Supporting Information for Publication

Discovery of Potent and Selective Inhibitors for G9a-Like Protein (GLP) Lysine Methyltransferase

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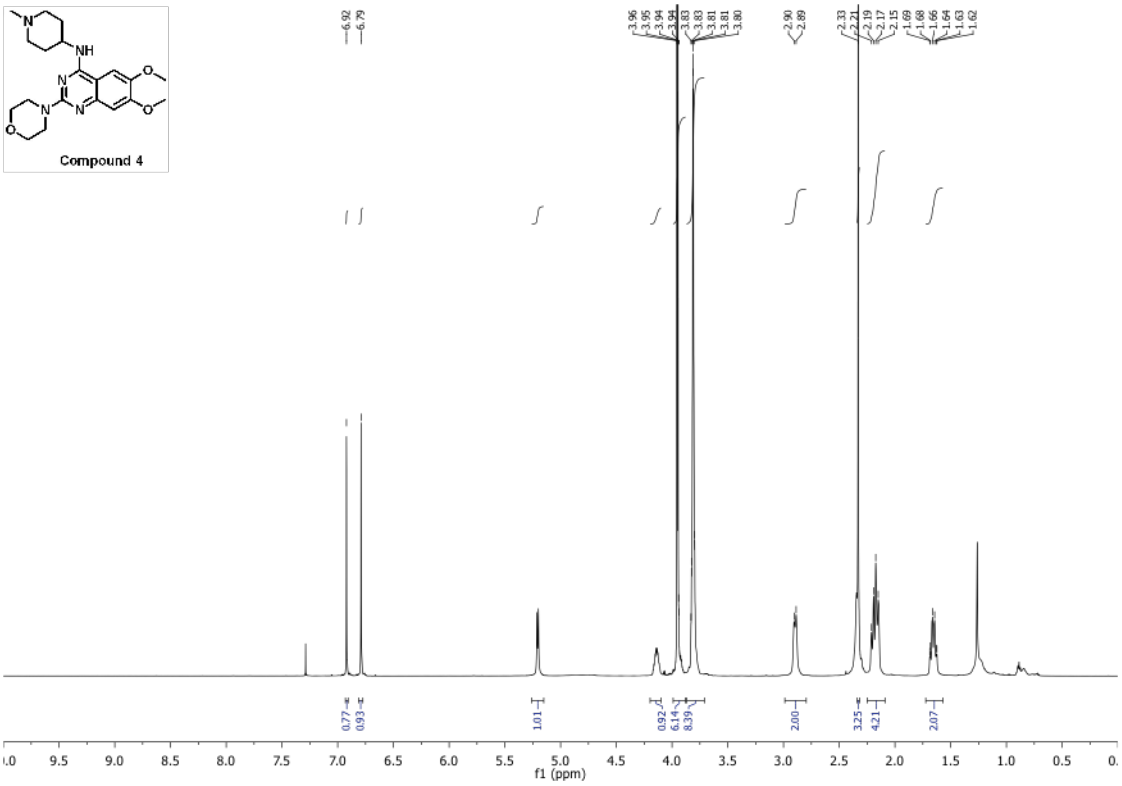
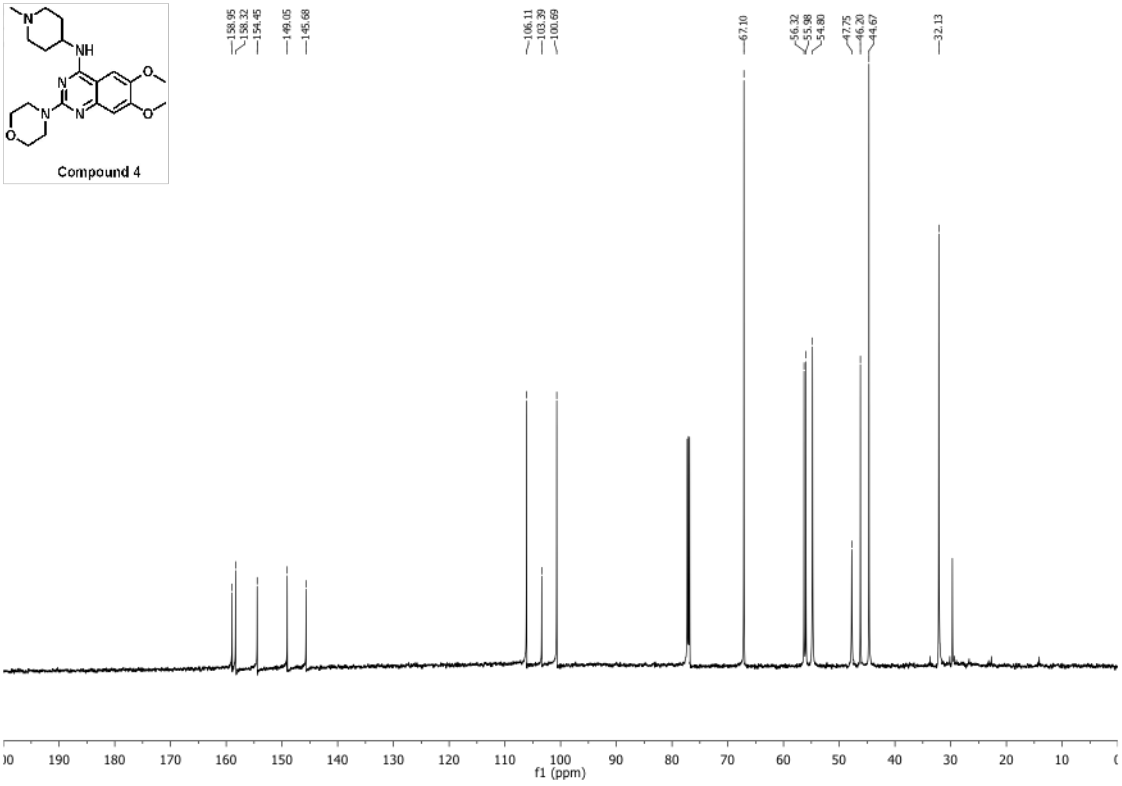
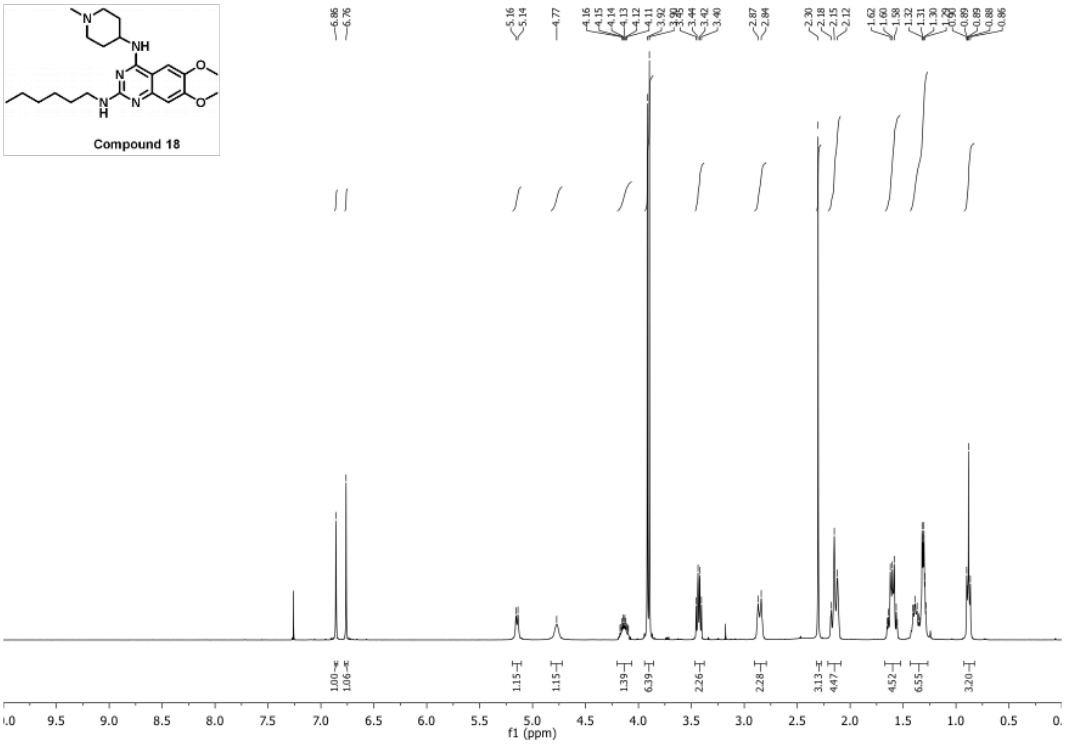
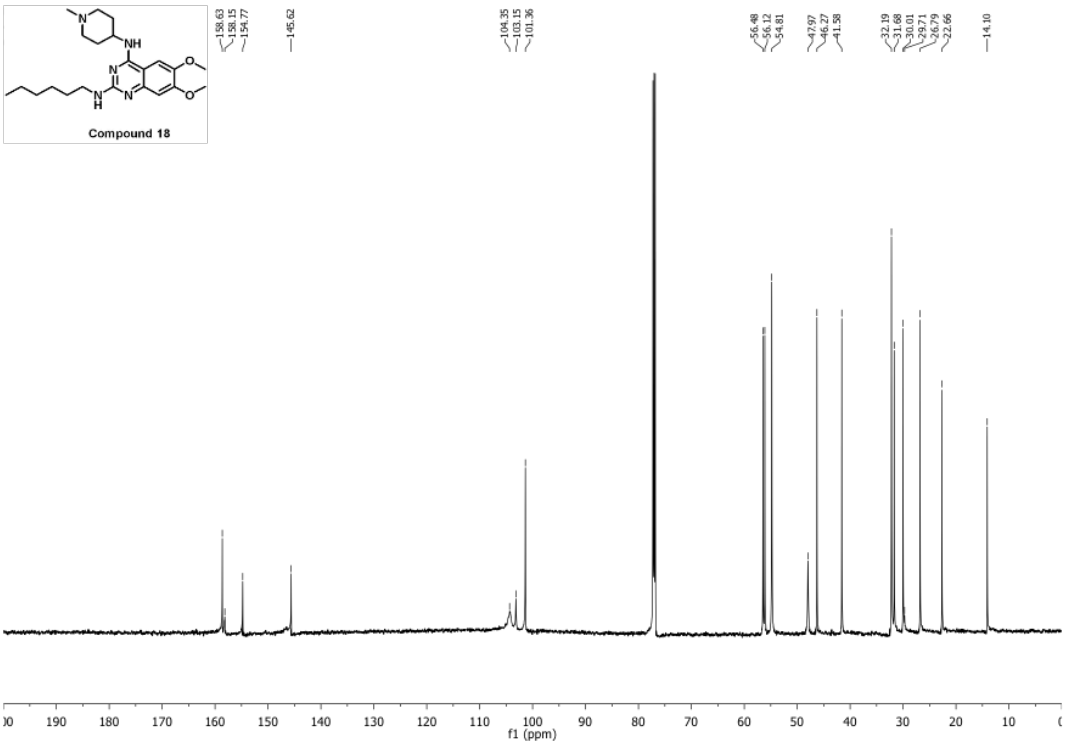
NMR spectra of compound **4**





^{1}H and ^{13}C NMR spectra of **18**





Supporting Table S1. Crystallography data and refinement statistics for 4.

	GLP-SAM/**4**	G9a-SAM/**4**
Data collection		
Space group	$P2_12_12_1$	P1211
Cell dimensions		
a, *b*, *c* (Å)	74.94, 95.78, 102.36	56.97, 82.30, 73.74
α, β, γ (°)	90.00, 90.00, 90.00	90.00, 89.97, 90.00
Molecule per asymmetric unit	2	2
Resolution (Å)	74.94-1.95 (2.06-1.95)*	82.30-2.60 (2.74-2.60)*
R_{sym}	0.146 (0.655)	0.207 (0.728)
$I/\sigma I$	10.5 (3.2)	4.9 (1.8)
Completeness (%)	99.8 (99.7)	100.0 (100.0)
Redundancy	6.8 (6.1)	3.9 (3.9)
Refinement		
Resolution (Å)	1.95	2.60
No. unique reflections	54301 (7802)	21095 (3083)
R_{work}/ R_{free}	0.160/0.198	0.171/0.234
No. atoms /average B-factor [Å2]	4640/25.2	4484/33.4
Protein	4174/25.1	4210/38.9
Zn	8/17.6	8/32.6
SAM	54/40.2	54/25.4
Compound	56/30.4	56/34.7
Other	8/42.5	0/0
Water	340/26.4	156/24.3
R.m.s deviations		

Bond lengths (Å)	0.008	0.010
Bond angles (º)	1.09	1.1
Ramachandran plot		
Most favoured (%)	95.9	95.8
Additional allowed (%)	4.1	3.4
Outliers (%)	0	0.8
Protein Data Bank entry	5TUZ	5TUY

*The values in parentheses refer to statistics in the highest bin.

Supporting Table S2. Crystallography data and refinement statistics for 18.

	GLP-SAM/**18**	G9a-SAM/**18**
Data collection		
Space group	$P2_12_12_1$	P1
Cell dimensions		
a, *b*, *c* (Å)	74.43,95.90,102.11	56.85, 67.75, 77.85
α, β, γ (°)	90.00, 90.00, 90.00	92.10,90.05,91.80
Molecule per asymmetric unit	2	4
Resolution (Å)	50.00-1.66 (1.69-1.66)*	50.00-1.72 (1.75-1.72)*
R_{sym}	0.118 (0.883)	0.075 (0.550)
$I/\sigma I$	25.2 (2.3)	23.9 (1.7)
Completeness (%)	100.00 (100.0)	96.4 (83.5)
Redundancy	6.8 (6.5)	3.1 (2.5)
Refinement		
Resolution (Å)	1.66	1.72
No. of reflections	84739 (1745)	117616(1275)
R_{work}/ R_{free}	0.170/0.192	0.206/0.247
No. atoms /average B-factor [Å2]	5094/22.4	9228/29.8
Protein	4338/21.0	8420/29.6
Zn	8/15.6	16/25.4
SAM	54/20.8	108/26.6
Compound	49/23.9	96/36.0
Water	645/32.1	588/32.1
R.m.s deviations		
Bond lengths (Å)	0.009	0.011

Bond angles (º)	1.448	1.488
Ramachandran plot		
Most favoured (%)	96.6	95.4
Additional allowed (%)	3.4	4.6
Outliers (%)	0	0
Protein Data Bank entry	5TTG	5TTF

*The values in parentheses refer to statistics in the highest bin.