

Preparation and Characterization of *h*-BN/Fe₃O₄/APTES-AMF/Cu^{II} Nanocomposite as a New and Efficient Catalyst for the One-Pot Three-Component Synthesis of 2-Amino-4-aryl(or heteroaryl)-7,7-dimethyl-5-oxo-5,6,7,8-tetrahydro-4*H*-chromene-3-carbonitriles

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Results and discussion

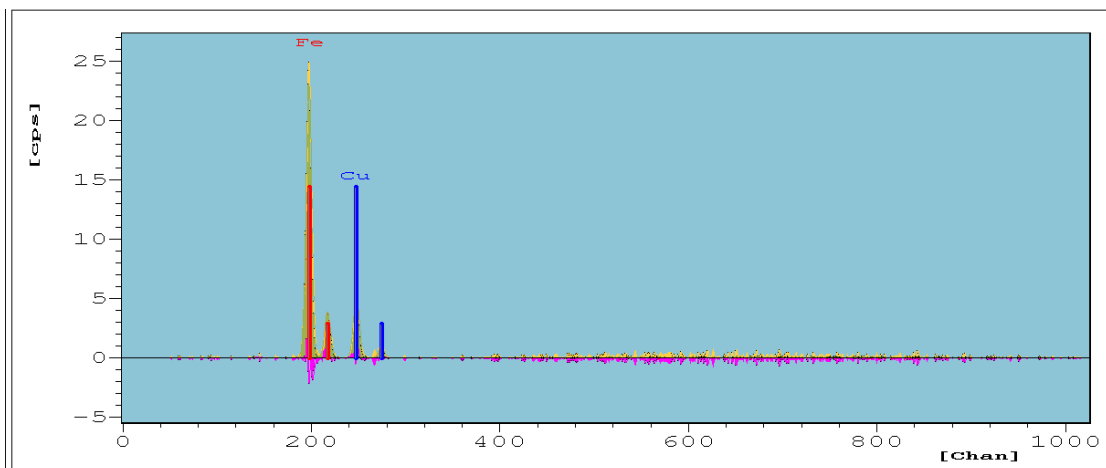


Fig. S1 ED-XRF spectrum of *h*-BN/Fe₃O₄/APTES-AMF/Cu^{II}.

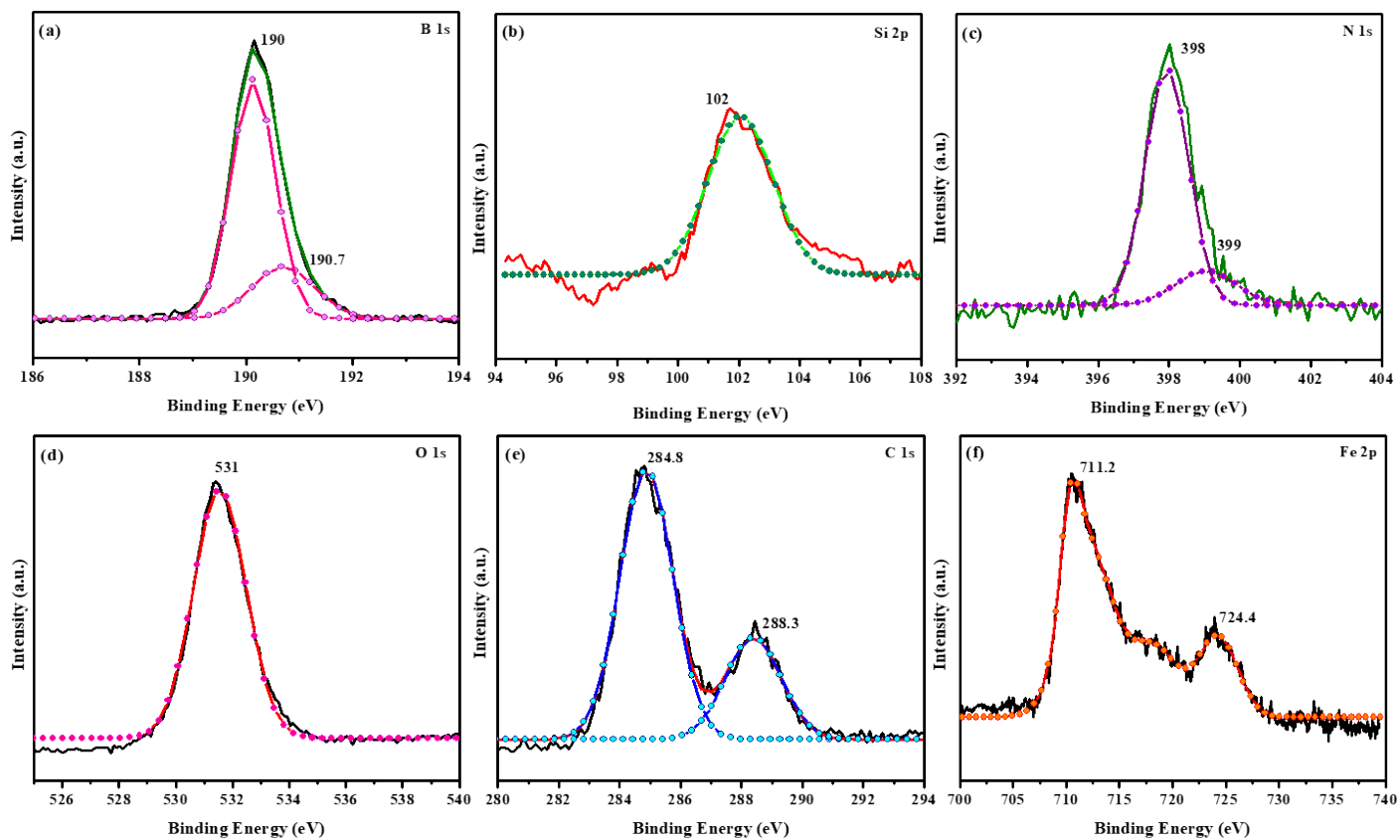
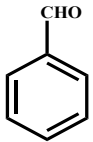
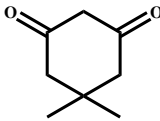

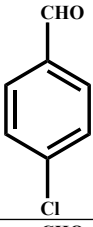
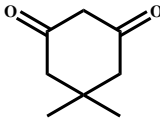

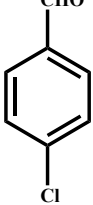
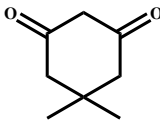

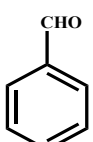
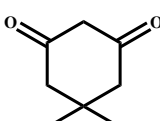
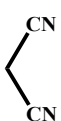
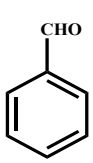
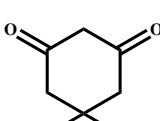

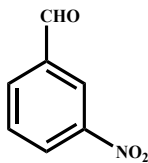
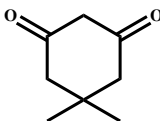

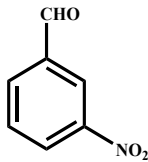
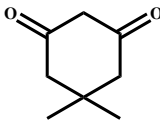

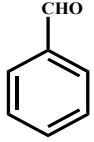
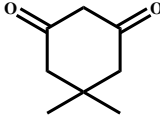

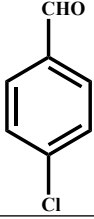
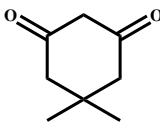

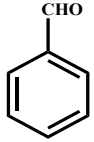
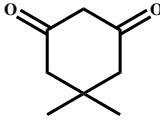

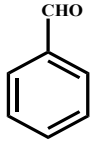
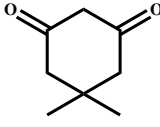



Fig. S2 Core level XPS spectra of (a) B 1s, (b) Si 2p, (c) N 1s, (d) O 1s, (e) C 1s and (f) Fe 2p.

Table S1 Comparison of the catalytic activity of *h*-BN/Fe₃O₄/APTES-AMF/Cu^{II} nanocatalyst with previously reported catalysts for the synthesis of 2-amino-4-aryl(or heteroaryl)-7,7-dimethyl-5-oxo-5,6,7,8-tetrahydro-4*H*-chromene-3-carbonitriles.

S.No.	Aromatic aldehyde	Dimedone	Malononitrile	Reaction conditions	Yield (%)	TOF (min ⁻¹)	Ref.
1.				CuFe ₂ O ₄ , EtOH, 60 °C, 8 min	93	–	58
2.				Sodium alginate, EtOH, reflux, 50 min	93	0.186	59
3.				<i>h</i> -BN/Fe ₃ O ₄ /APTES-AMF/Cu ^{II} , ethanol-water (1:1), r.t., 15 min	97	64.9	PW
4.				Ag ₃ [PMo ₁₂ O ₄₀], EtOH/H ₂ O, reflux, 90 min	97	–	60
5.				PC/AgNPs, H ₂ O/EtOH, reflux, 35 min	82	–	61
6.				[Cu(bpdo) ₂ .2H ₂ O] ²⁺ / _{montmorillonit} , H ₂ O/EtOH, reflux, 25 min	97	19.4	62

7.				<i>h</i> - BN/Fe ₃ O ₄ /APTE S-AMF/Cu ^{II} , ethanol-water (1:1), r.t., 15 min	97	64.9	PW
8.				Ni@Fe doped CeO ₂ chitosan, EtOH, 60 °C, 10 min	90	–	63
9.				MNPs-PhSO ₃ H, H ₂ O/EtOH, 100 °C, 15 min	90	–	64
10.				Bi-Su, H ₂ O/EtOH, 80 °C, 35 min	84	–	65
11.				<i>h</i> - BN/Fe ₃ O ₄ /APTE S-AMF/Cu ^{II} , ethanol-water (1:1), r.t., 15 min	98	65.6	PW

Catalyst recyclability test

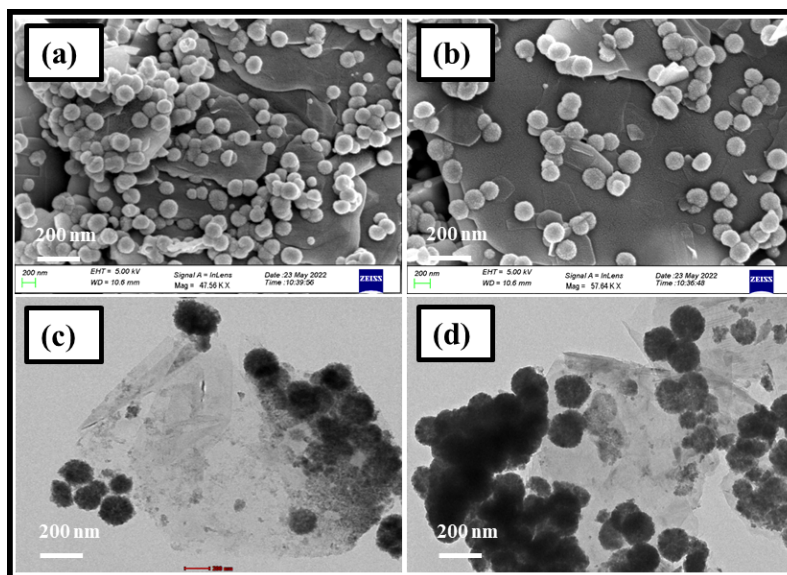


Fig. S3 FESEM micrographs of (a) fresh catalyst, (b) recovered catalyst after sixth cycle and TEM images of (c) fresh catalyst, (d) recovered catalyst after sixth run.

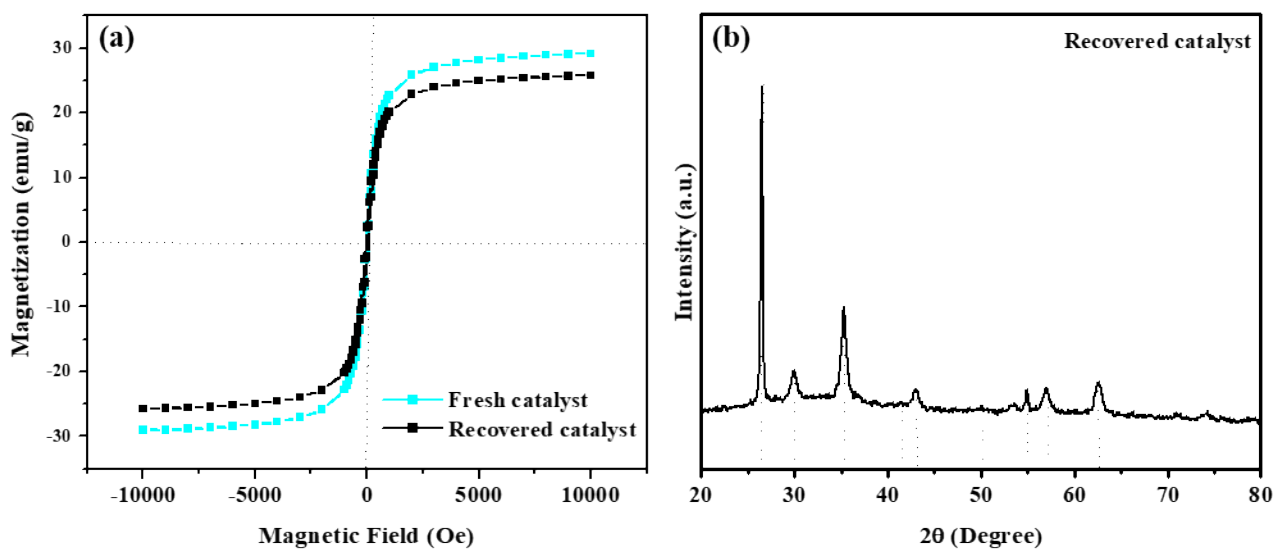
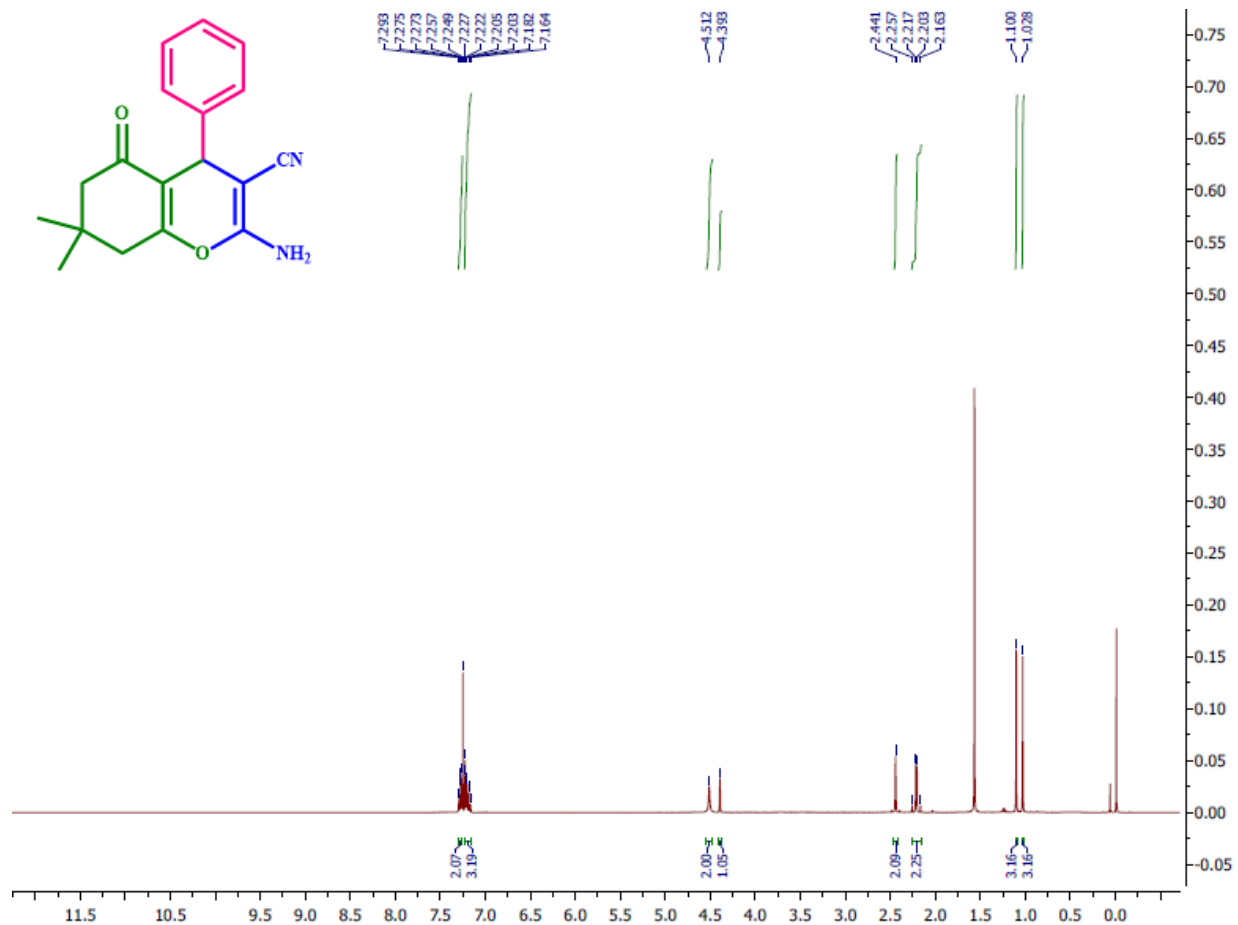


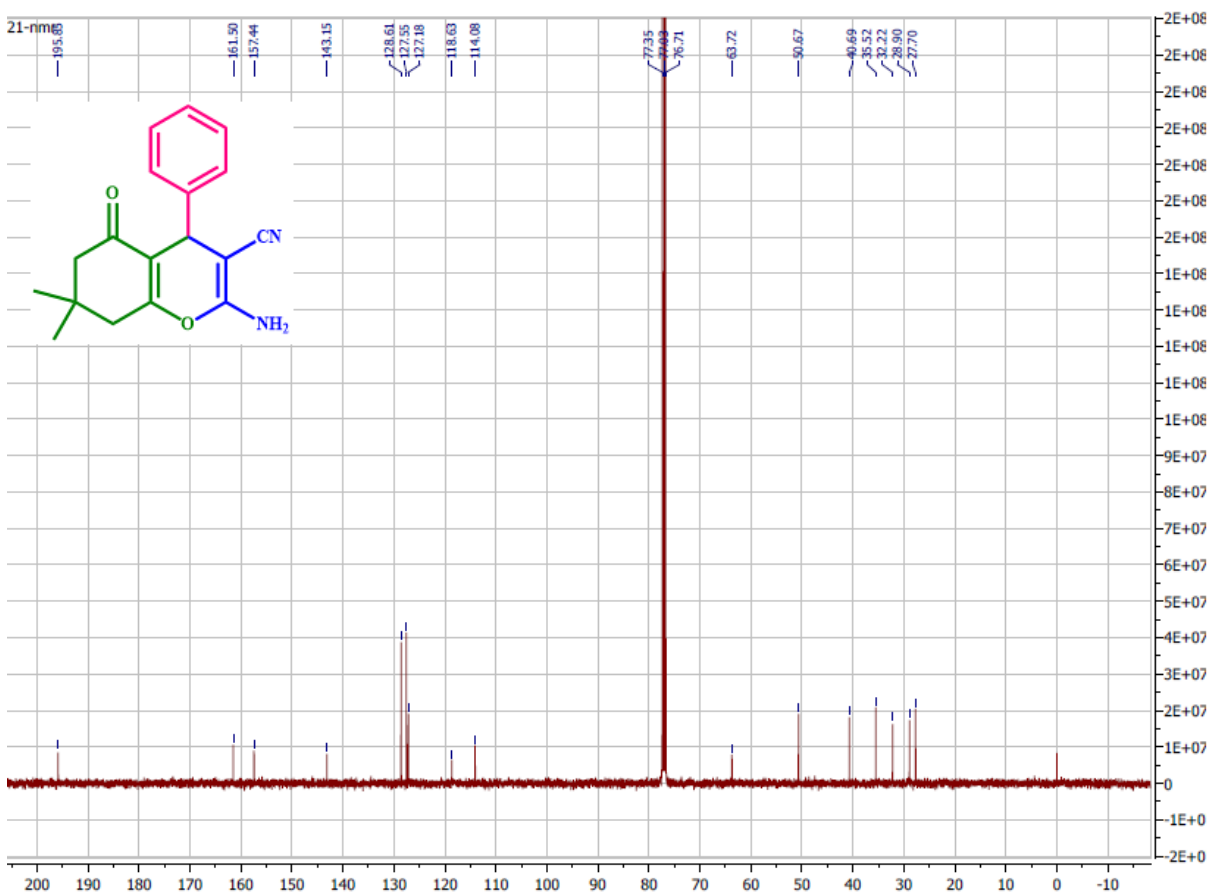
Fig. S4 (a) VSM and (b) XRD spectra of recovered h -BN/Fe₃O₄/APTES-AMF/Cu^{II} catalyst.

^1H and ^{13}C NMR spectra of 2-amino-4-aryl(or heteroaryl)-7,7-dimethyl-5-oxo-5,6,7,8-tetrahydro-4H-chromene-3-carbonitriles (4a-4o)

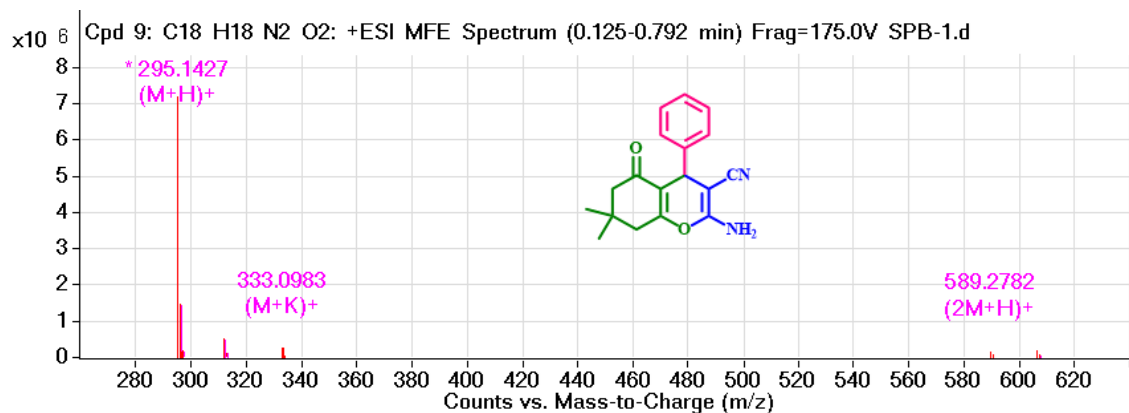
^1H NMR of 2-amino-4-phenyl-7,7-dimethyl-5-oxo-5,6,7,8-tetrahydro-4H-chromene-3-carbonitrile (4a)



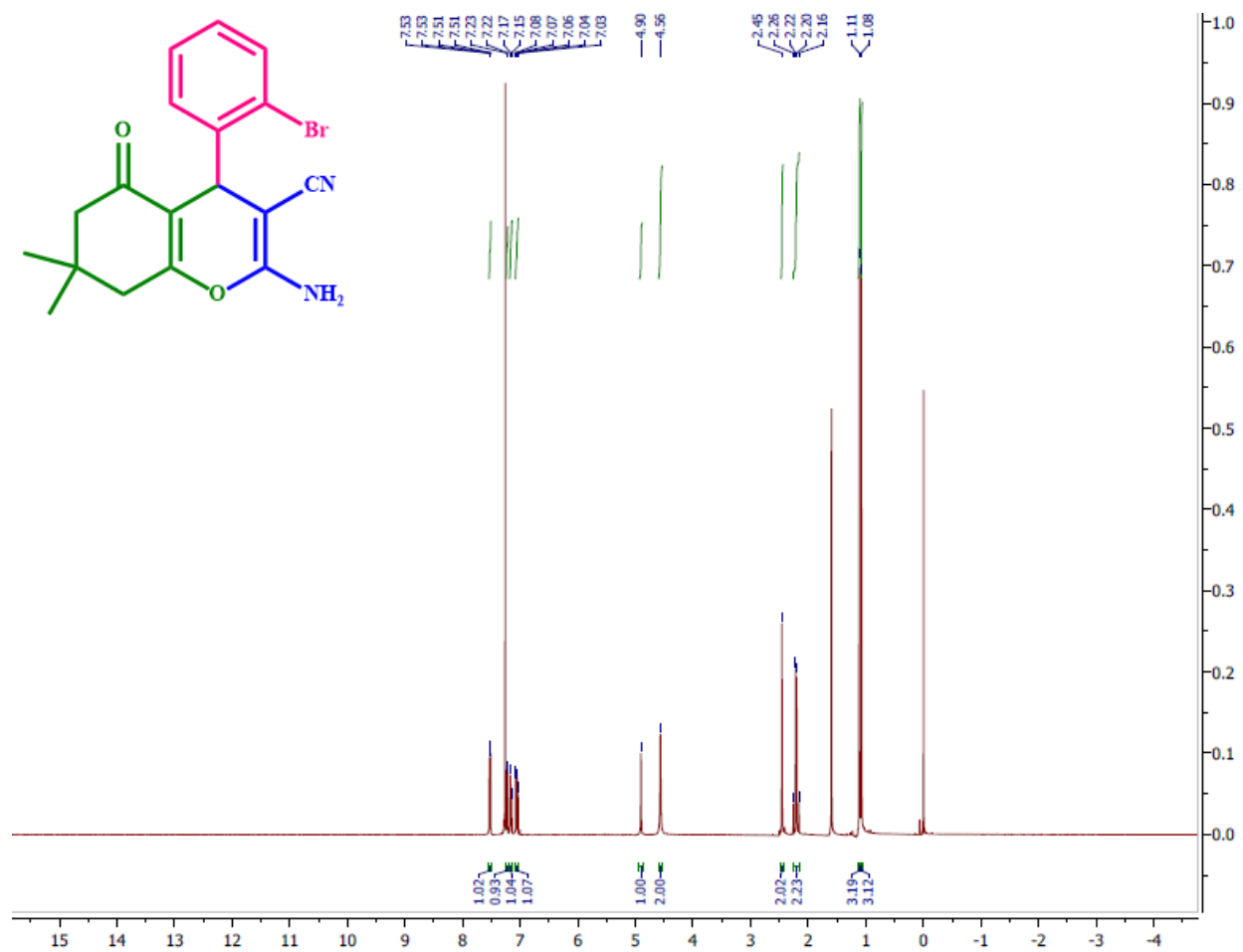
^{13}C NMR of 2-amino-4-phenyl-7,7-dimethyl-5-oxo-5,6,7,8-tetrahydro-4*H*-chromene-3-carbonitrile (4a)



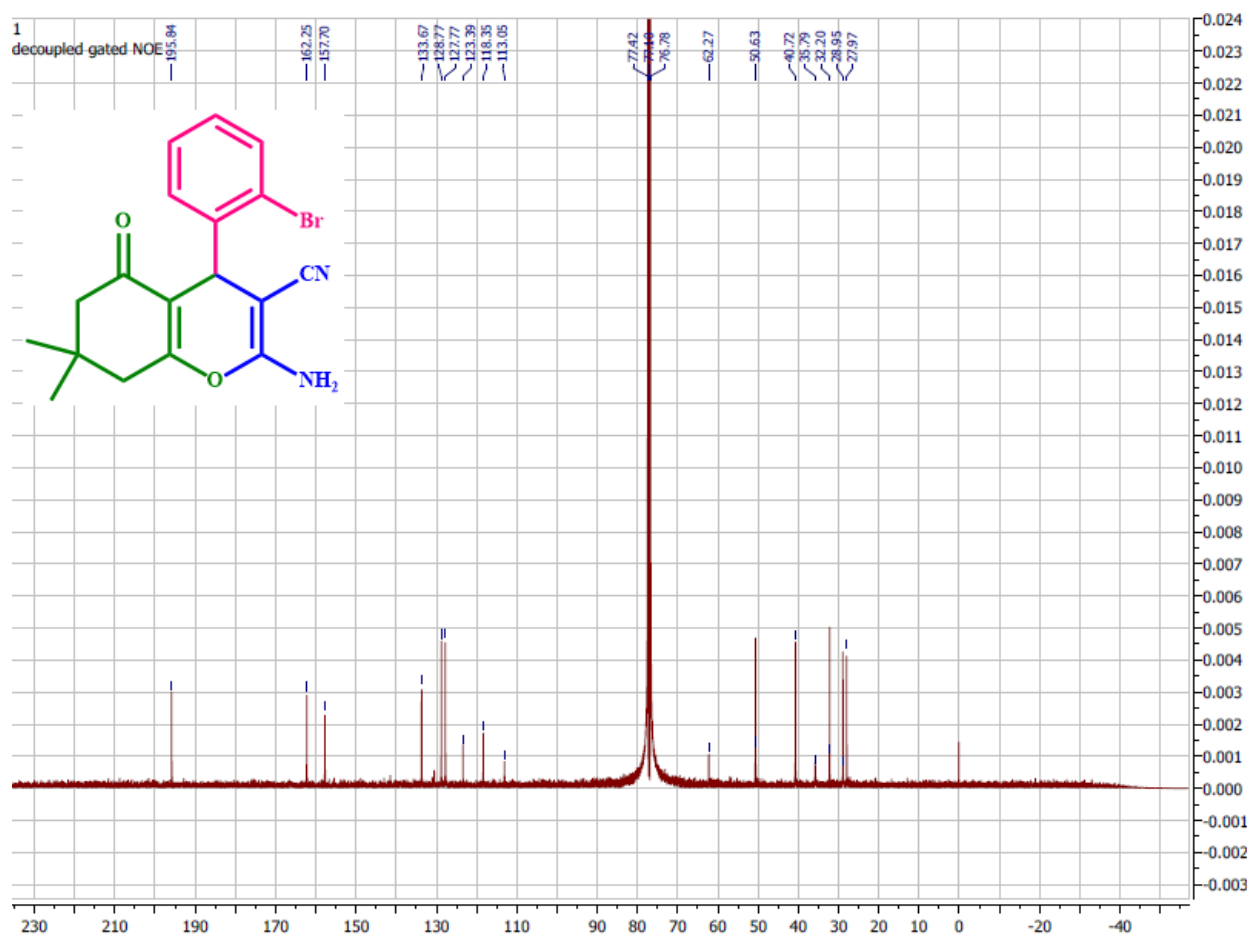
HRMS of 2-amino-4-phenyl-7,7-dimethyl-5-oxo-5,6,7,8-tetrahydro-4*H*-chromene-3-carbonitrile (4a)



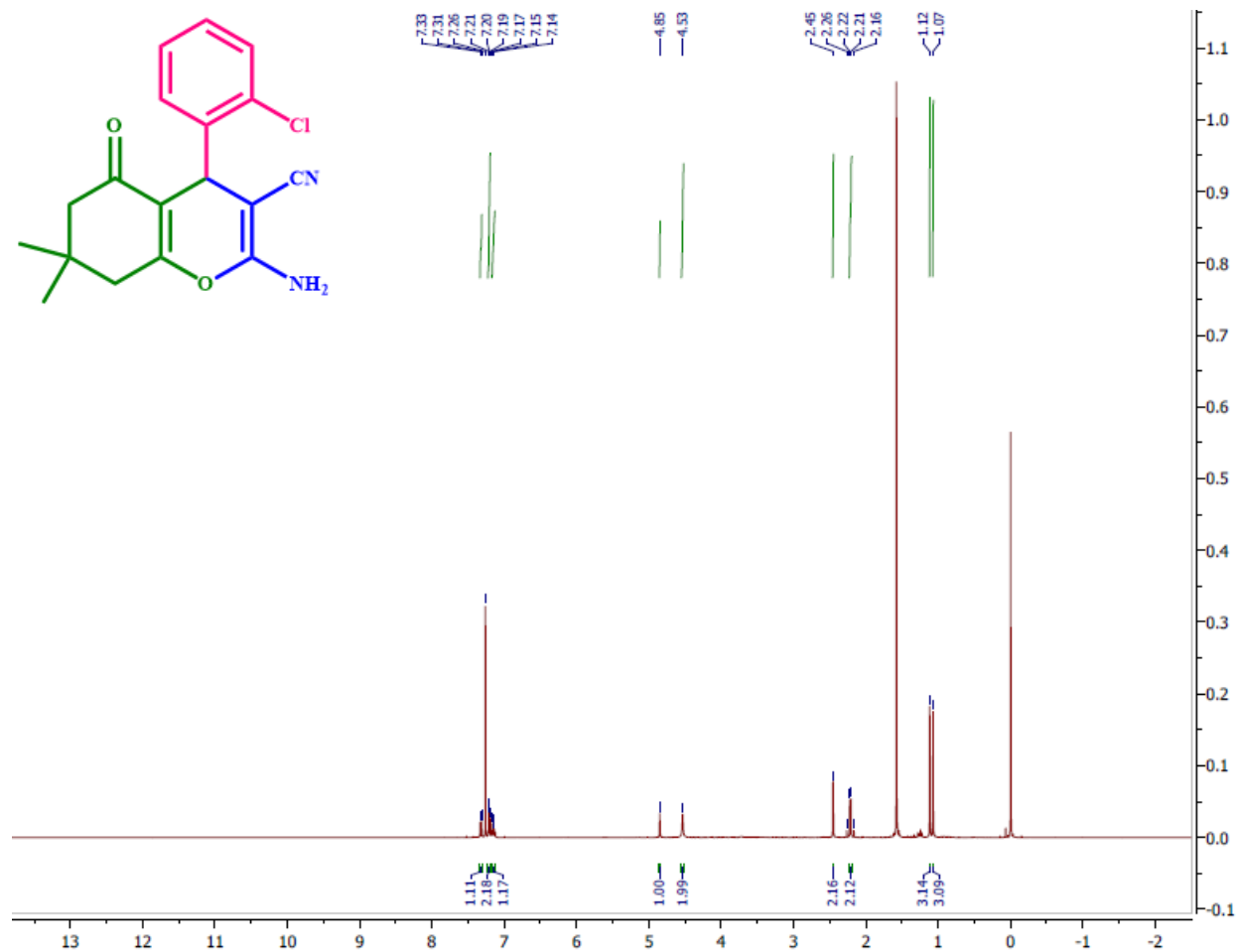
¹H NMR of 2-amino-4-(2-bromophenyl)-7,7-dimethyl-5-oxo-5,6,7,8-tetrahydro-4H-chromene-3-carbonitrile (4b)



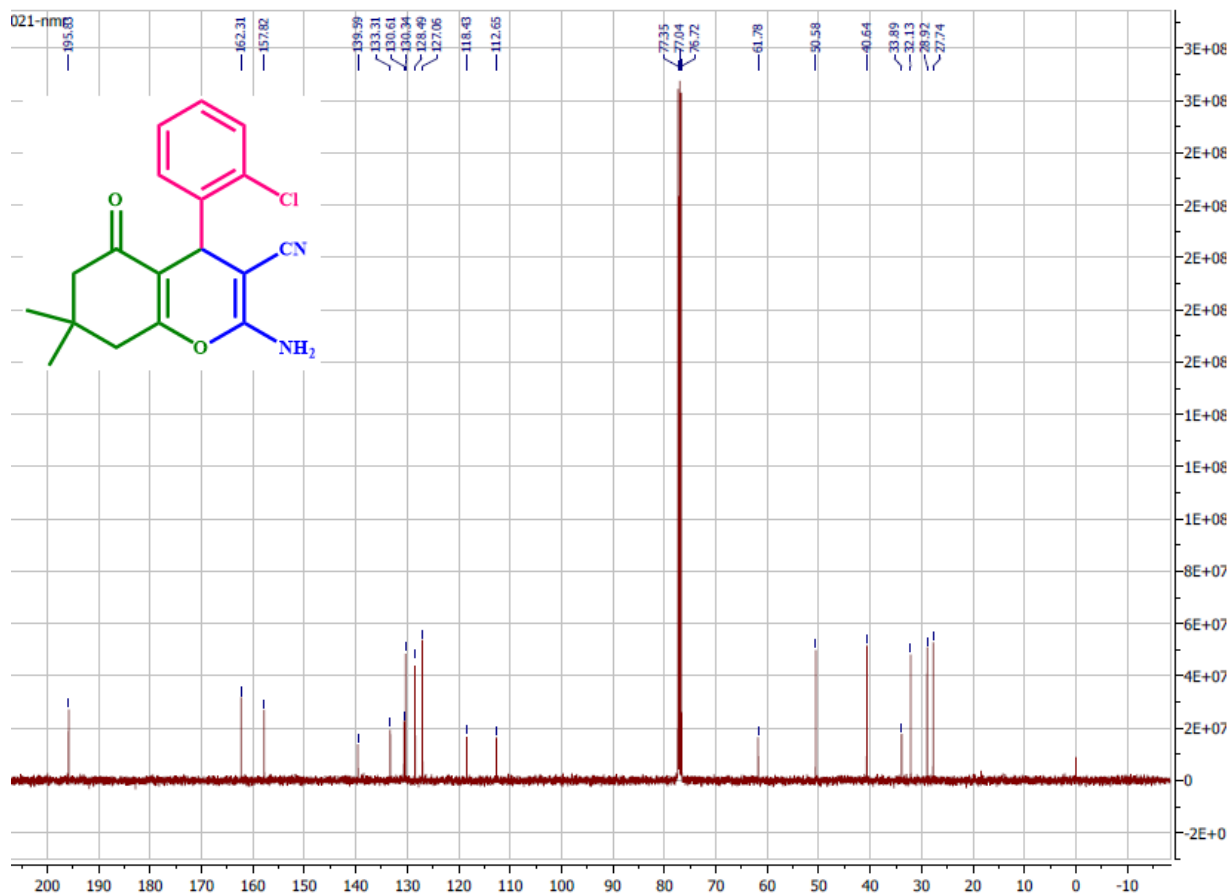
^{13}C NMR of 2-amino-4-(2-bromophenyl)-7,7-dimethyl-5-oxo-5,6,7,8-tetrahydro-4*H*-chromene-3-carbonitrile (4b)



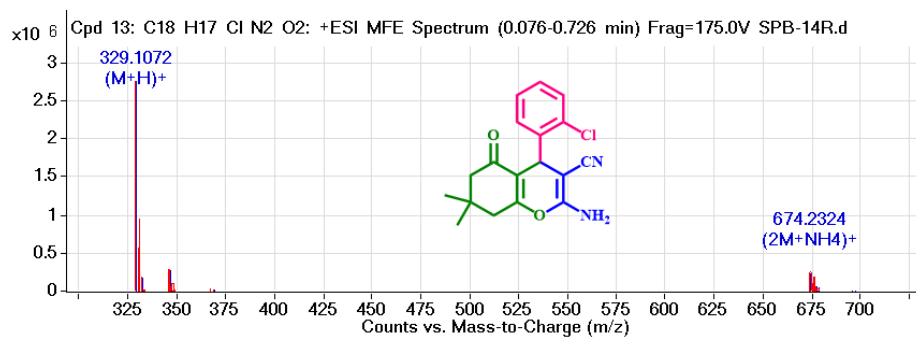
^1H NMR of 2-amino-4-(2-chlorophenyl)-7,7-dimethyl-5-oxo-5,6,7,8-tetrahydro-4*H*-chromene-3-carbonitrile (4c)



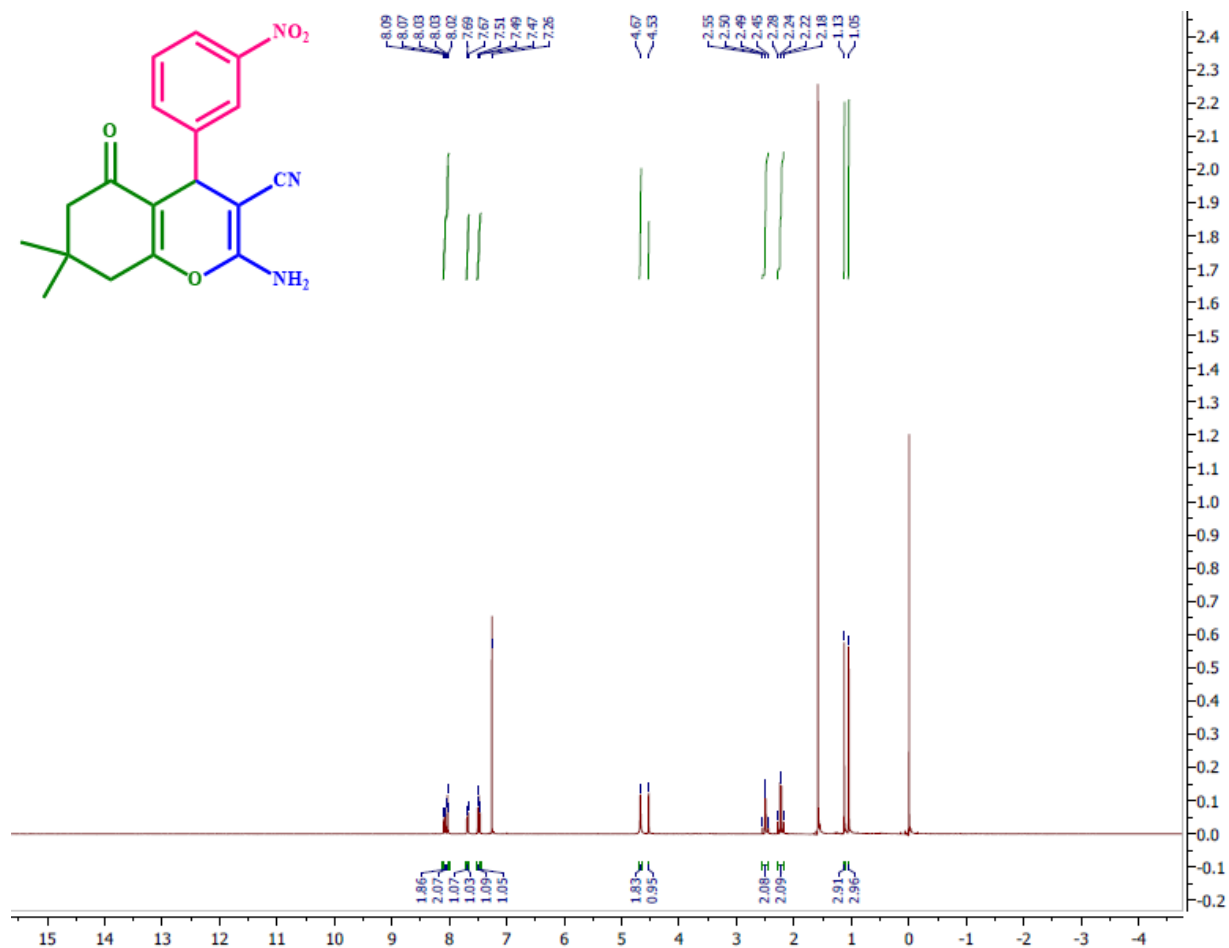
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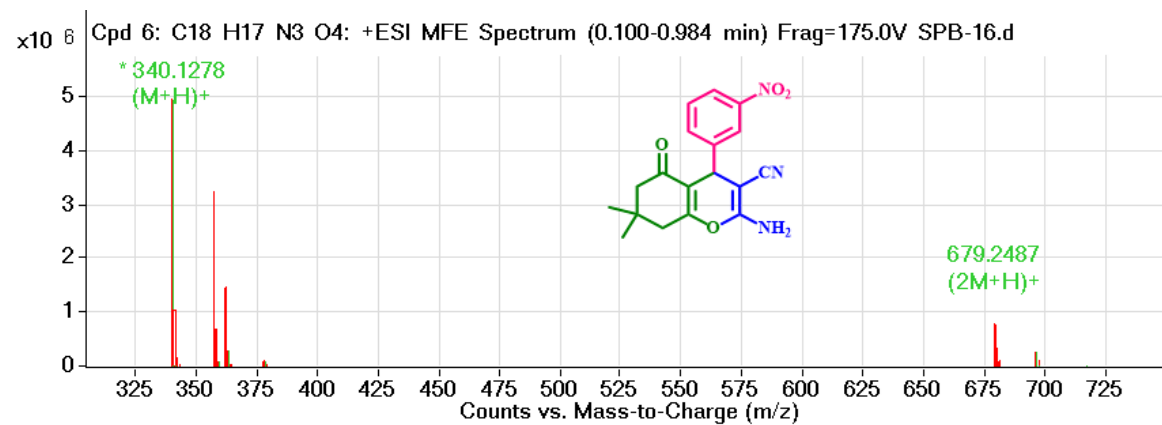
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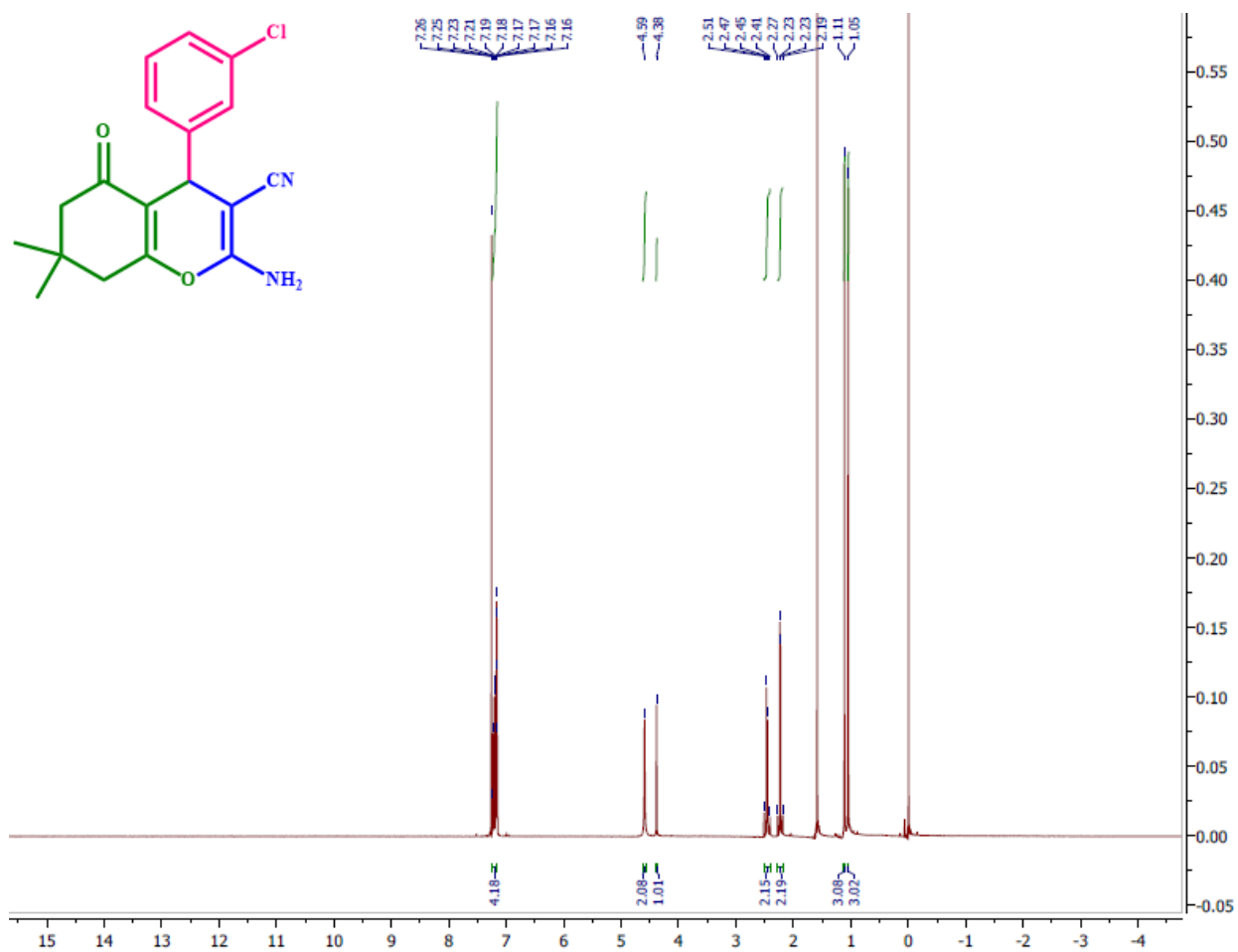
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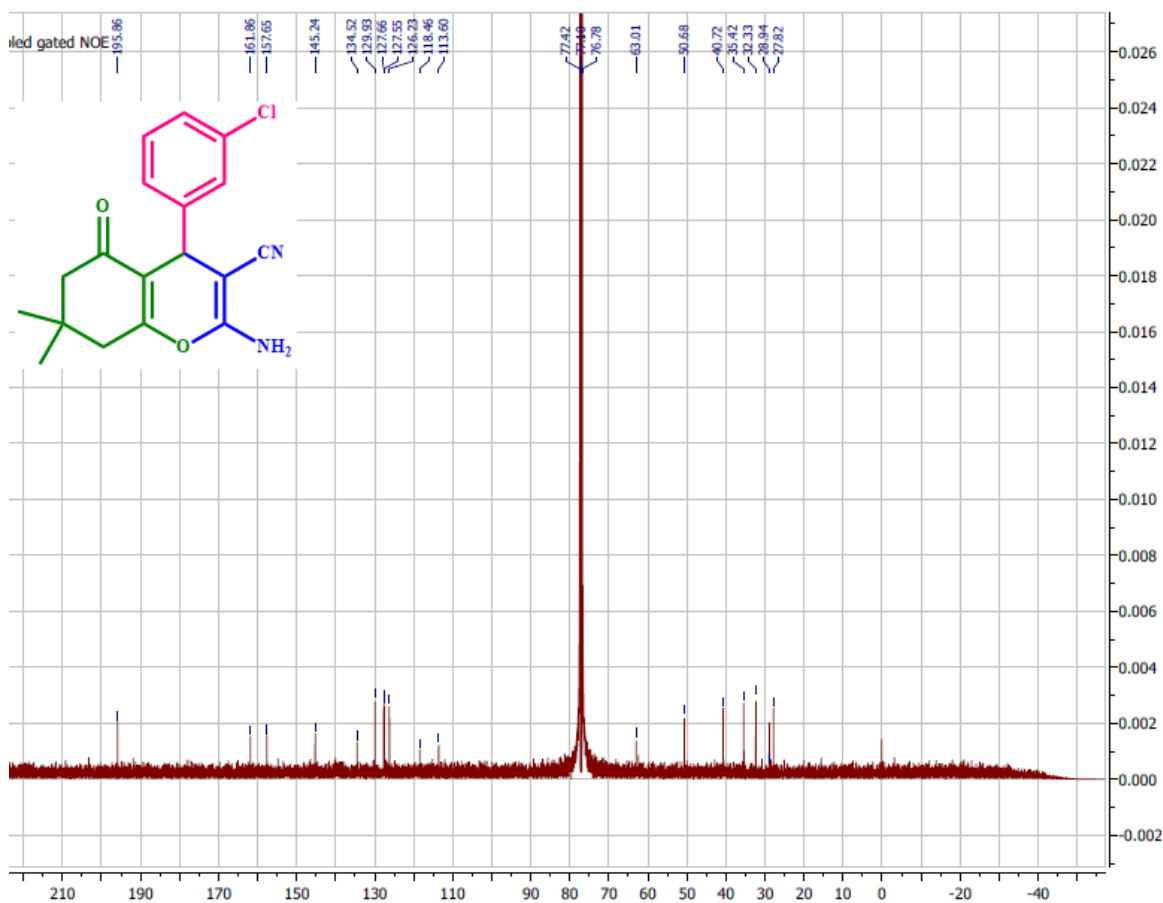
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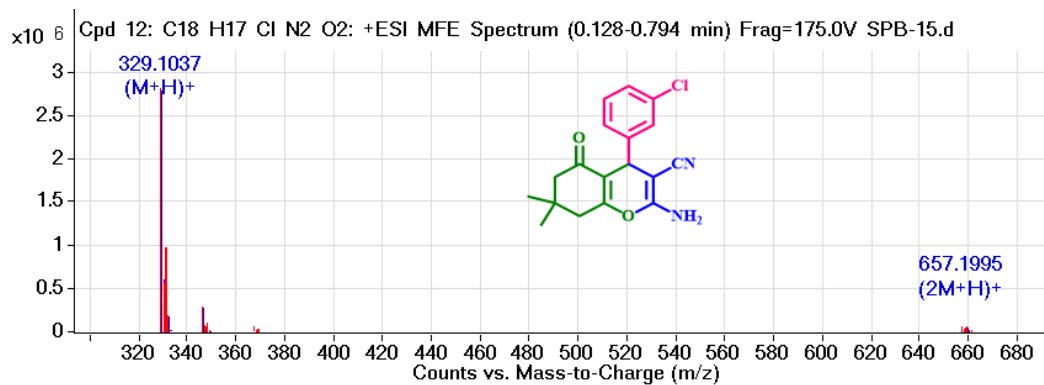
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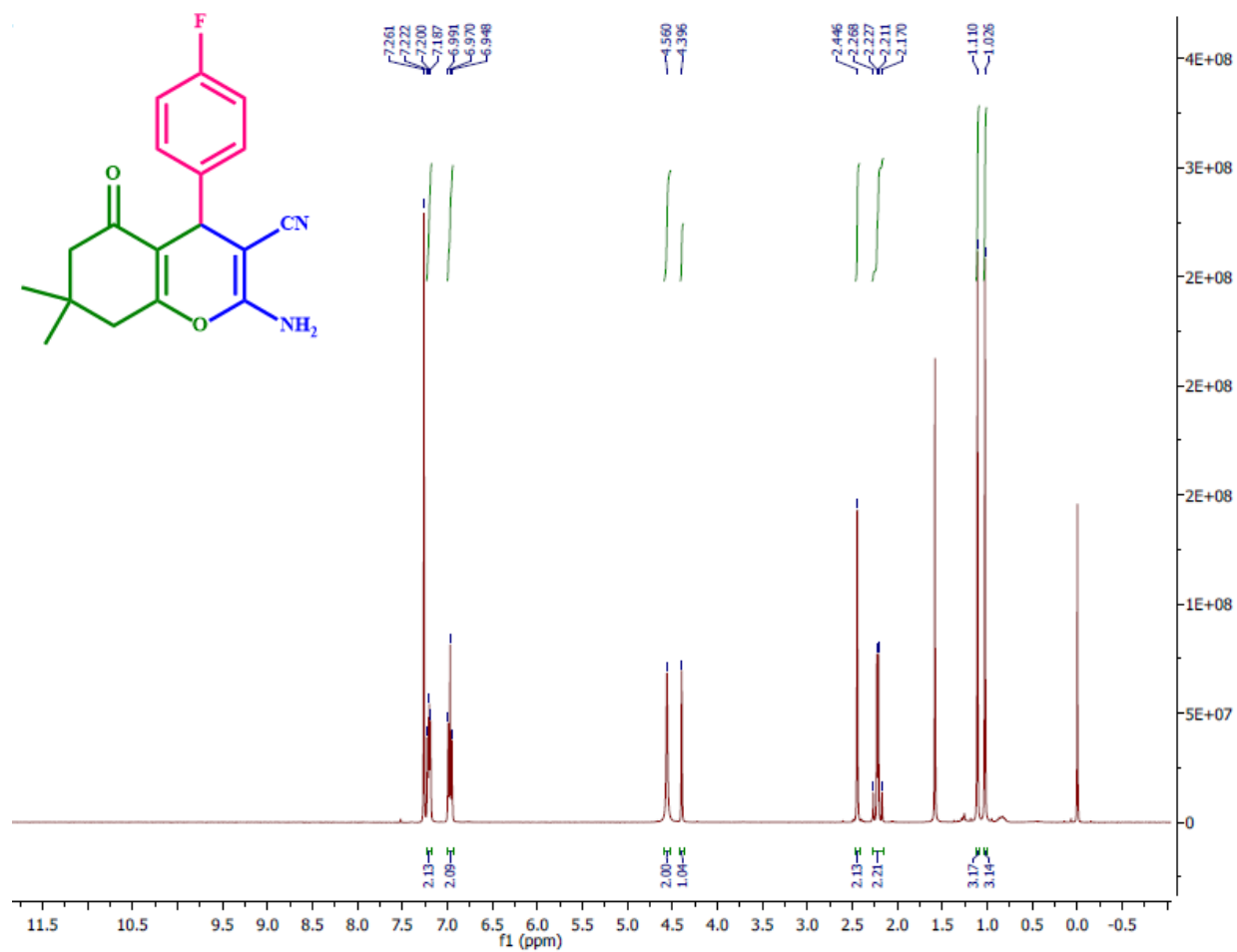
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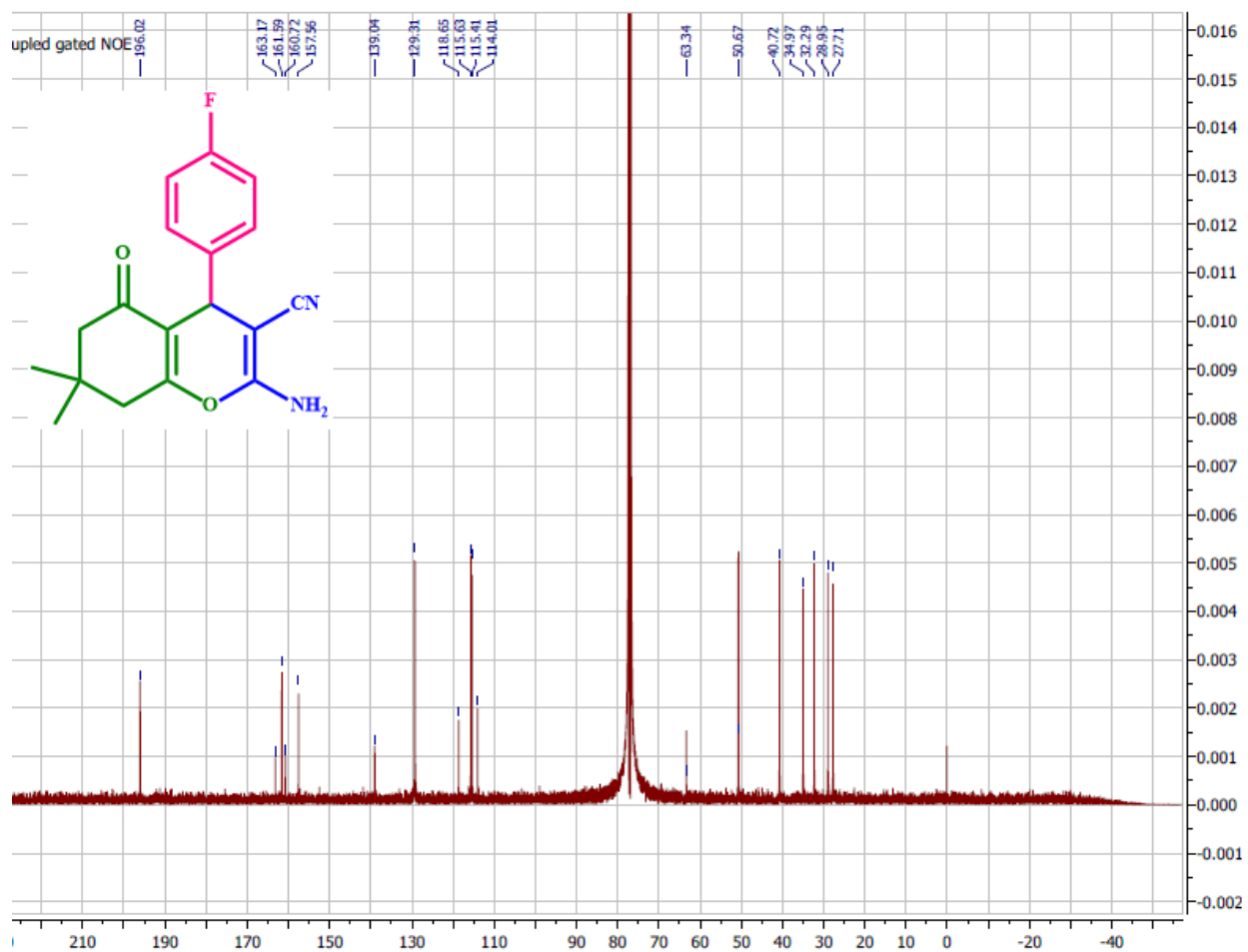
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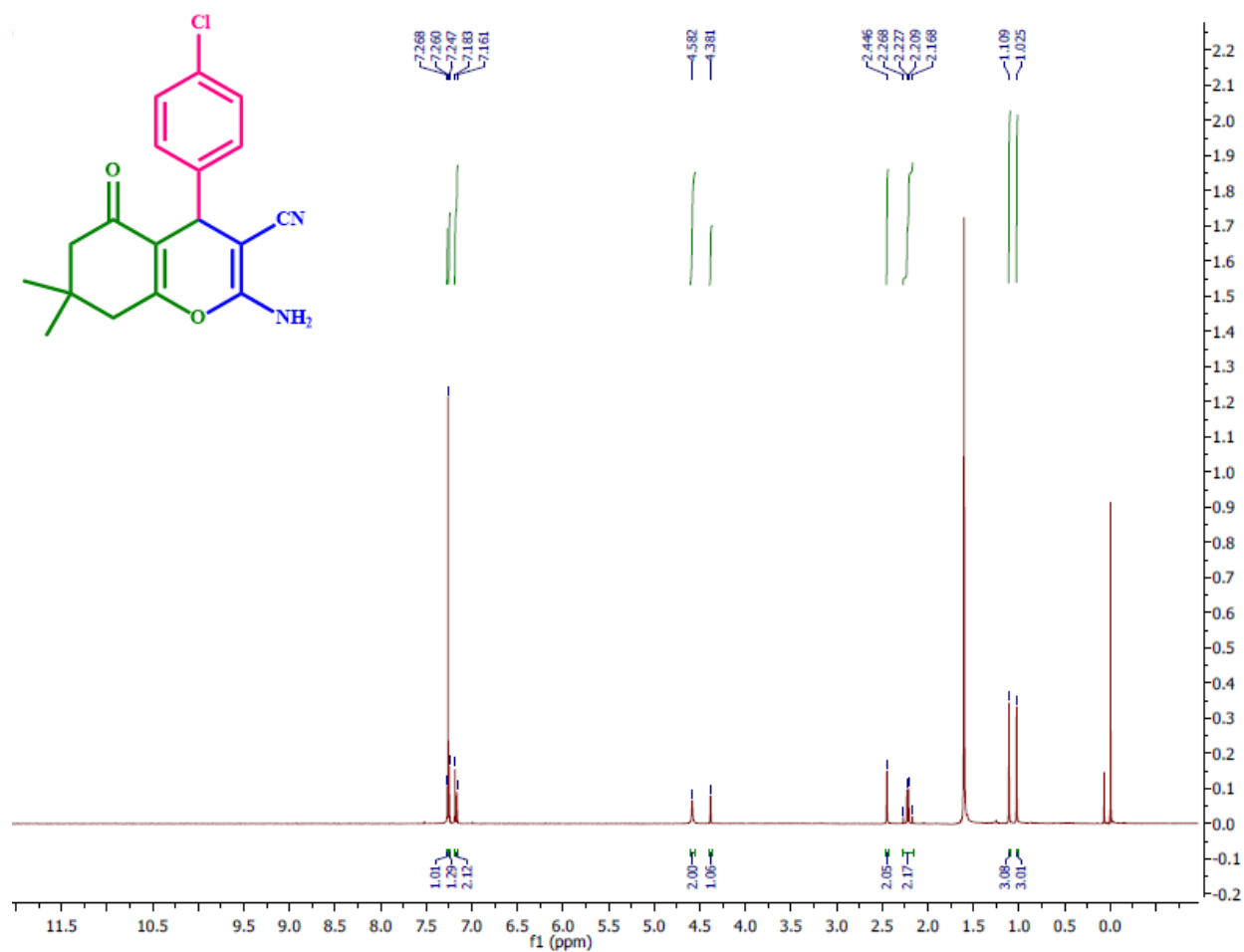
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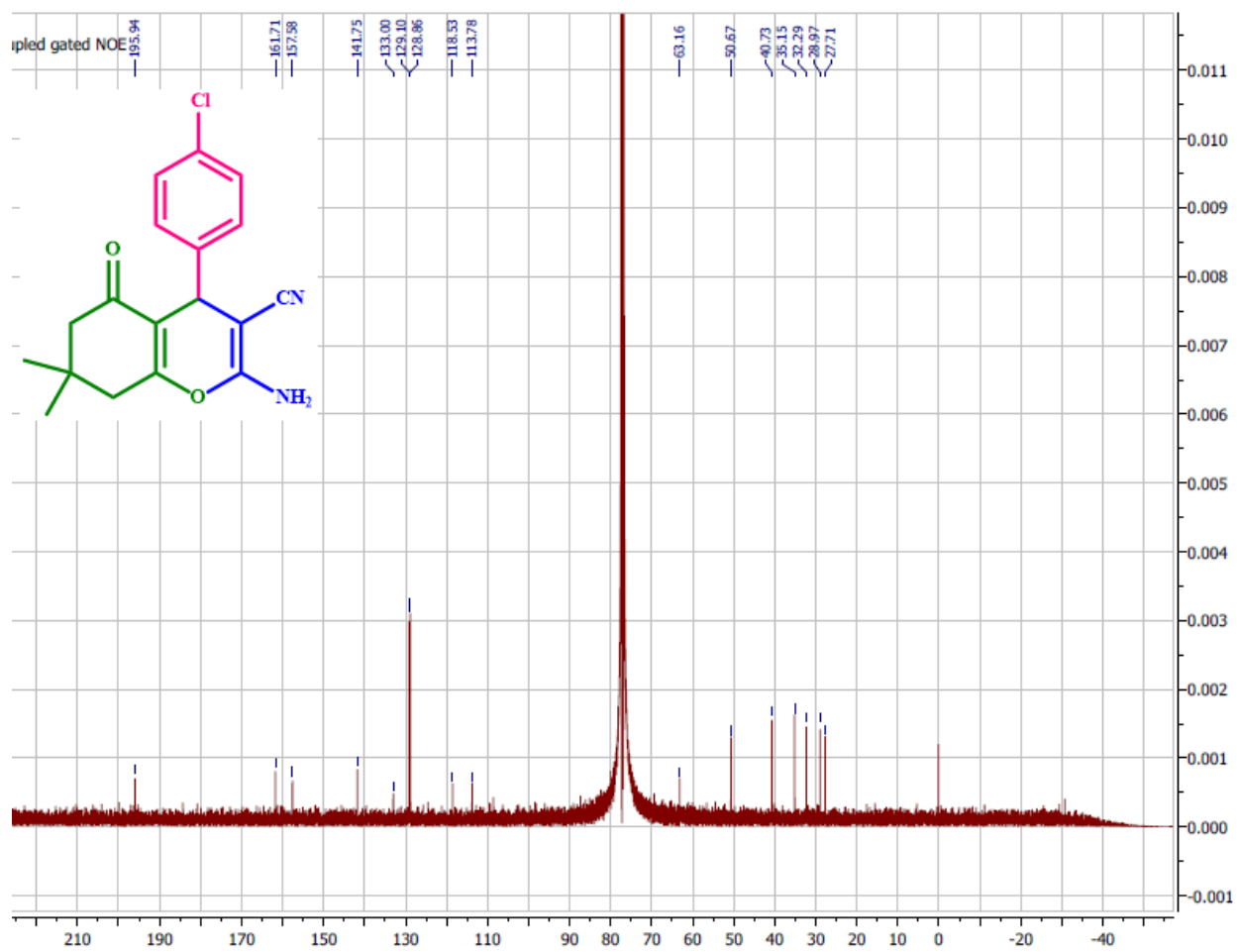
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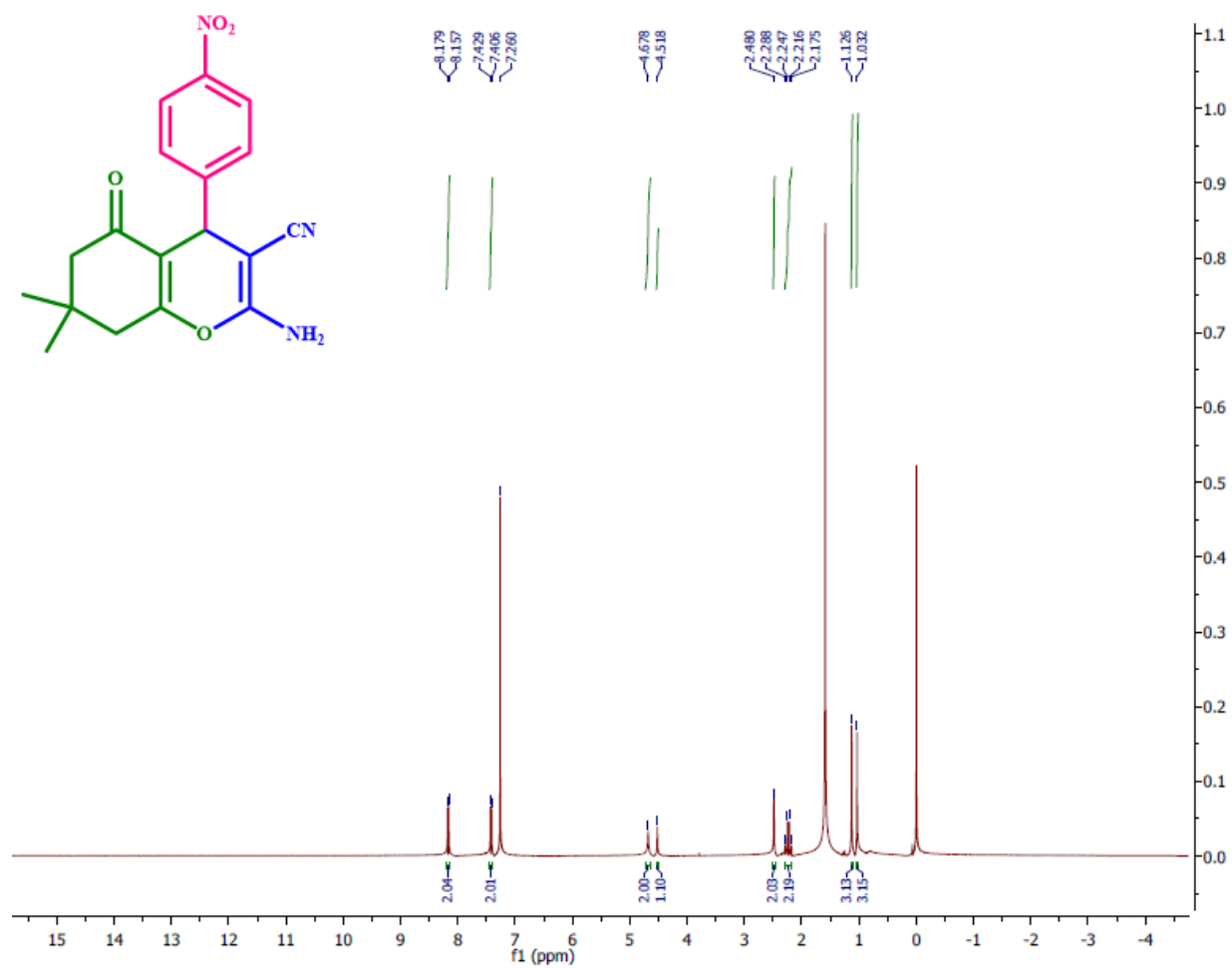
¹H NMR of 2-amino-4-(4-chlorophenyl)-7,7-dimethyl-5-oxo-5,6,7,8-tetrahydro-4*H*-chromene-3-carbonitrile (4g)



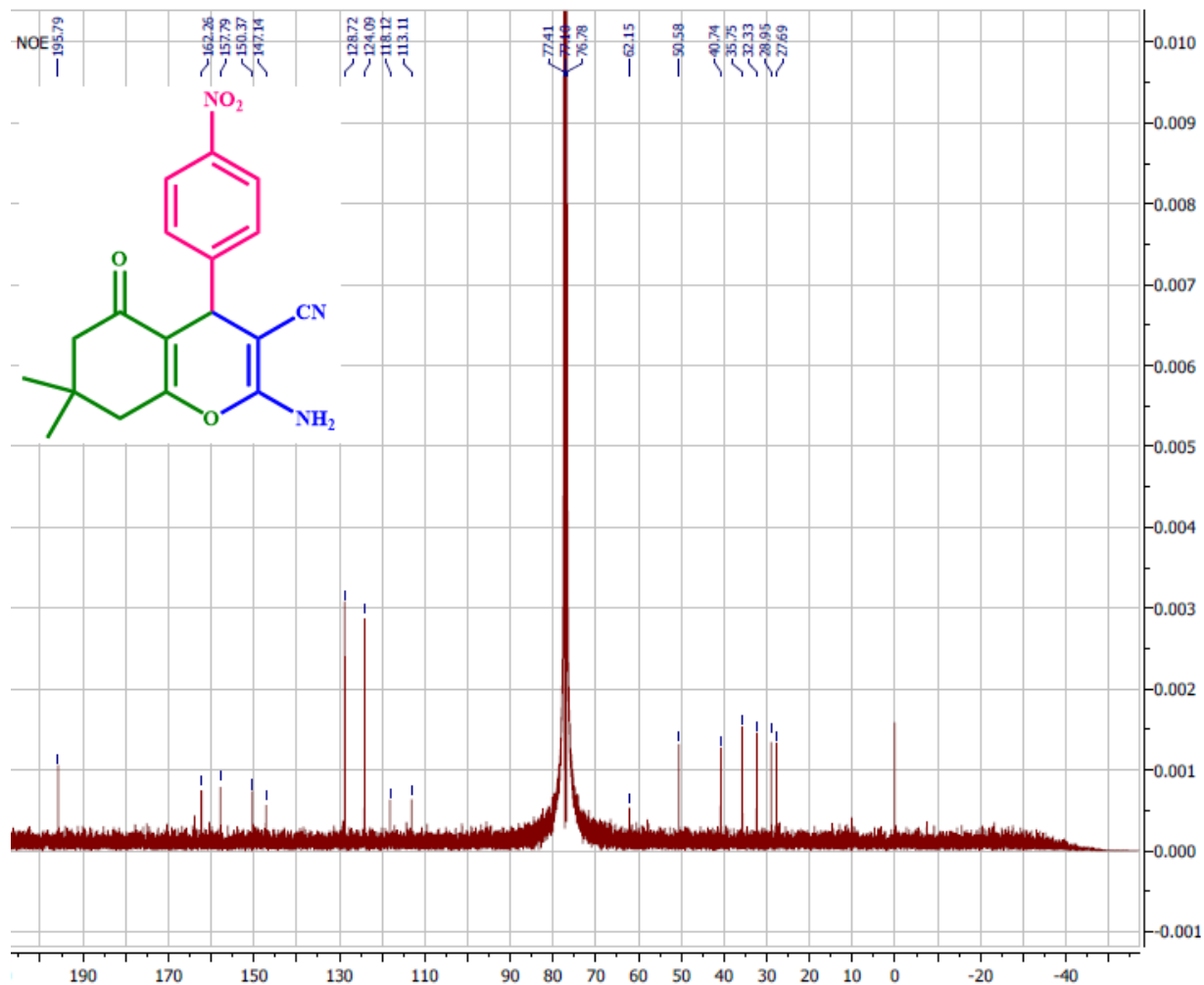
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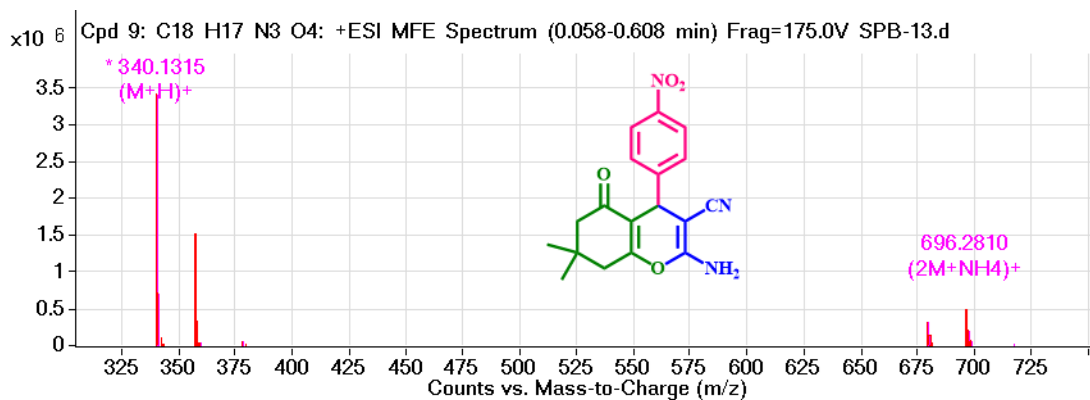
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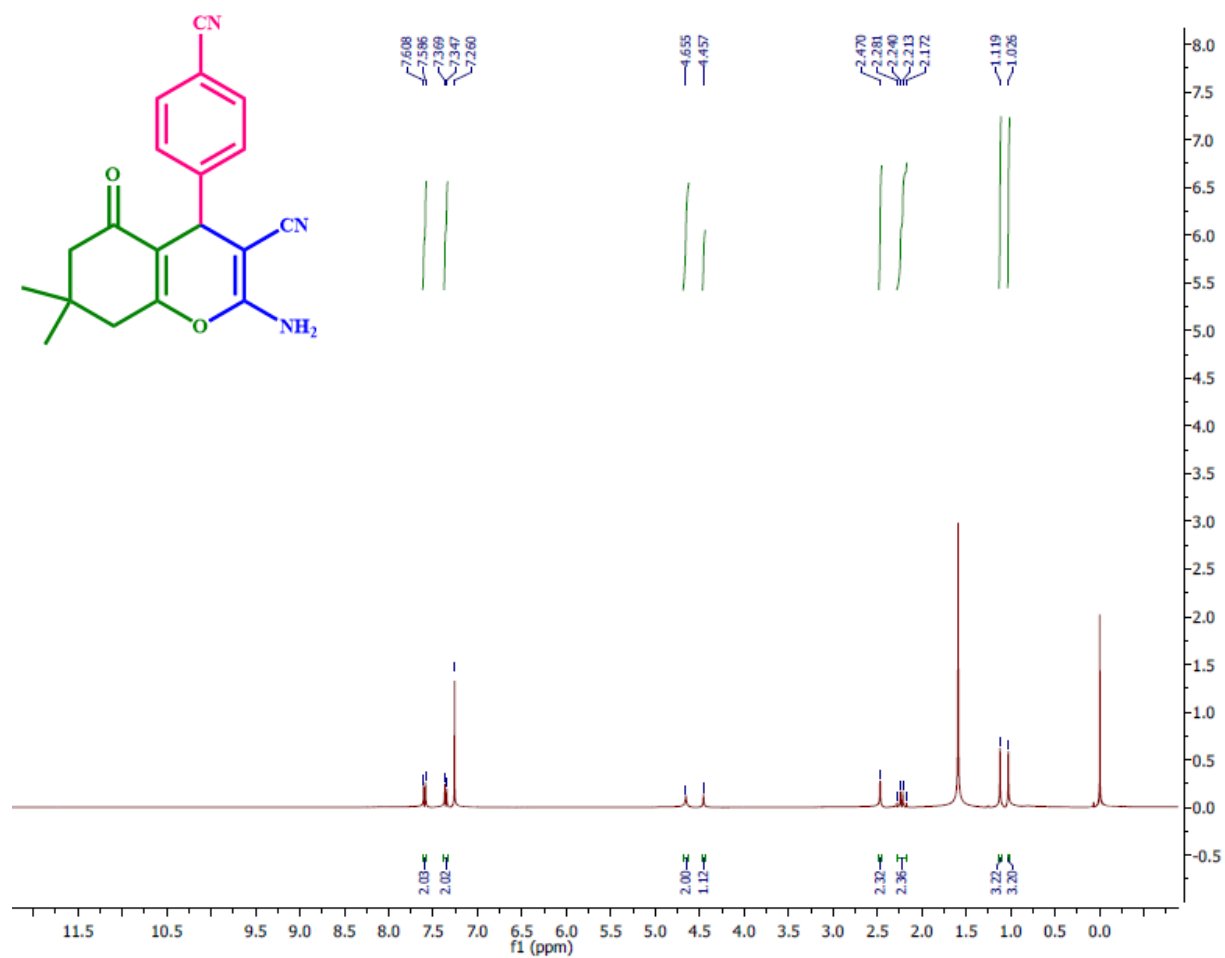
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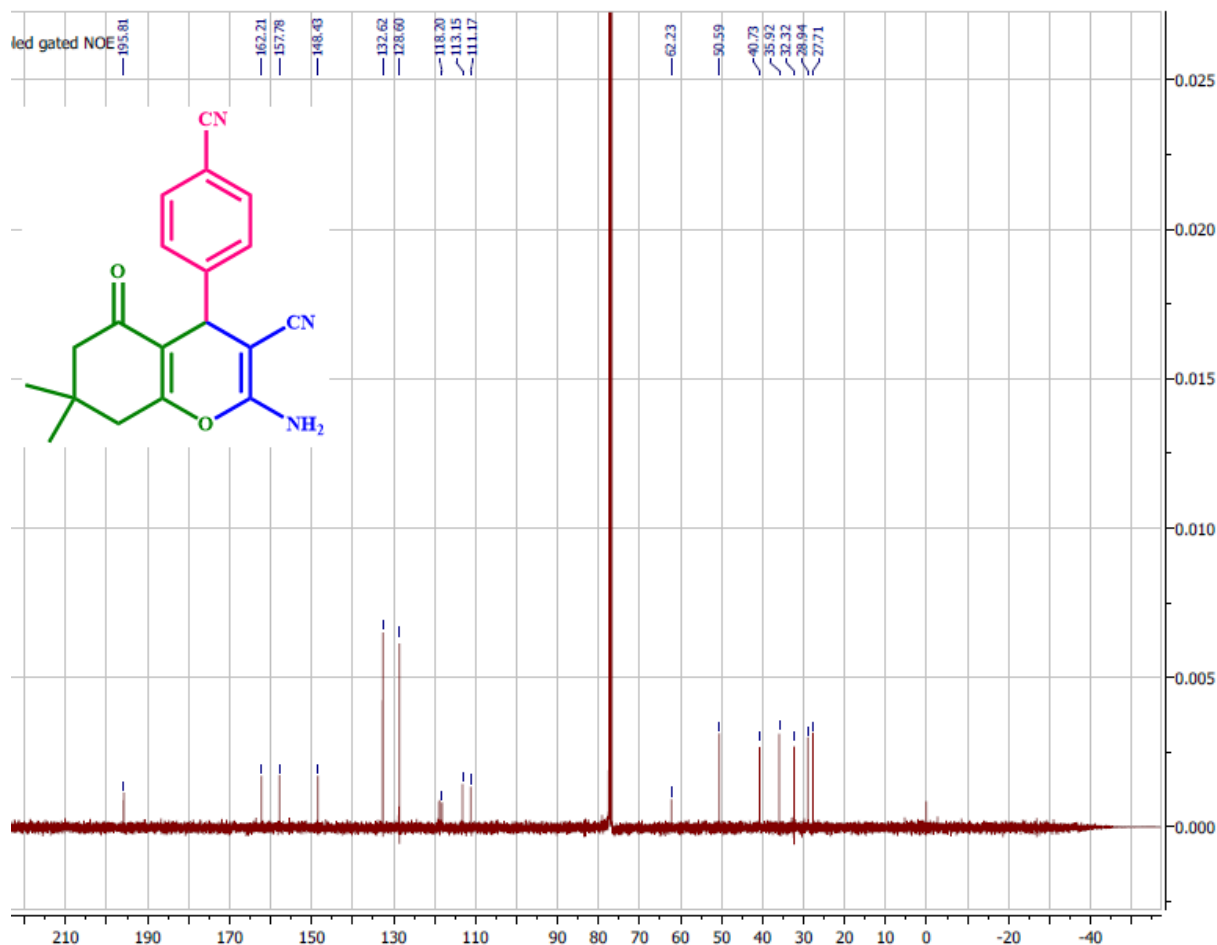
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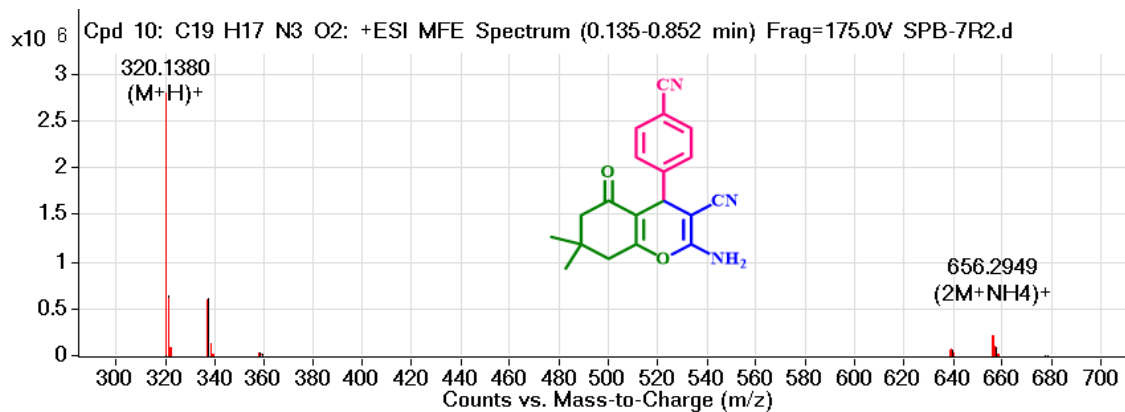
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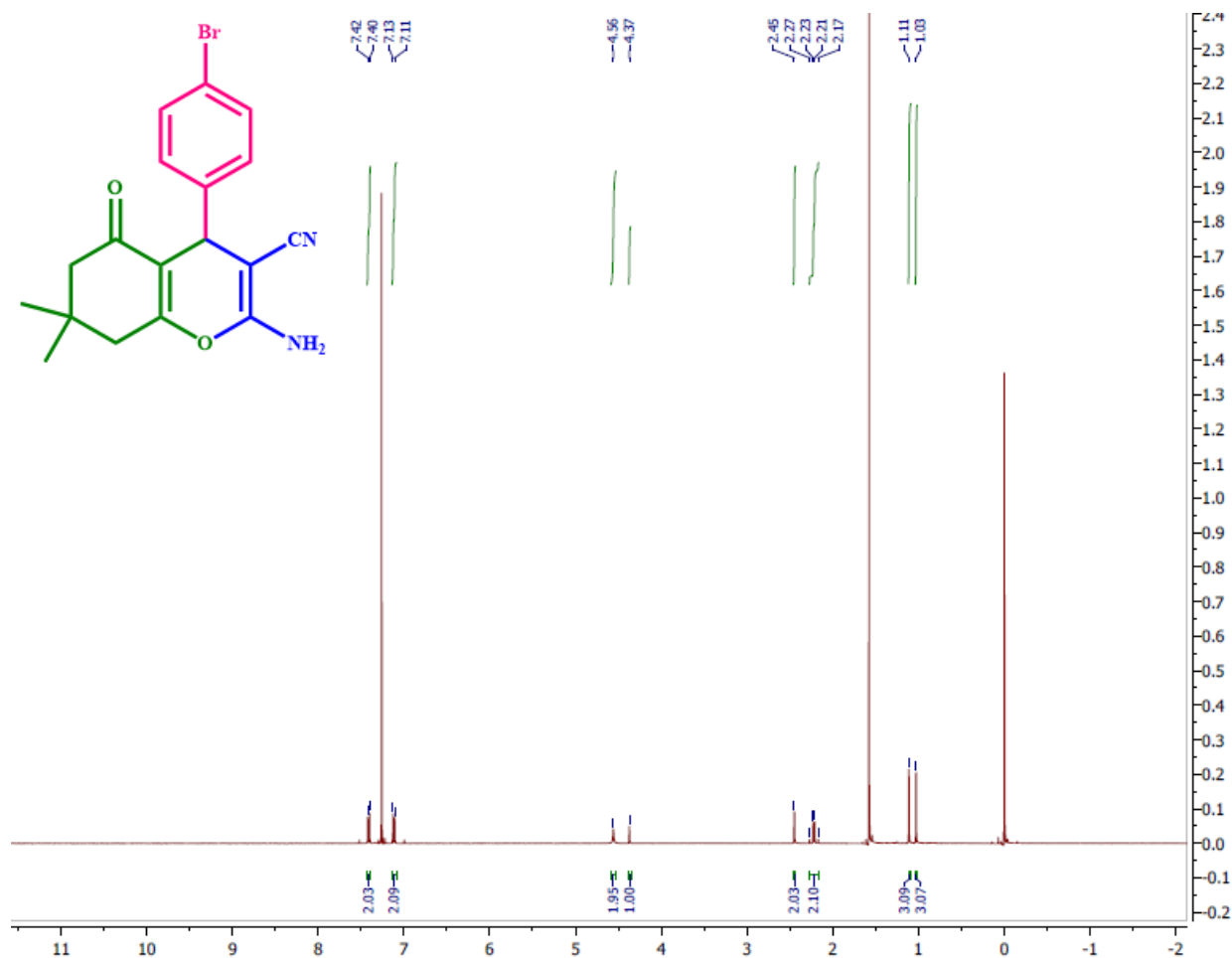
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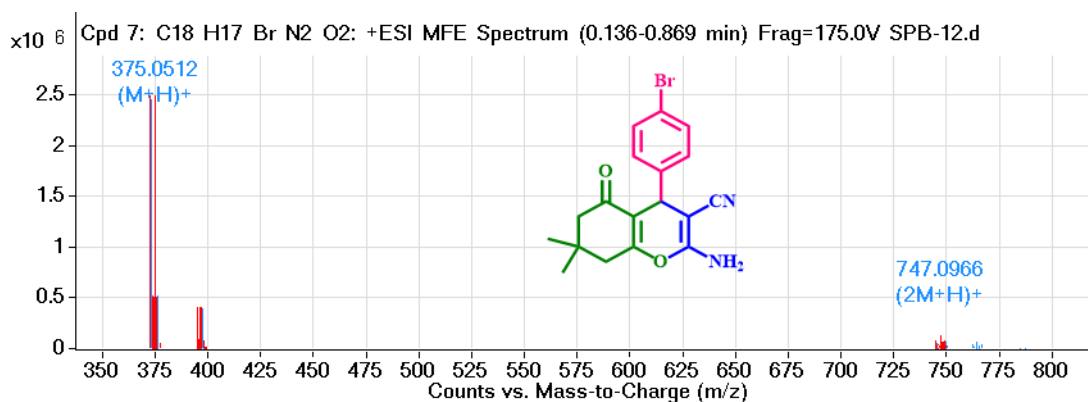
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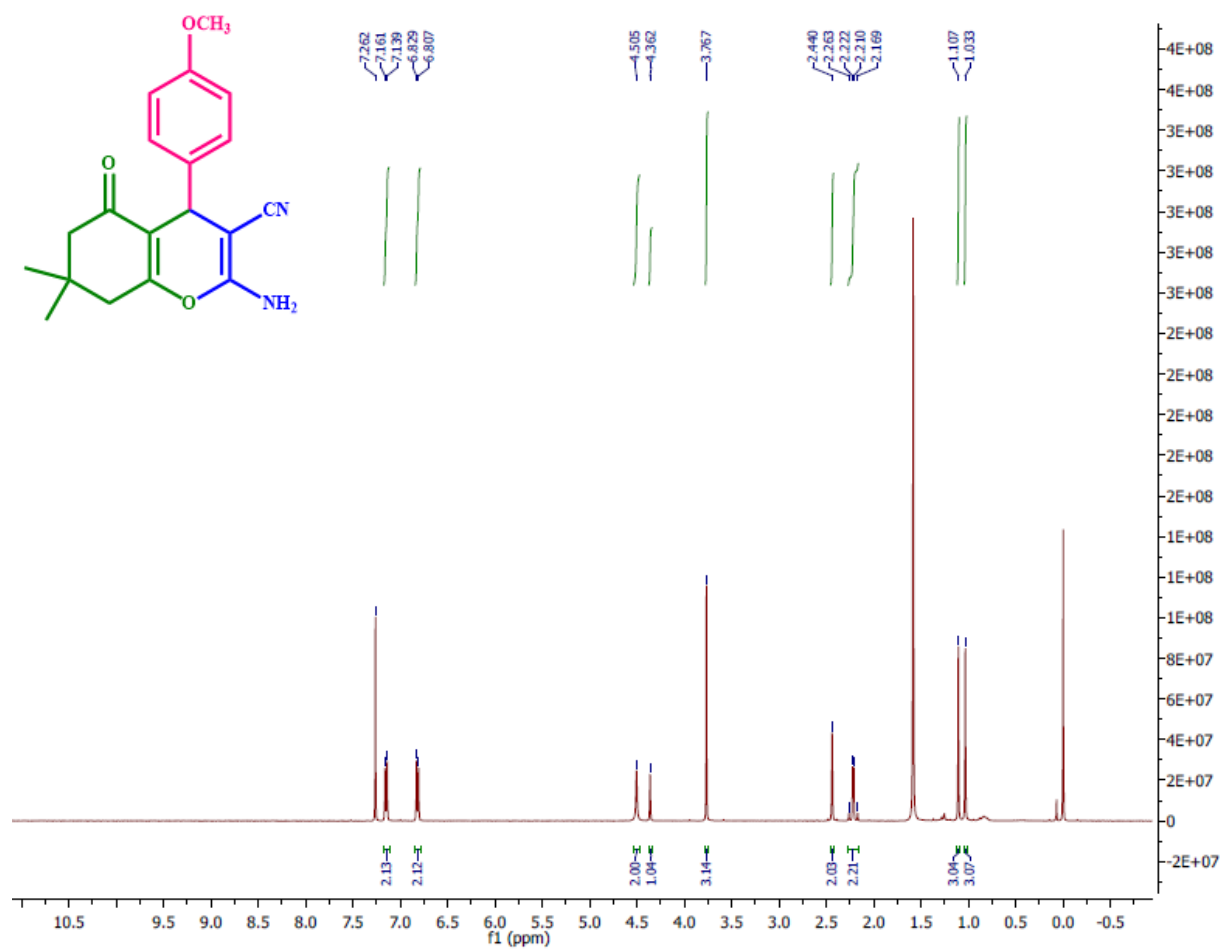
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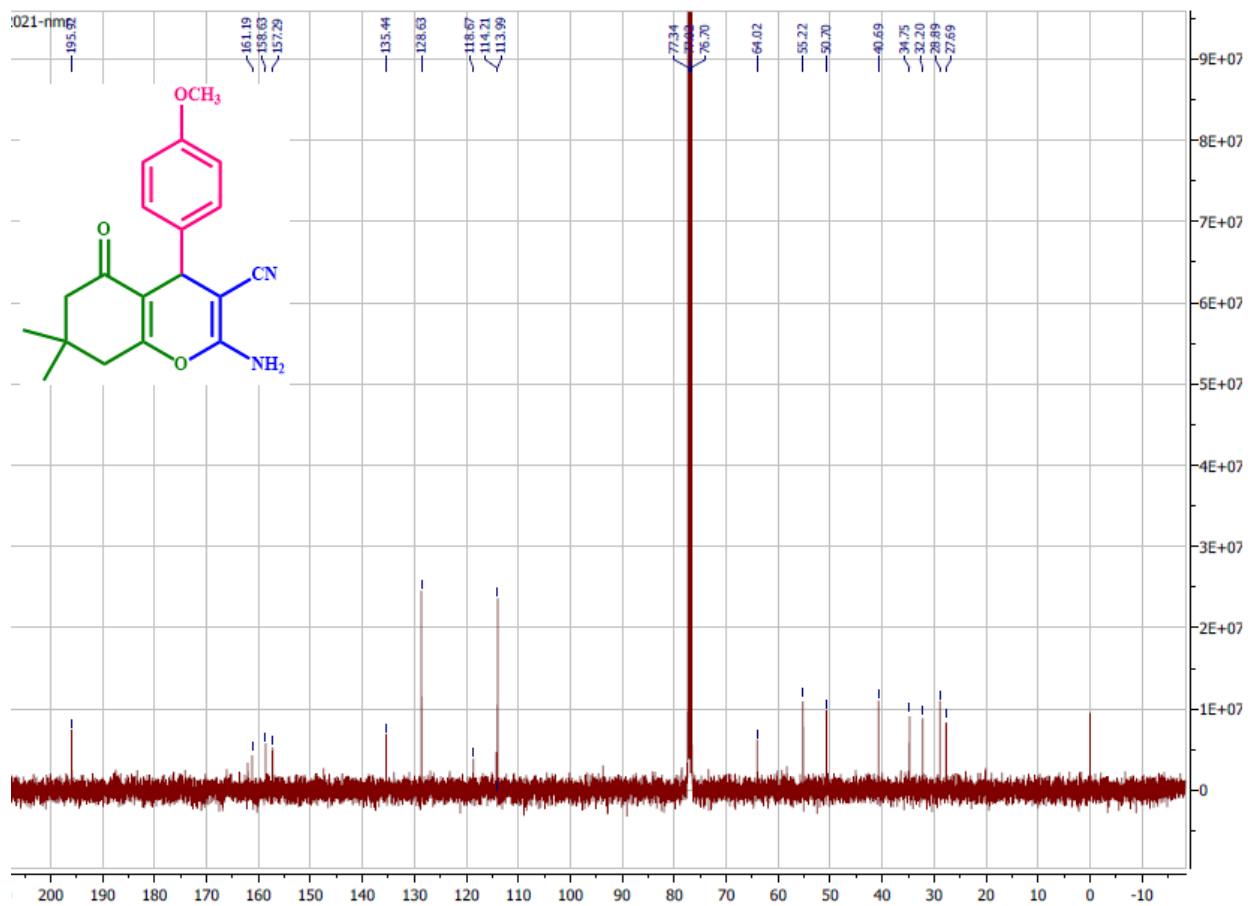
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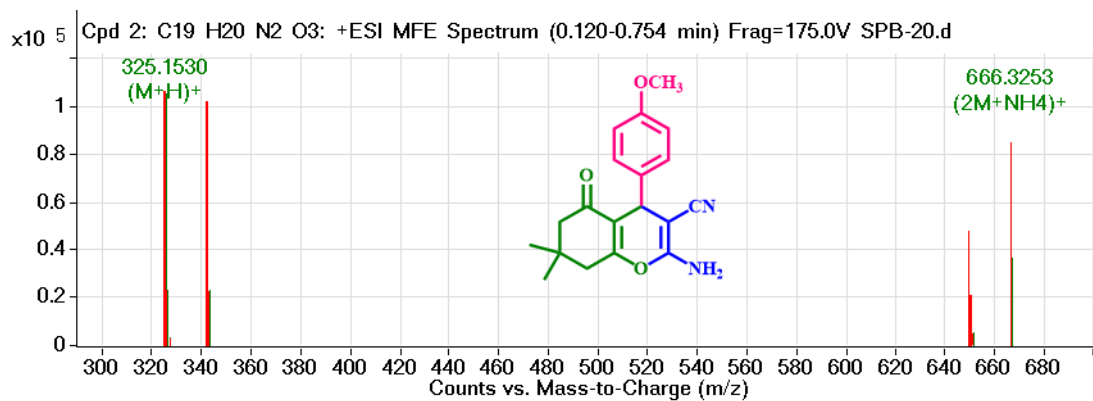
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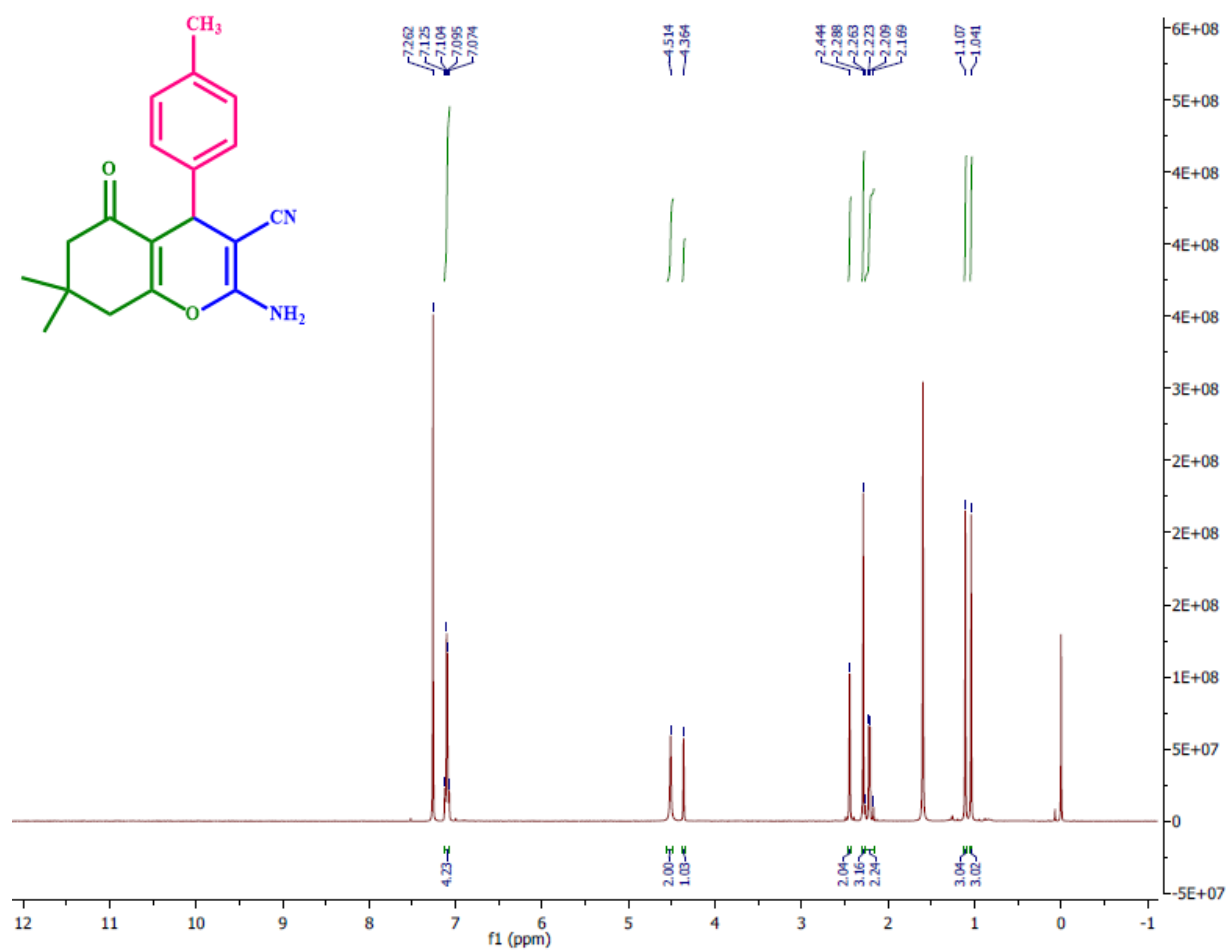
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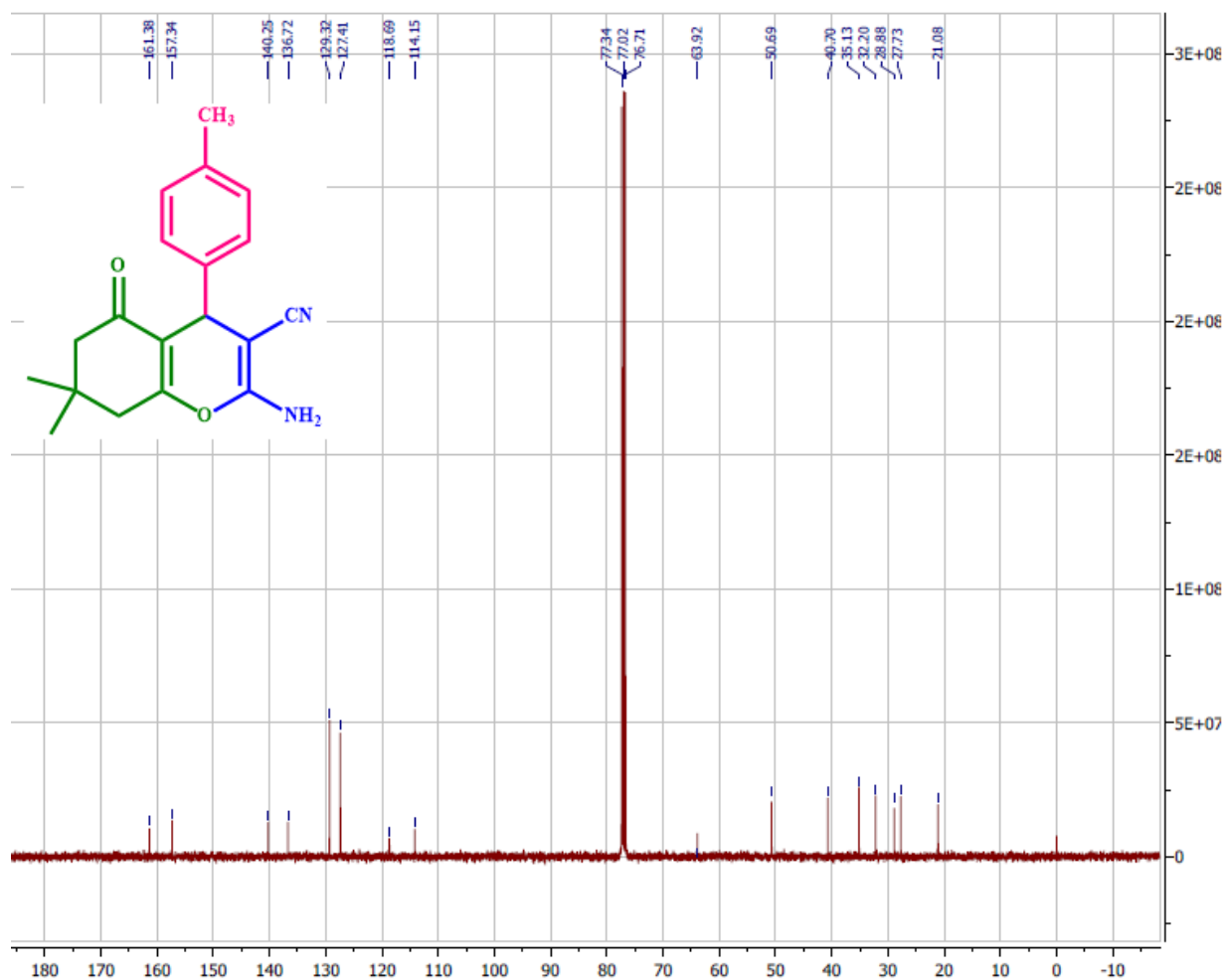
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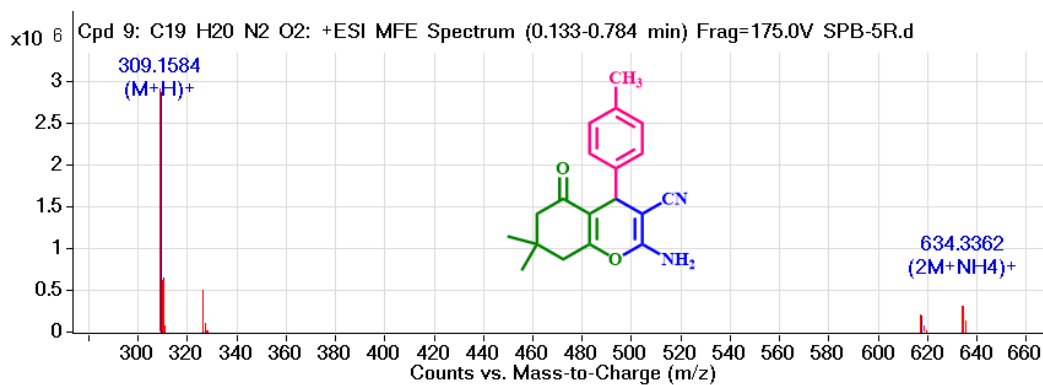
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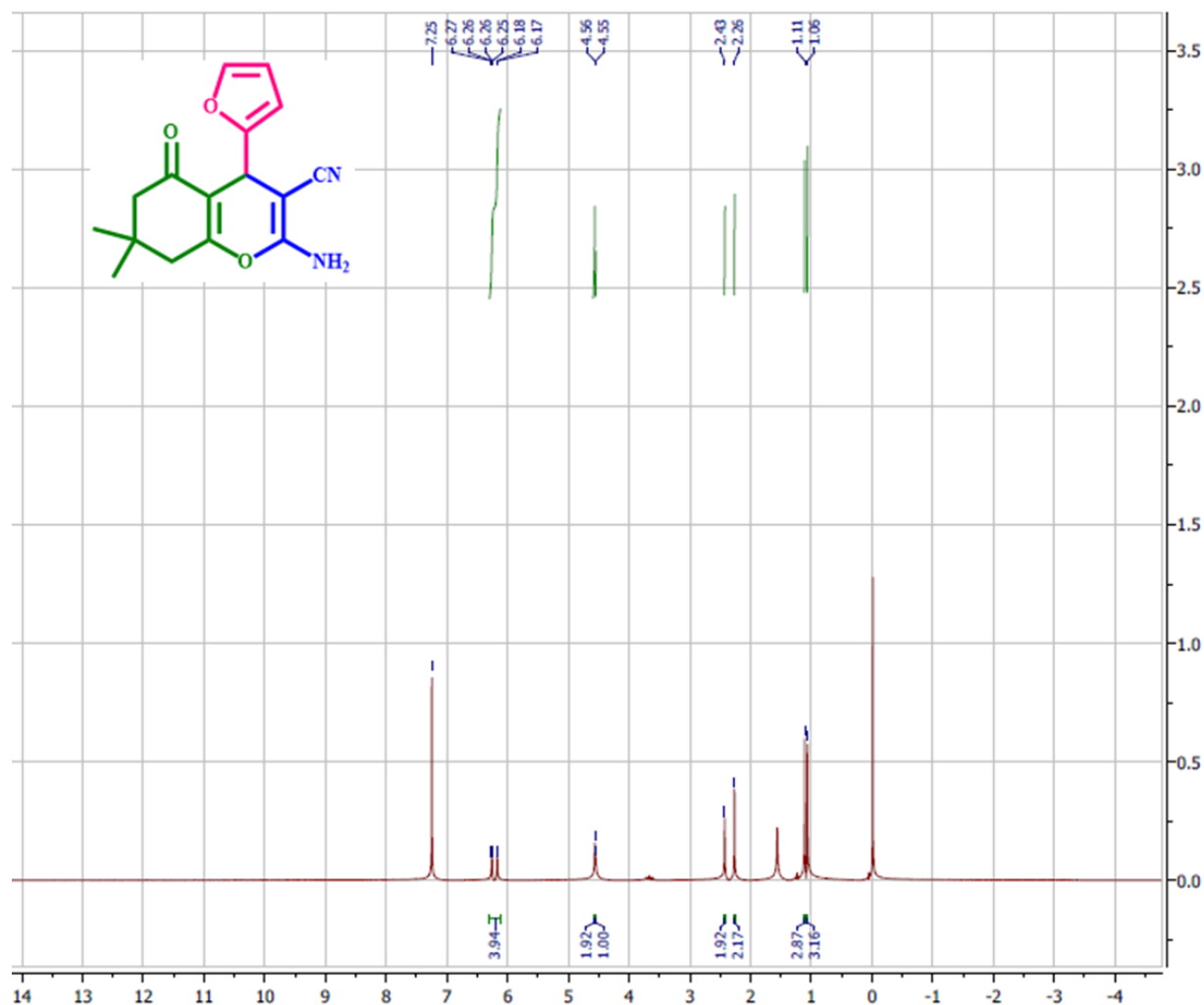
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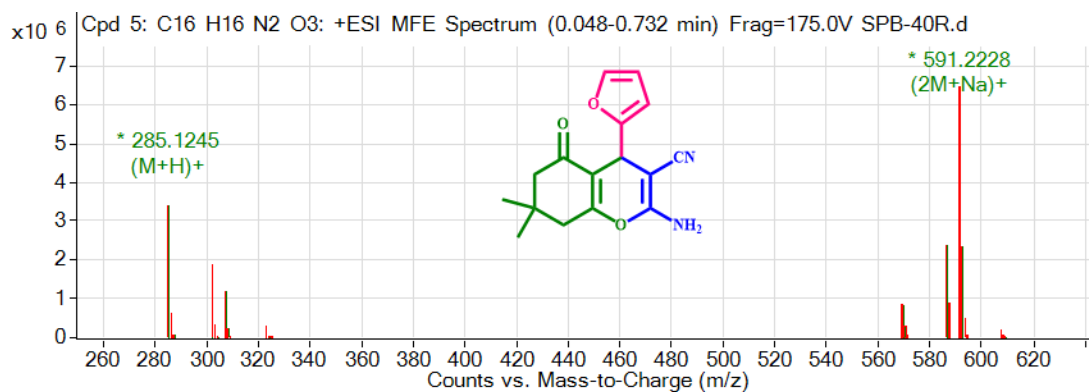
HRMS of 2-amino-4-(4-methylphenyl)-7,7-dimethyl-5-oxo-5,6,7,8-tetrahydro-4*H*-chromene-3-carbonitrile (4l)



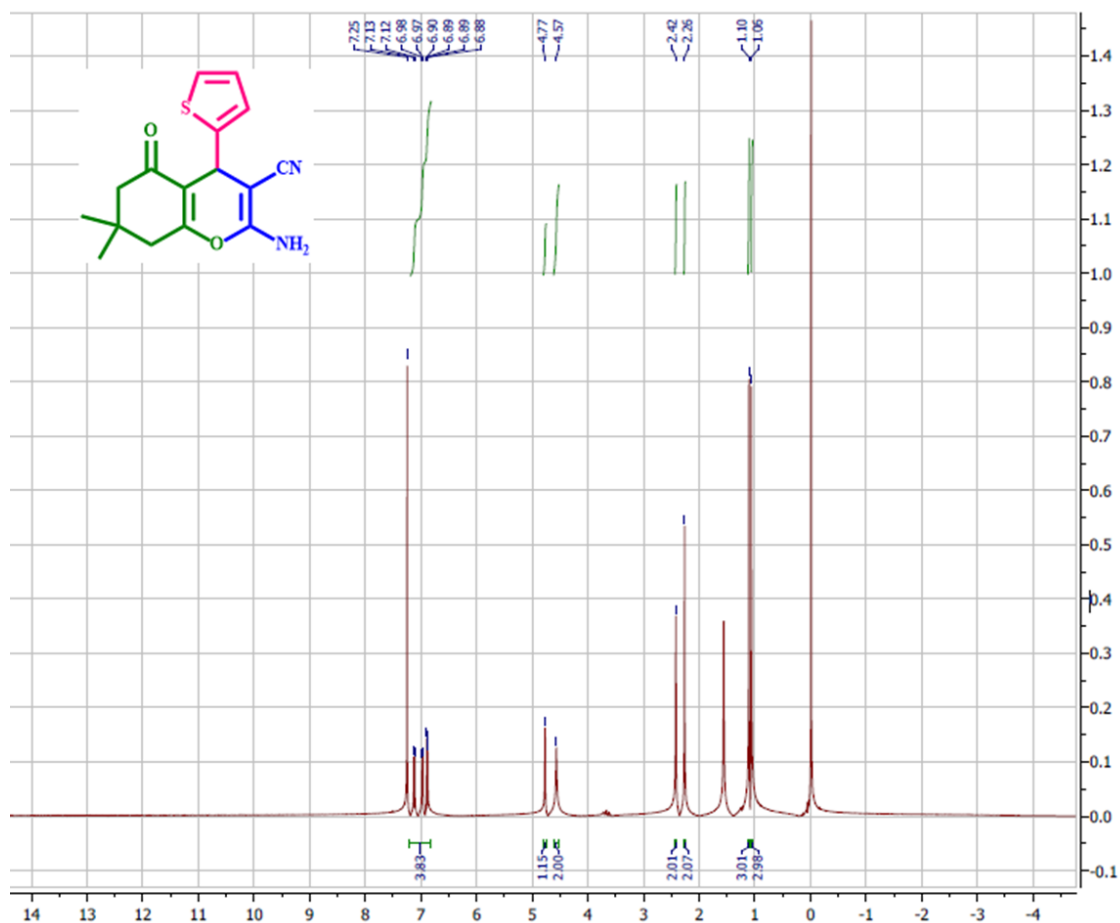
^1H NMR of 2-amino-4-(2-furyl)-7,7-dimethyl-5-oxo-5,6,7,8-tetrahydro-4*H*-chromene-3-carbonitrile (4m)



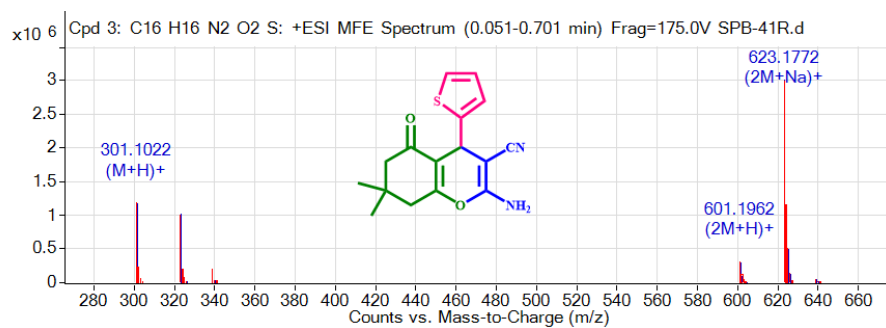
HRMS of 2-amino-4-(2-furyl)-7,7-dimethyl-5-oxo-5,6,7,8-tetrahydro-4*H*-chromene-3-carbonitrile (4m)



^1H NMR of 2-amino-4-(2-thienyl)-7,7-dimethyl-5-oxo-5,6,7,8-tetrahydro-4*H*-chromene-3-carbonitrile (4n)



HRMS of 2-amino-4-(2-thienyl)-7,7-dimethyl-5-oxo-5,6,7,8-tetrahydro-4*H*-chromene-3-carbonitrile (4n)



¹H NMR of 2-amino-4-styryl-7,7-dimethyl-5-oxo-5,6,7,8-tetrahydro-4H-chromene-3-carbonitrile (4o)

