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Chemistry & Drug Discovery

Supporting Information

Structure and Energetics of Ligand–Fluorine Interactions with Galectin-3 Backbone and Side-Chain Amides: Insight into Solvation Effects and Multipolar Interactions

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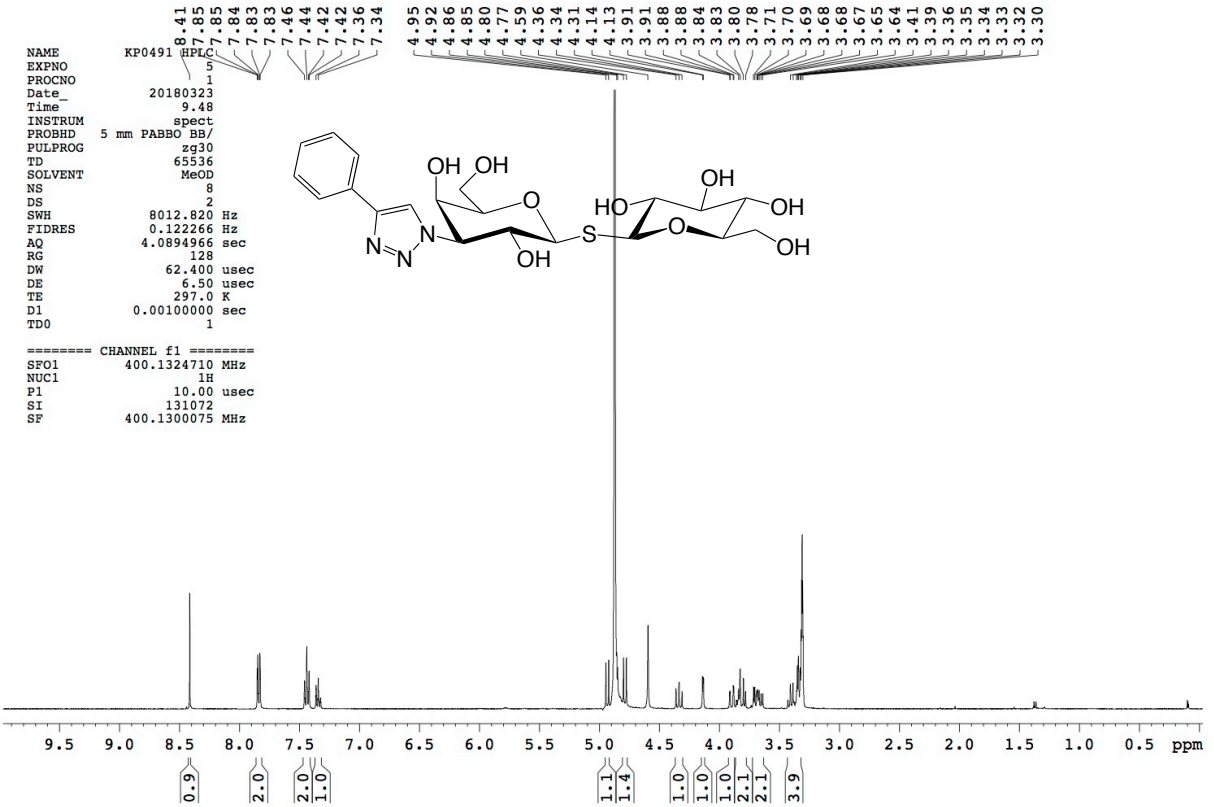
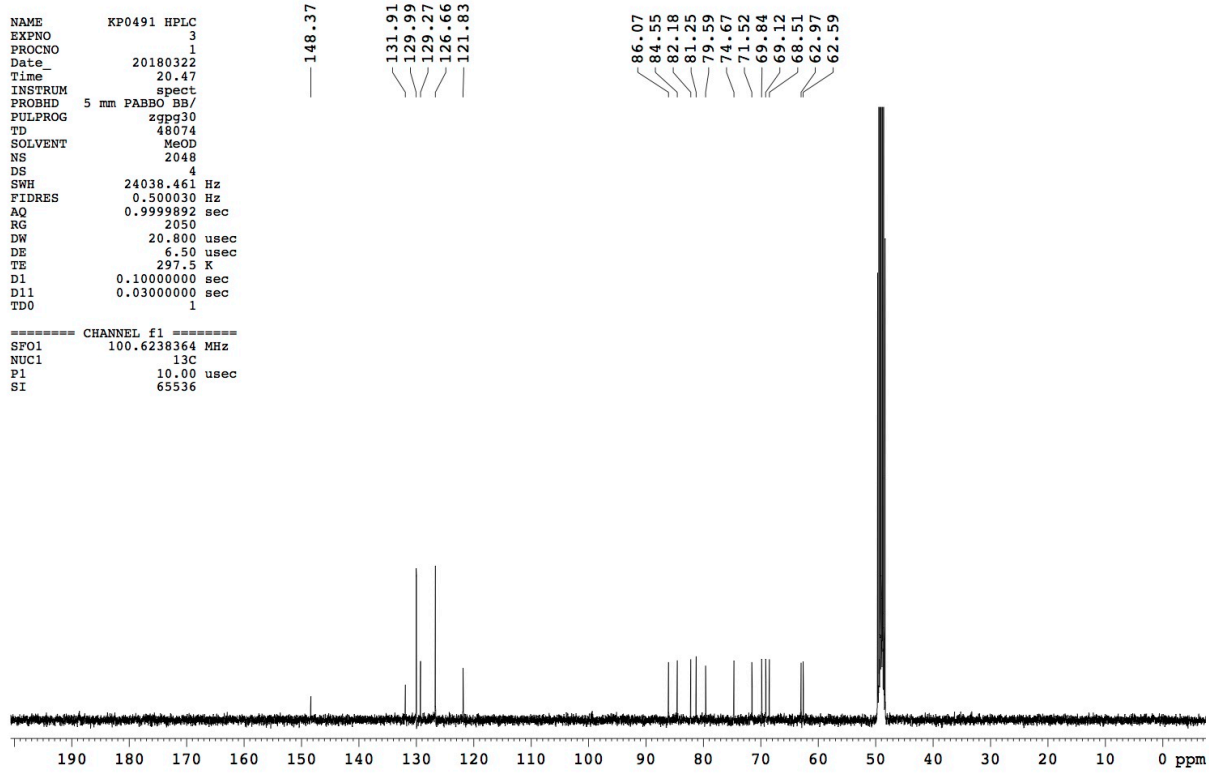
Figure S1: NMR spectrum of 3'-deoxy-3'-(4-phenyl-1*H*-1,2,3-triazol-1-yl)-β-D-galactopyranosyl 1-thio-β-D-glucopyranoside 9





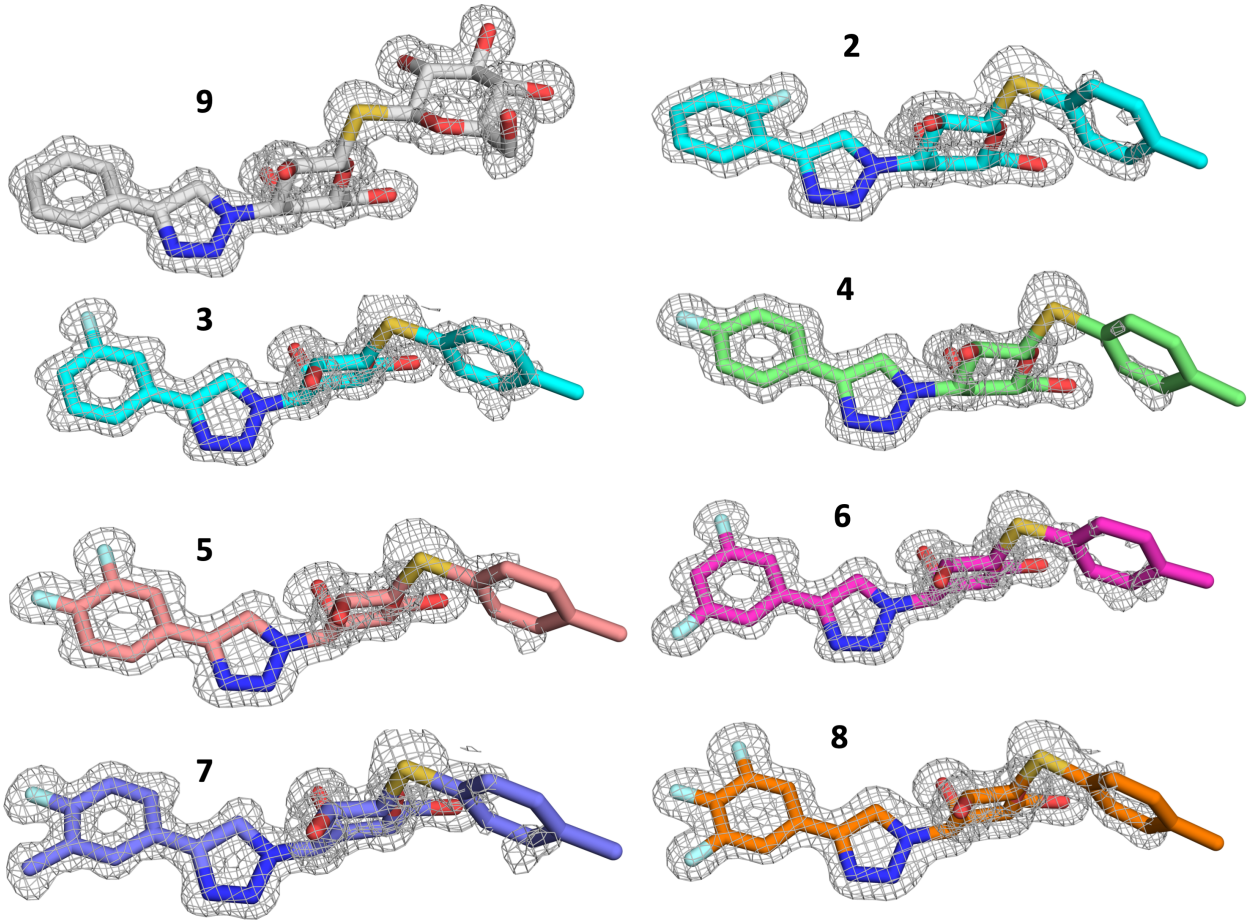


Figure S2: View of the ligands depicting their electron densities. The 2m|F_o|-D|F_c| electron density maps are contoured at 1.0 σ above the mean.

Table S1. Data processing and refinement statistics for the X-ray crystal structures.

Values in parentheses are for the highest resolution shell, unless noted otherwise.

compound	**2**	**3**	**4**	**5**
PDB code	6QLT	6QLN	6QLQ	6QLO
station	I911-3	I911-3	I911-3	I911-3
wavelength [Å]	0.9500	0.9500	0.9500	1.000
unit cell (Å)	a = 35.83 b = 57.44 c = 63.07	a = 36.91 b = 57.78 c = 62.78	a = 36.12 b = 57.48 c = 62.66	a = 36.39 b = 57.79 c = 62.85
space group	$P2_12_12_1$	$P2_12_12_1$	$P2_12_12_1$	$P2_12_12_1$
resolution range [Å]	27.65 - 1.15 (1.191 - 1.15)	27.59 - 1.0 (1.03 - 1.0)	27.51 - 1.079 (1.11 - 1.079)	30.79 - 1.18 (1.22 - 1.18)
completeness [%]	99.9 (99.9)	95.1 (91.9)	99.45 (95.8)	95.9 (92.1)
Total reflections **unique reflections**	278763 (26937) 46962 (4628)	418166 (39754) 69629 (6621)	331055 (30957) 56658 (5501)	257295(22594) 42509 (4033)
CC1/2	0.999 (0.359)	0.999 (0.752)	0.999 (0.173)	1 (0.768)
multiplicity	5.9 (5.8)	6.0 (6.0)	5.8 (5.6)	6.1 (5.6)
R_{merge} [%]	0.101 (1.8)	0.0602(0.8111)	0.115 (2.43)	0.0507(0.848)
mean I/σ(I)	13.4 (1.0)	17.4 (2.1)	10.2 (0.6)	21.4 (2.2)
Wilson B [Å^2]	10.11	7.32	9.55	10.27
refinement program	phenix.refine	phenix.refine	phenix.refine	phenix.refine
R_{model} (F) [%]	0.149 (0.303)	0.124 (0.217)	0.154 (0.357)	0.133 (0.218)
R_{free} (F) [%]	0.170 (0.318)	0.141 (0.232)	0.182 (0.379)	0.154 (0.248)
reflections used in refinement **(for R_{free})**	46961 (4628) 2280 (227)	69628 (6622) 3541 (316)	56502 (5353) 2907 (245)	42508 (4034) 2137 (196)
average B-factors [Å^2]	protein: 12.2 ligand: 19.9 solvent: 25.7	protein: 8.4 ligand: 11.9 solvent: 24.9	protein: 12.3 ligand: 23.0 solvent: 26.8	protein: 12.2 ligand: 17.9 solvent: 26.3
Ramachandran outliers [%]	0.0	0.0	0.0	0.0
rotamer outliers [%] **MolProbity clash score**	0.74 2.92	1.42 1.21	0.00 1.26	0.0 1.68
bond length rmsd from ideal [Å] **bond angle rmsd from ideal [°]**	0.014 1.59	0.012 1.71	0.006 0.97	0.009 1.09

compound	**6**	**7**	**8**	**9**
PDB code	6QLR	6QLU	6QLP	6QLS
station	I911-3	I911-3	ID23-1	BioMAX
wavelength [Å]	1.0000	0.9500	0.9762	0.635784
unit cell (Å)	a = 36.77 b = 57.82 c = 62.70	a = 36.90 b = 57.68 c = 62.89	a = 35.78 b = 57.27 c = 62.61	a = 36.48 b = 58.66 c = 63.12
space group	$P2_12_12_1$	$P2_12_12_1$	$P2_12_12_1$	$P2_12_12_1$
resolution range [Å]	31.4 - 0.97 (1.00 - 0.97)	27.6 - 1.1 (1.14 - 1.1)	31.1 - 1.08 (1.12 - 1.08)	22.1 - 1.04 1.08 - 1.04
completeness [%]	98.4 (88.0)	99.5 (96.0)	99.5 (98.2)	99.4 (96.3)
Total reflections **unique reflections**	341914 (23765) 78756 (7095)	315434 (20465) 55014 (5249)	264147 (23854) 55562 (5440)	422720 (39340) 64101 (6158)
CC1/2	0.999 (0.320)	1.000 (0.850)	1.000 (0.210)	0.999 (0.470)
multiplicity	4.3 (3.4)	5.7 (3.9)	4.8 (4.4)	6.6 (6.4)
R_{merge} [%]	0.058 (1.42)	0.048 (0.437)	0.056 (1.850)	0.091 (1.210)
mean I/σ(I)	13.8 (0.8)	22.3 (2.8)	12.2 (0.7)	9.0 (1.0)
Wilson B-factor [Å^2]	7.83	7.30	13.21	10.20
refinement program	phenix.refine	phenix.refine	phenix.refine	phenix.refine
R_{model} (F) [%]	0.137 (0.370)	0.123 (0.196)	0.153 (0.353)	0.136 (0.266)
R_{free} (F) [%]	0.156 (0.375)	0.149 (0.208)	0.171 (0.391)	0.159 (0.285)
reflections used in refinement **(for R_{free})**	78560 (6913) 3933 (316)	55009 (5245) 2728 (275)	55521 (5408) 2708 (281)	63976 (6104) 3303 (294)
average B-factors [Å^2]	protein: 9.5 ligand: 17.9 solvent: 25.2	protein: 8.5 ligand: 13.5 solvent: 22.4	protein: 18.1 ligand: 23.1 solvent: 28.3	protein: 11.5 ligand: 12.3 solvent: 27.7
Ramachandran outliers [%]	0.0	0.0	0.0	0.0
rotamer outliers [%] **MolProbity clash score**	0.0 2.06	0.00 1.28	0.74 2.90	0.0 2.80
bond length rmsd from ideal [Å] **bond angle rmsd from ideal [°]**	0.008 1.07	0.009 1.15	0.014 1.56	0.011 1.24