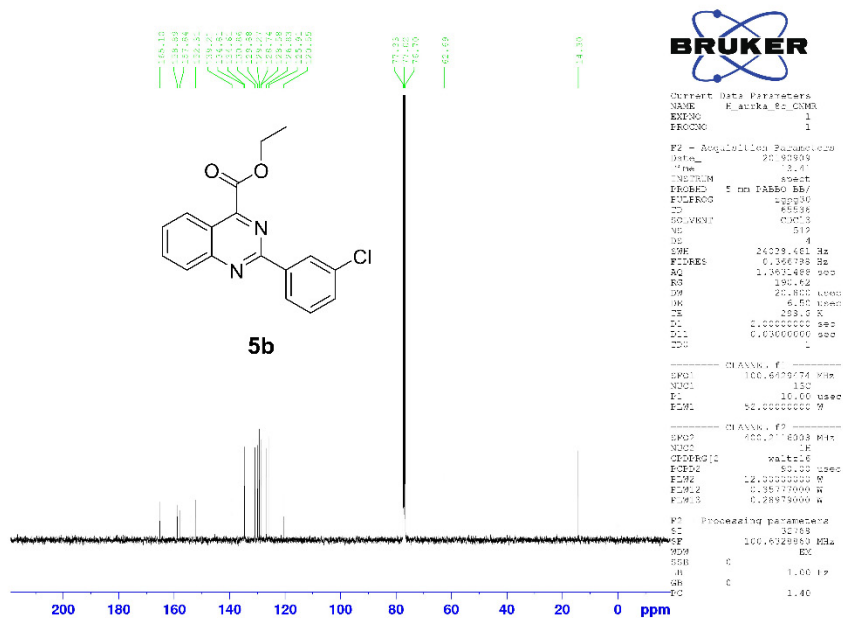
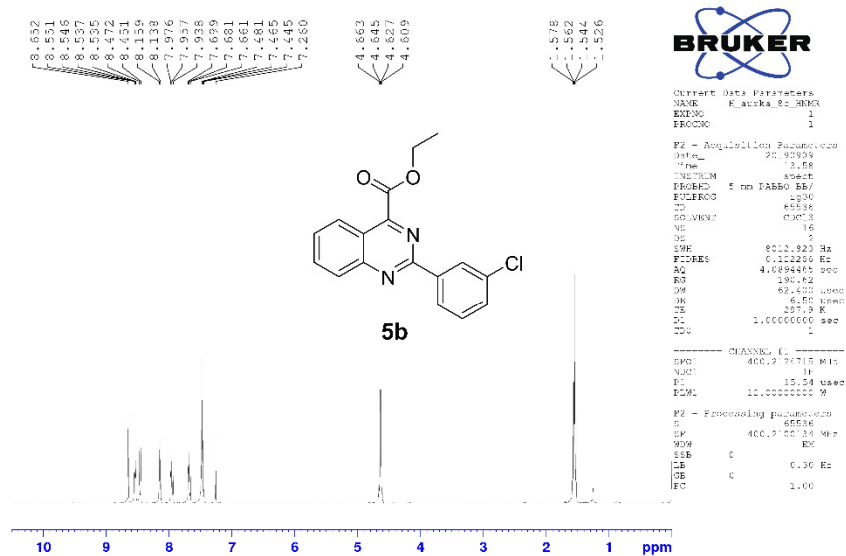


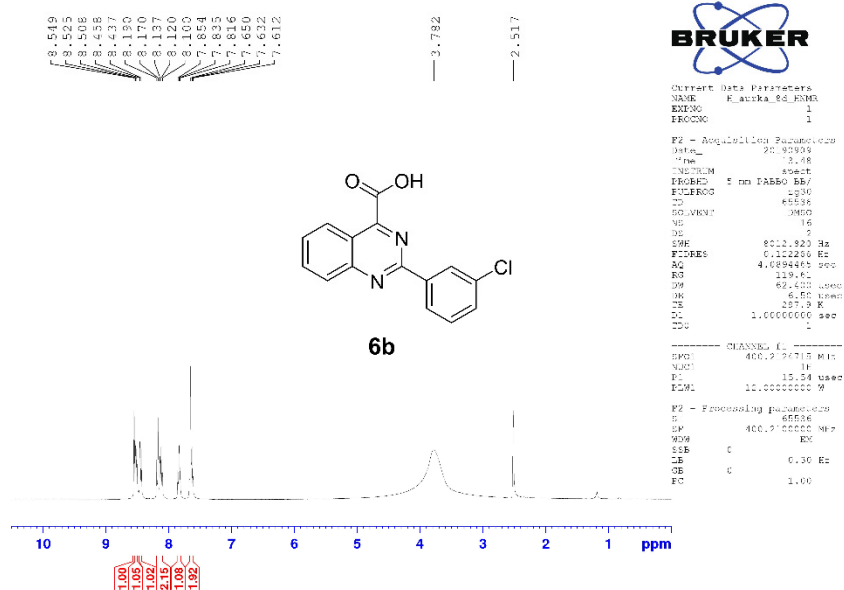
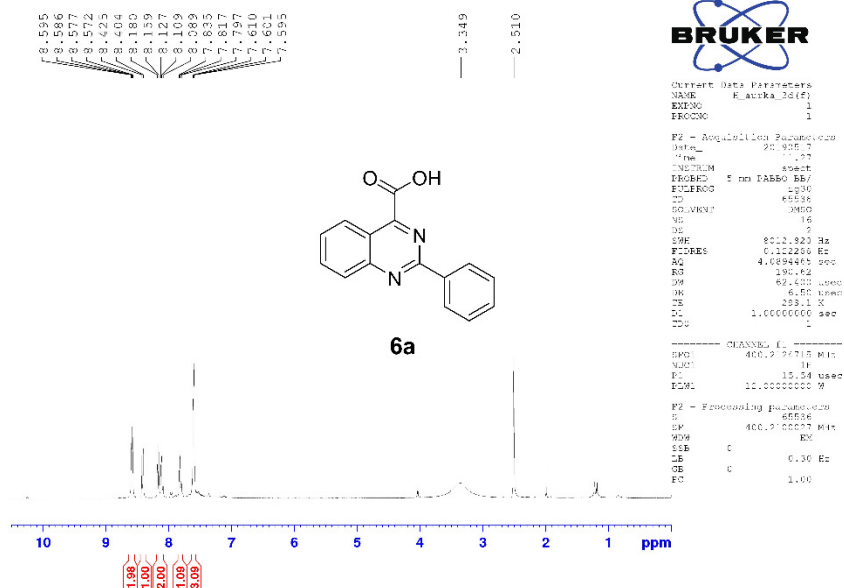
2-(3-Bromophenyl)-8-fluoroquinazoline-4-carboxylic Acid as a Novel and Selective Aurora A Kinase Inhibitory Lead with Apoptosis Properties: Design, Synthesis, In Vitro and In Silico Biological Evaluation

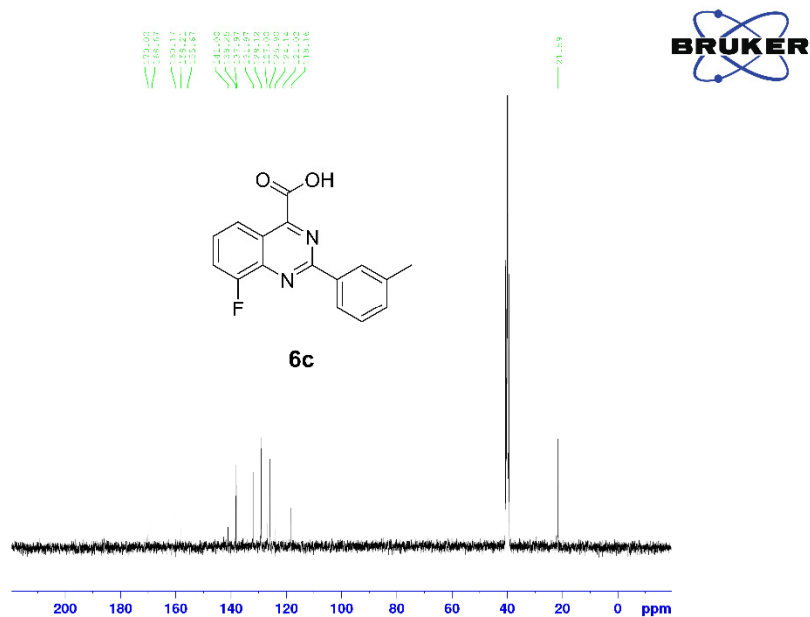
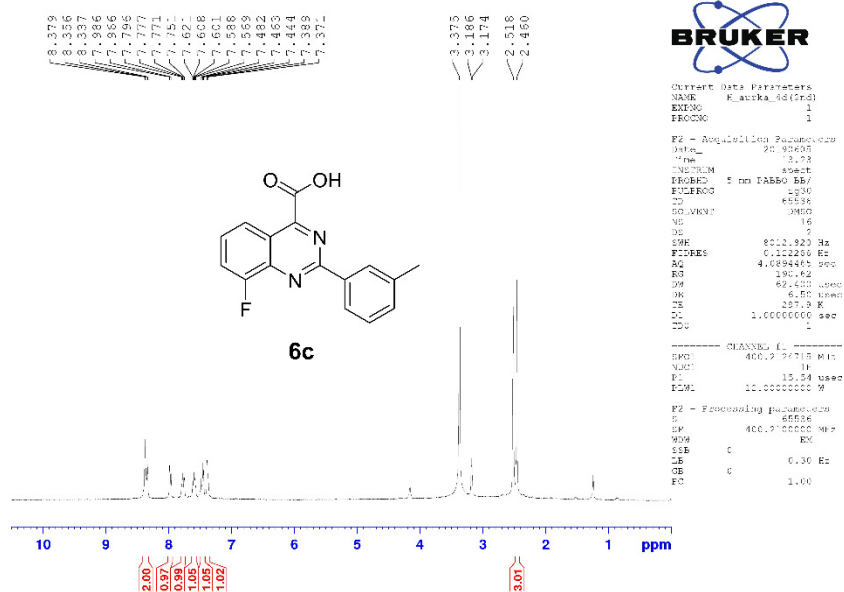
Supplementary Materials

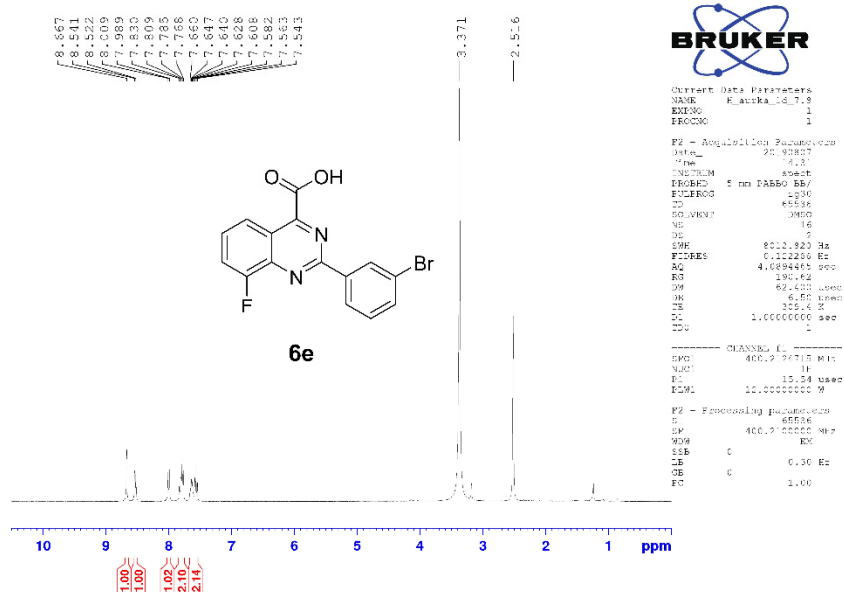
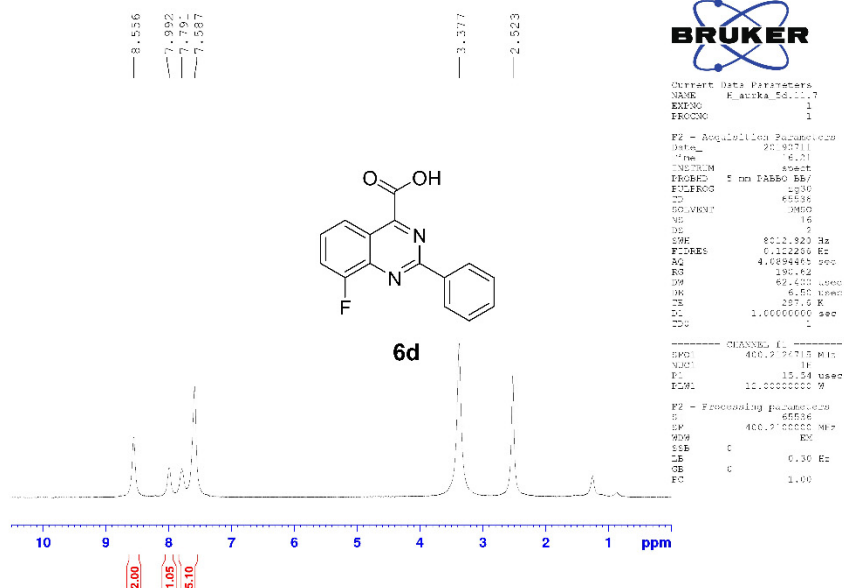
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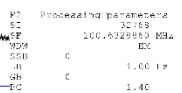
S1.1. ^1H NMR and ^{13}C NMR data.

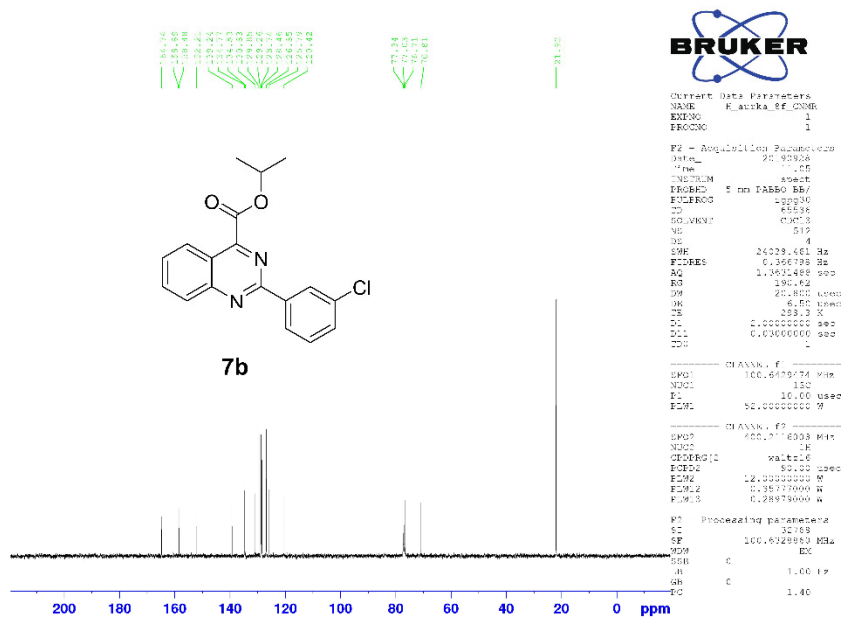
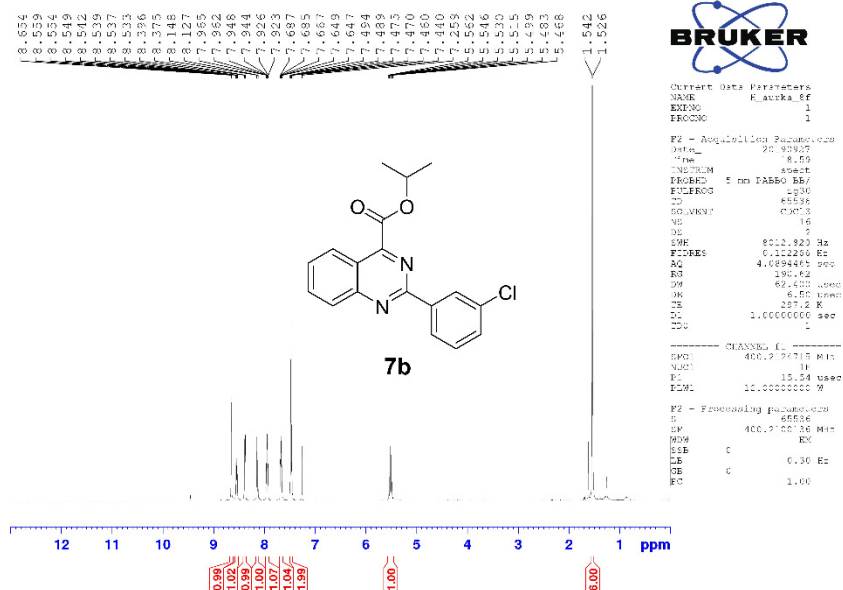






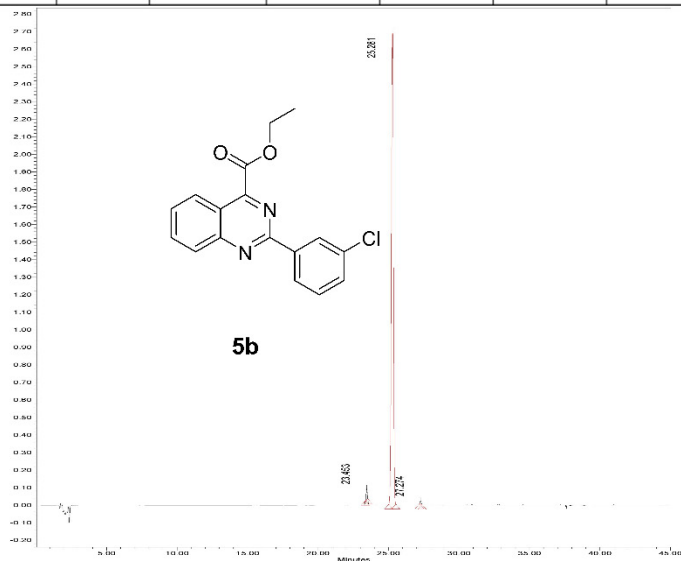




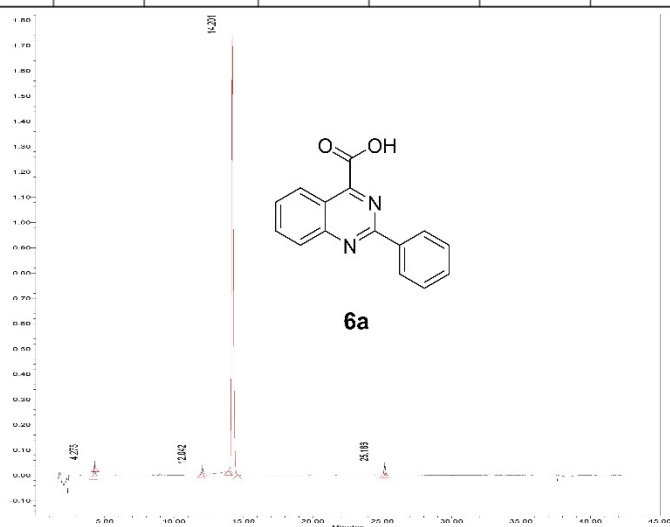


S1.2. HPLC purity data.

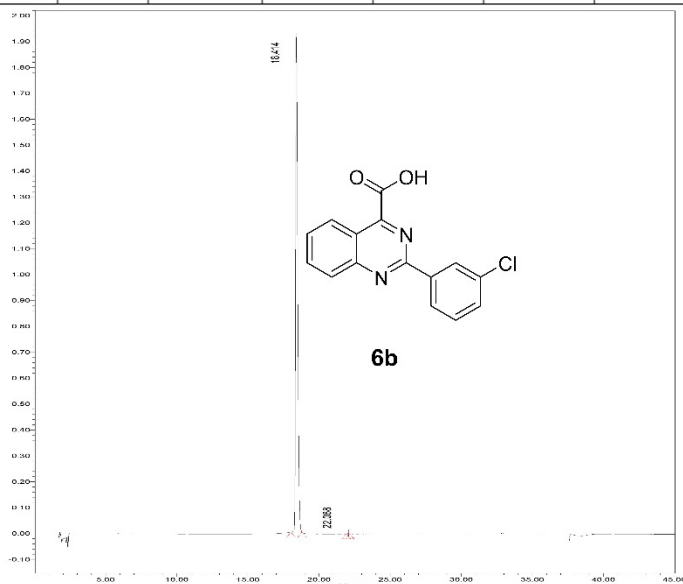
	Name	Retention Time (min)	Purity1 Angle	Purity1 Threshold	PDA Match1 Spect. Name	PDA Match1 Angle	PDA Match1 Threshold	PDA Match1 Lib. Name	Area (μV*sec)	% Area	Height (μV)	Int Type	Amount
1		23.453							359039	1.25	61587	bb	
2		25.281							28253726	98.39	2696270	bb	
3		27.274							102511	0.36	17051	bb	



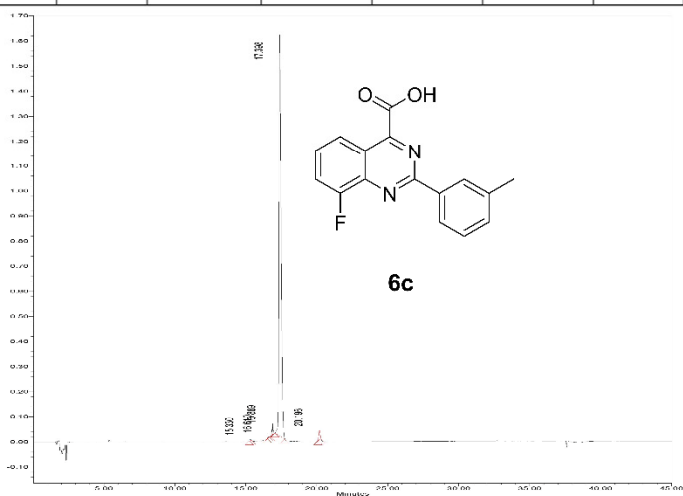
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1		4.275							69216	0.43	19709	bb	
2		12.042							84239	0.52	16232	bb	
3		14.201							15812613	97.79	1723518	bb	
4		25.186							203671	1.26	30833	bb	



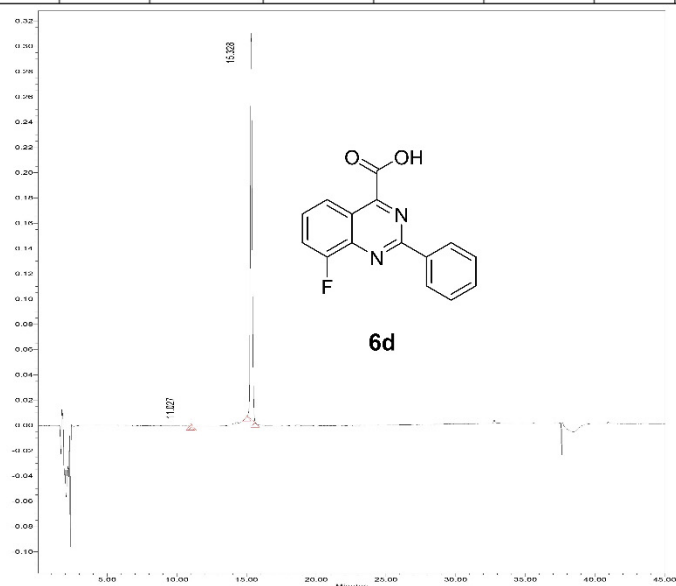
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1		18.414							19695683	99.93	1917425	bb	
2		22.068							13558	0.07	1639	bb	



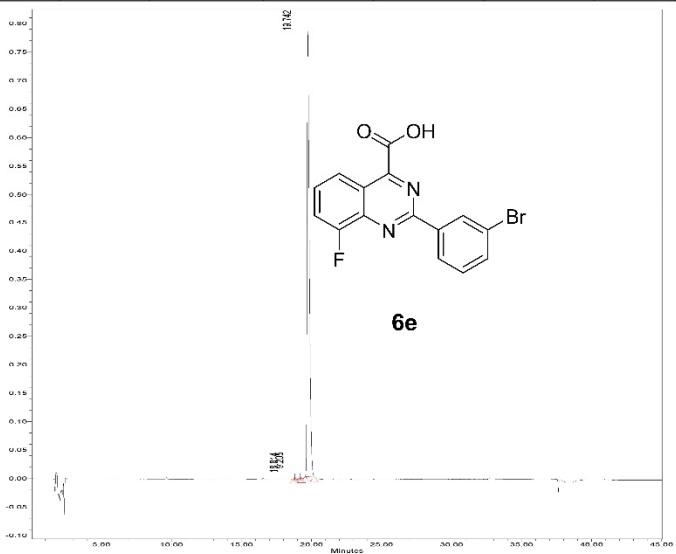
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1		15.330							25297	0.15	4601	bb	
2		16.610							18741	0.11	3390	bb	
3		16.889							199424	1.19	29974	bb	
4		17.398							16311815	97.03	1591978	bb	
5		20.196							256282	1.52	37135	bb	



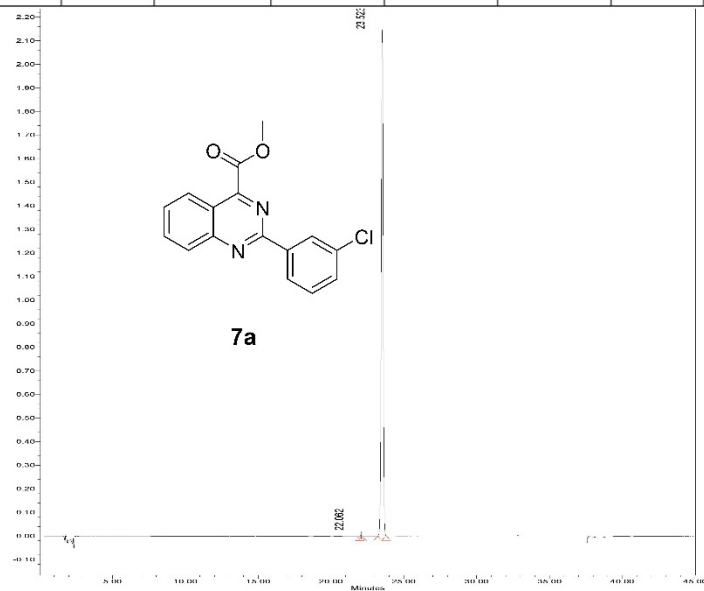
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1		11.027							5965	0.21	1155	bb		
2		15.328							2839909	99.79	303738	bb		



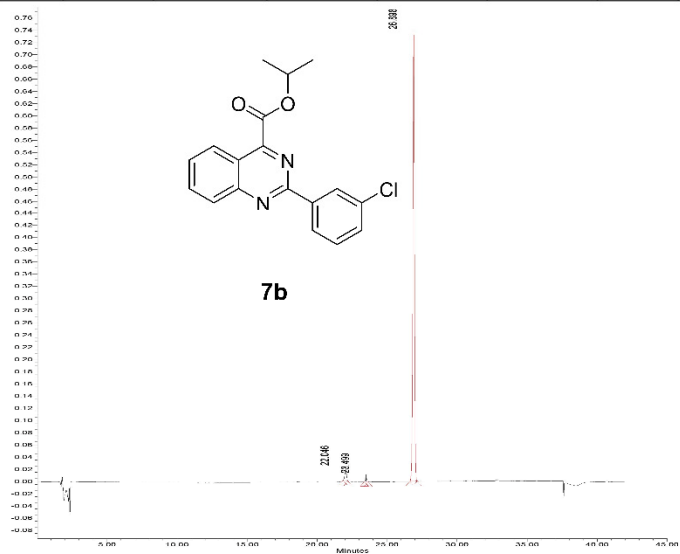
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1		18.814							4641	0.05	1212	bb		
2		19.205							7994	0.09	1605	bb		
3		19.742							8817287	99.86	786244	bb		



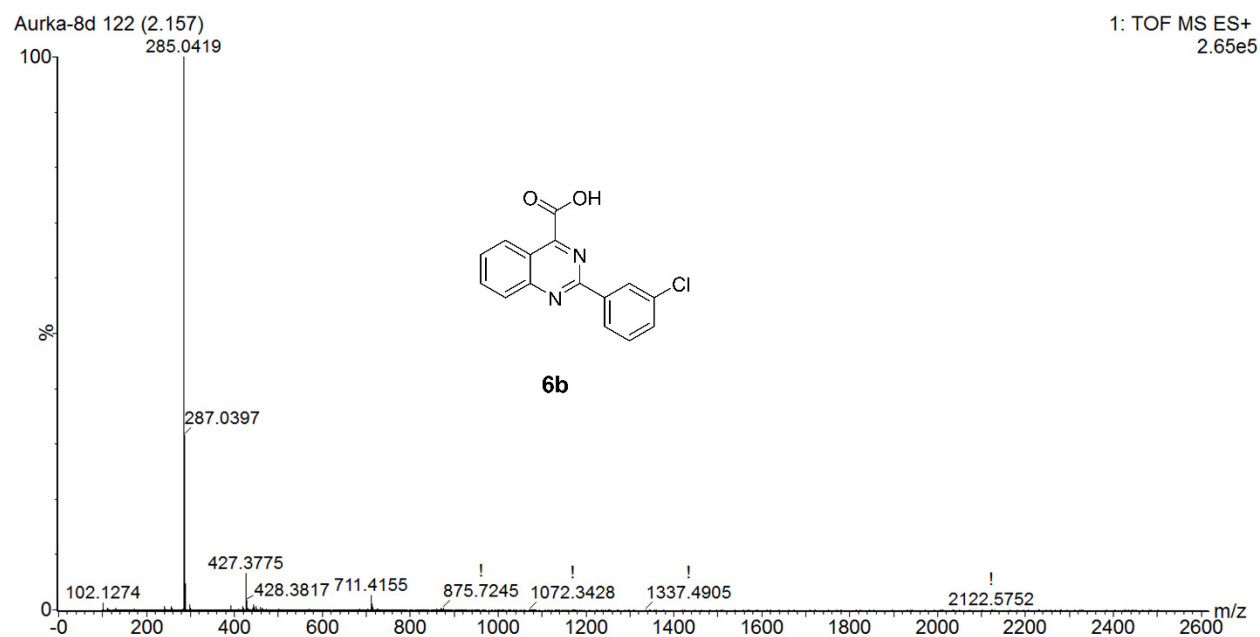
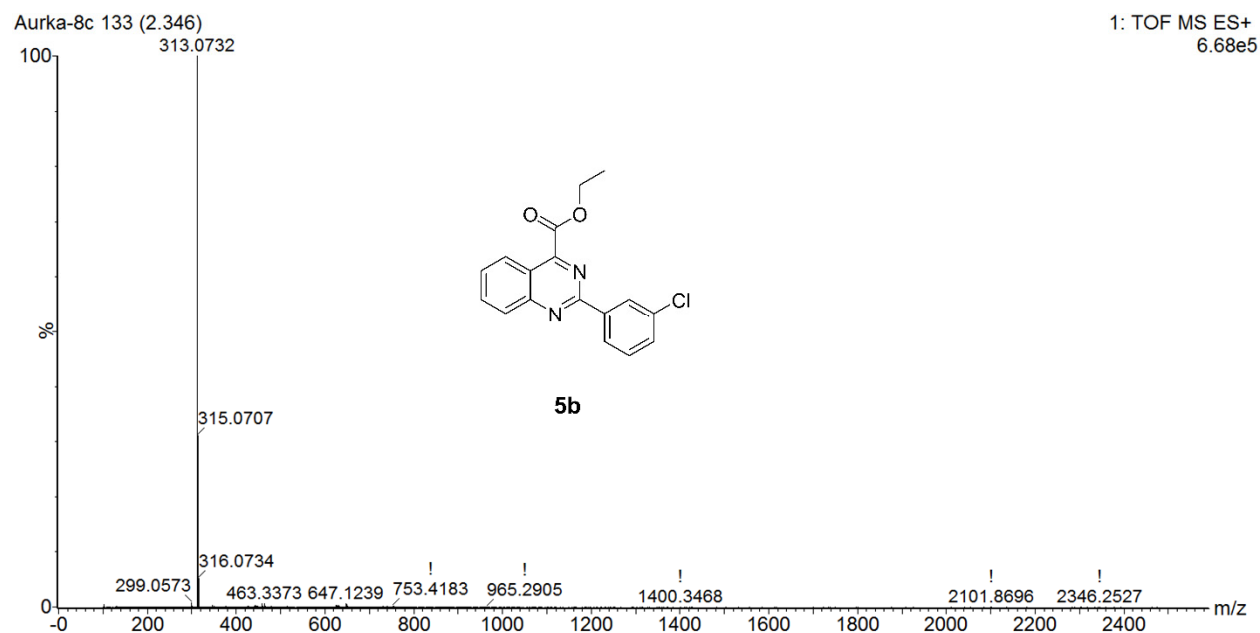
	Name	Retention Time (min)	Purity1 Angle	Purity1 Threshold	PDA Match1 Spect. Name	PDA Match1 Angle	PDA Match1 Threshold	PDA Match1 Lib. Name	Area (μV*sec)	% Area	Height (μV)	Int Type	Amount
1		22.062							9042	0.04	1651	bb	
2		23.523							20322738	99.96	2142776	bb	

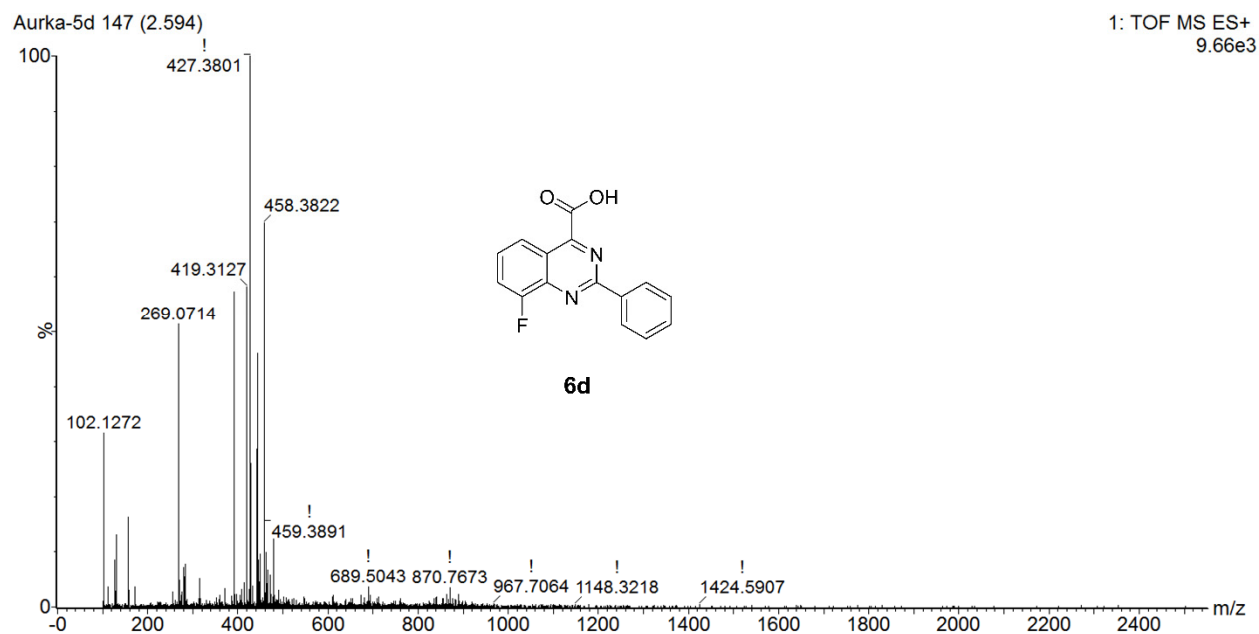
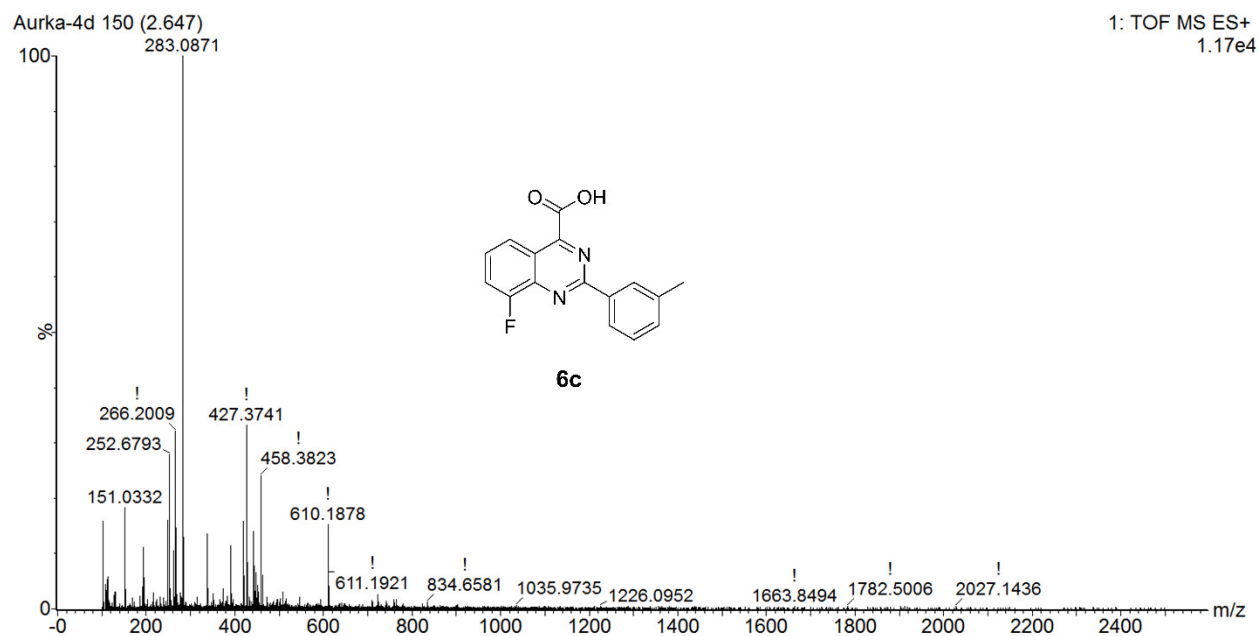


	Name	Retention Time (min)	Purity1 Angle	Purity1 Threshold	PDA Match1 Spect. Name	PDA Match1 Angle	PDA Match1 Threshold	PDA Match1 Lib. Name	Area (μV*sec)	% Area	Height (μV)	Int Type	Amount	Units
1		22.046							157671	2.48	16978	bb		
2		23.499							46452	0.73	6084	bb		
3		26.898							6157710	96.79	737125	bb		



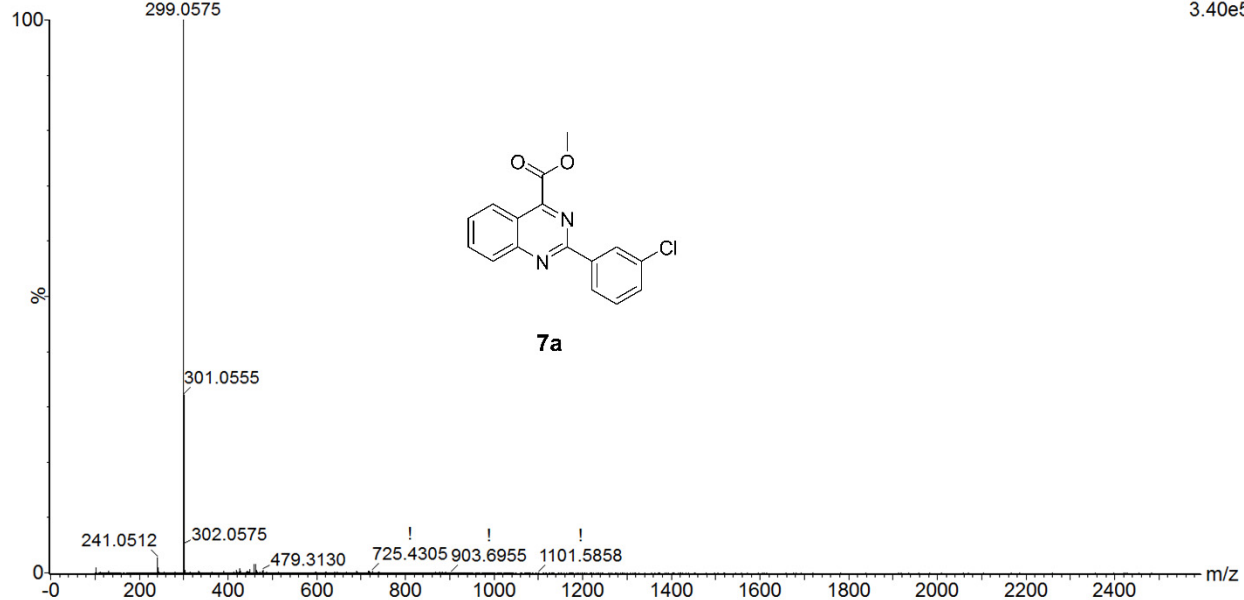
S1.3. Representative HRMS data.





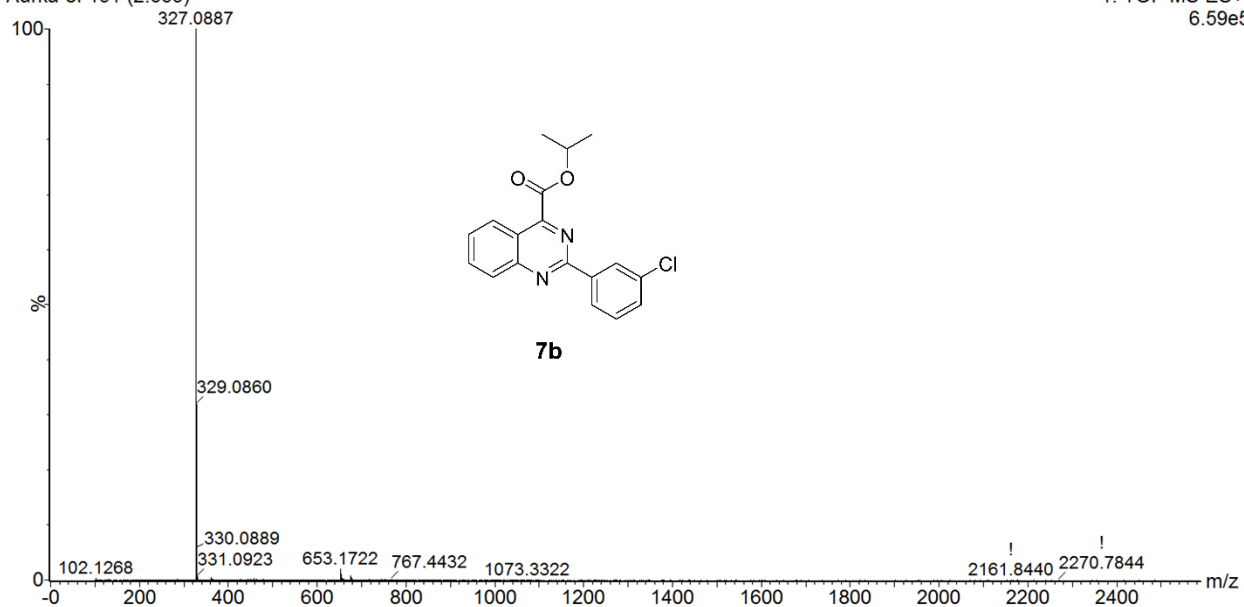
Aurka-8e 123 (2.174)

1: TOF MS ES+
3.40e5



Aurka-8f 151 (2.663)

1: TOF MS ES+
6.59e5



S2. In vitro screening

Table S1. NCI results of compound 5b.

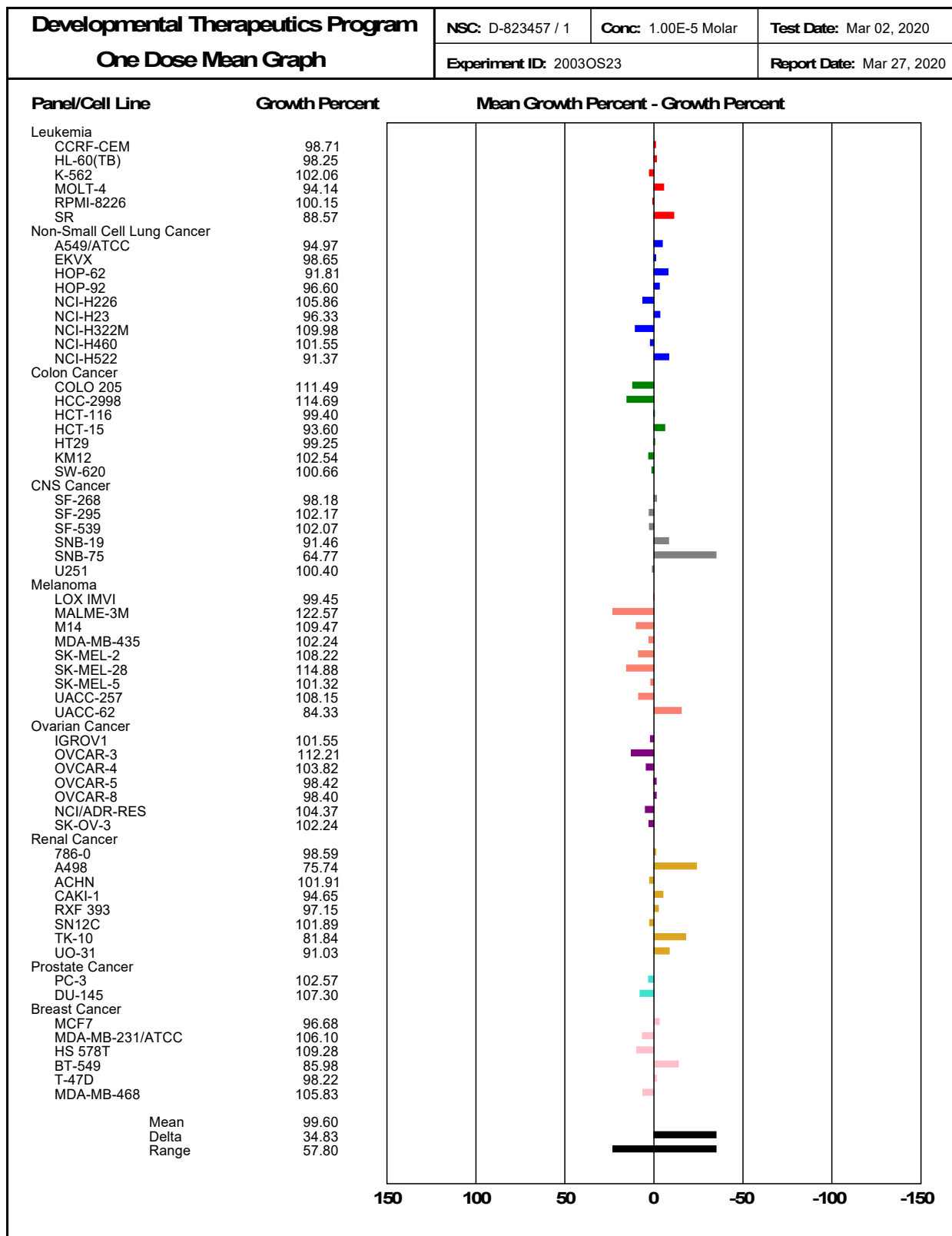


Table S2. NCI results of compound 6a.

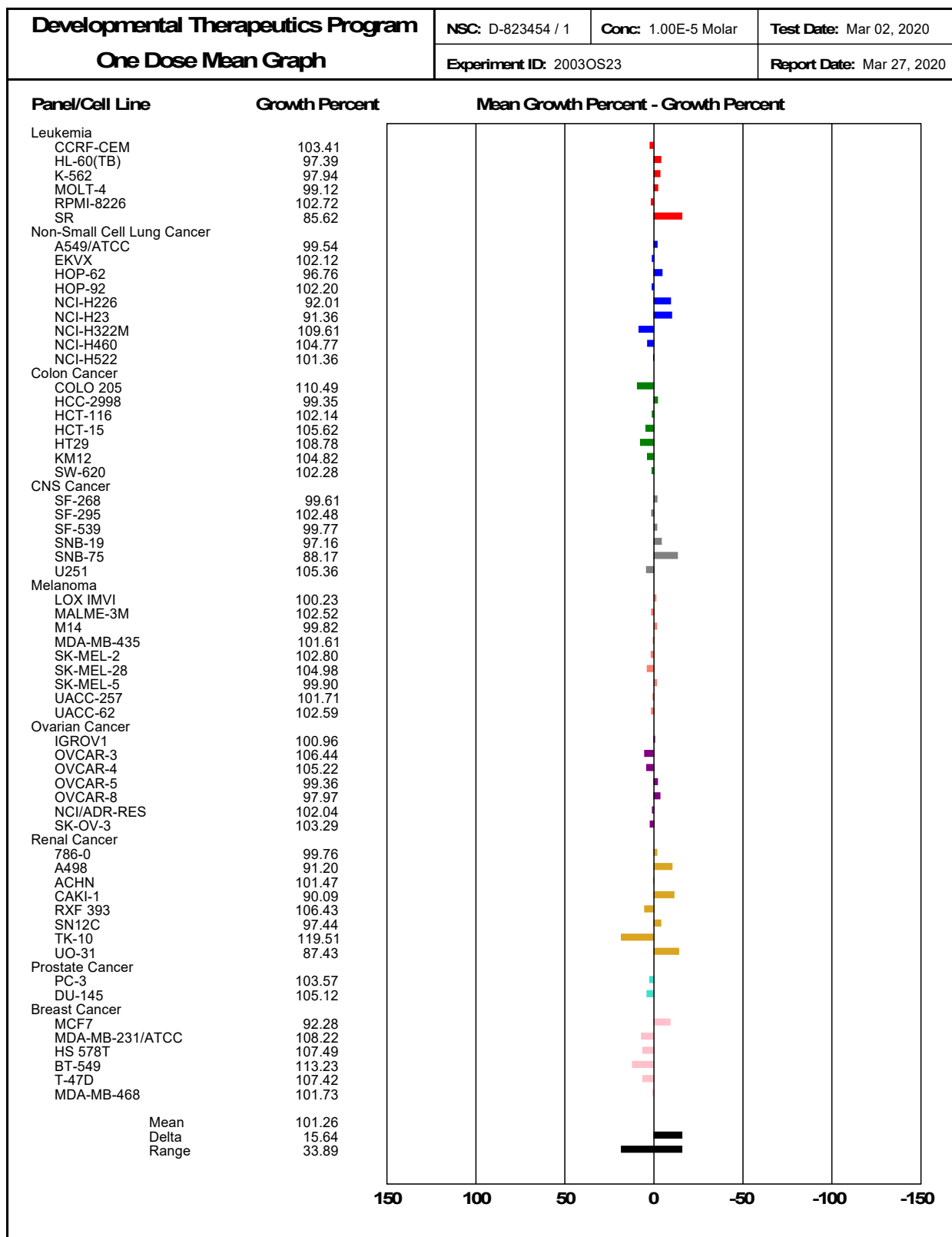


Table S3. NCI results of compound 6b.

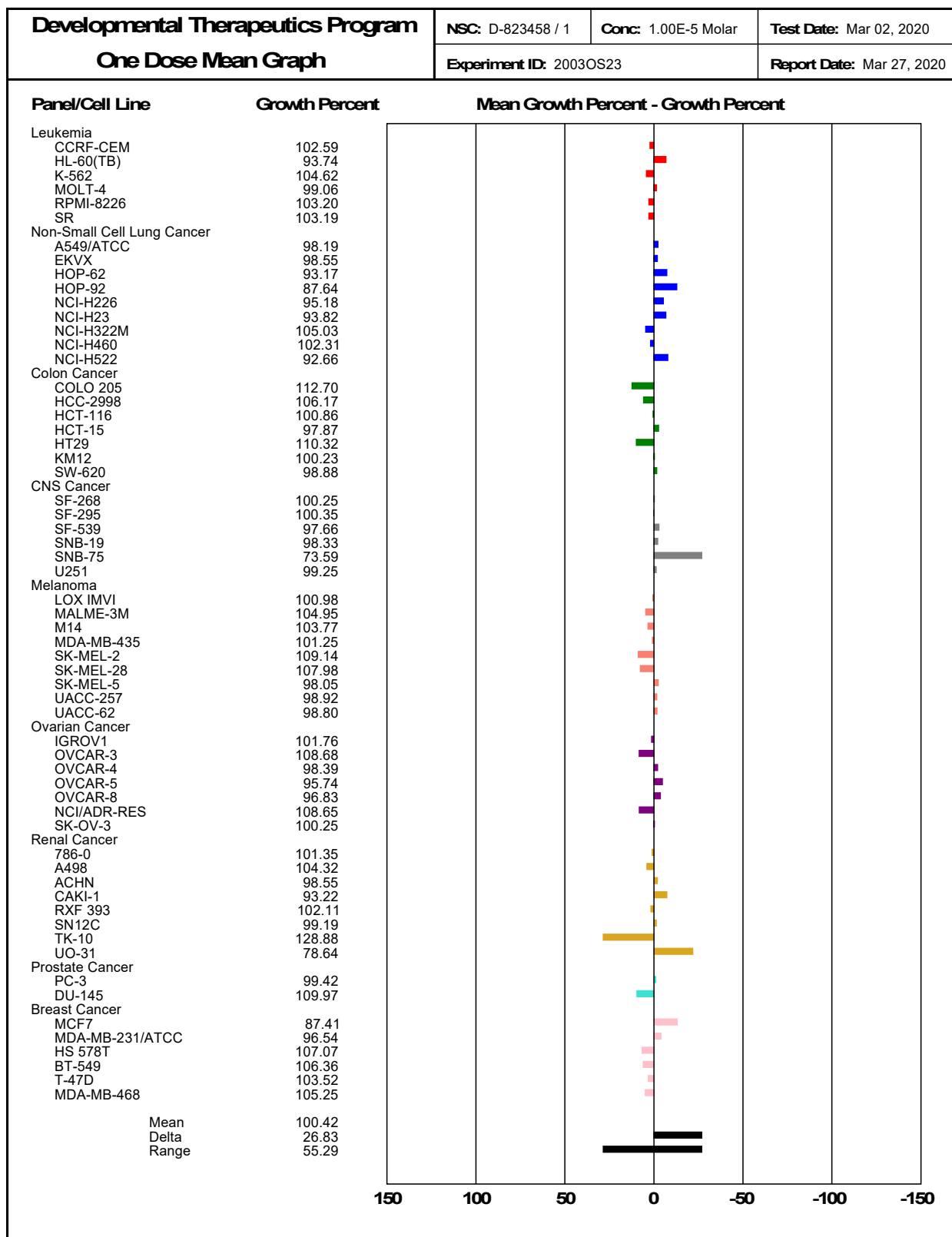


Table S4. NCI results of compound 6c.

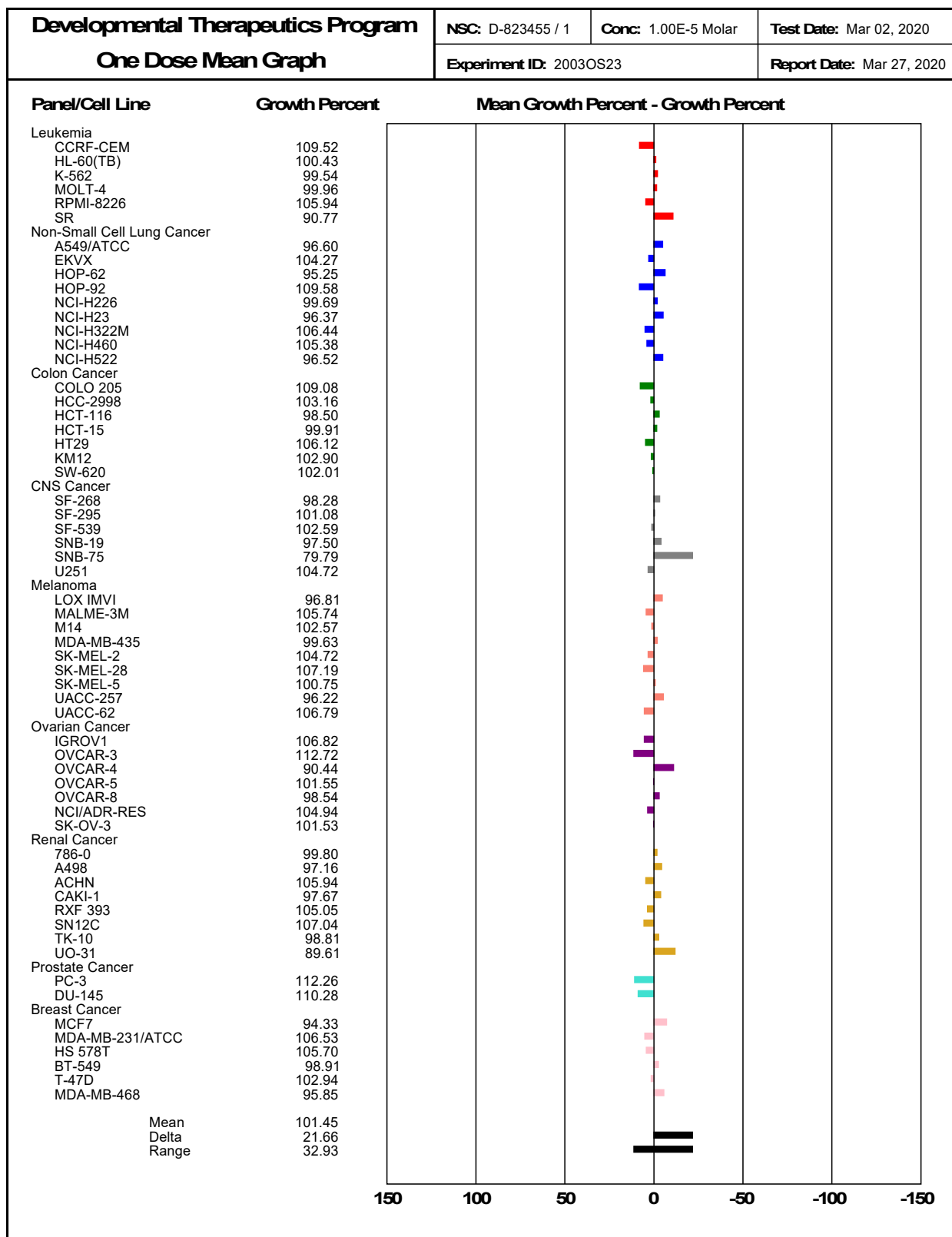


Table S5. NCI results of compound 6d.

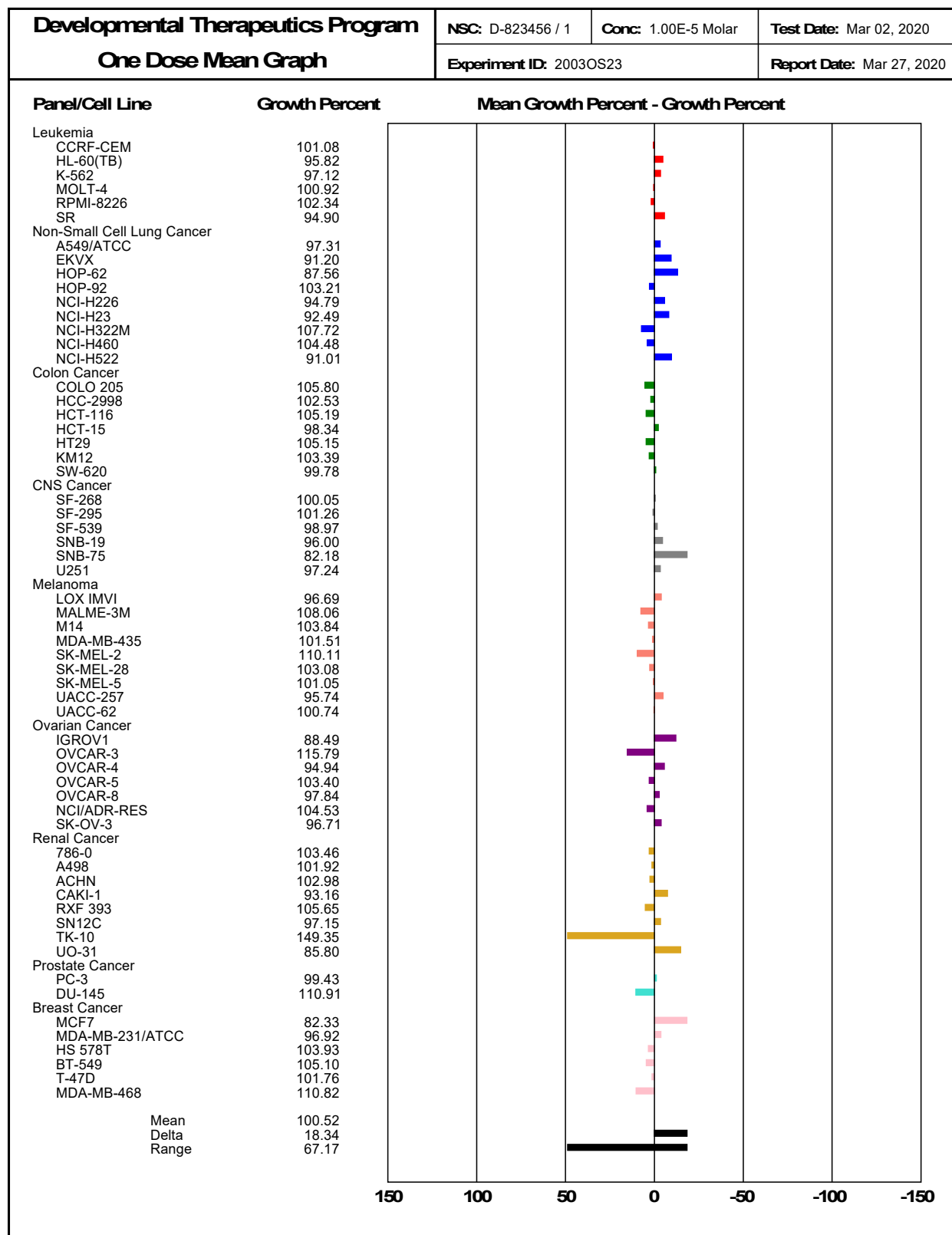


Table S6. NCI results of compound 6e.

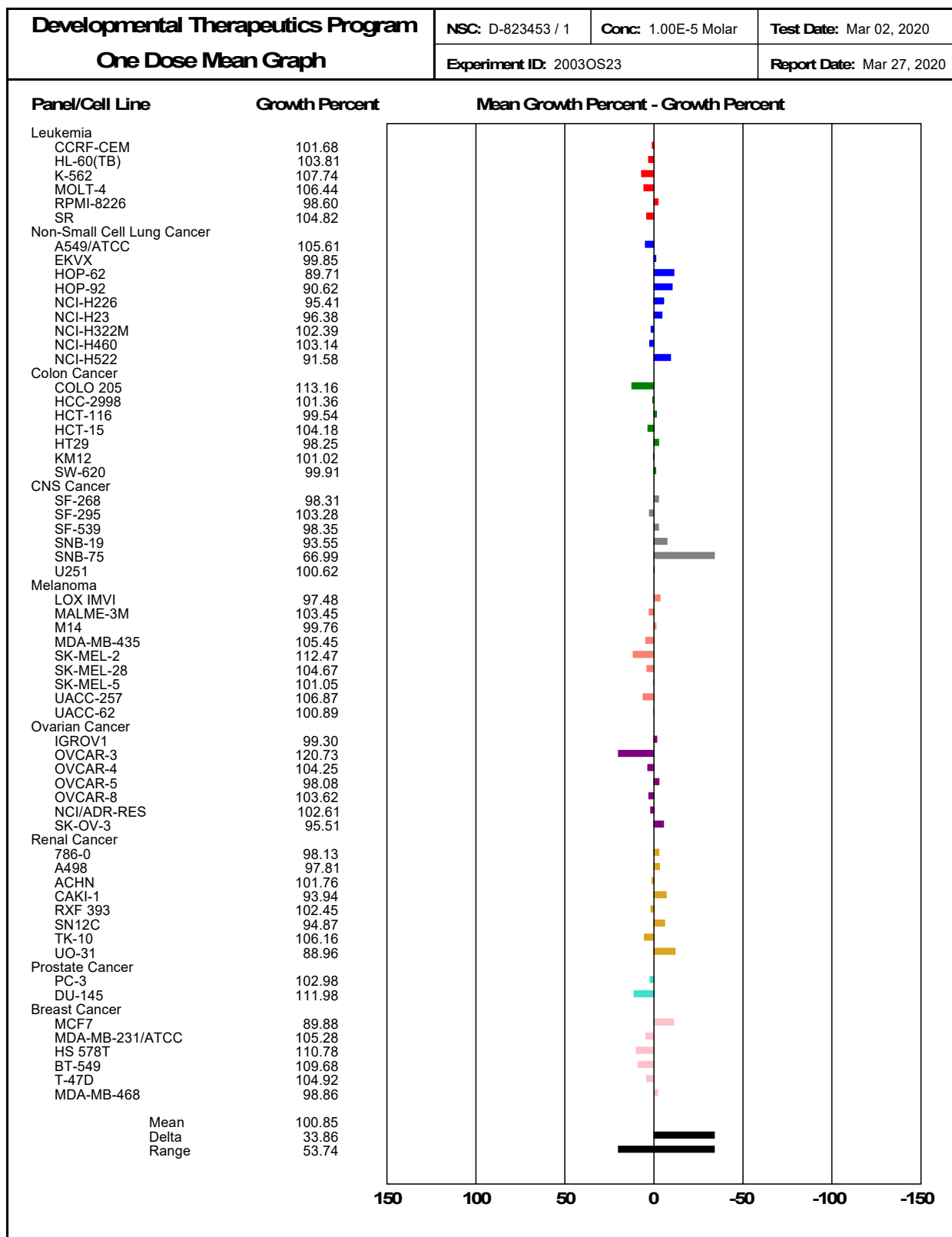


Table S7. NCI results of compound 7a.

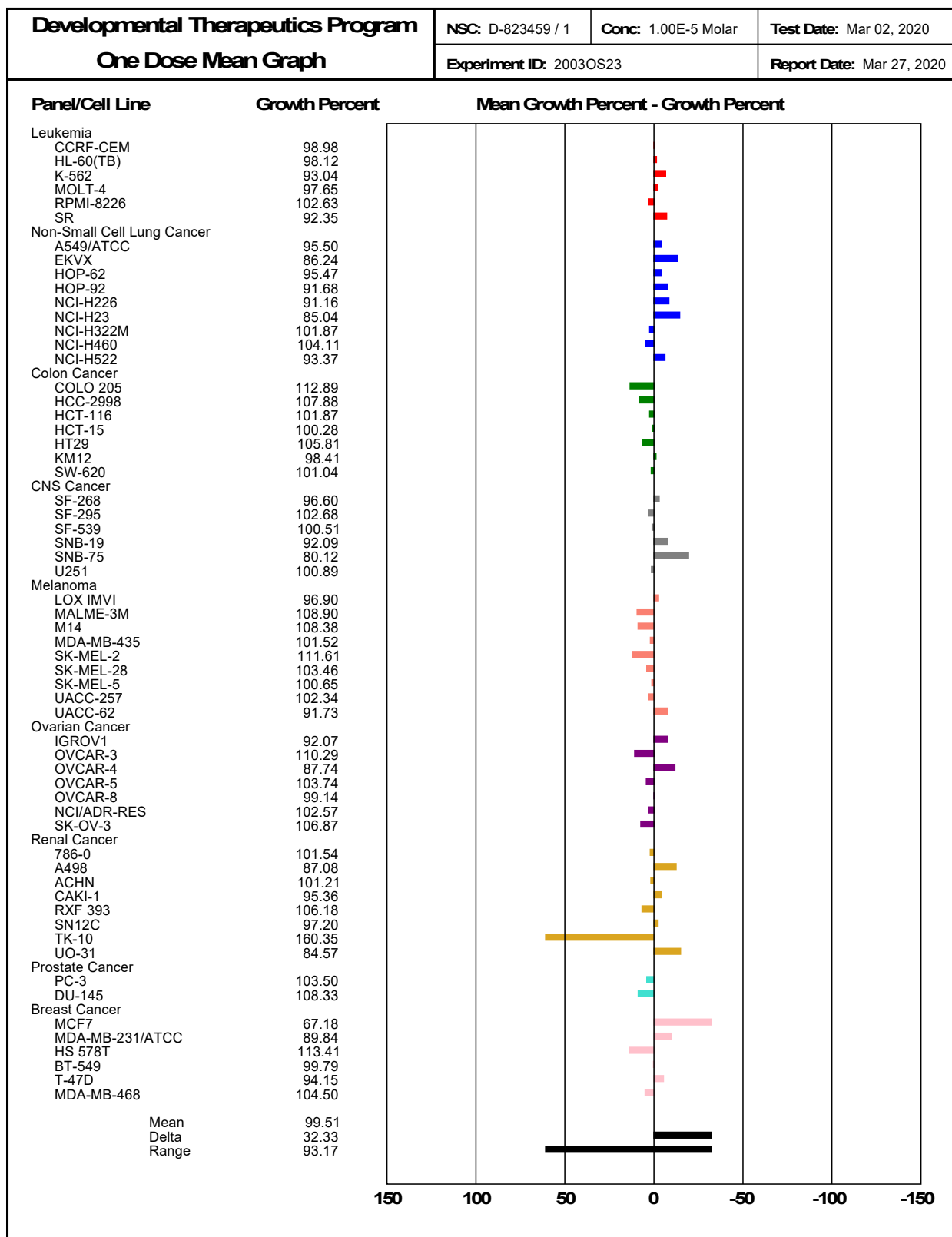


Table S8. NCI results of compound 7b.

