H57N2O4	C[C@]([C@H]1OC(C)=O)(CC2)[C@](C[C@@H]1[N+](C)CCCC3)([H])[C@@](CC4)([H])[C@@]2([H])[C@](C[C@@H]5N6CCC6)(C)[C@]4([H])C[C@@H]5OC(C)=O	10.2174/138955705402 3215	557	+1	4.334
Pipecuronium	C35H62N4O4	C[C@]([C@H]1OC(C)=O)(CC2)[C@](C[C@@H]1N3CC[N+](C)(C)CC3)([H])[C@@](CC4)([H])[C@@]2([H])[C@](C[C@@H]5N6CC[N+](C)(C)CC6)(C)[C@]4([H])C[C@@H]5OC(C)=O	10.2174/138955705402 3215	602	+2	0.628
Pancuronium	C35H60N2O4	C[C@]([C@H]1OC(C)=O)(CC2)[C@](C[C@@H]1[N+](C)CCCC3)([H])[C@@](CC4)([H])[C@@]2([H])[C@](C[C@@H]5[N+](C)CCCC6)(C)[C@]4([H])C[C@@H]5OC(C)=O	10.2174/138955705402 3215	572	+2	1.206
Jindal2001-DPJ-489	C32H54N2O2	C[C@]12C(C[C@@H]([N+](C)CCCC3)CC2)=CCC4C1CC[C@@]5(C)C4C[C@H]([N+](C)CCCC6)[C@@H]5OC(C)=O	10.1016/s0223-5234(00)01205-8	498	+2	-0.732
Jindal2002-DPJ-494	C30H53N3O	C[C@]12C(C[C@@H]([N+](C)CCCC3)CC2)=CCC4C1CC[C@@]5(C)C4C[C@H](N6CC[N+](C)(C)CC6)[C@@H]5O	10.1016/s0223-5234(02)01413-7	471	+2	-1.923
Jindal2002-DPJ-496	C32H55N3O2	C[C@]12C(C[C@@H]([N+](C)CCCC3)CC2)=CCC4C1CC[C@@]5(C)C4C[C@H](N6CC[N+](C)(C)CC6)[C@@H]5OC(C)=O	10.1016/s0223-5234(02)01413-7	513	+2	-1.021
Hu2012-8a	C29H52N2O3	C[C@@]12C(CCC3C2CC[C@@]4(C)C3C[C@H]([N+](C)CCOCC5)[C@@H]4OC(C)=O)C[C@@H]([N+](C)(C)CC1	10.1016/j.ejmech.2012.07.048	476	+2	-1.166
Hu2012-8b	C31H54N2O3	C[C@@]12C(CCC3C2CC[C@@]4(C)C3C[C@H]([N+](C)CCOCC5)[C@@H]4OC(C)=O)C[C@@H]([N+](C)CCCC6)CC1	10.1016/j.ejmech.2012.07.048	502	+2	0.099
Hu2012-8c	C32H57N3O3	C[C@@]12C(CCC3C2CC[C@@]4(C)C3C[C@H]([N+](C)CCOCC5)[C@@H]4OC(C)=O)C[C@@H](N6CC[N+](C)(C)CC6)CC1	10.1016/j.ejmech.2012.07.048	531	+2	1.565
Hu2012-8d	C32H56N2O3	C[C@@]12C(CCC3C2CC[C@@]4(C)C3C[C@H]([N+](C)CCOCC5)[C@@H]4OC(C)=O)C[C@@H]([N+](C)CCCC6)CC1	10.1016/j.ejmech.2012.07.048	516	+2	0.658
Hu2012-8e	C31H54N2O4	C[C@@]12C(CCC3C2CC[C@@]4(C)C3C[C@H]([N+](C)CCOCC5)[C@@H]4OC(C)=O)C[C@@H]([N+](C)CCOCC6)CC1	10.1016/j.ejmech.2012.07.048	518	+2	1.004
Hu2012-8f	C34H54N2O3	C[C@@]12C(CCC3C2CC[C@@]4(C)C3C[C@H]([N+](C)CCOCC5)[C@@H]4OC(C)=O)C[C@@H]([N+](C)(C6=CC=CC=C6)C)CC1	10.1016/j.ejmech.2012.07.048	538	+2	1.594
Hu2012-8g	C35H56N2O3	C[C@@]12C(CCC3C2CC[C@@]4(C)C3C[C@H]([N+](C)CCOCC5)[C@@H]4OC(C)=O)C[C@@H]([N+](C)(CC6=CC=CC=C6)C)CC1	10.1016/j.ejmech.2012.07.048	552	+2	1.253
Hu2015-24a	C32H56N2O3	C[C@@]12C(CCC3C2CC[C@@]4(C)C3C[C@H]([N+](C)CCCC5)[C@@H]4OC(C)=O)C[C@@H]([N+](C)CCOCC6)CC1	10.1016/j.steroids.2015.01.008	516	+2	0.658
Hu2015-24b	C31H54N2O3	C[C@@]12C(CCC3C2CC[C@@]4(C)C3C[C@H]([N+](C)CCCC5)[C@@H]4OC(C)=O)C[C@@H]([N+](C)CCOCC6)CC1	10.1016/j.steroids.2015.01.008	502	+2	0.099
Hu2015-24c	C32H57N3O3	C[C@@]12C(CCC3C2CC[C@@]4(C)C3C[C@H](N5CC[N+](C)(C)CC5)[C@@H]4OC(C)=O)C[C@@H]([N+](C)CCOCC6)CC1	10.1016/j.steroids.2015.01.008	531	+2	0.368
Hu2015-25a	C33H58N2O2	C[C@@]12C(CCC3C2CC[C@@]4(C)C3C[C@H]([N+](C)CCCC5)[C@@H]4OC(C)=O)C[C@@H]([N+](C)CCCC6)CC1	10.1016/j.steroids.2015.01.008	514	+2	0.312

Hu2015-25b	C32H56N2O2	C[C@@]12C(CCC3C2CC[C@@]4(C)C3C[C@H]([N+]5(C)CCCC5) [C@@H]4OC(C)=O)C[C@@H]([N+]6(C)CCCC6)CC1	10.1016/j.ster- oids.2015.01.008	500	+2	-0.248
Hu2015-25c	C33H59N3O2	C[C@@]12C(CCC3C2CC[C@@]4(C)C3C[C@H](N5CC[N+](C)(C) CC5)[C@@H]4OC(C)=O)C[C@@H]([N+]6(C)CCCC6)CC1	10.1016/j.ster- oids.2015.01.008	529	+2	0.022
Hu2015-26a	C32H56N2O2	C[C@@]12C(CCC3C2CC[C@@]4(C)C3C[C@H]([N+]5(C)CCCC 5)[C@@H]4OC(C)=O)C[C@@H]([N+]6(C)CCCC6)CC1	10.1016/j.ster- oids.2015.01.008	500	+2	-0.248
Hu2015-26b	C31H54N2O2	C[C@@]12C(CCC3C2CC[C@@]4(C)C3C[C@H]([N+]5(C)CCCC5) [C@@H]4OC(C)=O)C[C@@H]([N+]6(C)CCCC6)CC1	10.1016/j.ster- oids.2015.01.008	486	+2	-0.807
Hu2015-26c	C32H57N3O2	C[C@@]12C(CCC3C2CC[C@@]4(C)C3C[C@H](N5CC[N+](C)(C) CC5)[C@@H]4OC(C)=O)C[C@@H]([N+]6(C)CCCC6)CC1	10.1016/j.ster- oids.2015.01.008	515	+2	-0.537
Hu2015-27a	C33H59N3O2	C[C@@]12C(CCC3C2CC[C@@]4(C)C3C[C@H]([N+]5(C)CCCC 5)[C@@H]4OC(C)=O)C[C@@H](N6CC[N+](C)(C)CC6)CC1	10.1016/j.ster- oids.2015.01.008	529	+2	1.219
Hu2015-27b	C32H57N3O2	C[C@@]12C(CCC3C2CC[C@@]4(C)C3C[C@H]([N+]5(C)CCCC5) [C@@H]4OC(C)=O)C[C@@H](N6CC[N+](C)(C)CC6)CC1	10.1016/j.ster- oids.2015.01.008	515	+2	0.660
Hu2015-27c	C33H60N4O2	C[C@@]12C(CCC3C2CC[C@@]4(C)C3C[C@H](N5CC[N+](C)(C) CC5)[C@@H]4OC(C)=O)C[C@@H](N6CC[N+](C)(C)CC6)CC1	10.1016/j.ster- oids.2015.01.008	544	+2	0.929
Hu2015-28	C31H56N2O	C[C@@]12C(CCC3C2CC[C@@]4(C)C3C[C@H]([N+]5(C)CCCC 5)[C@@H]4O)C[C@@H]([N+]6(C)CCCC6)CC1	10.1016/j.ster- oids.2015.01.008	472	+2	-0.591
Hu2015-29	C31H57N3O	C[C@@]12C(CCC3C2CC[C@@]4(C)C3C[C@H](N5CC[N+](C)(C) CC5)[C@@H]4O)C[C@@H]([N+]6(C)CCCC6)CC1	10.1016/j.ster- oids.2015.01.008	487	+2	-0.880
Hu2015-30	C30H49N3O2	C[C@@]12C(CCC3C2CC[C@@]4(C)C3C[C@H](N5C=[N+](C)C= C5)[C@@H]4OC(C)=O)C[C@@H]([N+]6(C)CCCC6)CC1	10.1016/j.ster- oids.2015.01.008	483	+2	-2.523
Rao2016-1a	C37H62N2O2	C[C@@]12C(CCC3C2CC[C@@]4(C)C3C[C@H]([N+]5(CC=C)CC CCC5)[C@@H]4OC(C)=O)C[C@@H]([N+]6(CC=C)CCCC6)CC1	10.1111/ebdd.12711	566	+2	1.860
Rao2016-1b	C37H58N2O2	C[C@@]12C(CCC3C2CC[C@@]4(C)C3C[C@H]([N+]5(CC#C)CC CCC5)[C@@H]4OC(C)=O)C[C@@H]([N+]6(CC#C)CCCC6)CC1	10.1111/ebdd.12711	562	+2	0.512
Rao2016-1c	C34H57N2O2	C[C@@]12C(CCC3C2CC[C@@]4(C)C3C[C@H](N5CCCCC5)[C@ @H]4OC(C)=O)C[C@@H]([N+]6(CC=C)CCCC6)CC1	10.1111/ebdd.12711	525	+1	4.214
Rao2016-1d	C34H55N2O2	C[C@@]12C(CCC3C2CC[C@@]4(C)C3C[C@H](N5CCCCC5)[C@ @H]4OC(C)=O)C[C@@H]([N+]6(CC#C)CCCC6)CC1	10.1111/ebdd.12711	523	+1	3.540
Rao2016-2a	C37H63N3O2	C[C@@]12C(CCC3C2CC[C@@]4(C)C3C[C@H]([N+]5(CC=C)CC CCC5)[C@@H]4OC(C)=O)C[C@@H](N6CC[N+](C)(CC=C)CC6) CC1	10.1111/ebdd.12711	581	+2	2.767
Rao2016-2b	C37H59N3O2	C[C@@]12C(CCC3C2CC[C@@]4(C)C3C[C@H]([N+]5(CC#C)CC CCC5)[C@@H]4OC(C)=O)C[C@@H](N6CC[N+](C)(CC#C)CC6) C1	10.1111/ebdd.12711	577	+2	1.419
Rao2016-2c	C34H58N3O2	C[C@@]12C(CCC3C2CC[C@@]4(C)C3C[C@H](N5CCCCC5)[C@ @H]4OC(C)=O)C[C@@H](N6CC[N+](C)(CC=C)CC6)CC1	10.1111/ebdd.12711	540	+1	5.121
Rao2016-2d	C34H56N3O2	C[C@@]12C(CCC3C2CC[C@@]4(C)C3C[C@H](N5CCCCC5)[C@ @H]4OC(C)=O)C[C@@H](N6CC[N+](C)(CC#C)CC6)CC1	10.1111/ebdd.12711	538	+1	4.447
Rao2016-2e	C38H60N3O2	C[C@@]12C(CCC3C2CC[C@@]4(C)C3C[C@H](N5CCCCC5)[C@ @H]4OC(C)=O)C[C@@H](N6CC[N+](C)(CC7=CC=CC=C7)CC6)	10.1111/ebdd.12711	590	+1	6.650

		CC1					
Rao2016-2f	C39H63N3O2	C[C@@]12C(CCC3C2CC[C@@]4(C)C3C[C@H]([N+]5(C)CCCC5)[C@@H]4OC(C)=O)C[C@@H](N6CC[N+](C)(CC7=CC=CC=C7)CC6)CC1	10.1111/ebdd.12711	605	+2	3.522	
Rao2016-3a	C37H63N3O2	C[C@@]12C(CCC3C2CC[C@@]4(C)C3C[C@H](N5CC[N+](C)(C=C)CC5)[C@@H]4OC(C)=O)C[C@@H]([N+]6(CC=C)CCCCC6)CC1	10.1111/ebdd.12711	581	+2	1.571	
Rao2016-3b	C37H59N3O2	C[C@@]12C(CCC3C2CC[C@@]4(C)C3C[C@H](N5CC[N+](C)(C=C#C)CC5)[C@@H]4OC(C)=O)C[C@@H]([N+]6(CC#C)CCCCC6)CC1	10.1111/ebdd.12711	577	+2	0.222	
Rao2016-3c	C34H58N3O2	C[C@@]12C(CCC3C2CC[C@@]4(C)C3C[C@H](N5CC[N+](C)(C=C)CC5)[C@@H]4OC(C)=O)C[C@@H](N6CCCCC6)CC1	10.1111/ebdd.12711	540	+1	5.121	
Rao2016-3d	C34H56N3O2	C[C@@]12C(CCC3C2CC[C@@]4(C)C3C[C@H](N5CC[N+](C)(C=C#C)CC5)[C@@H]4OC(C)=O)C[C@@H](N6CCCCC6)CC1	10.1111/ebdd.12711	538	+1	4.447	
Rao2016-3e	C38H60N3O2	C[C@@]12C(CCC3C2CC[C@@]4(C)C3C[C@H](N5CC[N+](C)(C=C6=CC=CC=C6)CC5)[C@@H]4OC(C)=O)C[C@@H](N7CCCCC7)CC1	10.1111/ebdd.12711	590	+1	6.650	
Rao2016-3f	C39H63N3O2	C[C@@]12C(CCC3C2CC[C@@]4(C)C3C[C@H](N5CC[N+](C)(C=C6=CC=CC=C6)CC5)[C@@H]4OC(C)=O)C[C@@H]([N+]7(C)CCCCC7)CC1	10.1111/ebdd.12711	605	+2	2.326	
Rao2016-3g	C45H67N3O2	C[C@@]12C(CCC3C2CC[C@@]4(C)C3C[C@H](N5CC[N+](C)(C=C6=CC=CC=C6)CC5)[C@@H]4OC(C)=O)C[C@@H]([N+]7(CC8=CC=CC=C8)CCCCC7)CC1	10.1111/ebdd.12711	681	+2	4.944	
Rao2016-4a	C37H64N4O2	C[C@@]12C(CCC3C2CC[C@@]4(C)C3C[C@H](N5CC[N+](C)(C=C)CC5)[C@@H]4OC(C)=O)C[C@@H](N6CC[N+](C)(CC=C)C6)CC1	10.1111/ebdd.12711	596	+2	2.478	
Rao2016-4b	C37H60N4O2	C[C@@]12C(CCC3C2CC[C@@]4(C)C3C[C@H](N5CC[N+](C)(C=C#C)CC5)[C@@H]4OC(C)=O)C[C@@H](N6CC[N+](C)(CC#C)CC6)CC1	10.1111/ebdd.12711	592	+2	1.130	
Rao2016-4g	C45H68N4O2	C[C@@]12C(CCC3C2CC[C@@]4(C)C3C[C@H](N5CC[N+](C)(C=C6=CC=CC=C6)CC5)[C@@H]4OC(C)=O)C[C@@H](N7CC[N+](C)(CC8=CC=CC=C8)CC7)CC1	10.1111/ebdd.12711	696	+2	5.536	
CW 002	C52H68N2O12	O=C(OCCC[N@+]1(C)CCC(C=C(OC)C(OC)=C2)=C2[C@H]1CC3=CC(OC)=C(OC)C=C3)/C=C/C(OCCC[N@+]4(C)[C@H](CC5=C=C(OC)C(OC)=C5)C(C=C(OC)C(OC)=C6)=C6CC4)=O	10.1097/ALN.0b013e3 181dc1b5b	912	+2	2.663	
CW 011	C53H70N2O13	O=C(OCCC[N@+]1(C)CCC(C=C(OC)C(OC)=C2)=C2[C@H]1CC3=CC(OC)=C(OC)C=C3)/C=C/C(OCCC[N@+]4(C)[C@H](CC5=C=C(OC)=C(OC)C(OC)=C5)C(C=C(OC)C(OC)=C6)=C6CC4)=O	10.1097/ALN.0b013e3 181dc1b5b	942	+2	2.305	
CW 1759-50	C43H58N2O10	COC1=C(OC)C=C2C([C@@H](CC3=CC=C(OC)C=C3)[N+])(C)(CCCOCC/C=C/C(OCCC[N+]4(CCOCC4)CC5=CC=C(OC)C(OC)=C5)=O)O)CC2)=C1	10.1097/ALN.0000000 000002408	762	+2	2.268	
Patel1997-1	C58H80N2O14	O=C(CCCC/C=C/C(OCCC[N@+]([C@@H](C1=C2)CC(C=C3OC	10.1016/S0928-	1028	+2	3.121	

)=CC(OC)=C3OC)(CCC1=CC(OC)=C2OC)C=O)OCCC[N@+](C @@H](C(C4=C5)=CC(OC)=C5OC)CC(C=C6OC)=CC(OC)=C6OC) (CC4)C	0987(97)00020-1			
Patel1997-4	C60H88N2O16	COC(C(OC)=CC(CC[N+](CCCCOC(CCCC/C=C/C(OCCC[N+](CCC(C=C1OC)=CC(OC)=C1OC)(C)CCC(C=C2OC)=CC(OC)=C2OC)=O)=O)(C)CCC(C=C3OC)=CC(OC)=C3OC)=C4)=C4OC	10.1016/S0928- 0987(97)00020-1	1092	+2	-0.256
Patel1997-5	C56H82N2O16	COC(C(OC)=CC(CC[N+](CCCCOC(CCC(OCCC[N+](CCC(C=C1OC)=CC(OC)=C1OC)(C)CCC(C=C2OC)=CC(OC)=C2OC)=O)=O)(C)C CC(C=C3OC)=CC(OC)=C3OC)=C4)=C4OC	10.1016/S0928- 0987(97)00020-1	1038	+2	-1.590
Patel1997-6	C60H88N2O14	C[N+](CCCCOC(CC/C=C/C(CCC(OCCC[N+](C)(C)CCC(C=C1OC)=C(C=C1OC)CCC(C=C2OC)=CC(OC)=C2OC)=O)=O)(C)CCC(C=C3O C)=C(C=C3OC)CCC(C=C4OC)=CC(OC)=C4OC	10.1016/S0928- 0987(97)00020-1	1060	+2	0.902
Patel1997-8	C56H76N2O14	O=C(CCCC/C=C/C(OCCC[N@+](C@H](C(C=C1OC)=CC(OC)= C1OC)C2=CC(OC)=C3OC)(CCC2=C3)C)=O)OCCC[N@+](C@ H](C(C=C4OC)=CC(OC)=C4OC)C(C5=C6)=CC(OC)=C6OC)(CC5) C	10.1016/S0928- 0987(97)00020-1	1000	+2	2.363
Patel1997-9	C58H80N2O12S2	O=C(CC/C=C/C(CCC(SCCC[N@+](C@H](C1=C2)CC(C=C3OC)=CC(OC)=C3OC)(CCC1=CC(OC)=C2OC)C=O)SCCC[N@+](C @@H](C(C4=C5)=CC(OC)=C5OC)CC(C=C6OC)=CC(OC)=C6OC) (CC4)C	10.1016/S0928- 0987(97)00020-1	1060	+2	3.741
Patel1997-12	C60H84N2O14	CC(COC(CC/C=C/C(CCC(OCC(C)C[N@+](C@H](C1=C2)CC(C =C3OC)=CC(OC)=C3OC)(CCC1=CC(OC)=C2OC)C=O)=O)C[N@ +]4(C@H](C(C(C4)=C5)=CC(OC)=C5OC)CC(C=C6OC)=CC(O C)=C6OC)C	10.1016/S0928- 0987(97)00020-1	1056	+2	3.434
Clara2020-m-1a	C24H34N4	C[N+](CCCC1)CC2=CC(N=N/C3=CC(C[N+](4(C)CCCC4)=CC=C 3)=CC=C2	10.1016/j.ejmech.2020. 112403	378	+2	-2.202
Clara2020-m-1b	C26H38N4	C[N+](CCCC1)CC2=CC(N=N/C3=CC(C[N+](4(C)CCCC4)C)=CC =C3)=CC=C2	10.1016/j.ejmech.2020. 112403	406	+2	-1.084
Clara2020-m-1c	C28H42N4	C[N+](CCCC1)CC2=CC(N=N/C3=CC(C[N+](4(C)CCCC4)C)= CC=C3)=CC=C2	10.1016/j.ejmech.2020. 112403	434	+2	0.034
Clara2020-m-1d	C26H34N4	C[N+](CC=CCC1)CC2=CC(N=N/C3=CC(C[N+](4(C)CCCC4)C)= CC=C3)=CC=C2	10.1016/j.ejmech.2020. 112403	402	+2	-1.652
Clara2020-p-1a	C24H34N4	C[N+](CCCC1)CC2=CC=C(N=N/C3=CC=C(C[N+](4(C)CCCC4)C =C3)C=C2	10.1016/j.ejmech.2020. 112403	378	+2	-2.202
Clara2020-p-1b	C26H38N4	C[N+](CCCC1)CC2=CC=C(N=N/C3=CC=C(C[N+](4(C)CCCC4) C)C=C3)C=C2	10.1016/j.ejmech.2020. 112403	406	+2	-1.084
Clara2020-p-1c	C28H42N4	C[N+](CCCC1)CC2=CC=C(N=N/C3=CC=C(C[N+](4(C)CCCC 4)C)C=C3)C=C2	10.1016/j.ejmech.2020. 112403	434	+2	0.034
Clara2020-p-1d	C26H34N4	C[N+](CC=CCC1)CC2=CC=C(N=N/C3=CC=C(C[N+](4(C)CCC=CC 4)C)C=C3)C=C2	10.1016/j.ejmech.2020. 112403	402	+2	-1.652
Clara2020-m-5b	C19H24N3	C[N+](CCCC1)CC2=CC=CC(N=N/C3=CC=CC=C3)=C2	10.1016/j.ejmech.2020. 112403	294	+2	1.383

AV 391	C54H71ClN2O15	<chem>C[N+]1([C@@H](C(C=C2OC)=CC(OC)=C2OC)C(C(C1)=C3)=C(OC)C(OC)=C3OC)CCCOC/C(Cl)=C/C(OCCC[N+]1)(CCC4=C(C(OC)=C5OC)(C)[C@@H](C4=C5)CC(C=C6OC)=CC(OC)=C6OC)=O)=O</chem>	asaabstracts.com	1022	+2	1.863
AV 069	C54H71FN2O15	<chem>C[N+]1([C@@H](C(C=C2OC)=CC(OC)=C2OC)C(C(C1)=C3)=C(OC)C(OC)=C3OC)CCCOC/C(F)=C/C(OCCC[N+]1)(CCC4=C(C(OC)=C5OC)(C)[C@@H](C4=C5)CC(C=C6OC)=CC(OC)=C6OC)=O)=O</chem>	asaabstracts.com	1006	+2	1.263
NB 802-33	C54H71ClN2O15	<chem>C[N+]1([C@@H](C(C=C2OC)=CC(OC)=C2OC)C(C(C1)=C3)=CC(OC)=C3OC)CCCOC/C(Cl)=C/C(OCCC[N+]1)(CCC4=CC(O)C)=C5OC)(C)[C@@H](C4=C5OC)CC(C=C6OC)=CC(OC)=C6OC)=O)=O</chem>	asaabstracts.com	1022	+2	1.863
AV 001	C53H70N2O14	<chem>C[N+]1([C@@H](C(C=C2OC)=CC(OC)=C2OC)C(C(C1)=C3)=CC(OC)=C3OC)CCCOC/C=C/C(OCCC[N+]1)(CCC4=CC(OC)=C5OC)(C)[C@@H](C4=C5)CC(C=C6OC)=CC(OC)=C6OC)=O)=O</chem>	asaabstracts.com	958	+2	1.568
AV 003	C51H66N2O12	<chem>C[N+]1([C@@H](C(C=C2OC)=CC=C2OC)C(C(C1)=C3)=CC(O)C)=C3OC)CCCOC/C=C/C(OCCC[N+]1)(CCC4=CC(OC)=C5OC)(C)[C@@H](C4=C5)CC(C=C6OC)=CC=C6OC)=O)=O</chem>	asaabstracts.com	898	+2	2.284
NB 720-71	C55H73ClN2O16	<chem>C[N+]1([C@@H](C(C=C2OC)=CC(OC)=C2OC)C(C(C1)=C3)=C(OC)C(OC)=C3OC)CCCOC/C(Cl)=C/C(OCCC[N+]1)(CCC4=C(C(OC)=C5OC)(C)[C@@H](C4=C5OC)CC(C=C6OC)=CC(OC)=C6OC)=O)=O</chem>	asaabstracts.com	1052	+2	1.505

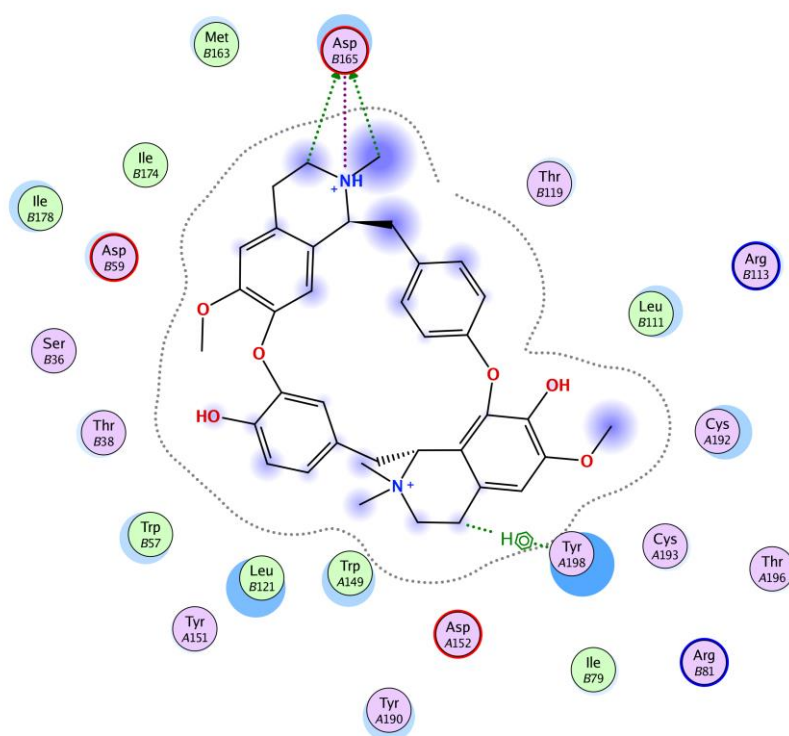


Figure S1. The binding modes of *d*-tubocurarine observed in the cryo-EM structure (PDB ID: 7SMS).