

Electronic Supplementary Information

Green Synthesis of Magnetic Fe₂O₃ Nanoparticle with *Chenopodium glaucum* L. as Recyclable Heterogeneous Catalyst for One-Pot Reactions and Heavy Metal Adsorption

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1. Results and Discussion

1.1. Preparation of 2-amino-4-aryl-4H-benzo[g]chromene-3-carbonitrile derivatives (4a-l) using magnetic CG-Fe₂O₃ nanoparticles

The catalyst screening was carried out to identify the optimal concentration of CG-Fe₂O₃ NPs for the reactions to occur with higher efficiency. Experimental results, as shown in **Table ST1**, show varying CG-Fe₂O₃ NPs concentrations affect reaction time and isolated yield. Optimal concentrations obtained higher yields: 92% at 5 and 7 mmol% concentration in 9 and 8 minutes, respectively. The increase in the quantity of catalyst exhibits minimal impact on the yield percentage within the same timeframe which indicates that 7 mmol% is an optimal range of CG-Fe₂O₃ NPs concentration for efficient reactions.

Table ST2. Optimizing the reaction conditions.

| Fe ₂ O ₃ -NPs (mmol%) | Time (min.) | Isolated Yield ^{a,*} (%) |
|---|-------------|-----------------------------------|
| 0 | 6 | 55% |
| 3 | 5 | 76% |
| 5 | 9 | 92% |
| 7 | 8 | 92% |
| 9 | 8 | 93% |

^aYield refers to extraction of all crops. *Reaction conditions: β -naphthol (1 eq.), benzaldehyde (1 eq.), malononitrile (1 eq.) at 100 watts.

According to the screening of different solvents for the condensation reaction which involves β -naphthol **1** (5 mmol), benzaldehyde **2a** (5 mmol), along with malononitrile **3** (5 mmol) using CG-Fe₂O₃ NPs (7 mmol%) at 100 watts for 8 minutes, glycerol emerged as the most efficient solvent which gives higher yield of xanthene in shorter time as compared to others as shown in **Table ST2**.

Table ST2. Solvent screening for the synthesis of xanthene derivative **4a**.

| Solvent | Time (min.) | Isolated Yield ^{a,*} (%) |
|---------------------|-------------|-----------------------------------|
| Ethanol | 9 | 92% |
| Methanol | 11 | 82% |
| Water | 15 | 35% |
| Acetonitrile | 14 | 70% |
| Glycerol | 7 | 95% |
| Polyethylene glycol | 20 | 75% |
| Ethylene glycol | 17 | 77% |

^aYield refers to extraction of all crops. *Reaction conditions: β -naphthol (1 eq.), benzaldehyde (1 eq.), malononitrile (1 eq.), and CG-Fe₂O₃ NPs (7 mmol%) at 100 watts.

In **Table ST3**, we discussed the optimization of the reaction power for a reaction performed in glycerol using CG-Fe₂O₃ NPs. It was observed that as the power increased, there was a significant rise in yield over time. However, excessive power elevation resulted in a decrease in product yield due to product decomposition at higher power.

Table ST3. The influence of power on the percentage yield of **4a** utilizing CG-Fe₂O₃ NPs in glycerol.

| Watt | Time (min.) | Isolated Yield ^{a,*} (%) |
|------------|-------------|-----------------------------------|
| 90 | 12 | 87% |
| 100 | 7 | 95% |
| 110 | 7 | 93% |
| 120 | 6 | 97% |
| 130 | 6 | 96% |

^aYield refers to extraction of all crops. *Reaction conditions: β -naphthol (1 eq.), benzaldehyde (1 eq.), malononitrile (1 eq.), and CG-Fe₂O₃ NPs (7 mmol%).

Using the optimized conditions, we examined the reusability of CG-Fe₂O₃ NPs in the reaction. After filtration from the previous reaction, the nanoparticles were washed with dry ethyl acetate and vacuum dried before reuse for xanthene derivative synthesis. Remarkably, product **4a** was obtained with a high yield of 97%. The catalyst retained good activity over three runs, with no notable decrease in yield observed (**Table ST4**), confirming its continued effectiveness.

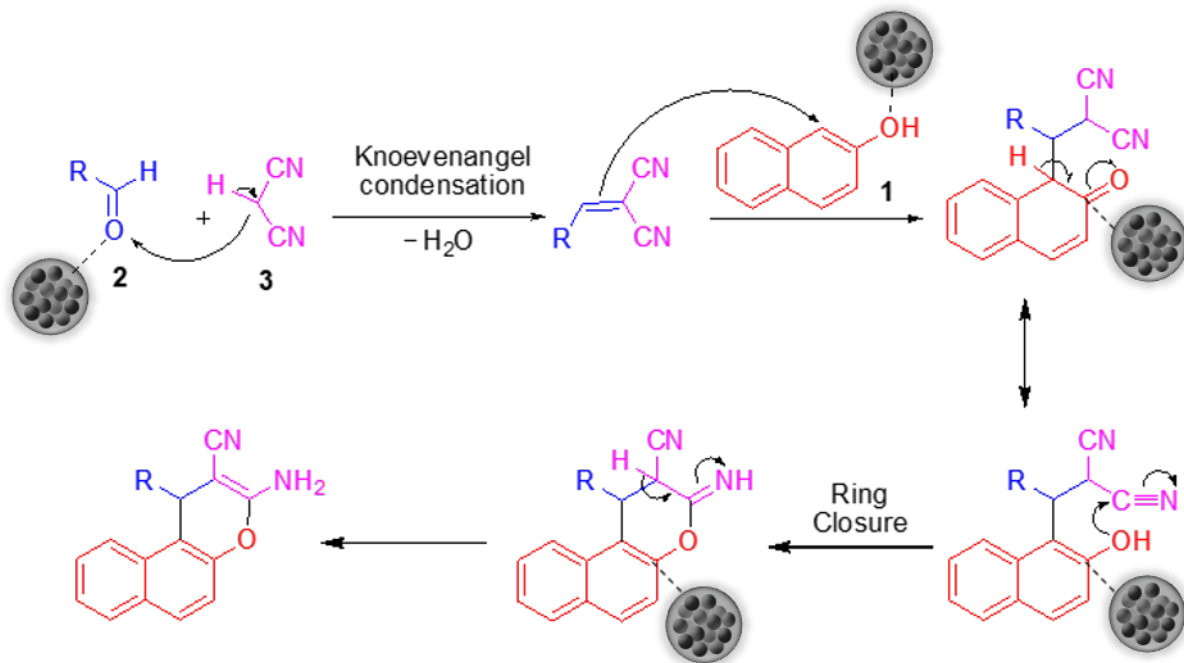
Table ST4. Reusability of CG-Fe₂O₃ NPs in synthesis of xanthene **4a** utilizing in glycerol.

| Run | Isolate Yield ^{a,*} (%) |
|-------|----------------------------------|
| Fresh | 97% |
| 1 | 96% |
| 2 | 94% |

^aYield refers to extraction of all crops. *Reaction conditions: β -naphthol (1 eq.), benzaldehyde (1 eq.), malononitrile (1 eq.), and CG-Fe₂O₃ NPs (7 mmol%) at 120 watts for 6 min.

1.2. Plausible Mechanism

As per the literature, the proposed mechanism as shown in **Scheme S1** involves Knoevenagel condensation between substituted-benzaldehyde **2** and malononitrile **3**, followed by Michael addition with β -naphthol **1** to form a dihydrochromene intermediate. Tautomerization and intramolecular cyclization then yield the final chromene product through consecutive steps of deprotonation, nucleophilic attack, tautomerization, and ring closure.



Scheme S1. Mechanism of synthesis of xanthene derivatives (**4a-l**) with magnetic CG-Fe₂O₃ NPs under MW irradiations.

2. Materials and Methods

2.1. Chemicals

All chemicals utilized in this study were procured from Sigma-Aldrich (Punjab, India) and were employed without further distillation. Solvents were sourced from Loba Chemie (Punjab, India).

2.2. Analytical instruments

The melting points of synthesized products were determined using a digital melting point apparatus *via* the open capillary method. FT-Infrared (FT-IR) spectra were obtained using the attenuated total reflection (ATR) mode on a Perkin Elmer Spectrum II instrument. ¹H-NMR and ¹³C-NMR spectra were recorded on a Bruker Avance NEO 500 MHz FT-NMR instrument with CDCl₃ as the solvent, at 300 and 400 MHz, respectively, referencing chemical shifts (δ) to tetramethyl silane (TMS) as an internal standard. The thin-layer chromatography (TLC) technique, coupled with visualization in a UV chamber, monitored reaction progress and assessed compound purity. The magnetic characteristics of the adsorbents were assessed using a vibrating sample magnetometer (VSM, 7410 Series, Lake Shore). The zero point charge (ZPC) and the hydrodynamic dimensions of the particles were measured using a Zetasizer Nano-ZS90 instrument (Chandigarh University,

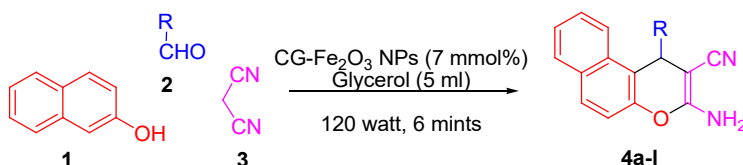
India). Metal ion concentrations were determined using an inductively coupled plasma optical emission spectrometer (ICP-OES, 5110 ICP-OES, Agilent Technologies, PAU, Ludhiana).

2.3. Synthesis of CG-Fe₂O₃ Nanoparticles

Combine 0.4 M ferric chloride and 0.2 M ferrous sulfate solution under nitrogen atmosphere, stirred for 15 minutes at 70 °C. Then slowly added *C. glaucum* until pH 11. Filtered precipitates, washed with acetone and water until pH 7. Dried at 70 °C for 24 hrs, then calcinated at 500 °C for 5 hrs to obtain CG-Fe₂O₃ NPs.

2.4. Synthesis of xanthene derivatives (4a-l)

A mixture composed of β -naphthol **1** (5 mmol), substituted benzaldehyde **2** (5 mmol), along with malononitrile **3** (5 mmol), in the presence of CG-Fe₂O₃ NPs (7 mmol%) was subjected to MW irradiation at 120 watt for 6 minutes in glycerol (5 mL) (**Scheme S2**). After completion of the reaction, the mixture was cooled to room temperature, recover magnetic nanoparticles *via* magnet, filtered off the solution, then washed with distilled water, and subsequently, the resulting solid was recrystallized using ethanol to afford the pure crystals with an efficiency of 90-95%. All reactions were monitored using TLC with silica gel-coated plates (ethyl acetate: hexane/ 6:4/ v:v).



Scheme S2. Synthesis of xanthene derivatives (**4a-l**) under MW irradiations using CG-Fe₂O₃ NPs.

In a similar manner, different aldehydes **2b-l** will undergo reaction with β -naphthol **1**, and malononitrile **3** using the same protocol. The progress of the reactions will be monitored through TLC and melting point analysis (**Table ST5**). These reactions proceed smoothly, even in the presence of various electron-donating (-Me and -OMe) as well as electron-withdrawing substituents (-NO₂) on the aldehyde, facilitating efficient reactions. The effectiveness of this approach is remarkable, yielding high percentages (92-97%) for the final products.

Table ST5. Synthesis of xanthene derivatives **4a-l** utilizing CG-Fe₂O₃ NPs in glycerol.

| Entry | R ₁ | R _f | Isolated Yield ^a (%) | Melting Point (°C) | Literature Melting Point (°C) | Reference |
|-----------|---|----------------|---------------------------------|--------------------|-------------------------------|-----------|
| 4a | C ₆ H ₅ | 0.66 | 95 | 208-209 | 210-211 | [25] |
| 4b | 3-NO ₂ C ₆ H ₄ | 0.78 | 97 | 210-211 | 212-214 | [25] |
| 4c | 4-NO ₂ C ₆ H ₄ | 0.75 | 95 | 178-179 | 179-182 | [17] |
| 4d | 2-Cl C ₆ H ₄ | 0.69 | 93 | 233-234 | 231-232 | [6] |
| 4e | 4-Cl C ₆ H ₄ | 0.70 | 97 | 230-231 | 231-232 | [14] |
| 4f | 4-CH ₃ C ₆ H ₄ | 0.58 | 97 | 203-205 | 202-204 | [25] |
| 4g | 4-CH ₃ O C ₆ H ₄ | 0.63 | 98 | 192-194 | 192-195 | [25] |
| 4h | 2-OH C ₆ H ₄ | 0.71 | 96 | 245-248 | 253-255 | [6] |
| 4i | 2-Thiophenyl | 0.60 | 97 | 267-268 | 265-269 | [6] |
| 4j | 2-Furyl | 0.54 | 96 | 265-267 | 267-269 | [17] |
| 4k | 4-NMe ₂ C ₆ H ₄ | 0.78 | 97 | 209-211 | 210-212 | [5] |
| 4l | 4-OH, 3-OMe C ₆ H ₃ | 0.65 | 96 | 163-165 | 160-164 | [6] |

^aYield refers to extraction of all crops.

2.5. Isotherm studies

Table ST6. Adsorption values of Hg²⁺ metal ions using CG-Fe₂O₃ nanoparticles.

| S. No. | C _i (mg/l) | C _e (mg/l) | log C _e | ln C _e | q _e (mg/g) |
|--------|-----------------------|-----------------------|--------------------|-------------------|-----------------------|
| 1 | 10 | 3.1 | 0.491 | 1.131 | 9.857 |
| 2 | 30 | 8.6 | 0.934 | 2.152 | 30.571 |
| 3 | 50 | 15.2 | 1.182 | 2.721 | 49.714 |
| 4 | 100 | 41.3 | 1.616 | 3.721 | 83.857 |
| 5 | 250 | 151.8 | 2.181 | 5.023 | 140.286 |
| 6 | 500 | 391.7 | 2.593 | 5.970 | 154.714 |

Table ST7. Adsorption values of Pb²⁺ metal ions using CG-Fe₂O₃ nanoparticles.

| S. No. | C _i (mg/L) | C _e (mg/L) | log C _e | ln C _e | q _e (mg/g) |
|--------|-----------------------|-----------------------|--------------------|-------------------|-----------------------|
| 1 | 10 | 4.2 | 0.623 | 1.435 | 8.286 |
| 2 | 30 | 9.2 | 0.964 | 2.219 | 29.714 |

| | | | | | |
|---|-----|-------|-------|-------|---------|
| 3 | 50 | 17.5 | 1.243 | 2.862 | 46.429 |
| 4 | 100 | 43.2 | 1.635 | 3.766 | 81.143 |
| 5 | 250 | 160.8 | 2.206 | 5.080 | 127.429 |
| 6 | 500 | 401.3 | 2.603 | 5.995 | 141.000 |

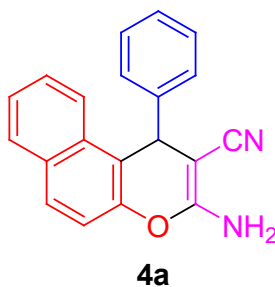
Table ST8. Parameters of Langmuir's and Freundlich's isotherm models using CG-Fe₂O₃ nanoparticles.

| Heavy metal ion | Langmuir's isotherm model | | | Freundlich isotherm model | | |
|--------------------|---------------------------|-----------|----------------|---------------------------|-----------|----------------|
| | Slope | intercept | R ² | Slope | intercept | R ² |
| Hg ²⁺ | 0.297 | 0.003 | 0.992 | 0.237 | 0.919 | 0.907 |
| Pb ²⁺ | 0.472 | -0.0005 | 0.951 | 0.248 | 0.821 | 0.865 |

Table ST9. The feasibility of the adsorption process derived from Langmuir's isotherm model using CG-Fe₂O₃ nanoparticles.

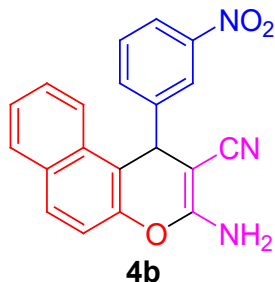
| C ₀ (mg/L) | Hg ²⁺ ; b = 0.29 | Pb ²⁺ ; b = 0.47 |
|-----------------------|-----------------------------|-----------------------------|
| | R _L | R _L |
| 10 | 0.256 | 0.175 |
| 30 | 0.103 | 0.066 |
| 50 | 0.065 | 0.041 |
| 100 | 0.033 | 0.021 |
| 250 | 0.014 | 0.009 |
| 500 | 0.007 | 0.004 |

2.6. Characterization of synthesized xanthene derivatives

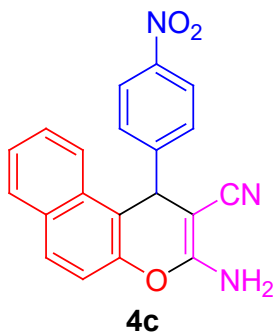


2-Amino-4-phenyl-4H-benzo[h]chromene-3-carbonitrile (4a): Yield 95%, colourless crystals, MP 208-209 °C; Lit. MP (210-211 °C). FT-IR spectrum, ν , cm⁻¹: 2182.36 (C≡N), 3338.00 (N-H), 3432.74 (sp² hybridized C-H bonds), 1589.45 (C=C aromatic stretching vibrations). ¹H-NMR spectrum, δ , ppm (*J*, Hz): 7.14-7.95 (Ar-H), 5.30 (*s*, 1H, CH), 6.98 (*s*, 1H, NH₂). ¹³C-NMR

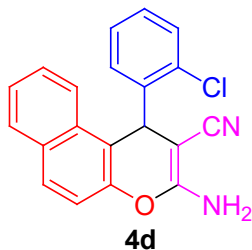
spectrum, δ , ppm: 159.61, 146.74, 145.60, 130.73, 130.07, 129.39, 128.60, 128.36, 126.97, 126.89, 126.50, 124.83, 123.52, 121.37, 120.39, 116.69, 115.58, 57.83, 38.00.



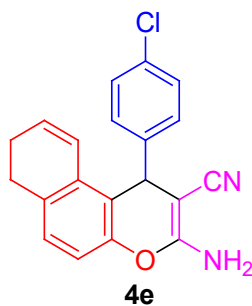
2-Amino-4-(3-nitrophenyl)-4H-benzo[h]chromene-3-carbonitrile (4b): Yield 97%, colourless crystals, MP 210-211 °C; Lit. MP (212-214 °C). FT-IR spectrum, ν , cm^{-1} : 2190.31 ($\text{C}\equiv\text{N}$), 3353.48 (N-H), 3463.45 (sp^2 hybridized C-H bonds), 1589.63 ($\text{C}=\text{C}$ aromatic stretching vibrations). ^1H -NMR spectrum, δ , ppm (J , Hz): 7.37-8.10 (Ar-H), 5.62 (s , 1H, CH), 7.18 (s , 1H, NH_2). ^{13}C -NMR spectrum, δ , ppm: 159.92, 147.90, 147.76, 146.90, 133.58, 130.76, 130.28, 129.94, 129.83, 128.47, 127.27, 125.01, 123.35, 121.69, 120.11, 116.74, 114.47, 56.98.



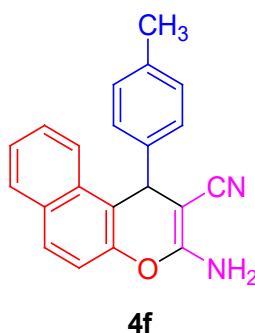
2-Amino-4-(4-nitrophenyl)-4H-benzo[h]chromene-3-carbonitrile (4c): Yield 97%, colorless crystals, MP 178-179 °C; Lit. MP (179-182 °C). FT-IR spectrum, ν , cm^{-1} : 2190.14 ($\text{C}\equiv\text{N}$), 3331.02 (N-H), 3426.62 (sp^2 hybridized C-H bonds), 1588.39 ($\text{C}=\text{C}$ aromatic stretching vibrations). ^1H -NMR spectrum, δ , ppm (J , Hz): 7.36-8.14 (Ar-H), 5.55 (s , 1H, CH), 7.15 (s , 1H, NH_2). ^{13}C -NMR spectrum, δ , ppm: 159.81, 152.82, 146.80, 146.08, 130.73, 129.92, 129.87, 128.46, 128.12, 127.22, 124.99, 123.99, 123.28, 121.24, 119.99, 116.74, 114.32, 56.51.



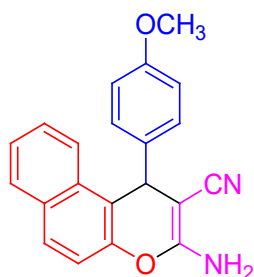
2-Amino-4-(2-chlorophenyl)-4-H-benzo[g] chromene-3-carbonitrile (4d): Yield 93.6%, colorless crystals, MP 233-234 °C; Lit. MP (231-232 °C). FT-IR spectrum, ν , cm^{-1} : 3173.28 ($\text{C}\equiv\text{N}$), 3298.17 (N-H), 3419.28 (sp^2 hybridized C-H bonds), 1568.91 ($\text{C}=\text{C}$ aromatic stretching vibrations). ^1H -NMR (250 MHz, DMSO- d_6) δ (ppm): 7.22-8.22 (Ar-H), 5.38 (s, 1H, CH), 6.96 (s, 1H, NH_2). ^{13}C -NMR (62.9 MHz, DMSO- d_6) δ (ppm): 160.22, 152.08, 146.71, 146.46, 130.66, 129.64, 129.33, 128.94, 128.85, 127.70, 124.44, 123.96, 123.02, 120.18, 119.66, 116.27, 114.12, 56.56.



2-Amino-4-(4-chlorophenyl)-4-H-benzo[g] chromene-3-carbonitrile (4e): Yield 97.9%, Yellow crystals, MP 230-231 °C; Lit. MP (231-232 °C). FT-IR spectrum, ν , cm^{-1} : 3466.53 ($\text{C}\equiv\text{N}$), 3328.22 (N-H), 3431.81 (sp^2 hybridized C-H bonds), 1577.14 ($\text{C}=\text{C}$ aromatic stretching vibrations). ^1H -NMR (250 MHz, DMSO- d_6) δ (ppm): 7.08-7.97 (Ar-H), 7.08 (s, 1H, CH), 5.36 (s, 1H, NH_2). ^{13}C -NMR (62.9 MHz, DMSO- d_6) δ (ppm): 159.79, 146.85, 144.62, 131.28, 130.86, 130.07, 129.73, 128.84, 128.71, 128.54, 127.21, 123.50, 120.43, 116.86, 115.08, 57.54, 39.92, 37.51.

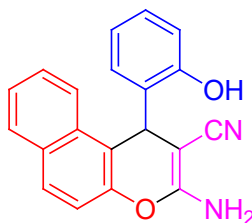


2-Amino-4-p-tolyl-4H-benzo[h]chromene-3-carbonitrile (4f): Yield 97%, colorless crystals, MP 203-205 °C; Lit. MP (202-204 °C). FT-IR spectrum, ν , cm^{-1} : 2187.77 ($\text{C}\equiv\text{N}$), 3336.16 (N-H), 3426.95 (sp^2 hybridized C-H bonds), 1591.27 ($\text{C}=\text{C}$ aromatic stretching vibrations). ^1H -NMR spectrum, δ , ppm (J , Hz): 7.04-7.93 (Ar-H), 5.25 (s, 1H, CH), 6.95 (s, 1H, NH_2). ^{13}C -NMR spectrum, δ , ppm: 159.50, 146.65, 142.69, 135.56, 130.70, 130.08, 129.27, 129.11, 128.31, 126.89, 126.77, 124.75, 123.53, 120.42, 119.56, 116.65, 115.67, 57.98, 37.56.



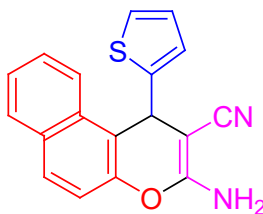
4g

2-Amino-4-(4-methoxyphenyl)-4-H-benzo[h] chromene-3-carbonitrile (4g): Yield 98%, yellow crystals, MP 192-194 °C; Lit. MP (192-195 °C). FT-IR spectrum, ν , cm^{-1} : 2188.25 ($\text{C}\equiv\text{N}$), 3343.94 (N-H), 3430.57 (sp^2 hybridized C-H bonds), 1588.73 ($\text{C}=\text{C}$ aromatic stretching vibrations). ^1H -NMR spectrum, δ , ppm (J , Hz): 6.76-7.79 (Ar-H), 4.61 (*s*, 1H, CH), 5.18 (*s*, 1H, NH_2). ^{13}C -NMR spectrum, δ , ppm: 158.52, 158.46, 147.04, 136.76, 131.41, 130.79, 129.52, 128.47, 128.21, 127.17, 125.07, 120.01, 120.37, 116.65, 115.23, 114.29, 62.56, 55.19.



4h

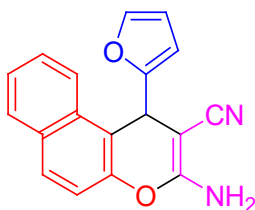
2-Amino-4-(2-hydroxyphenyl)-4-H-benzo[h] chromene-3-carbonitrile (4h): Yield 90%, Yellow crystals, MP 245-248 °C; Lit. MP (253-255 °C). FT-IR spectrum, ν , cm^{-1} : 3264.93 ($\text{C}\equiv\text{N}$), 3333.15 (N-H), 3415.64 (sp^2 hybridized C-H bonds), 1579.96 ($\text{C}=\text{C}$ aromatic stretching vibrations). ^1H NMR (500 MHz, DMSO- d_6) δ (ppm): 6.99-8.20 (Ar-H), 4.74 (*s*, 1H, CH), 5.21 (*s*, 1H, NH_2). ^{13}C -NMR (62.9 MHz, DMSO- d_6) δ (ppm): 157.92, 158.15, 147.24, 136.13, 131.25, 130.55, 129.10, 128.34, 128.45, 127.38, 125.87, 123.81, 120.52, 116.12, 115.24, 114.87, 55.26.



4i

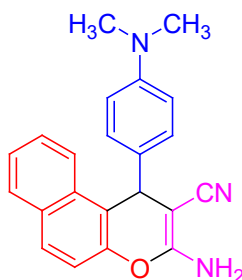
2-Amino-4-(thiophen-2-yl)-4-H-benzo[h]chromene-3-carbonitrile (4i): Yield 97%, yellow crystals, MP 267-268 °C; Lit. MP (265-269 °C). FT-IR spectrum, ν , cm^{-1} : 3187.81 ($\text{C}\equiv\text{N}$), 3316.27

(N-H), 3465.18 (sp^2 hybridized C-H bonds), 1597.38 (C=C aromatic stretching vibrations). ^1H NMR (500 MHz, DMSO- d_6) δ (ppm): 6.88-8.19 (Ar-H), 4.99 (*s*, 1H, CH), 5.37 (*s*, 1H, NH₂). ^{13}C -NMR (62.9 MHz, DMSO- d_6) δ (ppm): 156.82, 157.93, 146.91, 135.90, 130.86, 130.37, 130.07, 127.15, 127.93, 127.11, 125.53, 123.81, 120.17, 115.94, 115.13, 114.72, 55.15.



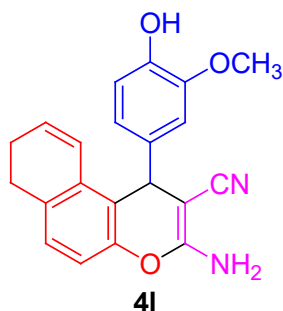
4j

2-Amino-4-(furan-2-yl)-4-H-benzo[h]chromene-3-carbonitrile (4j): Yield 96%, yellow crystals, MP 265-267 °C; Lit. MP (267-269 °C). FT-IR spectrum, ν , cm^{-1} : 3227.51 (C \equiv N), 3327.07 (N-H), 3417.26 (sp^2 hybridized C-H bonds), 1583.18 (C=C aromatic stretching vibrations). ^1H NMR (500 MHz, DMSO- d_6) δ (ppm): 6.27-7.89 (Ar-H), 5.19 (*s*, 1H, CH), 5.27 (*s*, 1H, NH₂). ^{13}C -NMR (62.9 MHz, DMSO- d_6) δ (ppm): 157.02, 158.23, 147.61, 136.83, 129.99, 130.27, 130.19, 128.29, 128.13, 127.38, 125.09, 123.88, 116.04, 116.73, 114.37, 55.15.



4k

2-amino-1-(4-(dimethylamino)phenyl)-4-H-benzo[h]chromene-3-carbonitrile (4k): Yield 97%, white crystals, MP 209-211 °C; Lit. MP (210-212 °C). FT-IR spectrum, ν , cm^{-1} : 3465.72 (C \equiv N), 3318.37 (N-H), 3437.43 (sp^2 hybridized C-H bonds), 1585.37 (C=C aromatic stretching vibrations). ^1H NMR (500 MHz, DMSO- d_6) δ (ppm): 7.67-7.17 (Ar-H), 5.76 (*s*, 1H, CH), 5.12 (*s*, 1H, NH₂). ^{13}C -NMR (62.9 MHz, DMSO- d_6) δ (ppm): 158.52, 153.40, 148.04, 146.34, 143.95, 138.16, 134.78, 133.46, 132.33, 130.54, 129.68, 128.54, 127.02, 124.42, 123.03, 122.43, 122.43, 121.94, 119.03, 67.54, 56.93, 44.83.



2-Amino-1-(4-hydroxy-3-methoxyphenyl)-1H-benzo[ff]chromene-2-carbonitrile (41): Yield 96%, yellow crystals, MP 163-165 °C; Lit. MP (160-164 °C) FT-IR spectrum, ν , cm^{-1} : 2218.35 ($\text{C}\equiv\text{N}$), 3127.74 (N-H), 3421.67 (sp^2 hybridized C-H bonds), 3362.14 (O-H bending), 1585.85 ($\text{C}=\text{C}$ aromatic stretching vibrations). ^1H -NMR spectrum, δ , ppm (J , Hz): 6.40-7.76 (Ar-H), 5.24 (*s*, 1H, CH), 6.40 (*s*, 1H, NH_2), 3.95 (*s*, 1H, OCH_3). ^{13}C -NMR spectrum, δ , ppm: 159.34, 153.42, 152.17, 147.07, 134.61, 129.83, 129.03, 128.93, 127.77, 126.52, 126.37, 124.00, 123.60, 117.78, 115.24, 114.42, 113.64, 110.46, 109.50, 56.22.

3. SEM Characterization

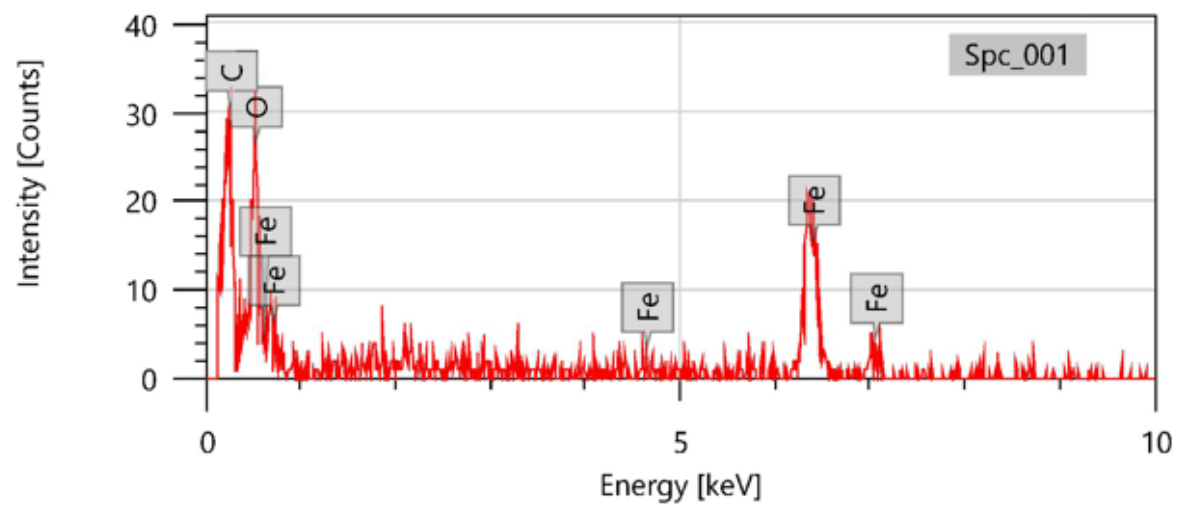


Figure S1. Energy-Dispersive X-ray Spectroscopy (EDS) spectra of CG-Fe₂O₃ NPs.

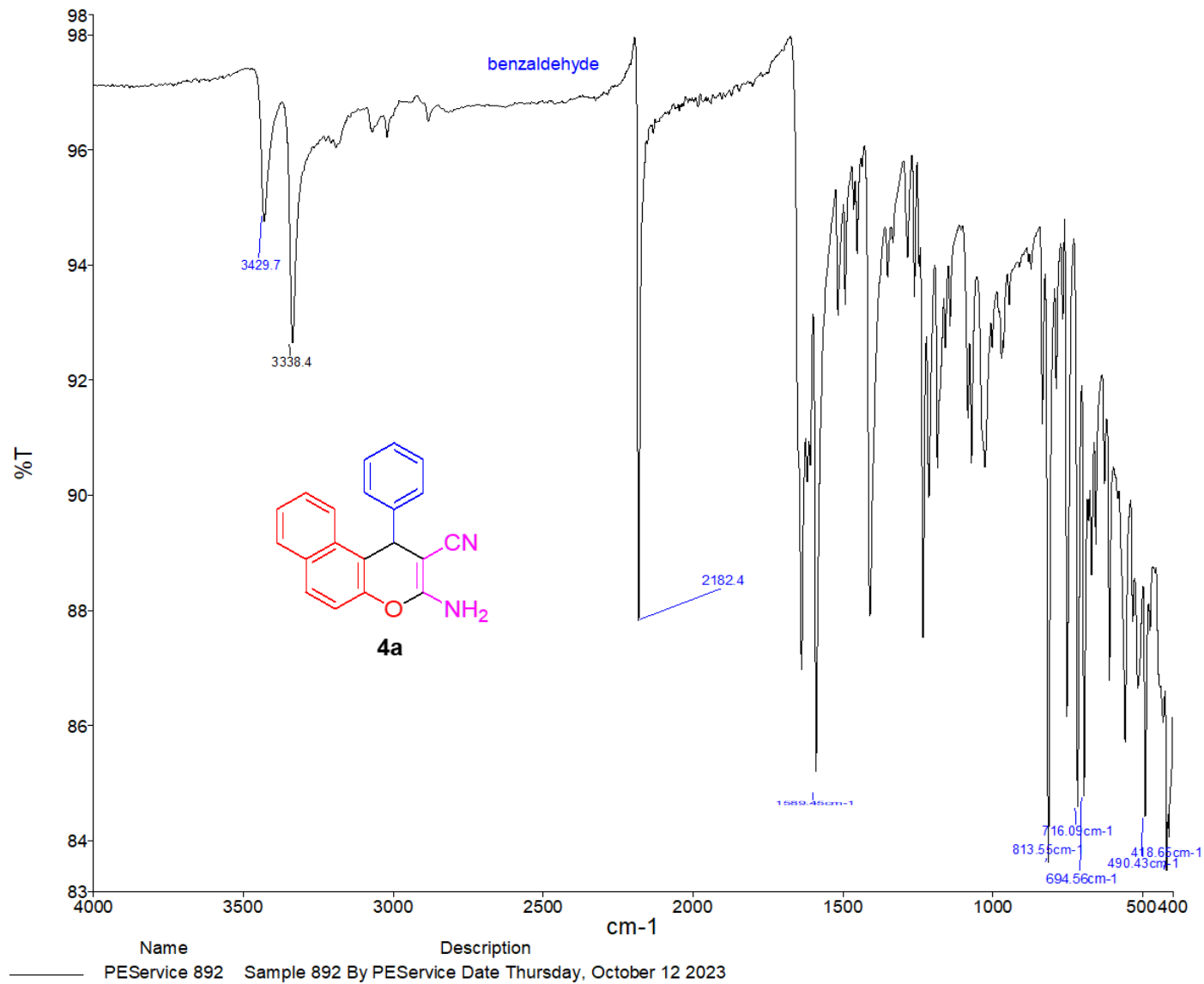


Figure S2. FT-IR spectrum of 2-Amino-4-phenyl-4H-benzo[h]chromene-3-carbonitrile (**4a**).

R2

1H_8scan DMSO {D:\Spectra} nmr 47

BRUKER
AVANCE NEO
500 MHz NMR
SPECTROMETER
SAIF, P.U.

Current Data Parameters
NAME Nov07-2023
EXPNO 470
PROCNO 1

F2 - Acquisition Parameters
Date_ 20231108
Time 3.43 h
INSTRUM Avance Neo 500
PROBHD Z119470 0333 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 64
DS 0
SWH 14705.883 Hz
FIDRES 0.448788 Hz
AQ 2.2282240 sec
RG 95.7854
DW 34.000 usec
DE 6.79 usec
TE 300.2 K
D1 1.00000000 sec
TD0 1
SFO1 500.1730885 MHz
NUC1 1H
P0 3.33 usec
P1 10.00 usec
PLW1 20.93000031 W

F2 - Processing parameters
SI 65536
SF 500.1699987 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

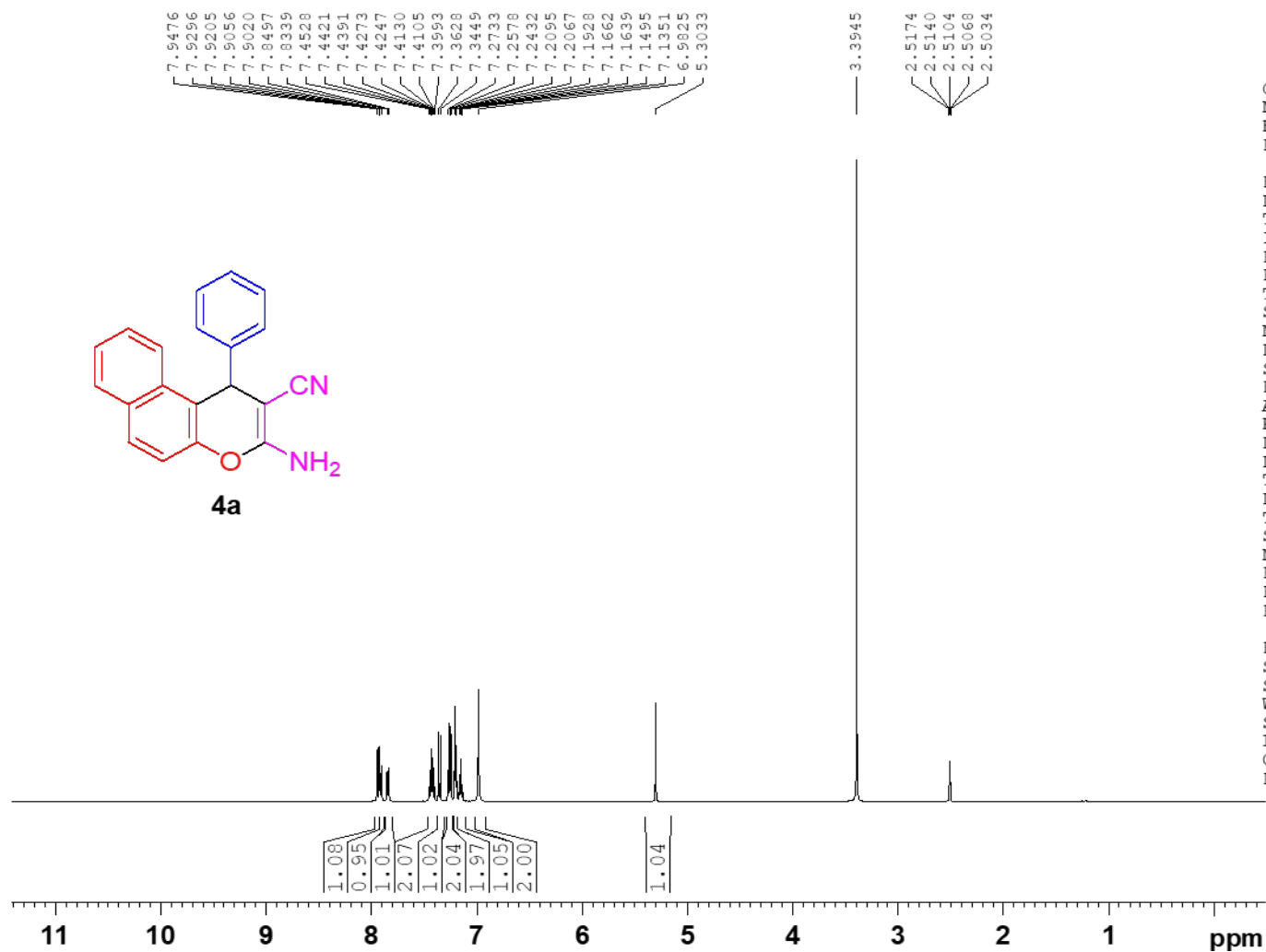


Figure S3. ¹H-NMR spectrum of 2-Amino-4-phenyl-4H-benzo[h]chromene-3-carbonitrile (**4a**).

R II
C13CPD DMSO {D:\Spectra} nmr 20

BRUKER
AVANCE NEO
500 MHz NMR SPECTROMETER
SAIF, PANJAB UNIVERSITY,
CHANDIGARH

Current Data Parameters
NAME Dec06-2023
EXPNO 201
PROCNO 1

F2 - Acquisition Parameters
Date_ 20231206
Time 15.34 h
INSTRUM Avance Neo 500
PROBHD z119470_0333 (zpgpg30)
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 512
DS 4
SWH 37037.035 Hz
FIDRES 1.130281 Hz
AQ 0.8847360 sec
RG 101
DW 13.500 usec
DE 6.50 usec
TE 300.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.7804233 MHz
NUC1 13C
P0 3.33 usec
P1 10.00 usec
PLW1 83.14099884 W
SFO2 500.1720007 MHz
NUC2 1H
CPDPRG[2] waltz65
PCPD2 80.00 usec
PLW2 20.93000031 W
PLW12 0.32703000 W
PLW13 0.16449000 W

F2 - Processing parameters
SI 32768
SF 125.7679179 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

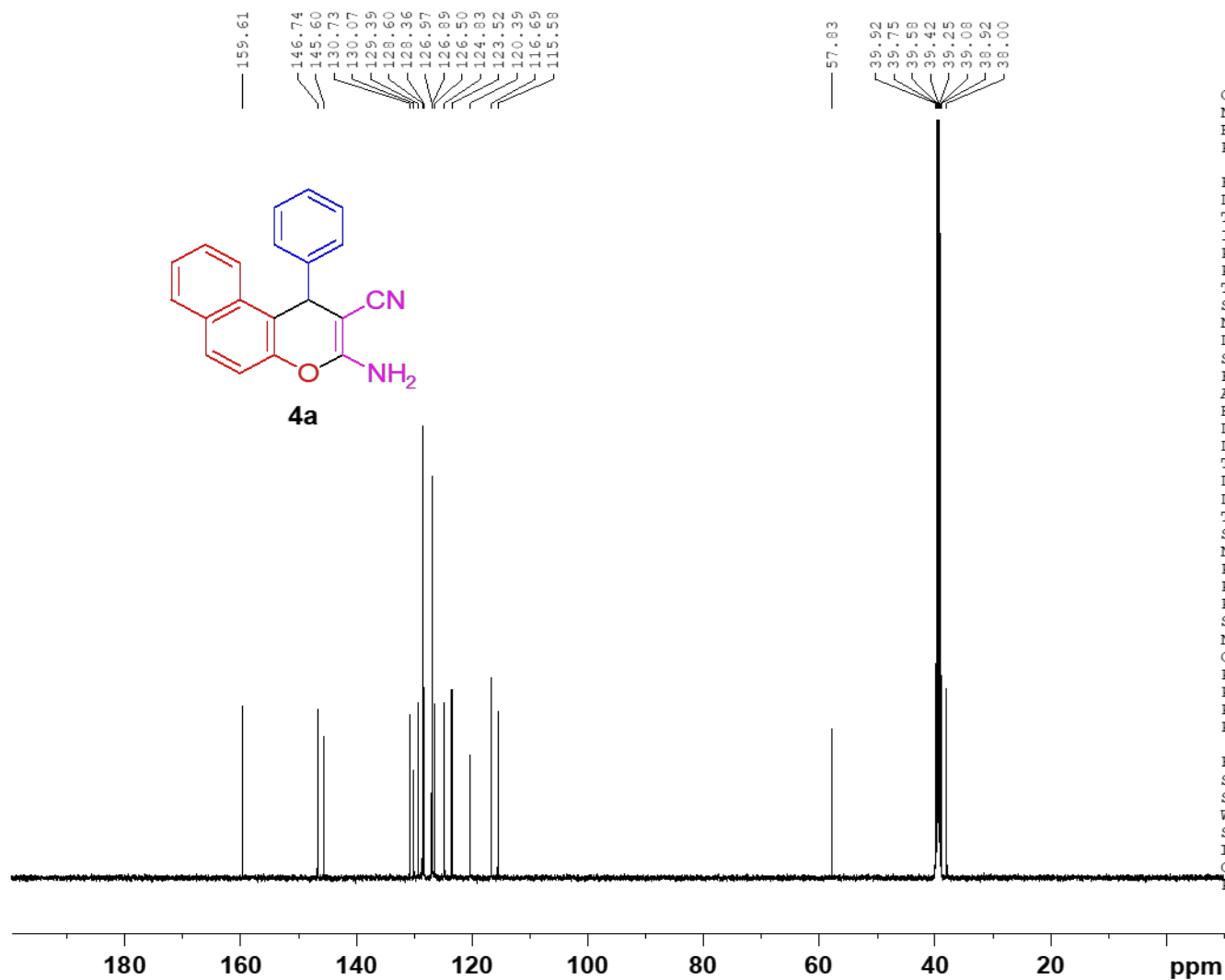


Figure S4. ¹³C-NMR spectrum of 2-Amino-4-phenyl-4H-benzo[h]chromene-3-carbonitrile (4a).

R II
C13CPD DMSO {D:\Spectra} nmr 20

BRUKER
AVANCE NEO
500 MHz NMR SPECTROMETER
SAIF, PANJAB UNIVERSITY,
CHANDIGARH

Current Data Parameters
NAME Dec06-2023
EXPNO 201
PROCNO 1

F2 - Acquisition Parameters
Date_ 20231206
Time 15.34 h
INSTRUM Avance Neo 500
PROBHD z119470_0333 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 512
DS 4
SWH 37037.035 Hz
FIDRES 1.130281 Hz
AQ 0.8847360 sec
RG 101
DW 13.500 usec
DE 6.50 usec
TE 300.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.7804233 MHz
NUC1 13C
P0 3.33 usec
P1 10.00 usec
PLW1 83.14099884 W
SFO2 500.1720007 MHz
NUC2 1H
CPDPRG[2] waltz65
PCPD2 80.00 usec
PLW2 20.93000031 W
PLW12 0.32703000 W
PLW13 0.16449000 W

F2 - Processing parameters
SI 32768
SF 125.7679179 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

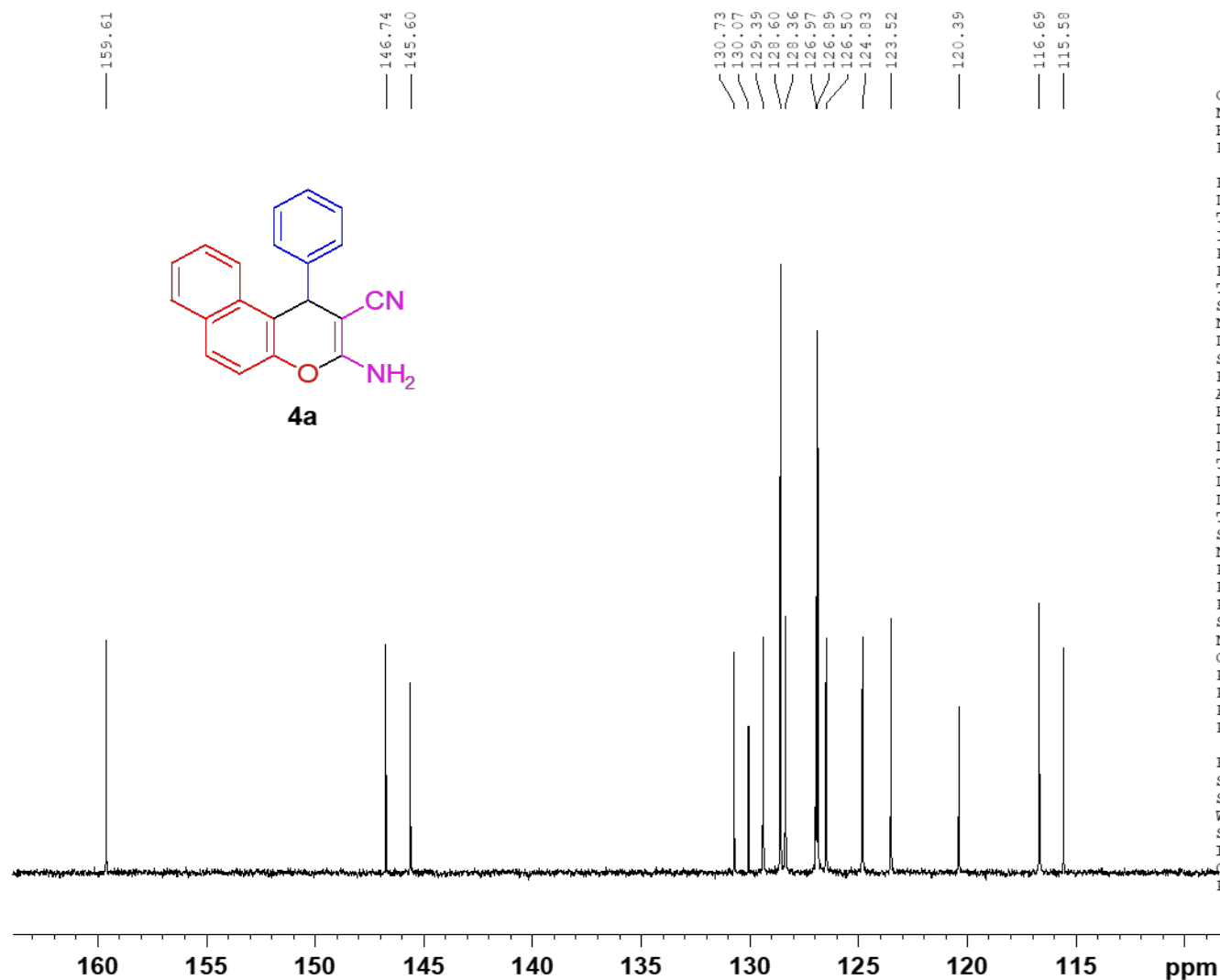


Figure S5. ¹³C-NMR expanded spectrum of 2-Amino-4-phenyl-4H-benzo[h]chromene-3-carbonitrile (4a).

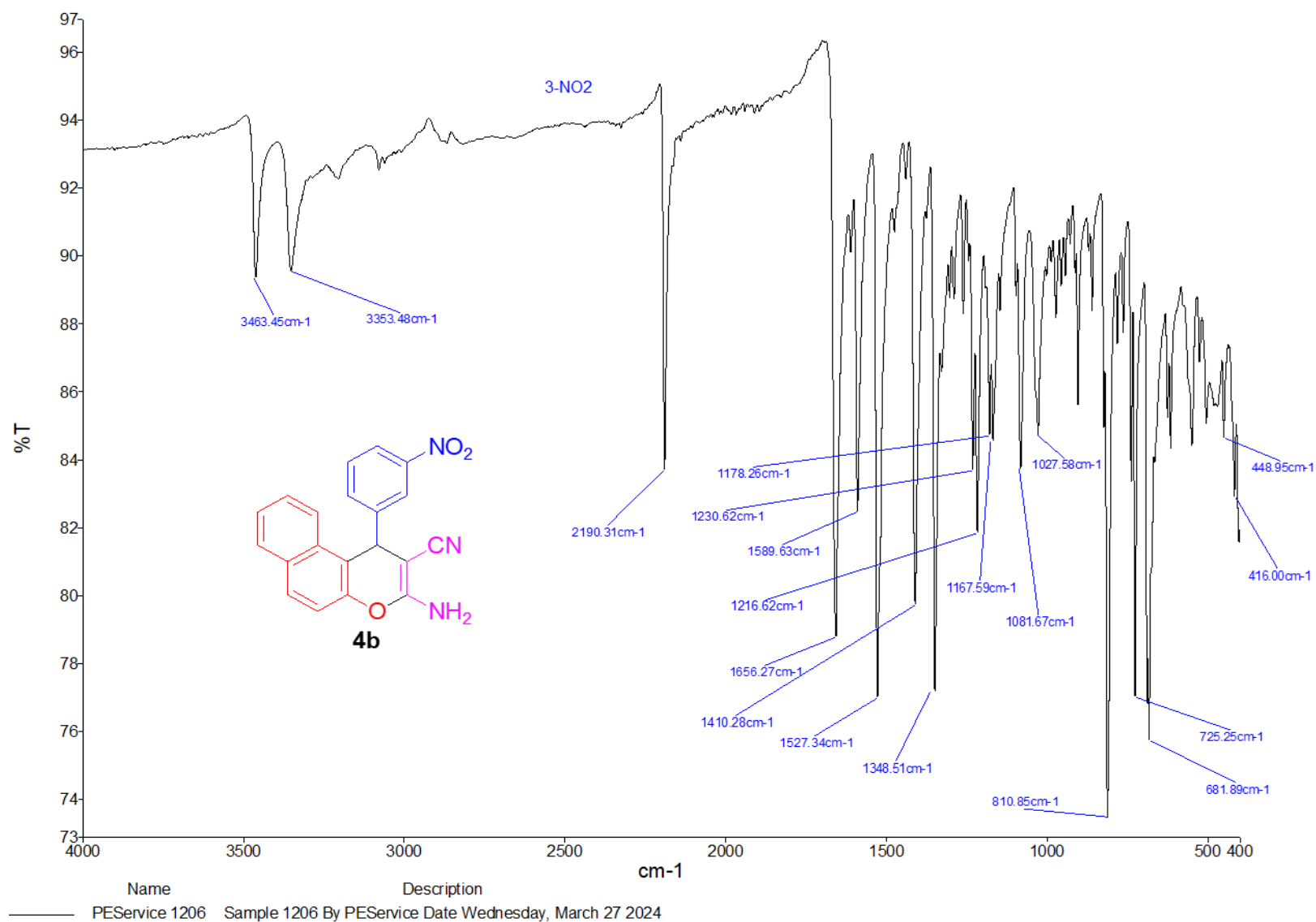


Figure S6. FT-IR spectrum of 2-Amino-4-(3-nitrophenyl)-4H-benzo[h]chromene-3-carbonitrile (**4b**).

9-1025
8-0990
8-0955
8-0133
8-0105
7-9970
7-9941
7-9572
7-9532
7-9899
7-8822
7-8686
7-8518
7-6800
7-6644
7-5554
7-5395
7-5237
7-4565
7-4425
7-4282
7-4259
7-4075
7-3911
7-3772
7-3730
7-1901
5-1628

```
Current Data Parameters
NAME           Mar15-2024
EXPNO           100
PROCNO           1
```

```
F2 - Processing parameters
SI                65536
SF                500.1700040 MHz
WDW               EM
SSB               0
LB                0.30 Hz
GB                0
PC                1.00
```

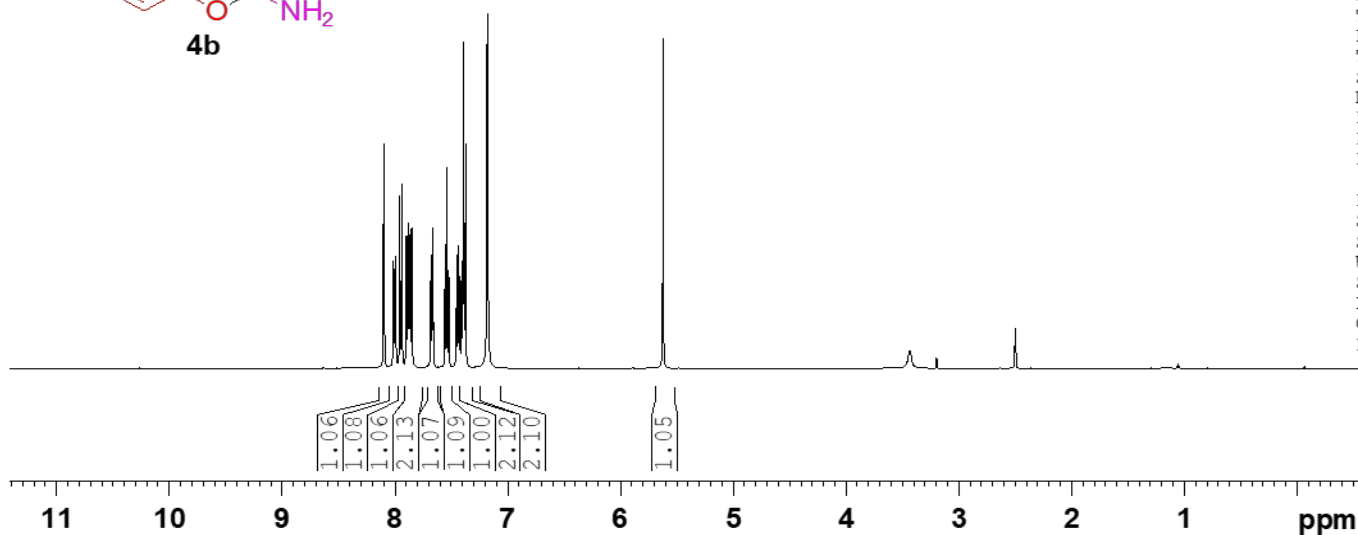


Figure S7. ^1H -NMR spectrum of 2-Amino-4-(3-nitrophenyl)-4H-benzo[h]chromene-3-carbonitrile (**4b**).

3NO2
1H_8scan DMSO {D:\Spectra} nmr 10

BRUKER
AVANCE NEO
500 MHz NMR
SPECTROMETER
SAIF, P.U.

Current Data Parameters
NAME Mar15-2024
EXPNO 100
PROCNO 1

F2 - Acquisition Parameters
Date_ 20240315
Time_ 9.45 h
INSTRUM Avance Neo 500
PROBHD Z119470_0333 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 0
SWH 14705.883 Hz
FIDRES 0.448788 Hz
AQ 2.2282240 sec
RG 46.858
DW 34.000 usec
DE 6.79 usec
TE 300.2 K
D1 1.00000000 sec
TD0 1
SFO1 500.1730885 MHz
NUC1 1H
P0 3.33 usec
P1 10.00 usec
PLW1 20.93000031 W

F2 - Processing parameters
SI 65536
SF 500.1700040 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

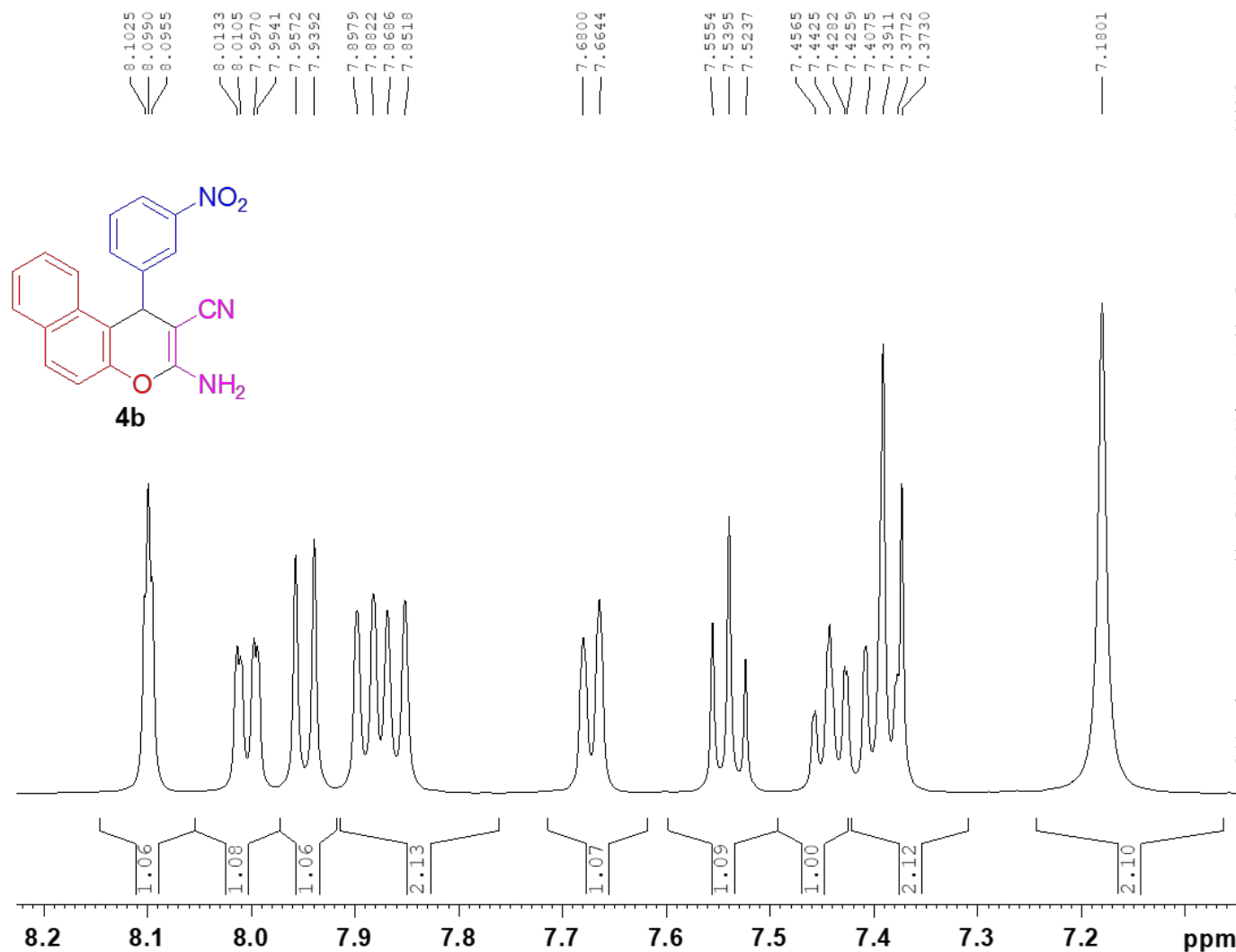
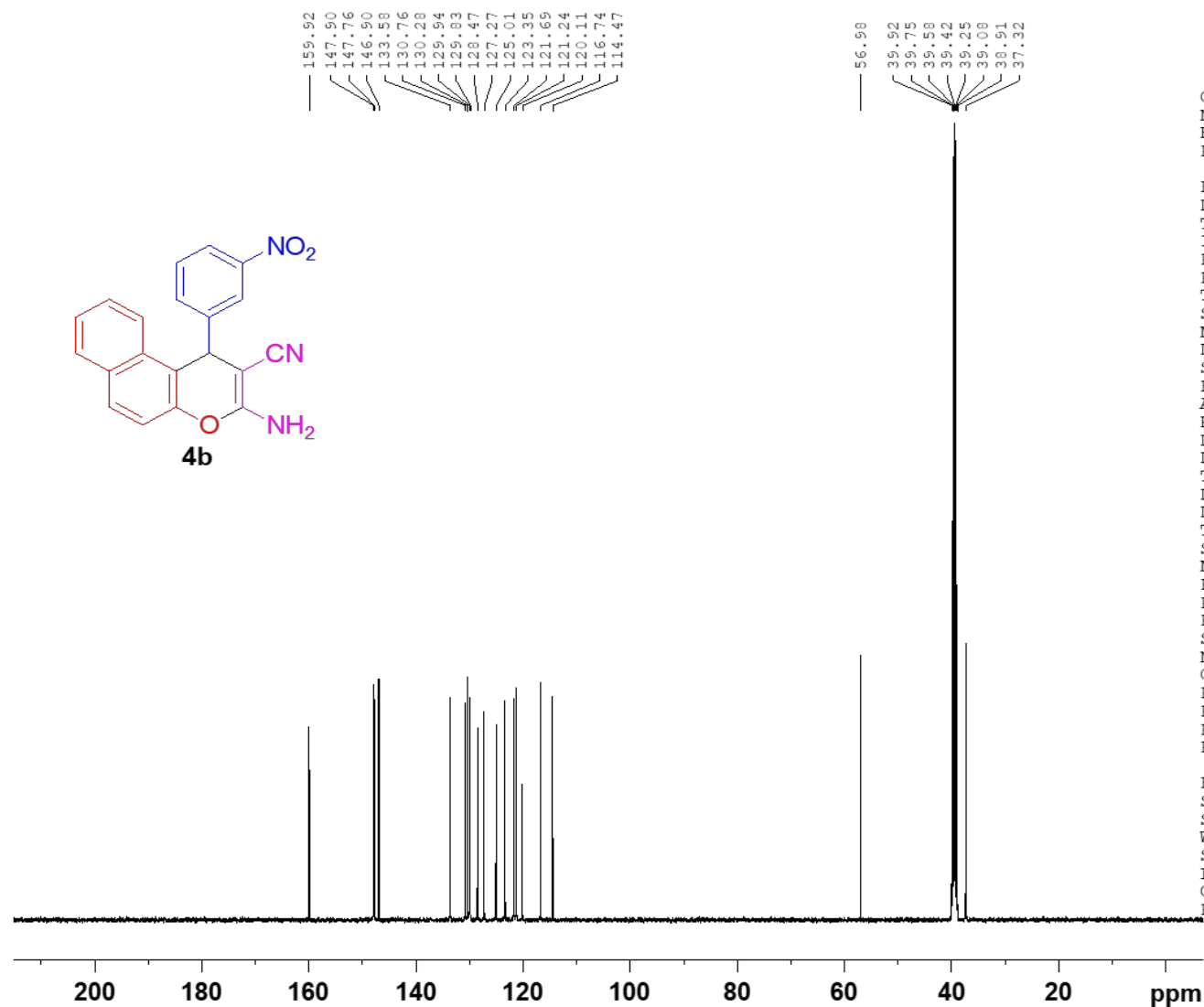
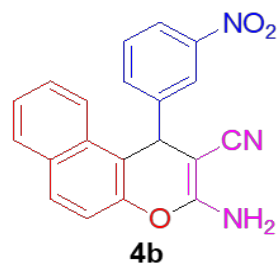


Figure S8. ¹H-NMR expanded spectrum of 2-Amino-4-(3-nitrophenyl)-4H-benzo[h]chromene-3-carbonitrile (**4b**).

3NO2
C13CPD DMSO {D:\Spectra} nmr 10



BRUKER
AVANCE NEO
500 MHz NMR SPECTROMETER
SAIF, PANJAB UNIVERSITY,
CHANDIGARH

Current Data Parameters
NAME Mar15-2024
EXPNO 101
PROCNO 1

F2 - Acquisition Parameters
Date_ 20240315
Time_ 11.21 h
INSTRUM Avance Neo 500
PROBHD Z119470_0333 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 256
DS 4
SWH 37037.035 Hz
FIDRES 1.130281 Hz
AQ 0.8847360 sec
RG 101
DW 13.500 usec
DE 6.50 usec
TE 300.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.7804233 MHz
NUC1 13C
P0 3.33 usec
P1 10.00 usec
PLW1 83.14099884 W
SFO2 500.1720007 MHz
NUC2 1H
CPDPRG2 waltz65
PCPD2 80.00 usec
PLW2 20.93000031 W
PLW12 0.32703000 W
PLW13 0.16449000 W

F2 - Processing parameters
SI 32768
SF 125.7679185 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Figure S9. ¹³C-NMR spectrum of 2-Amino-4-(3-nitrophenyl)-4H-benzo[h]chromene-3-carbonitrile (**4b**).

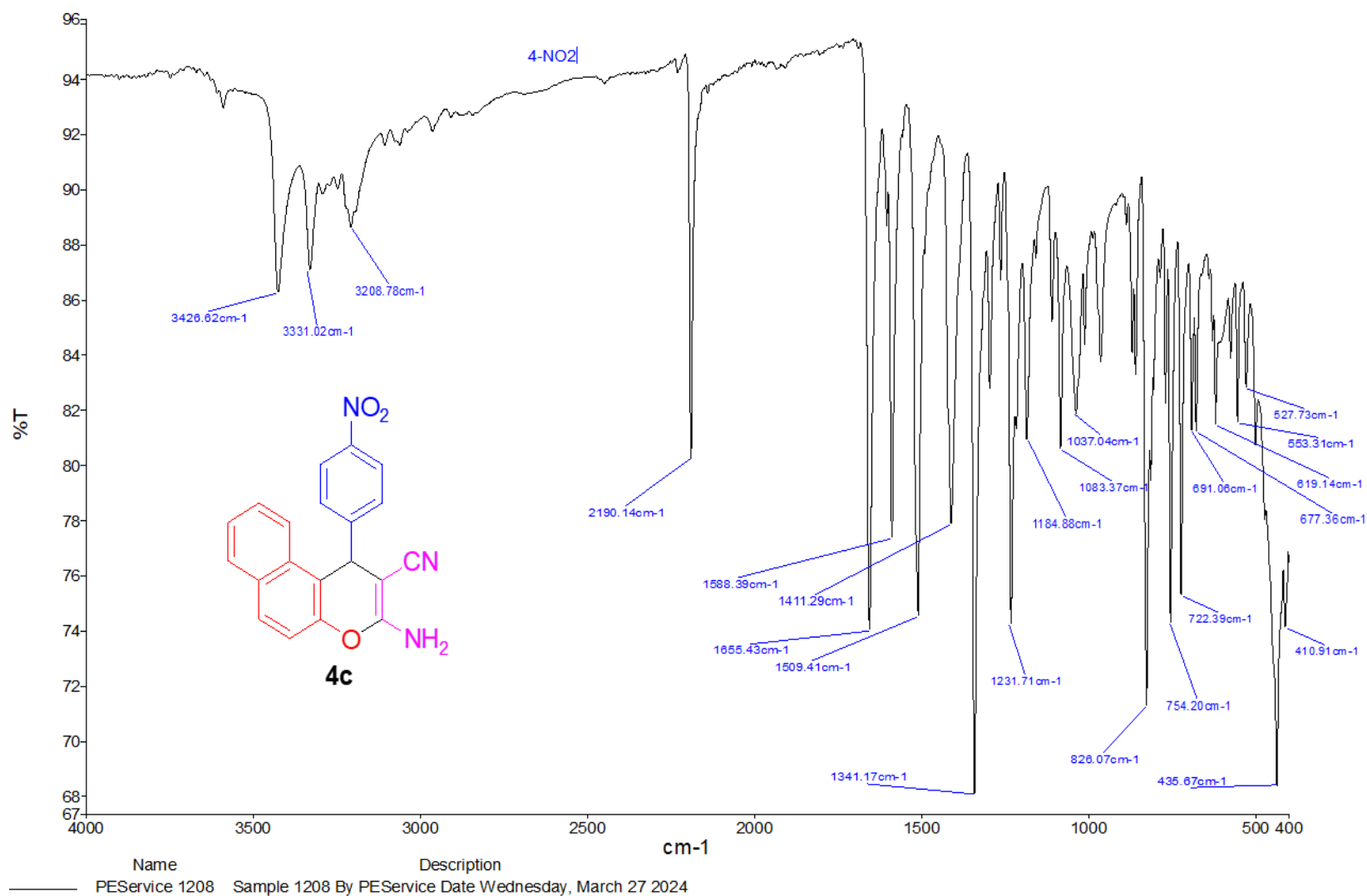


Figure S10. FT-IR spectrum of 2-Amino-4-(4-nitrophenyl)-4H-benzo[h]chromene-3-carbonitrile (**4c**).

4-NO2

1H_8scan DMSO {D:\Spectra} nmr 39

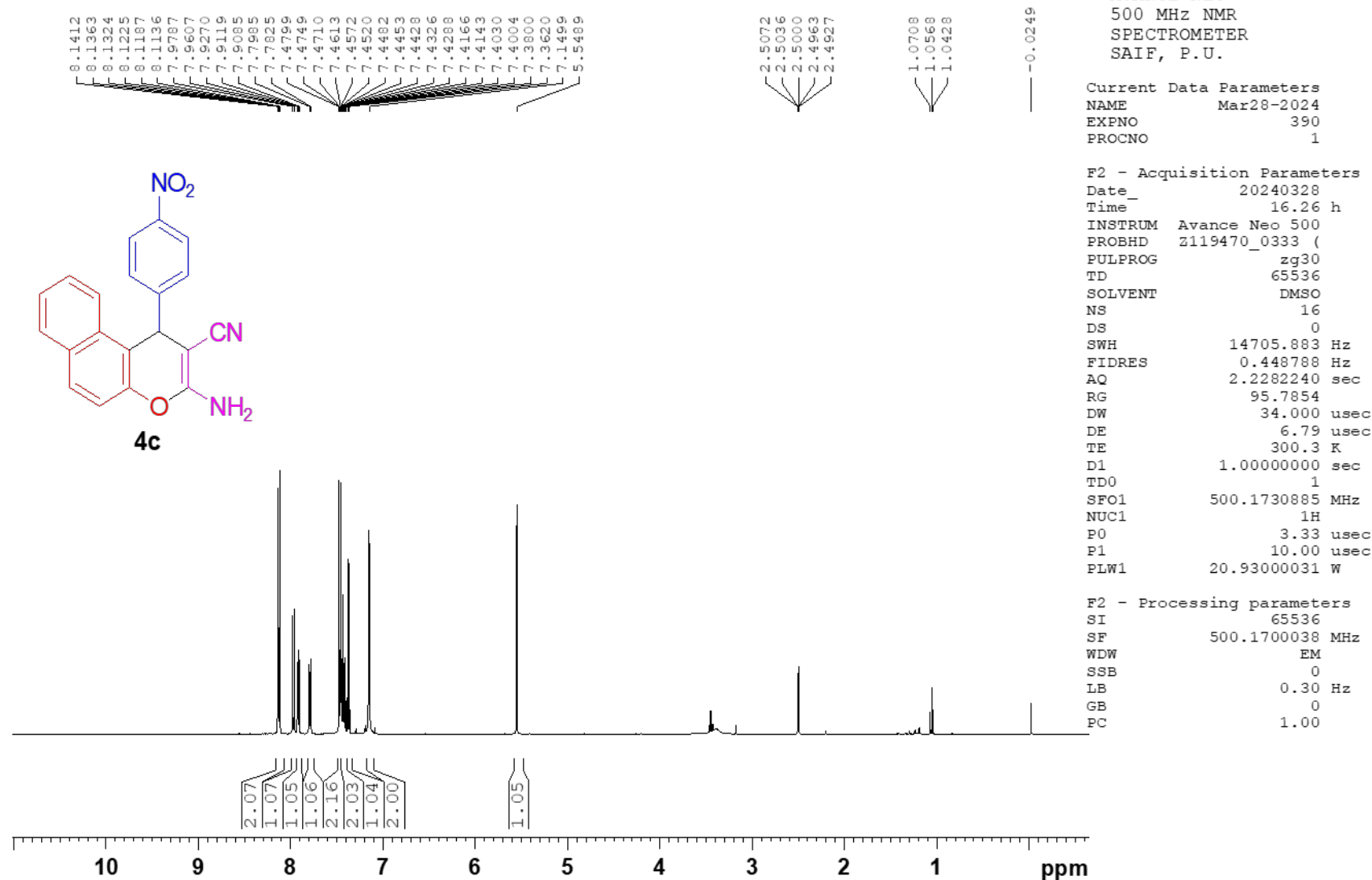


Figure S11. ¹H-NMR spectrum of 2-Amino-4-(4-nitrophenyl)-4H-benzo[h]chromene-3-carbonitrile (**4c**).

4-NO2

1H_8scan DMSO {D:\Spectra} nmr 39

BRUKER
AVANCE NEO
500 MHz NMR
SPECTROMETER
SAIF, P.U.

Current Data Parameters
NAME Mar28-2024
EXPNO 390
PROCNO 1

F2 - Acquisition Parameters
Date_ 20240328
Time 16.26 h
INSTRUM Avance Neo 500
PROBHD z119470_0333 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 0
SWH 14705.883 Hz
FIDRES 0.448788 Hz
AQ 2.2282240 sec
RG 95.7854
DW 34.000 usec
DE 6.79 usec
TE 300.3 K
D1 1.00000000 sec
TD0 1
SFO1 500.1730885 MHz
NUC1 1H
P0 3.33 usec
P1 10.00 usec
PLW1 20.93000031 W

F2 - Processing parameters
SI 65536
SF 500.1700038 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

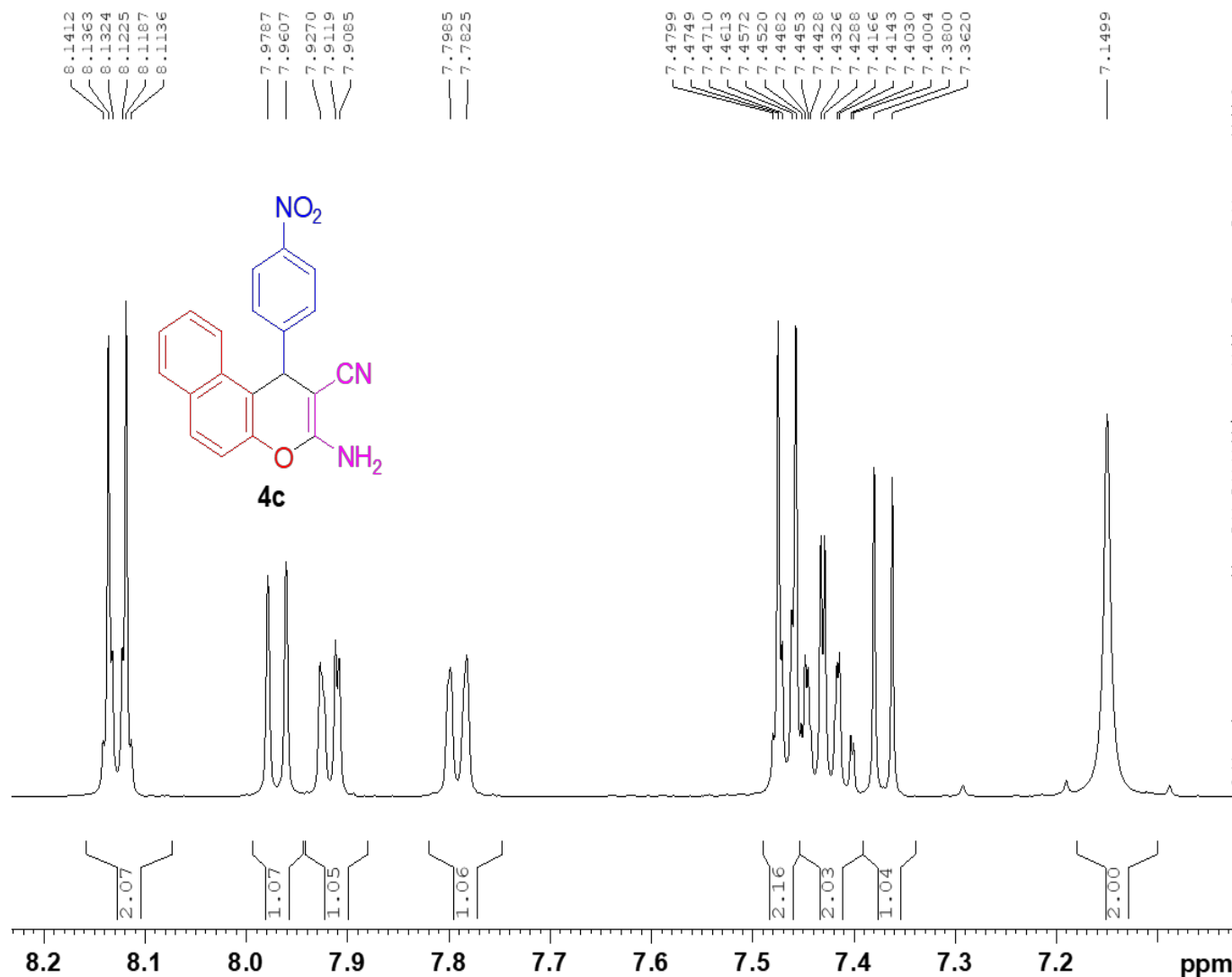
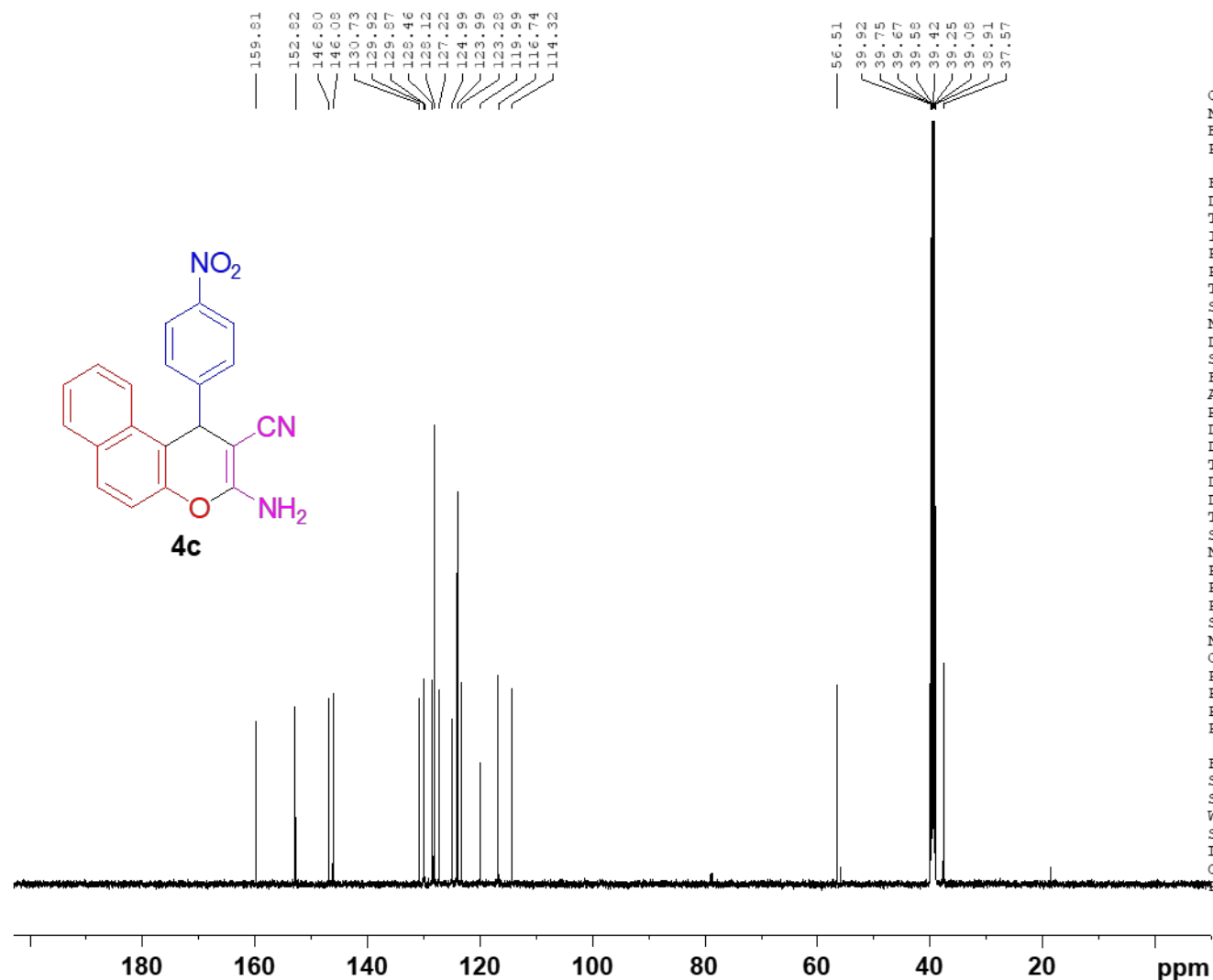


Figure S12. ¹H-NMR expanded spectrum of 2-Amino-4-(4-nitrophenyl)-4H-benzo[h]chromene-3-carbonitrile (4c).

4-NO2
C13CPD DMSO {D:\Spectra} nmr 39



BRUKER
AVANCE NEO
500 MHz NMR SPECTROMETER
SAIF, PANJAB UNIVERSITY,
CHANDIGARH

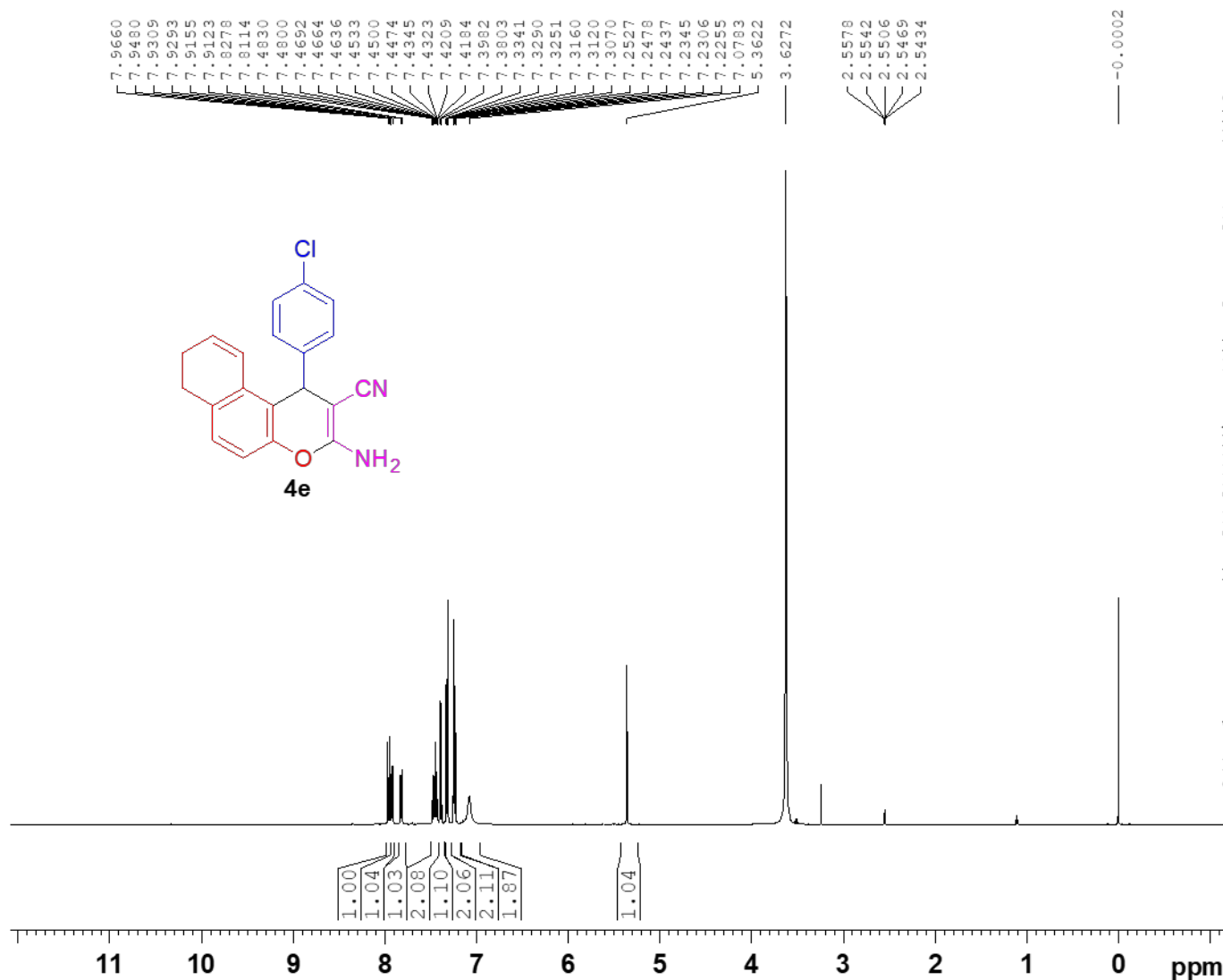
Current Data Parameters
NAME Mar28-2024
EXPNO 391
PROCNO 1

F2 - Acquisition Parameters
Date_ 20240329
Time 9.02 h
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PROBHD Z119470_0333 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 256
DS 4
SWH 37037.035 Hz
FIDRES 1.130281 Hz
AQ 0.8847360 sec
RG 101
DW 13.500 usec
DE 6.50 usec
TE 300.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.7804233 MHz
NUC1 13C
P0 3.33 usec
P1 10.00 usec
PLW1 83.14099884 W
SFO2 500.1720007 MHz
NUC2 1H
CPDPRG[2] waltz65
PCPD2 80.00 usec
PLW2 20.93000031 W
PLW12 0.32703000 W
PLW13 0.16449000 W

F2 - Processing parameters
SI 32768
SF 125.7679207 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Figure S13. ¹³C-NMR spectrum of 2-Amino-4-(4-nitrophenyl)-4H-benzo[h]chromene-3-carbonitrile (**4c**).

4CL
1H_8scan DMSO {D:\Spectra} nmr 22



BRUKER
AVANCE NEO
500 MHz NMR
SPECTROMETER
SAIF, P.U.

Current Data Parameters
NAME Jul30-2024
EXPNO 220
PROCNO 1

F2 - Acquisition Parameters
Date 20240730
Time 19.21 h
INSTRUM Avance Neo 500
PROBHD Z119470_0333 (PULPROG zg30)
TD 65536
SOLVENT DMSO
NS 16
DS 0
SWH 14705.883 Hz
FIDRES 0.448788 Hz
AQ 2.2282240 sec
RG 32.6666
DW 34.000 usec
DE 6.79 usec
TE 300.2 K
D1 1.00000000 sec
TD0 1
SFO1 500.1730885 MHz
NUC1 1H
P0 3.33 usec
P1 10.00 usec
PLW1 20.93000031 W

F2 - Processing parameters
SI 65536
SF 500.1699787 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Figure S14. ¹H-NMR spectrum of 2-Amino-4-(4-chlorophenyl)-4-H-benzo[g] chromene-3-carbonitrile (**4e**).

4CL
1H_8scan DMSO {D:\Spectra} nmr 22

BRUKER
AVANCE NEO
500 MHz NMR
SPECTROMETER
SAIF, P.U.

Current Data Parameters
NAME Jul30-2024
EXPNO 220
PROCNO 1

F2 - Acquisition Parameters
Date 20240730
Time 19.21 h
INSTRUM Avance Neo 500
PROBHD Z119470_0333 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 0
SWH 14705.883 Hz
FIDRES 0.448788 Hz
AQ 2.2282240 sec
RG 32.6666
DW 34.000 usec
DE 6.79 usec
TE 300.2 K
D1 1.00000000 sec
TD0 1
SFO1 500.1730885 MHz
NUC1 1H
P0 3.33 usec
P1 10.00 usec
PLW1 20.93000031 W

F2 - Processing parameters
SI 65536
SF 500.1699787 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

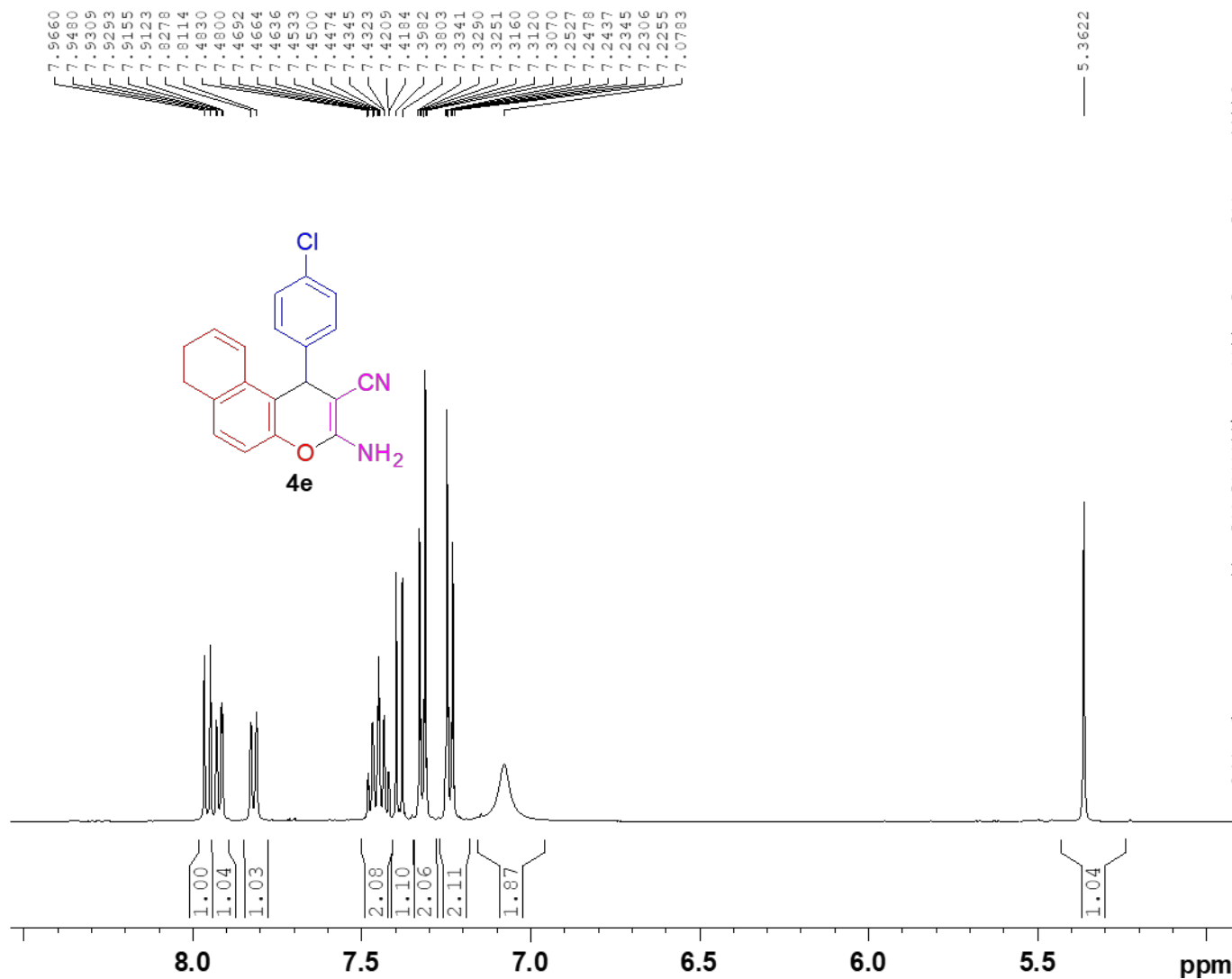


Figure S15. ¹H-NMR expanded spectrum of 2-Amino-4-(4-chlorophenyl)-4-H-benzo[g] chromene-3-carbonitrile (**4e**).

4CL
C13CPD DMSO {D:\Spectra} nmr 22

BRUKER
AVANCE NEO
500 MHz NMR SPECTROMETER
SAIF, PANJAB UNIVERSITY,
CHANDIGARH

Current Data Parameters
NAME Jul30-2024
EXPNO 221
PROCNO 1

F2 - Acquisition Parameters
Date_ 20240730
Time_ 19.47 h
INSTRUM Avance Neo 500
PROBHD Z119470_0333 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 512
DS 4
SWH 37037.035 Hz
FIDRES 1.130281 Hz
AQ 0.8847360 sec
RG 101
DW 13.500 usec
DE 6.50 usec
TE 300.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.7804233 MHz
NUC1 13C
P0 3.33 usec
P1 10.00 usec
PLW1 83.14099884 W
SFO2 500.1720007 MHz
NUC2 1H
CPDPRG[2] waltz65
PCPD2 80.00 usec
PLW2 20.93000031 W
PLW12 0.32703000 W
PLW13 0.16449000 W

F2 - Processing parameters
SI 32768
SF 125.7679005 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

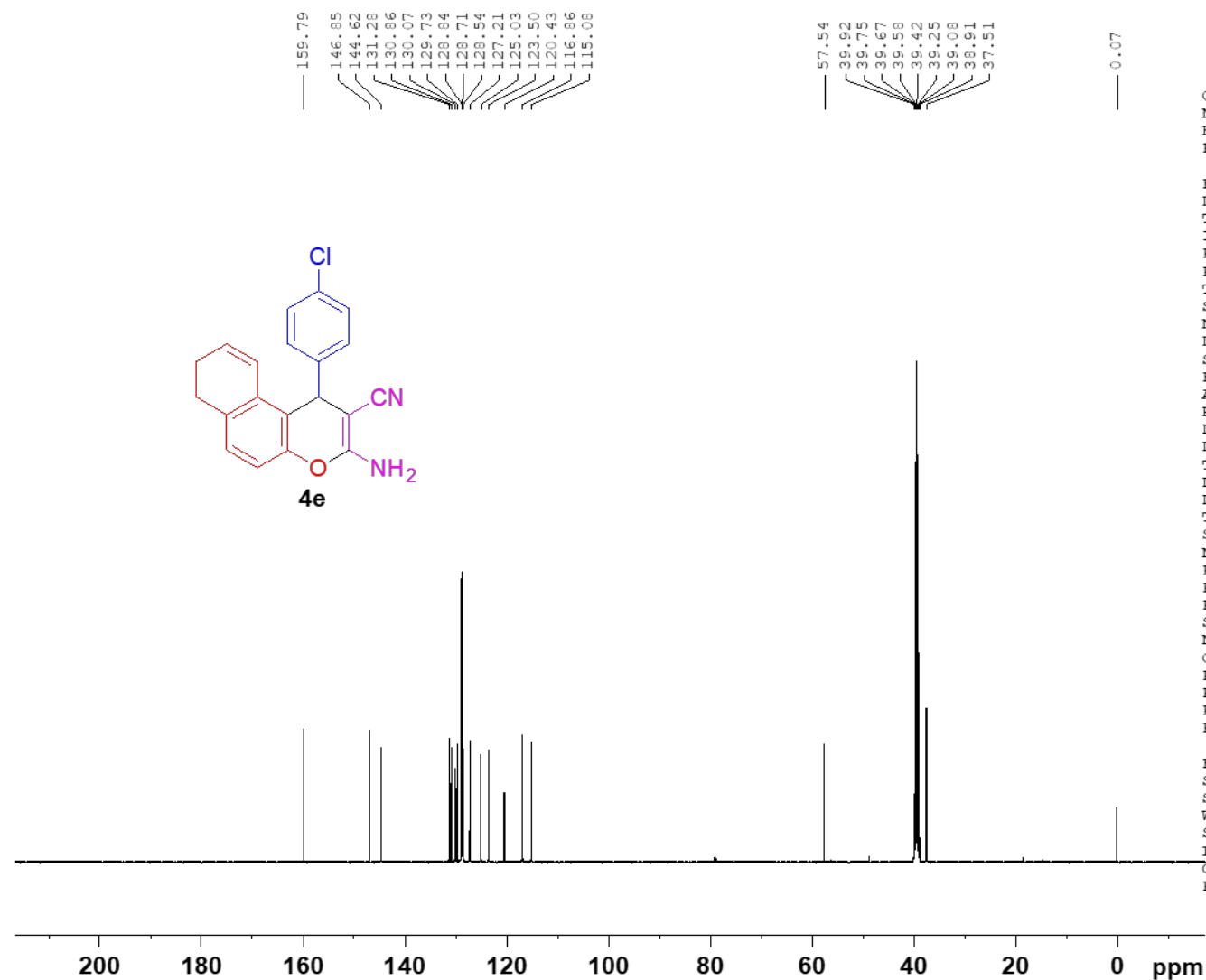


Figure S16. ¹³C-NMR spectrum of 2-Amino-4-(4-chlorophenyl)-4-H-benzo[g] chromene-3-carbonitrile (**4e**).

4CL
C13CPD DMSO {D:\Spectra} nmr 22

BRUKER
AVANCE NEO
500 MHz NMR SPECTROMETER
SAIF, PANJAB UNIVERSITY,
CHANDIGARH

Current Data Parameters
NAME Jul30-2024
EXPNO 221
PROCNO 1

F2 - Acquisition Parameters
Date_ 20240730
Time 19.47 h
INSTRUM Avance Neo 500
PROBHD Z119470_0333 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 512
DS 4
SWH 37037.035 Hz
FIDRES 1.130281 Hz
AQ 0.8847360 sec
RG 101
DW 13.500 usec
DE 6.50 usec
TE 300.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.7804233 MHz
NUC1 13C
P0 3.33 usec
P1 10.00 usec
PLW1 83.14099884 W
SFO2 500.1720007 MHz
NUC2 1H
CPDPRG[2] waltz65
PCPD2 80.00 usec
PLW2 20.93000031 W
PLW12 0.32703000 W
PLW13 0.16449000 W

F2 - Processing parameters
SI 32768
SF 125.7679005 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

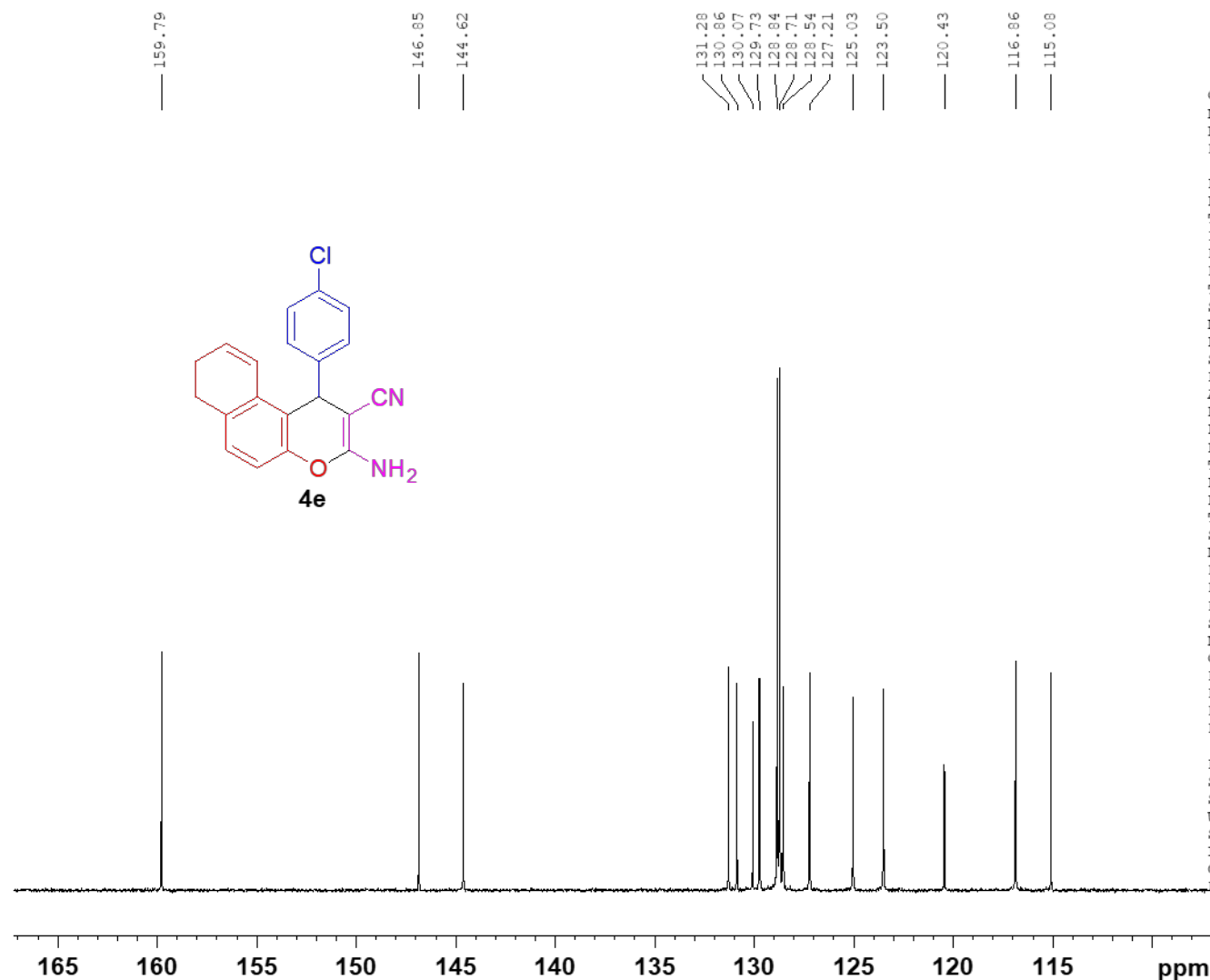


Figure S17. ^{13}C -NMR expanded spectrum of 2-Amino-4-(4-chlorophenyl)-4-H-benzo[g] chromene-3-carbonitrile (**4e**).

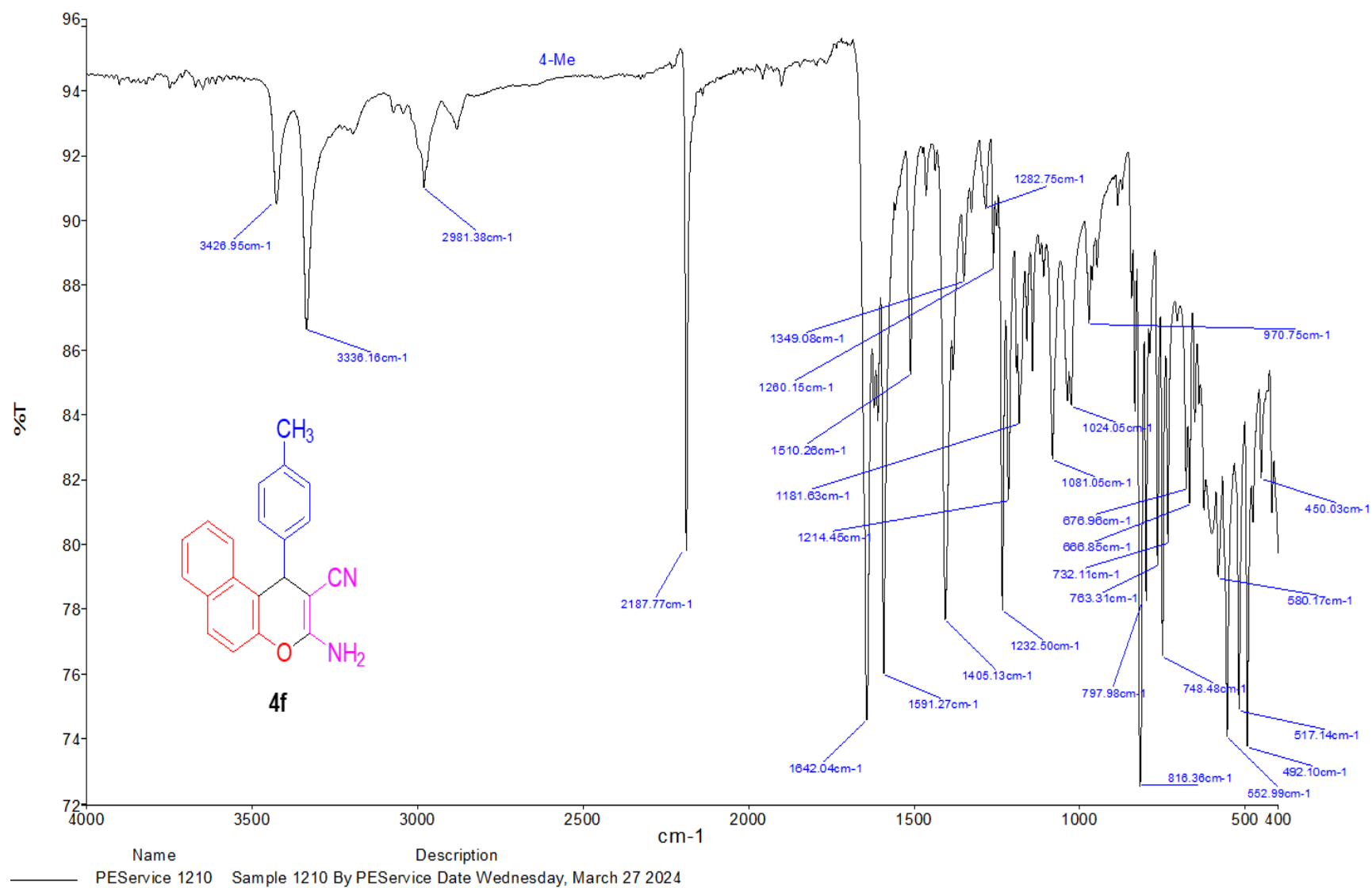


Figure S18. FT-IR spectrum of 2-Amino-4-p-tolyl-4H-benzo[h]chromene-3-carbonitrile (**4f**).

4Me
1H_8scan DMSO {D:\Spectra} nmr 9

BRUKER
AVANCE NEO
500 MHz NMR
SPECTROMETER
SAIF, P.U.

Current Data Parameters
NAME Mar15-2024
EXPNO 90
PROCNO 1

F2 - Acquisition Parameters
Date_ 20240315
Time 9.43 h
INSTRUM Avance Neo 500
PROBHD Z119470_0333 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 0
SWH 14705.883 Hz
FIDRES 0.448788 Hz
AQ 2.2282240 sec
RG 48.9649
DW 34.000 usec
DE 6.79 usec
TE 300.2 K
D1 1.00000000 sec
TD0 1
SFO1 500.1730885 MHz
NUC1 1H
P0 3.33 usec
P1 10.00 usec
PLW1 20.93000031 W

F2 - Processing parameters
SI 65536
SF 500.1699986 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

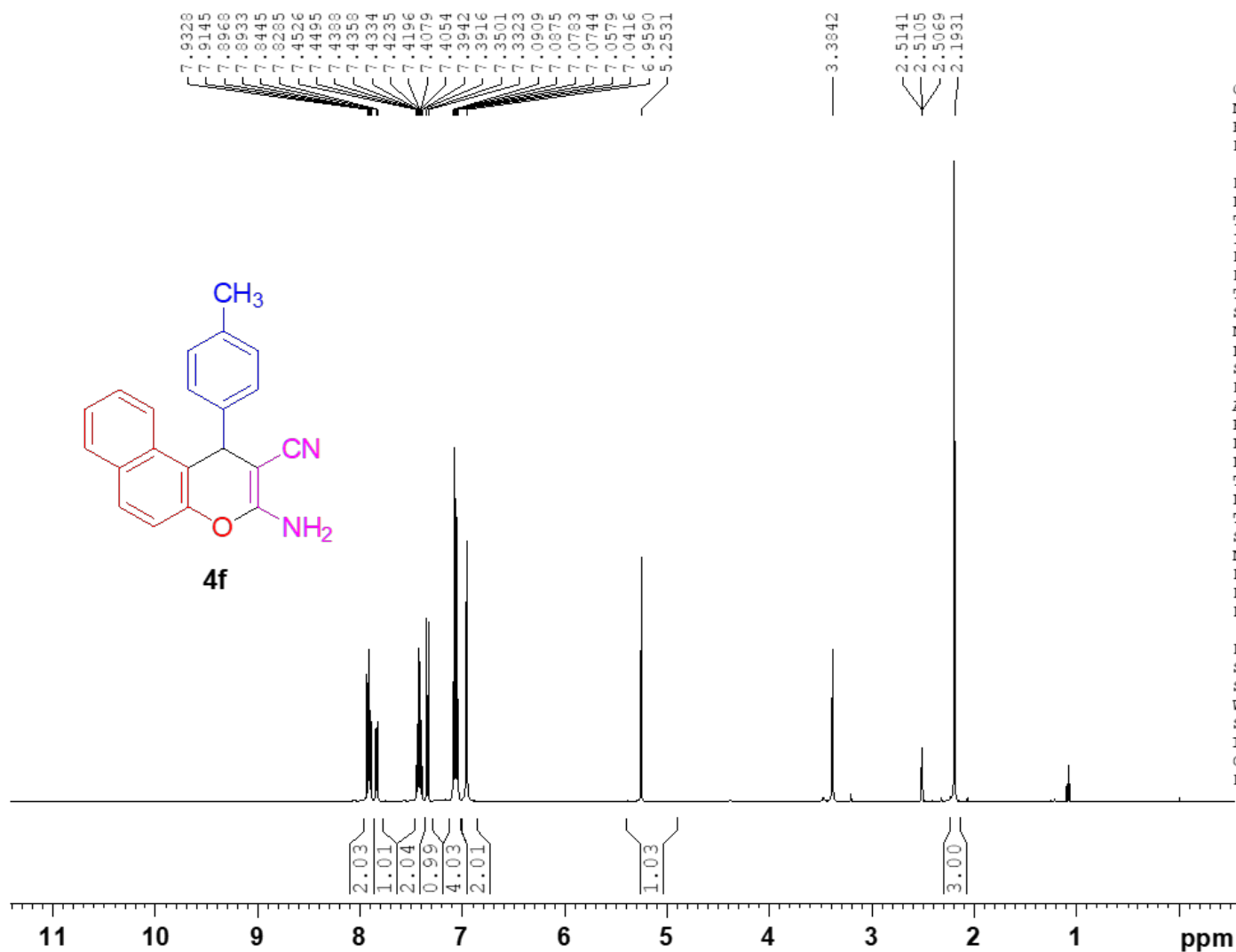


Figure S19. ¹H-NMR spectrum of 2-Amino-4-p-tolyl-4H-benzo[h]chromene-3-carbonitrile (**4f**).

4Me
1H_8scan DMSO {D:\Spectra} nmr 9

BRUKER
AVANCE NEO
500 MHz NMR
SPECTROMETER
SAIF, P.U.

Current Data Parameters
NAME Mar15-2024
EXPNO 90
PROCNO 1

F2 - Acquisition Parameters
Date_ 20240315
Time 9.43 h
INSTRUM Avance Neo 500
PROBHD Z119470_0333 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 0
SWH 14705.883 Hz
FIDRES 0.448788 Hz
AQ 2.2282240 sec
RG 48.9649
DW 34.000 usec
DE 6.79 usec
TE 300.2 K
D1 1.00000000 sec
TD0 1
SFO1 500.1730885 MHz
NUC1 1H
P0 3.33 usec
P1 10.00 usec
PLW1 20.93000031 W

F2 - Processing parameters
SI 65536
SF 500.1699986 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

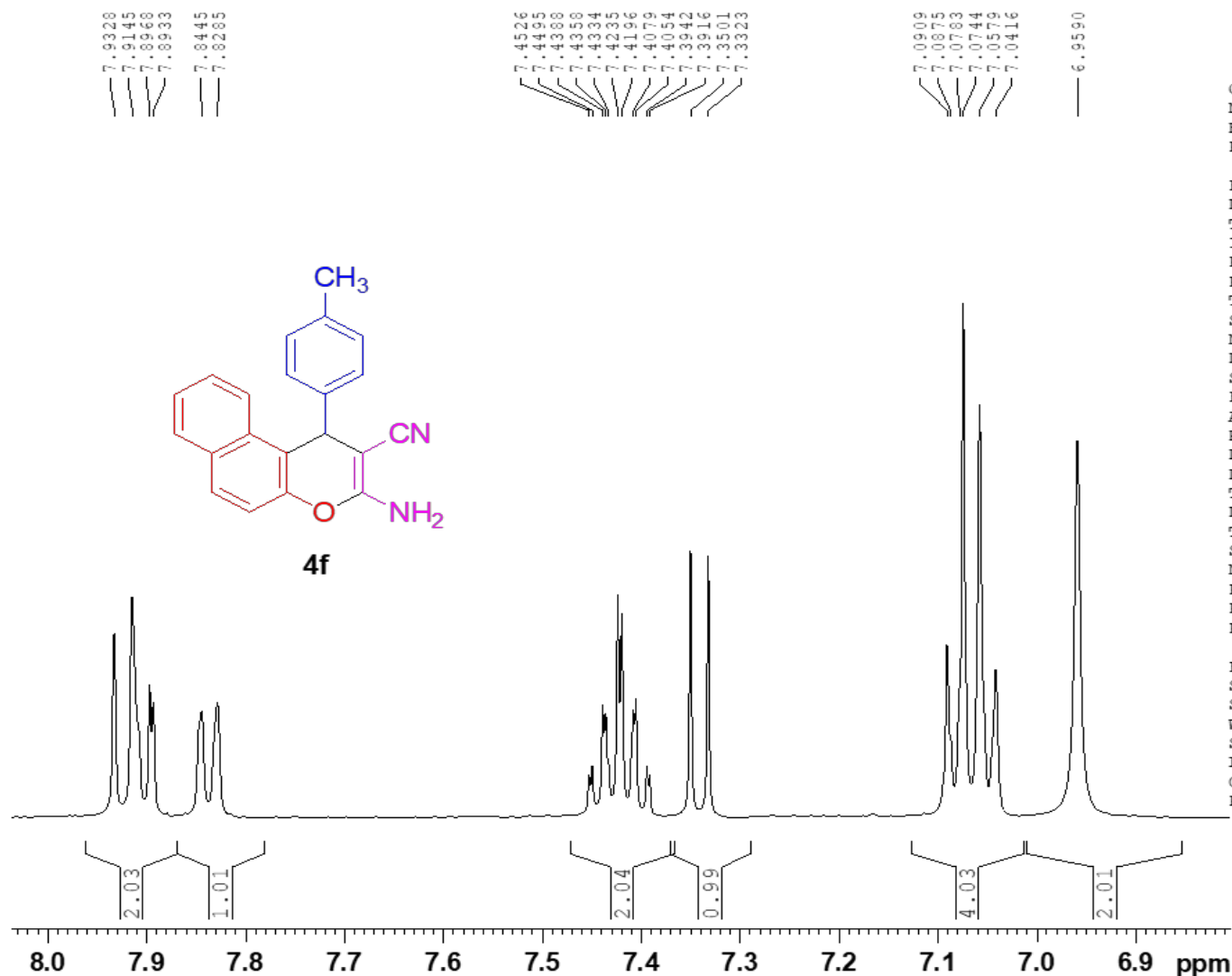
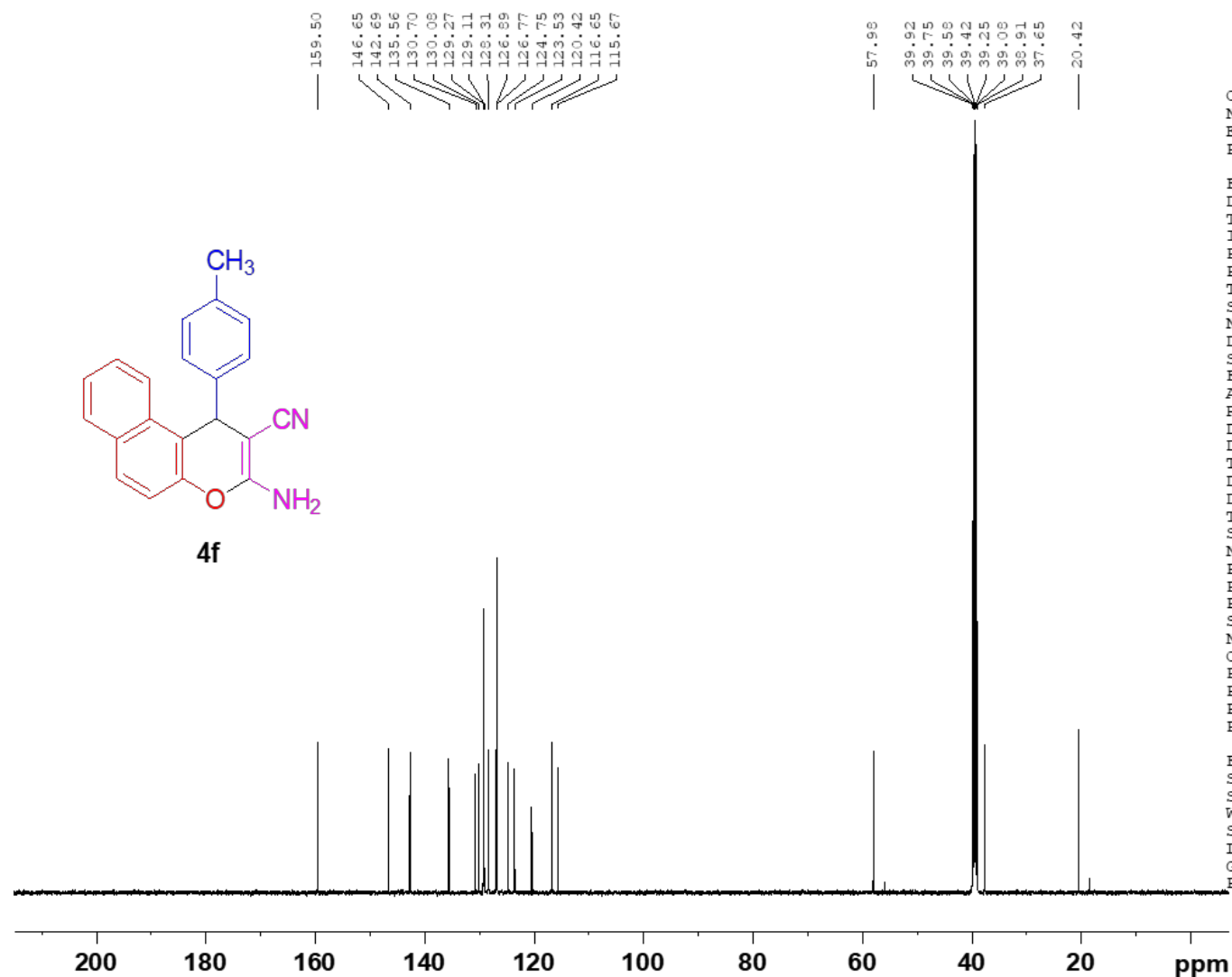


Figure S20. ¹H-NMR expanded spectrum of 2-Amino-4-p-tolyl-4H-benzo[h]chromene-3-carbonitrile (**4f**).

4Me

C13CPD DMSO {D:\Spectra} nmr 9



BRUKER
 AVANCE NEO
 500 MHz NMR SPECTROMETER
 SAIF, PANJAB UNIVERSITY,
 CHANDIGARH

Current Data Parameters
 NAME Marl5-2024
 EXPNO 91
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20240315
 Time_ 11.07 h
 INSTRUM Avance Neo 500
 PROBHD Z119470_0333 (
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 256
 DS 4
 SWH 37037.035 Hz
 FIDRES 1.130281 Hz
 AQ 0.8847360 sec
 RG 101
 DW 13.500 usec
 DE 6.50 usec
 TE 300.2 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1
 SFO1 125.7804233 MHz
 NUC1 13C
 P0 3.33 usec
 P1 10.00 usec
 PLW1 83.14099884 W
 SFO2 500.1720007 MHz
 NUC2 1H
 CPDPRG[2] waltz65
 PCPD2 80.00 usec
 PLW2 20.93000031 W
 PLW12 0.32703000 W
 PLW13 0.16449000 W

F2 - Processing parameters
 SI 32768
 SF 125.7679206 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

Figure S21. ^{13}C -NMR spectrum of 2-Amino-4-p-tolyl-4H-benzo[h]chromene-3-carbonitrile (4f).

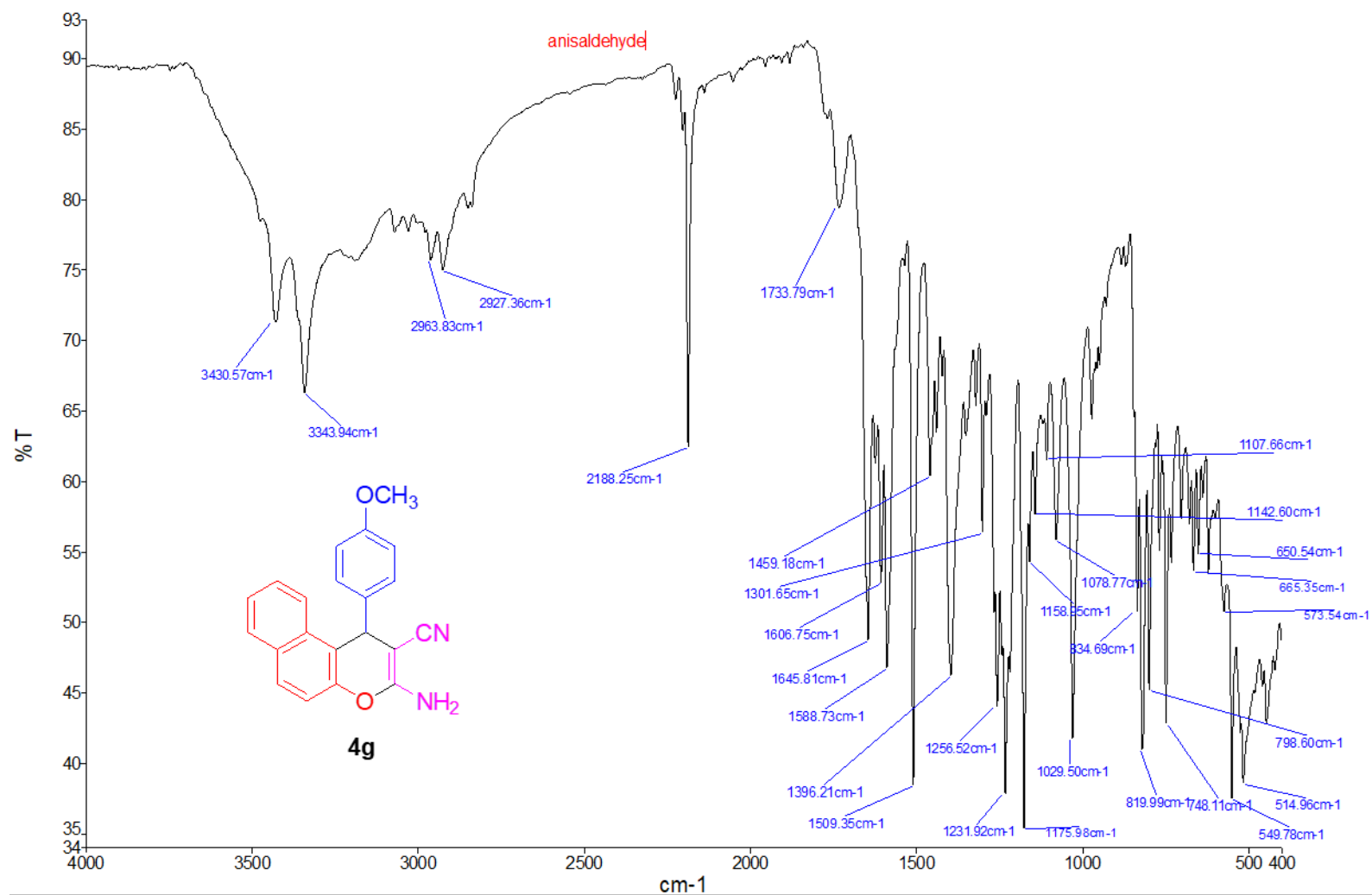
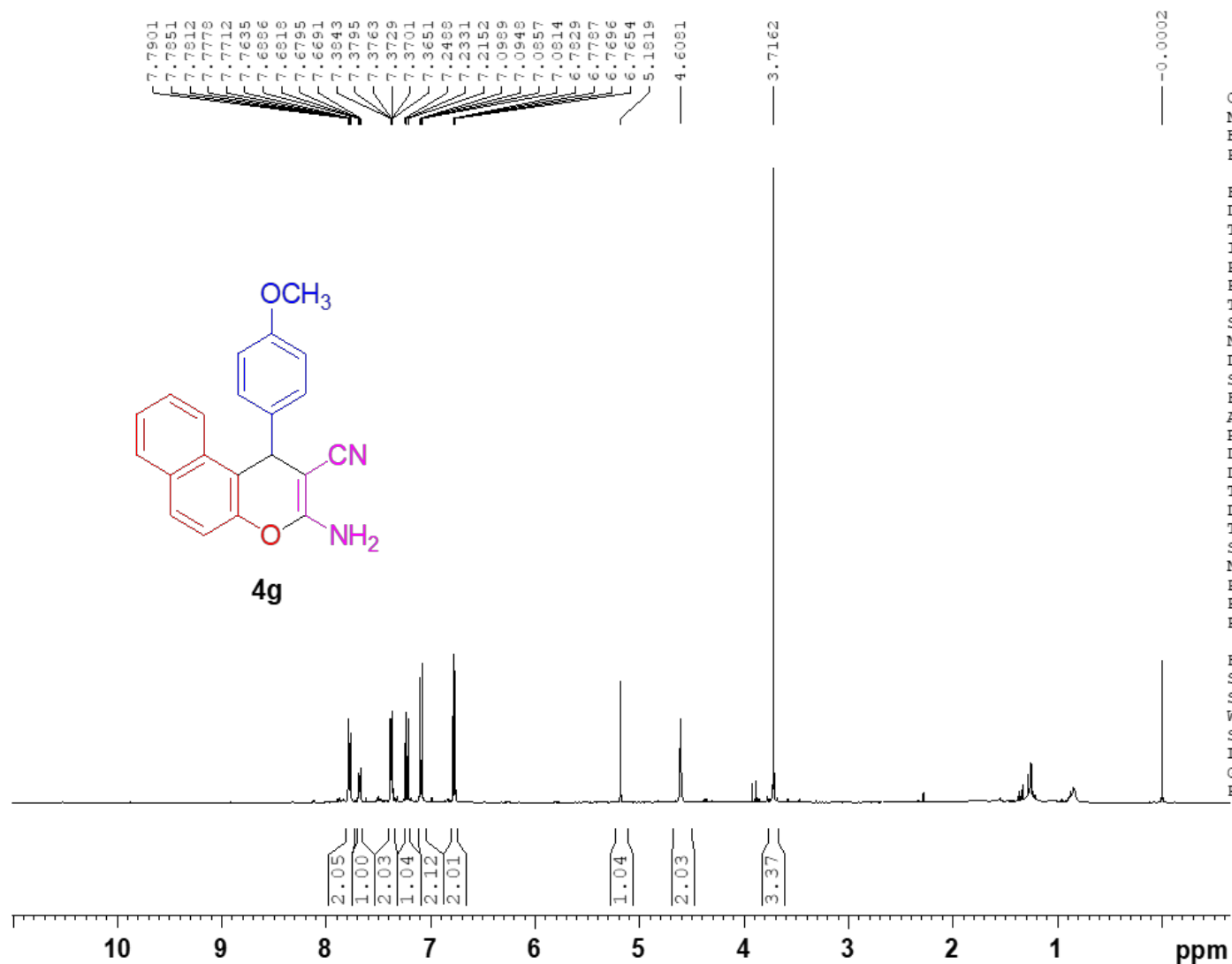


Figure S22. FT-IR spectrum of 2-Amino-4-(4-methoxyphenyl)-4-H-benzo[h] chromene-3-carbonitrile (**4g**).

Ani
1H_8scan CDCl3 {D:\Spectra} nmr 36



BRUKER
AVANCE NEO
500 MHz NMR
SPECTROMETER
SAIF, P.U.

Current Data Parameters
NAME Mar28-2024
EXPNO 360
PROCNO 1

F2 - Acquisition Parameters
Date_ 20240328
Time 16.14 h
INSTRUM Avance Neo 500
PROBHD Z119470_0333 (zg30)
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 0
SWH 14705.883 Hz
FIDRES 0.448788 Hz
AQ 2.2282240 sec
RG 95.7854
DW 34.000 usec
DE 6.79 usec
TE 300.2 K
D1 1.00000000 sec
TD0 1
SFO1 500.1730885 MHz
NUC1 1H
P0 3.33 usec
P1 10.00 usec
PLW1 20.93000031 W

F2 - Processing parameters
SI 65536
SF 500.1700174 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Figure S23. ¹H-NMR spectrum of 2-Amino-4-(4-methoxyphenyl)-4-H-benzo[h] chromene-3-carbonitrile (**4g**).

Ani
1H_8scan CDCl3 {D:\Spectra} nmr 36

BRUKER
AVANCE NEO
500 MHz NMR
SPECTROMETER
SAIF, P.U.

Current Data Parameters
NAME Mar28-2024
EXPNO 360
PROCNO 1

F2 - Acquisition Parameters
Date 20240328
Time 16.14 h
INSTRUM Avance Neo 500
PROBHD z119470_0333 (z)
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 0
SWH 14705.883 Hz
FIDRES 0.448788 Hz
AQ 2.2282240 sec
RG 95.7854
DW 34.000 usec
DE 6.79 usec
TE 300.2 K
D1 1.00000000 sec
TD0 1
SFO1 500.1730885 MHz
NUC1 1H
P0 3.33 usec
P1 10.00 usec
PLW1 20.93000031 W

F2 - Processing parameters
SI 65536
SF 500.1700174 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

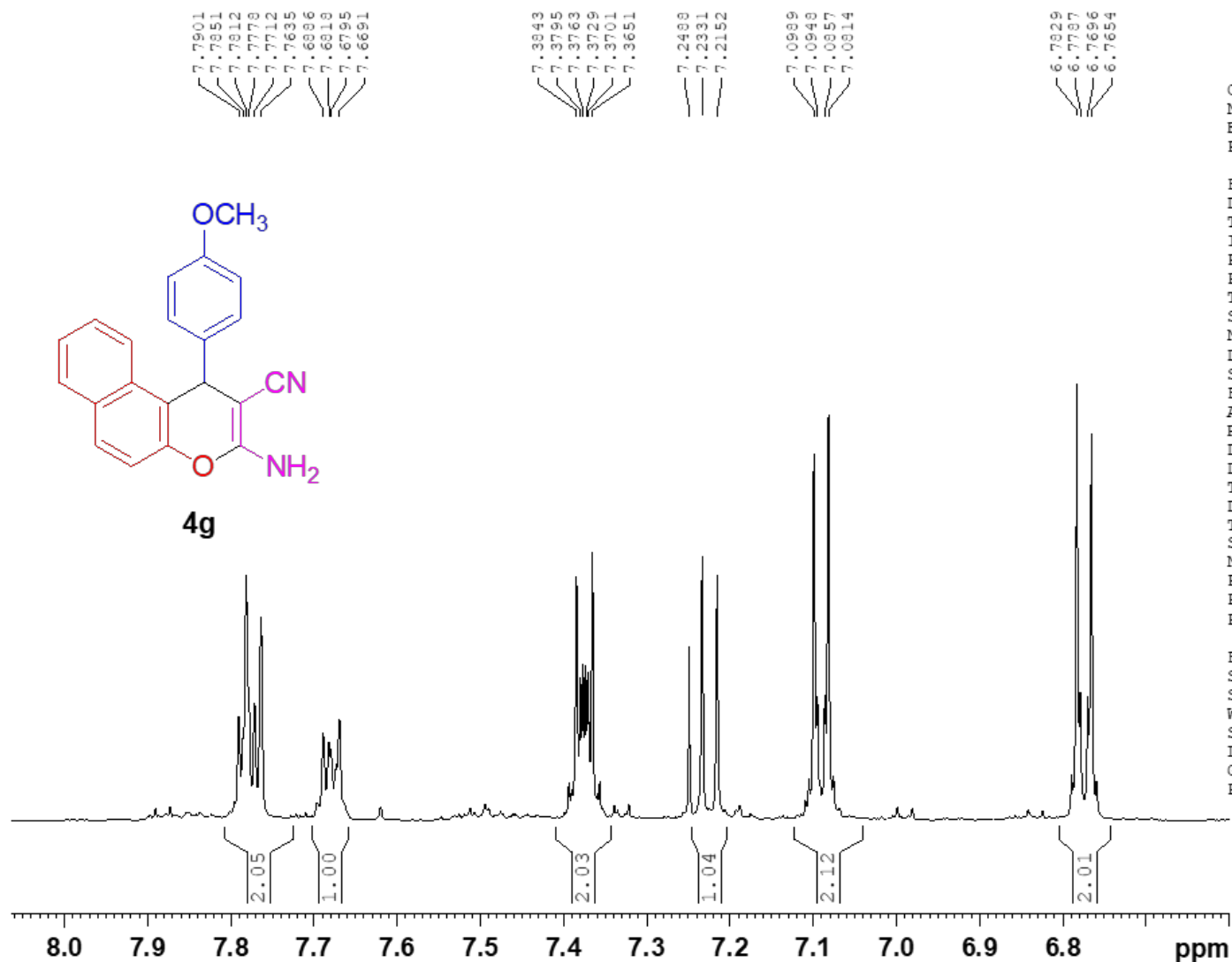


Figure S24. ¹H-NMR expanded spectrum of 2-Amino-4-(4-methoxyphenyl)-4-H-benzo[h] chromene-3-carbonitrile (**4g**).

Ani
C13CPD CDC13 {D:\Spectra} nmr 36

BRUKER
AVANCE NEO
500 MHz NMR SPECTROMETER
SAIF, PANJAB UNIVERSITY,
CHANDIGARH

Current Data Parameters
NAME Mar28-2024
EXPNO 361
PROCNO 1

F2 - Acquisition Parameters
Date_ 20240329
Time_ 8.01 h
INSTRUM Avance Neo 500
PROBHD Z119470_0333 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 37037.035 Hz
FIDRES 1.130281 Hz
AQ 0.8847360 sec
RG 101
DW 13.500 usec
DE 6.50 usec
TE 300.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.7804233 MHz
NUC1 13C
P0 3.33 usec
P1 10.00 usec
PLW1 83.14099884 W
SFO2 500.1720007 MHz
NUC2 1H
CPDPRG[2] waltz65
PCPD2 80.00 usec
PLW2 20.93000031 W
PLW12 0.32703000 W
PLW13 0.16449000 W

F2 - Processing parameters
SI 32768
SF 125.7678491 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

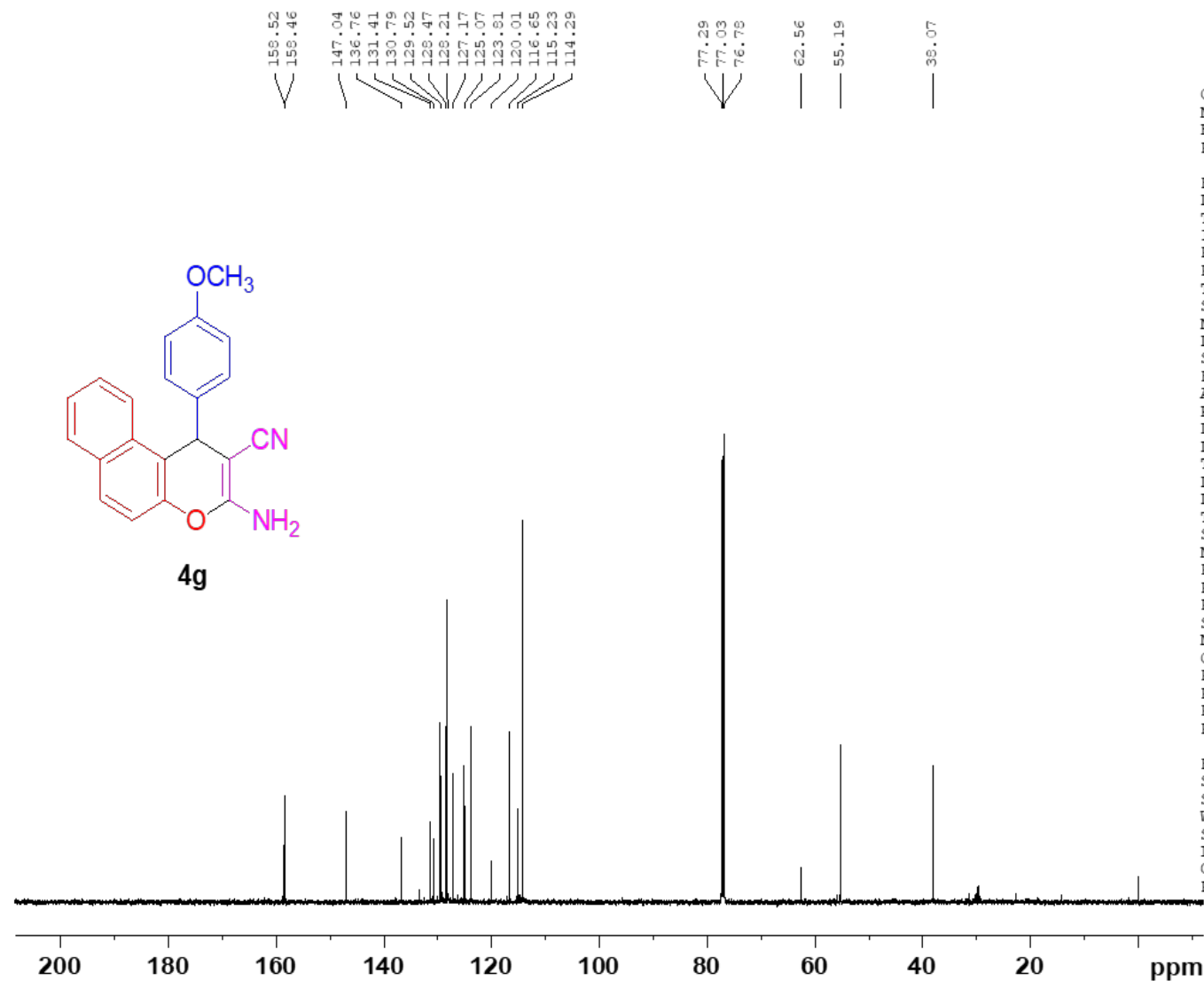


Figure S25. ¹³C-NMR spectrum of 2-Amino-4-(4-methoxyphenyl)-4-H-benzo[h] chromene-3-carbonitrile (4g).

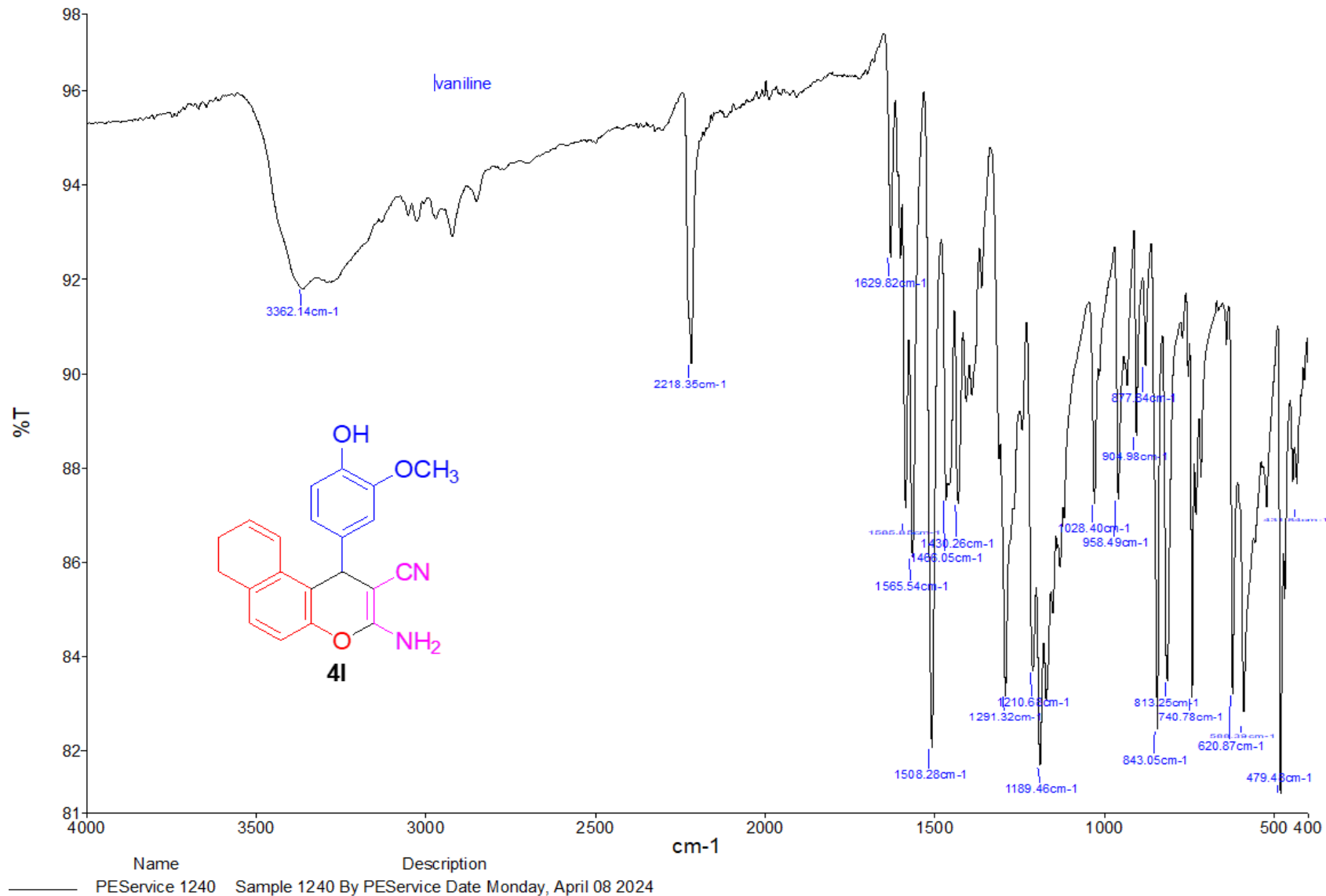


Figure S26. FT-IR spectrum of 2-Amino-1-(4-hydroxy-3-methoxyphenyl)-1H-benzo[f]chromene-2-carbonitrile (**4I**).

Va
1H_8scan CDC13 {D:\Spectra} nmr 32

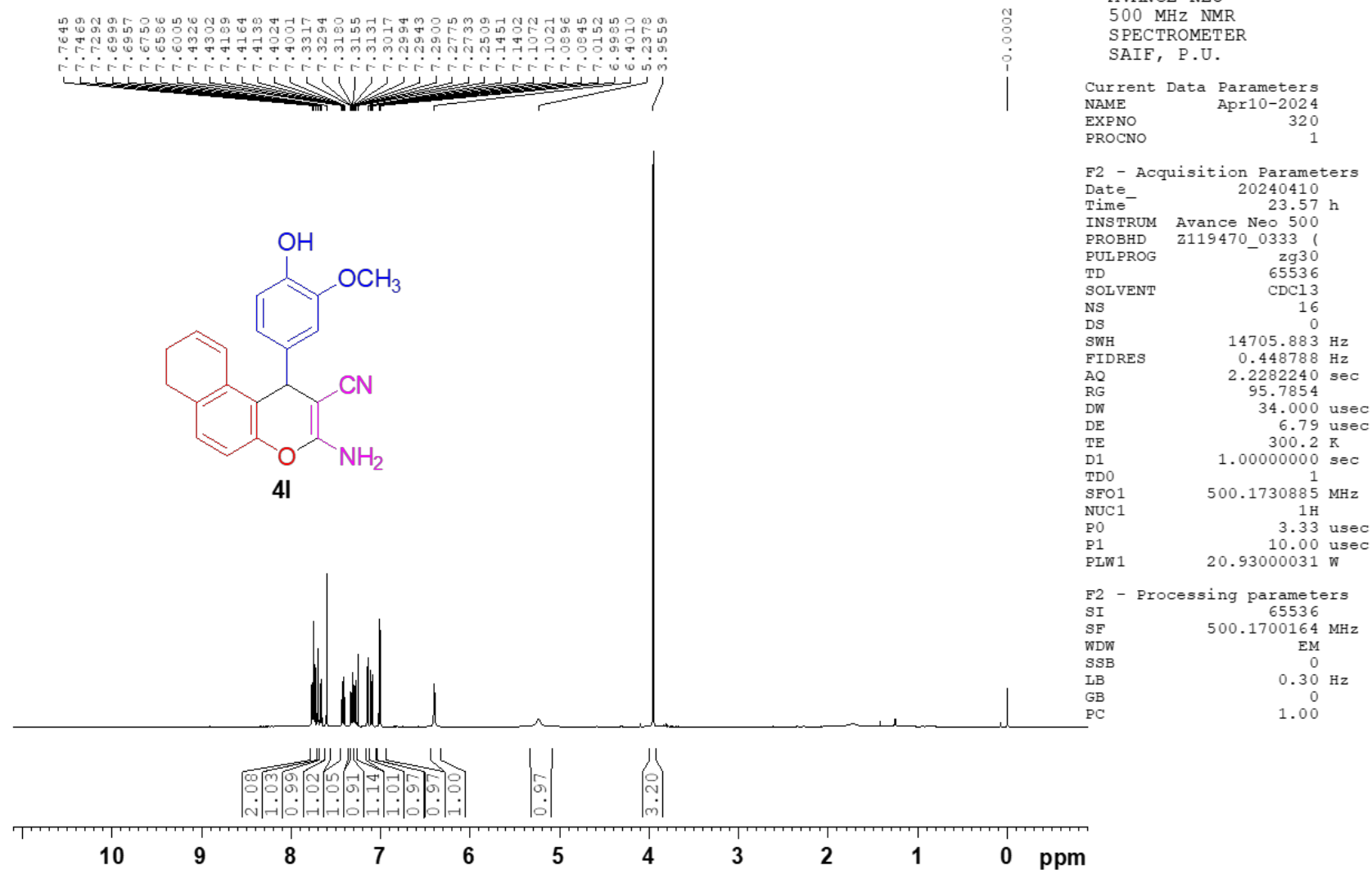


Figure S27. ¹H-NMR spectrum of 2-Amino-1-(4-hydroxy-3-methoxyphenyl)-1H-benzo[f]chromene-2-carbonitrile (**4l**).

Va
1H_8scan CDCl3 {D:\Spectra} nmr 32

BRUKER
AVANCE NEO
500 MHz NMR
SPECTROMETER
SAIF, P.U.

Current Data Parameters
NAME Apr10-2024
EXPNO 320
PROCNO 1

F2 - Acquisition Parameters
Date_ 20240410
Time_ 23.57 h
INSTRUM Avance Neo 500
PROBHD Z119470_0333 (z)
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 0
SWH 14705.883 Hz
FIDRES 0.448788 Hz
AQ 2.2282240 sec
RG 95.7854
DW 34.000 usec
DE 6.79 usec
TE 300.2 K
D1 1.00000000 sec
TD0 1
SFO1 500.1730885 MHz
NUC1 1H
P0 3.33 usec
P1 10.00 usec
PLW1 20.93000031 W

F2 - Processing parameters
SI 65536
SF 500.1700164 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

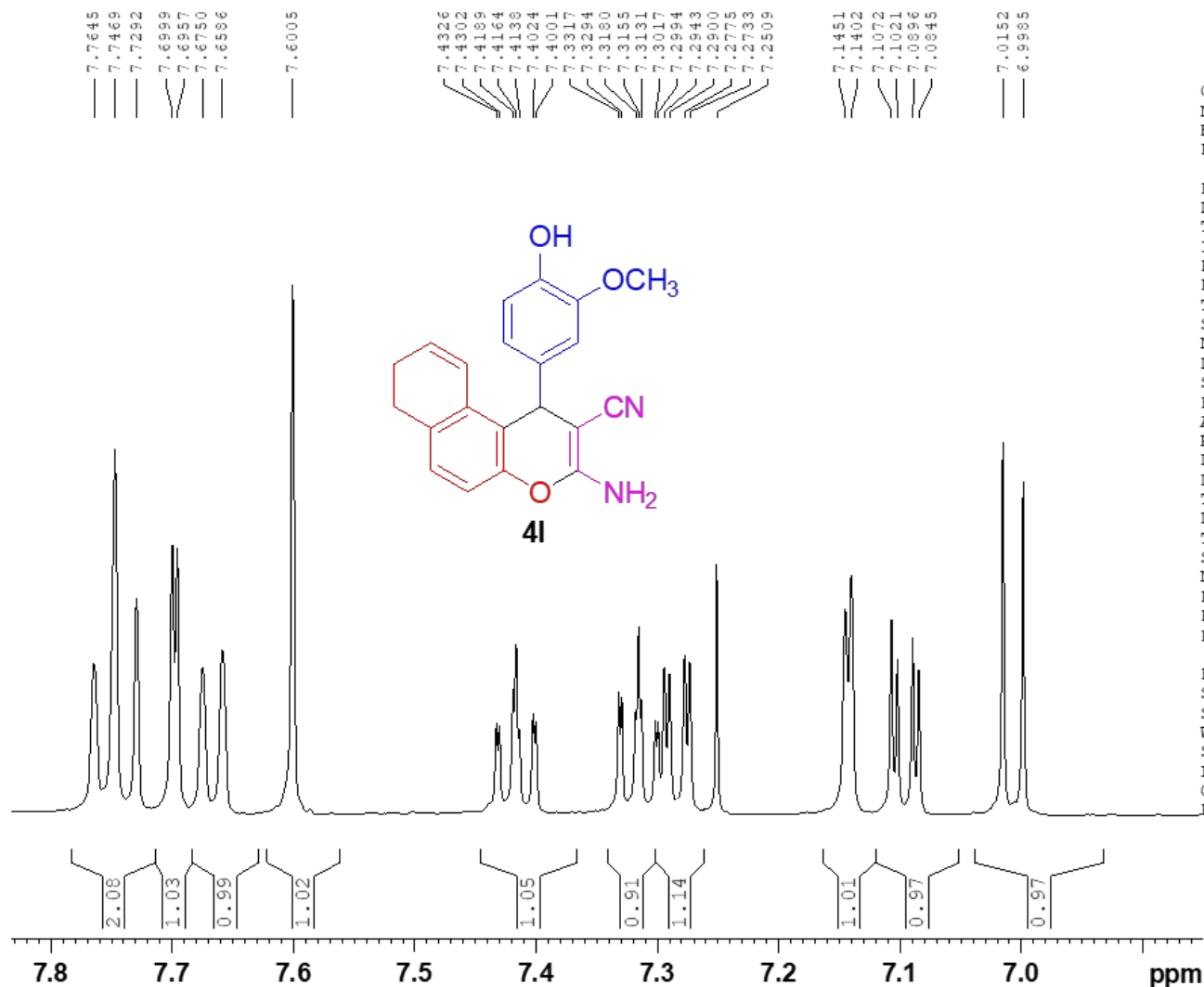


Figure S28. ¹H-NMR expanded spectrum of 2-Amino-1-(4-hydroxy-3-methoxyphenyl)-1H-benzo[f]chromene-2-carbonitrile (4I).

Va
C13CPD CDCl3 {D:\Spectra} nmr 32

BRUKER
AVANCE NEO
500 MHz NMR SPECTROMETER
SAIF, PANJAB UNIVERSITY,
CHANDIGARH

Current Data Parameters
NAME Apr10-2024
EXPNO 321
PROCNO 1

F2 - Acquisition Parameters
Date_ 20240411
Time 0.24 h
INSTRUM Avance Neo 500
PROBHD z119470_0333 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 37037.035 Hz
FIDRES 1.130281 Hz
AQ 0.8847360 sec
RG 101
DW 13.500 usec
DE 6.50 usec
TE 300.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.7804233 MHz
NUC1 13C
P0 3.33 usec
P1 10.00 usec
PLW1 83.14099884 W
SFO2 500.1720007 MHz
NUC2 1H
CPDPRG[2] waltz65
PCPD2 80.00 usec
PLW2 20.93000031 W
PLW12 0.32703000 W
PLW13 0.16449000 W

F2 - Processing parameters
SI 32768
SF 125.7678465 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

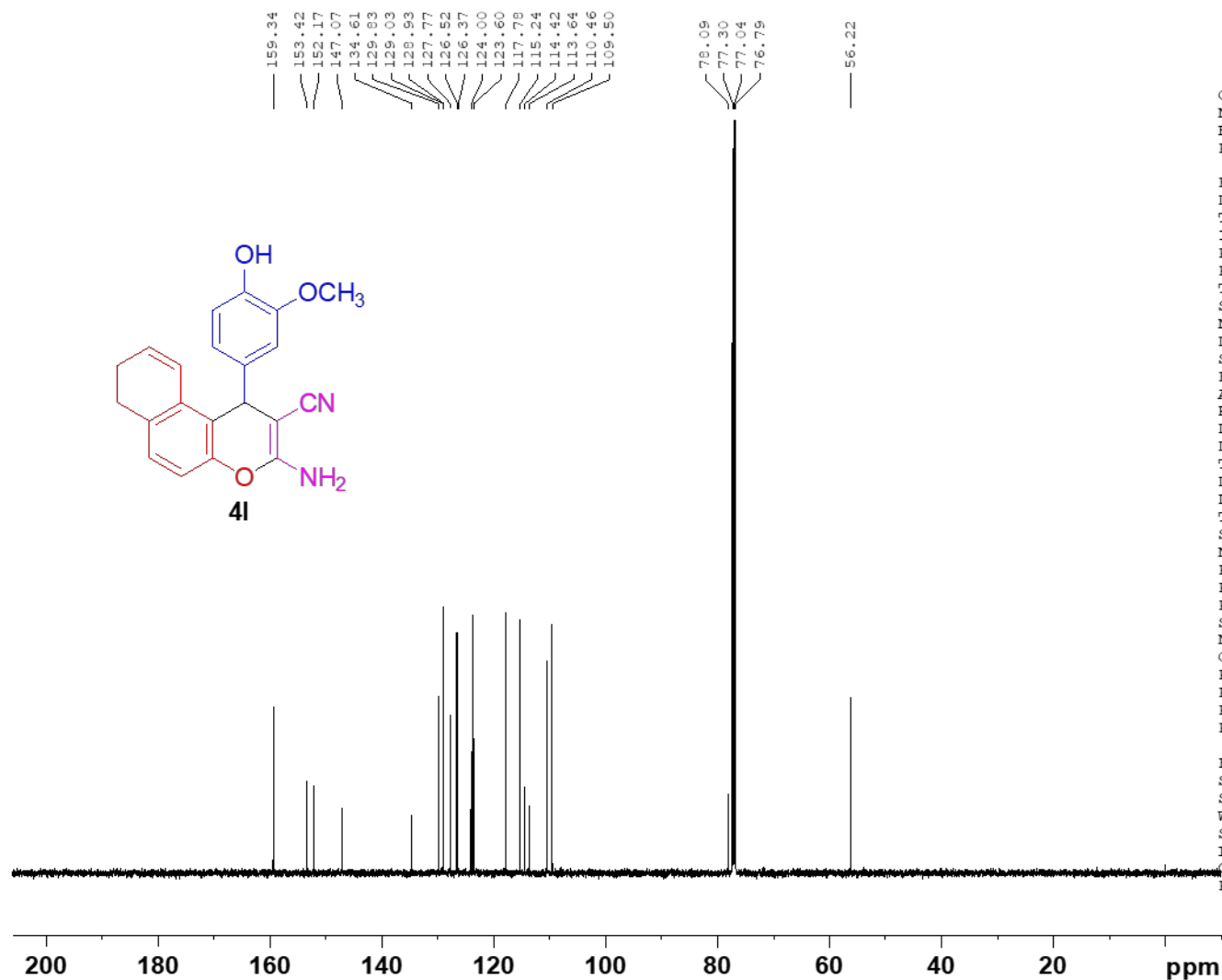


Figure S29. ¹³C-NMR spectrum of 2-Amino-1-(4-hydroxy-3-methoxyphenyl)-1H-benzo[f]chromene-2-carbonitrile (**4l**).