Supporting Information: A Virtual Screen Discovers Novel, Fragment-Sized Inhibitors of *Mycobacterium tuberculosis* InhA

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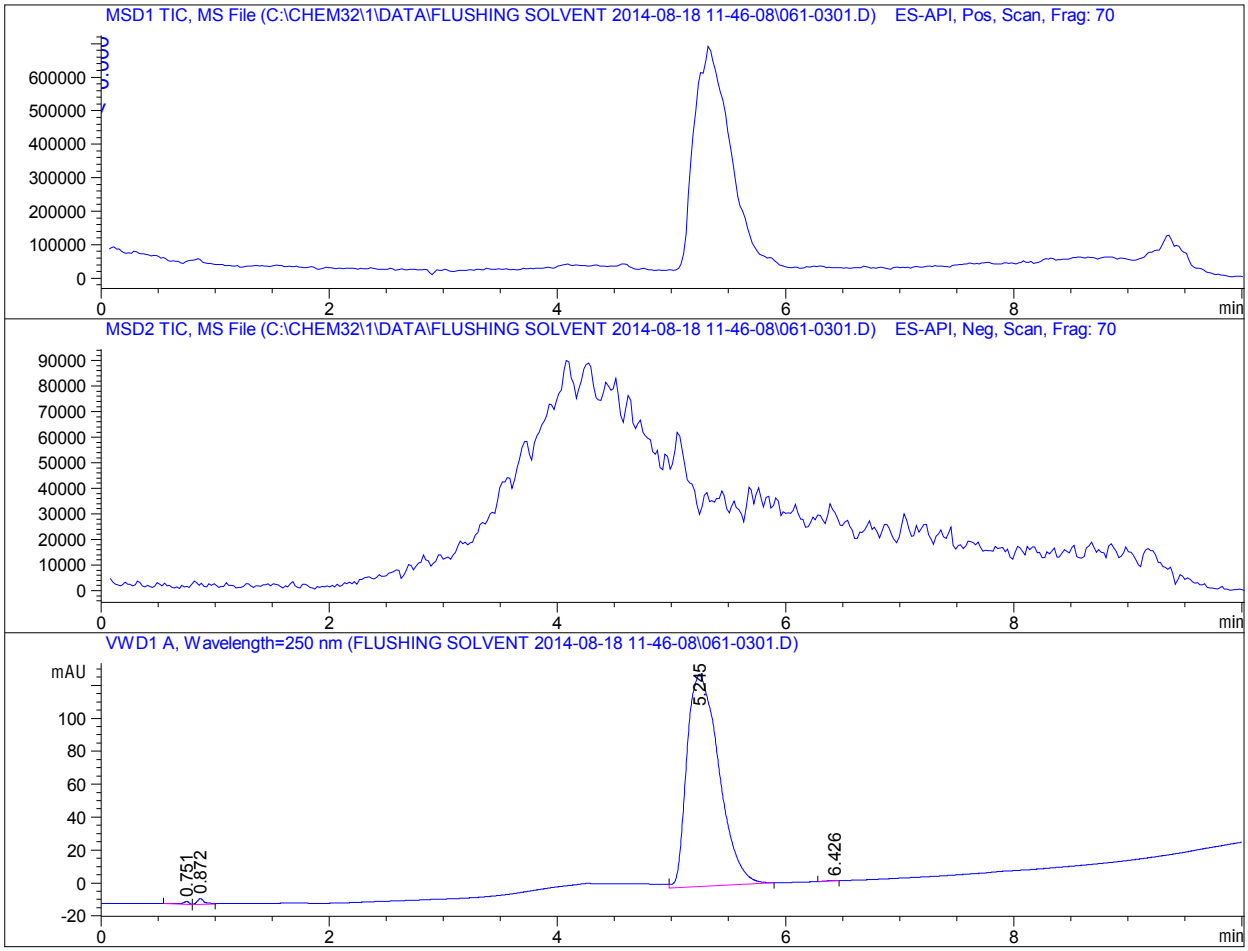


Signal 3: VWD1 A, Wavelength=250 nm

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	0.751	BB	0.0606	7.39936	1.77554	0.2924
2	0.872	BV	0.0649	16.23327	3.58137	0.6415
3	5.245	VB	0.2830	2505.29712	128.74850	99.0092
4	6.426	BB	0.1322	1.43855	1.70840e-1	0.0569
Totals :				2530.36830	134.27625	

Figure S1. LC-MS (Liquid Chromatography coupled with Mass Spectroscopy) indicates the sample of NCI 99389 was 99% pure. The top image shows the peaks for positively charged ions, the middle image displays the negatively charged ions, and the bottom image displays all peaks detected at 250 nm. The table contains the retention times and area under the curve values for all peaks detected at 250 nm, with peak 3 corresponding to the expected mass/charge of NCI 99389.

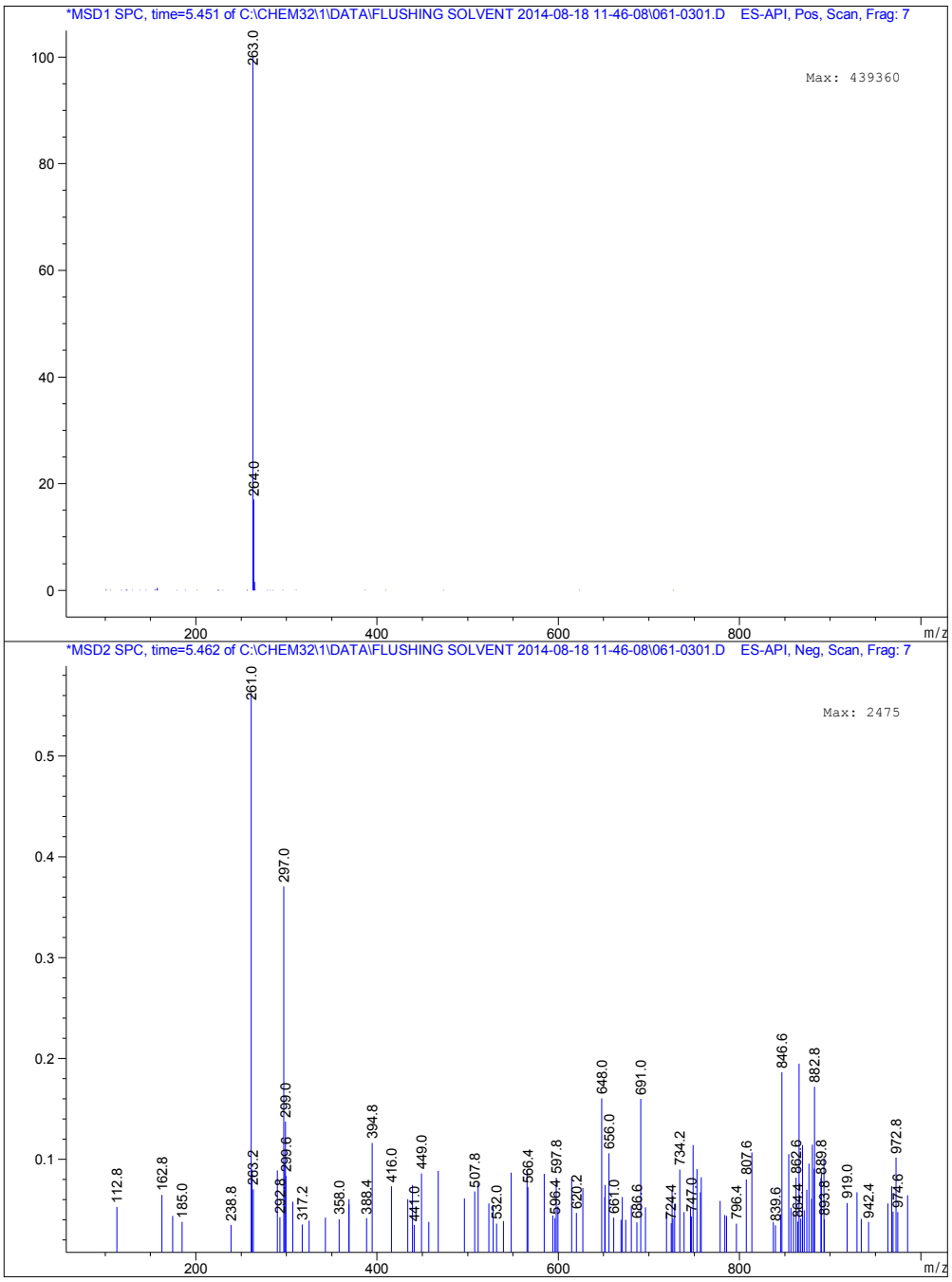


Figure S2. Mass spectra shows the mass of 263 $(M+1)^+$, which is consistent with NCI 99389. The top image displays the mass per charge for positively charged ions, while the bottom image shows the mass per charge for negatively charged ions.

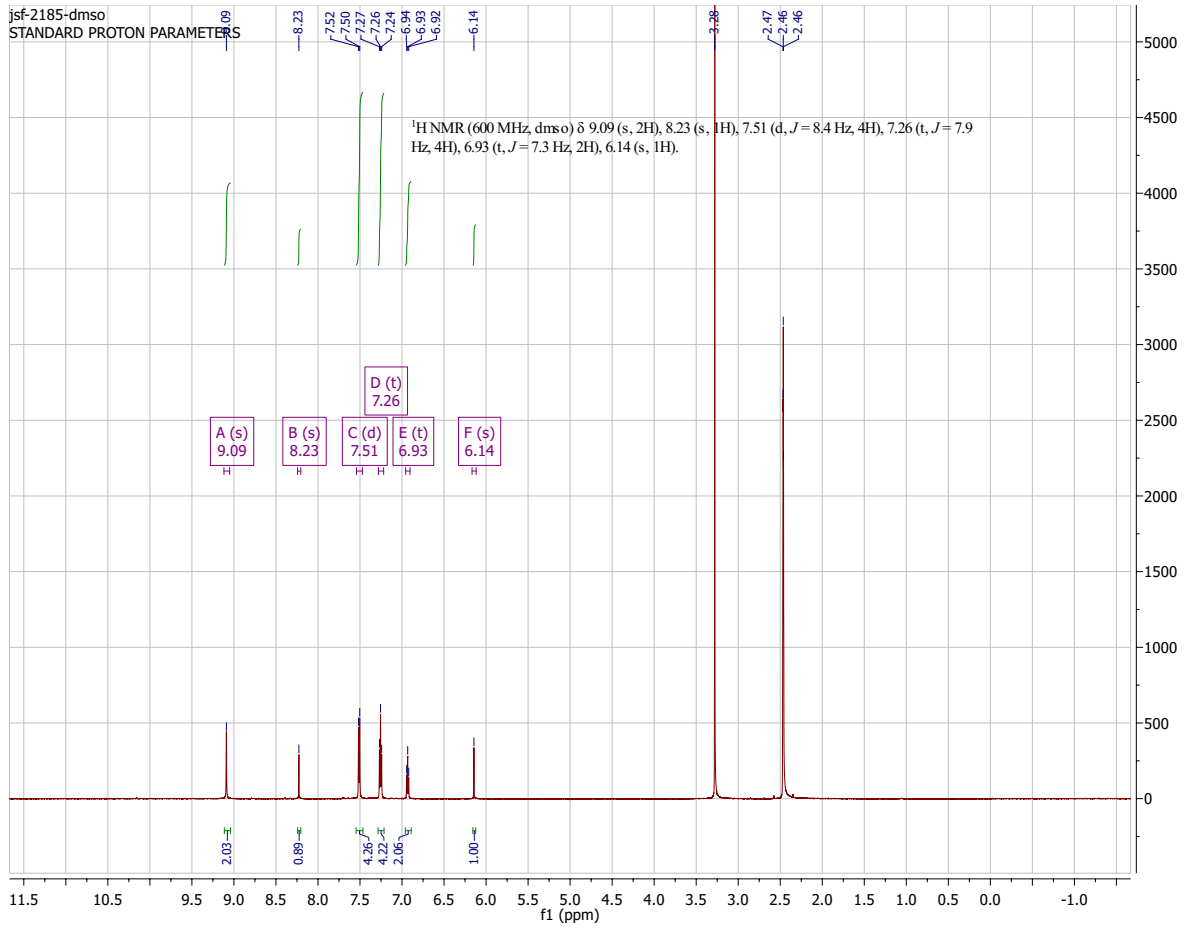
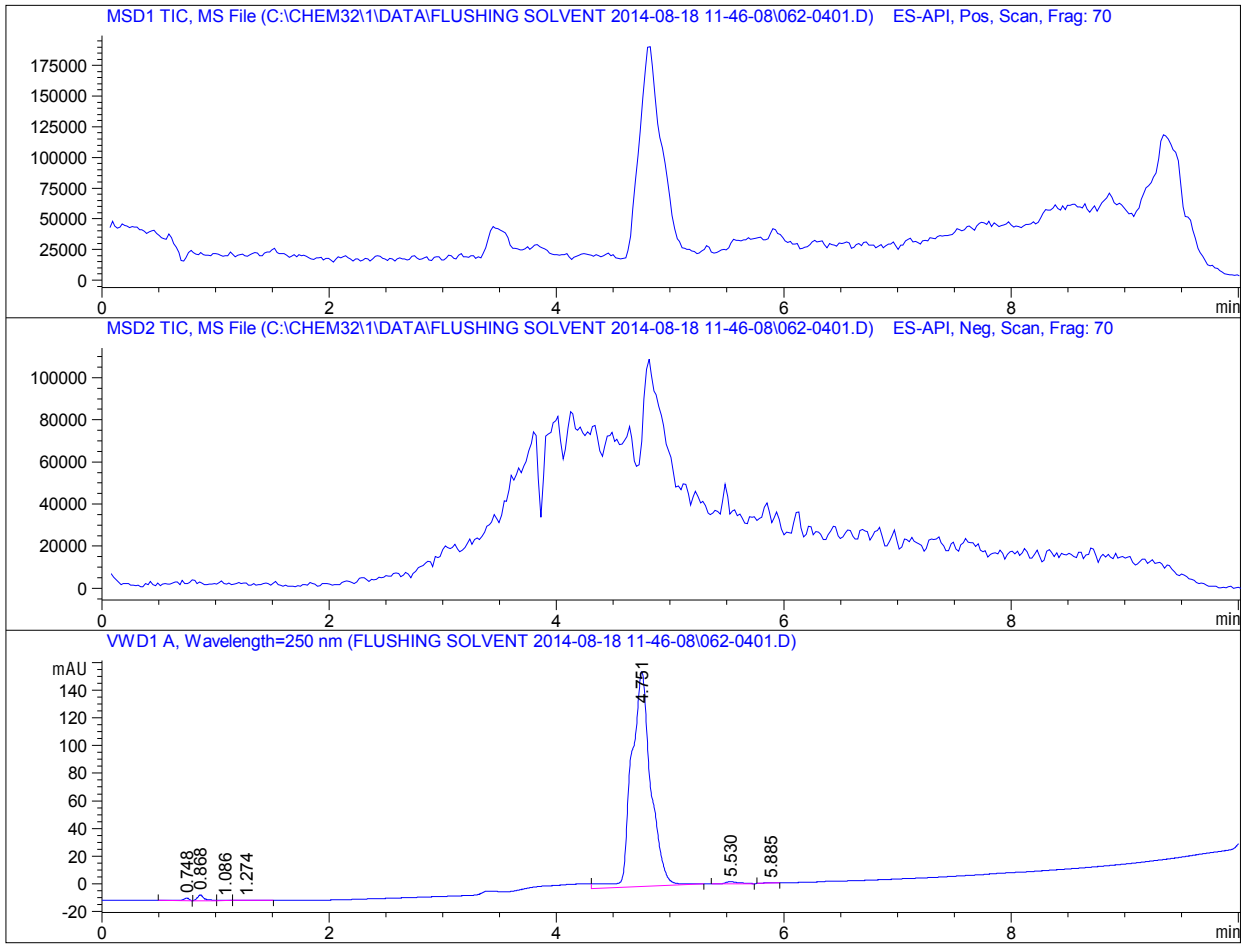


Figure S3. Proton NMR indicates the sample of NCI 99389 had the expected 2D structure. The compound was dissolved in deuterated DMSO and produced the following signal, using a 600 MHz NMR machine: δ 9.09 (s, 2H), 8.23 (s, 1H), 7.51 (d, J = 8.4 Hz, 4H), 7.26 (t, J = 7.9 Hz, 4H), 6.93 (t, J = 7.3 Hz, 2H), 6.14 (s, 1H).



Signal 1: VWD1 A, Wavelength=250 nm

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	0.748	BB	0.0601	7.45916	1.88903	0.3988
2	0.868	BV	0.0654	17.38281	4.10563	0.9293
3	1.086	VV	0.1032	2.03760	2.92832e-1	0.1089
4	1.274	VB	0.1999	2.55657	1.73470e-1	0.1367
5	4.751	VB	0.1594	1826.92542	155.10576	97.6640
6	5.530	BB	0.1154	12.12564	1.54783	0.6482
7	5.885	BB	0.1075	2.13630	3.21764e-1	0.1142
Totals :				1870.62349	163.43631	

Figure S4. LC-MS indicates the sample of NCI 111591 was > 97% pure. The top image shows the peaks for positively charged ions, the middle image displays the negatively charged ions, and the bottom image displays all peaks detected at 250 nm. The table contains the retention times and area under the curve values for all peaks detected at 250 nm, with peak 5 corresponding to the expected mass/charge of NCI 111591.

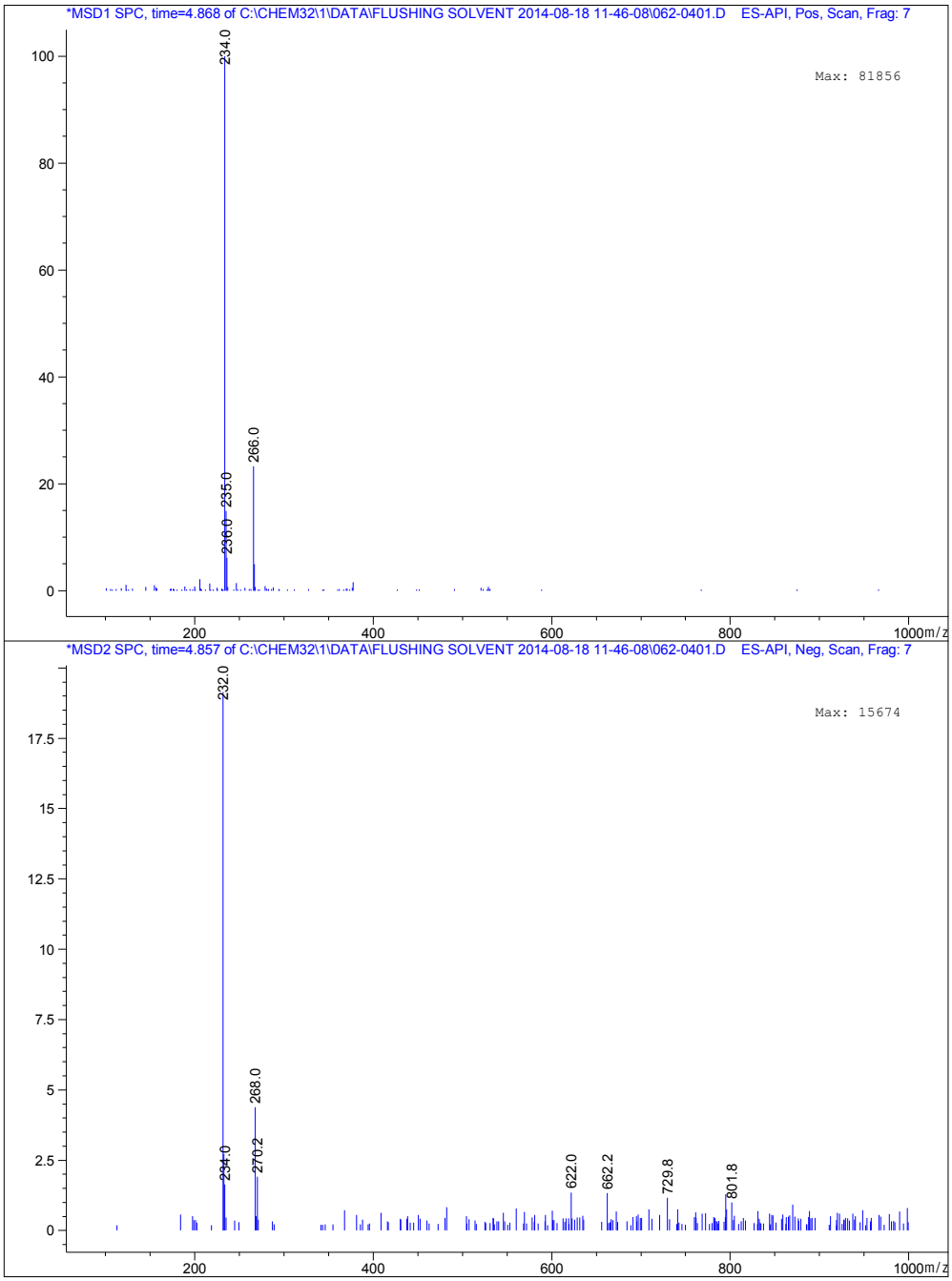


Figure S5. Mass spectra shows the mass of 234 $(M+1)^+$, which is consistent with NCI 111591. The top image displays the mass/charge for positively charged ions, while the bottom image shows the mass/charge for negatively charged ions.

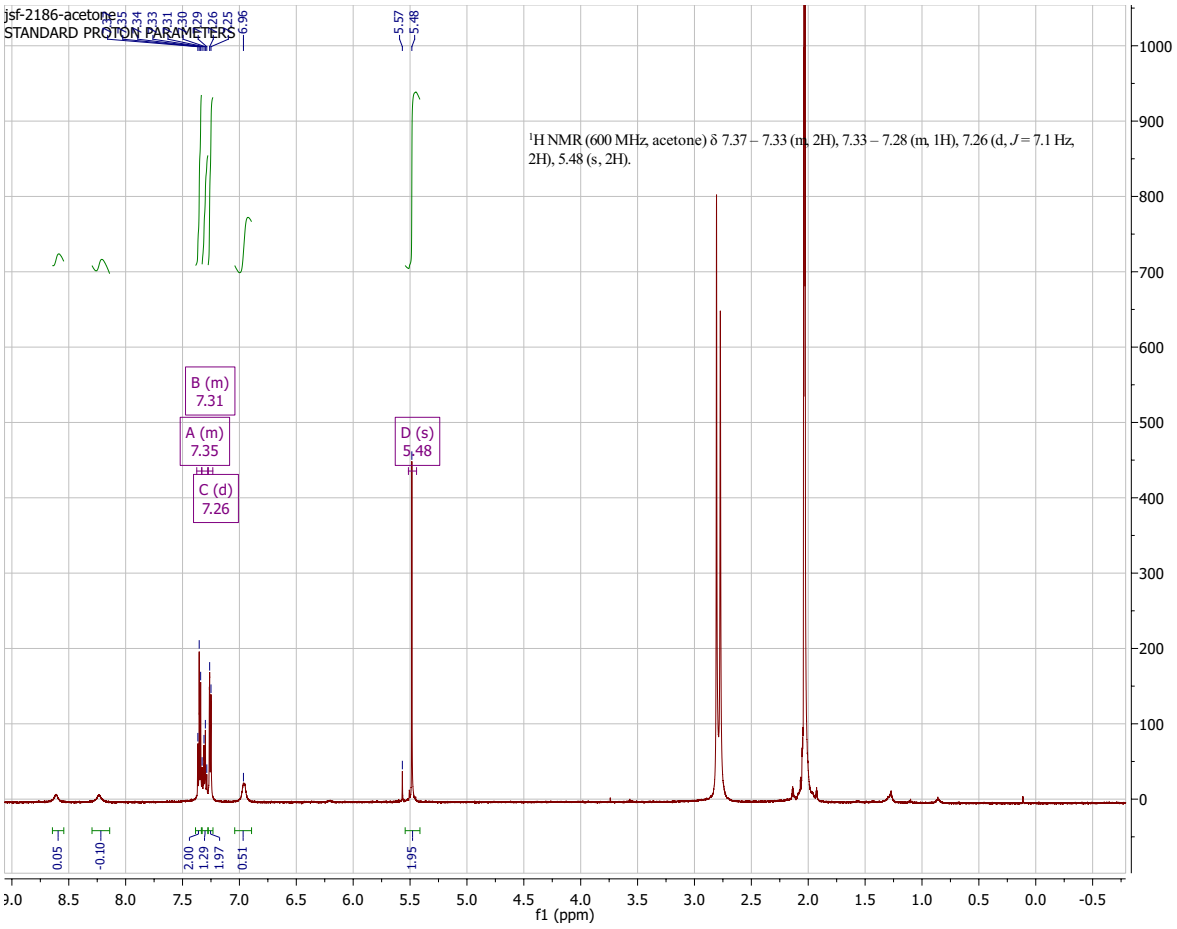


Figure S6. Proton NMR demonstrates that the sample of NCI 111591 had the expected 2D structure. The compound was dissolved in deuterated acetone and produced the following signal, using a 600 MHz NMR machine: δ 7.37 - 7.33 (m, 2H), 7.33 - 7.28 (m, 1H), 7.26 (d, J = 7.1 Hz, 2H), 5.48 (s, 2H).

Table S1. Tanimoto Similarity of Each Novel Inhibitor Compared to the Other 7 New Inhibitors

NCI ID	111590	111588	99389	111591	135809	196166	112144	111589
111590	1.00	0.78	0.39	0.71	0.39	0.54	0.39	0.83
111588	0.78	1.00	0.45	0.78	0.46	0.55	0.48	0.84
99389	0.39	0.45	1.00	0.49	0.43	0.41	0.33	0.41
111591	0.71	0.78	0.49	1.00	0.57	0.48	0.38	0.72
135809	0.39	0.46	0.43	0.57	1.00	0.36	0.34	0.45
196166	0.54	0.55	0.41	0.48	0.36	1.00	0.41	0.48
112144	0.39	0.48	0.33	0.38	0.34	0.41	1.00	0.41
111589	0.83	0.84	0.41	0.72	0.45	0.48	0.41	1.00
Average Similarity to Other 7 Inhibitors	0.6	0.6	0.4	0.6	0.4	0.5	0.4	0.6
Maximum Similarity to the Other 7	0.8	0.8	0.5	0.8	0.6	0.6	0.5	0.8
Scaffold # Using a Cutoff > 0.7	2	2	1	2	4	5	3	2