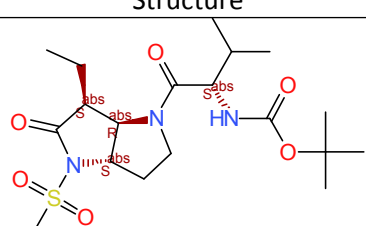
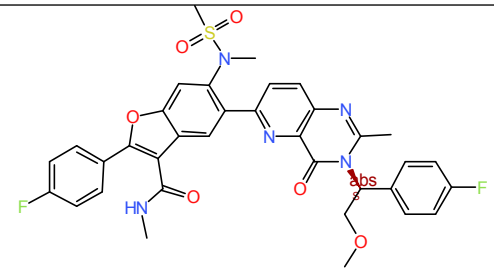
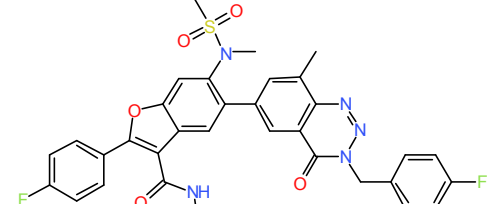
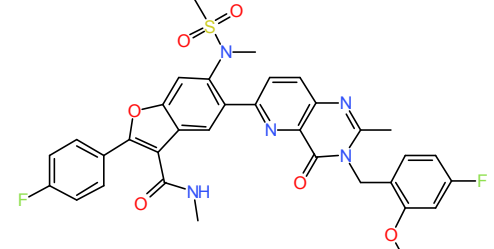
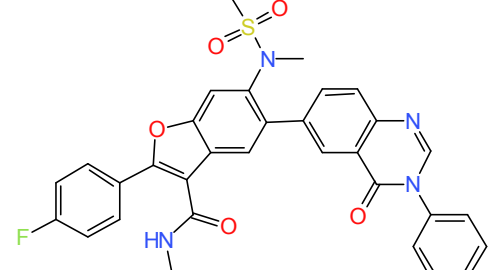
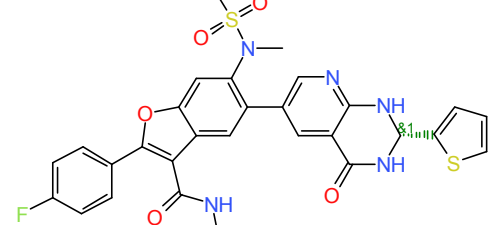
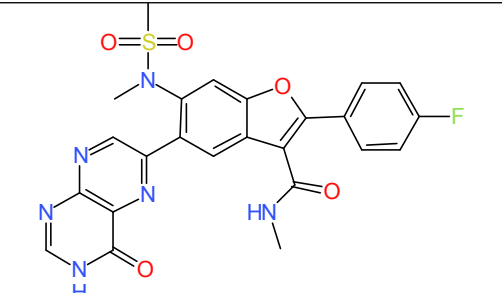
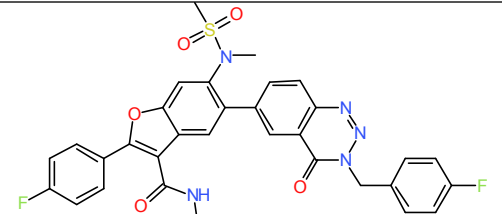
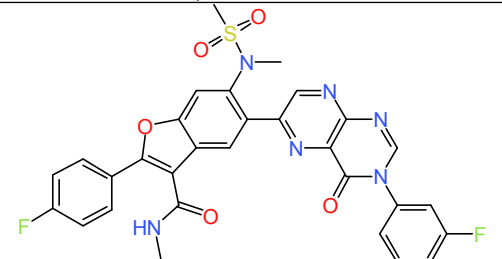
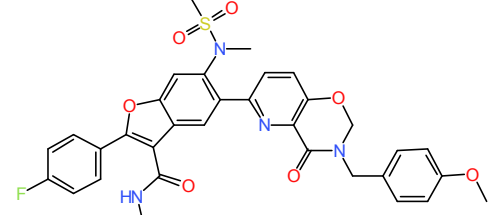
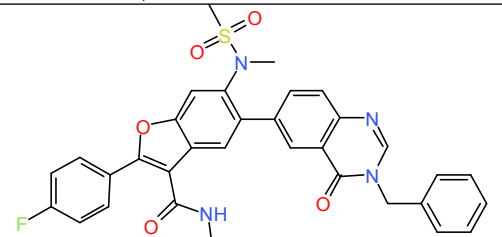
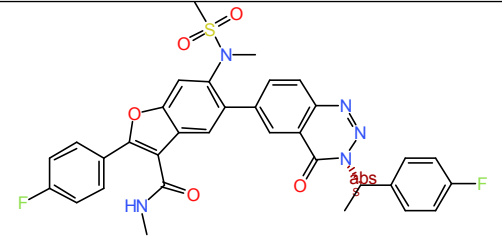
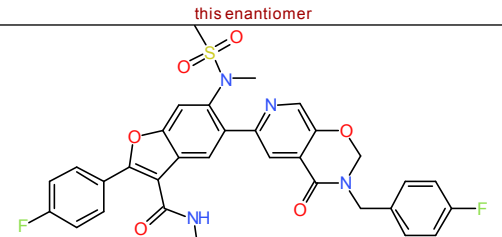
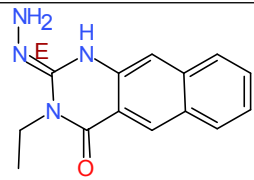
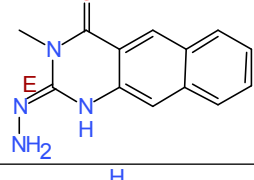
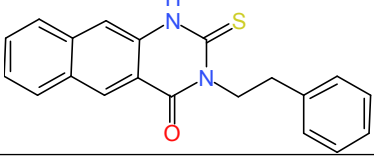
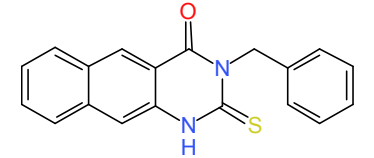
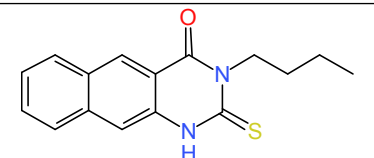
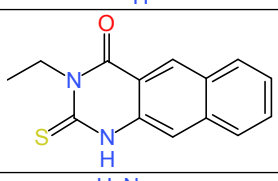
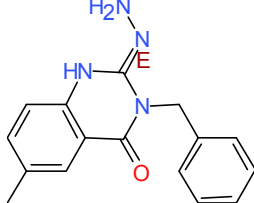
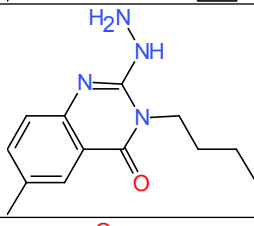
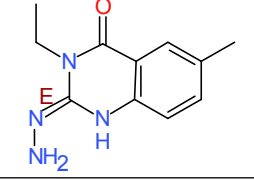
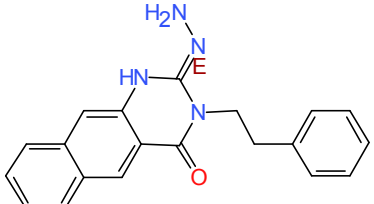


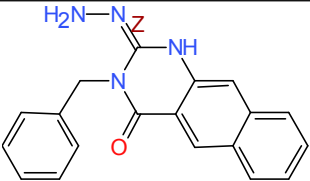
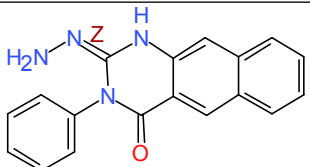
S1 Table: Dataset of training set of the HCV NS3/4A serine protease inhibitors consist of synthesized compounds with biological activity values (pIC_{50}), predicted pIC_{50} and predicted Z-score.

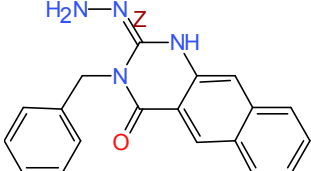
No.	Structure	Molecule	pIC_{50}	PRED	Z-SCORE	Ref.
1	 this enantiomer	CHEMBL419930	4.66	4.65	0.01	[28]
2	 this enantiomer	CHEMBL4107186	8.3	8.38	0.15	[29]
3	 this enantiomer	CHEMBL3978278	8.15	7.74	0.71	[29]
4	 this enantiomer	CHEMBL3972861	7.62	8.16	0.94	[29]
5	 this enantiomer	CHEMBL3969256	8.55	7.29	2.19	[29]
6	 racemate	CHEMBL3966786	6.4	7.23	1.45	[29]

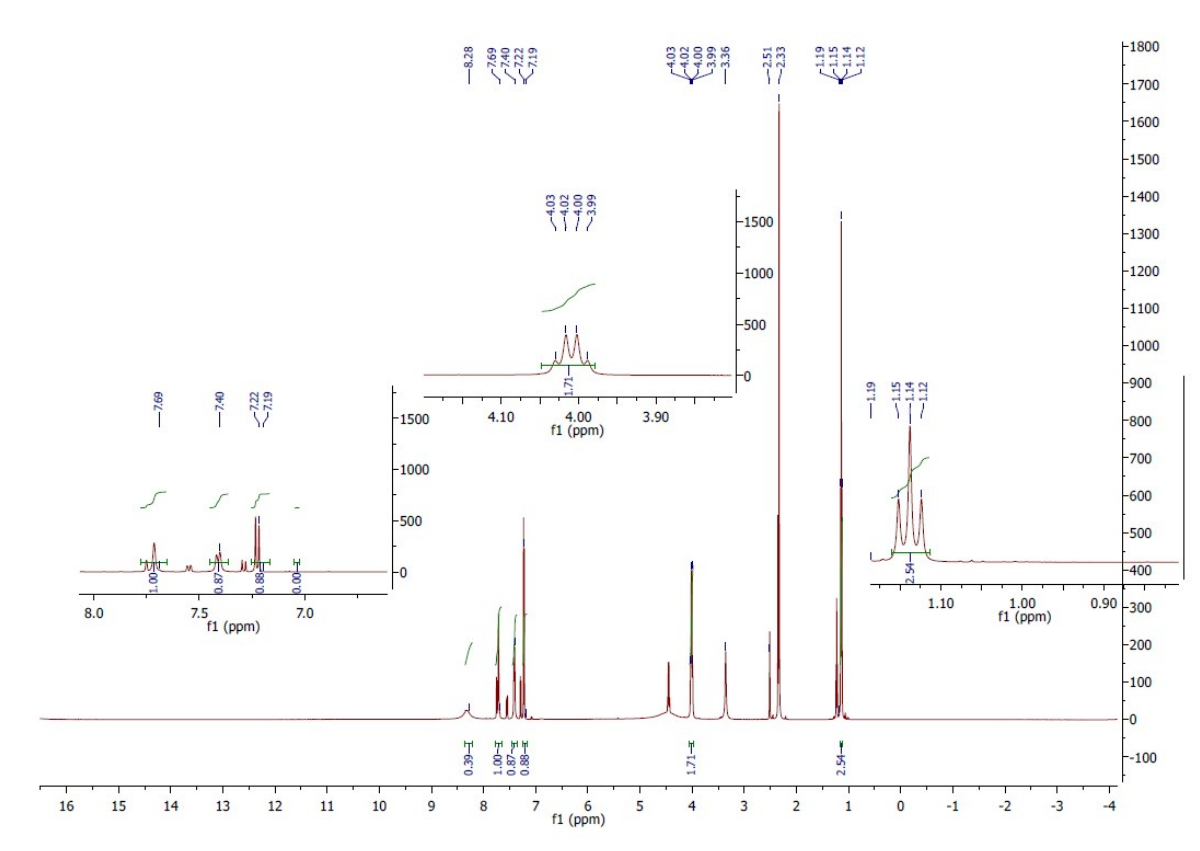
7		CHEMBL3960822	6.25	6.96	1.23	[29]
8		CHEMBL3960796	7.98	7.88	0.18	[29]
9		CHEMBL3959793	8.3	7.86	0.76	[29]
10		CHEMBL3957232	8.52	8.11	0.71	[29]
11		CHEMBL3949897	8.2	7.54	1.15	[29]
12		CHEMBL3936097	7.46	7.72	0.45	[29]
13		CHEMBL3932292	8.15	8.07	0.14	[29]

14		CHEMBL3925629	7.45	8.35	1.56	[29]
15		CHEMBL3913311	5.77	6.91	1.97	[29]
16		CHEMBL3913046	7.11	6.97	0.24	[29]
17		CHEMBL3910003	8.43	7.49	1.63	[29]
18		CHEMBL3904432	6.89	6.48	0.71	[29]
19		CHEMBL116118	4	4.32	0.55	[28]
20		CHEMBL112200	4.57	4.65	0.14	[28]
21		9	5.04	4.58	0.8	

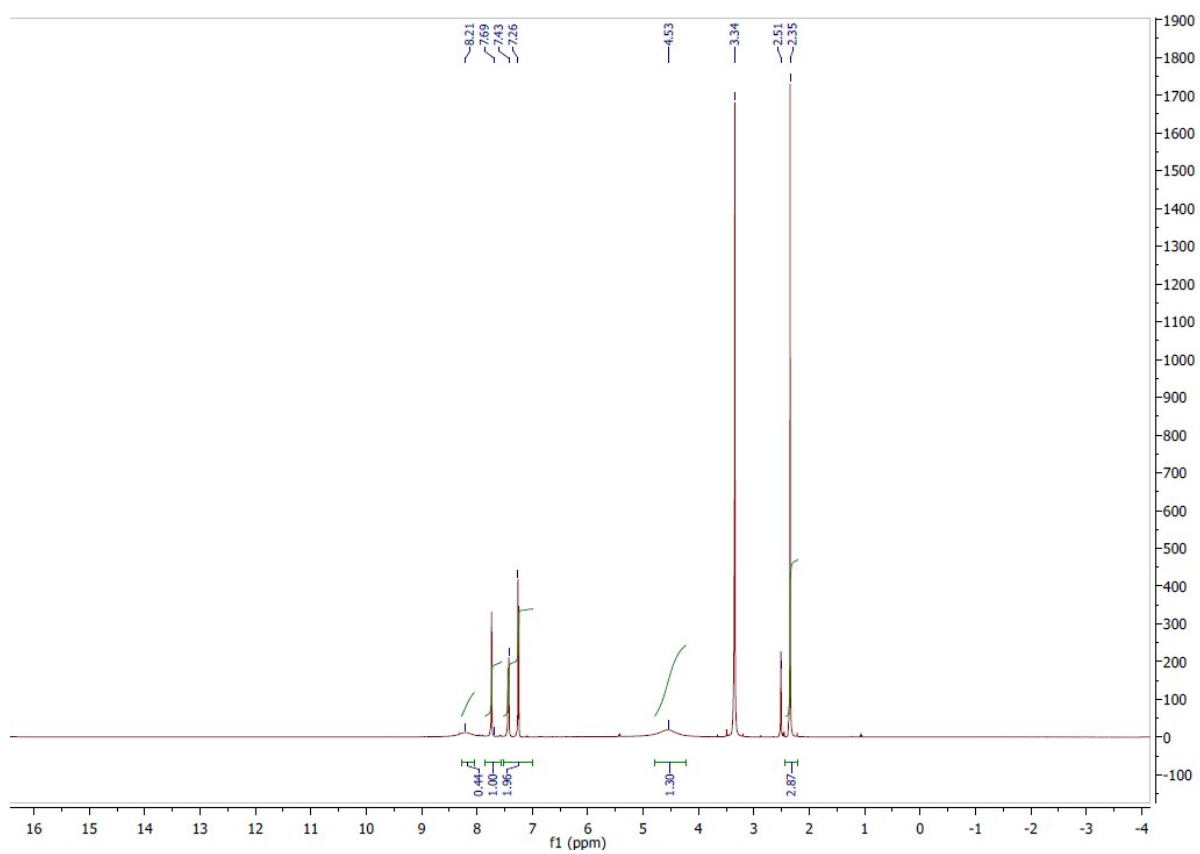
22		8	4.1	4.18	0.14	
23		7	4.65	4.05	1.04	
24		6	4.5	5.03	0.93	
25		5	4.43	4.82	0.68	
26		3	5.03	4.63	0.69	
27		2	5.19	4.23	1.66	
28		17	4.53	4.63	0.17	
29		16	4.63	4.35	0.48	
30		15	3.75	4.07	0.56	
31		13	4.84	4.97	0.23	

32		12	3.65	4.76	1.93	
33		11	4.47	4.49	0.04	

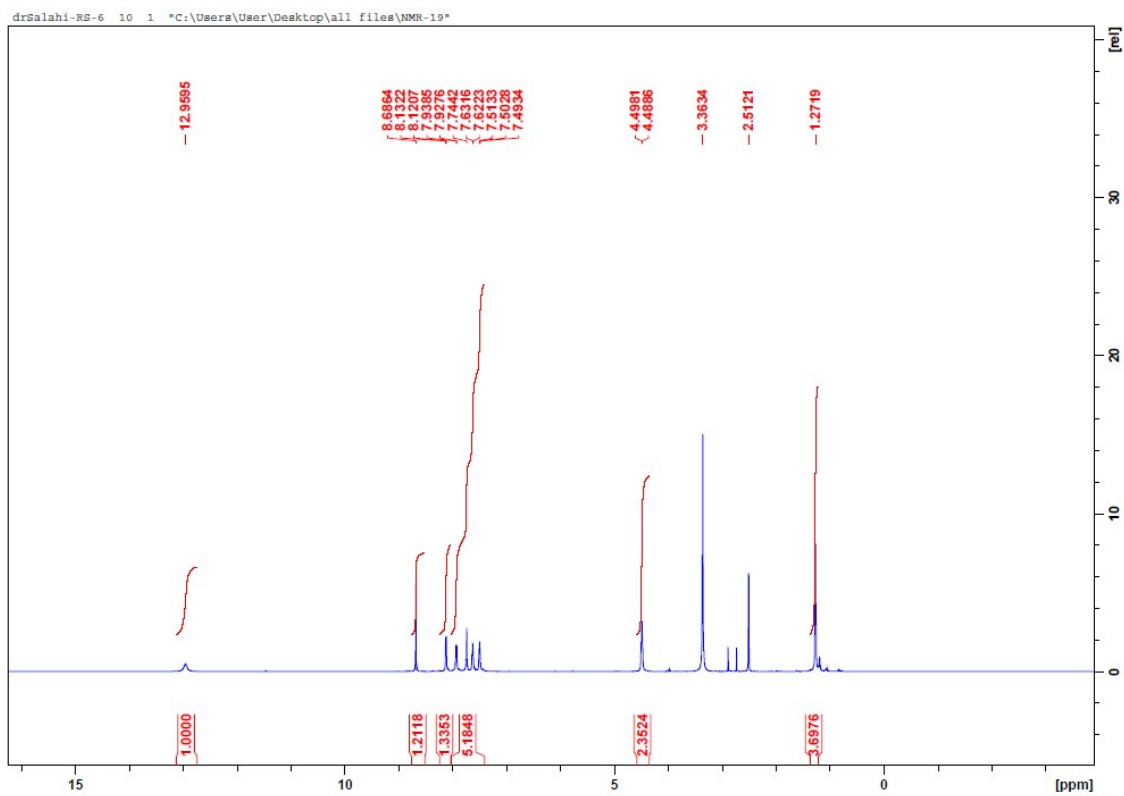
9		1	4.59	3.95	0.64	
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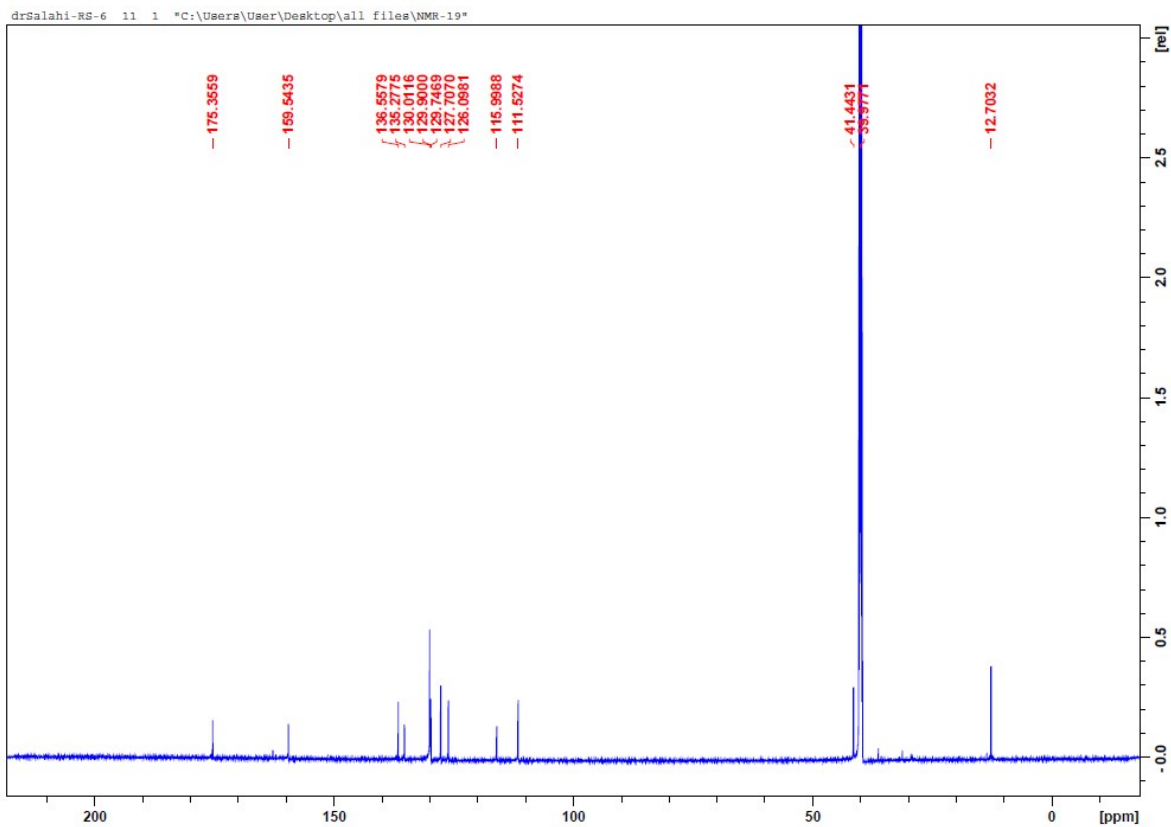
¹H-NMR for compound 15



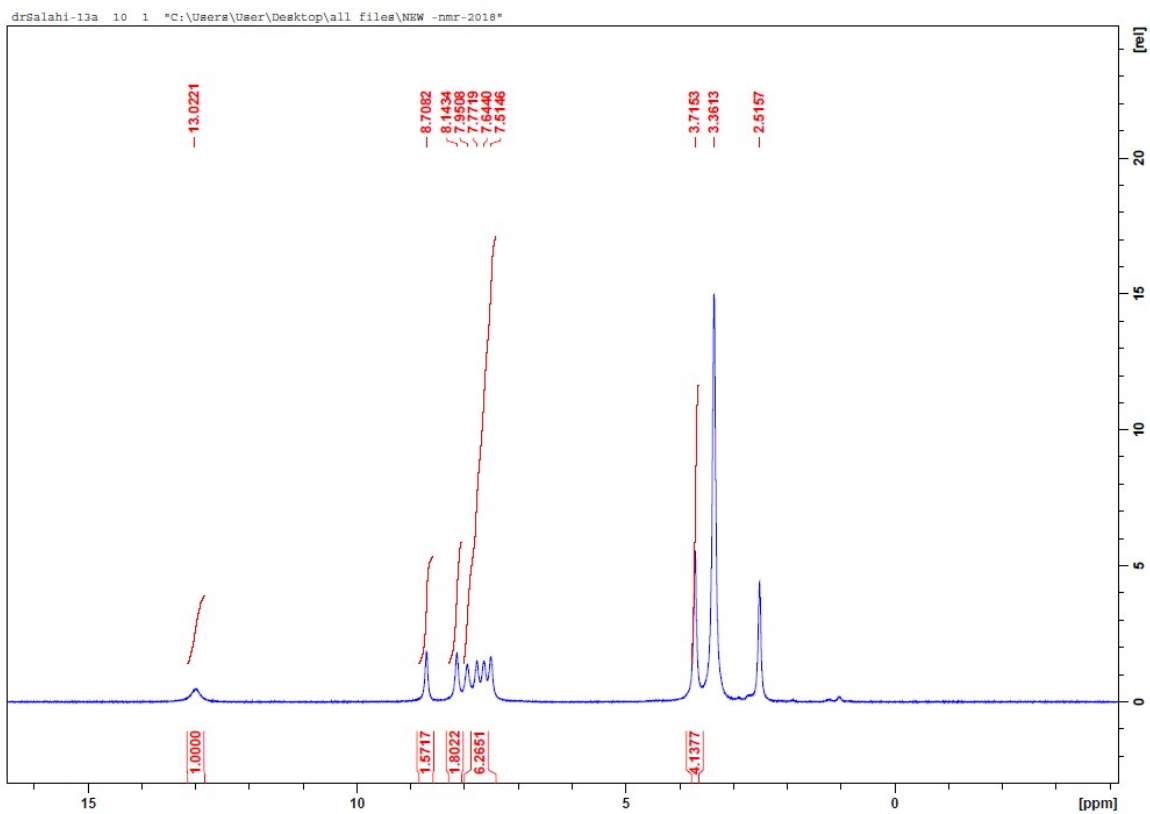
¹H-NMR for compound 14



¹H-NMR for compound 2



^{13}C -NMR for compound 2



$^1\text{H-NMR}$ for compound 1