Molecular mechanism of substrate specificity for heparan sulfate 2-*O*-sulfotransferase

Supplementary Information

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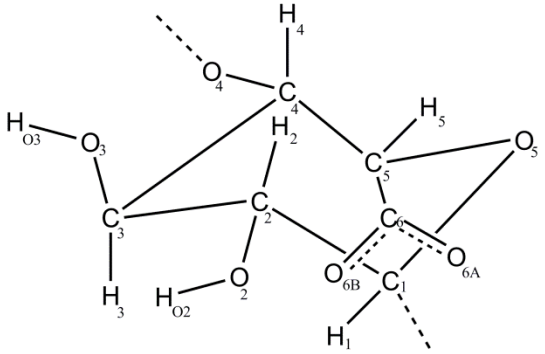
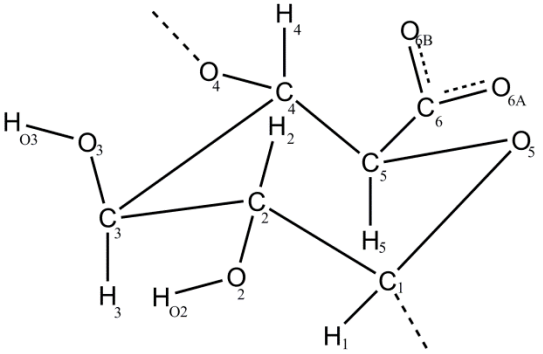
Running title: Crystal of ternary complex of 2OST

(a)



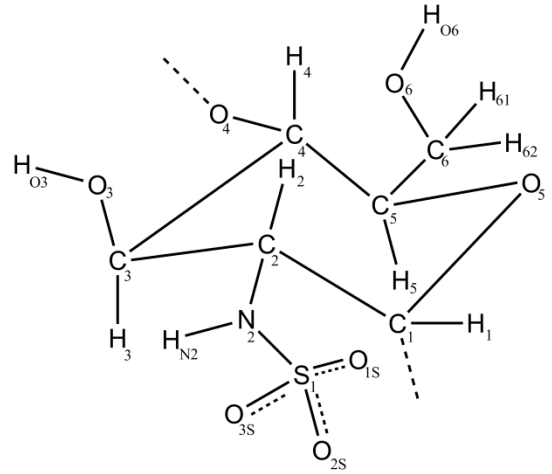
O_4 = -0.5010 C_2 = 0.2382 H_4 = 0.0856 H_5 = 0.1276
C_4 = 0.2610 O_2 = -0.7473 C_5 = -0.0540 O_5 = -0.5075
C_3 = 0.0201 H_{O2} = 0.4869 C_6 = 0.8627 C_1 = 0.3259
O_3 = -0.7292 H_2 = 0.1084 O_{6A} = -0.8366 H_1 = 0.1070
H_{O3} = 0.4902 H_3 = 0.0986 O_{6B} = -0.8366

(b)



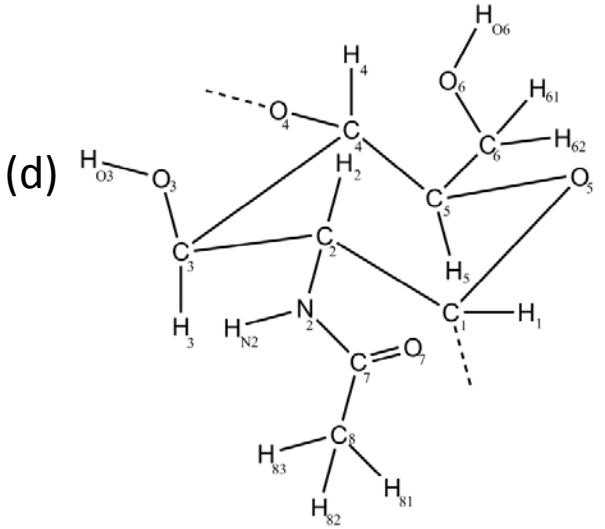
O_4 = -0.4735 C_2 = 0.1529 H_4 = 0.1085 H_5 = 0.0733
C_4 = 0.1990 O_2 = -0.7409 C_5 = 0.1480 O_5 = -0.5506
C_3 = 0.1668 H_{O2} = 0.4752 C_6 = 0.8056 C_1 = 0.3569
O_3 = -0.7607 H_2 = 0.1394 O_{6A} = -0.9005 H_1 = 0.0896
H_{O3} = 0.4989 H_3 = 0.1129 O_{6B} = -0.9005

(c)



O_4 = -0.5020 S_1(S6) = 1.3142 H_3 = 0.0710 H_{61} = 0.0402
C_4 = -0.2608 O_{1S}(O) = -0.7205 H_4 = 0.1630 H_{62} = 0.0402
C_3 = 0.4935 O_{2S}(O) = -0.7205 C_5 = 0.4255 H_5 = 0.0792
O_3 = -0.7214 O_{3S}(O) = -0.7205 C_6 = 0.1715 O_5 = -0.6106
H_{O3} = 0.4526 H_{N2}(H) = 0.4045 O_6 = -0.7553 C_1 = 0.4562
C_2 = 0.0053 H_2 = 0.1117 H_{6O} = 0.4744 H_1 = 0.1098
N_2(NT) = -0.8012

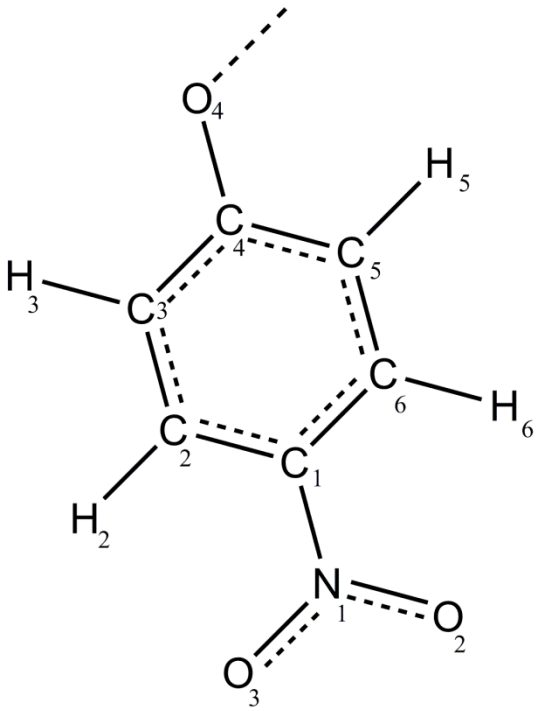
(d)



O_4 = -0.4993 C_7 = 0.9301 H_2 = 0.1523 H_{61} = 0.0463
C_4 = -0.1034 O_7 = -0.7187 H_3 = 0.1077 H_{62} = 0.0463
C_3 = 0.3669 C_8 = -0.7376 H_4 = 0.1463 H_5 = 0.1024
O_3 = -0.7116 H_{81} = 0.2034 C_5 = 0.3081 O_5 = -0.5152
H_{O3}= 0.4545 H_{82} = 0.2034 C_6 = 0.1614 C_1 = 0.3106
C_2 = 0.0065 H_{83} = 0.2034 O_6 = -0.7400 H_1 = 0.1198
N_2 = -0.7008 H_{N2} = 0.3858 H_{O6} = 0.4716

Supplemental Figure 1. Amber charges are given in (a) IdoA, (b) GlcA (c) GlcNS (d) GlcNAc, and (e) pnp. Amber atom types are indicated for non-standard atoms in parenthesis. Other relevant non-standard amber parameters are given in (f).

(e)



C_1 = 0.0946 C_2 = -0.1654 C_4 = 0.4776 H_5 = 0.1971
N_1(NO)= 0.7297 H_2 = 0.2042 O_4 = -0.5051 C_6 = -0.1654
O_2(O) = -0.4869 C_3 = -0.1473 C_5 = -0.1473 H_6 = 0.2042
O_3(O) = -0.4869 H_3 = 0.1971

(f)

Non-standard amber parameters used in the present study.

Mass

S6	32.06
NO	14.01

Bond	K_R	Req
NT-S6	300.0	1.696
S6-O	300.0	1.470
CA-NO	337.0	1.460
O -NO	337.0	1.220

Angle	θ	θeq
CT-OH-CA	50.0	116.90
CT-OH-CT	50.0	116.90
H2-CT-OH	50.0	110.90
OS-CT-OH	160.0	110.00
CA-NO-O	50.0	118.30
O -NO-O	50.0	123.40
NO-CA-CA	63.0	119.30
CT-NT-S6	100.0	116.60
NT-S6-O	50.0	105.20
S6-NT-H	50.0	107.30
O -S6-O	50.0	113.40

Dihedral	div	Vn/2	γ	n
X -S6-NT-X	6	1.80	0.0	3.
O -NO-CA-CA	1	2.50	180.0	-2.
O -NO-CA-CA	1	2.00	0.0	1.
NO-CA-CA-HA	1	2.50	180.0	-2.
NO-CA-CA-HA	1	2.00	0.0	1.

Improper	Vn/2	γ	n
X -X -NO-O	1.1	180.	2.

Non-bonded	R*	ε
S6	2.0000	0.2500
NO	1.8240	0.1700

Supplemental Figure 1. continued.