

## Supplementary Materials

### Synthesis and Bioinformatics Study of 2-Nitrocinnamaldehyde Derivatives as an Anti MCF-7 Breast Cancer Cells

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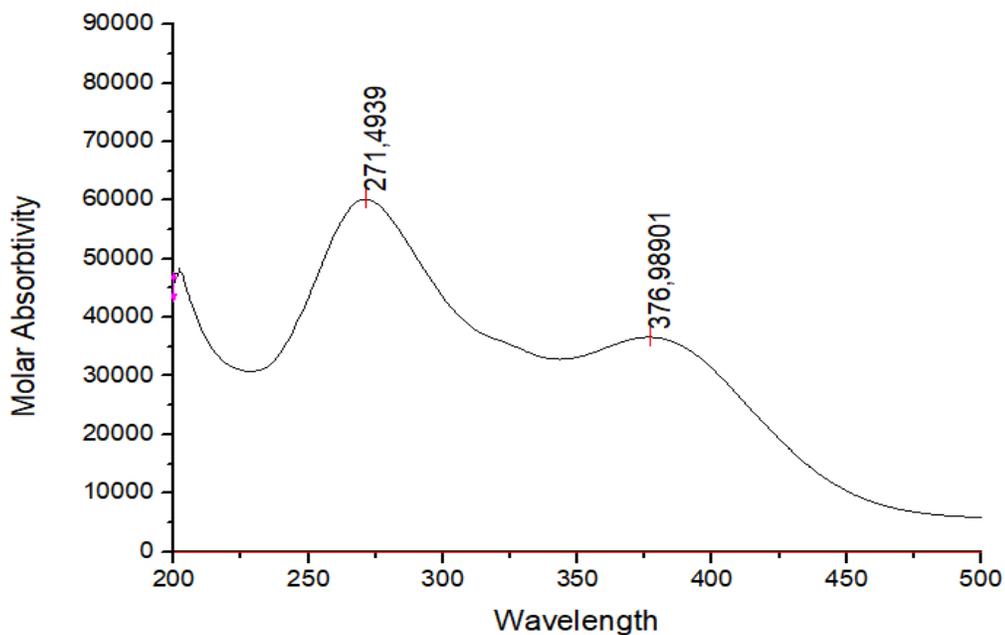
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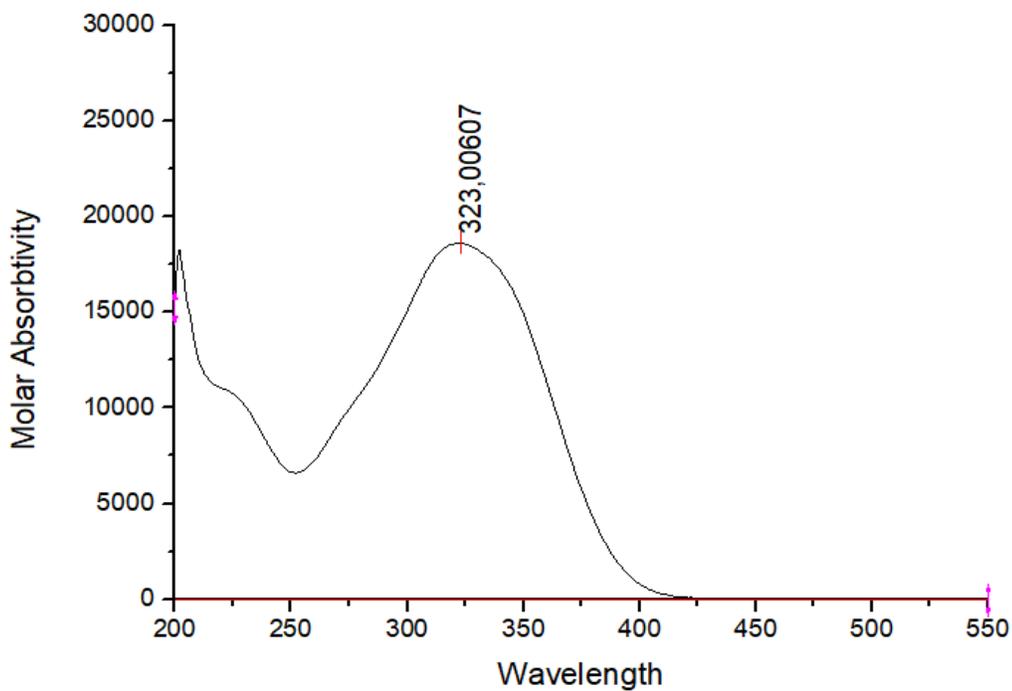
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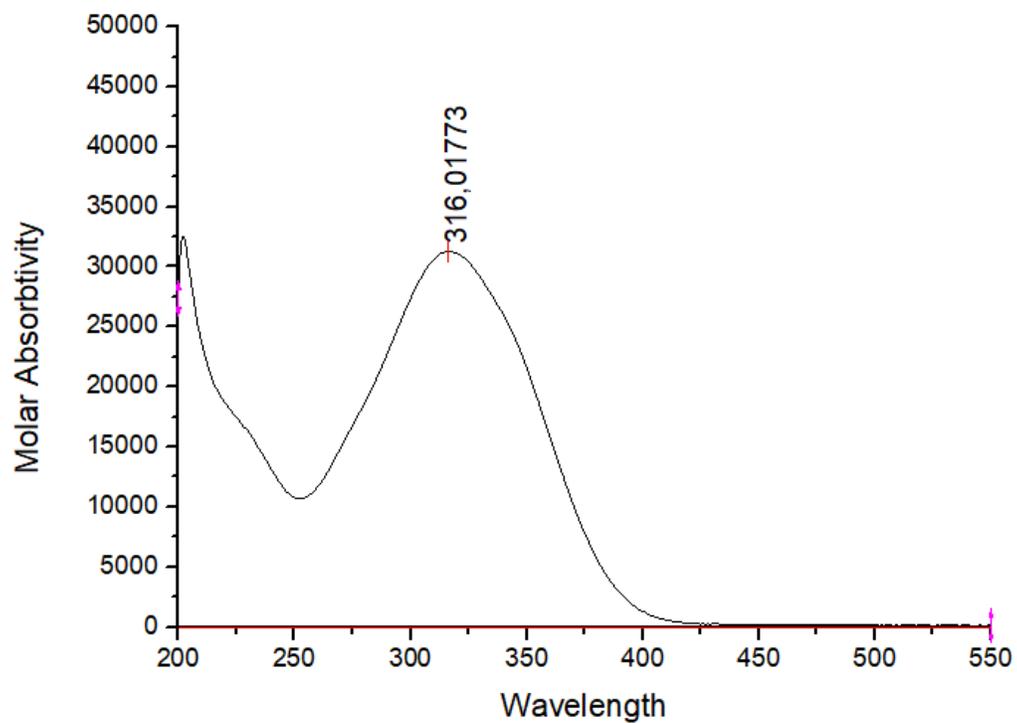
### A. UV-VIS Spectra of The Synthesized Compounds



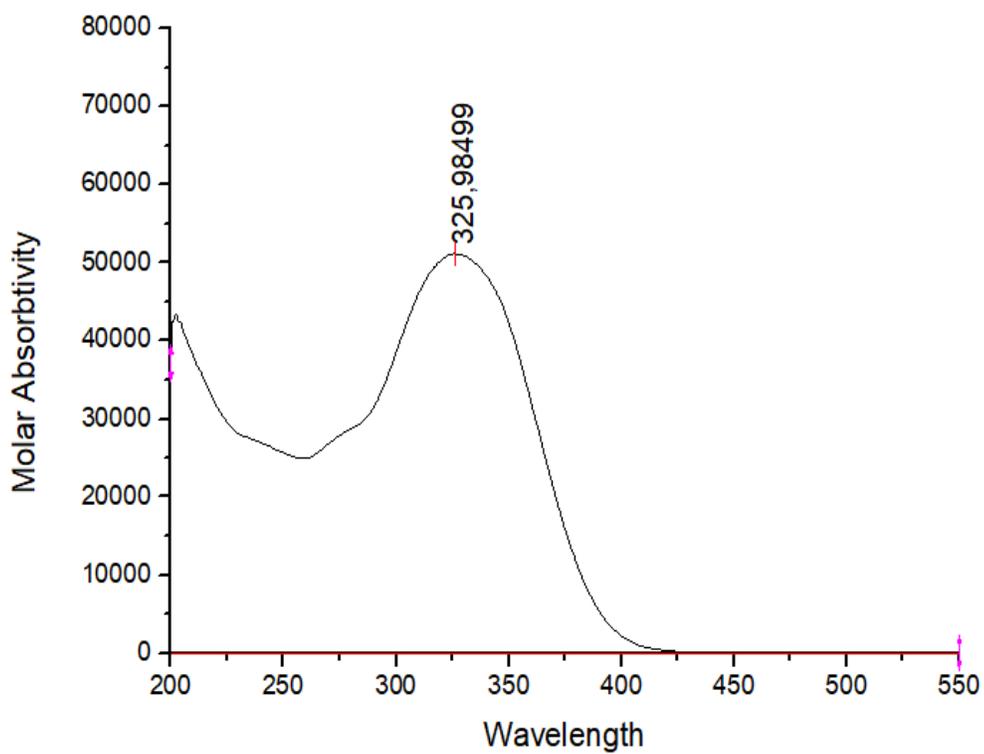
**Figure 1A** UV-Vis spectra of compound **9** at a concentration of  $1 \times 10^{-5}$  M in methanol.



**Figure 2A** UV-Vis spectra of compound **10** at a concentration of  $2 \times 10^{-5}$  M in methanol.



**Figure 3A** UV-Vis spectra of compound **11** at a concentration of  $1 \times 10^{-5}$  M in methanol.



**Figure 4A** UV-Vis spectra of compound **12** at a concentration of  $1 \times 10^{-5}$  M in methanol.

## B. FT-IR Spectra of The Synthesized Compounds

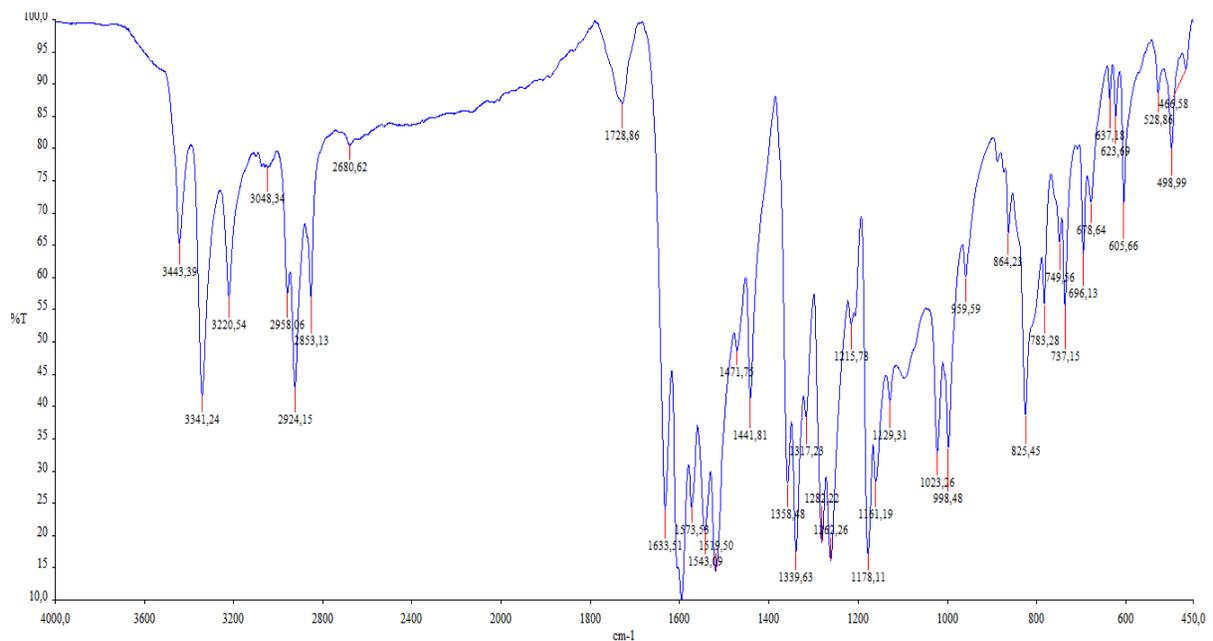


Figure 1B Infrared spectra of compound 9 in KBr plate.

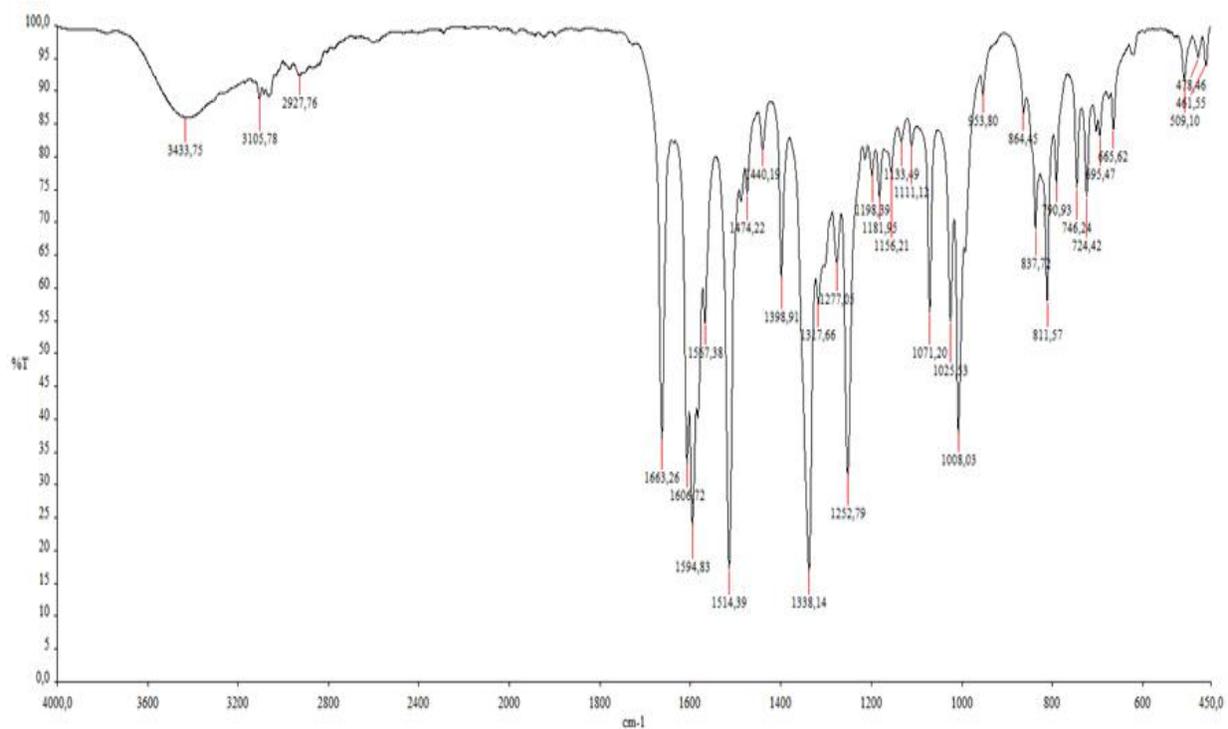
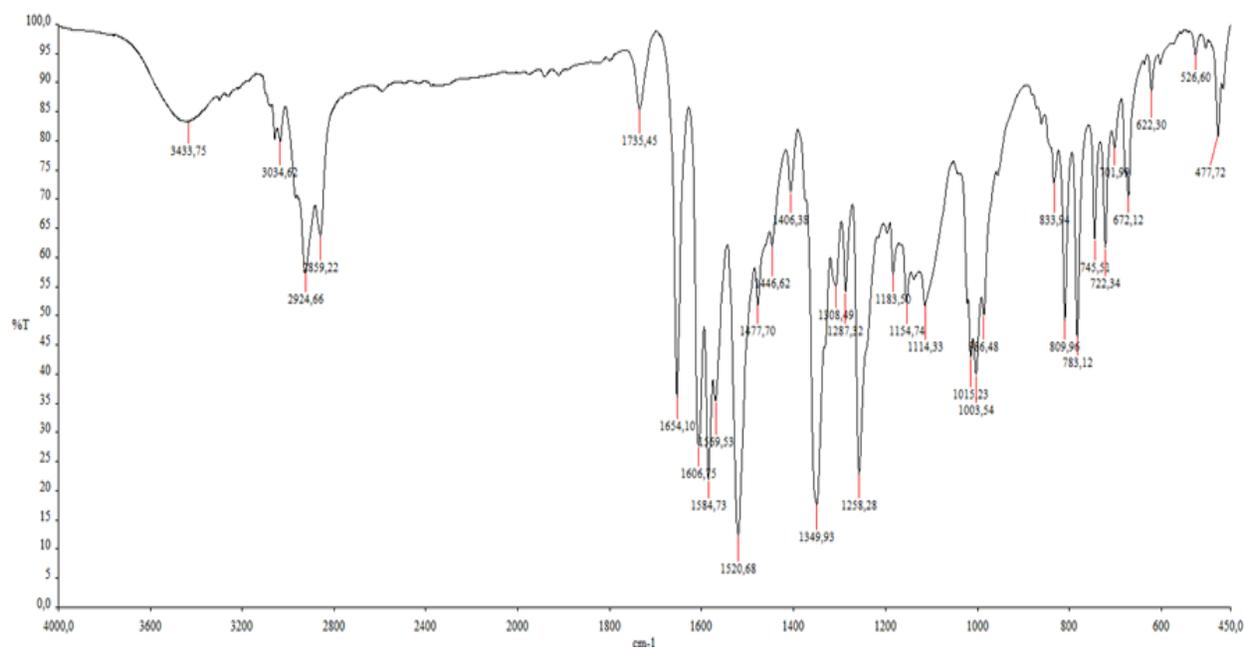
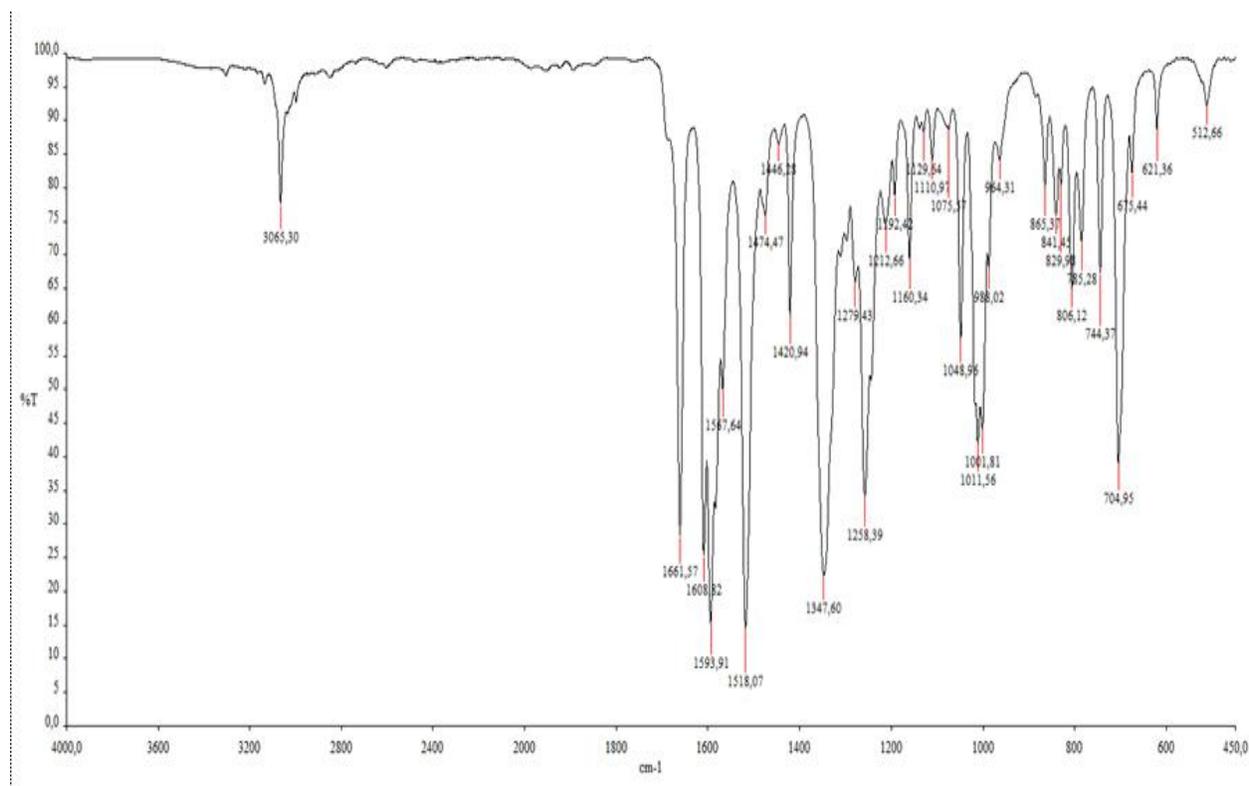


Figure 2B Infrared spectra of compound 10 in KBr plate.



**Figure 3B** Infrared spectra of compound **11** in KBr plate.



**Figure 4B** Infrared spectra of compound **12** in KBr plate.

### C. <sup>1</sup>H-NMR Spectra of The Synthesized Compounds

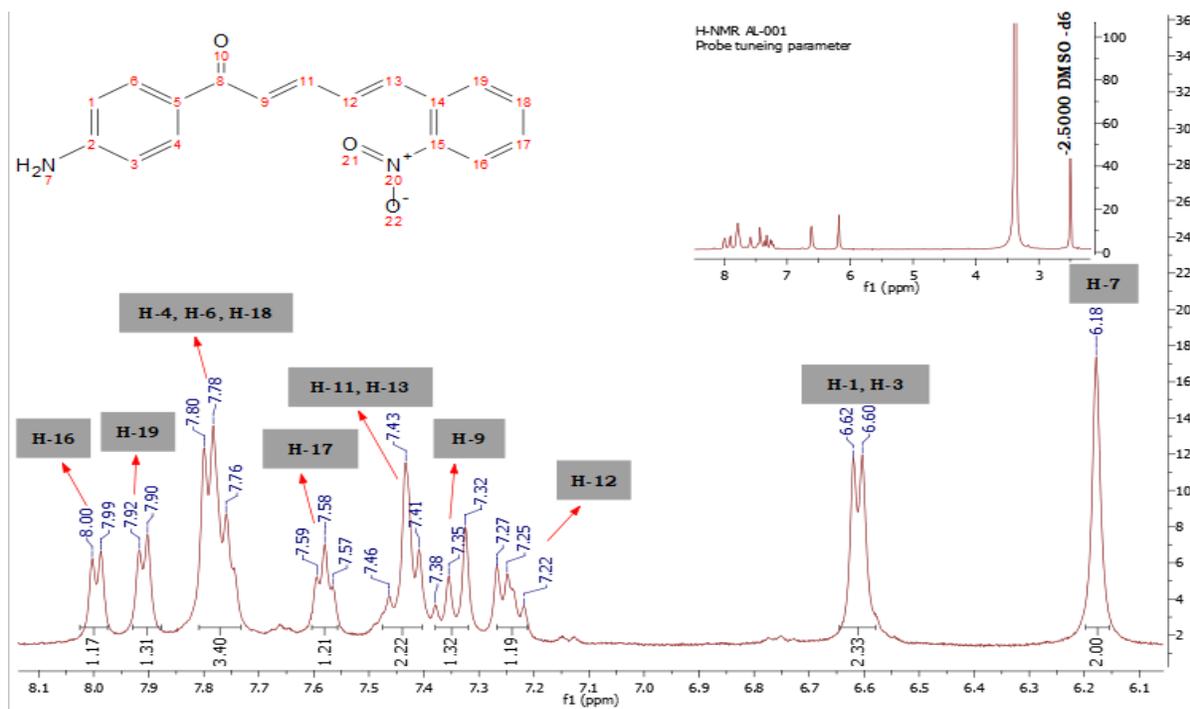


Figure 1C <sup>1</sup>H-NMR spectra of compound 9 (500 MHz, DMSO).

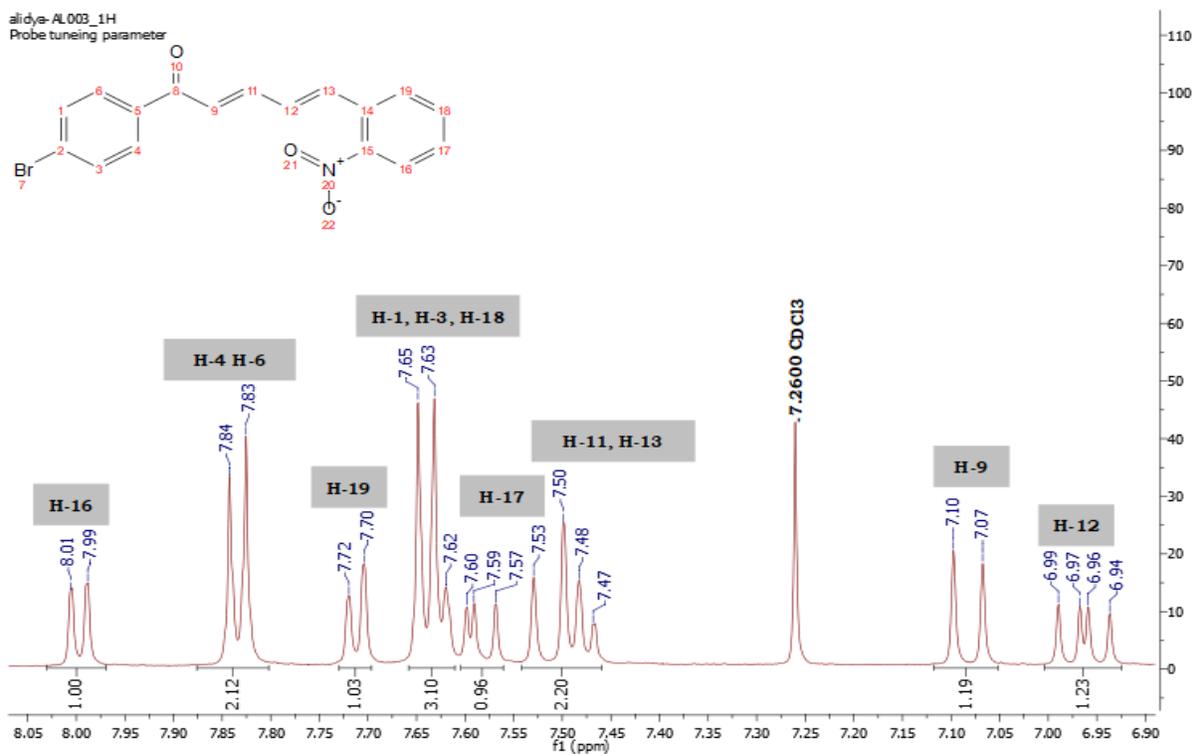


Figure 2C <sup>1</sup>H-NMR spectra of compound 10 (500 MHz, CDCl<sub>3</sub>).

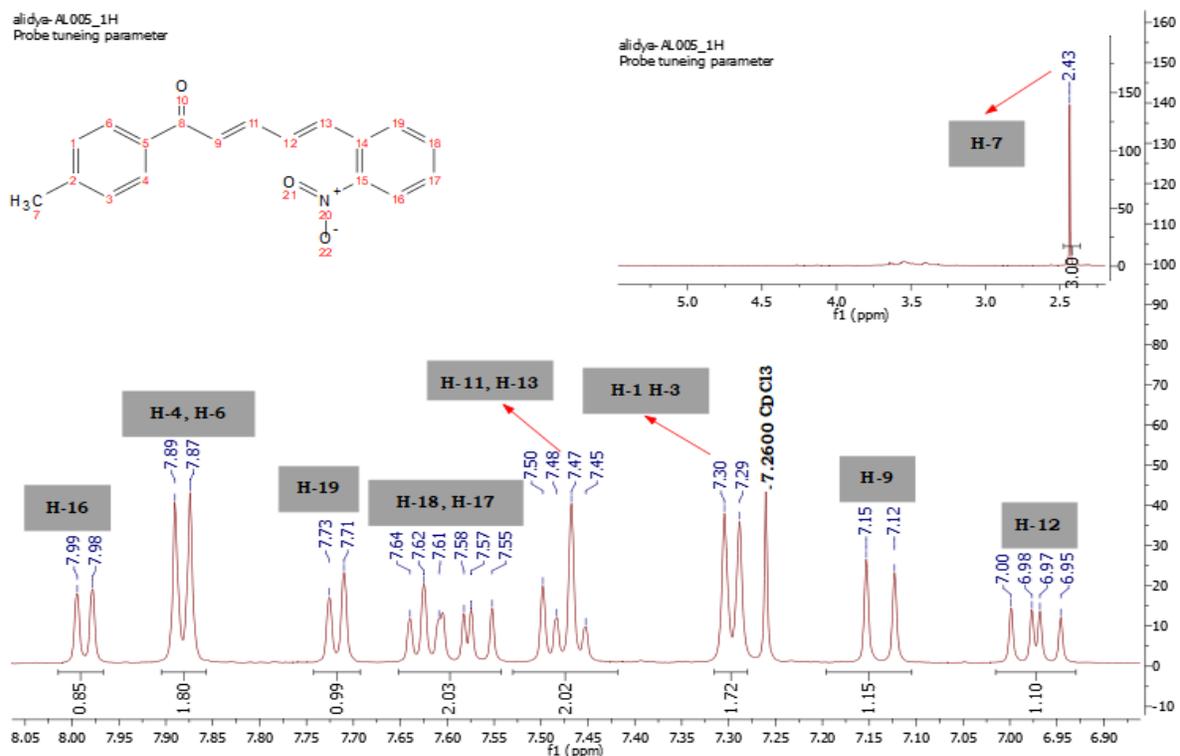


Figure 3C <sup>1</sup>H-NMR spectra of compound **11** (500 MHz, CDCl<sub>3</sub>).

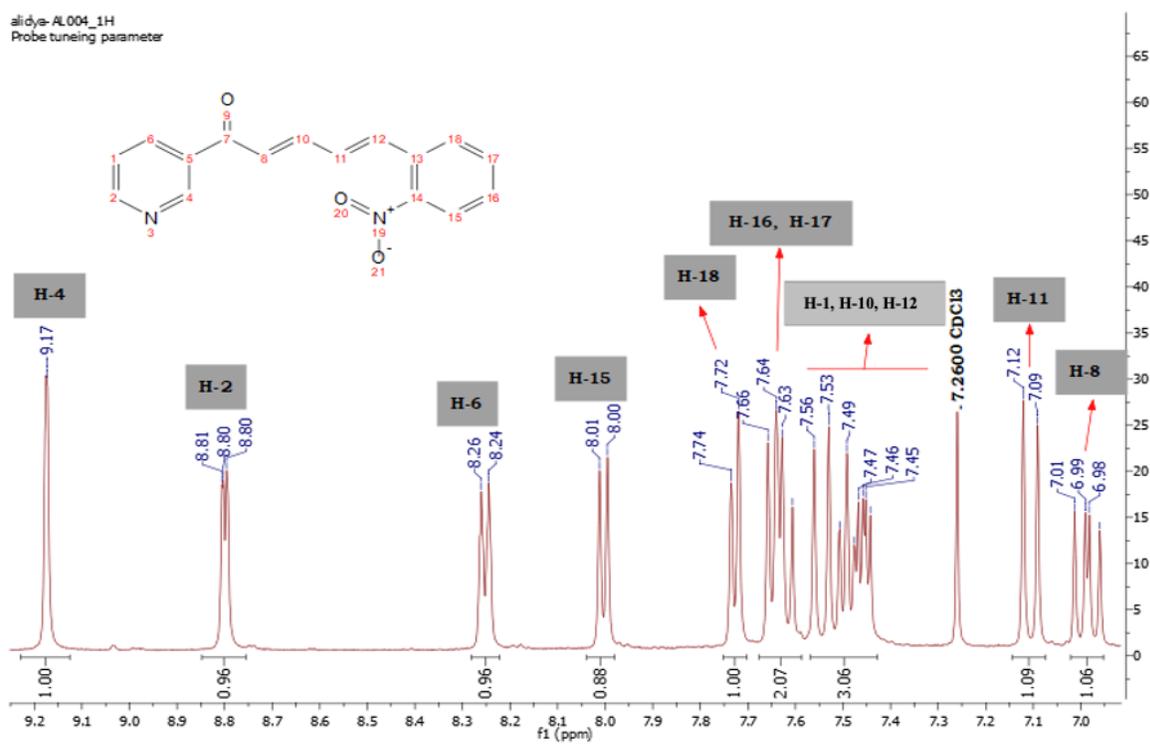


Figure 4C <sup>1</sup>H-NMR spectra of compound **12** (500 MHz, CDCl<sub>3</sub>).

## D. $^{13}\text{C}$ -NMR Spectra of The Synthesized Compounds

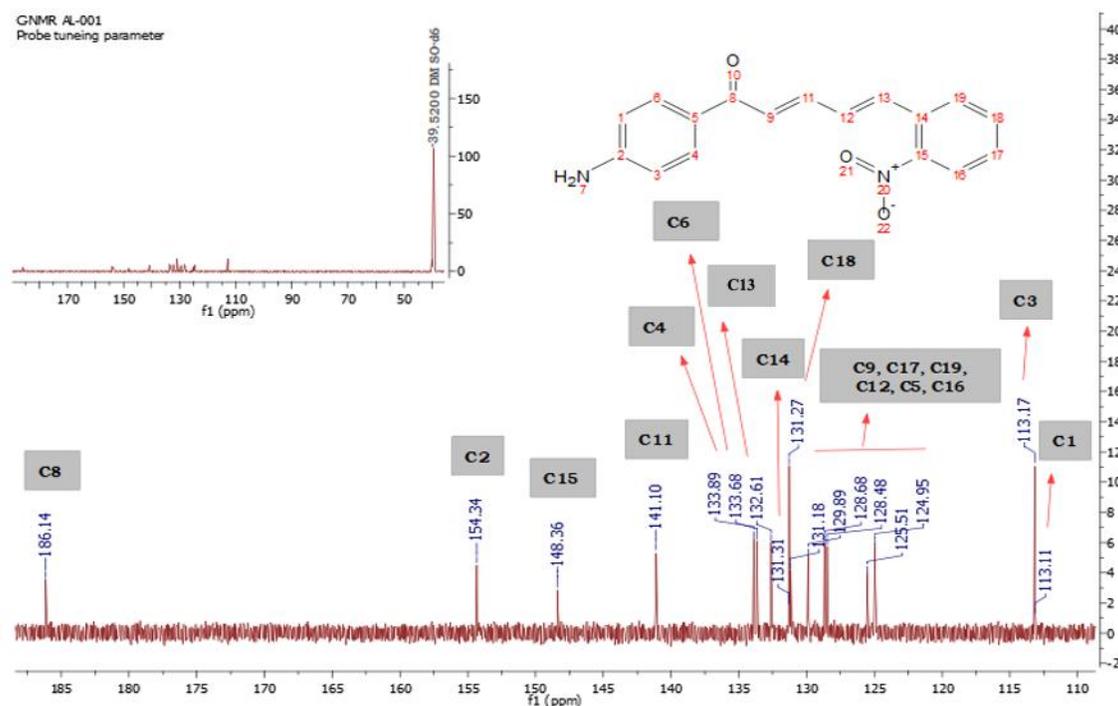


Figure 1D  $^{13}\text{C}$ -NMR spectra of compound 9 (125 MHz, DMSO).

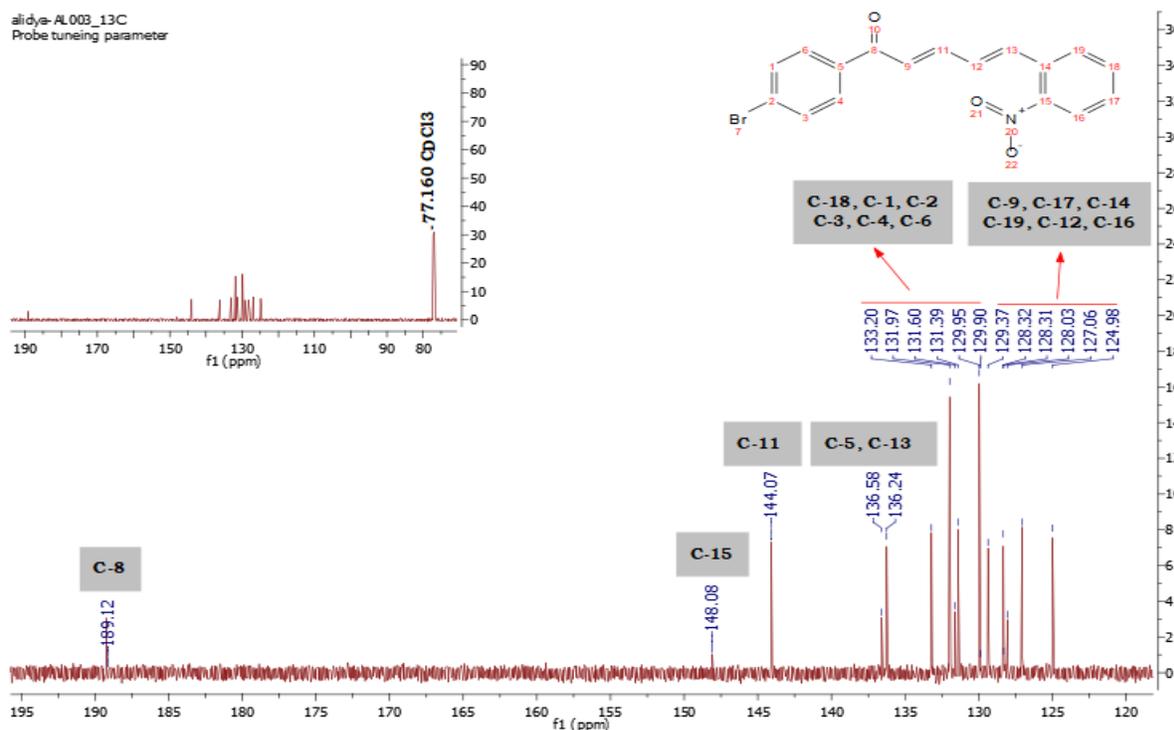


Figure 2D  $^{13}\text{C}$ -NMR spectra of compound 10 (125 MHz,  $\text{CDCl}_3$ ).

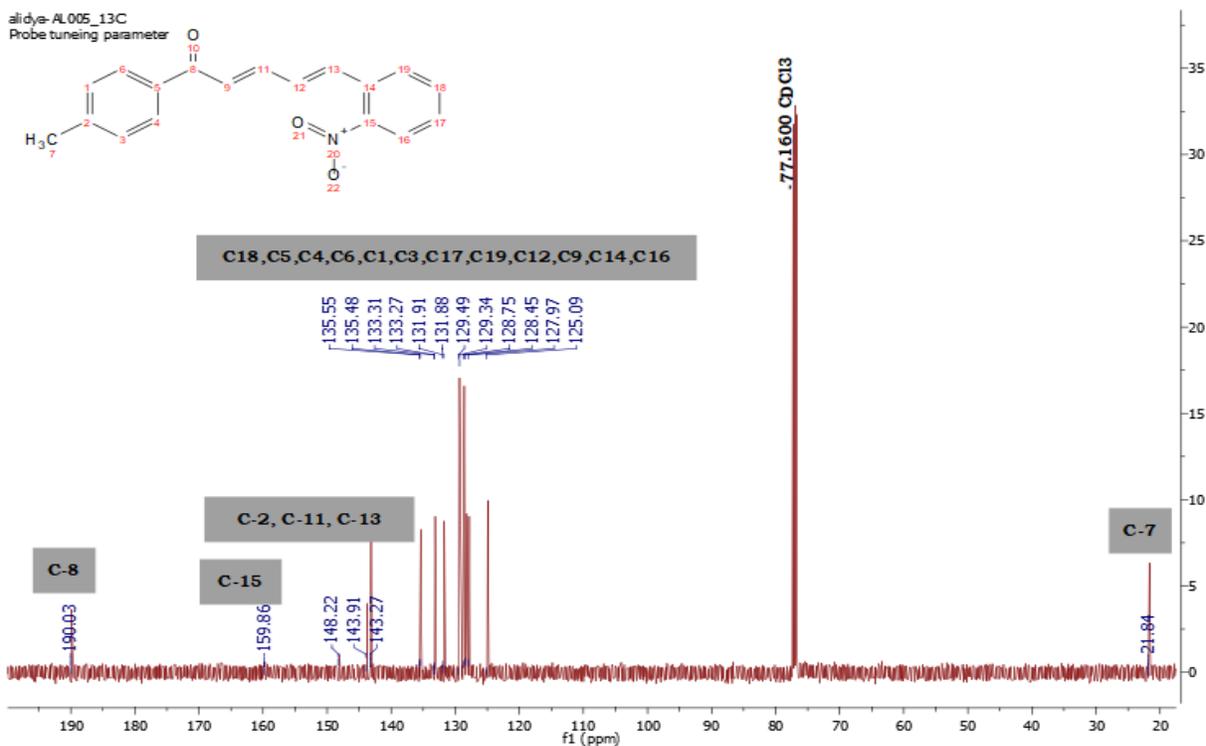


Figure 3D  $^{13}\text{C}$ -NMR spectra of compound **11** (125 MHz,  $\text{CDCl}_3$ ).

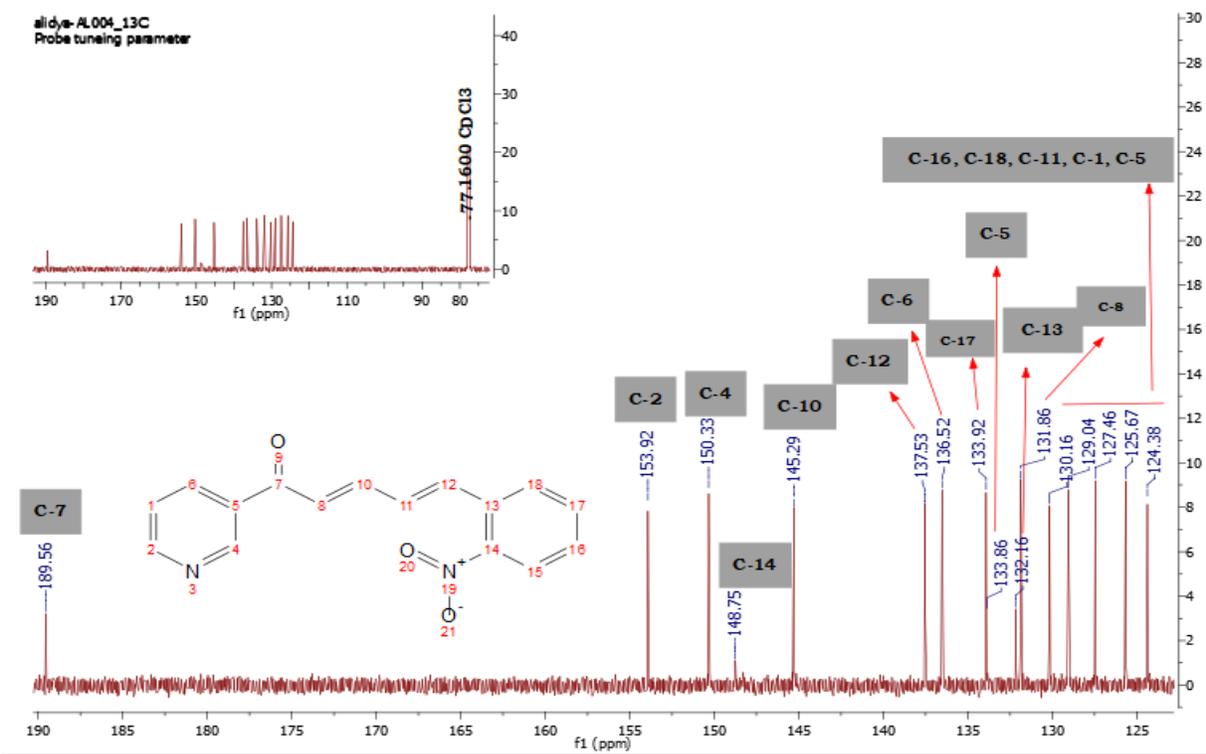


Figure 4D  $^{13}\text{C}$ -NMR spectra of compound **12** (125 MHz,  $\text{CDCl}_3$ ).

### E. Mass Spectra of The Synthesized Compounds

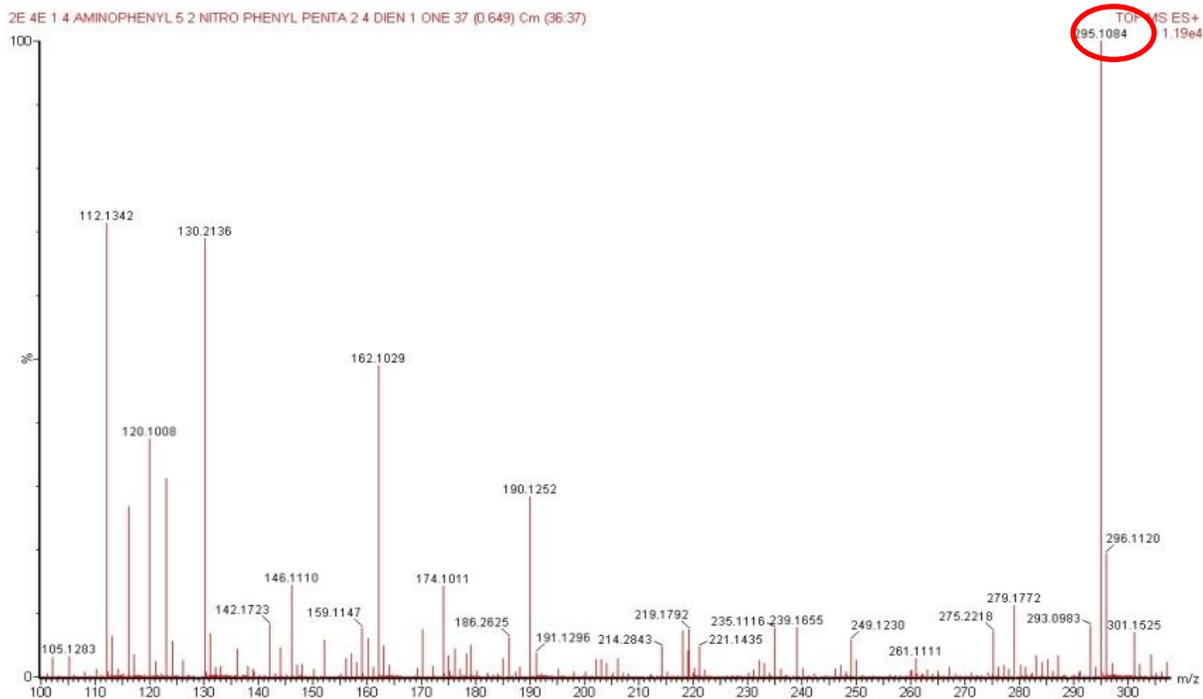


Figure 1E Mass spectra of compound 9 ToF-HRMS ES+.

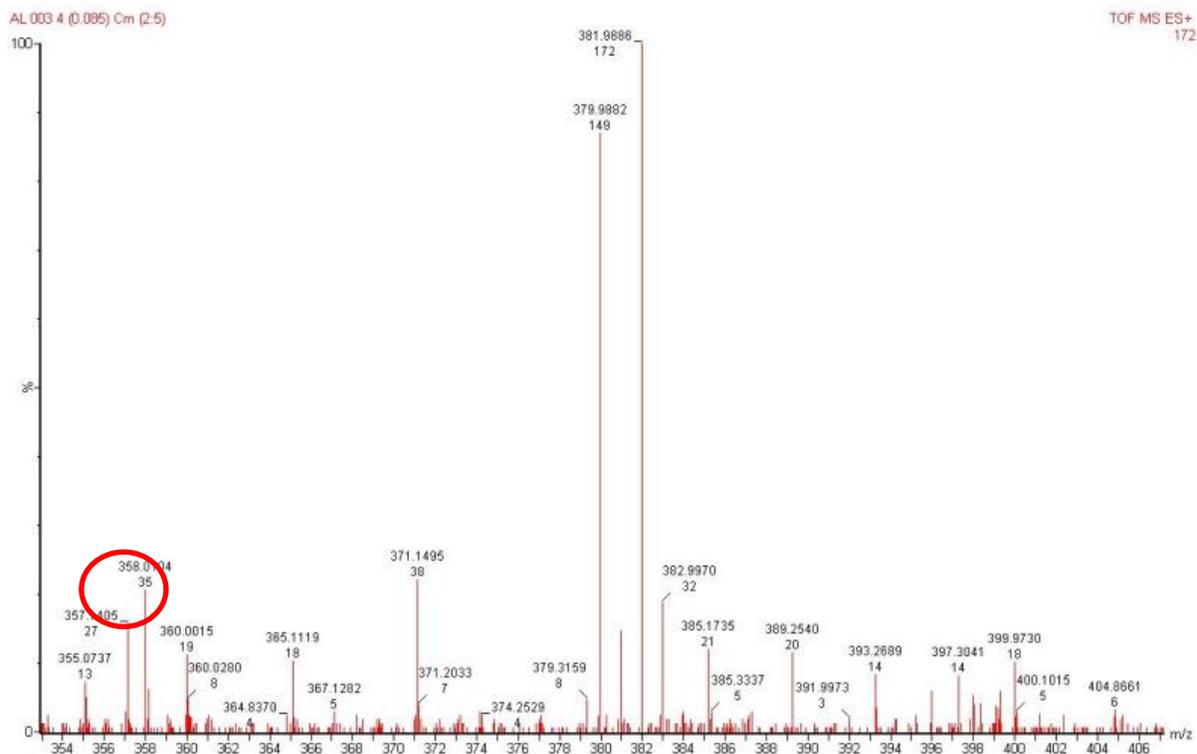
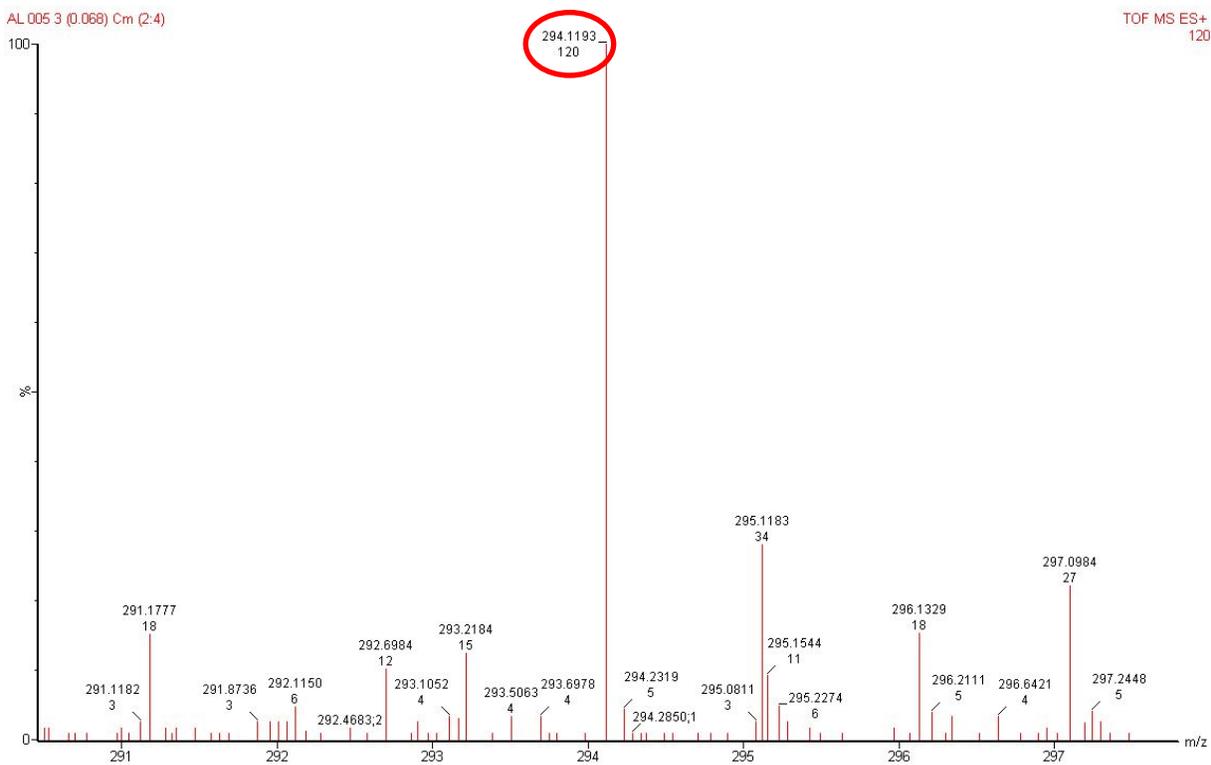
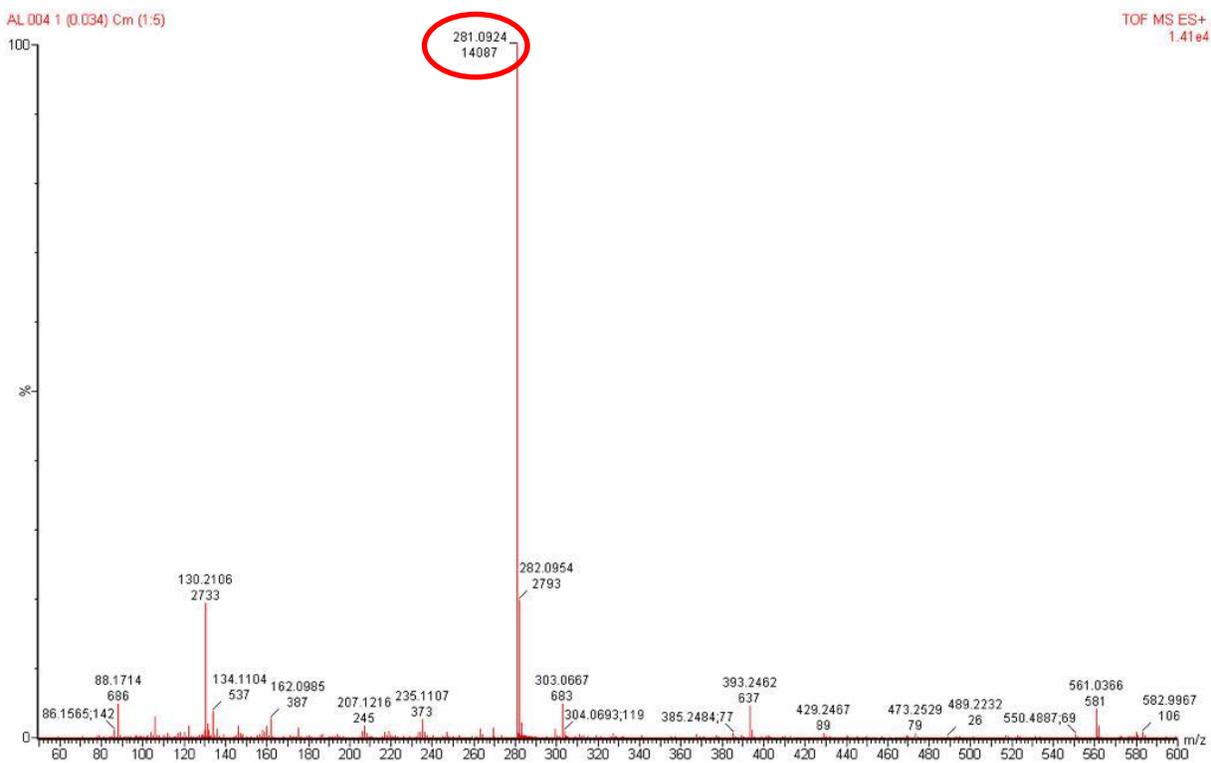


Figure 2E Mass spectra of compound 10 ToF-HRMS ES+.



**Figure 3E** Mass spectra of compound **11** ToF-HRMS ES<sup>+</sup>.



**Figure 4E** Mass spectra of compound **12** ToF-HRMS ES<sup>+</sup>.

## F. Results of MTT Assay Of The Compounds Against MCF-7 Cells

**Table 1F** Results of Absorbance of Compound **9** Against MCF-7 Cells.

	Media	Media + Cells	Cisplatin	Solvent (DMSO 2%)	Sample Concentration (µg/mL)							
					3.91	7.81	15.63	31.25	62.50	125.00	250.00	500.00
<b>Absorbance 570 nm</b>	0.5023	0.7987	0.6651	0.7611	0.7948	0.7892	0.7812	0.7775	0.8182	0.7507	0.6293	0.5176
	0.5081	0.7939	0.6497	0.8029	0.8090	0.7811	0.7899	0.7964	0.8280	0.7900	0.6396	0.5204
<b>Absorbance 600 nm</b>	0.6431	0.2254	0.4646	0.3000	0.2222	0.2173	0.2224	0.2227	0.3165	0.4251	0.5609	0.6044
	0.6522	0.2141	0.4571	0.2330	0.2193	0.2144	0.2113	0.2161	0.3062	0.3756	0.5662	0.6016
<b>Difference in Absorbance</b>	-0.1408	0.5733	0.2005	0.4611	0.5726	0.5719	0.5588	0.5548	0.5017	0.3256	0.0684	-0.0868
	-0.1441	0.5798	0.1926	0.5699	0.5897	0.5667	0.5786	0.5803	0.5218	0.4144	0.0734	-0.0812
<b>% Live Cells</b>		108.78	52.12	91.73	108.68	108.57	106.58	105.97	97.90	71.14	32.05	8.46
		109.77	50.92	108.27	111.28	107.78	109.59	109.85	100.96	84.63	32.81	9.31
<b>Average % of Living Cells</b>		109.28	51.52	100.00	109.98	108.18	108.09	107.91	99.43	77.89	32.43	8.88
<b>SEM</b>		0.49	0.60	8.27	1.30	0.40	1.50	1.94	1.53	6.75	0.38	0.43
<b>Normalization Data on % Living Cells</b>		109.28	51.52	100.00	109.98	108.18	108.09	107.91	99.43	77.89	32.43	8.88

**Table 2F** Results of Absorbance of Compound **10** Against MCF-7 Cells.

	Media	Media + Cells	Cisplatin	Solvent (DMSO 2%)	Sample Concentration (µg/mL)							
					3.91	7.81	15.63	31.25	62.50	125.00	250.00	500.00
<b>Absorbance 570 nm</b>	0.5012	0.8099	0.6649	0.8065	0.7926	0.8017	0.8215	0.8533	0.8682	0.8607	0.7856	0.6134
	0.5034	0.8054	0.6486	0.8004	0.8000	0.8053	0.8145	0.8412	0.8456	0.8655	0.7675	0.5808
<b>Absorbance 600 nm</b>	0.6420	0.1900	0.4680	0.1926	0.1878	0.1983	0.2063	0.2296	0.2564	0.2708	0.3247	0.5112
	0.6441	0.1876	0.4604	0.1911	0.1919	0.1942	0.2060	0.2250	0.2362	0.2805	0.3346	0.5250
<b>Difference in Absorbance</b>	-0.1408	0.6199	0.1969	0.6139	0.6048	0.6034	0.6152	0.6237	0.6118	0.5899	0.4609	0.1022
	-0.1407	0.6178	0.1882	0.6093	0.6081	0.6111	0.6085	0.6162	0.6094	0.5850	0.4329	0.0558
<b>% Live Cells</b>		101.10	44.88	101.31	99.10	98.91	100.48	101.61	100.03	97.12	79.97	32.29
		100.82	43.72	99.69	99.53	99.93	99.59	100.61	99.71	96.46	76.25	26.12
<b>Average % of Living Cells</b>		100.96	44.30	100.00	99.32	99.42	100.03	101.11	99.87	96.79	78.11	29.21
<b>SEM</b>		0.14	0.58	0.31	0.22	0.51	0.45	0.50	0.16	0.33	1.86	3.08
<b>Normalization Data on % Living Cells</b>		101.66	44.61	100.69	100.00	100.11	100.72	101.81	100.56	97.46	78.65	29.41

**Table 3F** Results of Absorbance of Compound **11** Against MCF-7 Cells.

	Media	Media + Cells	Cisplatin	Solvent (DMSO 2%)	Sample Concentration (µg/mL)							
					3.91	7.81	15.63	31.25	62.50	125.00	250.00	500.00
<b>Absorbance 570 nm</b>	0.4885	0.7876	0.6384	0.8074	0.8112	0.8098	0.8097	0.8108	0.7740	0.7415	0.7211	0.7269
	0.4723	0.7977	0.6485	0.8053	0.8044	0.8033	0.8033	0.8035	0.7920	0.7966	0.7433	0.7122
<b>Absorbance 600 nm</b>	0.6264	0.2094	0.4716	0.2250	0.2166	0.2197	0.2135	0.2099	0.2075	0.3553	0.3953	0.4269
	0.6011	0.2183	0.4985	0.2236	0.2188	0.2120	0.2139	0.2157	0.2154	0.3078	0.3962	0.4256
<b>Difference in Absorbance</b>	-0.1379	0.5782	0.1668	0.5824	0.5946	0.5901	0.5962	0.6009	0.5665	0.3862	0.3259	0.3000
	-0.1288	0.5794	0.1500	0.5817	0.5856	0.5913	0.5894	0.5878	0.5766	0.4888	0.3471	0.2866
<b>% Live Cells</b>		99.46	41.96	100.05	101.75	101.13	101.98	102.63	97.83	72.62	64.19	60.57
		99.63	39.61	99.95	100.50	101.29	101.03	100.80	99.24	86.97	67.16	58.70
<b>Average % of Living Cells</b>		99.55	40.78	100.00	101.13	101.21	101.50	101.72	98.53	79.79	65.58	59.64
<b>SEM</b>		0.08	1.17	0.05	0.63	0.08	0.48	0.92	0.71	7.17	1.48	0.94
<b>Normalization Data on % Living Cells</b>		98.44	40.330.8074	98.89	100.00	100.08	100.37	100.59	97.44	78.91	64.95	58.97

**Table 4F** Results of Absorbance of Compound **12** Against MCF-7 Cells.

	Media	Media + Cells	Cisplatin	Solvent (DMSO 2%)	Sample Concentration (µg/mL)							
					3.91	7.81	15.63	31.25	62.50	125.00	250.00	500.00
<b>Absorbance 570 nm</b>	0.4860	0.7896	0.6476	0.8011	0.7849	0.7820	0.7958	0.8032	0.7760	0.6790	0.6012	0.5297
	0.5057	0.7960	0.6521	0.7968	0.8-33	0.7965	0.7937	0.8018	0.7731	0.6849	0.6356	0.5363
<b>Absorbance 600 nm</b>	0.6239	0.2123	0.4773 6	0.2280	0.2041	0.2034	0.2113	0.2344	0.3411	0.4846	0.5488	0.5985
	0.6478	0.2082	0.4778	0.2250	0.2118	0.2115	0.2096	0.2352	0.3451	0.4678	0.5571	0.6148
<b>Difference in Absorbance</b>	-0.1379	0.5773	0.1740	0.5731	0.5808	0.5786	0.5845	0.5688	0.4349	0.1944	0.0524	-0.0688
	-0.1421	0.5878	0.1743	0.5718	0.5915	0.5850	0.5841	0.5666	0.4280	0.2171	0.0785	-0.0785
<b>% Live Cells</b>		100.68	44.07	100.09	101.17	100.86	101.69	99.49	80.69	46.94	27.01	9.99
		102.15	44.12	99.91	102.67	100.76	101.64	99.18	79.72	50.12	30.67	8.63
<b>Average % of Living Cells</b>		101.42	44.09	100.00	101.92	101.31	101.66	99.33	80.21	48.53	28.84	9.31
<b>SEM</b>		0.74	0.02	0.09	0.75	0.45	0.03	0.15	0.48	1.59	1.83	0.68
<b>Normalization Data on % Living Cells</b>		101.42	44.09	100.00	101.92	101.31	101.66	99.33	80.21	48.53	28.84	9.31

G. Calculated IC<sub>50</sub> of The Compounds Against MCF-7 Cells

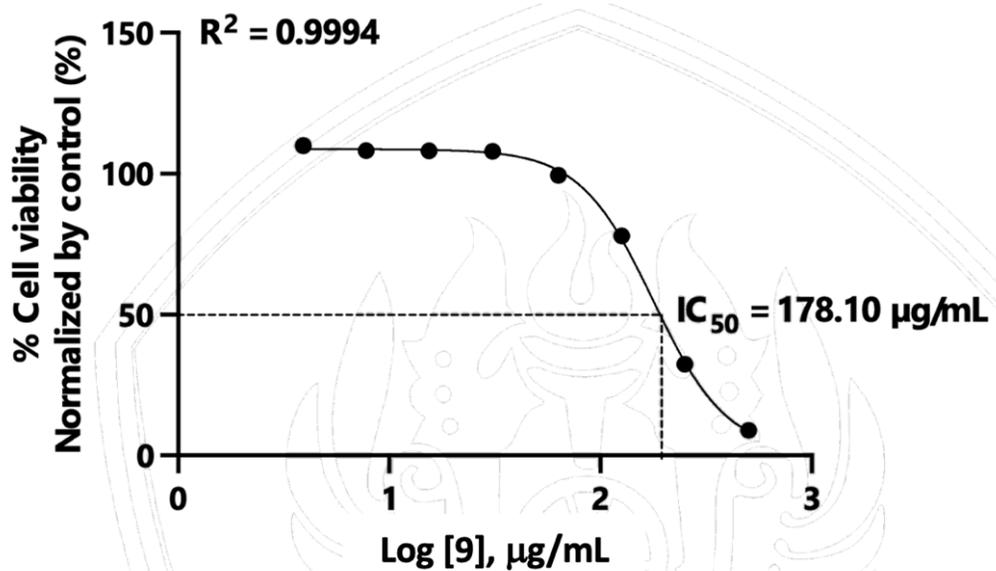


Figure 1G Calculated IC<sub>50</sub> of Compound 9 Against MCF-7 Cells.

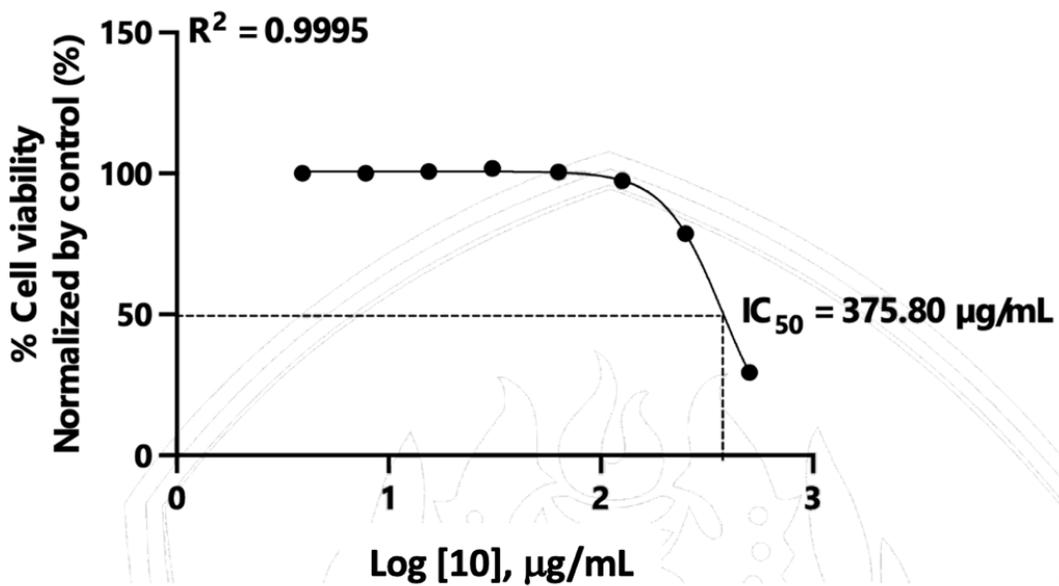


Figure 2G Calculated IC<sub>50</sub> of Compound 10 Against MCF-7 Cells.

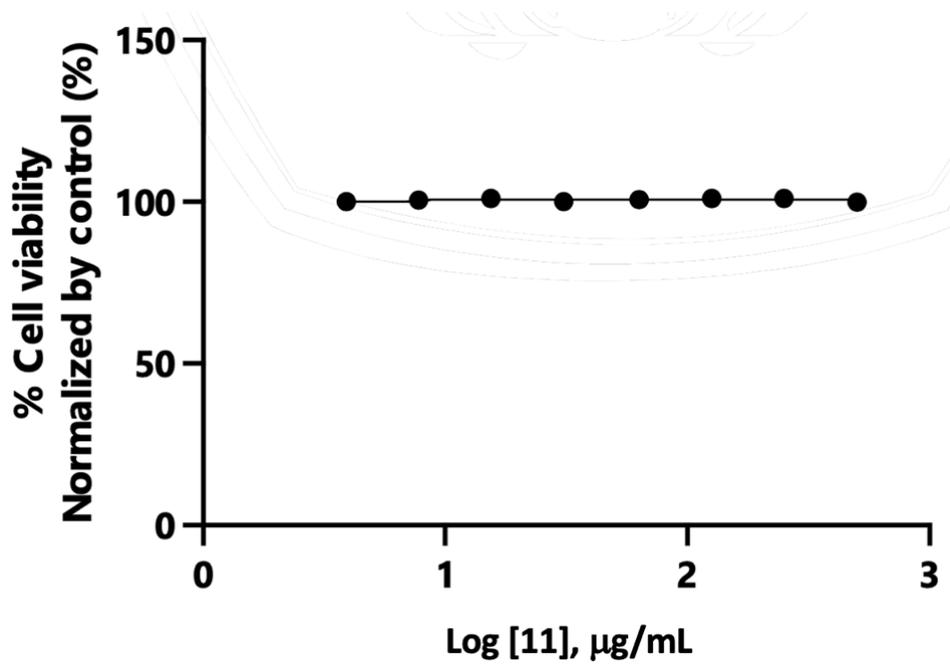


Figure 3G Calculated IC<sub>50</sub> of Compound 11 Against MCF-7 Cells.

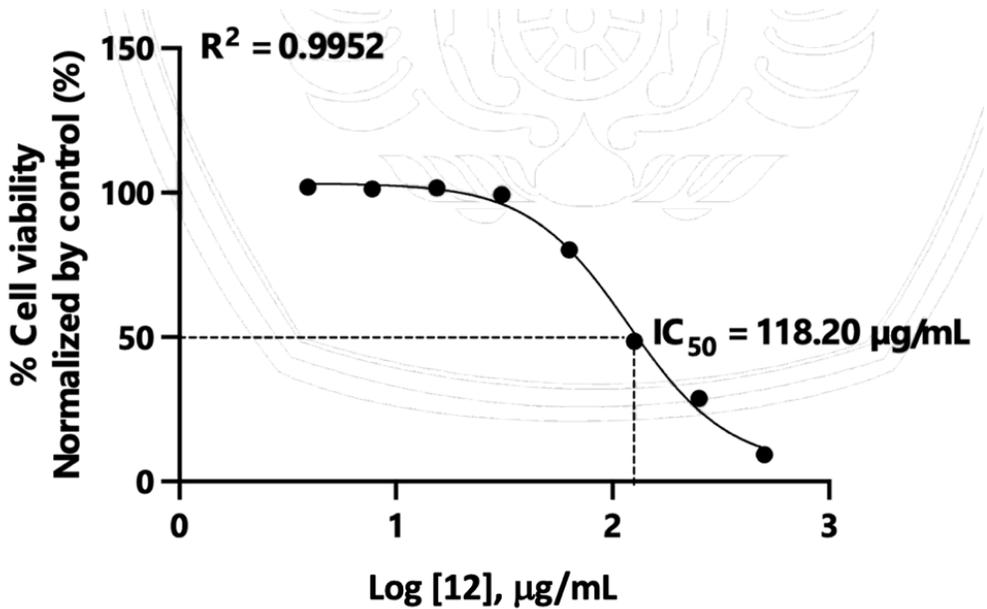
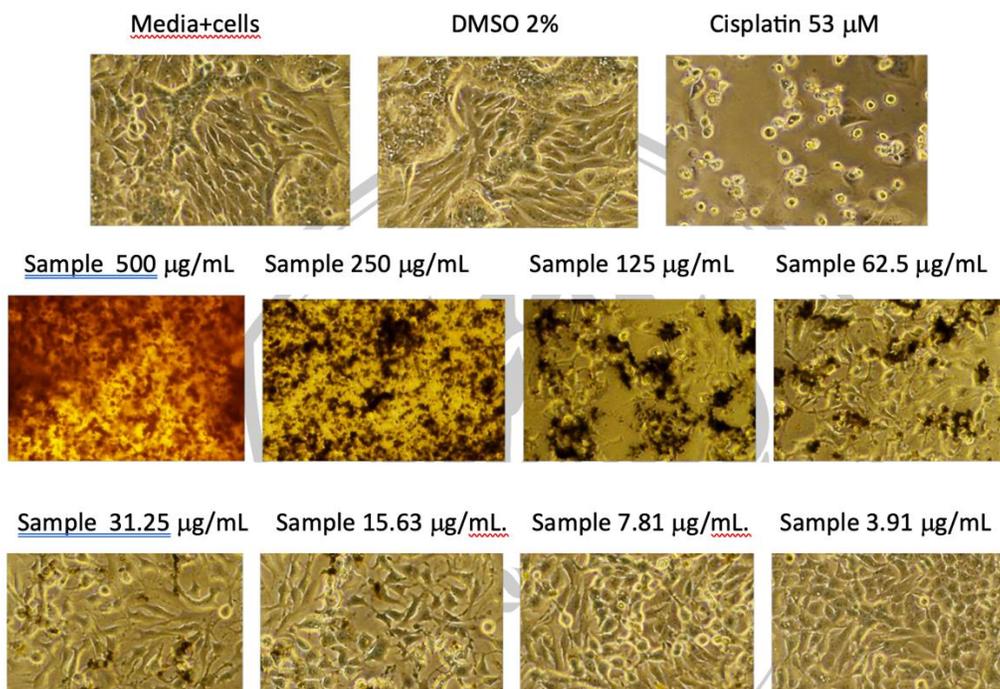
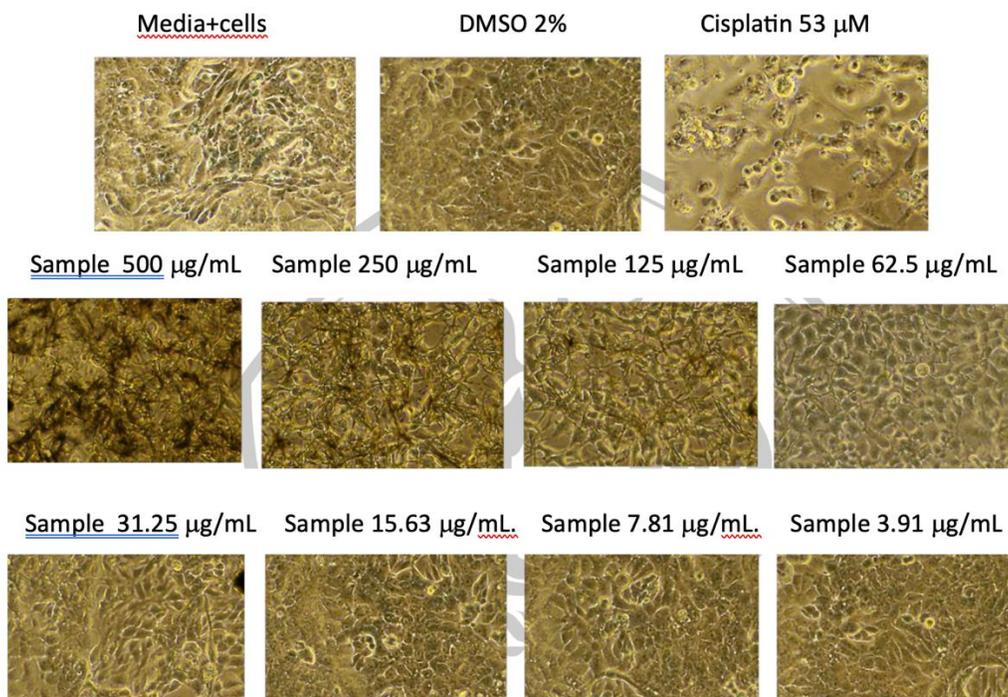


Figure 4G Calculated IC<sub>50</sub> of Compound 12 Against MCF-7 Cells.

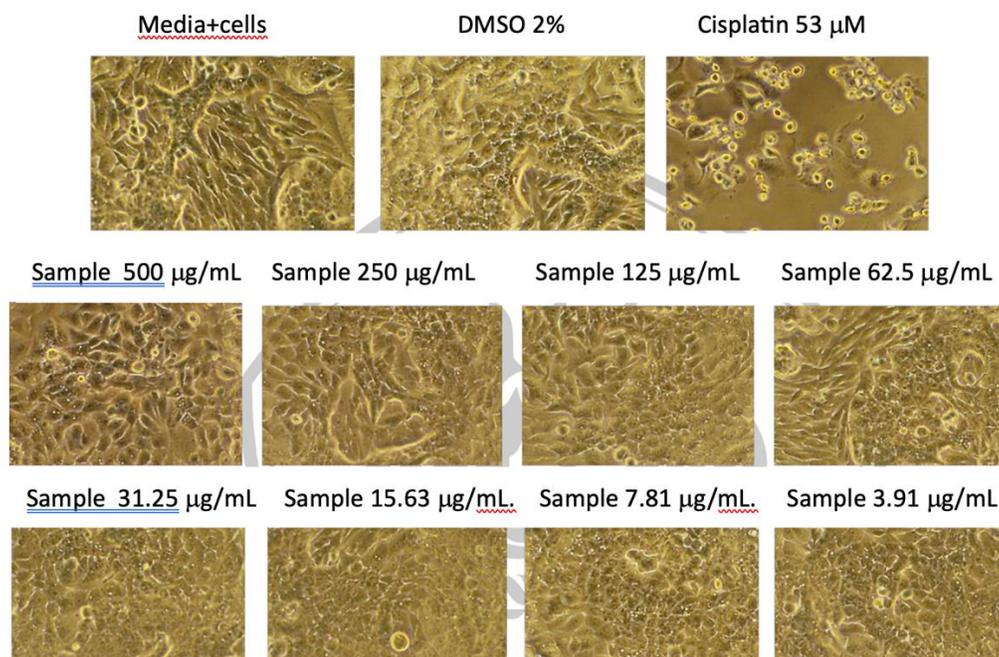
## H. Morphology of MCF-7 Cells Against The Compounds



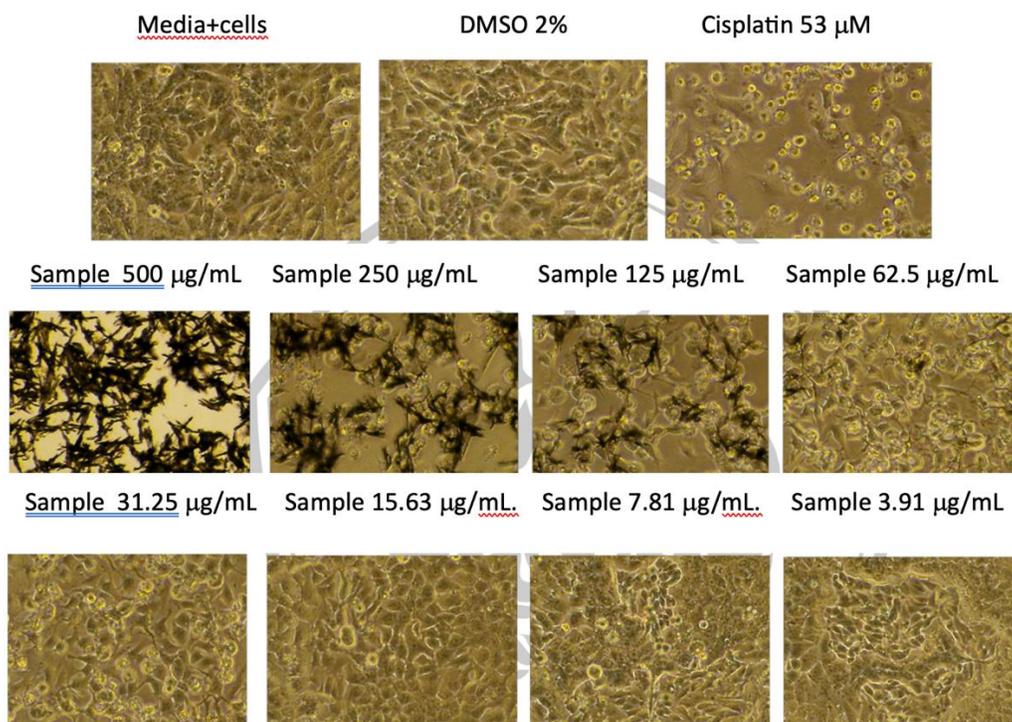
**Figure 1H** Morphology of MCF-7 Cells Against Compound 9.



**Figure 2H** Morphology of MCF-7 Cells Against Compound 10.



**Figure 3H** Morphology of MCF-7 Cells Against Compound 11.



**Figure 4H** Morphology of MCF-7 Cells Against Compound 12.