Supplementary Information (SI) for RSC Advances.
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Coumarin-Amino Acid Hybrids as Promising Anticancer Agents: Design, Synthesis, Docking Studies and Ck2 Inhibition

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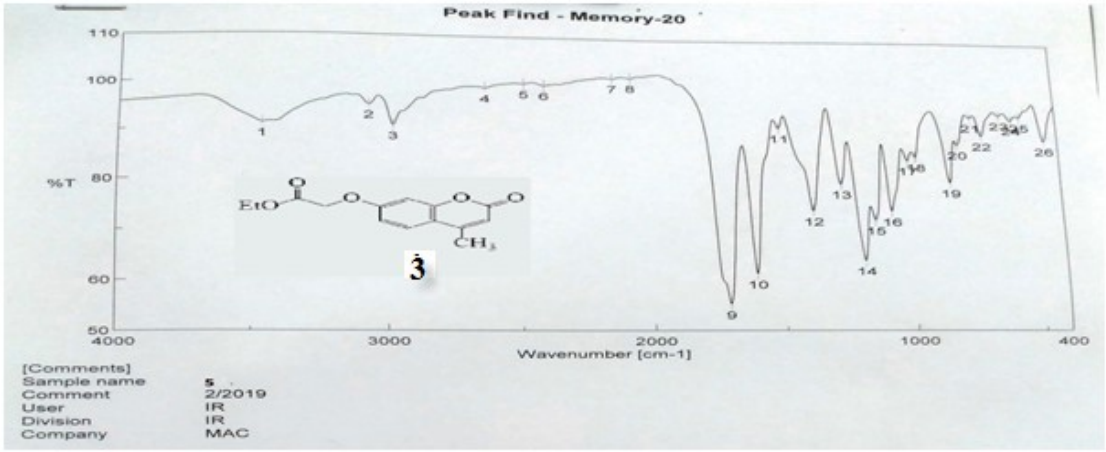
IR of Compound 3



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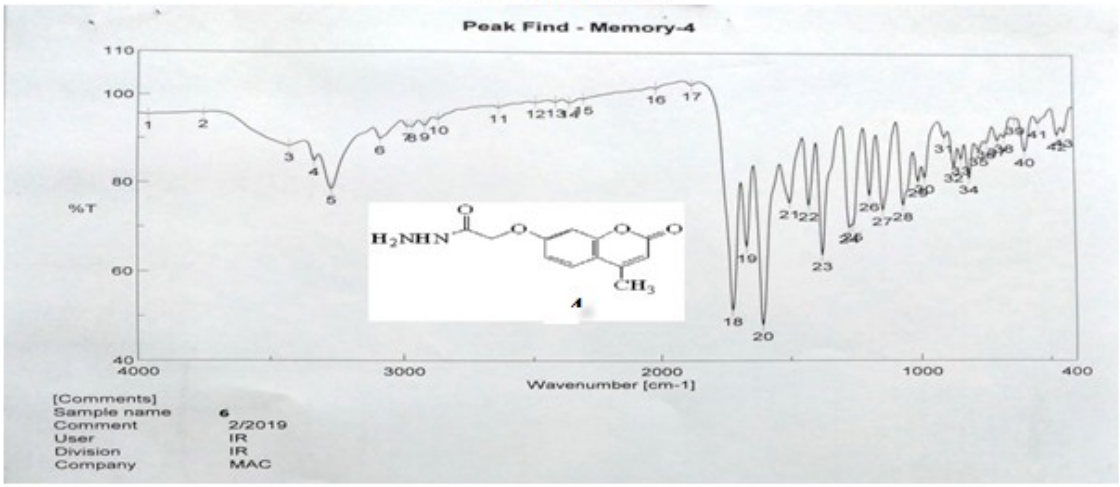
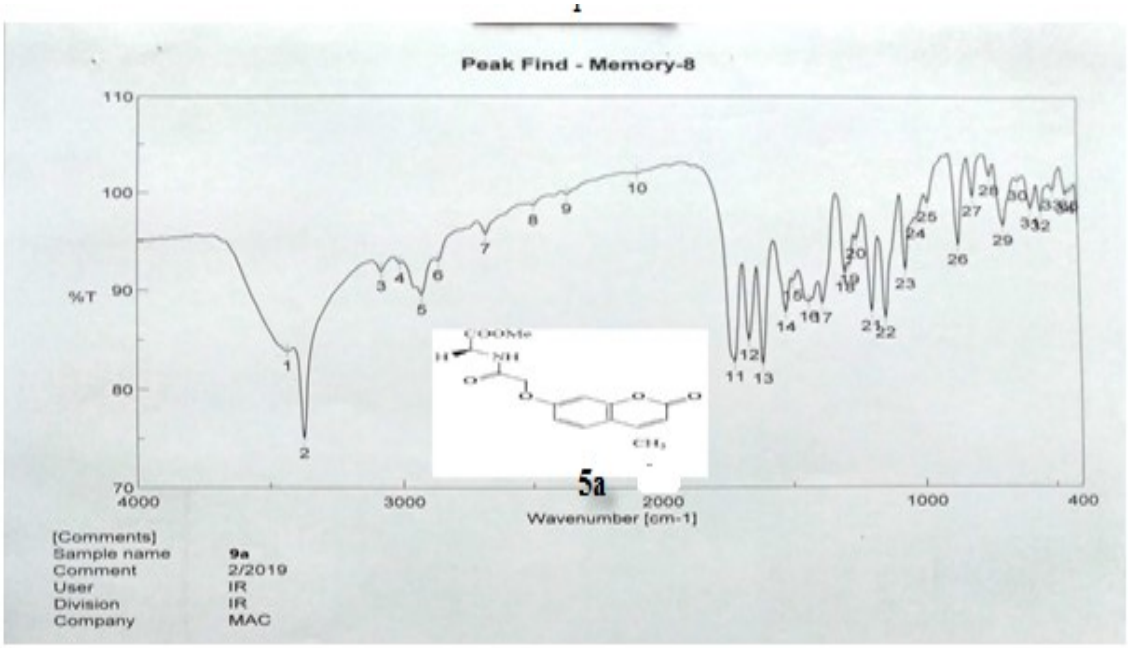


IR of Compound 5a



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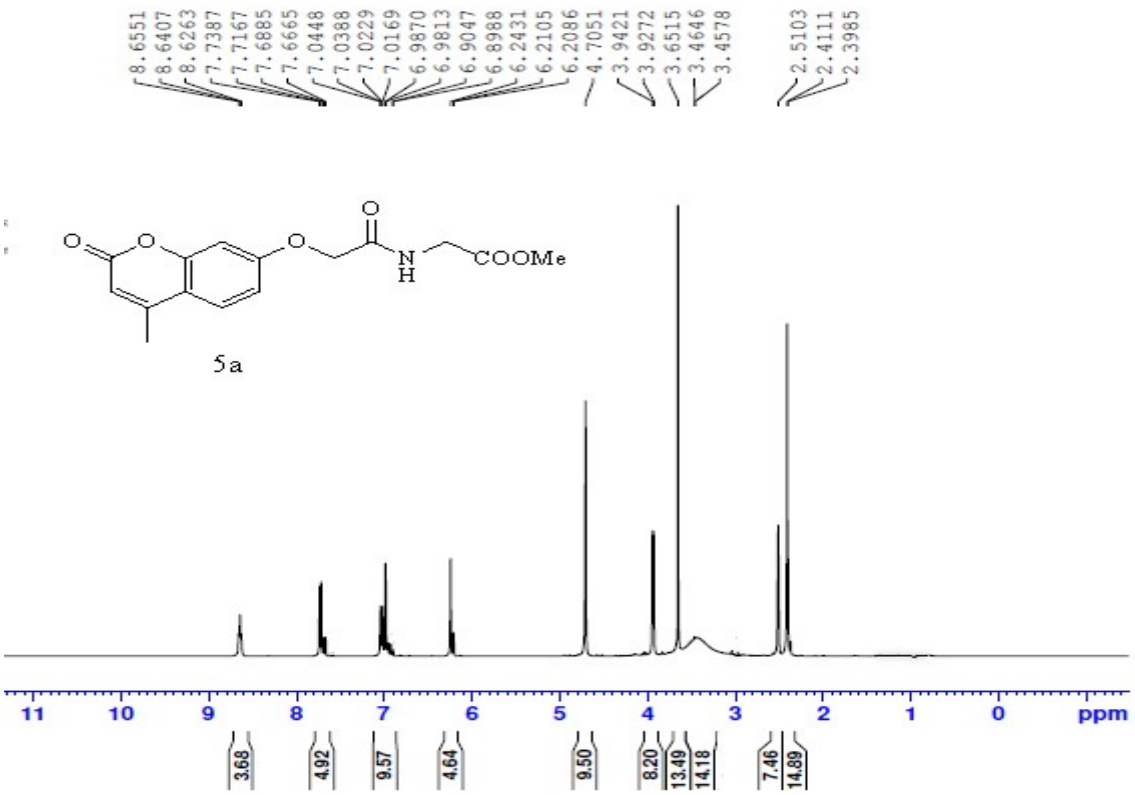

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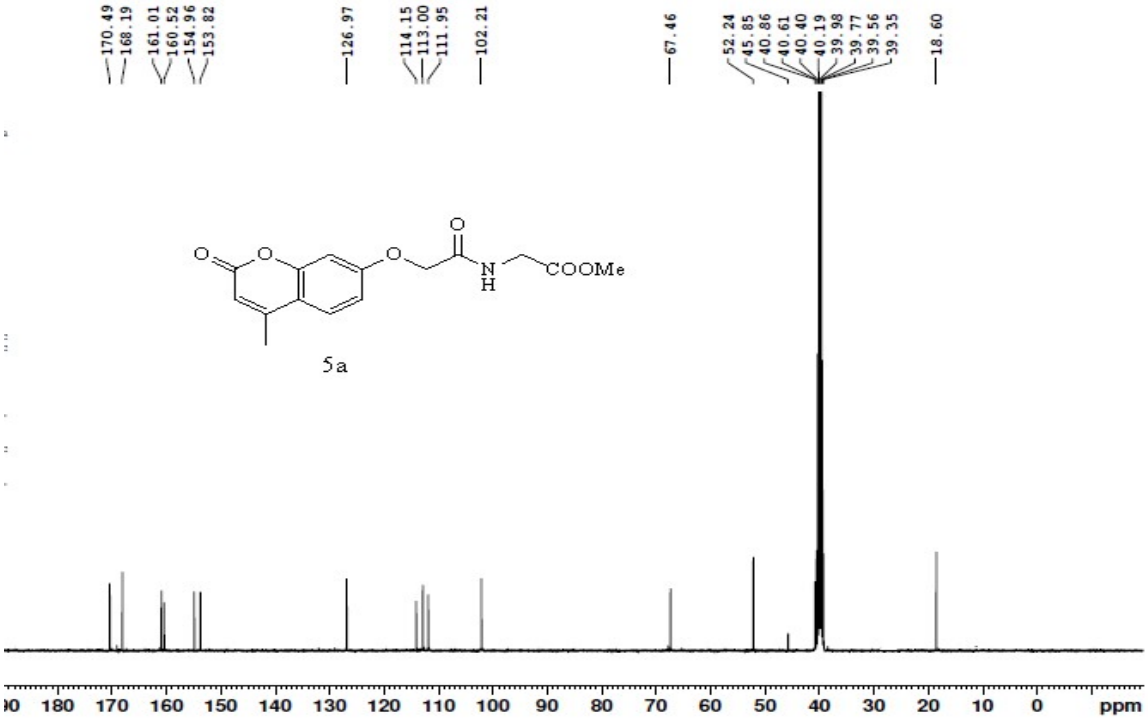

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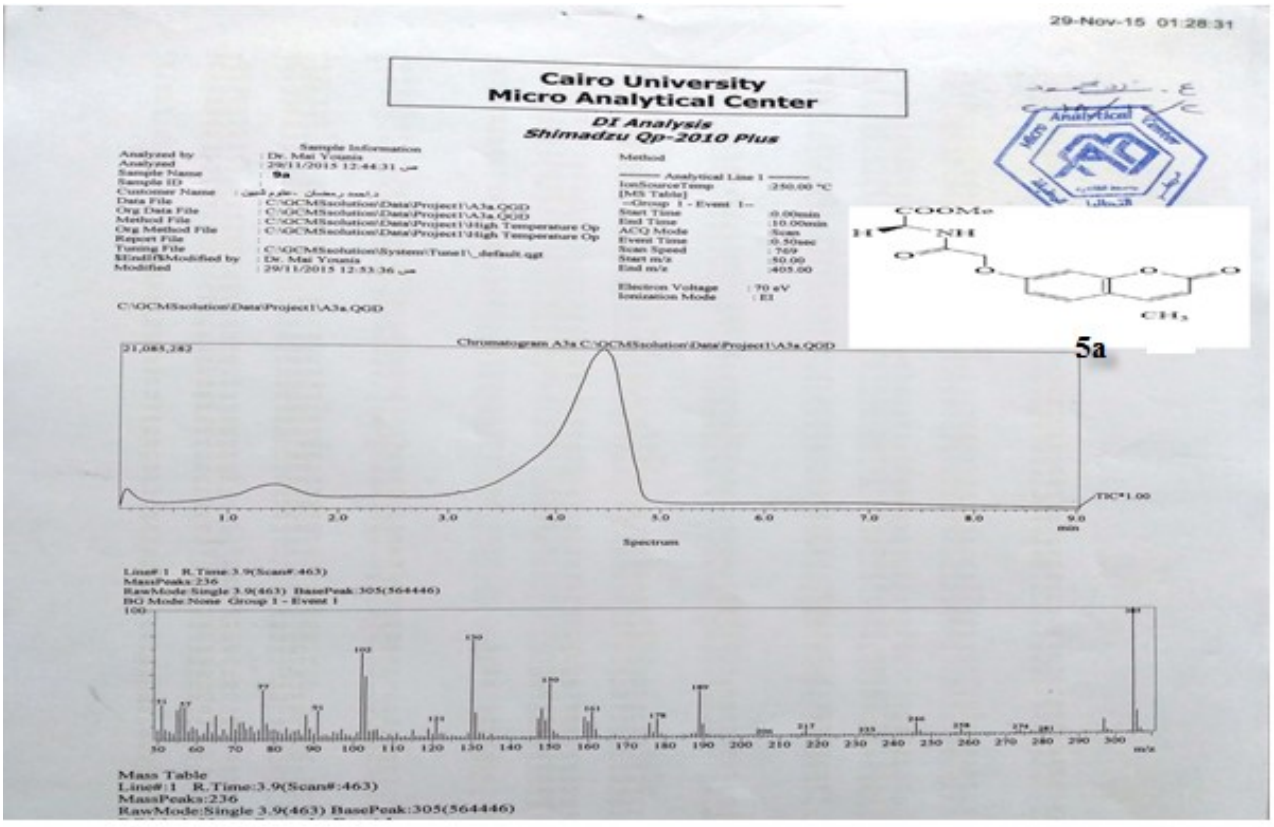

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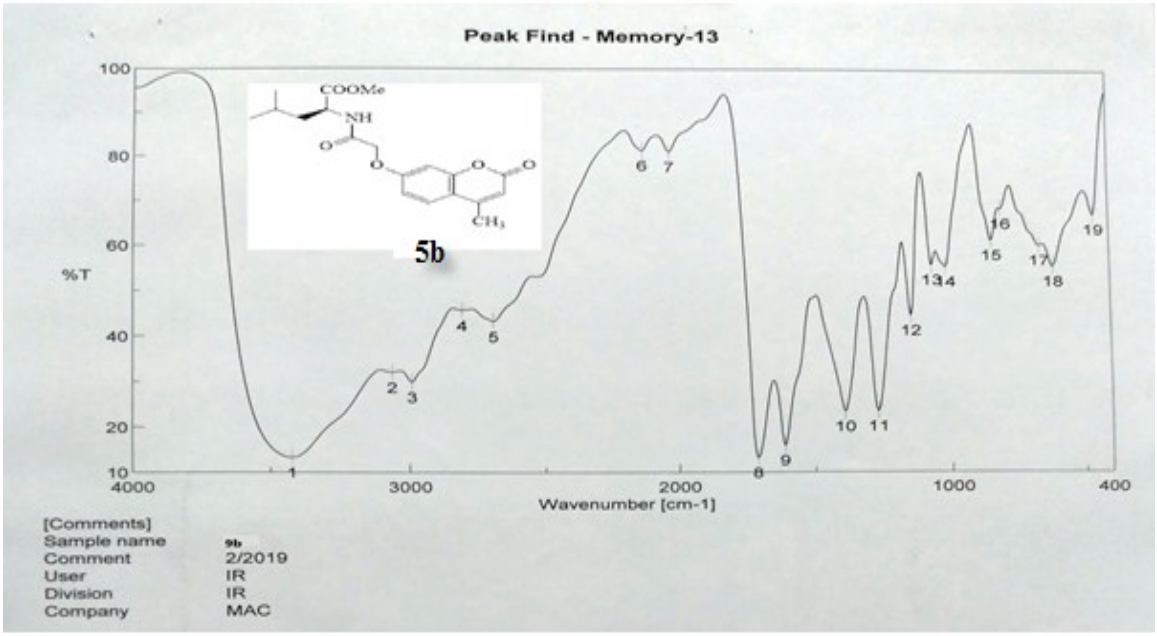

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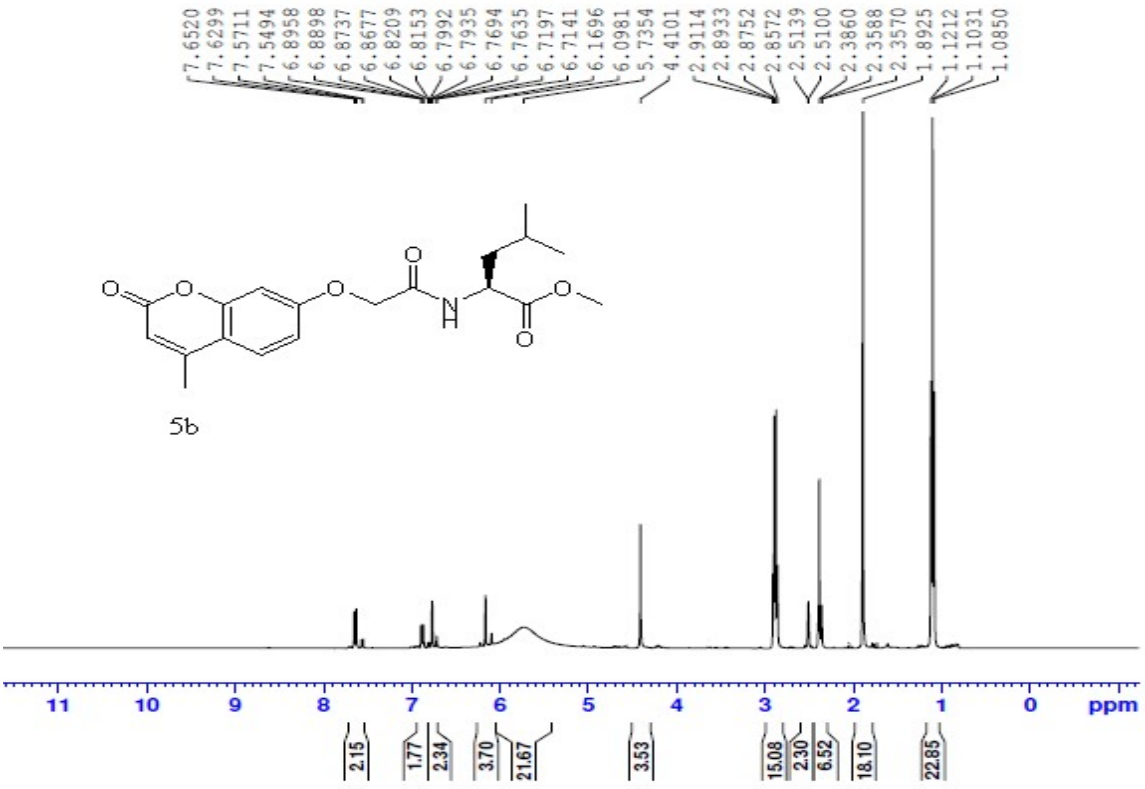

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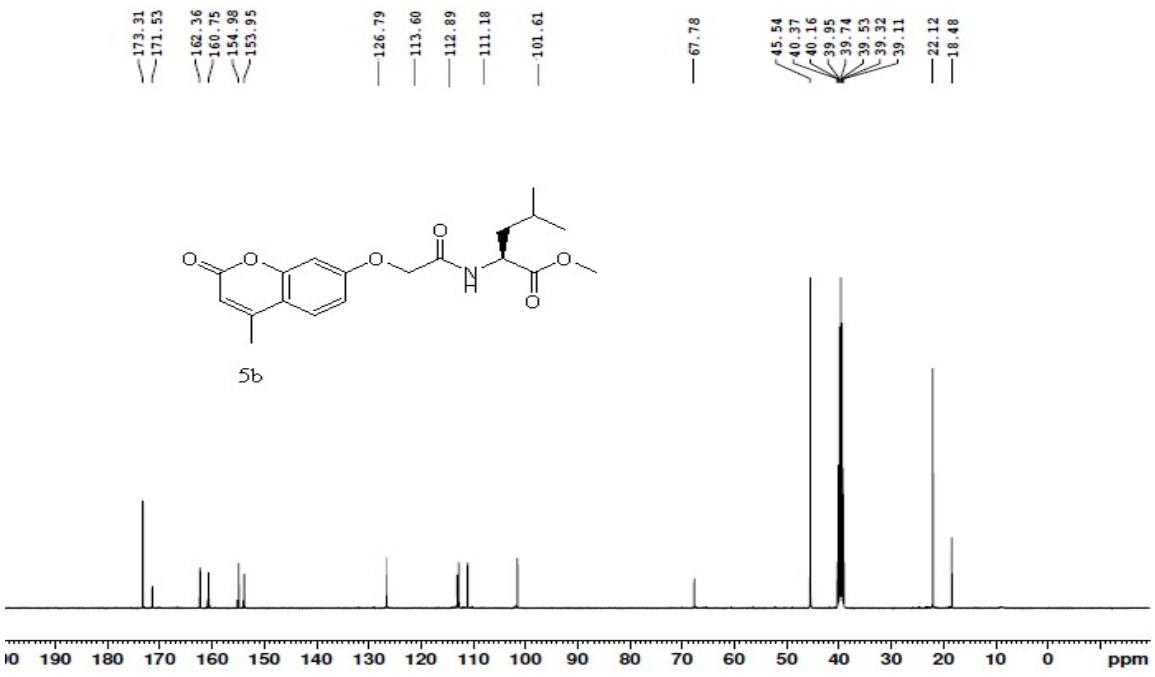

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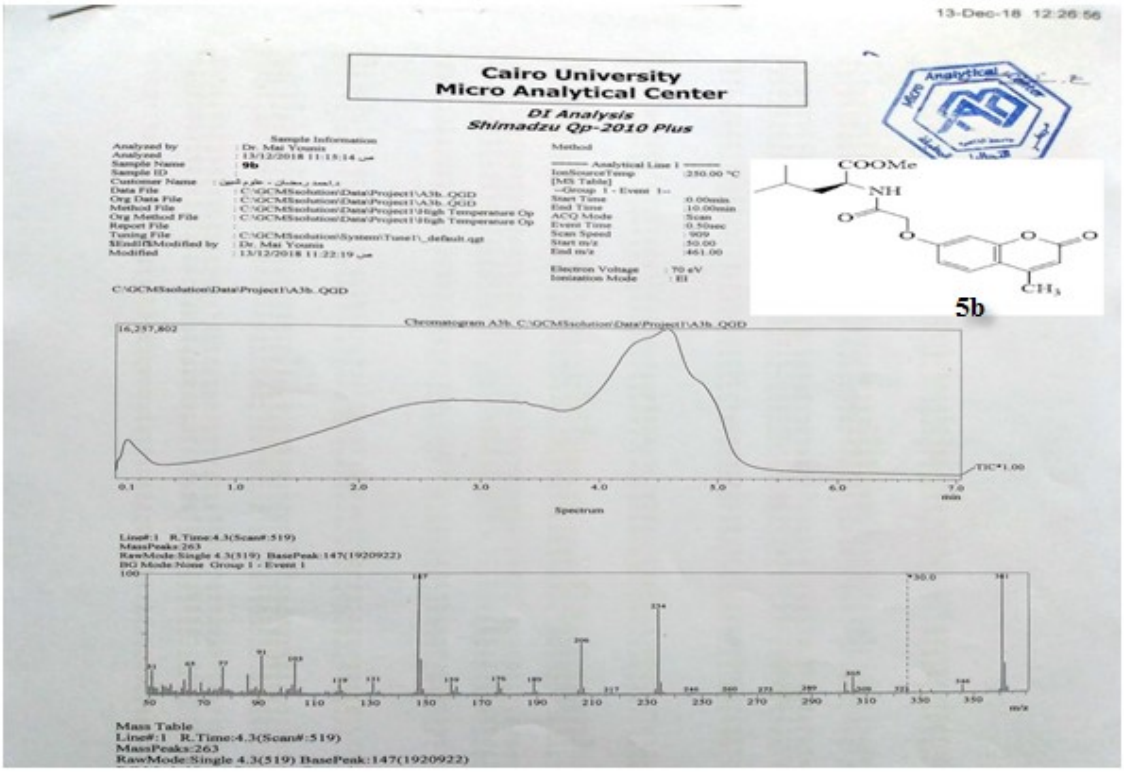

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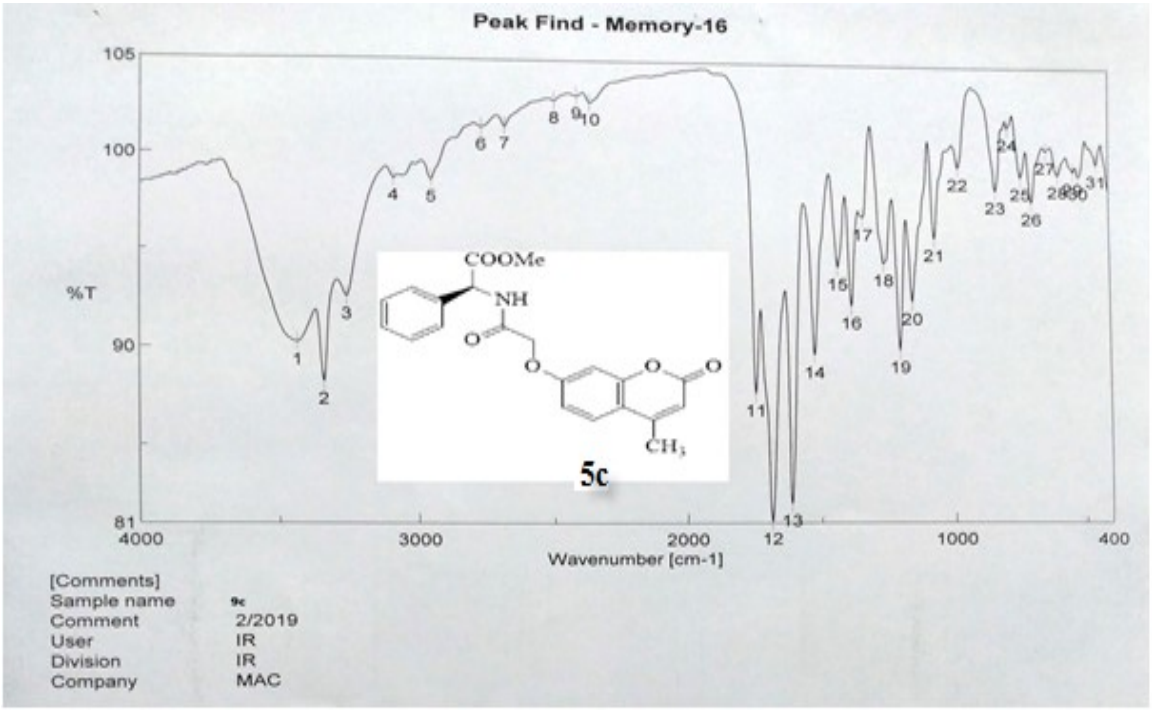

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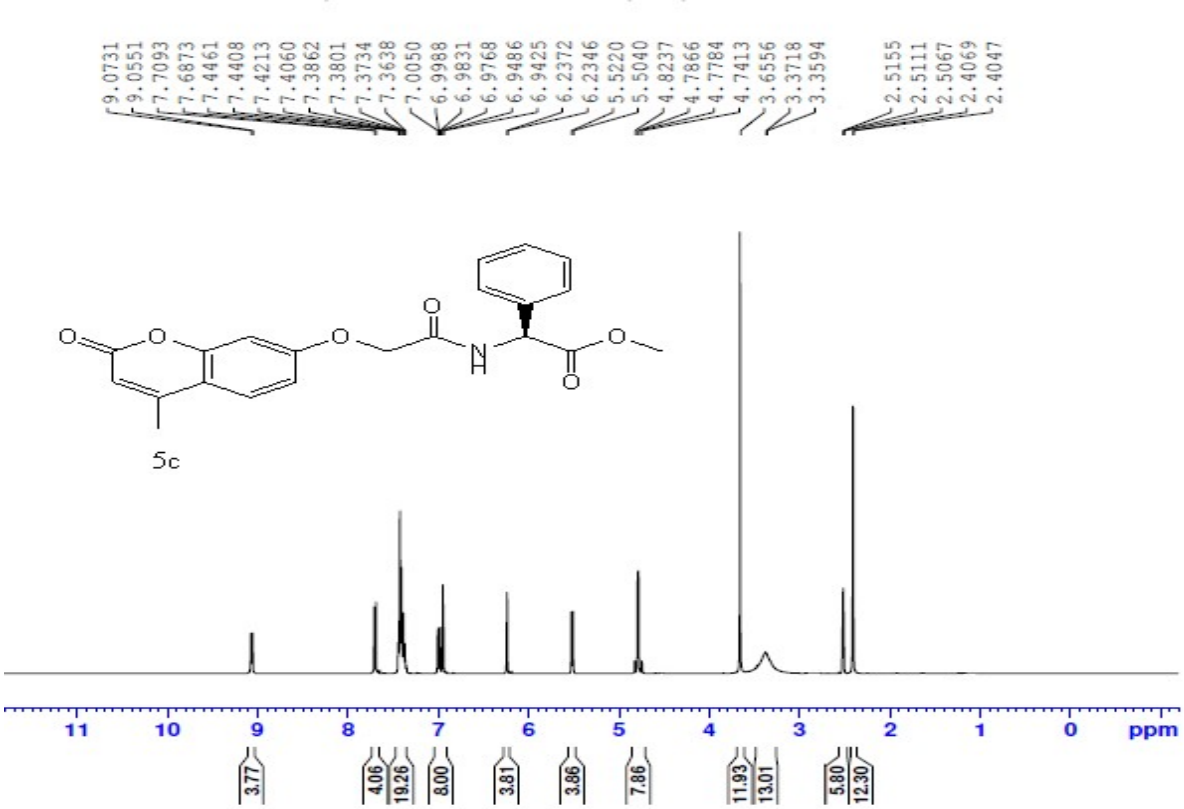

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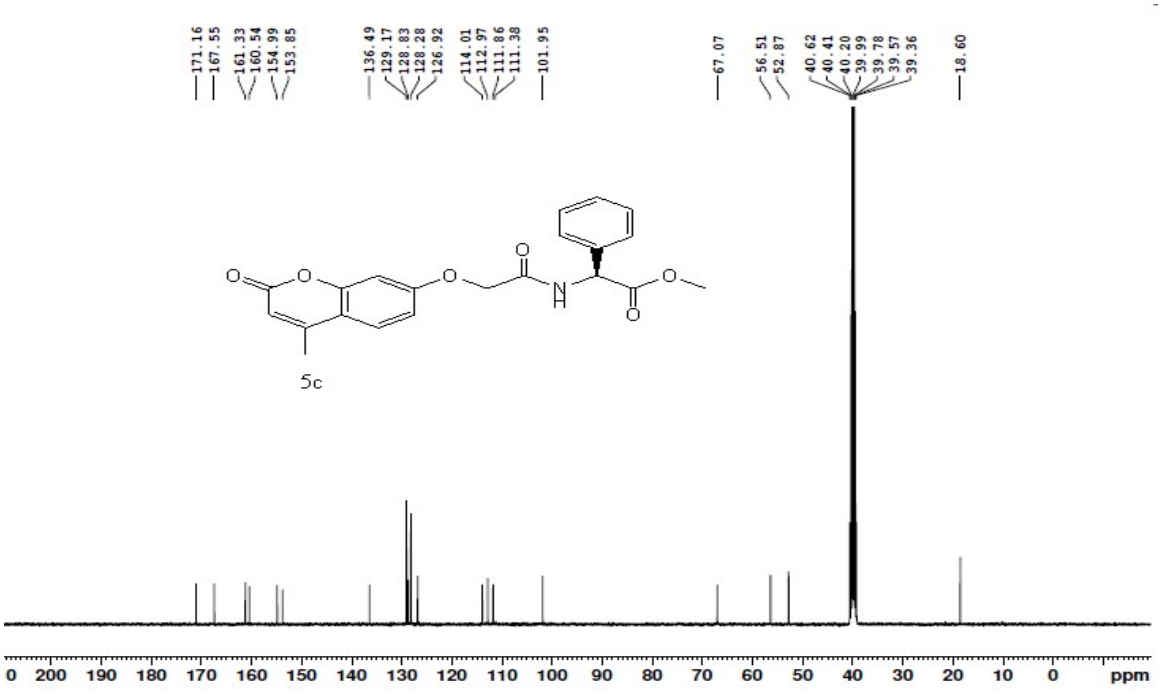

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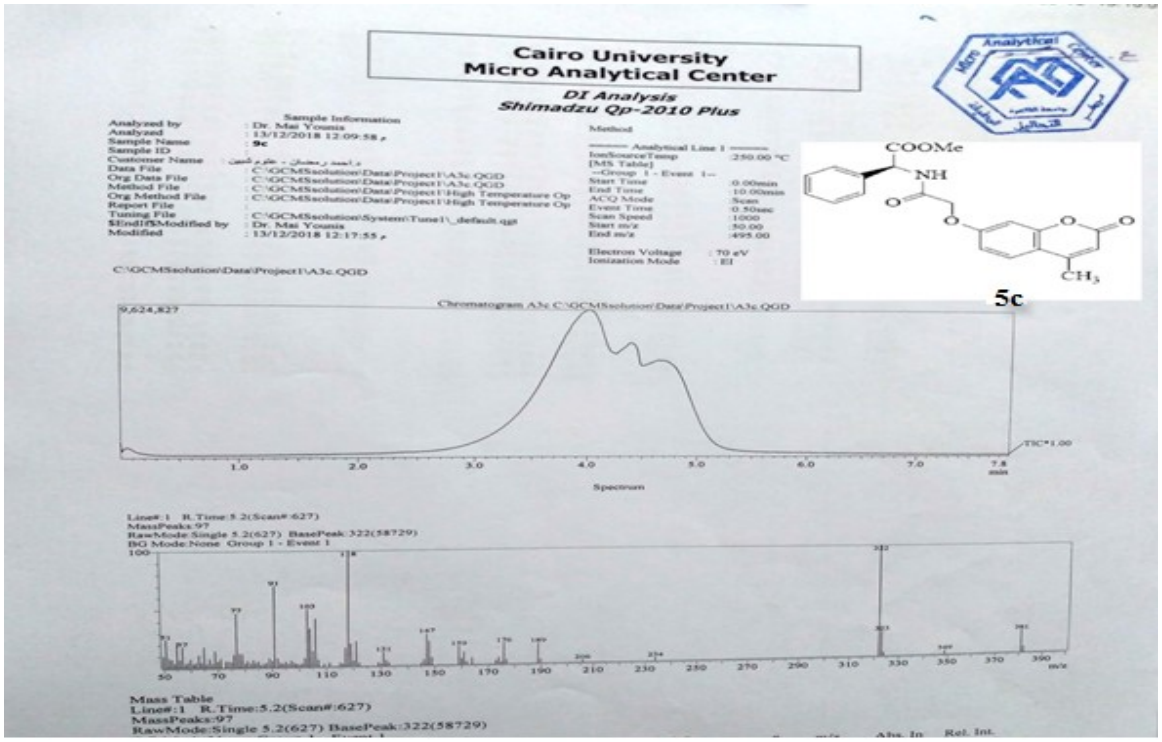

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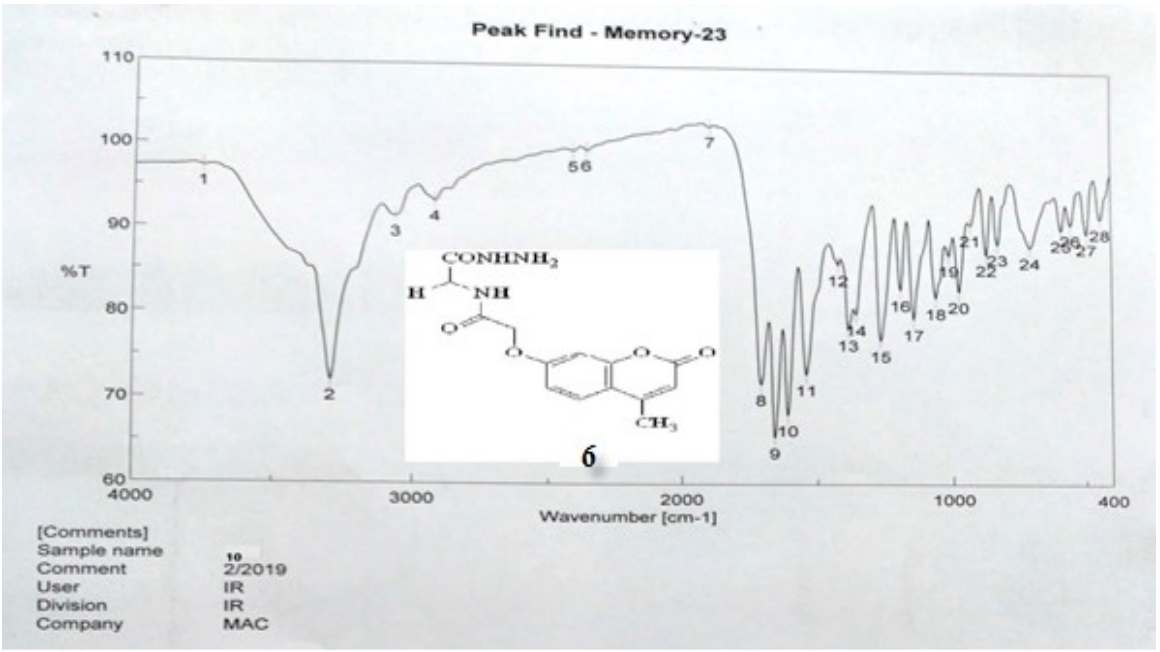

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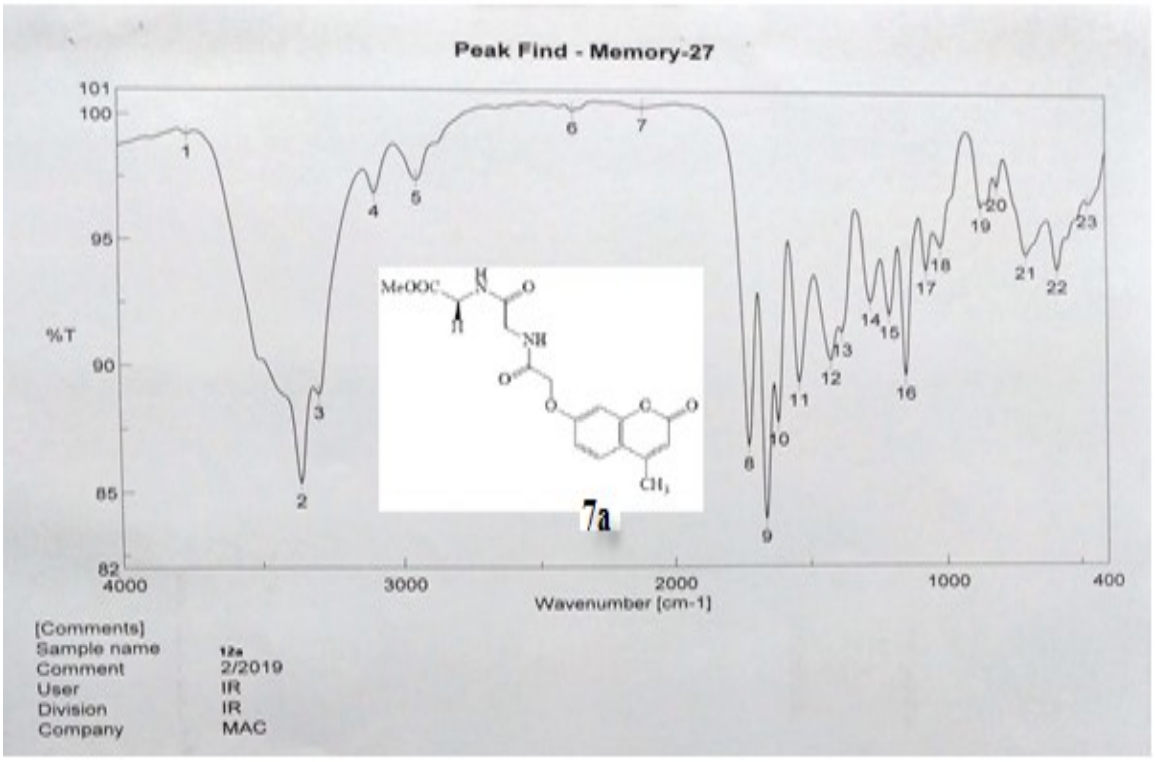

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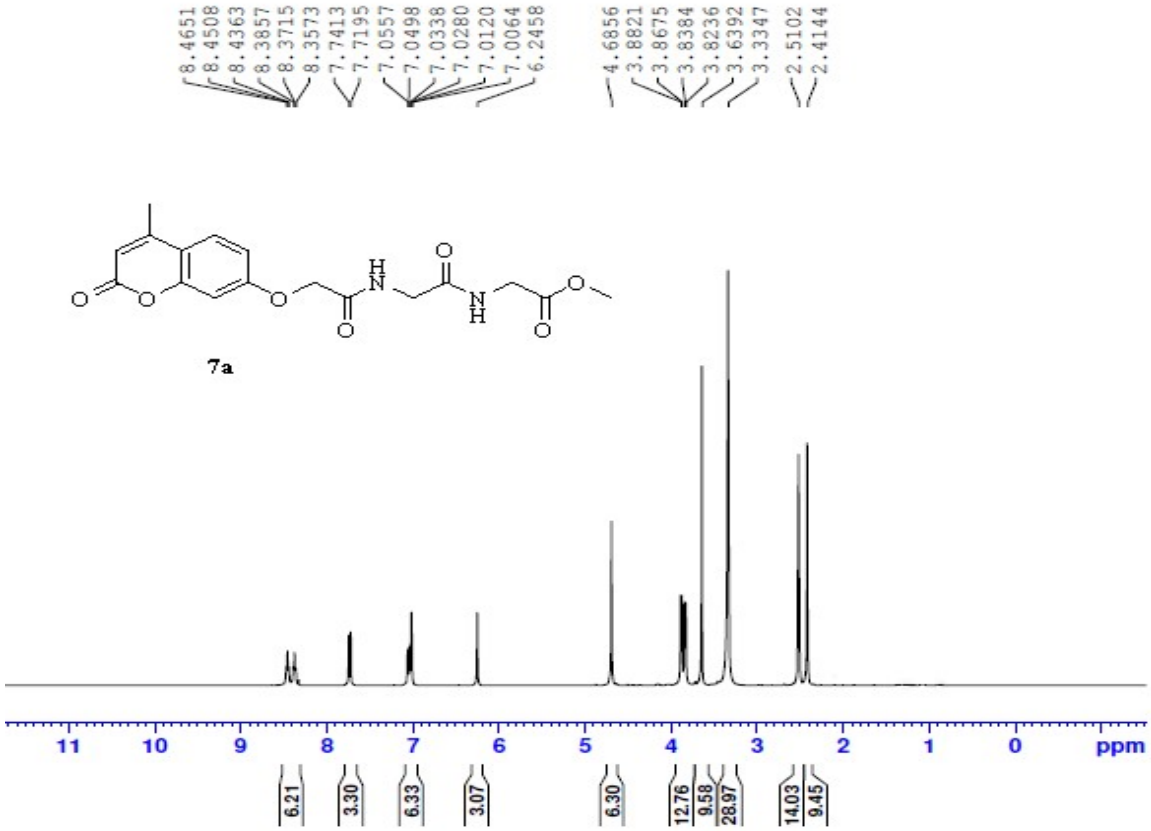

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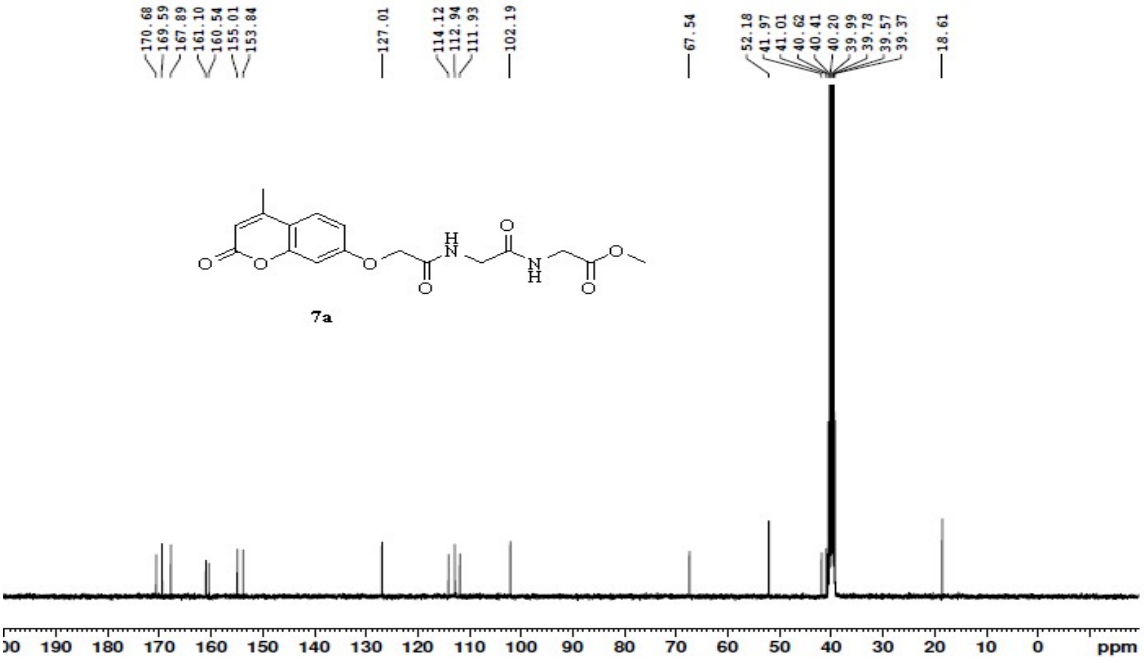

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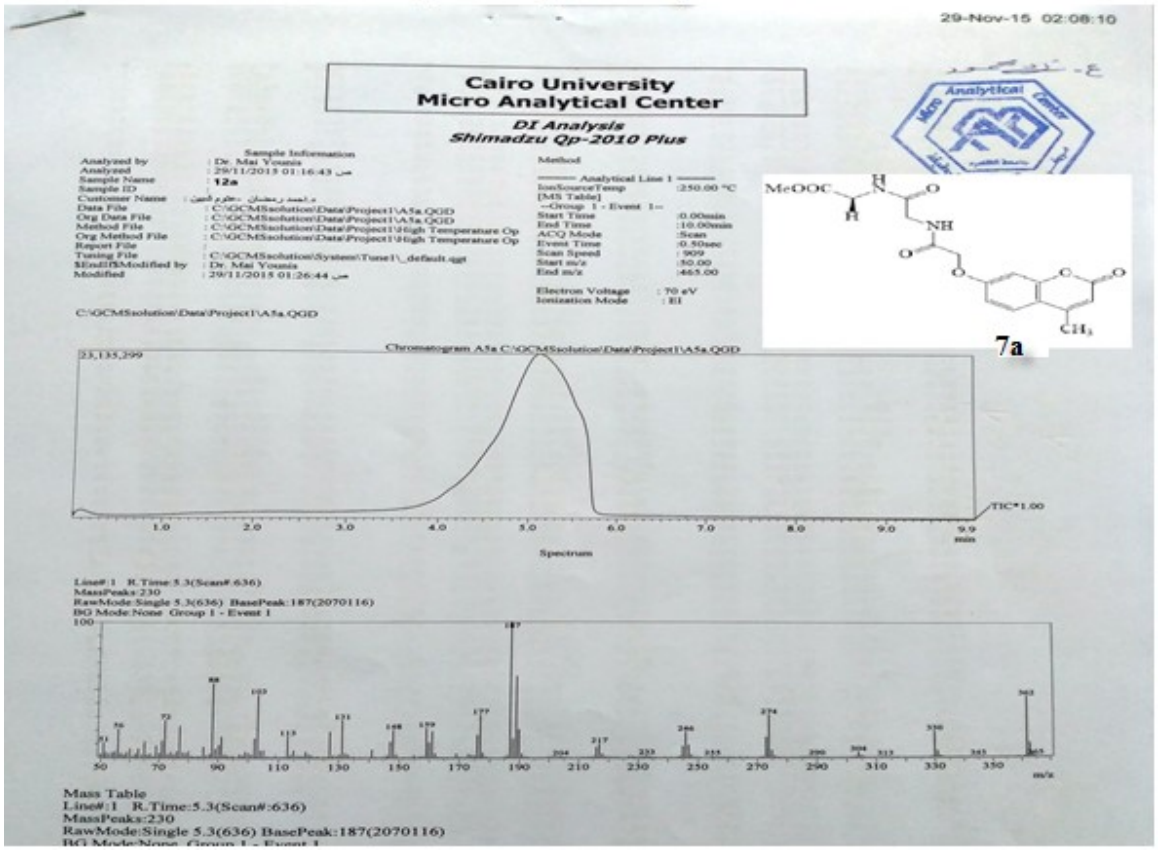

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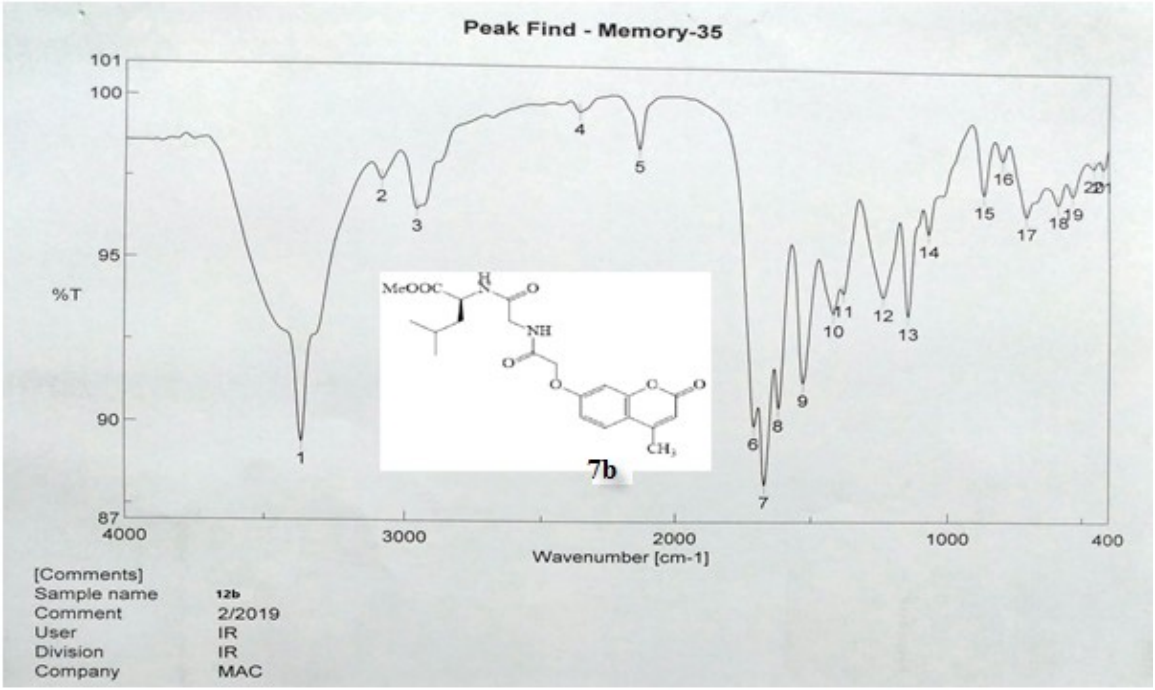

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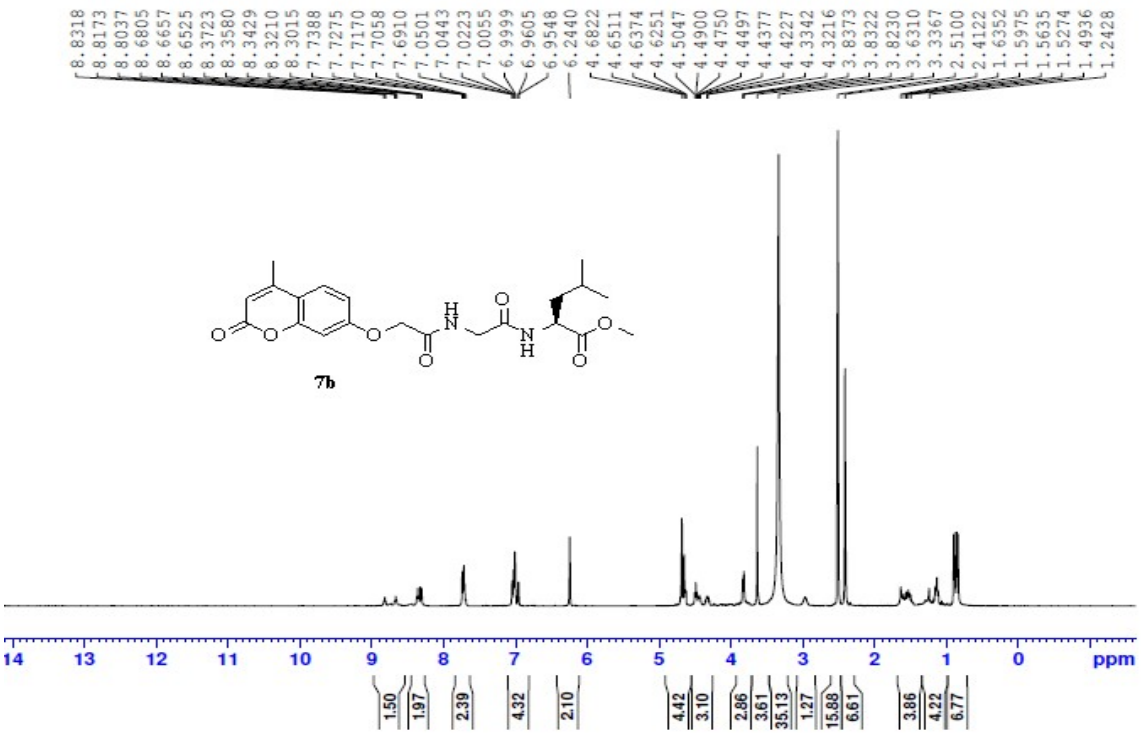

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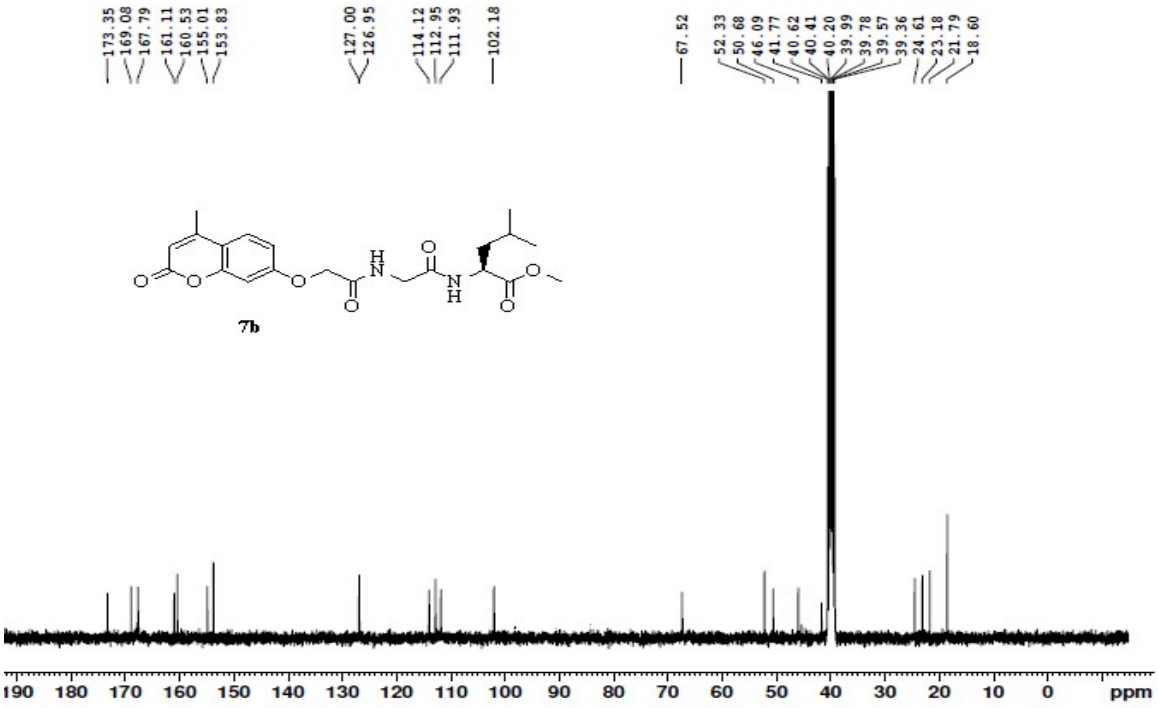

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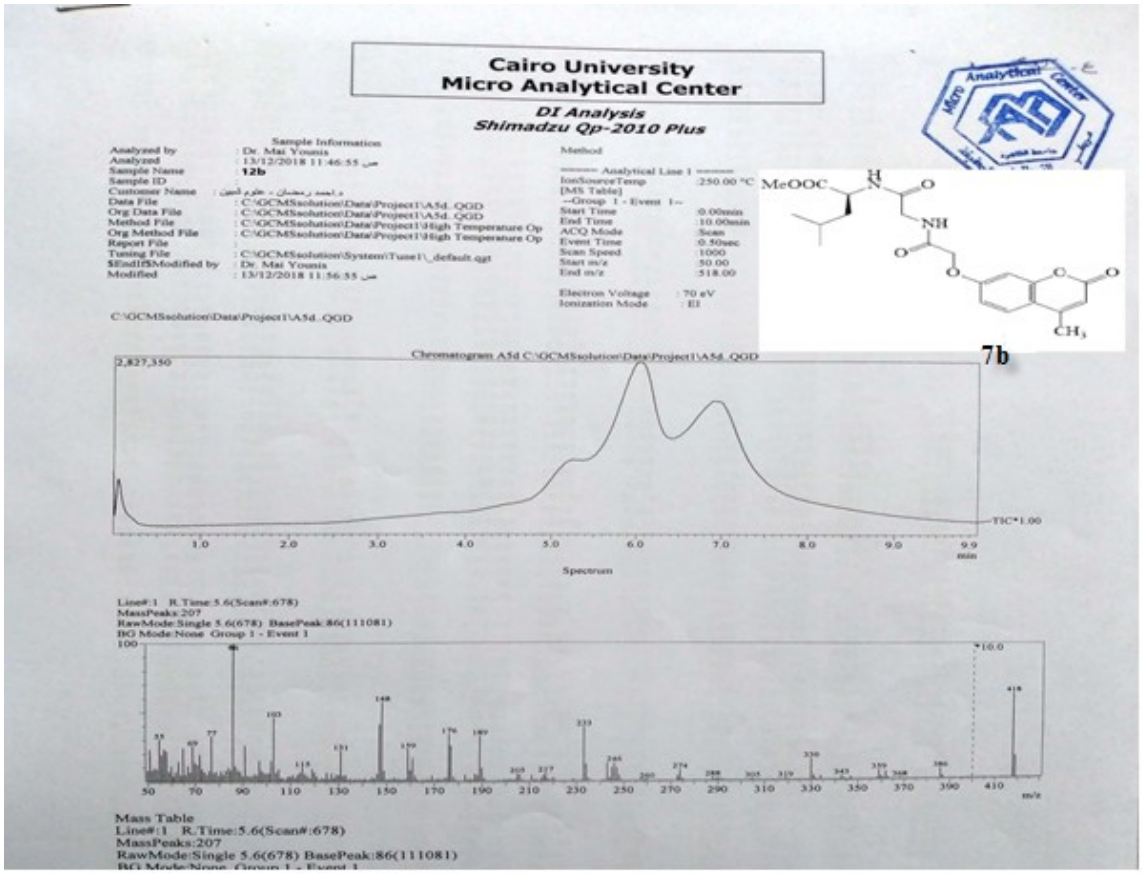

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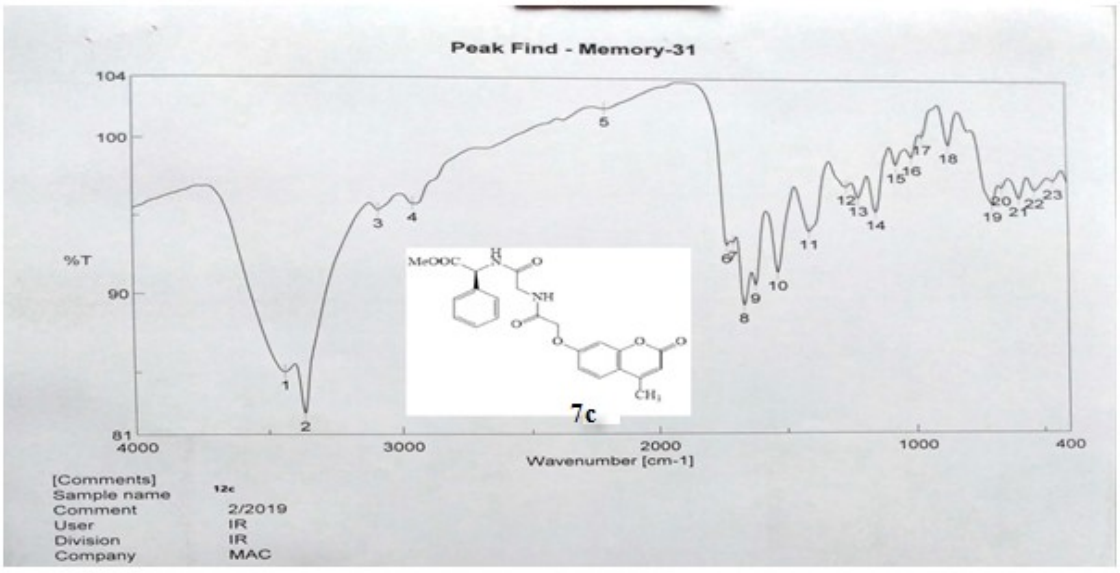

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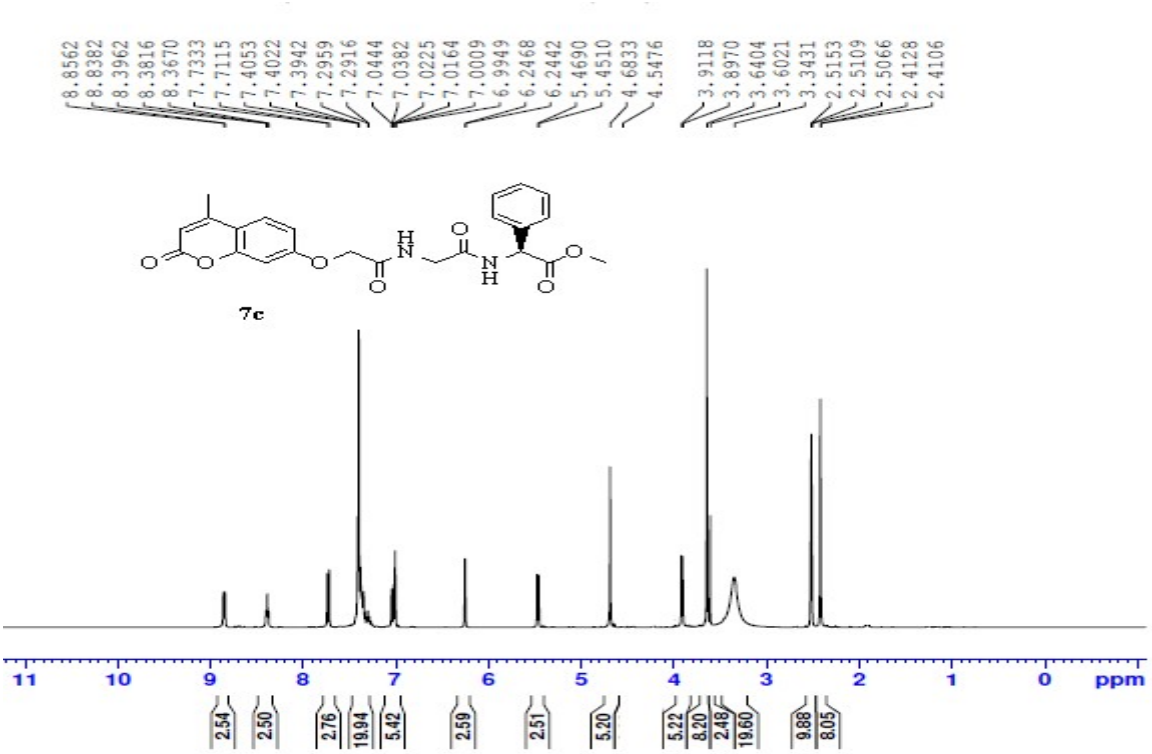

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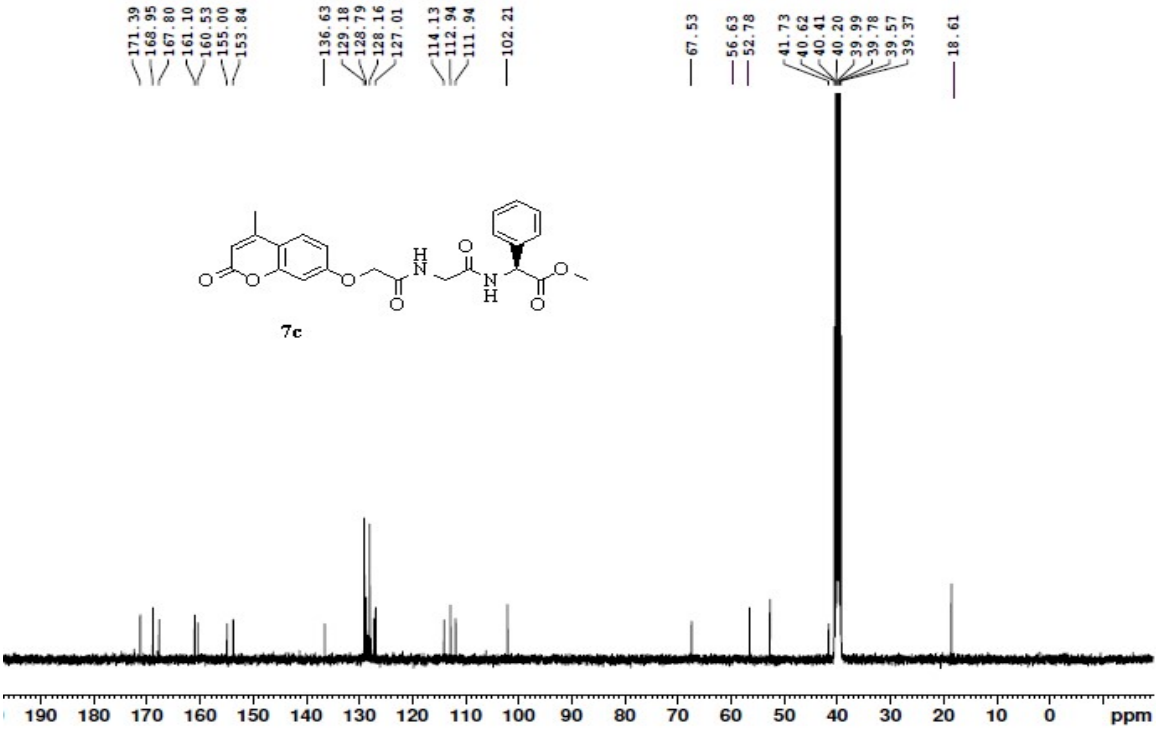

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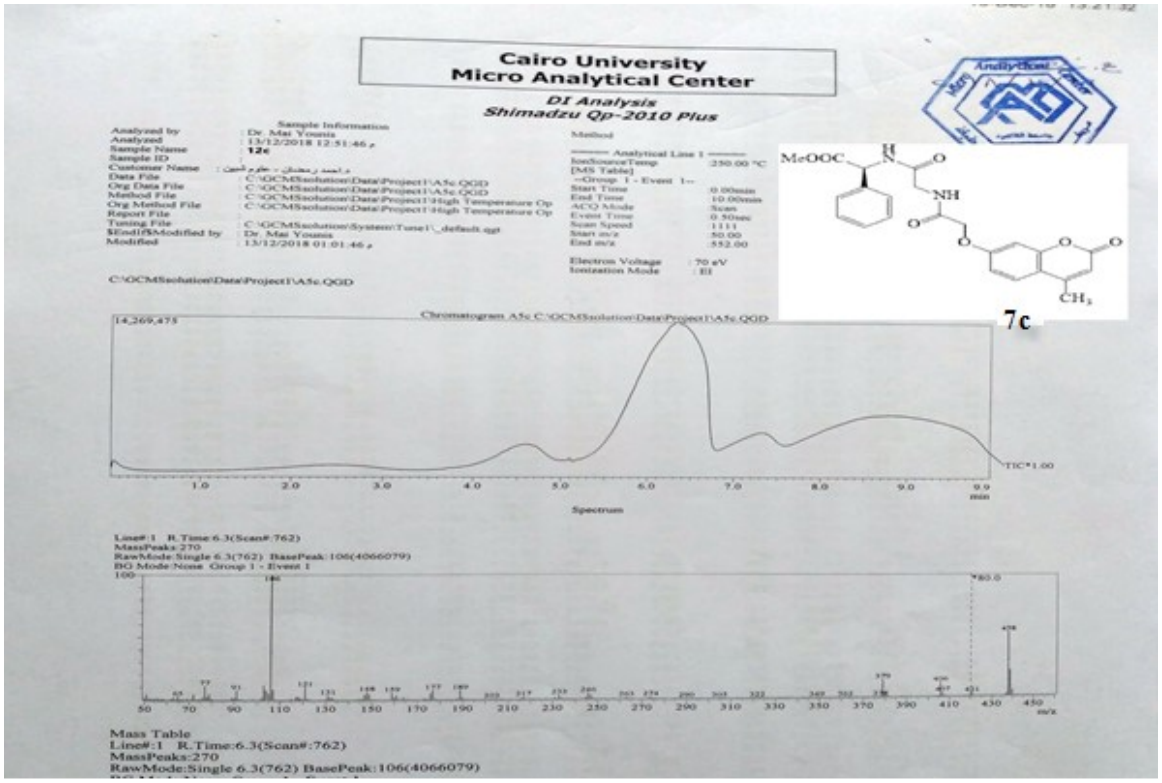

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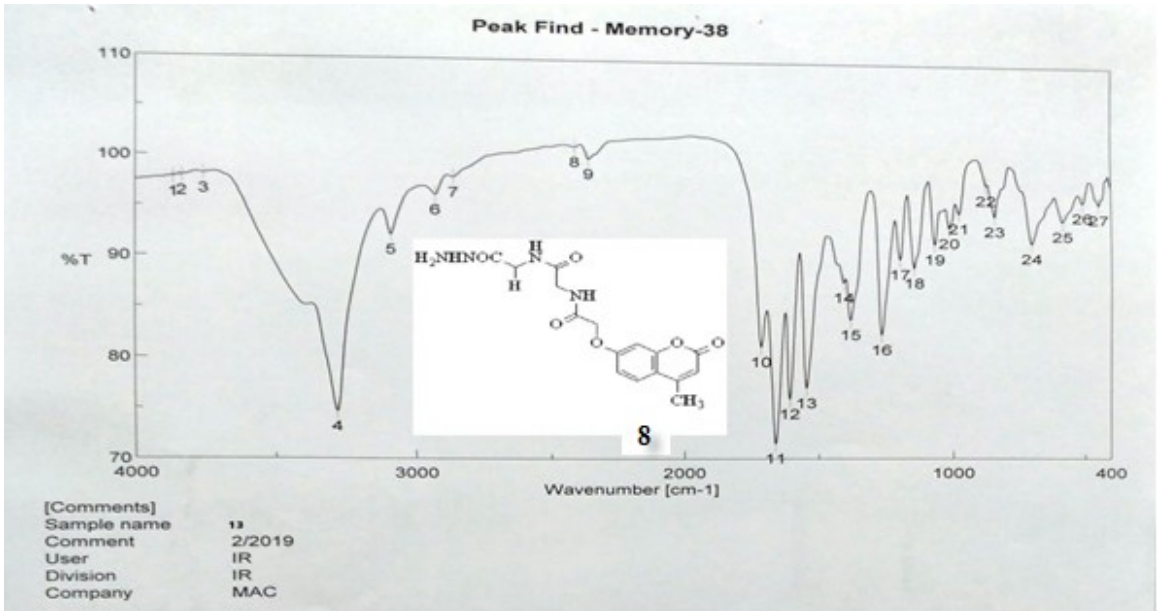

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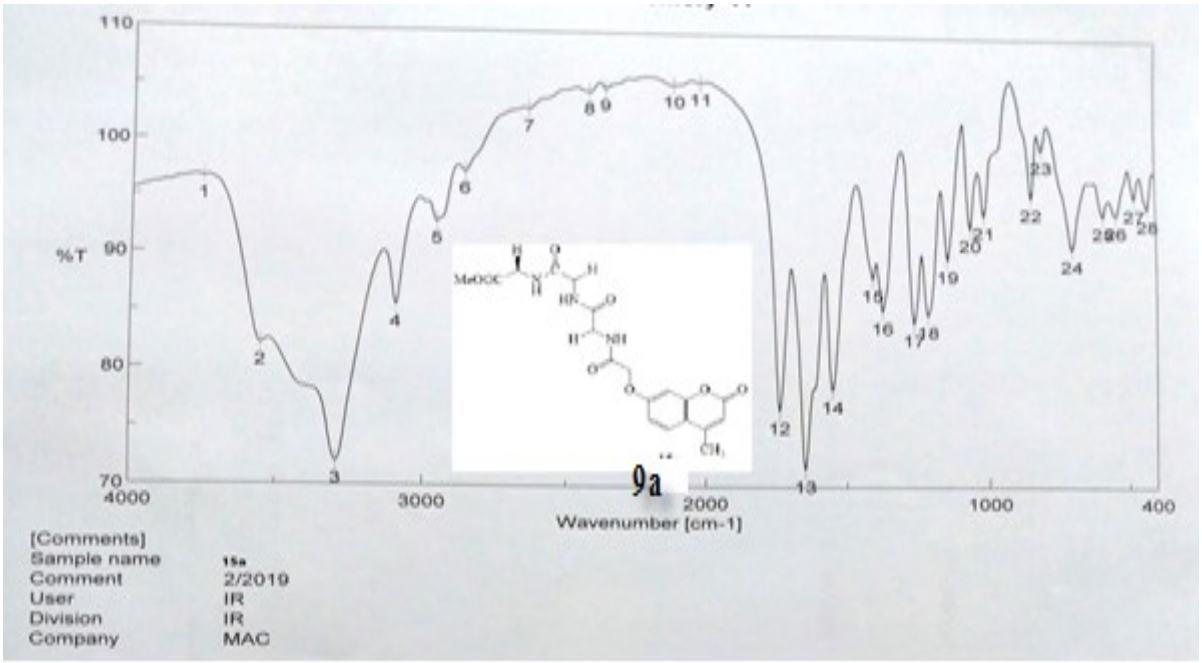

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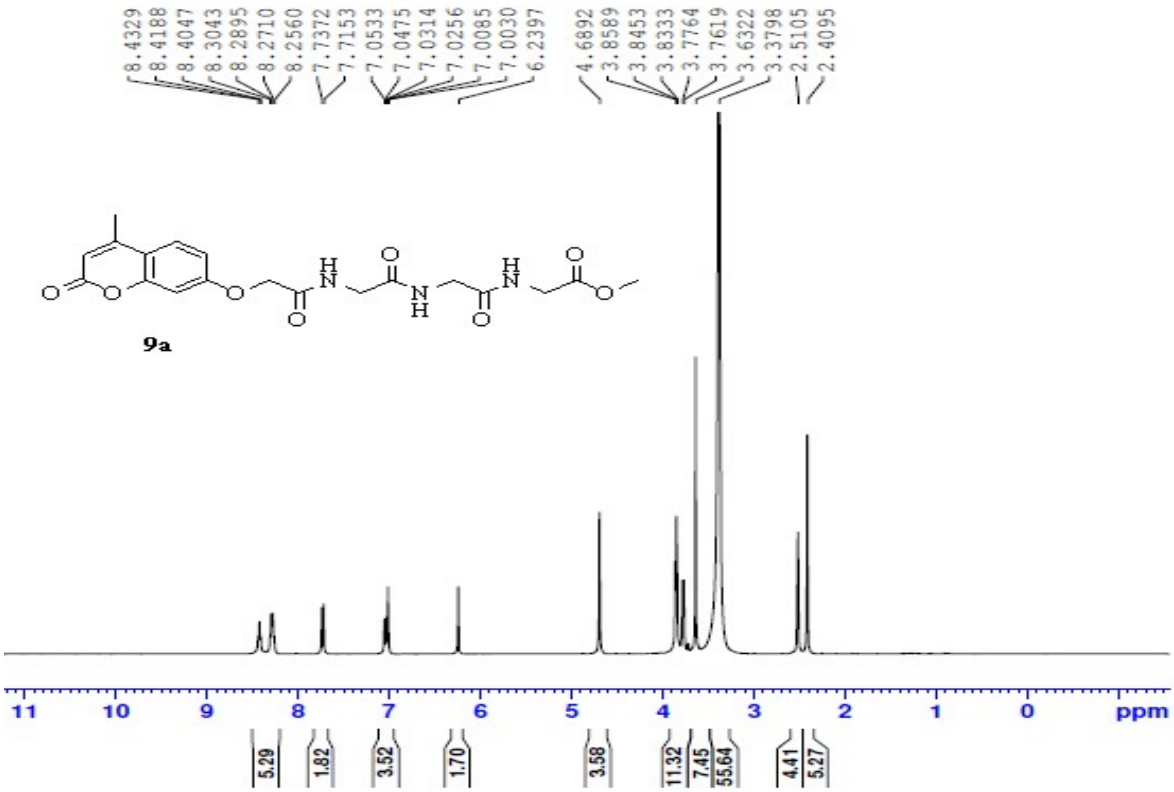

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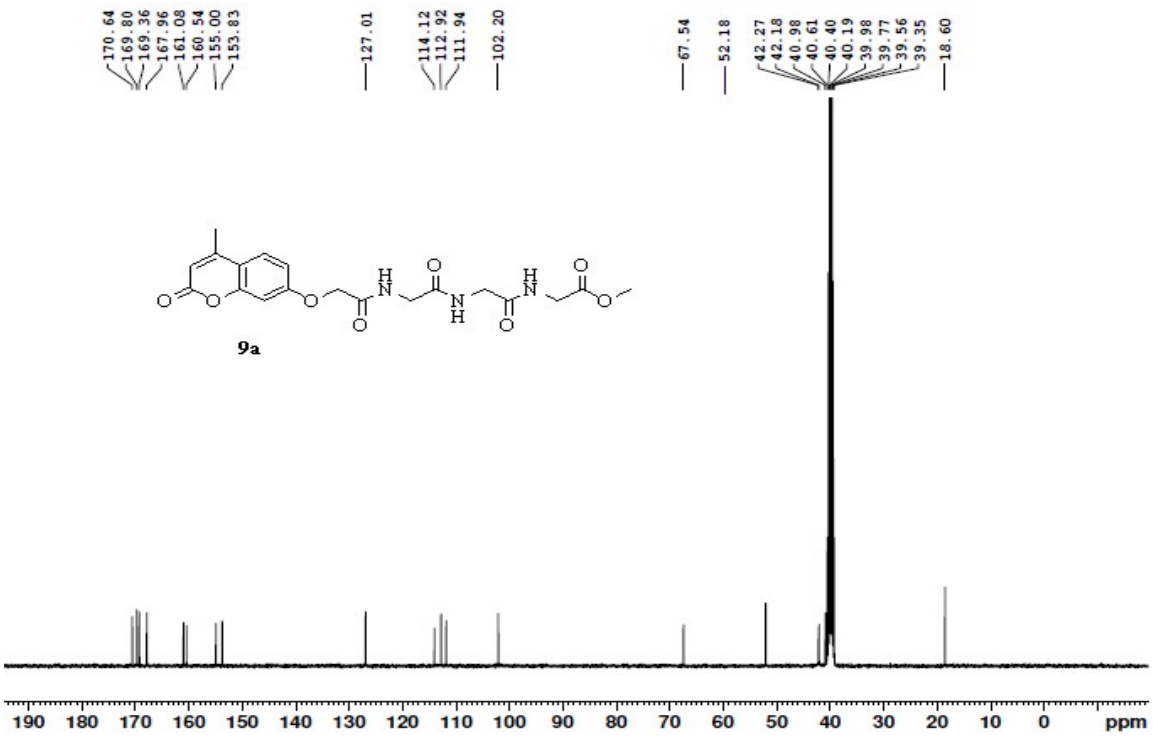

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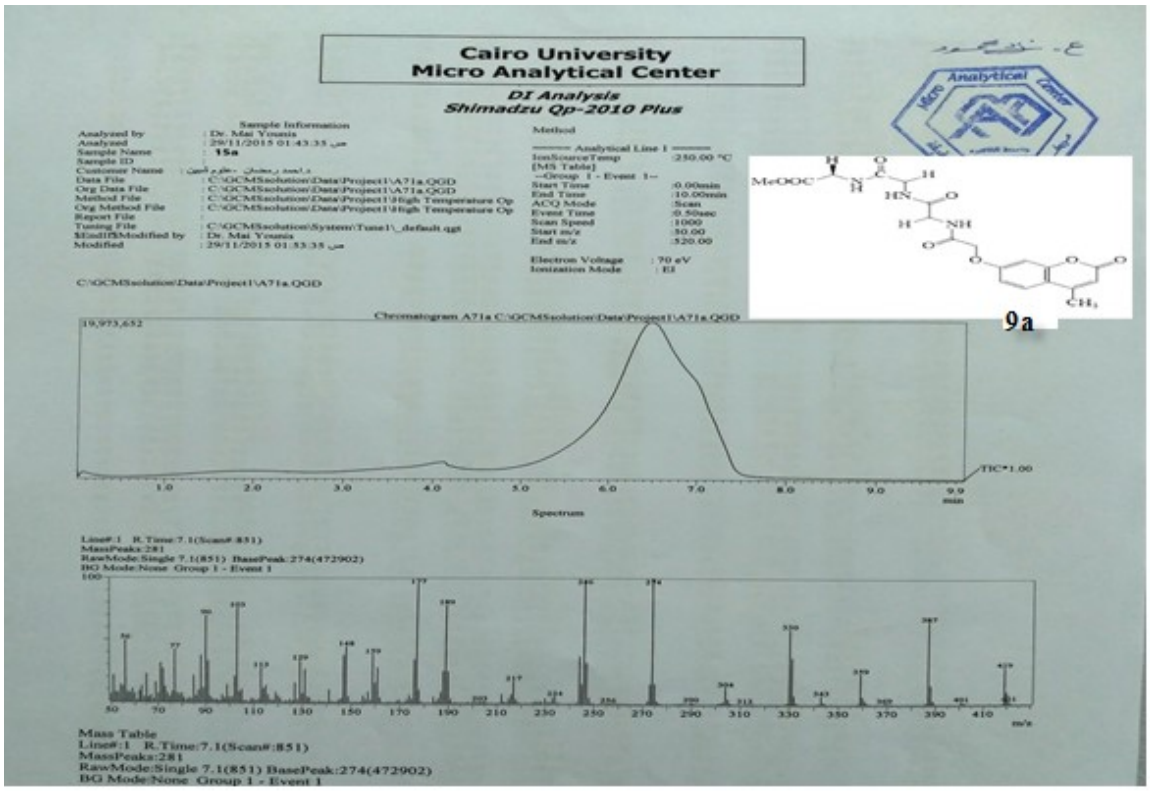

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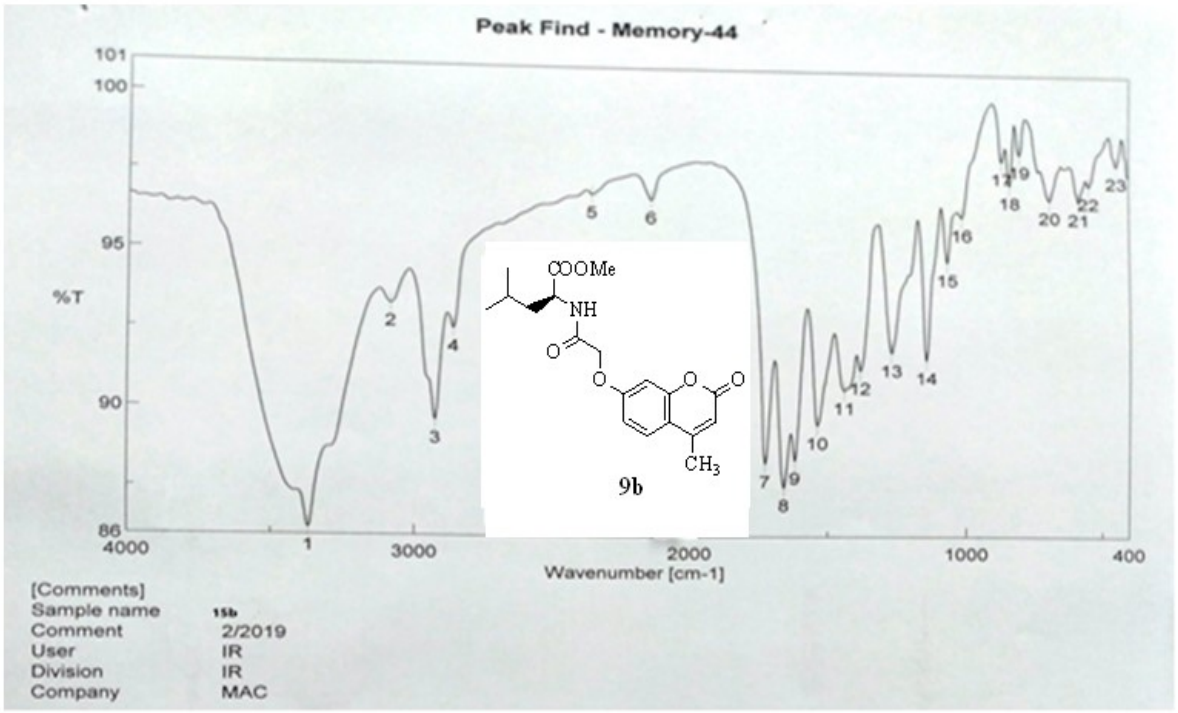

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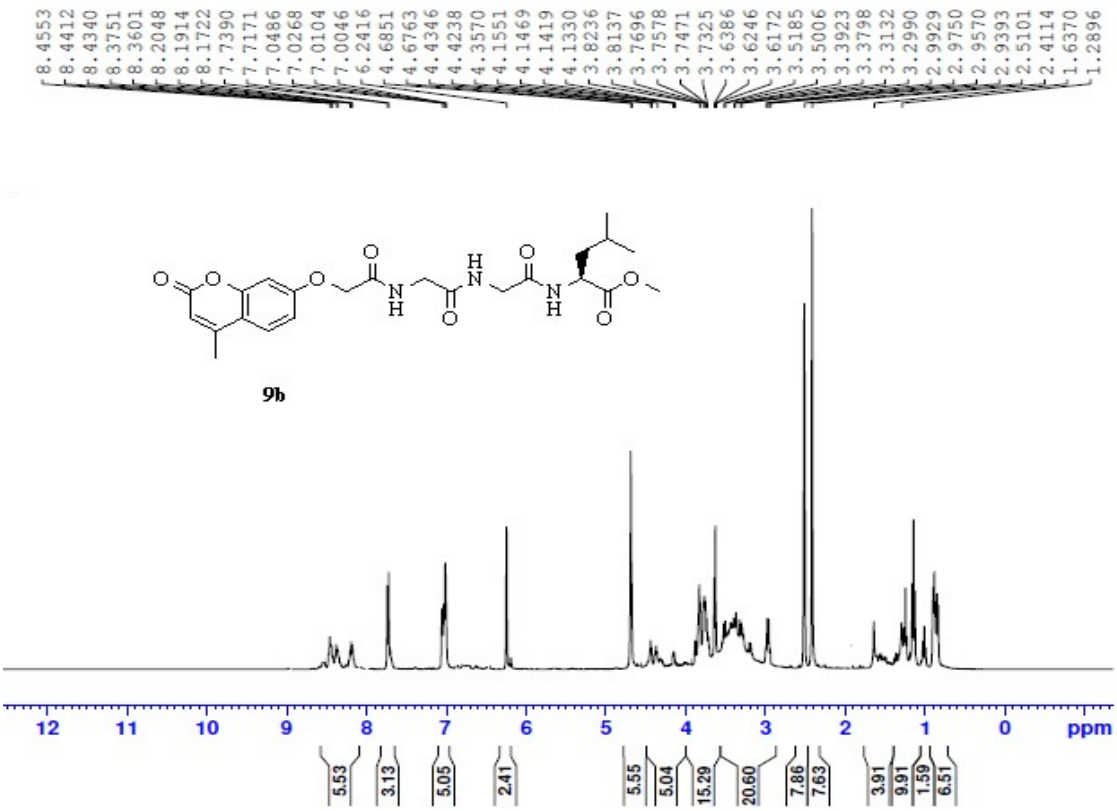

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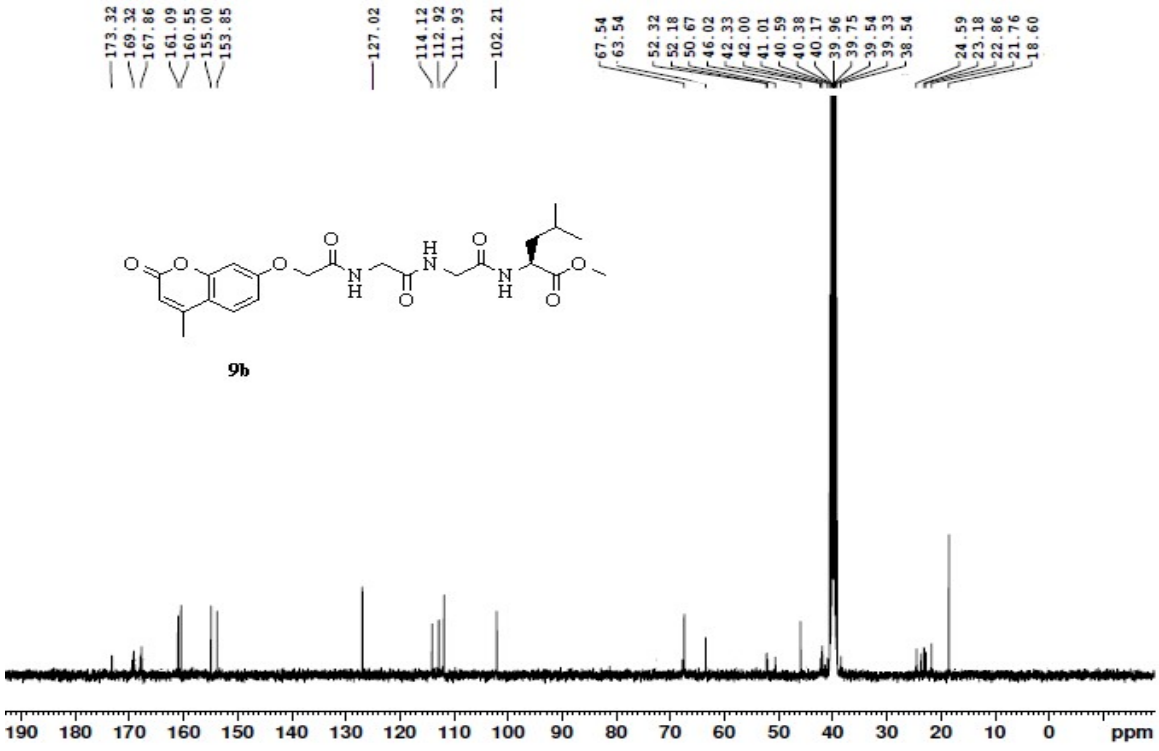

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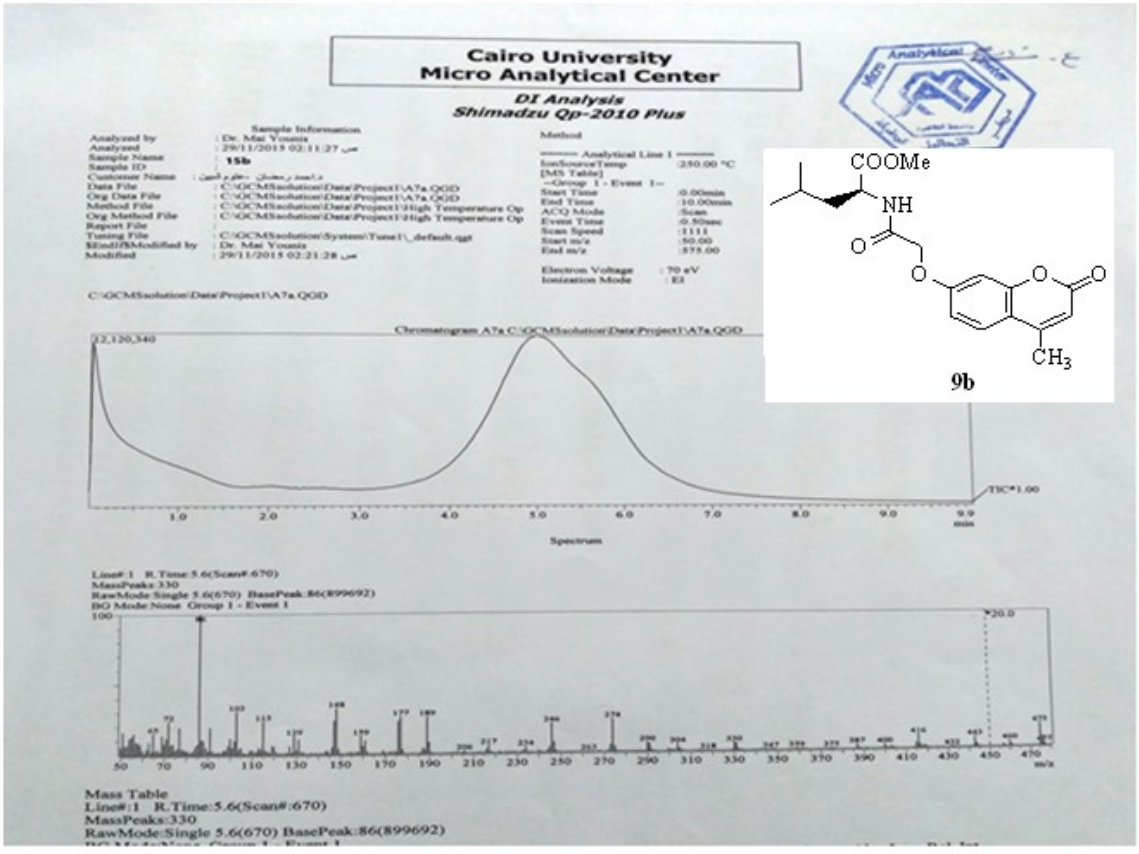

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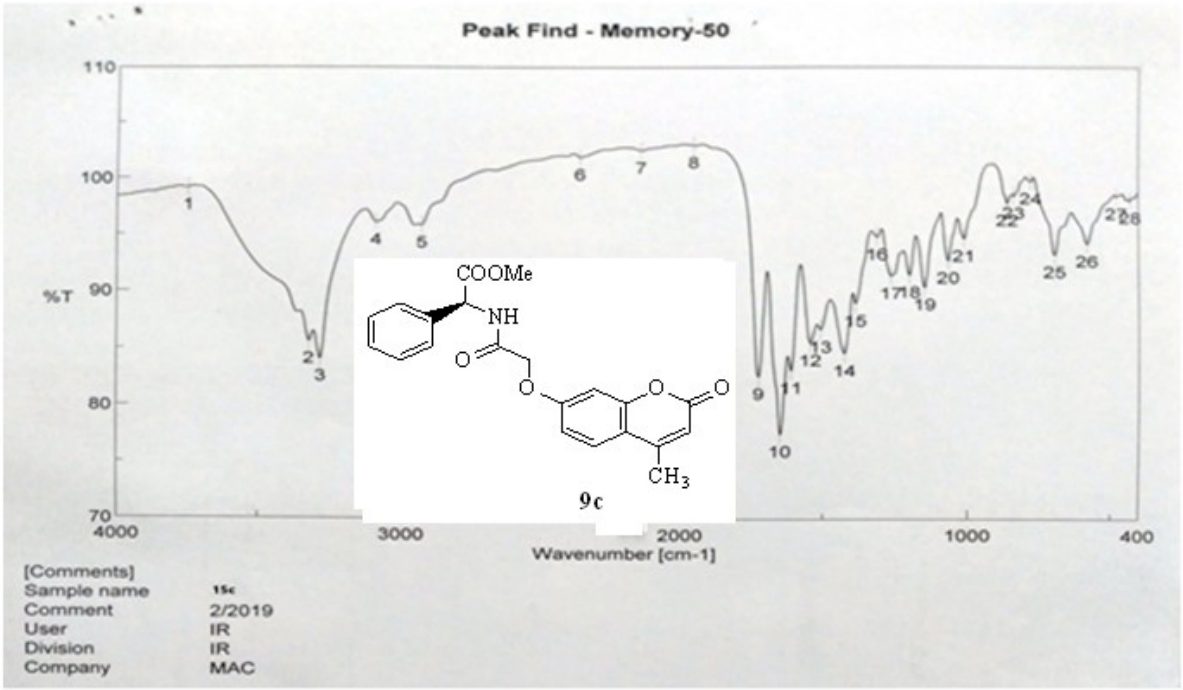

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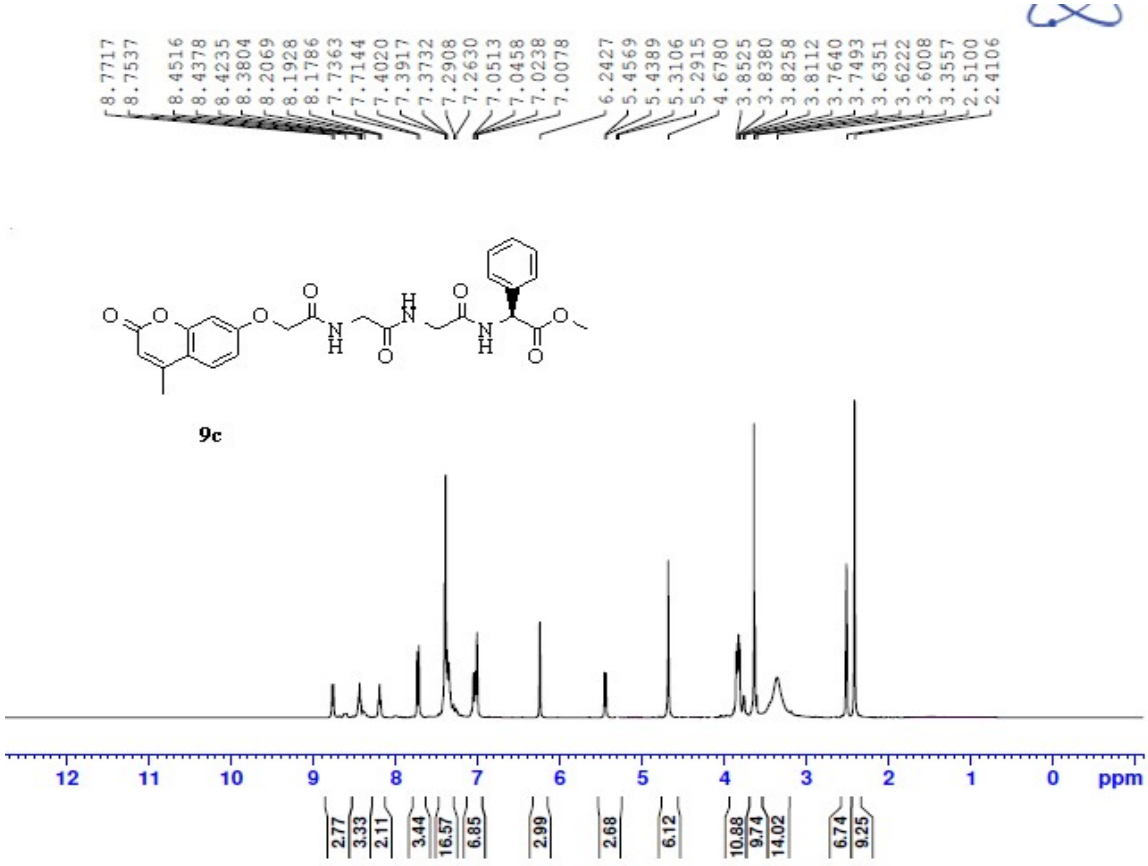

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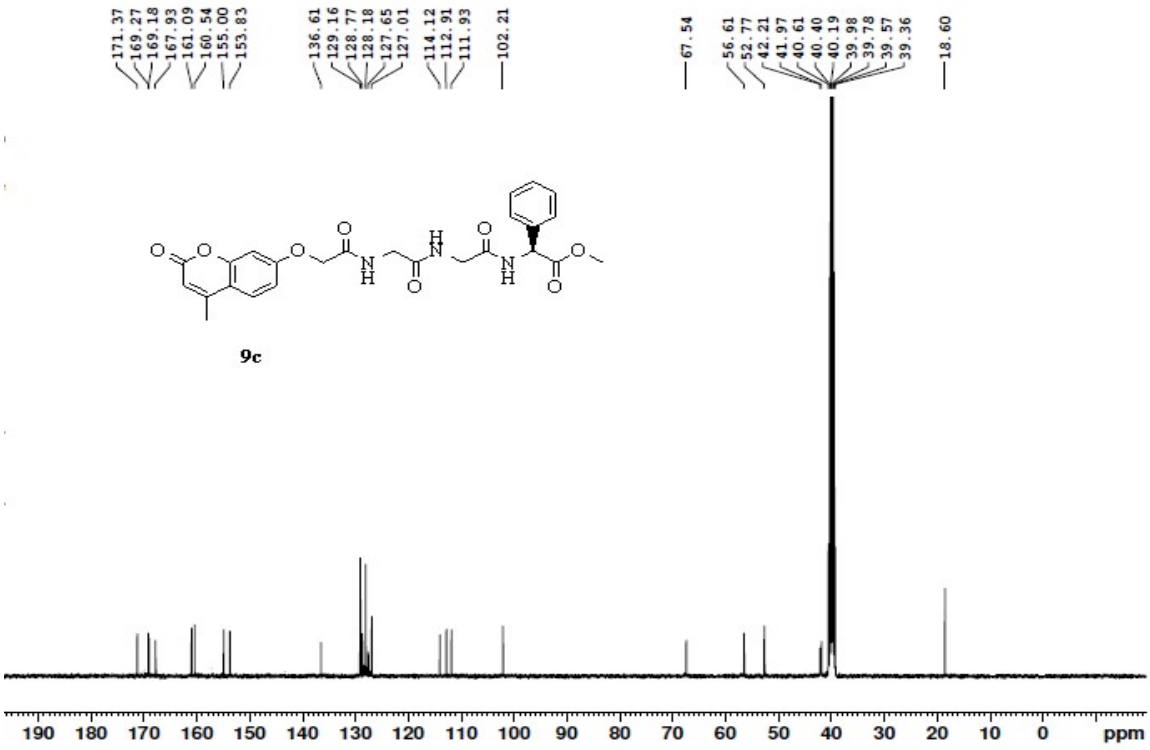

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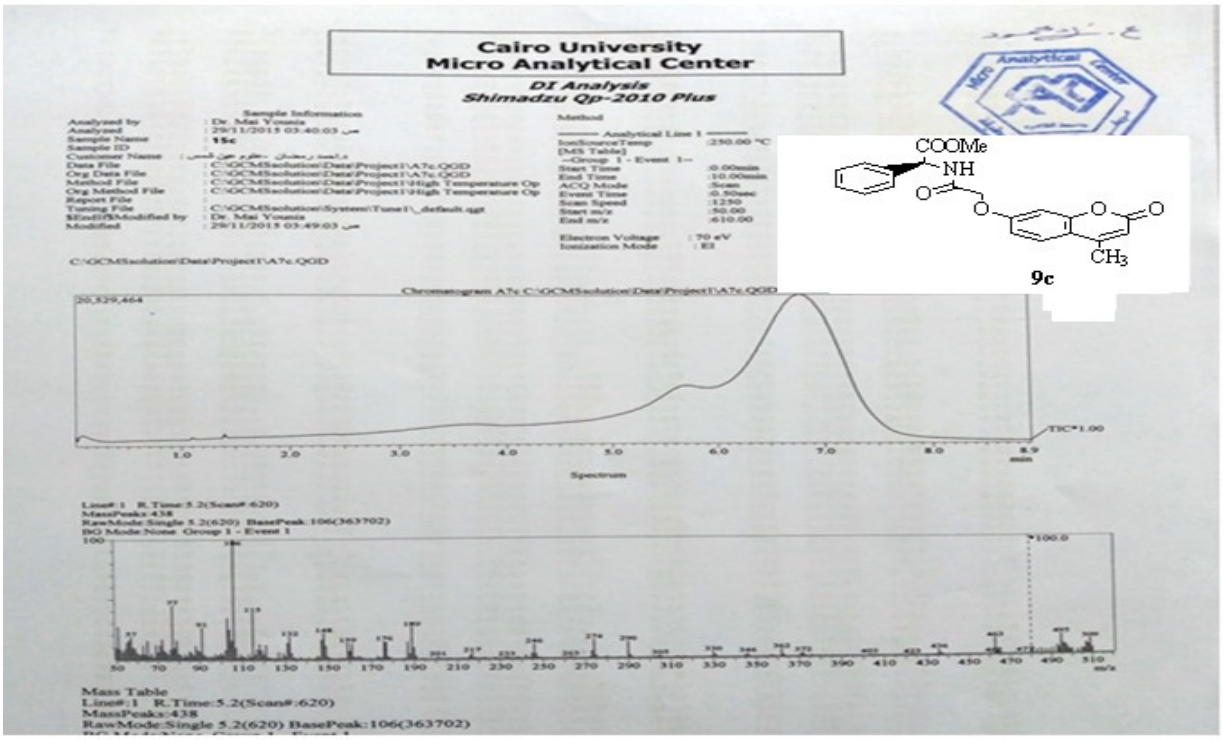

Table (1)

	[a]QPlogs	[b]Caco	[c]Percentage Human/ oral absorption	[d]QPlogKhsa	[e]LogBB	[f]MW	[g]HBD	[h]HBA	[i]QPlog(O/w)	[j]MDCK
5a	-3.646	181.355	64.010	-0.675	-1.579	305.287	0.250	7.000	0.770	144.494
5b	-3.646	199.349	81.479	-0.182	-1.548	361.394	0.250	7.000	2.410	140.667
5c	-4.417	155.169	81.879	-0.101	-1.557	381.384	0.250	7.000	2.331	133.414
6	-4.417	213.401	42.985	-0.809	-1.098	305.290	0.250	7.000	2.685	187.87
7a	-2.343	13.956	48.247	-0.971	-2.662	362.338	0.500	8.750	0.139	17.540
7b	-3.478	25.835	62.284	-0.471	-2.575	418.446	0.500	8.750	1.719	35.052
7c	-4.246	31.876	65.625	-0.407	-2.432	438.436	0.500	8.750	2.009	39.495
8	-2.077	31.762	23.323	-1.133	-2.437	362.341	3.500	9.750	-1.257	39.340
9a	-2.164	3.161	19.983	-1.288	-3.526	419.390	0.750	10.500	-0.504	6.110
9b	-3.497	3.481	29.567	-0.774	-3.709	475.497	0.750	10.500	1.005	8.221
9c	-4.058	2.585	28.675	-0.689	-3.821	495.488	0.750	10.500	1.248	6.389

[a]Predicted aqueous solubility; log S in mol/L (acceptable range; -6.5-0.5), [b]Predicted apparent Caco-2 cell permeability in nm/sec; (<25% is poor and >500% is great), [c]percentage of human oral absorption; (<25% is poor and >80% is high), [d]prediction of binding to human serum albumin; (acceptable range; -1.0-1.5), [e]prediction of brain/blood; (acceptable range; -3.0-1.2), [f]molecular weight (<500), [g]Hydrogen bond donor (<5), [h]Hydrogen bond acceptor (<10), [i]Prediction octanol/water partition coefficient lop p (acceptable range; -2.0-6.5), [j]Prediction apparent MDCK cell permeability in nm/sec; (<25% is poor and >500% is great), ADME; Absorption, distribution, metabolism and excretion