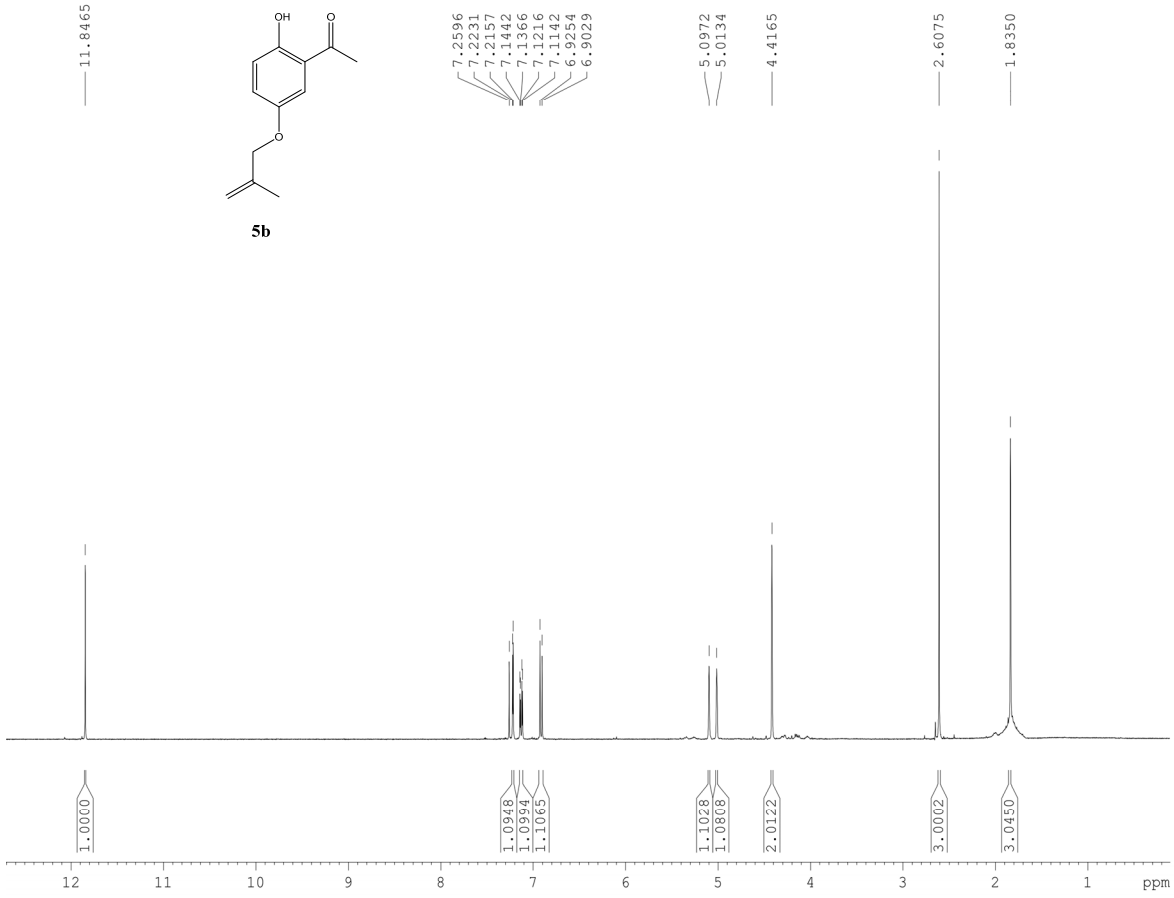
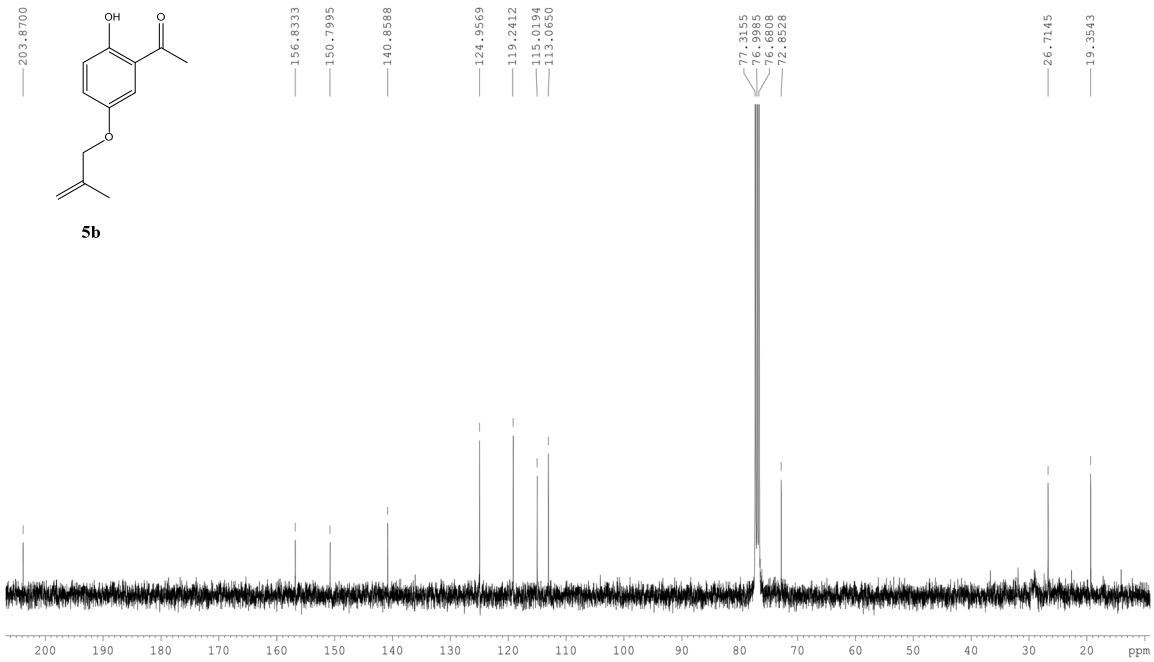
SpectraS1: ^{1}H and ^{13}C NMR of compounds 5b–5d and 6b-6c

^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound 5b



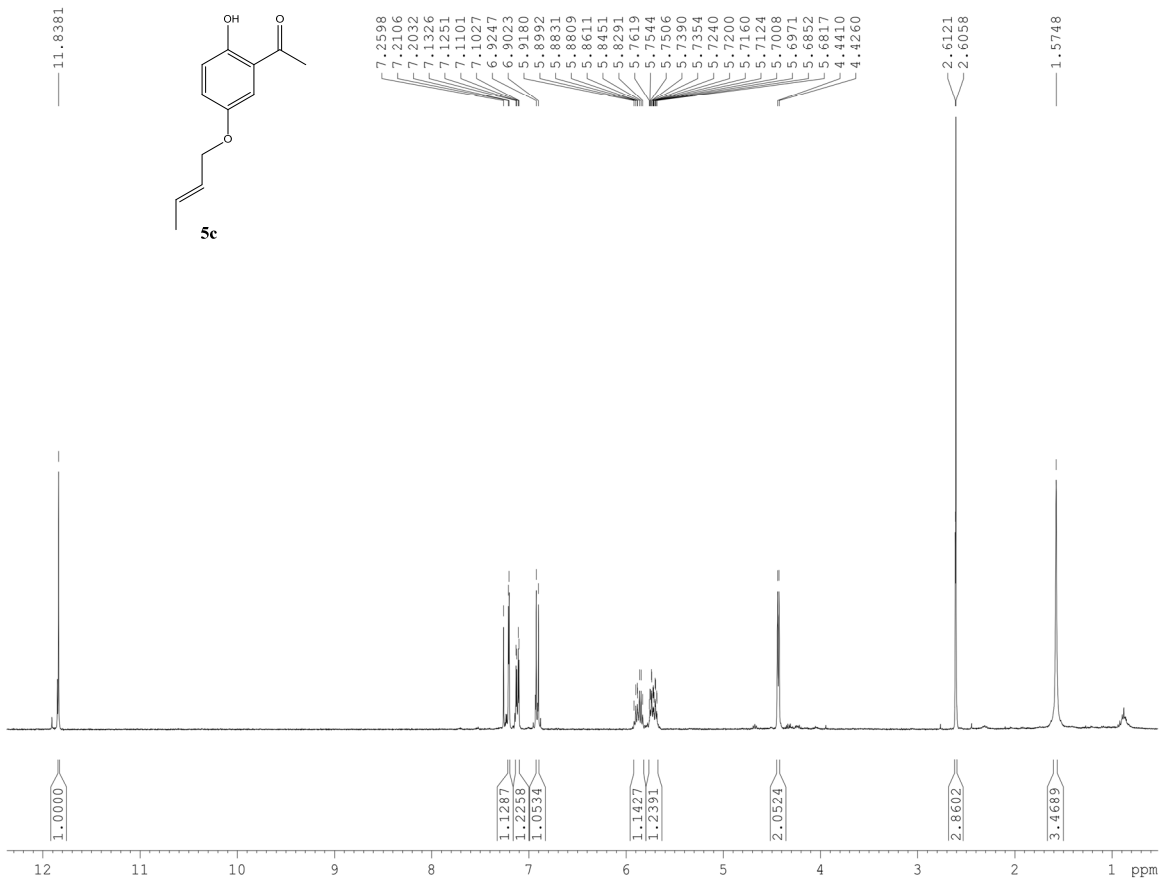
5b

^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound 5b

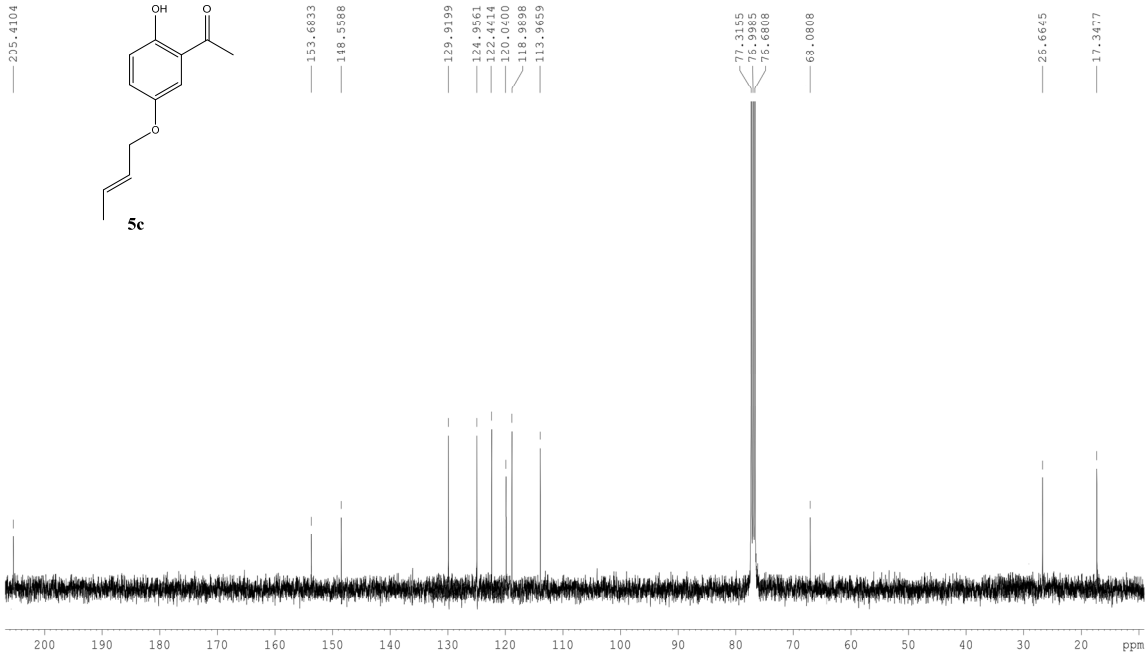


5b

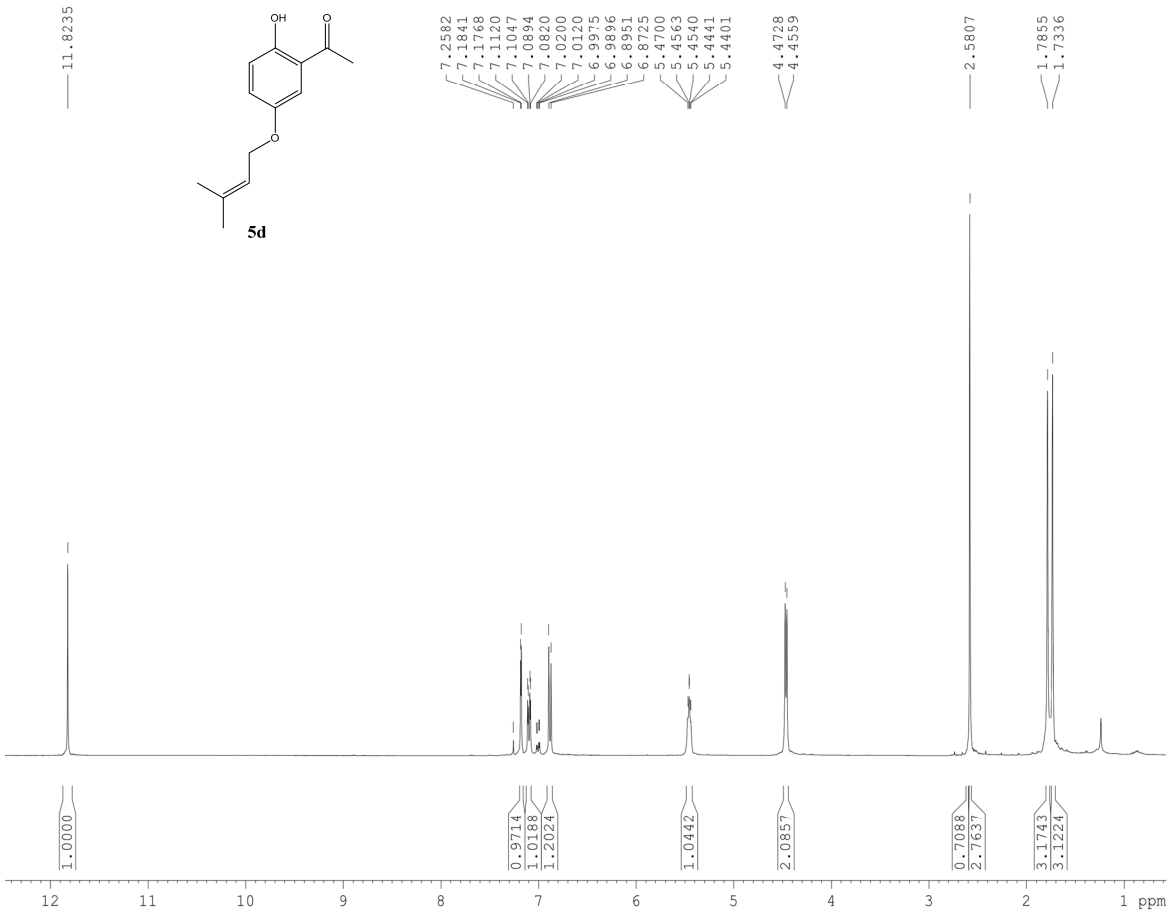
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound 5c



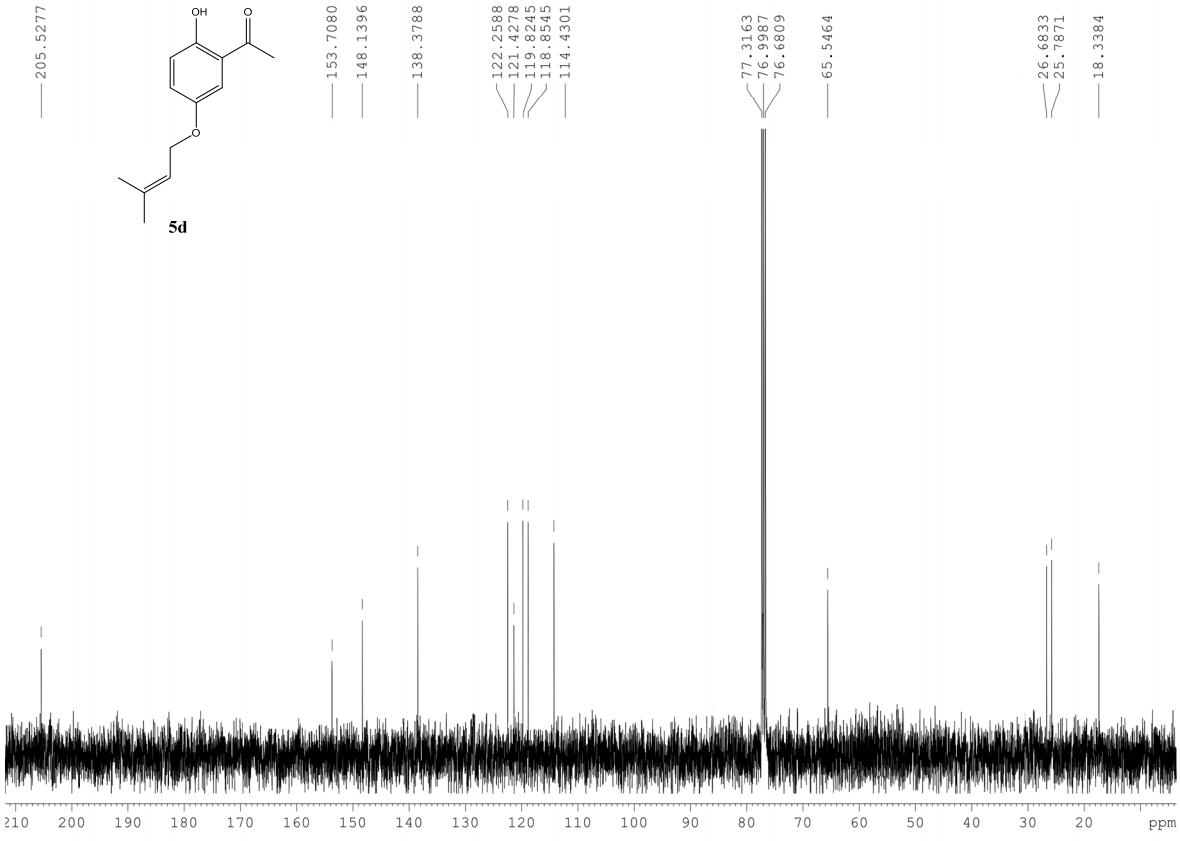
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound 5c



^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound 5d

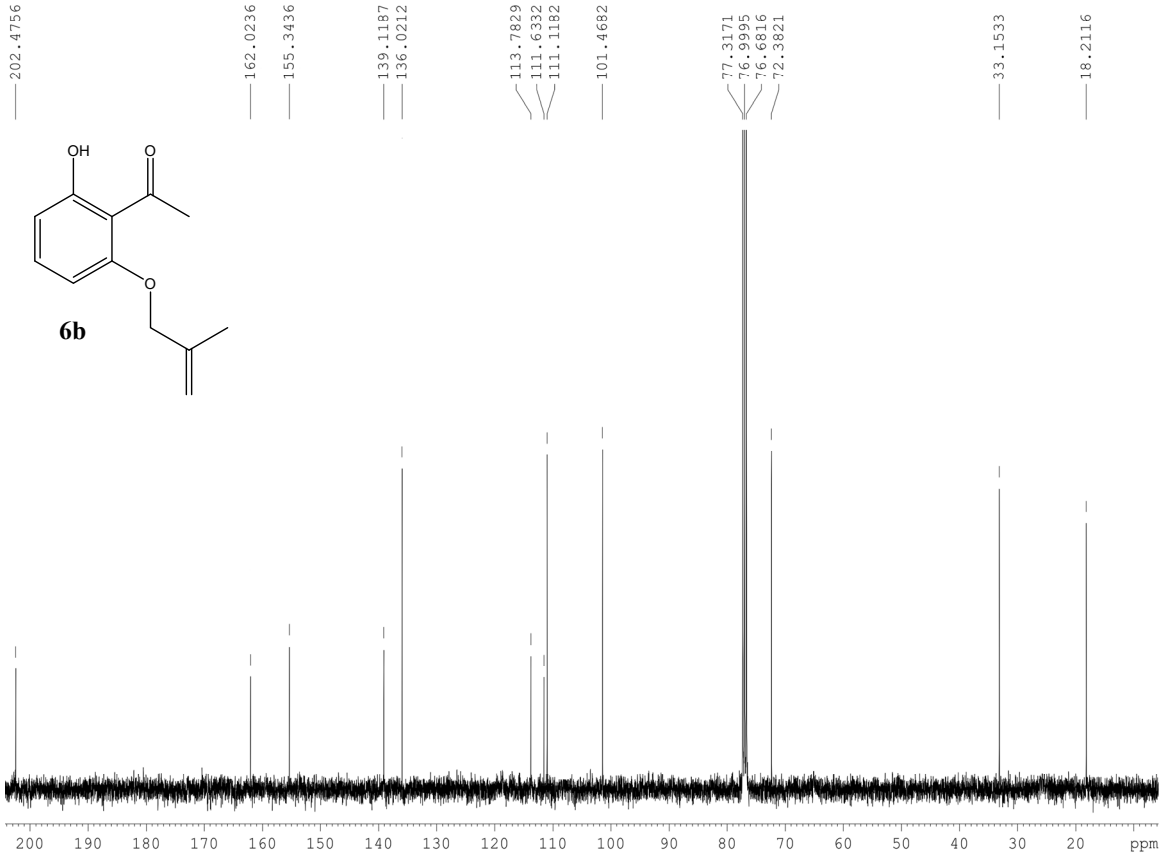


^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound 5d

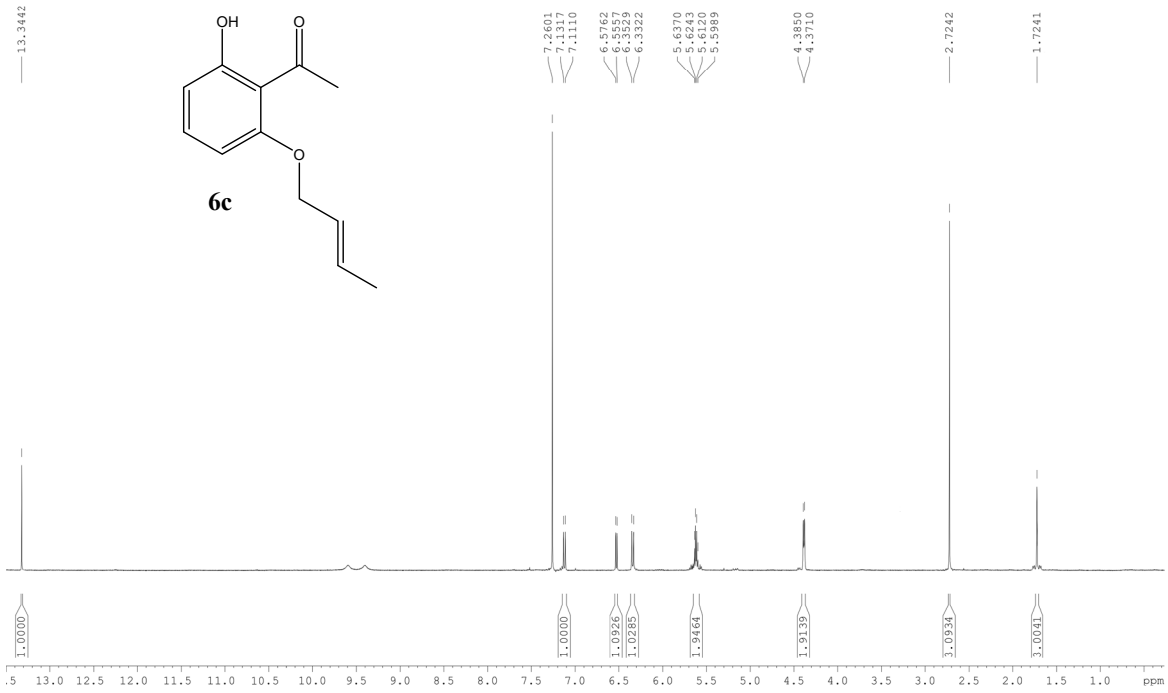


^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound 6b

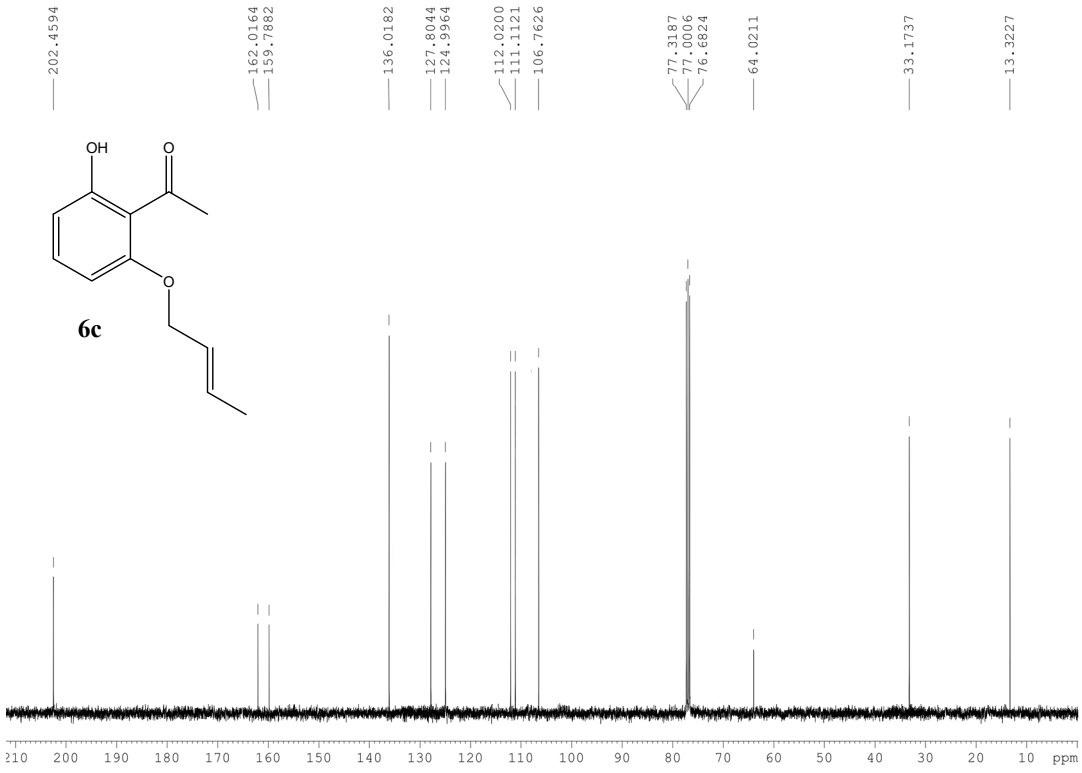
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound 6b



^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound 6c

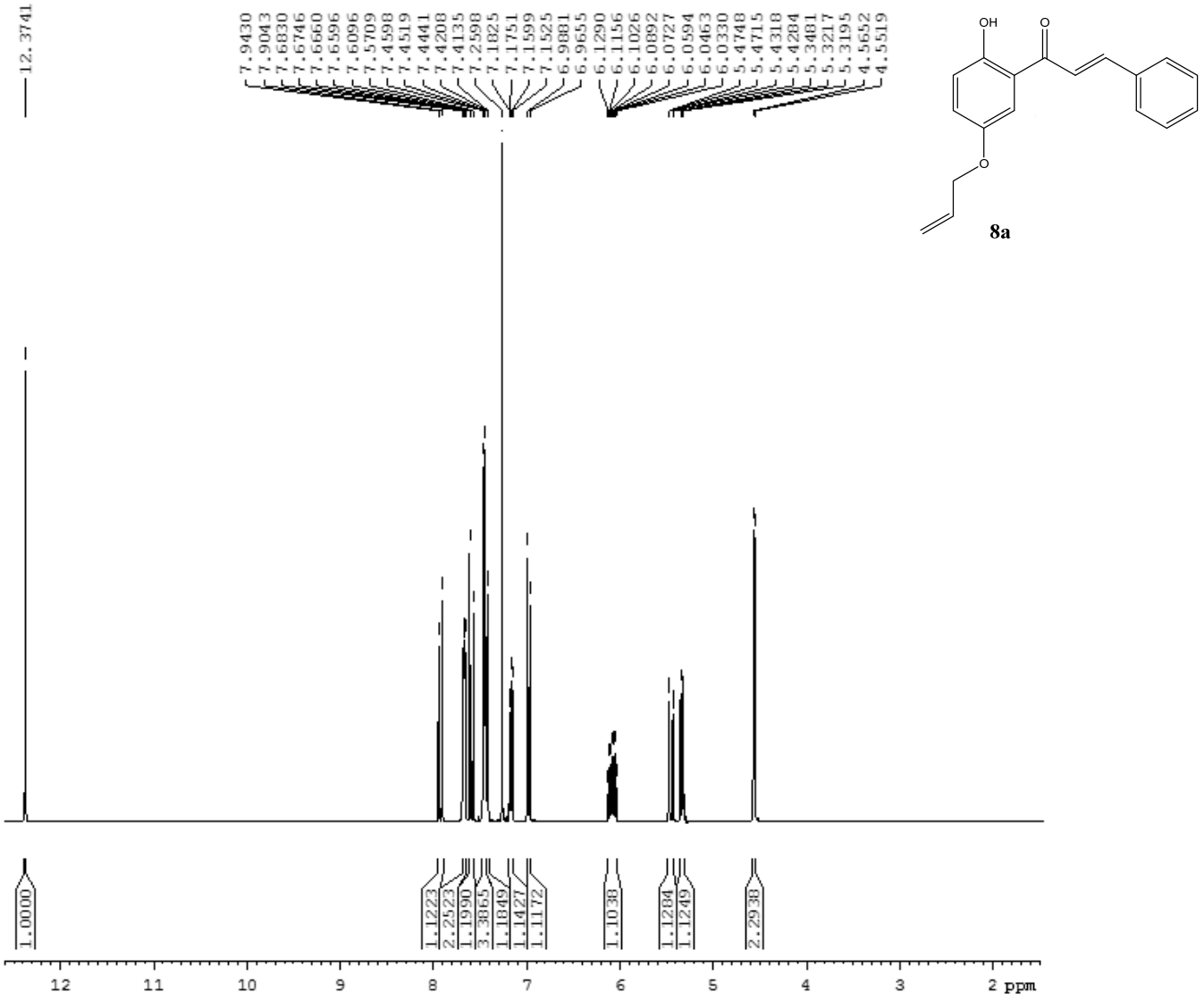


^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound 6c



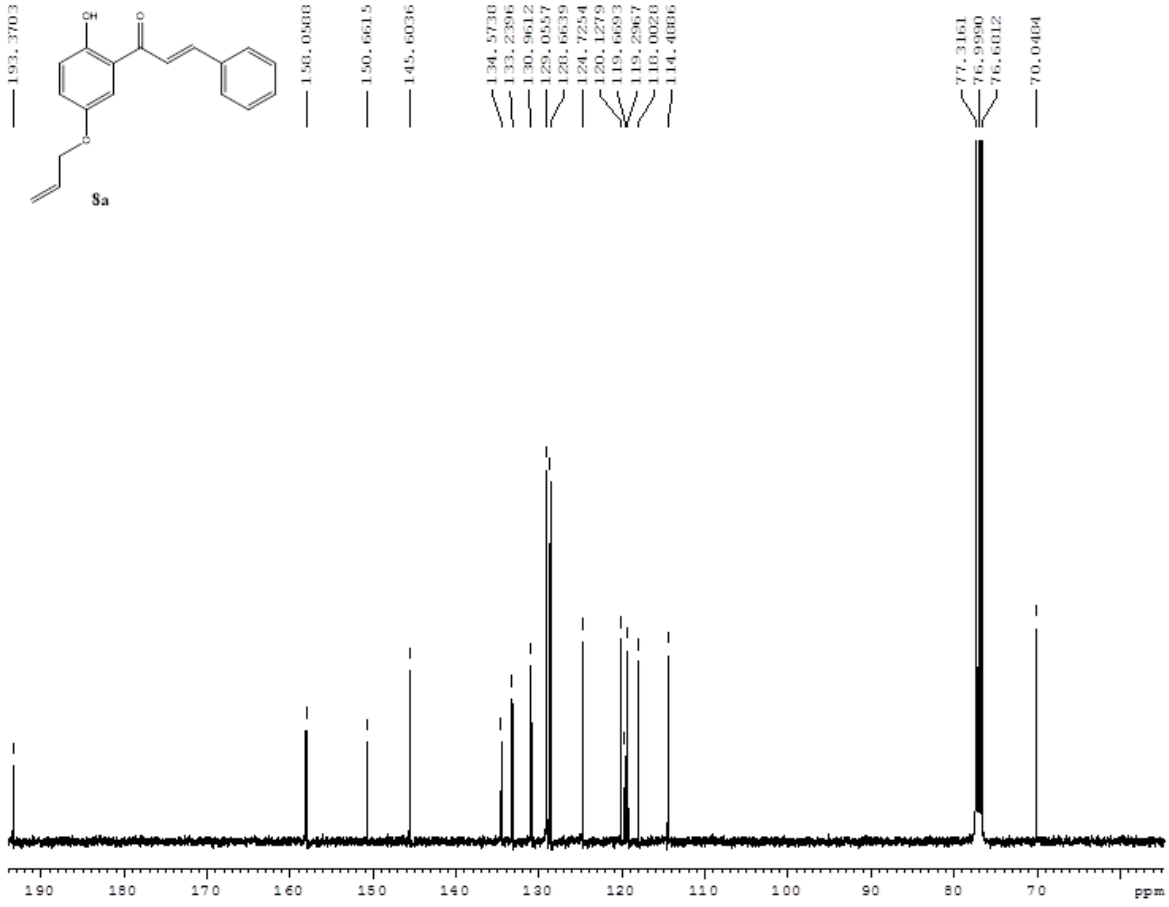
SpectraS2: ^{1}H, ^{13}C NMR, and MS of compounds 8a-8d and 9a-9d

^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound 8a

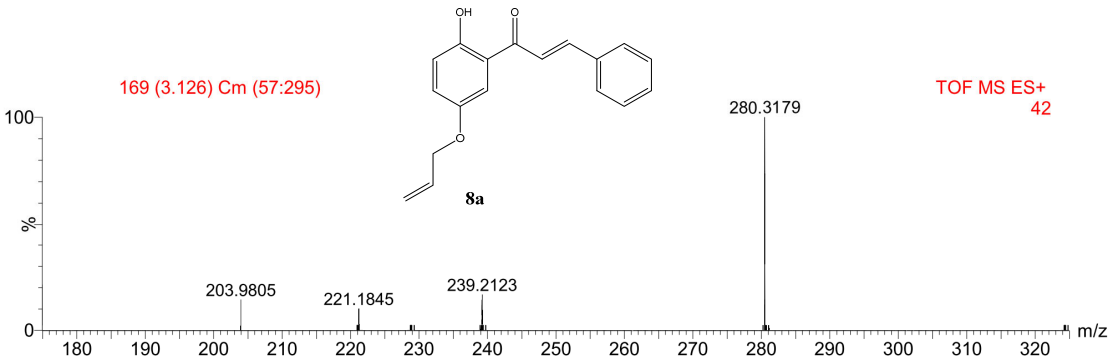


8a

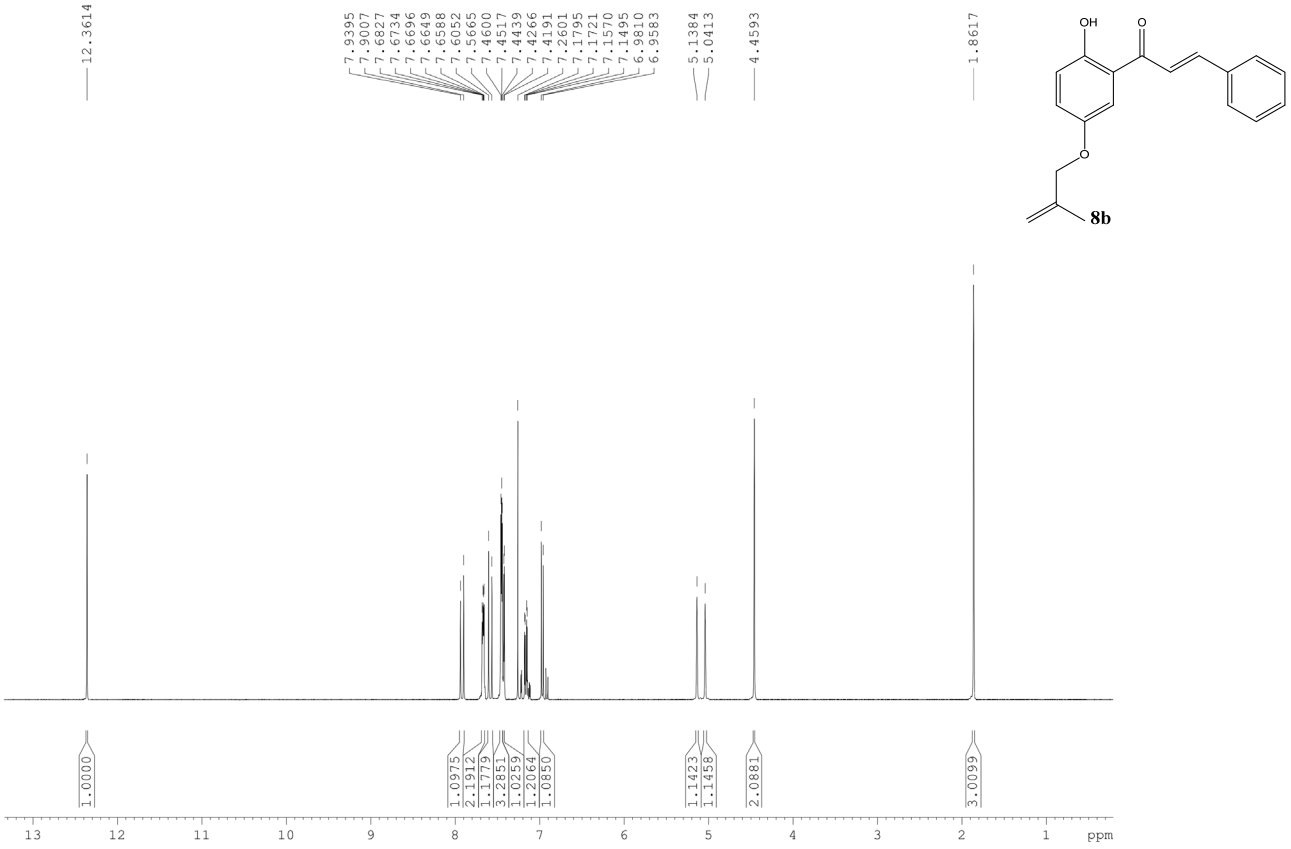
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound 8a



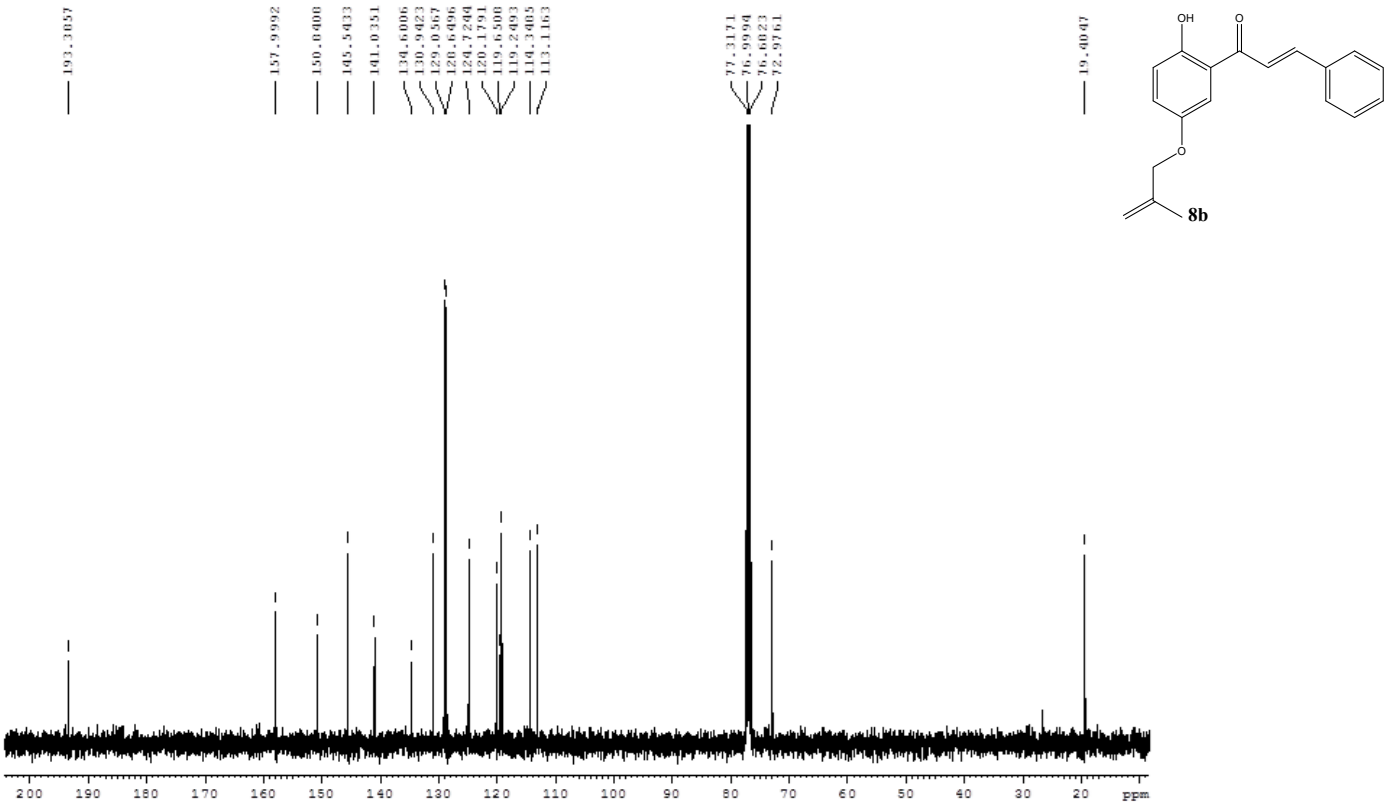
Mass of compound 8a



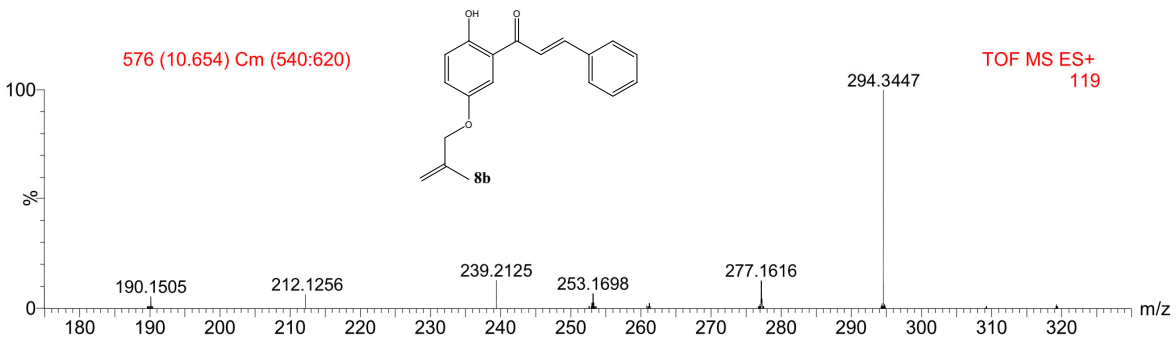
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound 8b



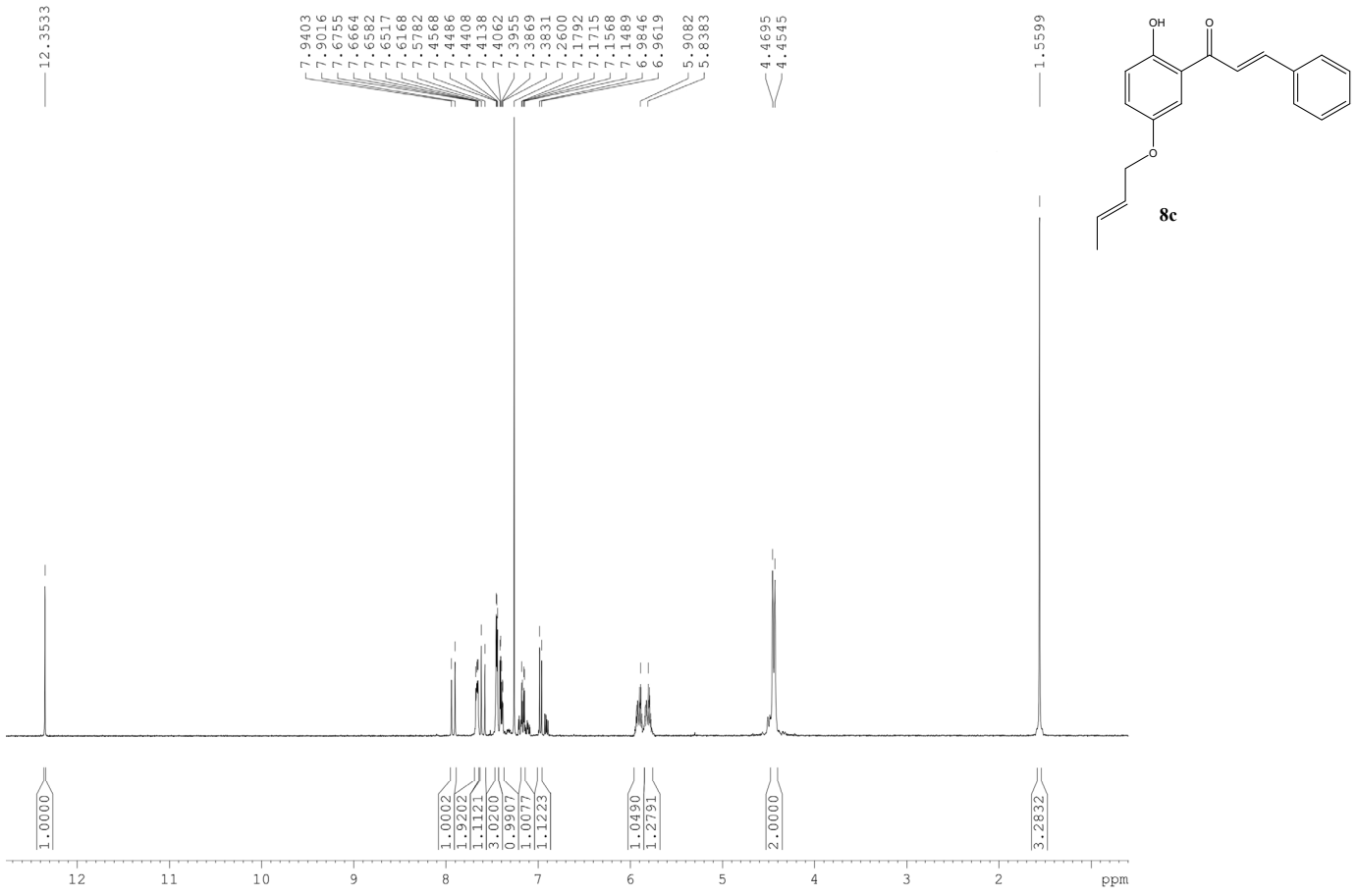
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound 8b



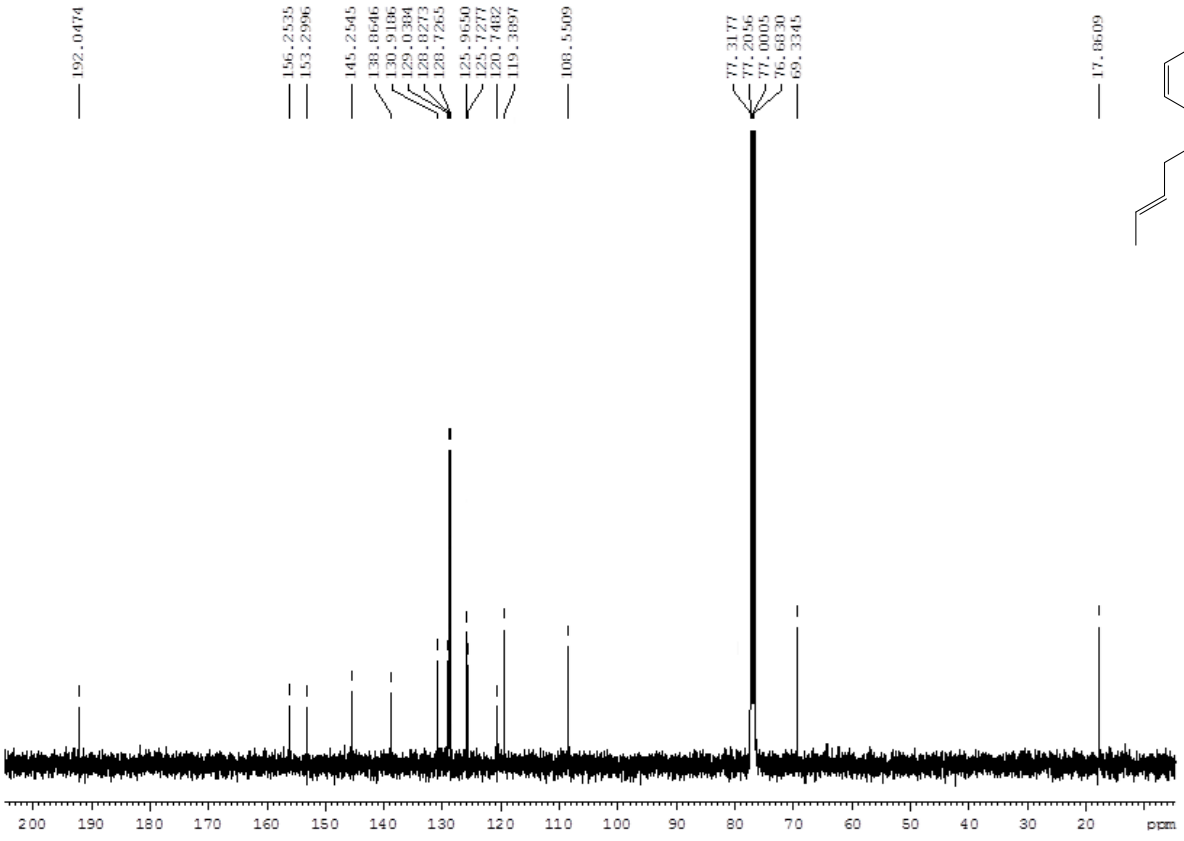
Mass of compound 8b



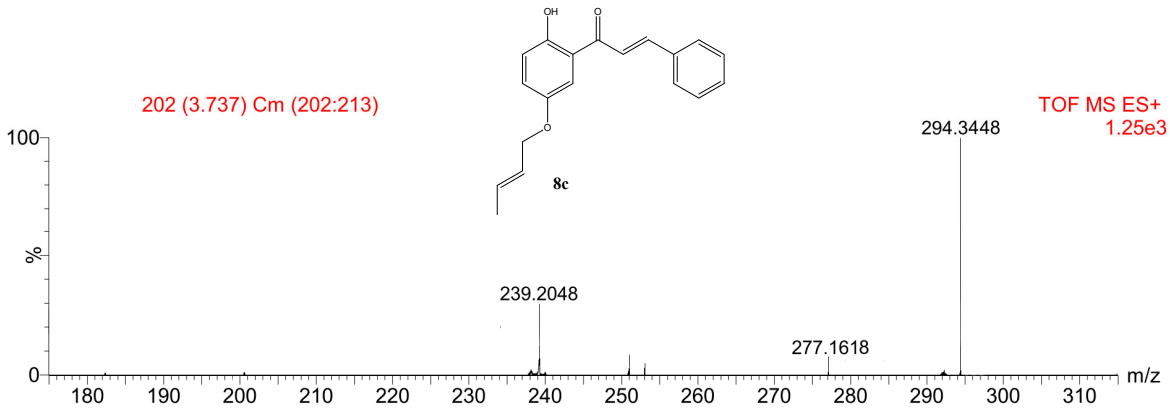
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound 8c



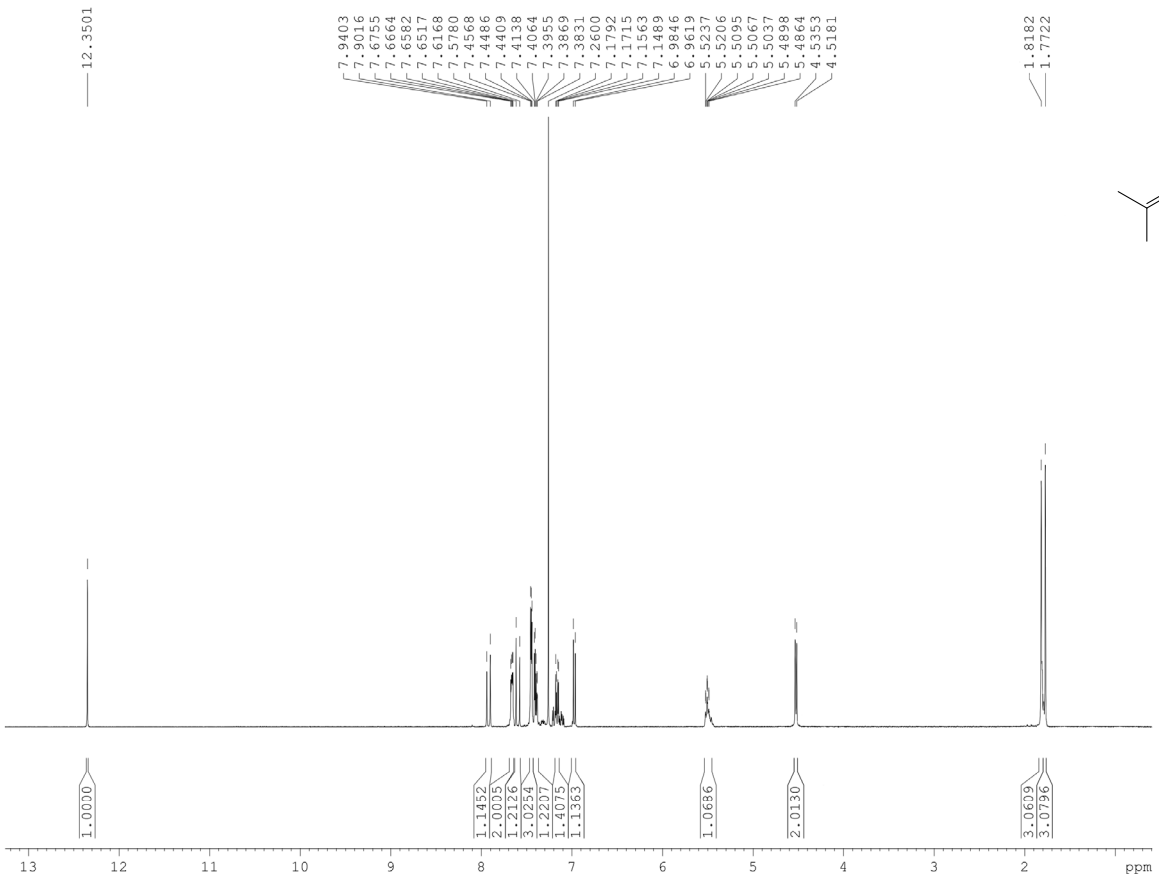
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound 8c

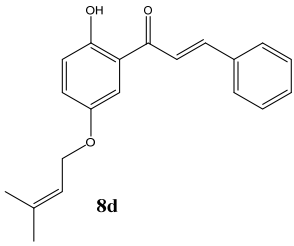


Mass of compound 8c



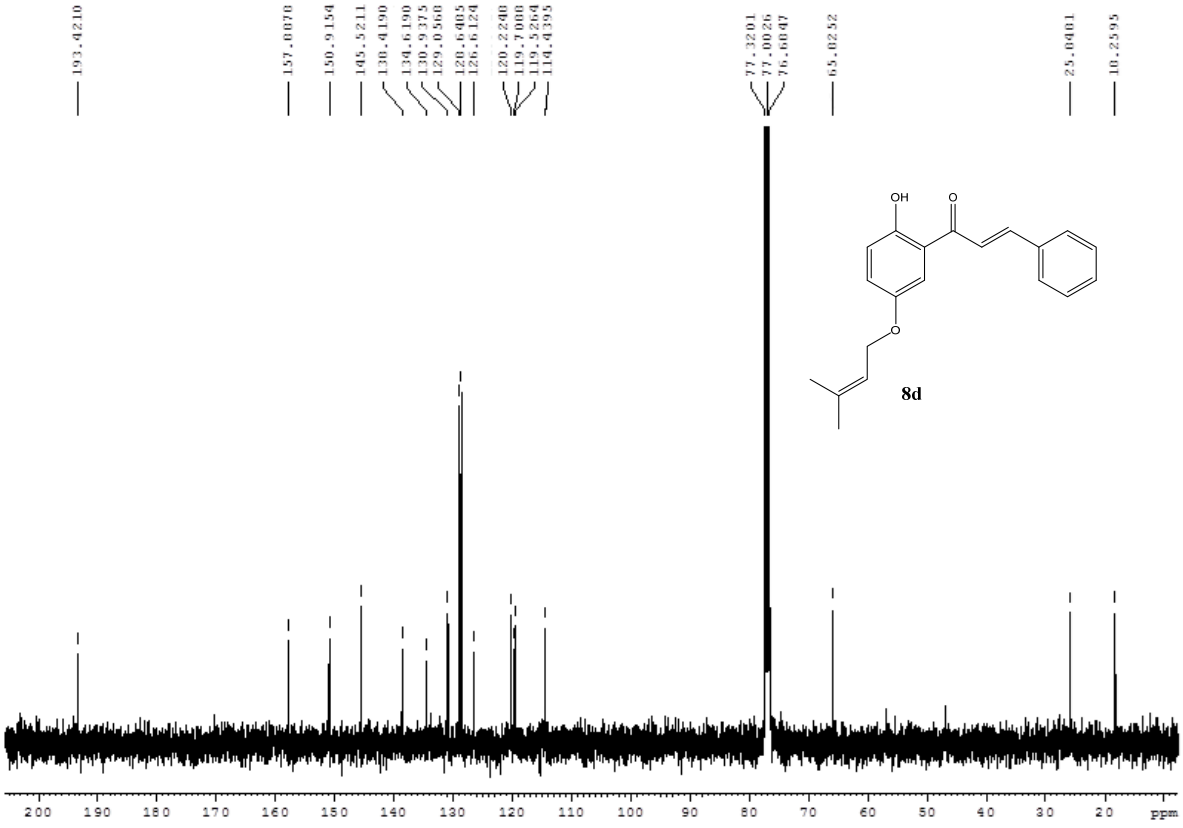
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound 8d



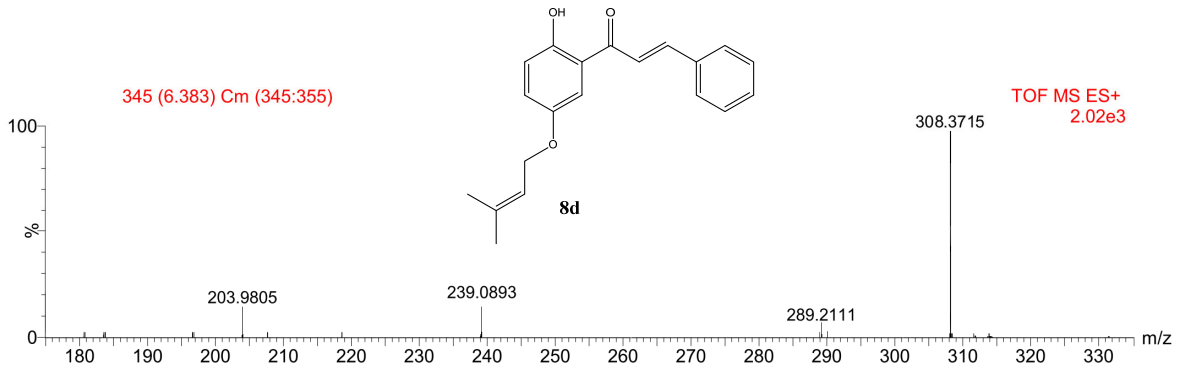


8d

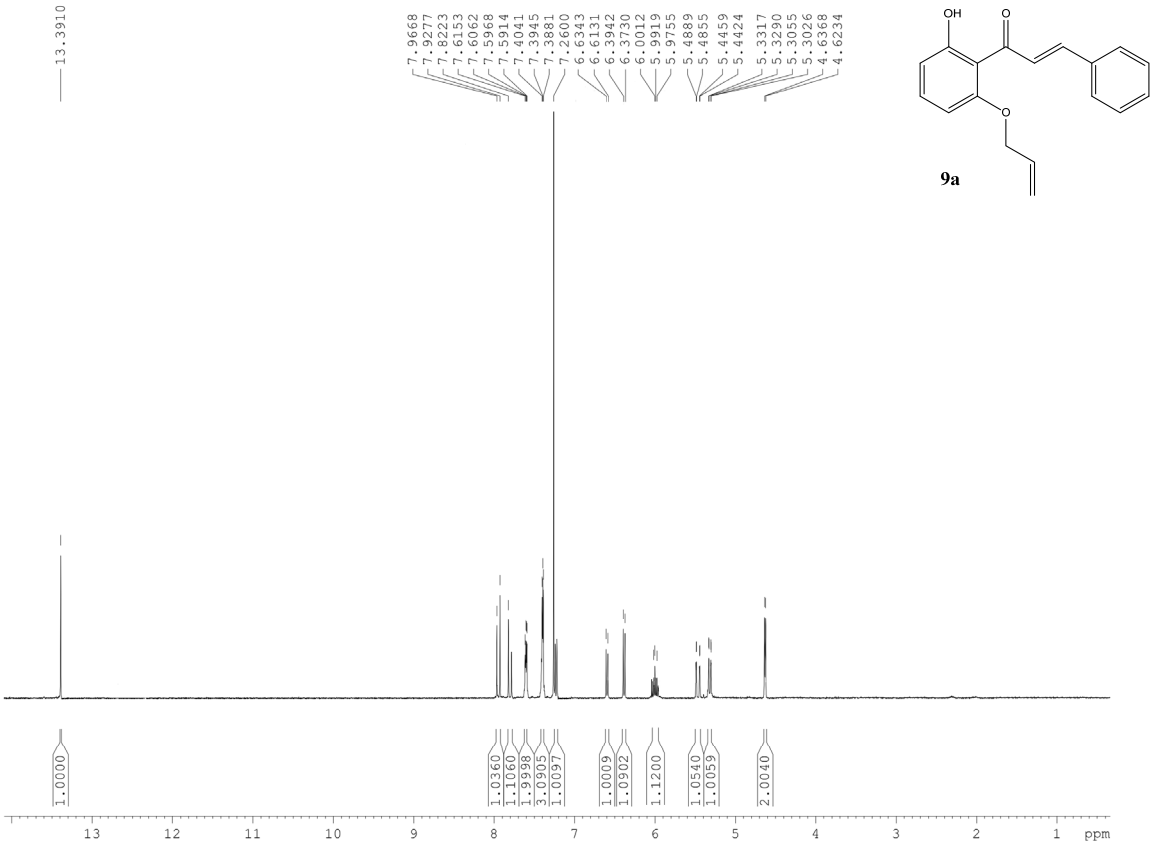
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound 8d



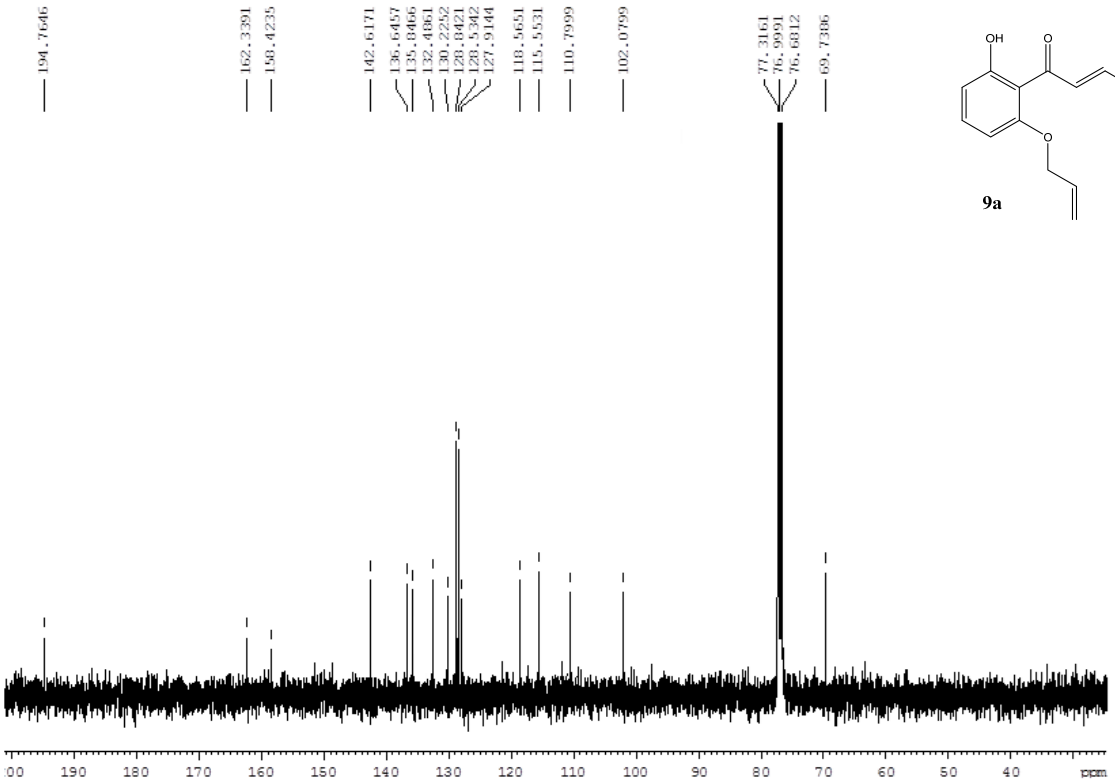
Mass of compound 8d



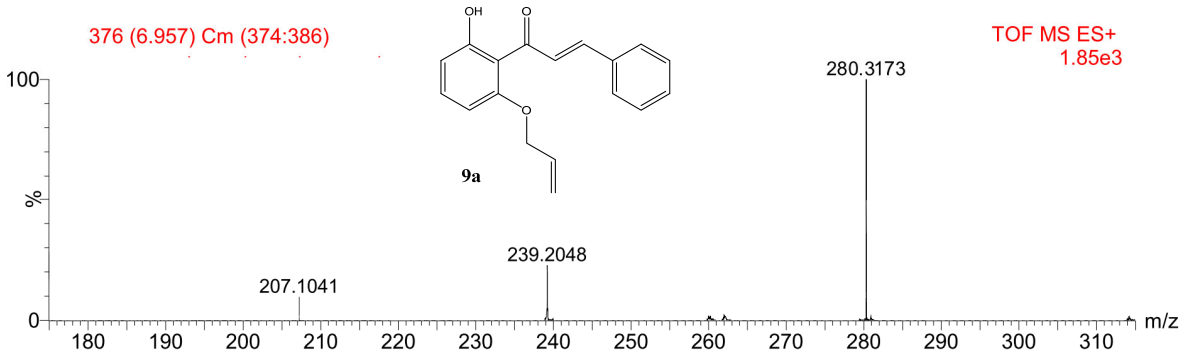
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound 9a



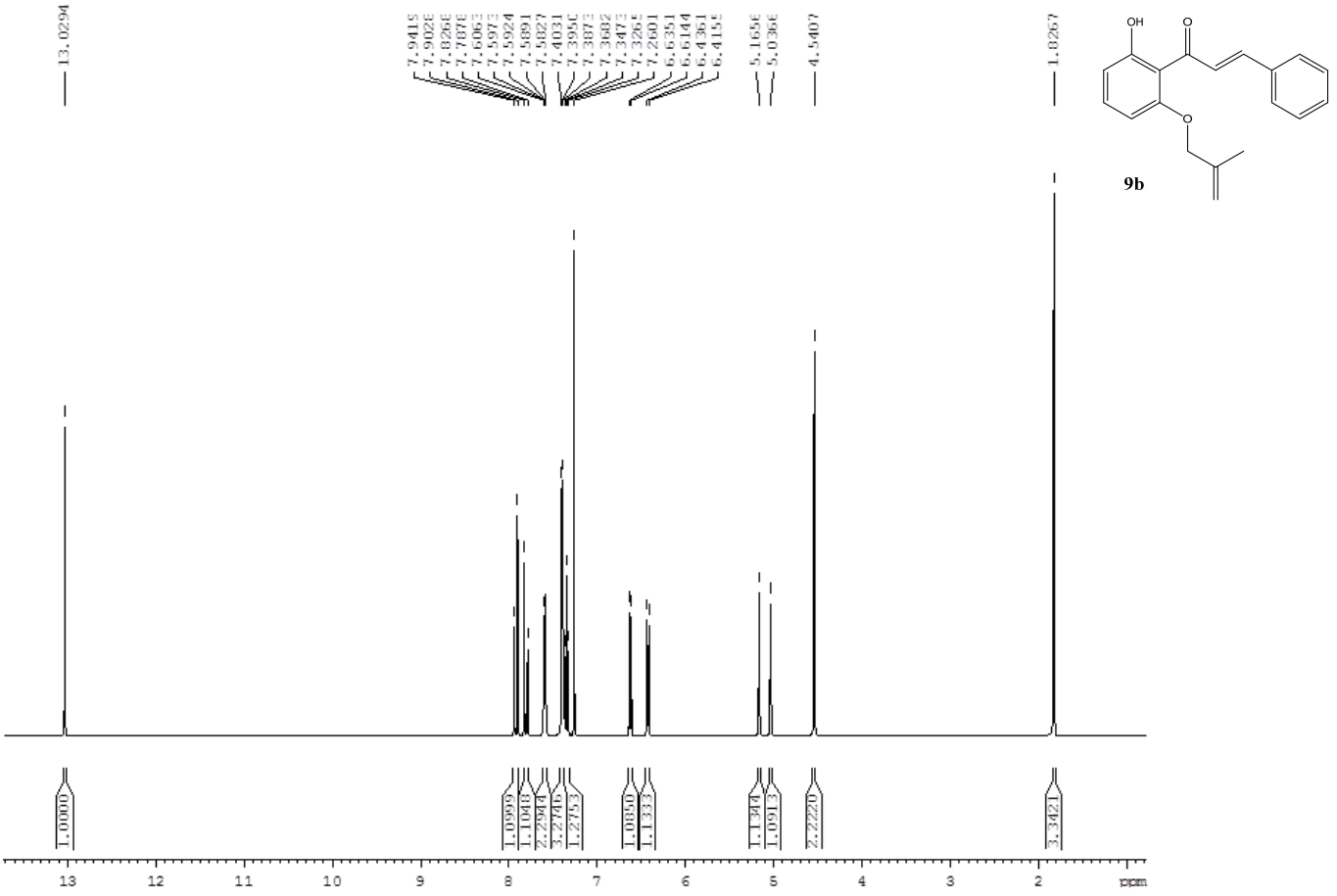
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound 9a



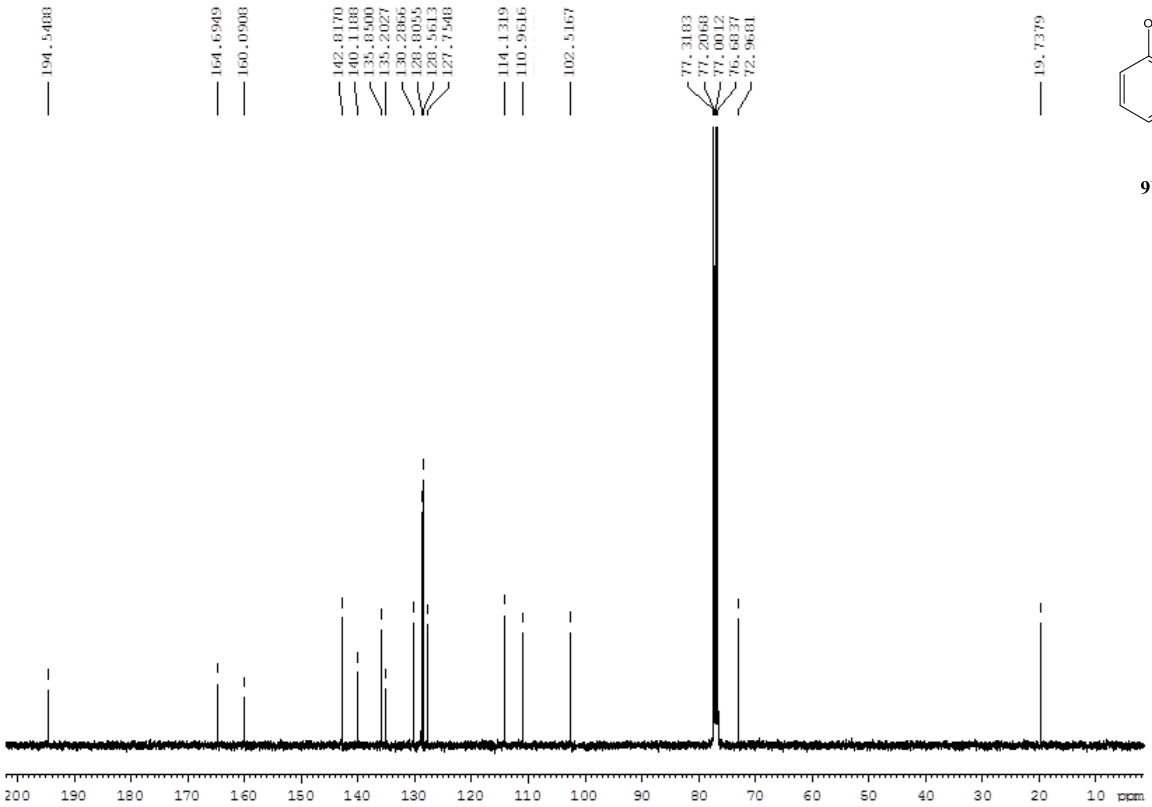
Mass of compound 9a



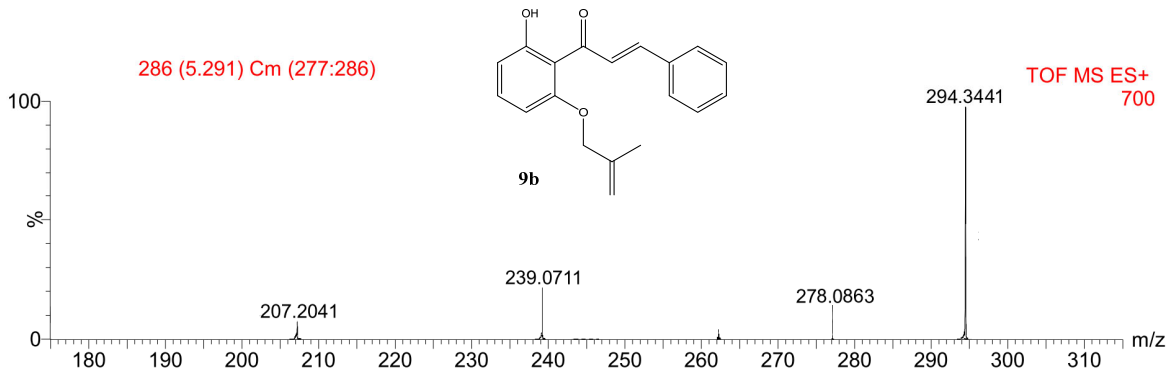
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound 9b



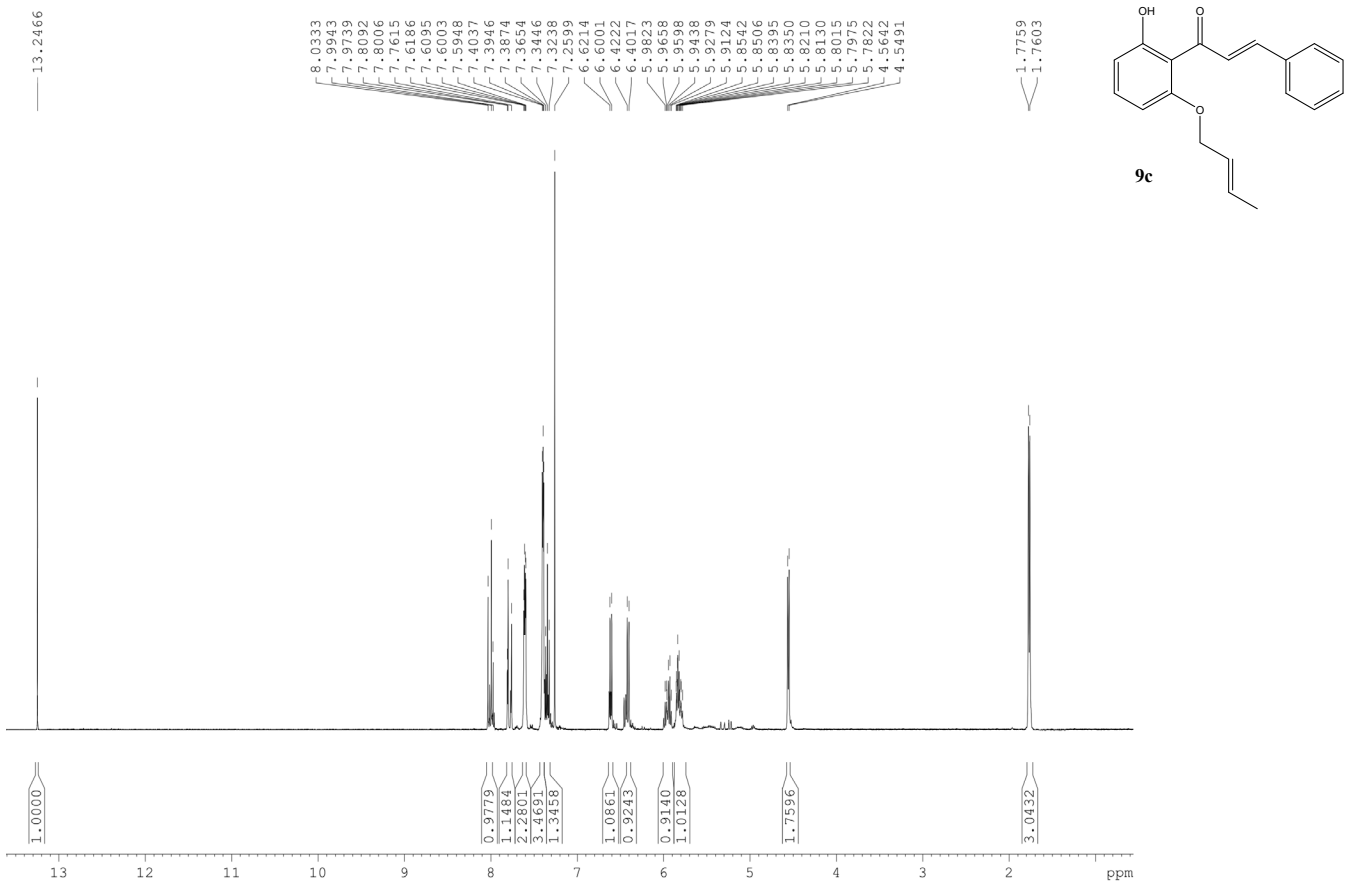
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound 9b



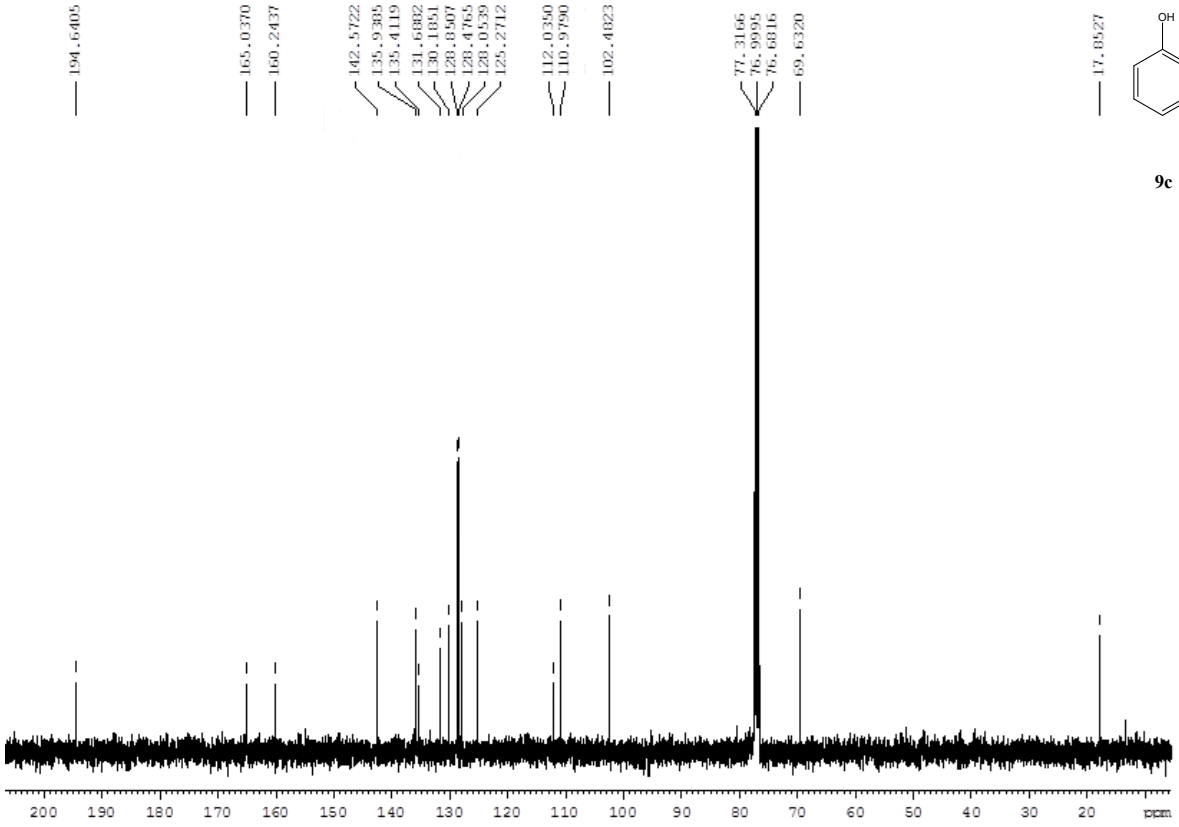
Mass of compound 9b



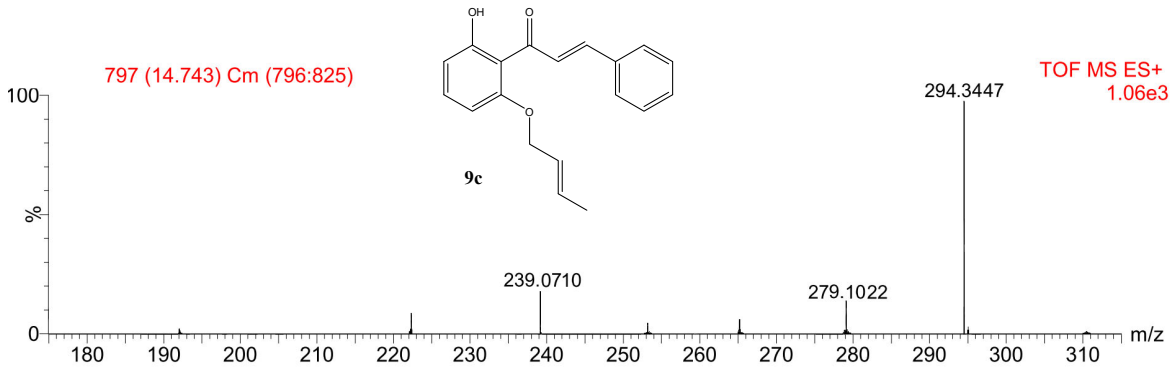
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound 9c



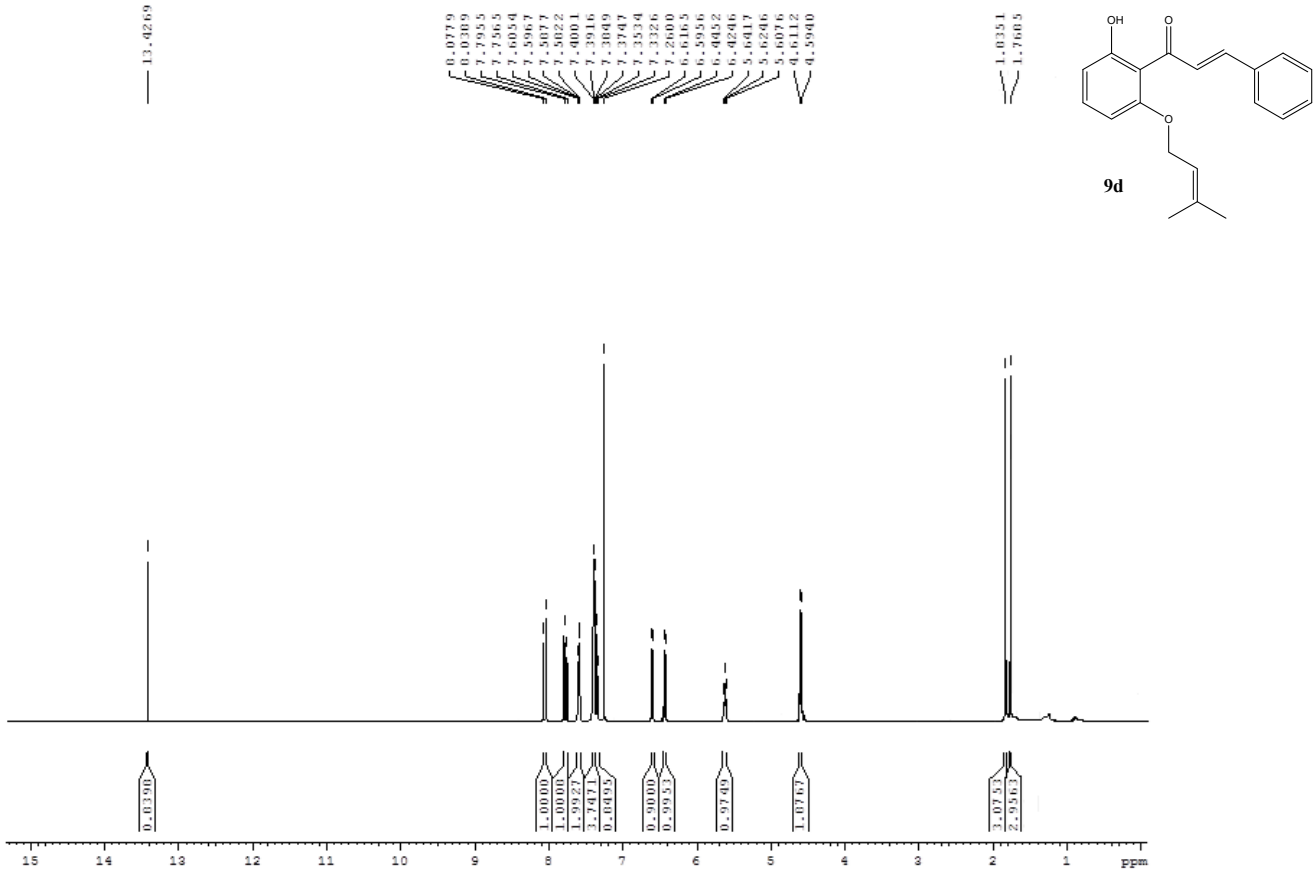
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound 9c



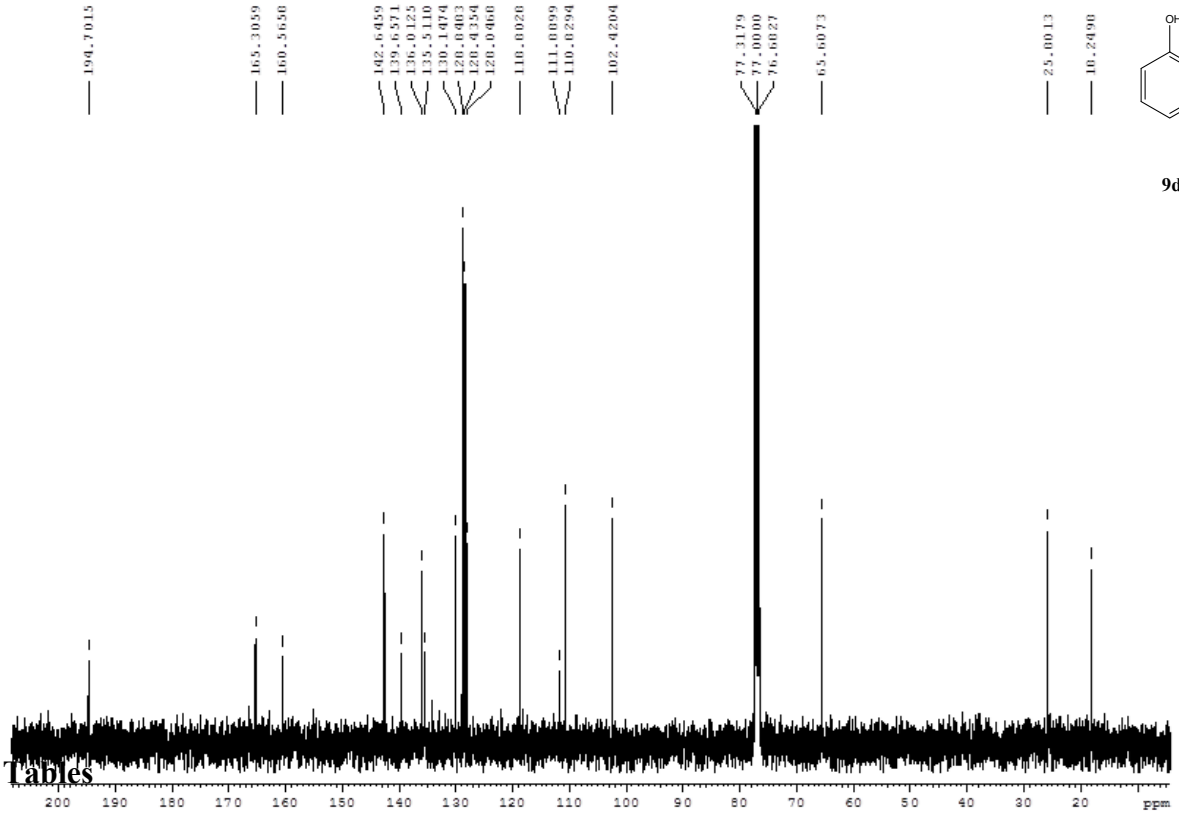
Mass of compound 9c



^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound 9d



^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound 9d



Tables

Mass of compound 9d

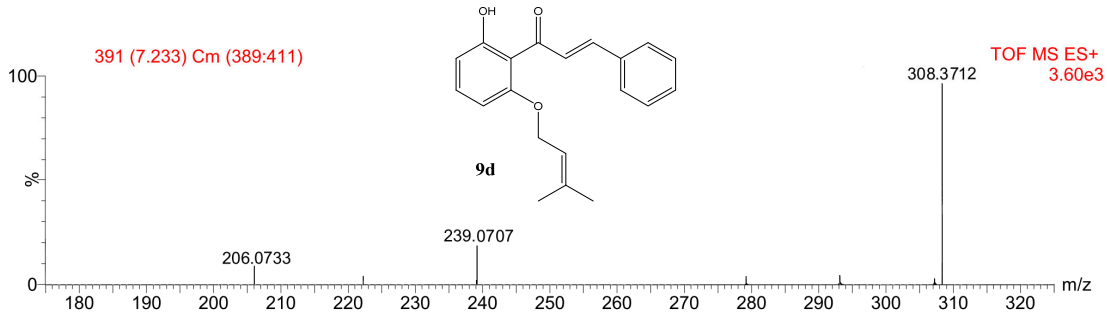


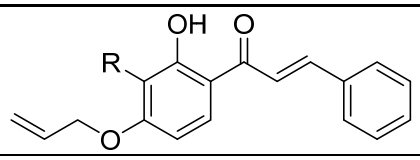
Table 1. Result of quantitative structure activity relationship in gas phase.

$pEC_{50} = 5.49(0.25) - 0.005(0.0008)MS + 0.464(0.46)C_{3'}$ $N= 12; r= 0.925; r^2= 0.856; SD= 0.032; F= 26.8; q^2= 0.832$					
Compound	**Descriptors**		**pEC_{50}**		**Residual**
	MS	**$C_{3'}$**	**Experimental**	**Calculated**	
7a	274.488	-0.436	3.804	3.783	0.021
7b	292.74	-0.439	3.643	3.682	-0.039
7c	294.889	-0.464	3.640	3.658	-0.018
7d	310.99	-0.397	3.609	3.601	0.008
8a	274.385	-0.254	3.930	3.869	0.062
8b	292.611	-0.23	3.741	3.780	-0.039
8c	294.79	-0.249	3.742	3.759	-0.017
8d	310.9	-0.246	3.663	3.672	-0.009
9a	273.381	-0.352	3.804	3.829	-0.024
9b	289.812	-0.379	3.707	3.726	-0.019
9c	293.786	-0.365	3.724	3.710	0.013
9d	310.067	-0.39	3.670	3.609	0.061

Table 2. Result of quantitative structure activity relationship in condensed phase.

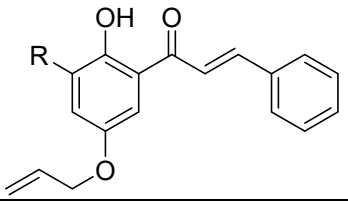
$pEC_{50} = 5.51(0.24) - 0.006(0.0008)MS + 0.472(0.13)C_{3'}$ $N= 12; r= 0.934; r^2= 0.871; SD= 0.029; F= 30.5; q^2= 0.852$					
Compound	**Descriptors**		**pEC_{50}**		**Residual**
	MS	**$C_{3'}$**	**Experimental**	**Calculated**	
7a	274.488	-0.448	3.804	3.781	0.023
7b	292.74	-0.459	3.643	3.675	-0.032
7c	294.889	-0.471	3.64	3.657	-0.017
7d	310.99	-0.395	3.609	3.604	0.005
8a	274.385	-0.251	3.930	3.875	0.056
8b	292.611	-0.242	3.741	3.778	-0.038
8c	294.79	-0.251	3.742	3.762	-0.020
8d	310.9	-0.256	3.663	3.670	-0.007
9a	273.381	-0.364	3.804	3.827	-0.023
9b	289.812	-0.382	3.707	3.728	-0.021
9c	293.786	-0.374	3.724	3.709	0.014
9d	310.067	-0.392	3.670	3.611	0.06

Table 3. Proposal compounds based in QSAR analysis based in **7a** core.



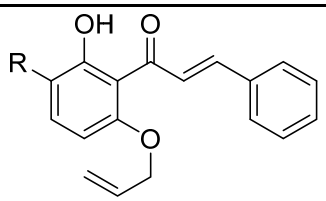
Compound	R	MS	$C_{3'}$	pIC_{50} Calc
Test_1	H	274.488	-0.448	3.781
Test_2	F	279.027	-0.014	3.829
Test_3	Cl	288.424	-0.451	3.57
Test_4	Br	293.425	-0.651	3.447
Test_5	CN	289.785	-0.548	3.517
Test_6	CHO	290.634	-0.463	3.551
Test_7	NO_2	293.698	-0.328	3.596
Test_8	Me	292.08	-0.135	3.695
Test_9	OH	282.496	0.023	3.826
Test_10	Ome	300.033	0.066	3.74
Test_11	NH_2	284.616	-0.088	3.761
Test_12	NMe_2	316.854	-0.043	3.589

Table 4. Proposal compounds based in QSAR analysis based in **8a** core.



Compound	R	MS	$C_{3'}$	pIC_{50} Calc
Test_1	H	274.385	-0.251	3.745
Test_2	F	277.802	0.289	3.98
Test_3	Cl	288.466	-0.112	3.726
Test_4	Br	293.738	-0.271	3.62
Test_5	CN	289.272	-0.214	3.673
Test_6	CHO	290.77	0.096	3.811
Test_7	NO_2	293.906	-0.171	3.666
Test_8	Me	292.317	0.184	3.843
Test_9	OH	281.185	0.278	3.954
Test_10	OMe	301.735	0.138	3.765
Test_11	NH_2	284.899	0.23	3.909
Test_12	NMe_2	320.063	0.154	3.662

Table 5. Proposal compounds based in QSAR analysis based in **9a** core.



Compound	R	MS	C_3	pIC_{50} Calc
Test_1	H	273.381	-0.364	3.827
Test_2	F	273.92	0.068	3.898
Test_3	Cl	283.853	-0.264	3.684
Test_4	Br	288.885	-0.466	3.56
Test_5	CN	285.025	-0.330	3.647
Test_6	CHO	286.103	-0.309	3.65
Test_7	NO_2	292.96	-0.258	3.633
Test_8	Me	290.964	0.028	3.777
Test_9	OH	278.041	0.148	3.910
Test_10	Ome	297.139	0.155	3.799
Test_11	NH_2	280.34	0.311	3.972
Test_12	NMe_2	317.798	0.100	3.650