Thienopyrimidine-Chalcones Hybrid Molecules Inhibits Fas-activated Serine/Threonine Kinase: An Approach to Ameliorates Antiproliferation in Human Breast Cancer Cells

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Running head: FASTK Inhibitors

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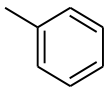
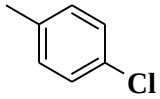
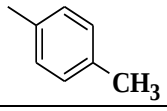
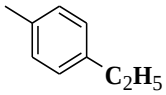
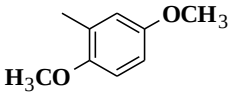
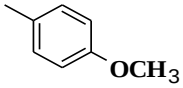
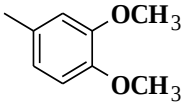
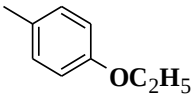
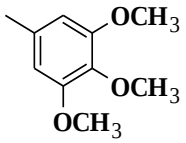
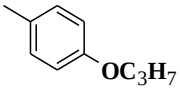
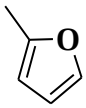
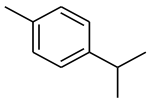
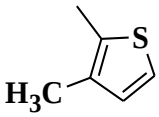
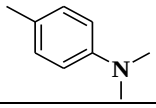
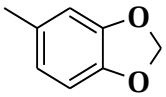
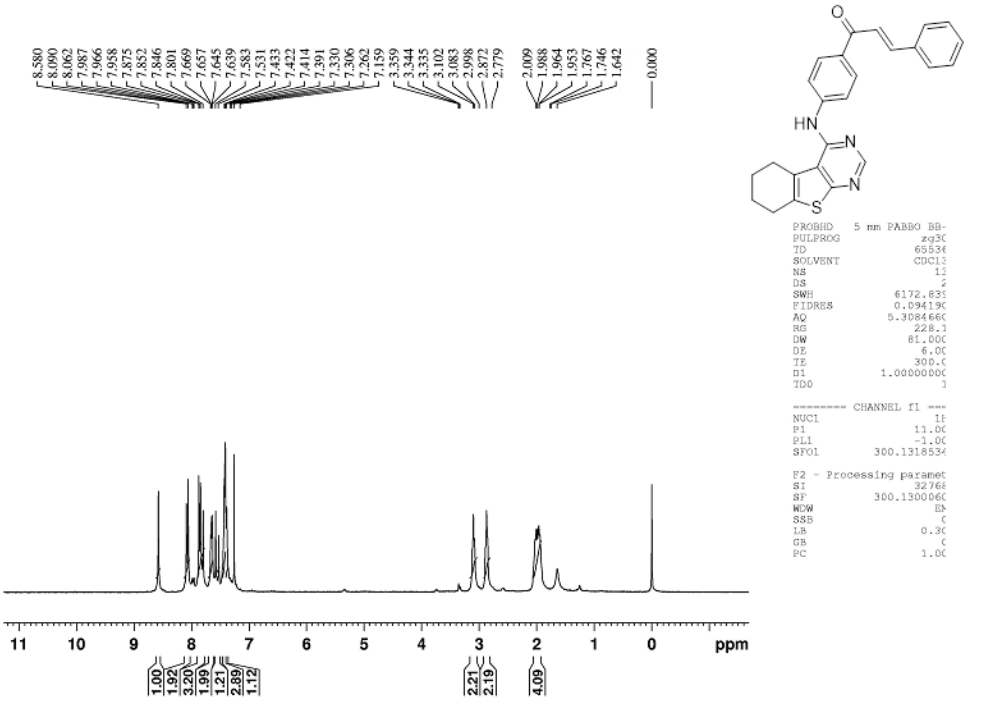
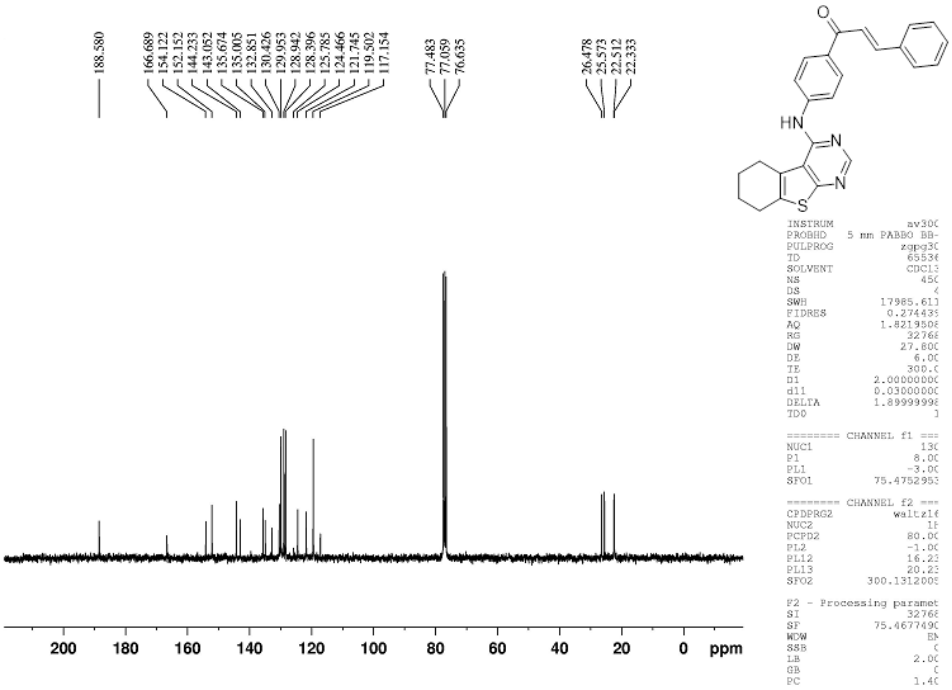
Table S1: Structures of Thienopyrimidine based chalcones and their binding affinity to FASTK and IC_{50} values.

Compound No.	R	IC_{50}, (μM), for FASTK Inhibition	Binding affinity (Ka), M^{-1}	Compound No.	R	IC_{50}, (μM), for FASTK Inhibition	Binding affinity (Ka), M^{-1}
2		0.32	7.6×10^5	10		0.17	1.16×10^7
3		> 1.0	3.08×10^4				
4		> 1.0	6.95×10^2	11		> 1.0	0.0237
5		> 1.0	2.43×10^2	12		0.15	2.98×10^7
6		> 1.0	2.68×10^4	13		> 1.0	ND
7		> 1.0	3.7×10^4	14		> 1.0	ND
8		> 1.0	1.1×10^4	15		> 1.0	1.67×10^4
9		> 1.0	3.08×10^3	16		> 1.0	ND

^{1}H NMR Compound 2



^{13}C NMR Compound 2



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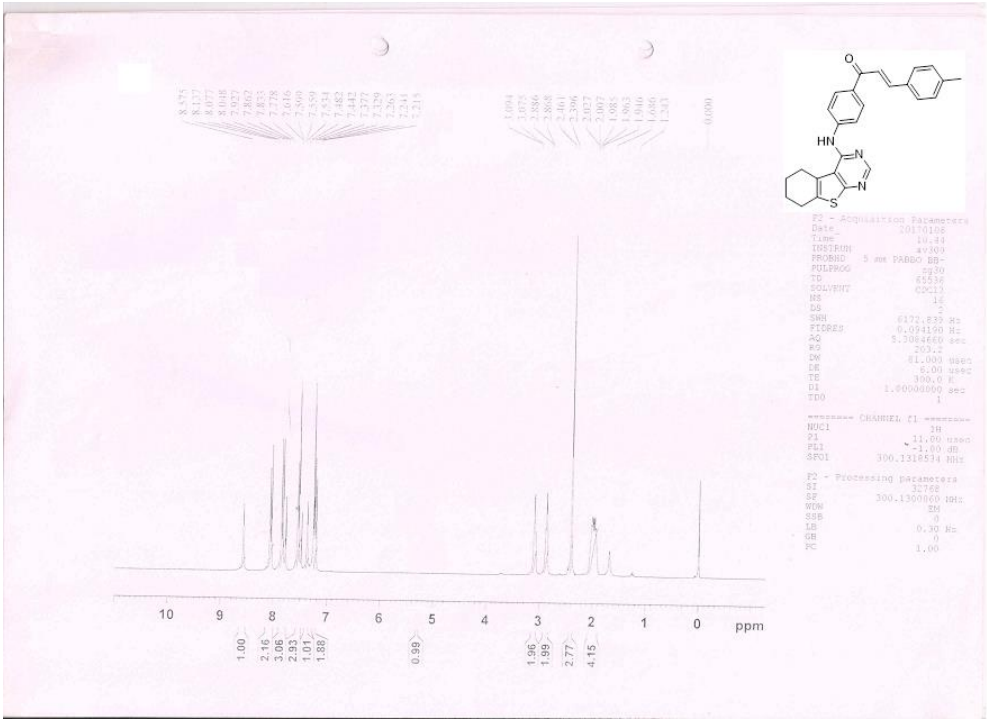
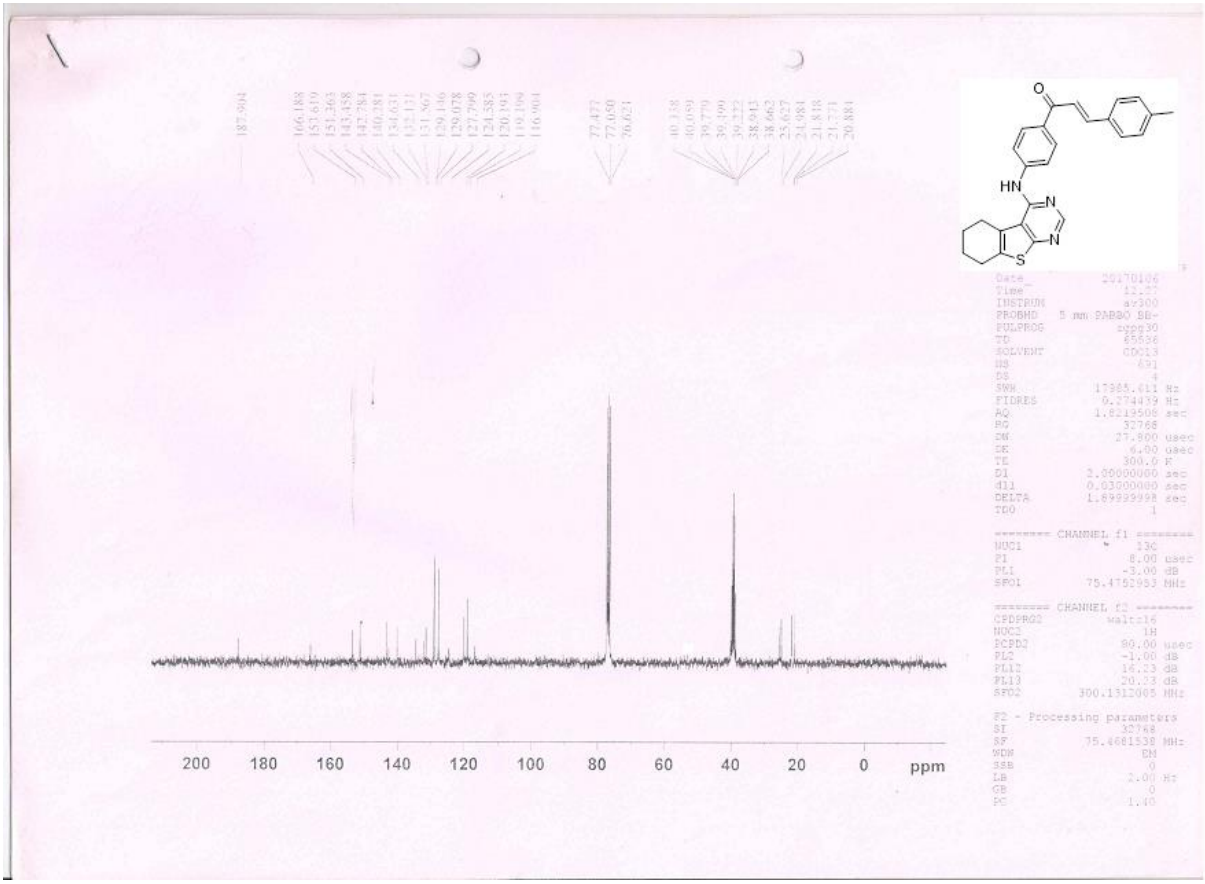


^{13}C NMR Compound 3



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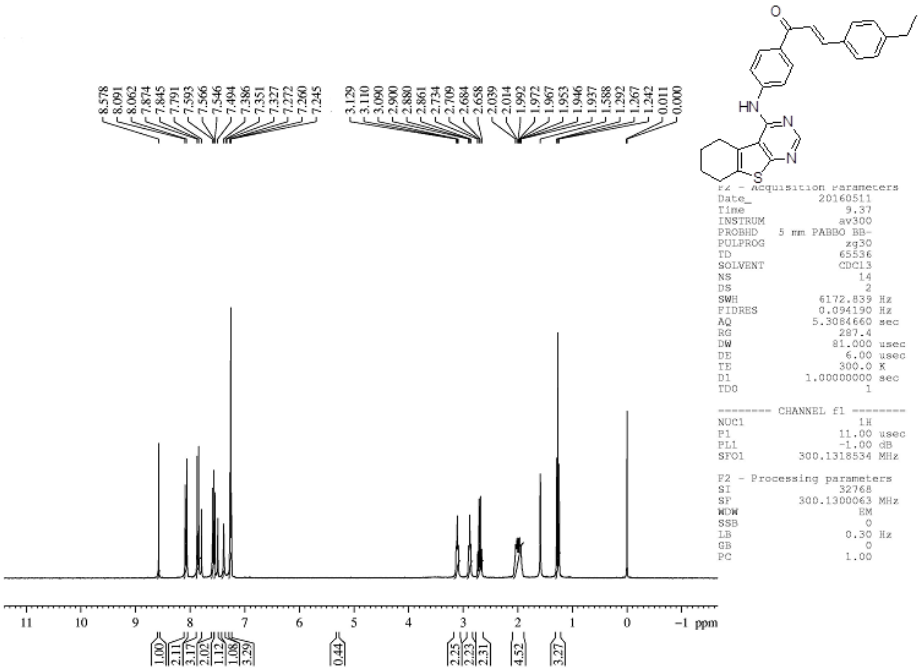

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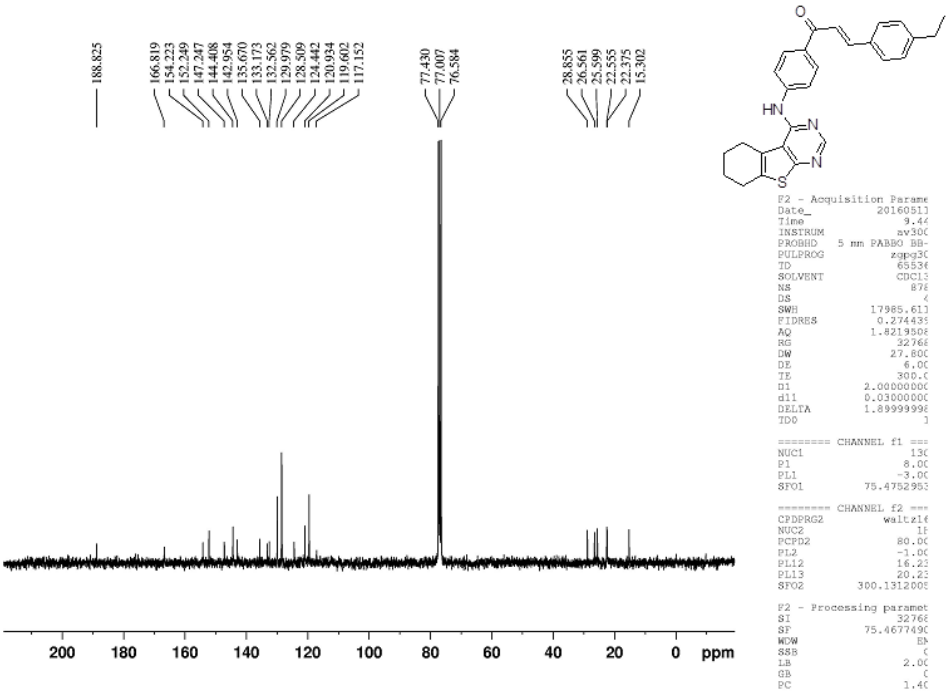

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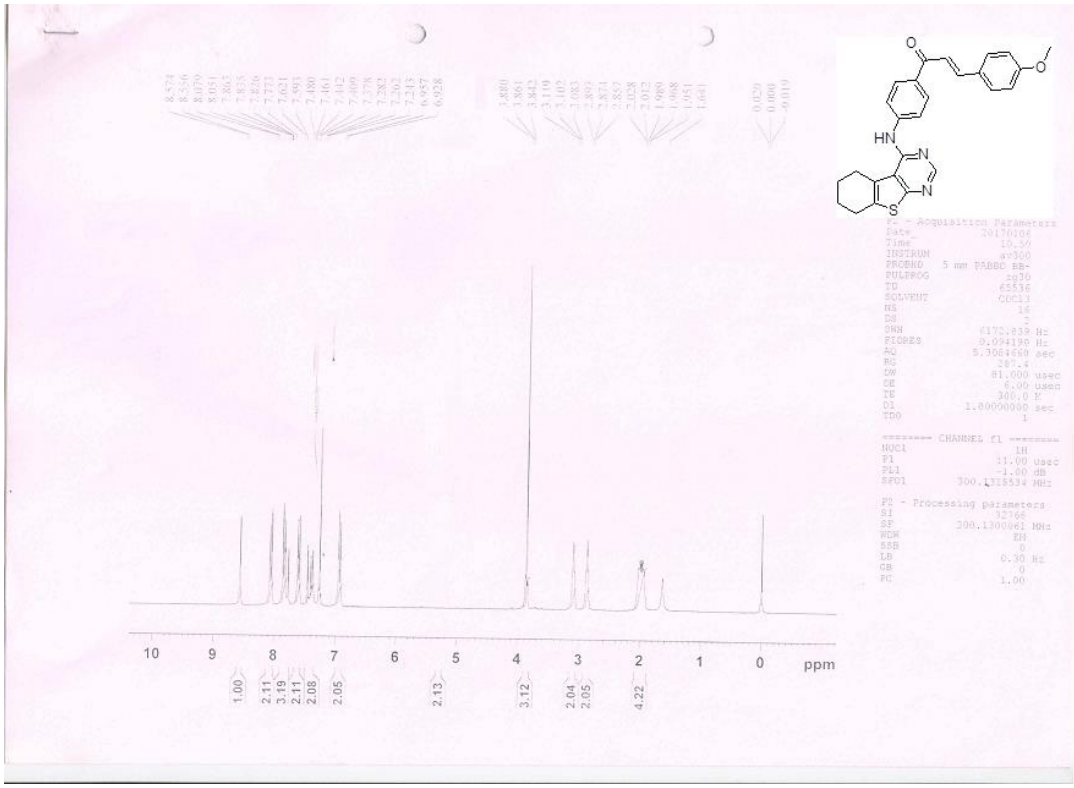

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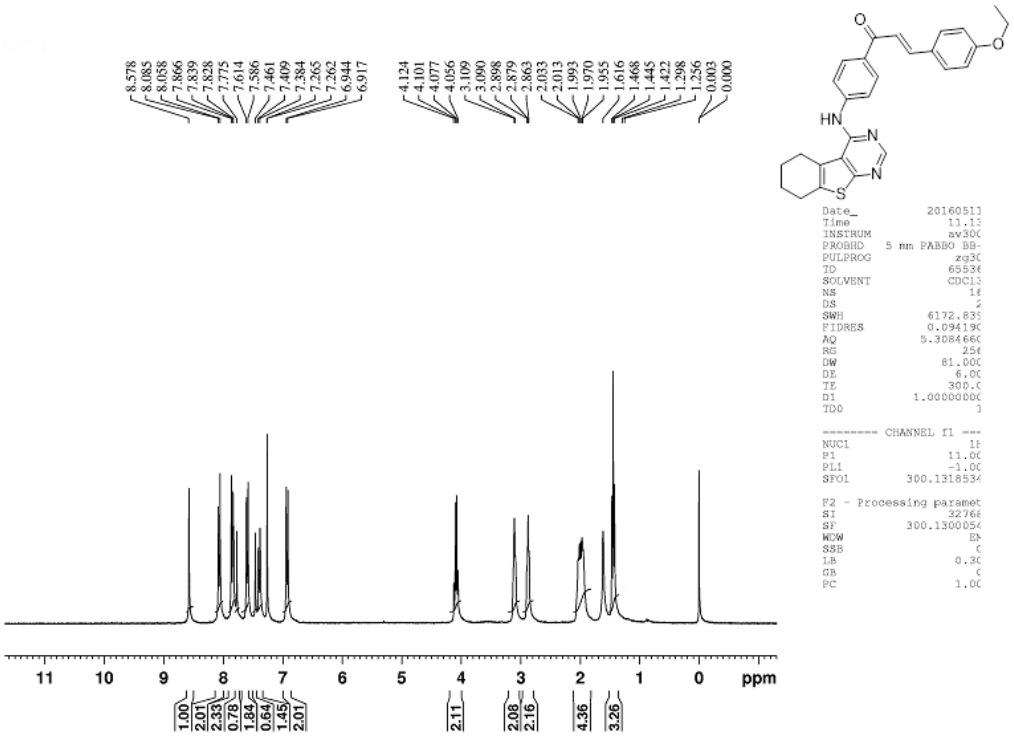

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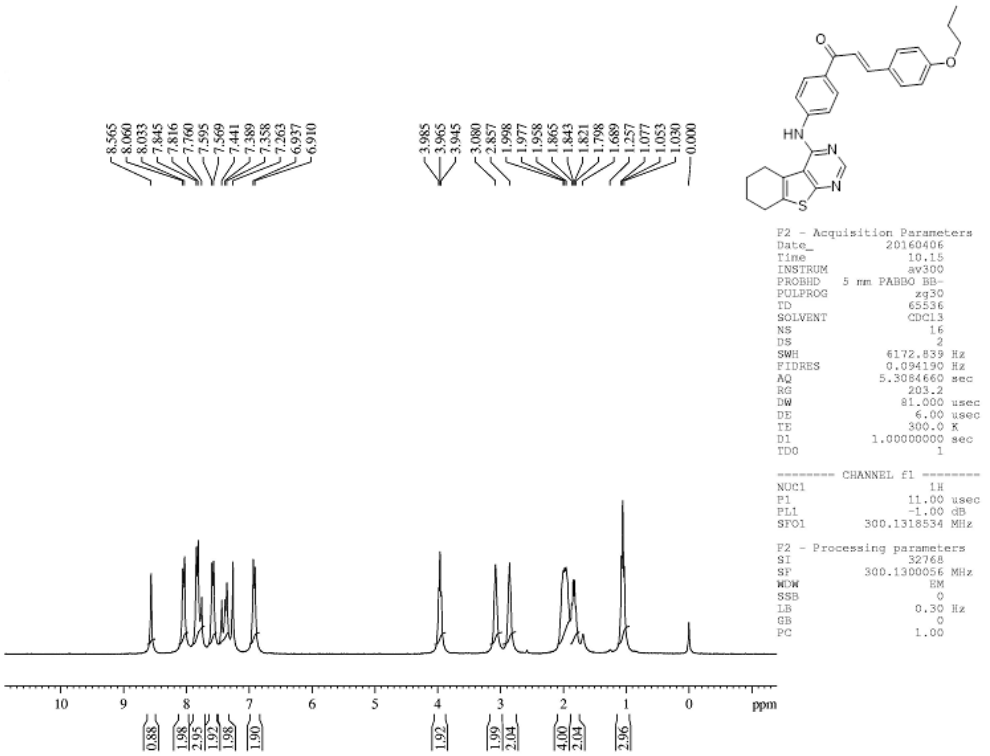

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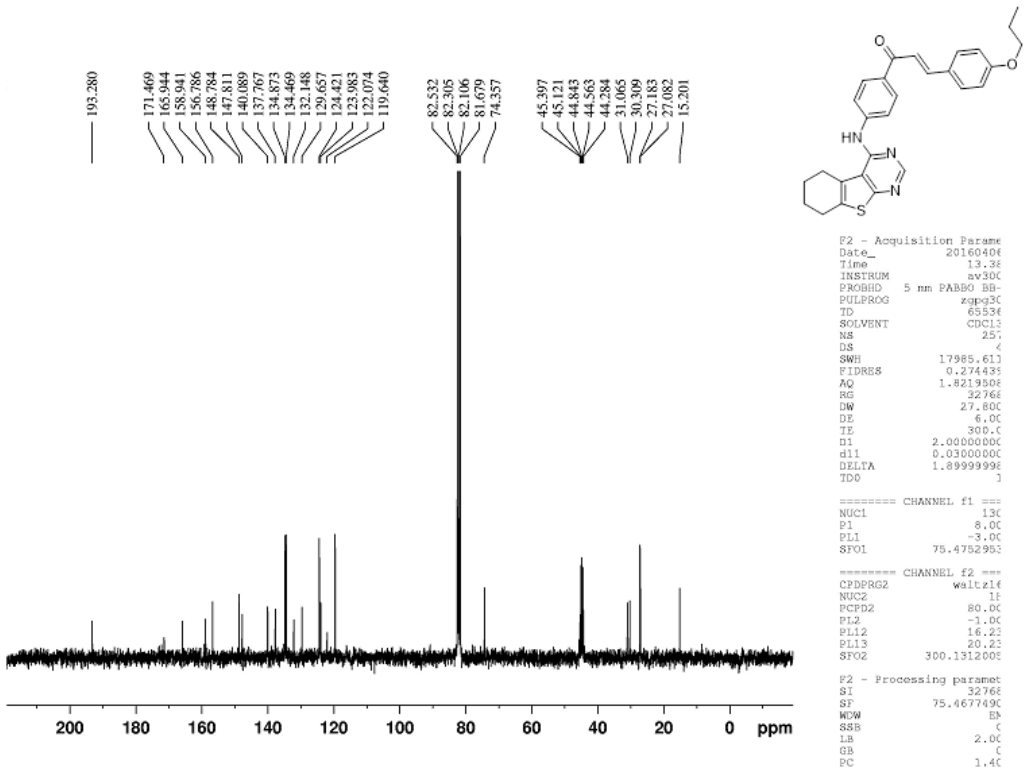
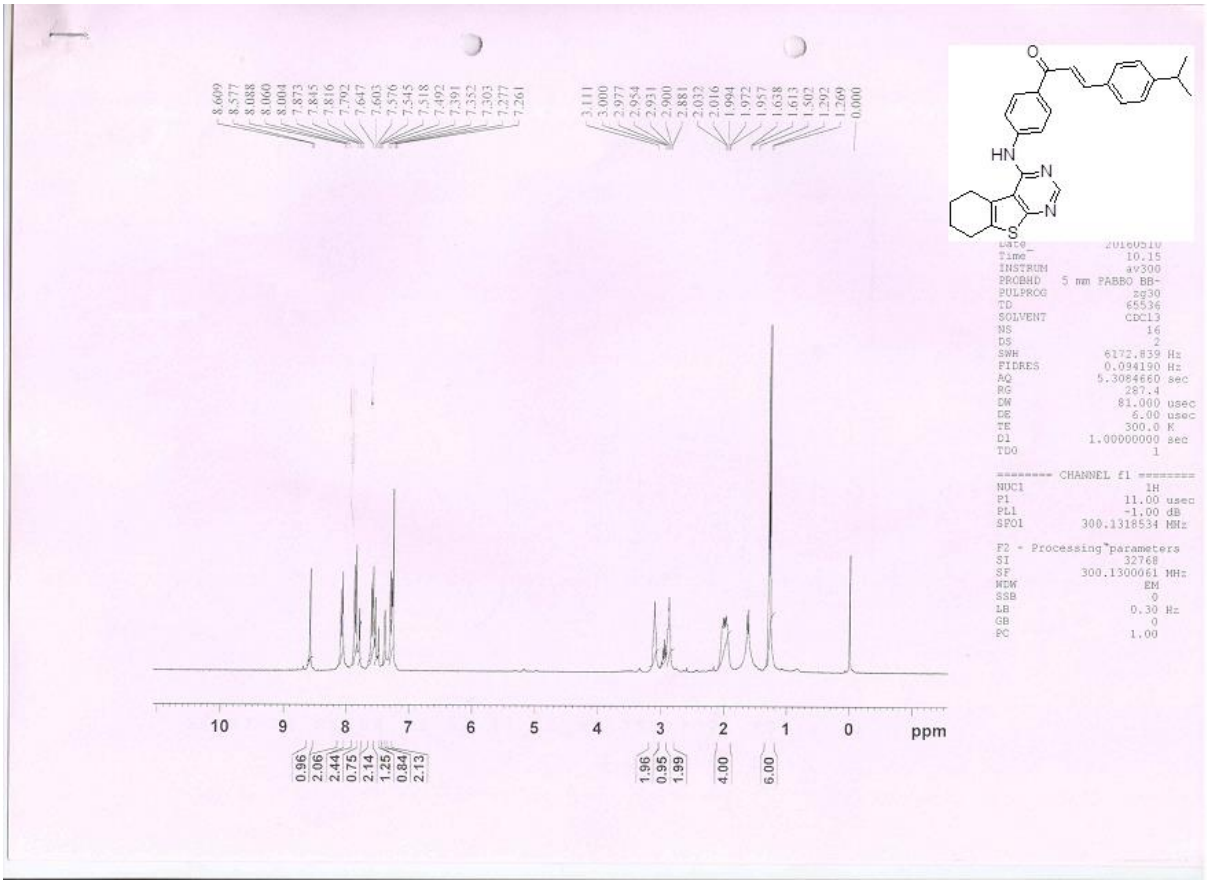
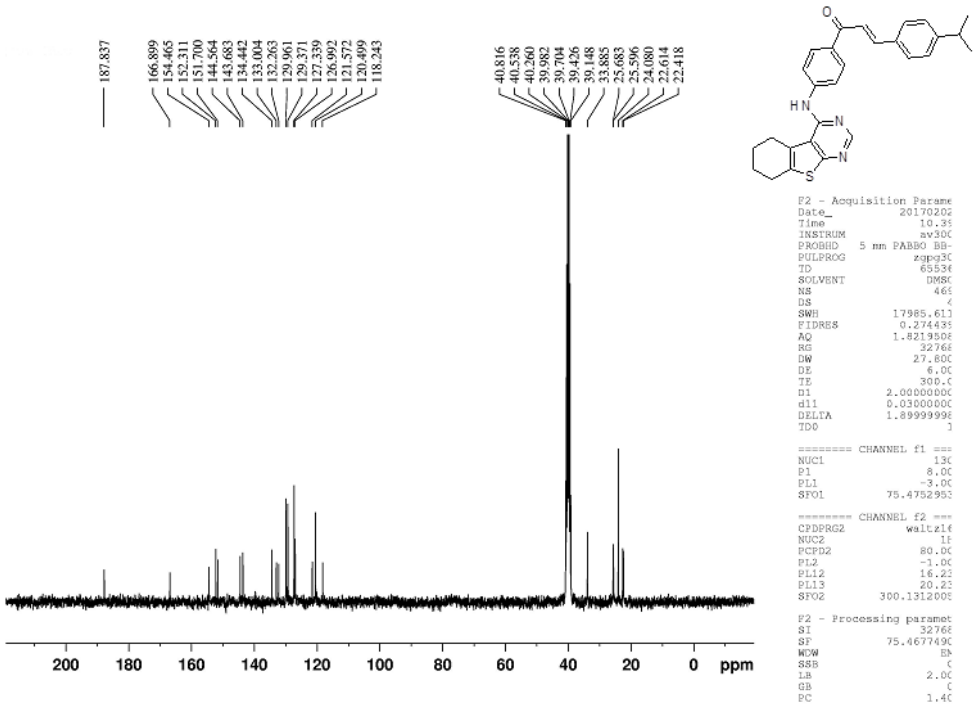


^{1}H NMR Compound 8



^{13}C NMR Compound 8



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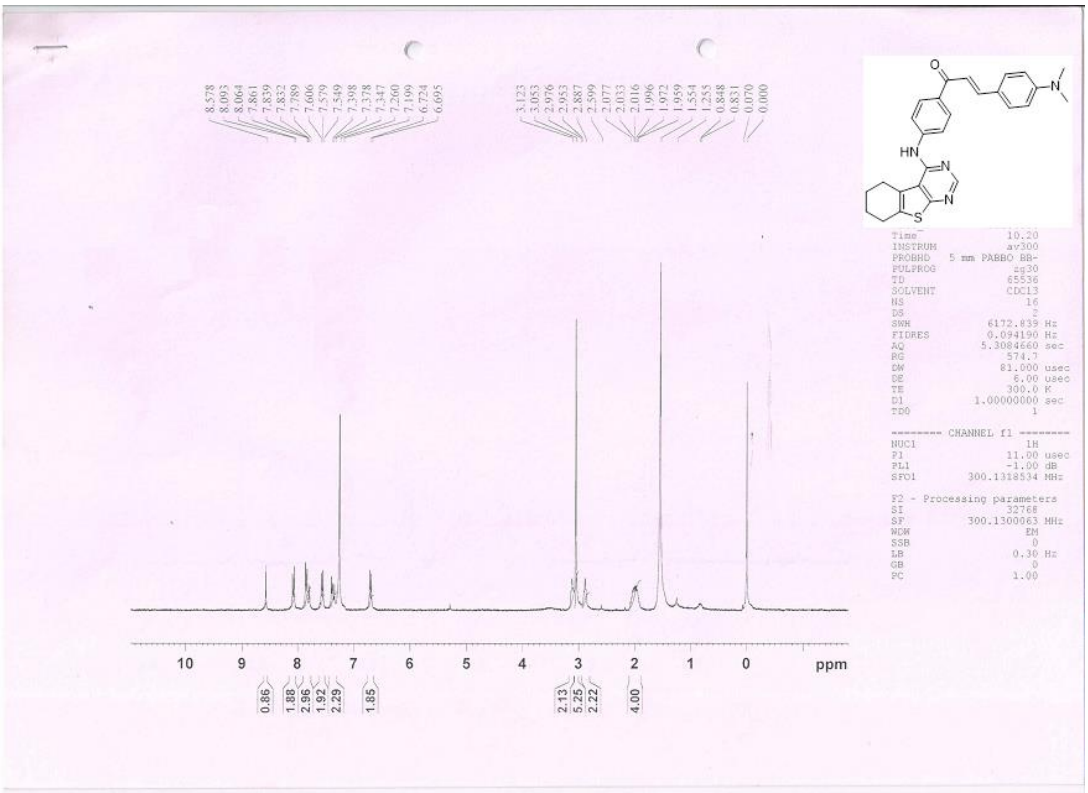

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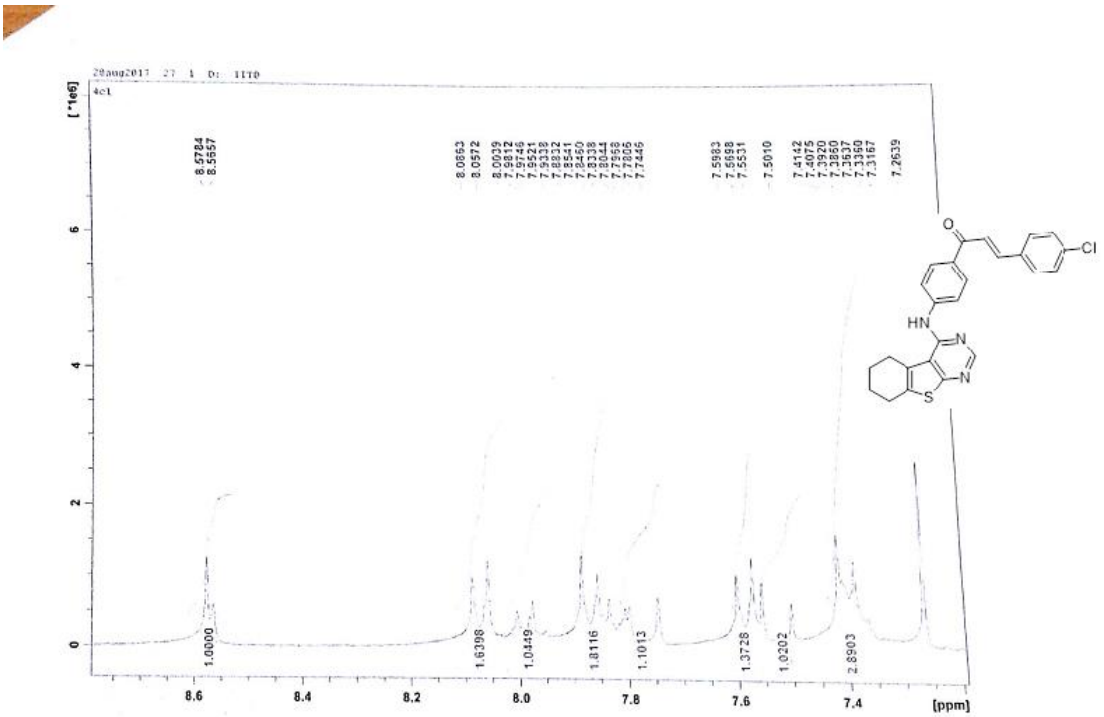

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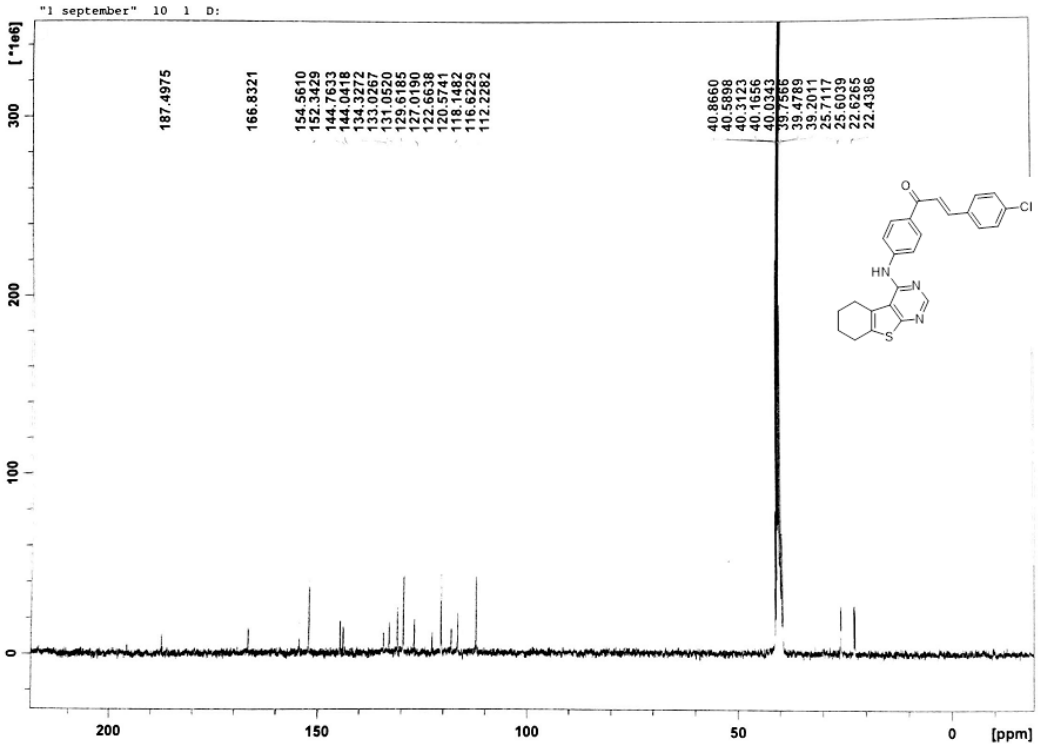

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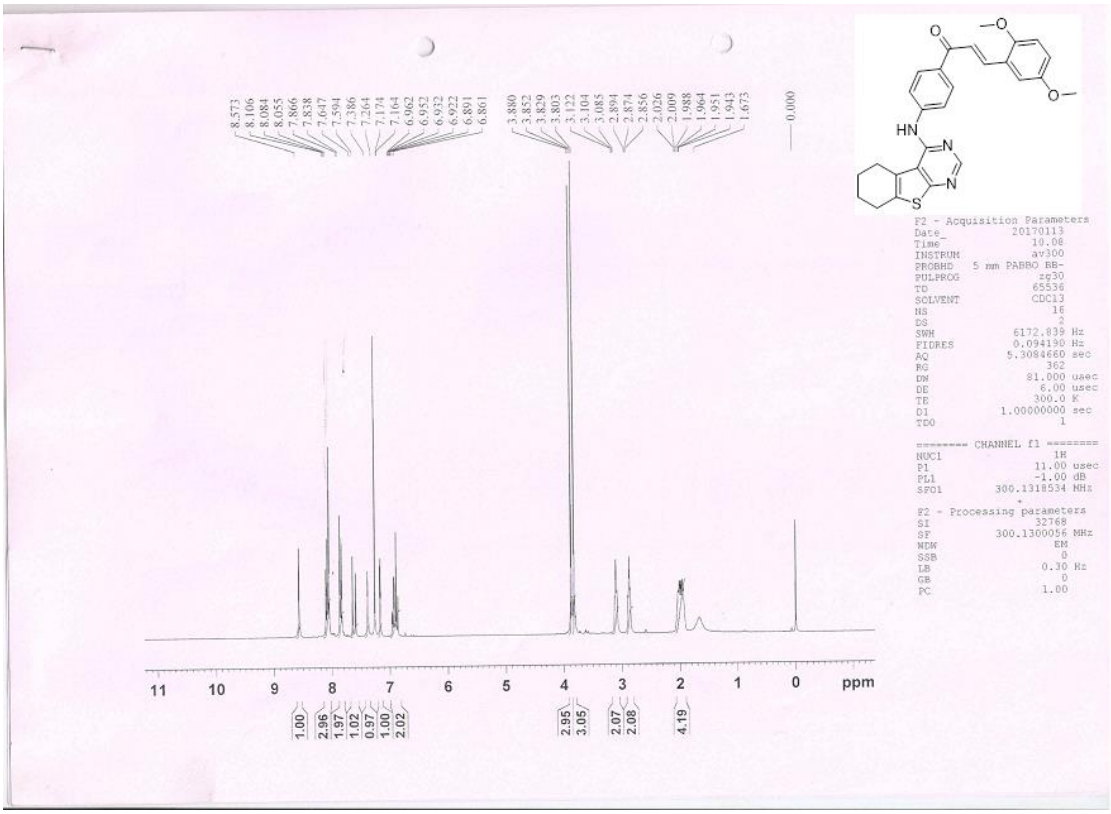

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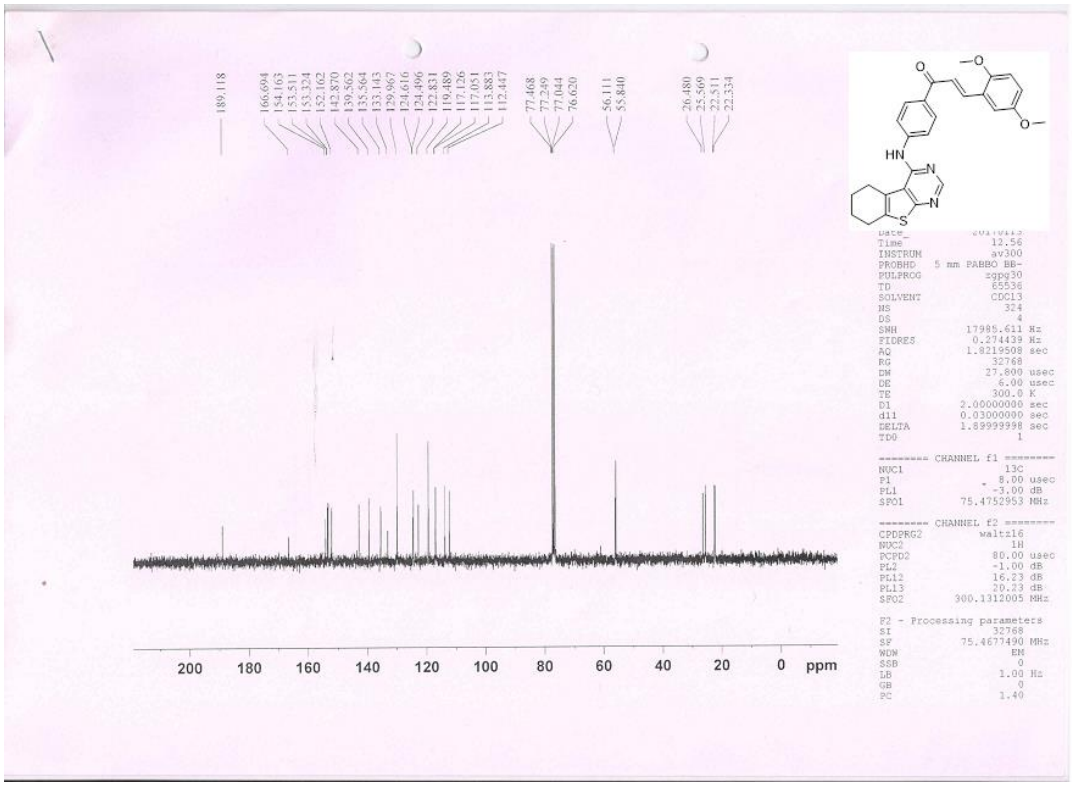

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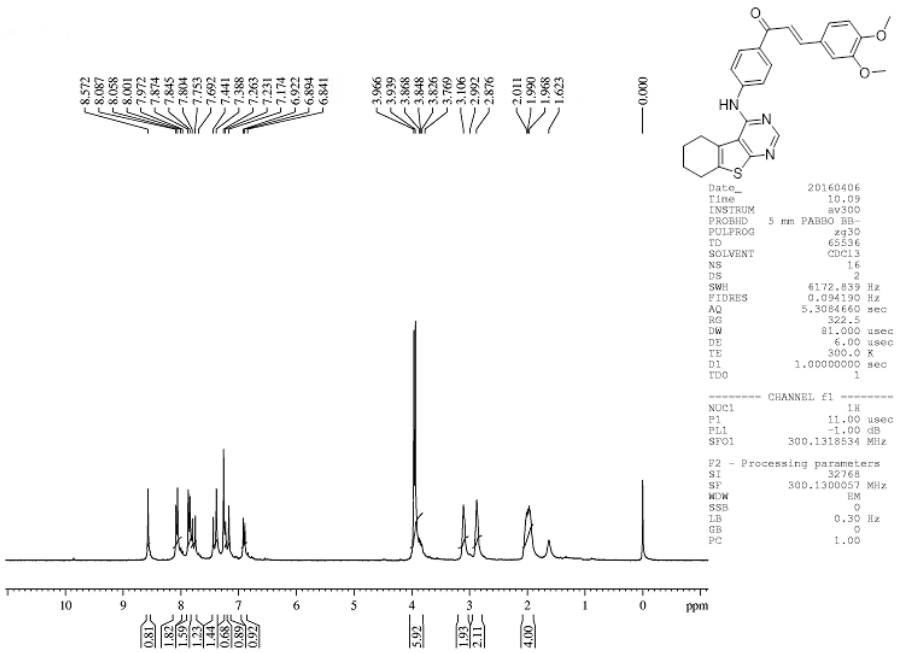

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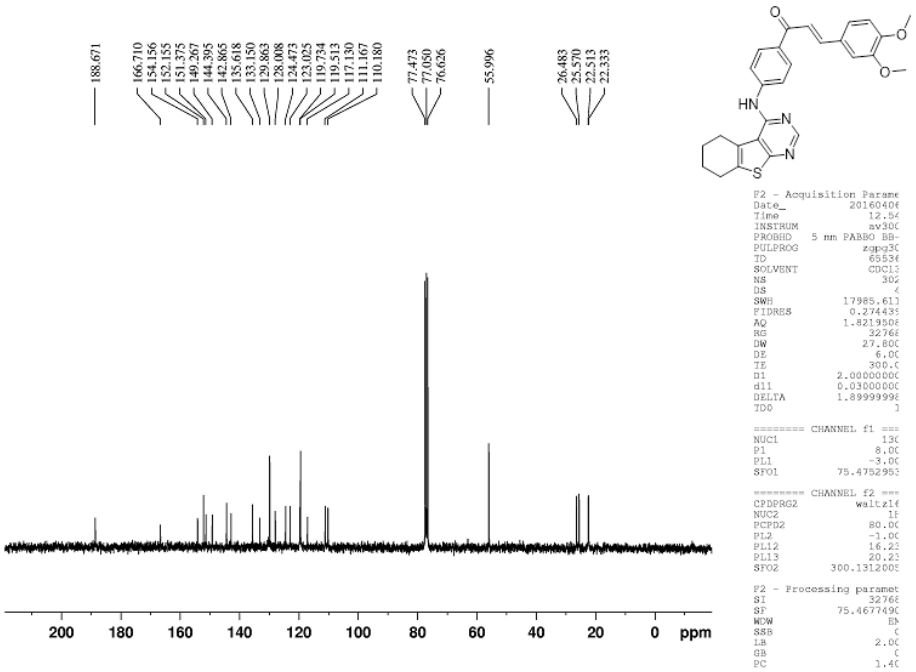

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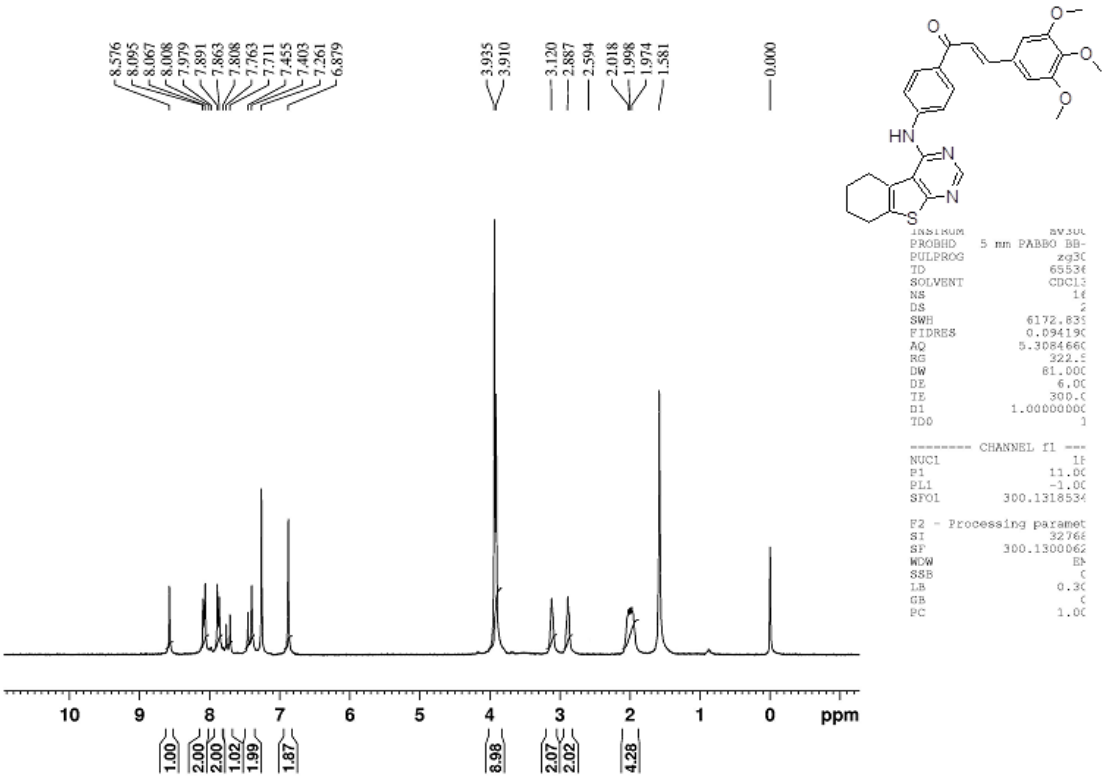
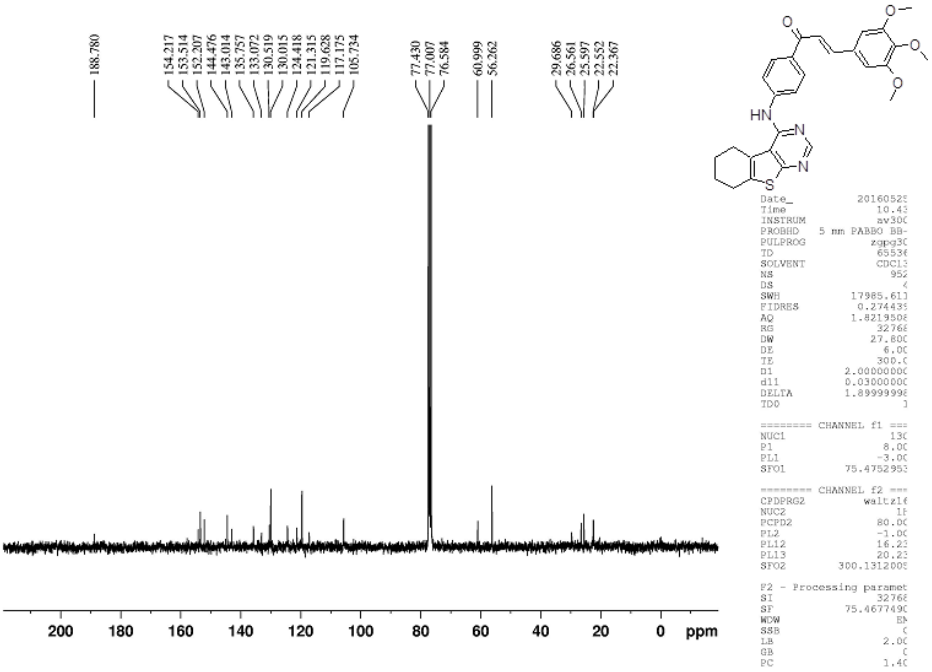


^{13}C NMR Compound 13



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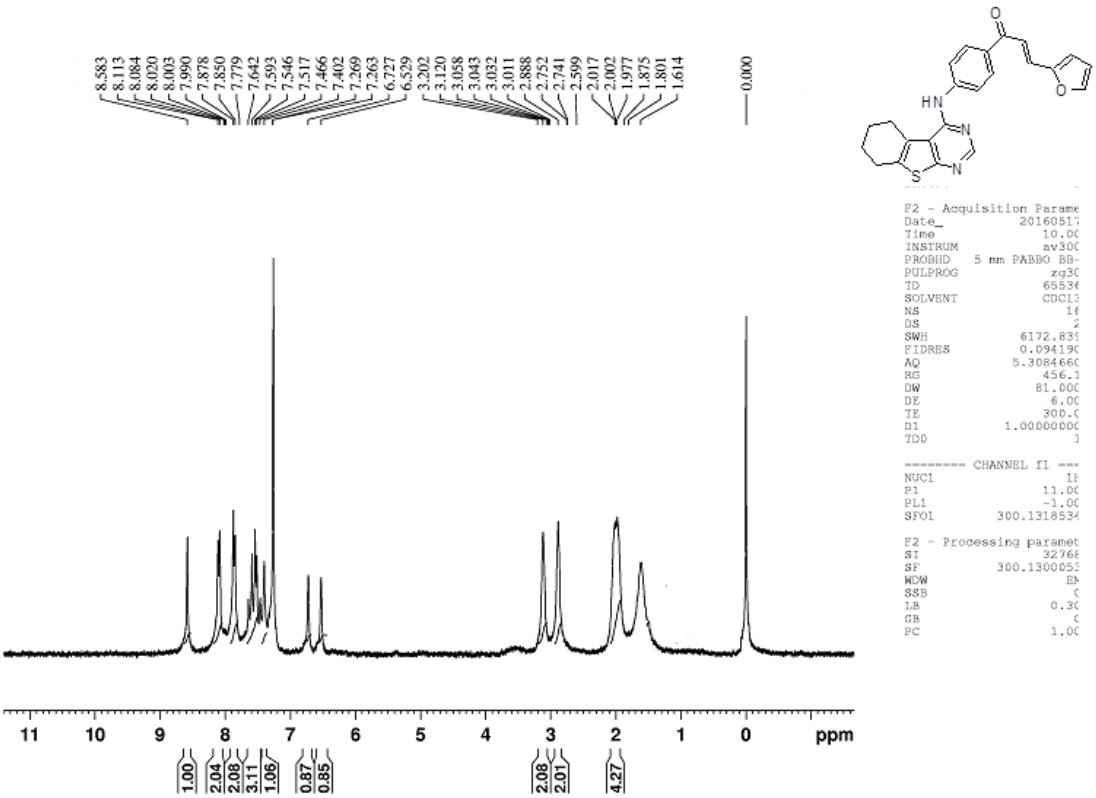

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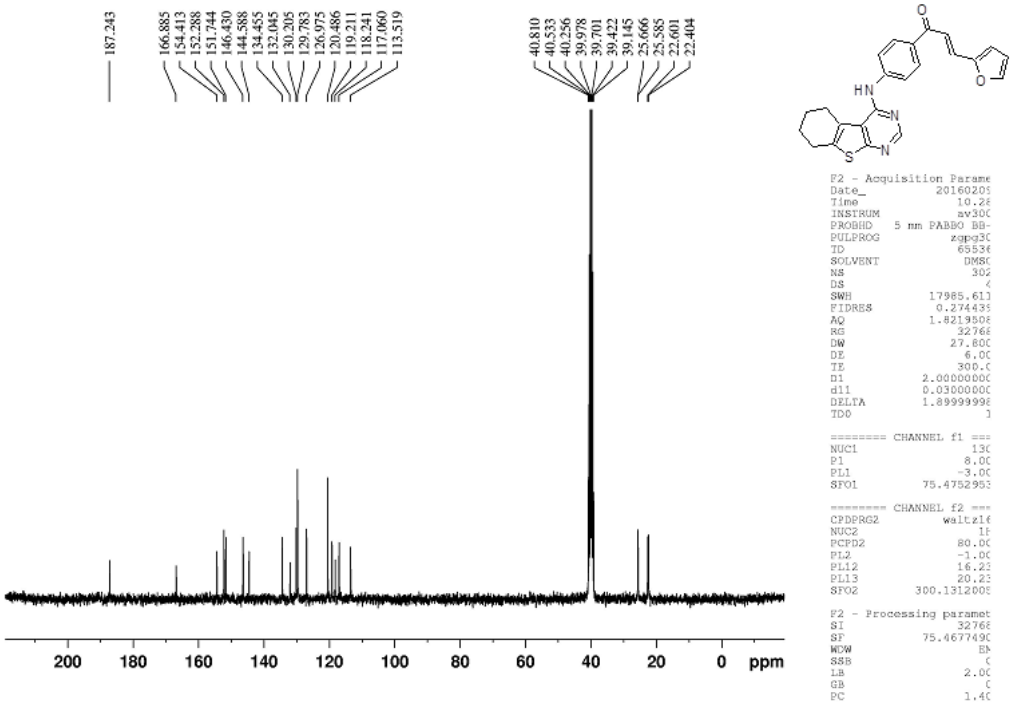
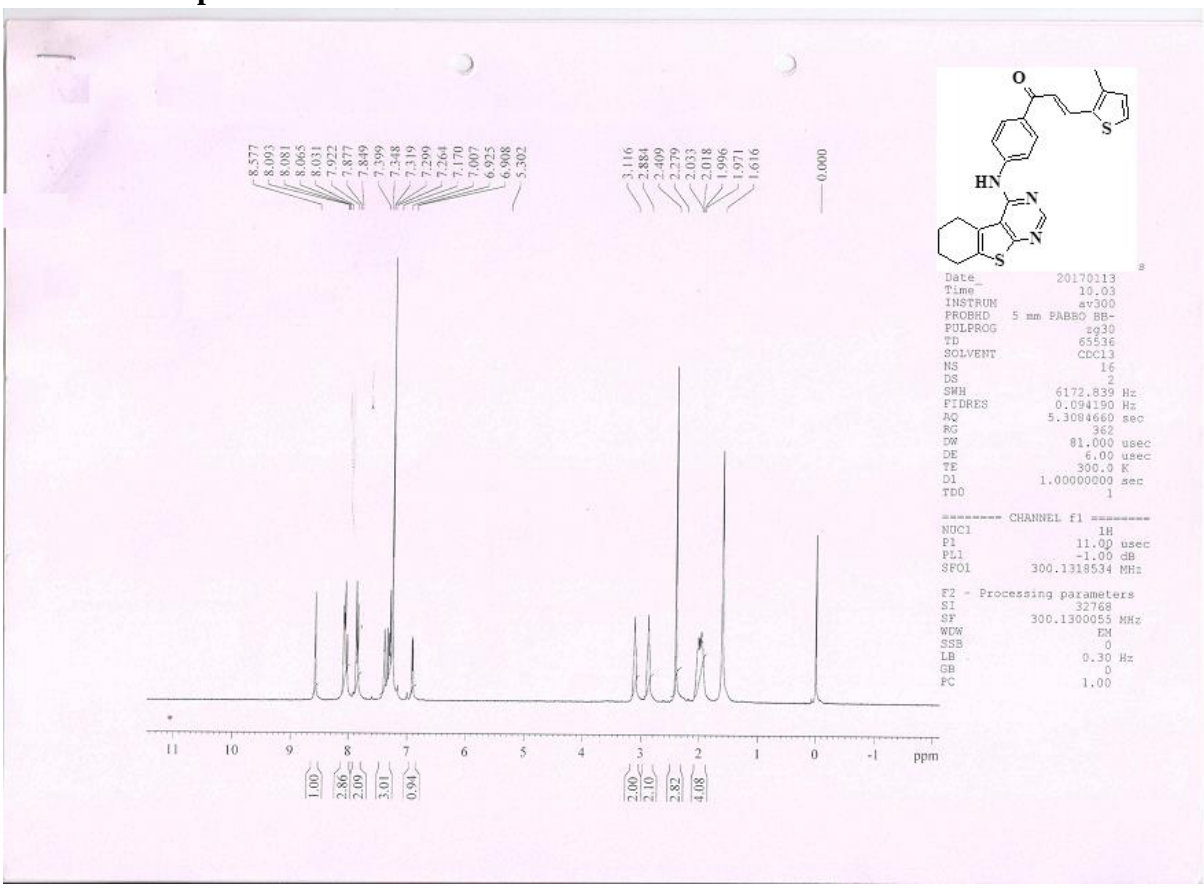


^{1}H NMR Compound 15



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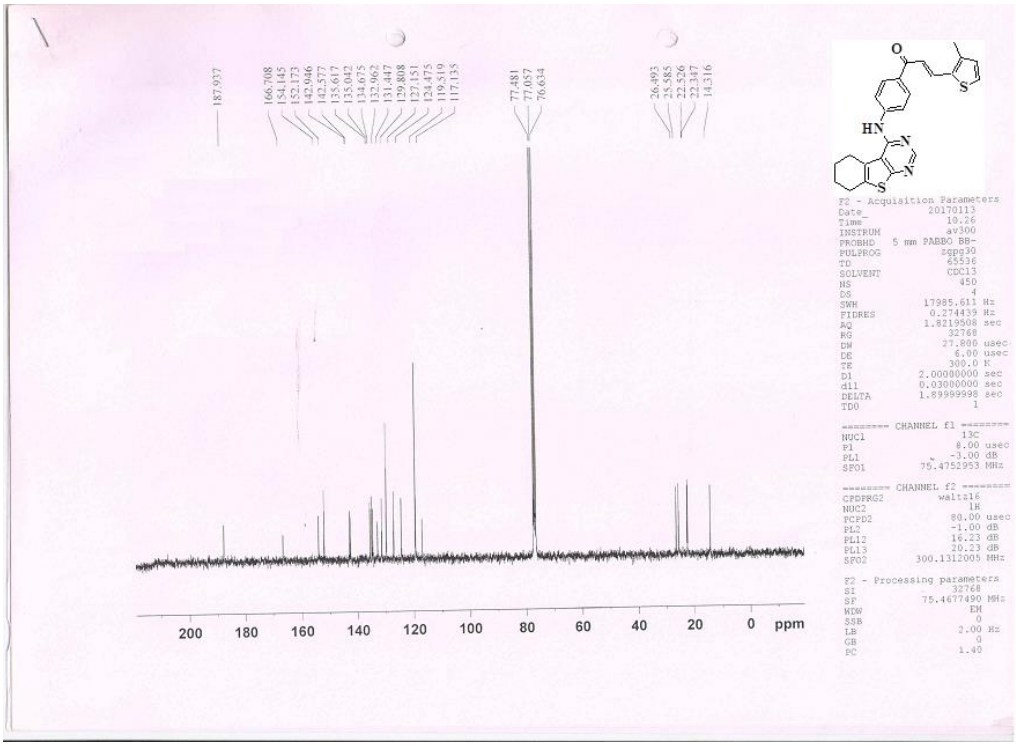
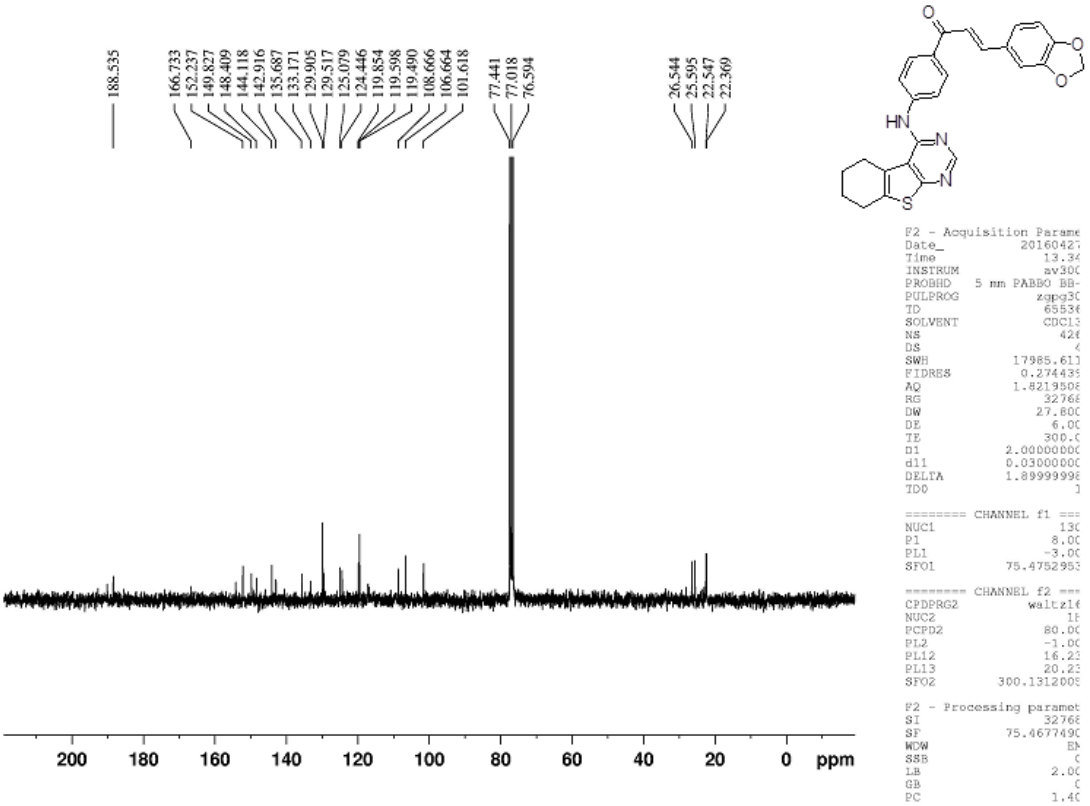
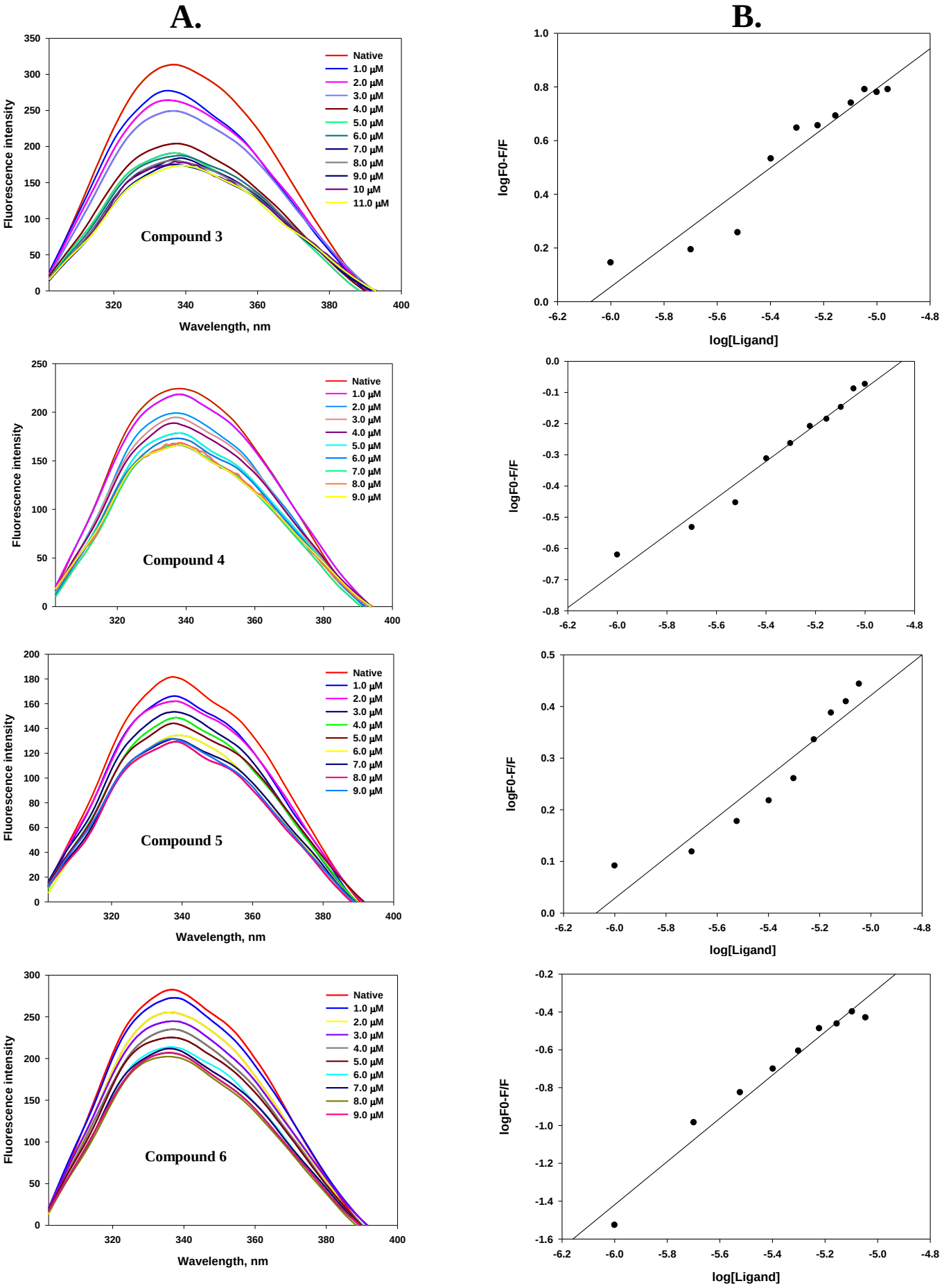
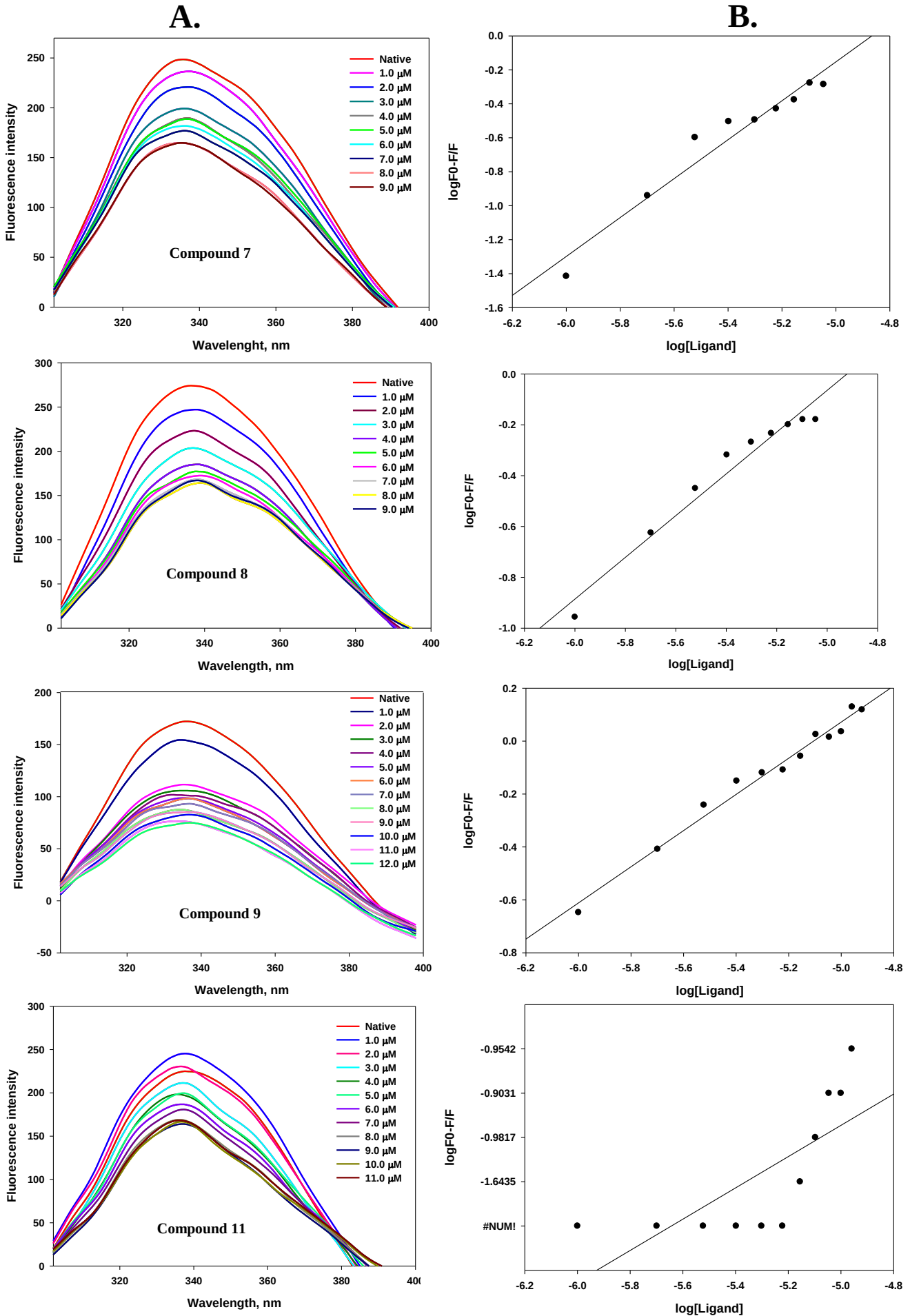


^{13}C NMR Compound 16




A.
B.
Fluorescence intensity
Wavelength, nm
Native
1.0 μM
2.0 μM
3.0 μM
4.0 μM
5.0 μM
6.0 μM
7.0 μM
8.0 μM
9.0 μM
10 μM
11.0 μM
Compound 3
Compound 4
Compound 5
Compound 6
logF0-F/F
log[Ligand]


A.
B.
Fluorescence intensity
Wavelenght, nm
Native
1.0 µM
2.0 µM
3.0 µM
4.0 µM
5.0 µM
6.0 µM
7.0 µM
8.0 µM
9.0 µM
Compound 7
logF0-F/F
log[Ligand]
Wavelength, nm
Compound 8
10.0 µM
11.0 µM
12.0 µM
Compound 9
Compound 11
-0.9542
-0.9031
-0.9817
-1.6435
#NUM!

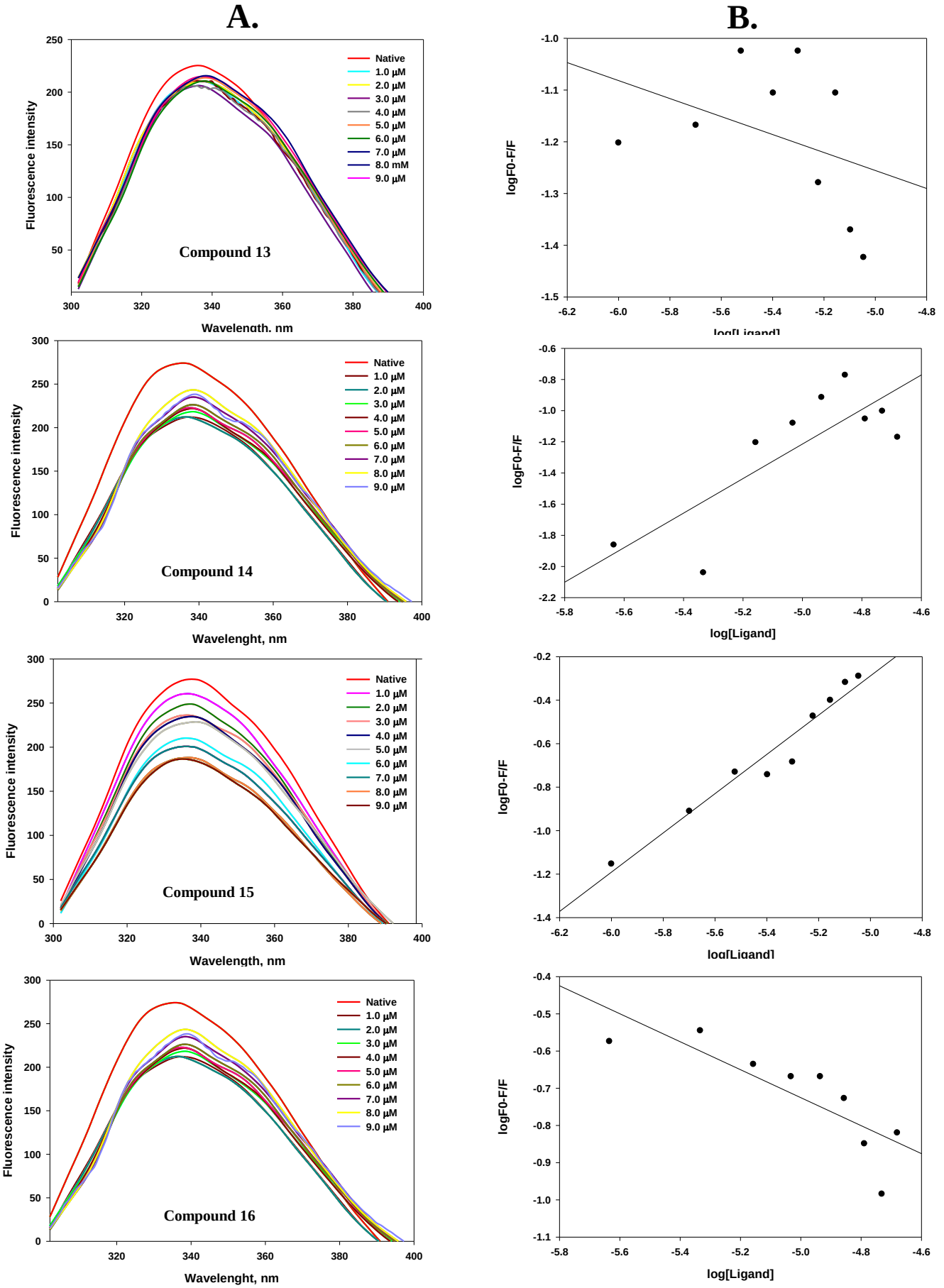


Figure S1: Binding studies of different compounds (Compound No. 3, 4, 5. 6, 7, 8, 9, 11, 13, 14, 15 and 16) with FATSK using fluorescence spectroscopy. **(A).** Panel represents fluorescence emission spectra and **(B).** Panel represents the Modified Stern-Volmer plot of different compounds.