



UNIVERSITAT DE
BARCELONA

Non-glycosidic analogues of alpha-galactosylceramide: Design, synthesis and biological activity

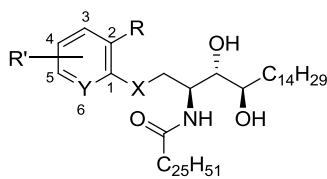
Roser Borràs Tudurí

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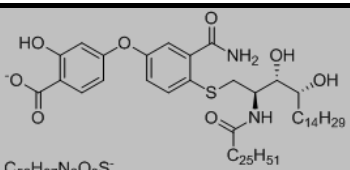
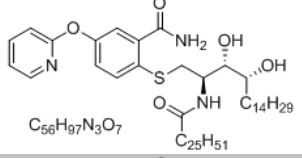
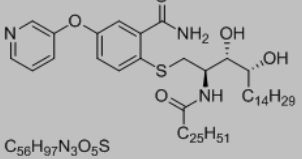
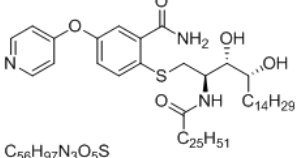
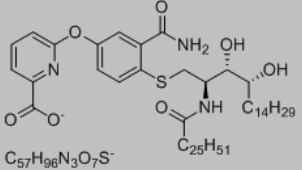
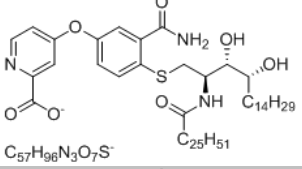
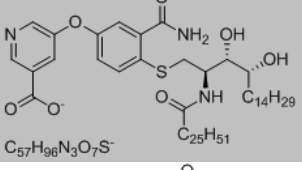
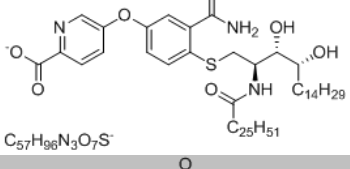
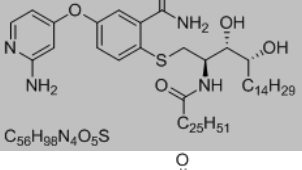
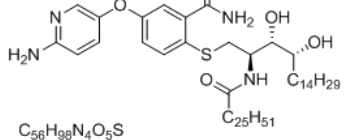
ANNEX 1. Library of compounds screened by Docking studies

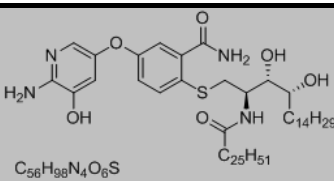
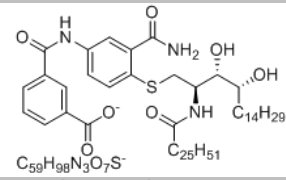
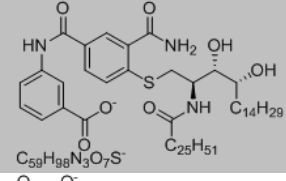
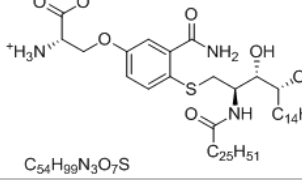
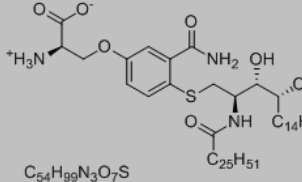
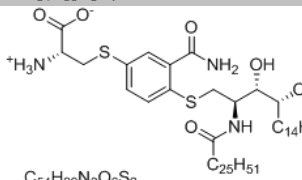
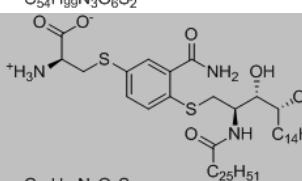
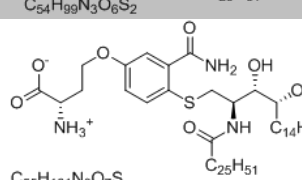
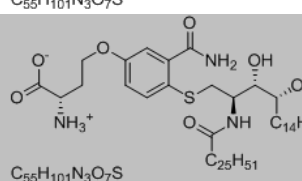
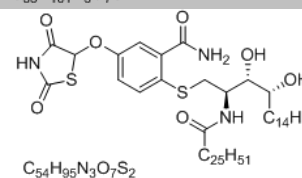


	X	Y (position)	R	R' (position)	
HS44	NH				<i>Inositol like with similar OHs configuration as glucose</i> $C_{50}H_{100}N_2O_7$
I-1a or DS-1	S	CH	CH ₂ OH	-	 $C_{51}H_{95}NO_4S$
DS-2	O	CH	CH ₂ OH	-	 $C_{51}H_{95}NO_5$
DS-3	S	CH	CONH ₂	-	 $C_{51}H_{94}N_2O_4S$
DS-4	O	CH	CONH ₂	-	 $C_{51}H_{94}N_2O_5$
DS-5	O	CH	COO ⁻	-	 $C_{51}H_{92}NO_6$
DS-6	S	N (6)	COO ⁻	-	 $C_{50}H_{91}N_2O_5S$
DS-7	O	N (6)	CONH ₂	-	 $C_{50}H_{93}N_3O_5$
DS-8	S	N (6)	CH ₂ OH	-	 $C_{50}H_{94}N_2O_4S$

	X	Y (position)	R	R' (position)	
DS-9	S	N (5)	CH ₂ OH	-	
DS-10	S	N (4)	CH ₂ OH	-	
DS-11	S	N (3)	CH ₂ OH	-	
DS-12	O	N (6)	CH ₂ OH	-	
DS-13	O	N (5)	CH ₂ OH	-	
DS-14	S	CH	SO ₂ NH ₂	-	
DS-15	O	CH	SO ₂ NH ₂	-	
DS-16	O	CH	CONH ₂	F (4)	
DS-17	O	CH	CONH(CH ₂) ₂ OH	F (4)	
DS-18	S	CH	C(NH)NH ₂	-	
DS-19	O	CH	C(NHMe) ⁺ NH ₂	-	

	X	Y (position)	R	R' (position)	
DS-20	S	CH	CONH ₂	Ph (4)	 C ₅₇ H ₉₈ N ₂ O ₄ S
DS-21	S	CH	CONH ₂	2Pyr (4)	 C ₅₆ H ₉₇ N ₃ O ₄ S
DS-22	S	CH	CONH ₂	(4-COO ⁻)-Ph (4)	 C ₅₈ H ₉₇ N ₂ O ₆ S ⁻
DS-23	S	CH	CONH ₂	(2-COO ⁻)-Ph (4)	 C ₅₈ H ₉₇ N ₂ O ₆ S ⁻
DS-24	S	CH	CONH ₂	OPh (4)	 C ₅₇ H ₉₈ N ₂ O ₅ S
DS-25	S	CH	CONH ₂	O-[(2-COO ⁻)-Ph] (4)	 C ₅₈ H ₉₇ N ₂ O ₇ S ⁻
DS-26	S	CH	CONH ₂	O-[(3-COO ⁻)-Ph] (4)	 C ₅₈ H ₉₇ N ₂ O ₇ S ⁻
DS-27	S	CH	CONH ₂	O-[(2-SO ₂ OH)-Ph] (4)	 C ₅₇ H ₉₈ N ₂ O ₈ S ₂
DS-28	S	CH	CONH ₂	O-[(3-COO ⁻ ,4-OH)-Ph] (4)	 C ₅₈ H ₉₇ N ₂ O ₈ S ⁻
DS-29	S	CH	CONH ₂	O-[(2-COO ⁻ ,3-OH)-Ph] (4)	 C ₅₈ H ₉₇ N ₂ O ₈ S ⁻

	X	Y (position)	R	R' (position)	
DS-30	S	CH	CONH ₂	O-[(4-COO ⁻ ,3-OH)-Ph] (4)	 <chem>C58H97N2O8S-</chem>
DS-31	S	CH	CONH ₂	O-2Pyr (4)	 <chem>C56H97N3O7</chem>
DS-32	S	CH	CONH ₂	O-3Pyr (4)	 <chem>C56H97N3O5S</chem>
DS-33	S	CH	CONH ₂	O-4Pyr (4)	 <chem>C56H97N3O5S</chem>
DS-34	S	CH	CONH ₂	O-[(3-COO ⁻)-2Pyr] (4)	 <chem>C57H96N3O7S-</chem>
DS-35	S	CH	CONH ₂	O-[(3-COO ⁻)-4Pyr] (4)	 <chem>C57H96N3O7S-</chem>
DS-36	S	CH	CONH ₂	O-[(5-COO ⁻)-3Pyr] (4)	 <chem>C57H96N3O7S-</chem>
DS-37	S	CH	CONH ₂	O-[(4-COO ⁻)-3Pyr] (4)	 <chem>C57H96N3O7S-</chem>
DS-38	S	CH	CONH ₂	O-[(5-NH ₂)-4Pyr] (4)	 <chem>C56H98N4O5S</chem>
DS-39	S	CH	CONH ₂	O-[(4-NH ₂)-3Pyr] (4)	 <chem>C56H98N4O5S</chem>

	X	Y (position)	R	R' (position)	
DS-40	S	CH	CONH ₂	O-[(4-NH ₂ ,5-OH)-3Pyr] (4)	 C ₅₆ H ₉₈ N ₄ O ₆ S
DS-41	S	CH	CONH ₂	NHCO-[(3-COO ⁻)-Ph] (4)	 C ₅₉ H ₉₈ N ₃ O ₇ S ⁻
DS-42	S	CH	CONH ₂	CONH-[(3-COO ⁻)-Ph] (4)	 C ₅₉ H ₉₈ N ₃ O ₇ S ⁻
DS-43	S	CH	CONH ₂	O-(S)Ser (4)	 C ₅₄ H ₉₉ N ₃ O ₇ S
DS-44	S	CH	CONH ₂	O-(R)Ser (4)	 C ₅₄ H ₉₉ N ₃ O ₇ S
DS-45	S	CH	CONH ₂	S-(R)Cys (4)	 C ₅₄ H ₉₉ N ₃ O ₆ S ₂
DS-46	S	CH	CONH ₂	S-(S)Cys (4)	 C ₅₄ H ₉₉ N ₃ O ₆ S ₂
DS-47	S	CH	CONH ₂	O-(S)homo-Ser (4)	 C ₅₅ H ₁₀₁ N ₃ O ₇ S
DS-48	S	CH	CONH ₂	O-(R)homo-Ser (4)	 C ₅₅ H ₁₀₁ N ₃ O ₇ S
DS-49	S	CH	CONH ₂	Thiazole-2,4-dione-5-O (4)	 C ₅₄ H ₉₅ N ₃ O ₇ S ₂