

## Electronic Supplementary Information

# 7-Substituted 8-aza-7-deazaadenosine for modification of the siRNA major groove

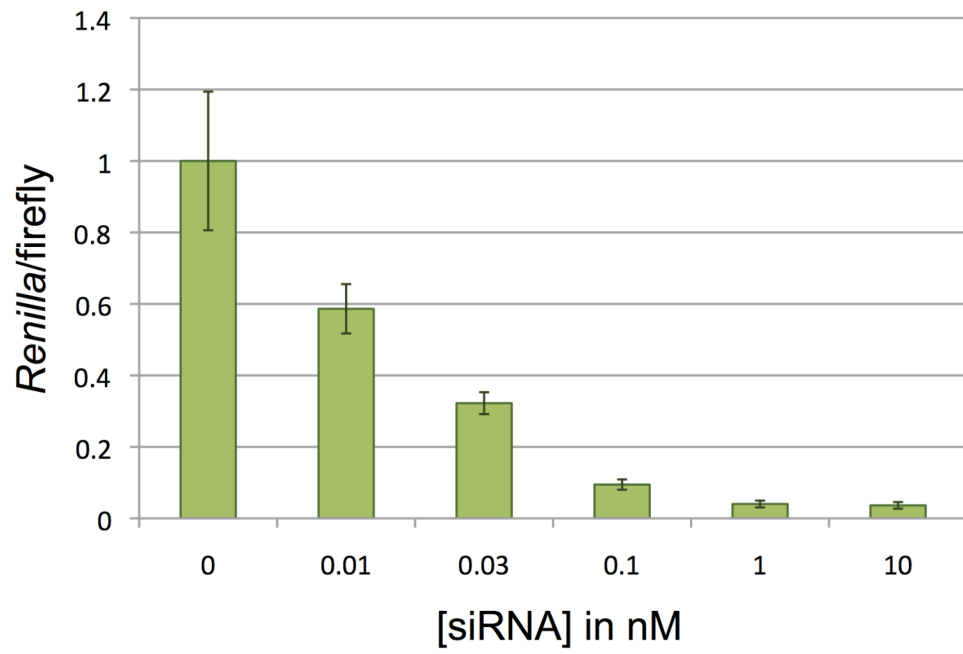
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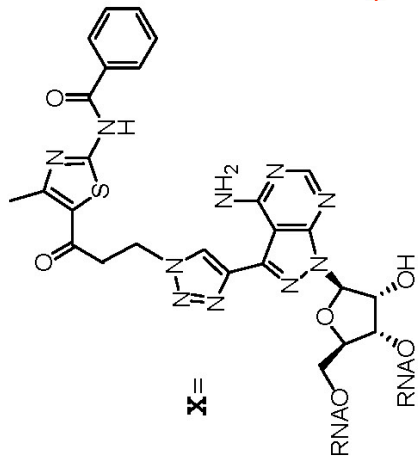
**Supplementary Information Table 1:**  $T_m$  data for all 12-bp RNA duplexes reported in **Figure 3**.

<b>X =</b>	<b>Y=</b>	<b>Ave <math>T_m</math> (°C)</b>	<b>Std Dev (°C)</b>	<b>Temp start (°C)</b>	<b>Temp end (°C)</b>
<b>Adenosine</b>	U	43.1	0.6	10	65
	C	34.2	0.5	10	60
	A	32.4	0.4	10	60
	G	32.5	0.5	10	60
<b>Propargyl</b>	U	41.4	1.0	12	60
	C	34.0	0.4	12	60
	A	32.7	0.2	12	60
	G	31.6	0.7	10	60
<b>Ethynyl</b>	U	39.8	0.2	10	65
	C	30.5	0.6	10	60
	A	30.9	0.3	10	60
	G	30.6	0.1	10	60
<b>Triazole I</b>	U	41.6	0.3	10	65
	C	33.2	0.7	10	60
	A	31.8	0.5	10	60
	G	31.5	0.4	10	60
<b>Triazole II</b>	U	40.3	0.5	10	65
	C	31.5	0.6	10	60
	A	30.7	0.2	10	60
	G	30.5	0.2	10	60
<b>Triazole III</b>	U	39.7	0.5	10	60
	C	32.1	0.3	14	60
	A	30.7	0.4	14	60
	G	30.4	0.8	14	60
<b>Triazole IV</b>	U	39.4	0.3	13	60
	C	31.2	0.2	13	60
	A	31.2	0.4	13	60
	G	30.5	0.5	13	60
<b>Triazole V</b>	U	34.9	1.4	15	65
	C	29.1	2.9	15	65
	A	27.5	0.4	10	50
	G	28.8	1.0	13	60
<b>Triazole VI</b>	U	35.9	0.6	15	65
	C	28.1	1.1	10	60
	A	28.0	0.6	10	50
	G	27.9	0.5	10	50



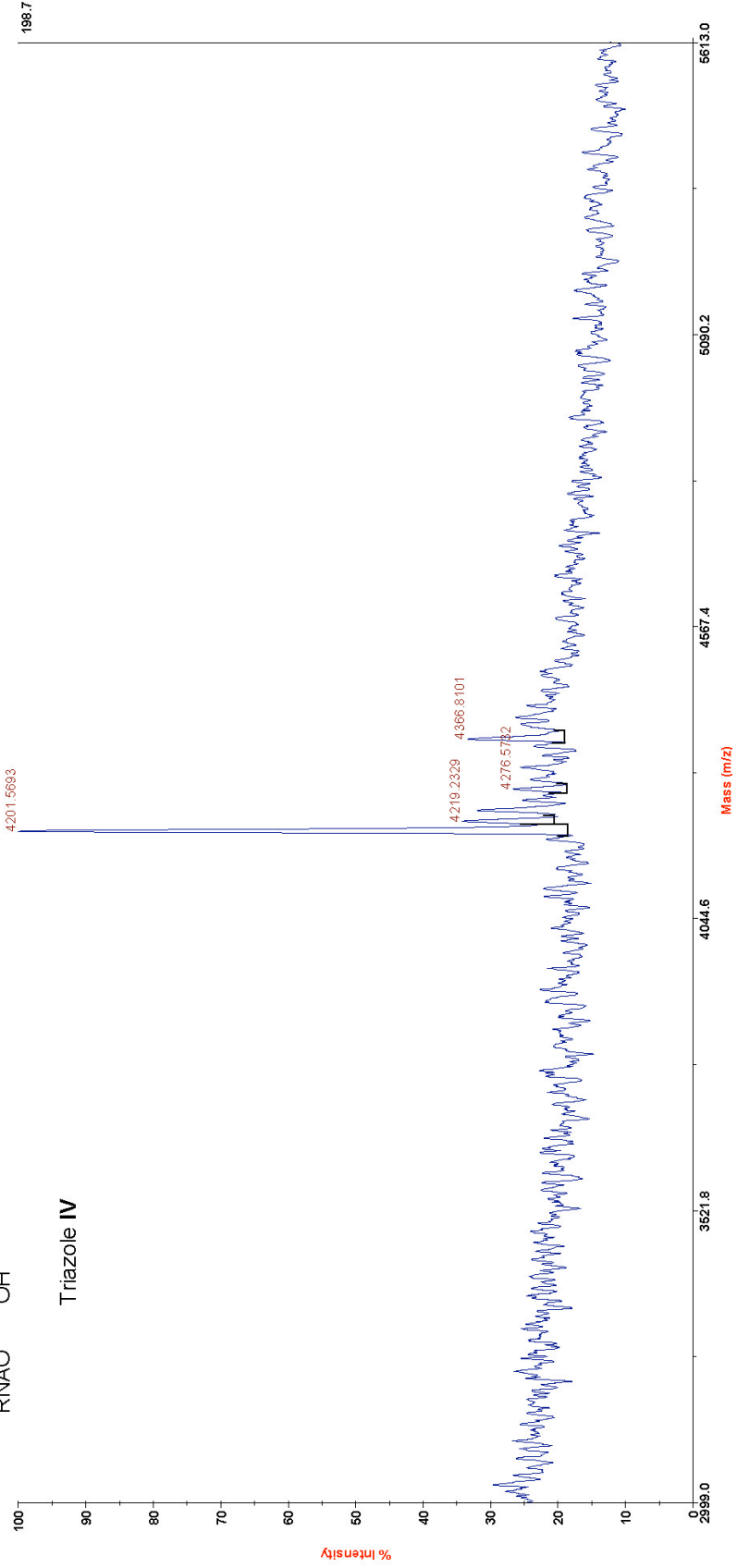
**Supplementary Figure 1:** Representative siRNA titration of the PIK3CB siRNA, modified with Triazole I at guide position 15.

5' -CAU UAX GGU GGG-3'



[M+H]<sup>+</sup>  
Calc. 4201.7  
Obs. 4201.6  
DNA standard = 4366.8 Da

4700 Linear Spec #1 MC=>SMS=>MC[BP = 4200.9, 199]



4700 Linear Spec #1 MC=>SM5=>SM5=>SM5=>SM5=>BC[BP = 4368.6, 35]

