

Direct Z-Scheme g-C₃N₅/Cu₃TiO₄ Heterojunction Enhanced Photocatalytic Performance of Chromene-3-Carbonitriles Synthesis under Visible Light Irradiation

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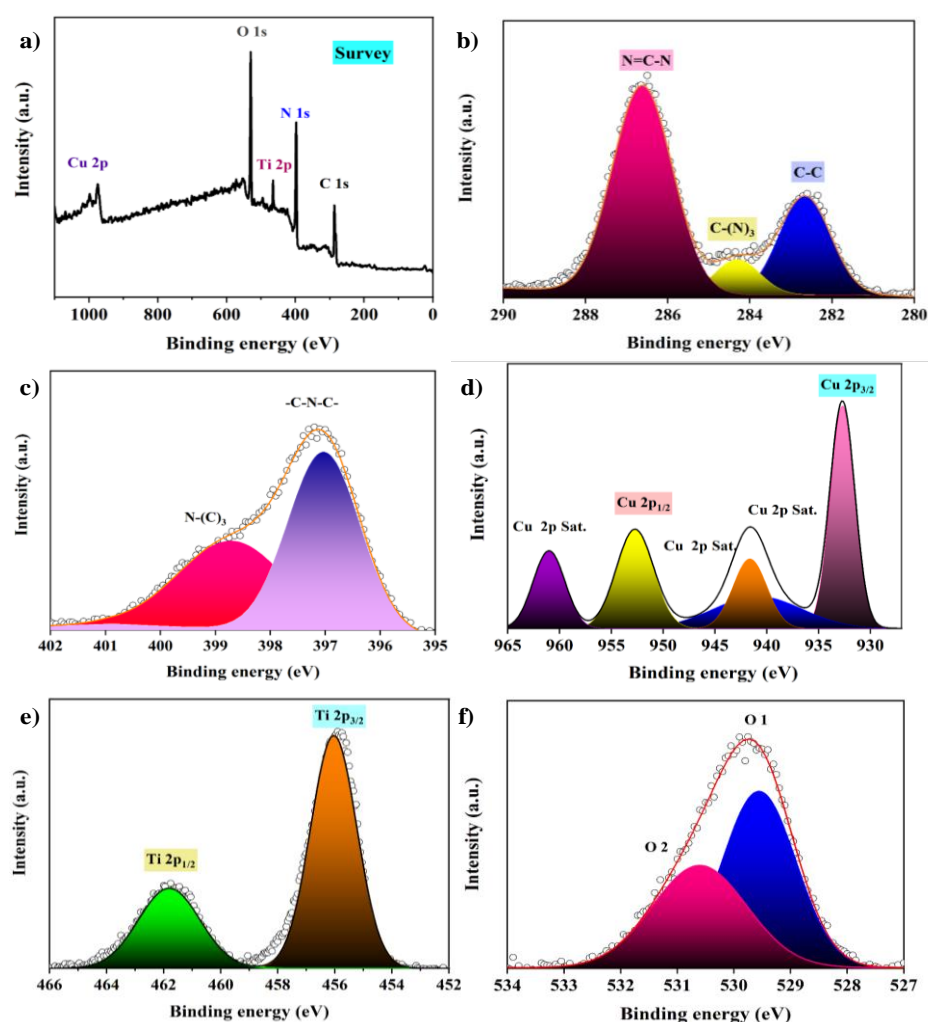
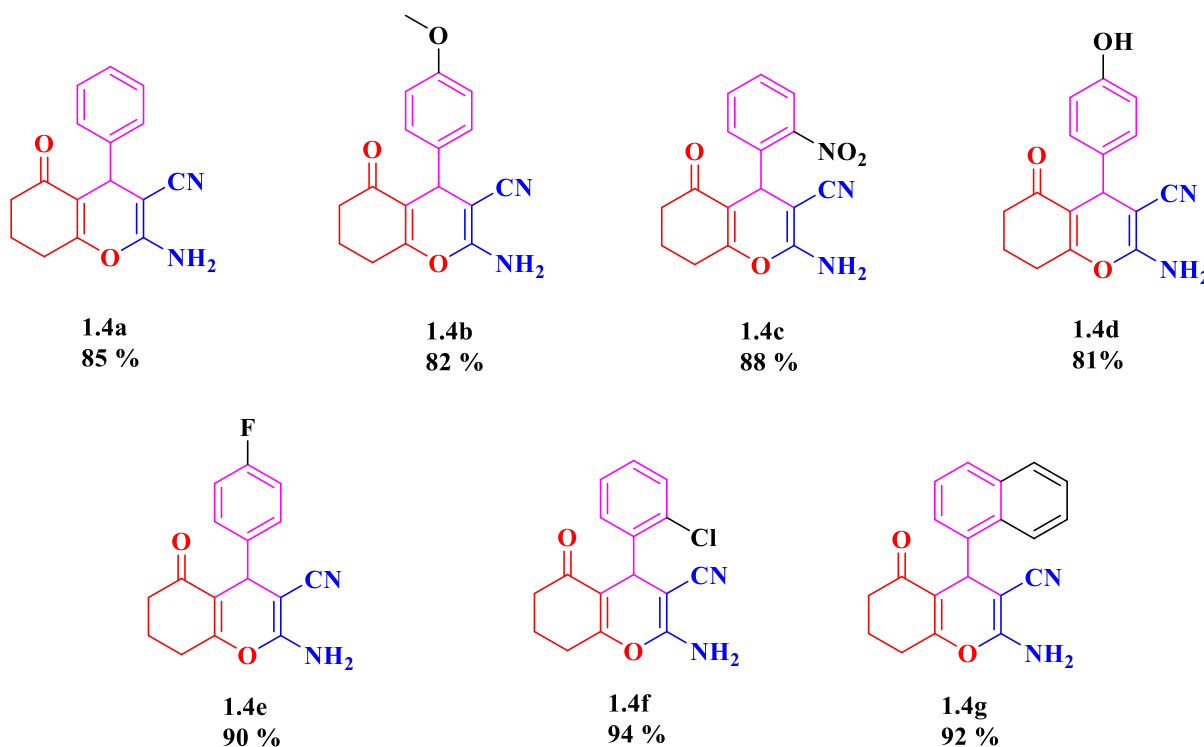
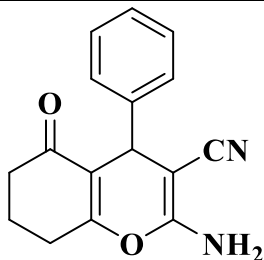
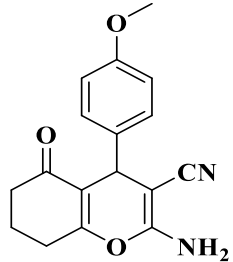
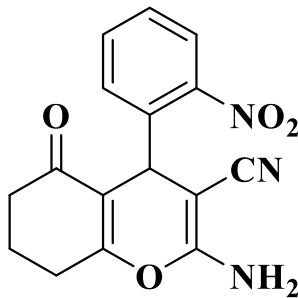
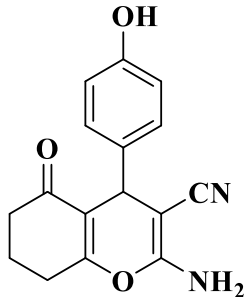
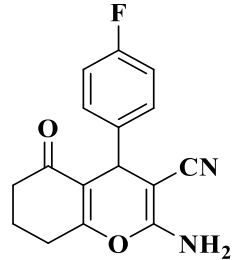
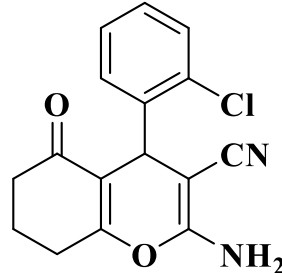


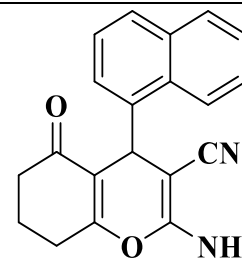
Figure S1. XPS analysis of 10% CN5CT nanocomposite (a) Survey (b) C 1s (c) N 1s (d) Cu 2p (e) Ti2p & f) O 1s.



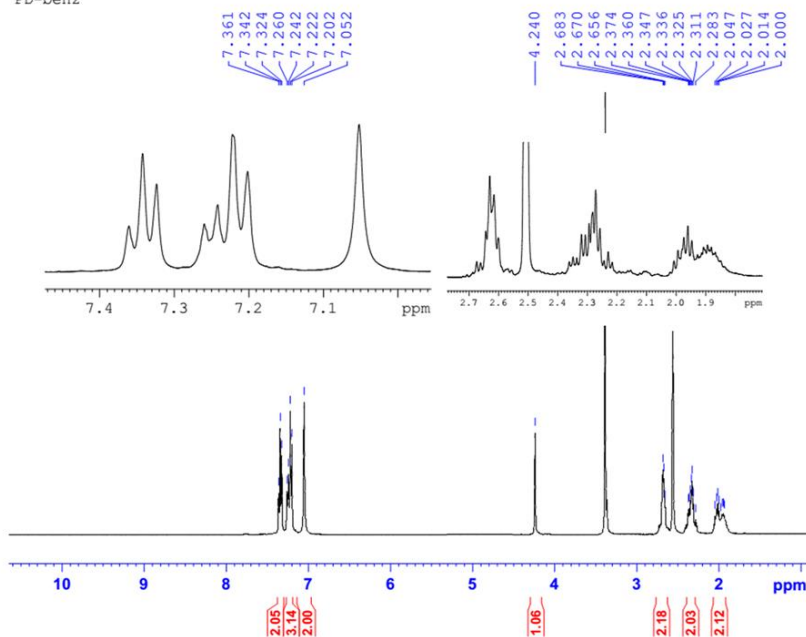
1.4a	2-amino-5-oxo-4-phenyl-5,6,7,8-tetrahydro-4H-chromene-3-carbonitrile	
Molecular Formula	C ₁₆ H ₁₄ N ₂ O ₂	
Molecular Weight (g/mol)	267.10	
Colour	white solid	
Melting point (°C)	206-208	
FT-IR, ν/cm ⁻¹	3039, 1447, 1334, 968, 754, 703.	
¹ H-NMR (400 MHz, CDCl ₃ , Me ₄ Si) (ppm): δ	1.91-2.04 (m, 2H), 2.28-2.37 (m, 2H), 2.65-2.68 (t, 2H), 4.24 (s, 1H), 7.05 (s, 2H), 7.20-7.24 (m, 3H), 7.32-7.35 (t, 2H).	
¹³ C-NMR (100 MHz, CDCl ₃ , Me ₄ Si) (ppm): δ	20.20, 26.99, 36.05, 57.39, 113.21, 119.81, 124.11, 129.05, 146.73, 152.78, 159.01, 165.58, 196.33.	
		
1.4b	2-amino-4-(4-methoxyphenyl)-5-oxo-5,6,7,8-tetrahydro-4H-chromene-3-carbonitrile	
Molecular Formula	C ₁₇ H ₁₆ N ₂ O ₃	
Molecular Weight (g/mol)	297.11	
Colour	Light white solid	
Melting point (°C)	236-238	
FT-IR, ν/cm ⁻¹	3111, 1700, 1649, 1513, 1441, 1219, 1083, 777, 533.	
¹ H-NMR (400 MHz, CDCl ₃ , Me ₄ Si) (ppm): δ	1.91-1.96 (m, 2H), 2.22-2.30 (t, 2H), 2.50-2.56 (t, 2H), 3.59 (s, 3H), 4.31 (s, 1H), 4.48 (s, 2H), 6.74-6.76 (d, 2H), 7.08-7.10 (d, 2H).	
¹³ C-NMR (100 MHz, CDCl ₃ , Me ₄ Si) (ppm): δ	20.14, 27.01, 36.84, 55.24, 113.41, 113.97, 115.48, 118.77, 128.66, 128.95, 135.51, 157.35, 158.63, 162.97, 196.11.	
		
1.4c	2-amino-4-(2-nitrophenyl)-5-oxo-5,6,7,8-tetrahydro-4H-chromene-3-carbonitrile	

Molecular Formula	C ₁₆ H ₁₃ N ₃ O ₄	
Molecular Weight (g/mol)	311.09	
Colour	white solid	
Melting point (°C)	232-234	
FT-IR, ν/cm ⁻¹	2059, 1520, 1448, 1334, 968, 831, 747.	
¹ H-NMR (400 MHz, CDCl ₃ , Me ₄ Si) (ppm): δ	1.84-1.95 (m, 2H), 2.13-2.26 (m, 2H), 2.58-2.61 (t, 2H), 4.93 (s, 1H), 7.16 (s, 2H), 7.37-7.45 (m, 2H), 7.63-7.67 (t, 1H), 7.80-7.82 (d, 1H).	
¹³ C-NMR (100 MHz, CDCl ₃ , Me ₄ Si) (ppm): δ	20.18, 26.97, 36.05, 57.41, 113.21, 119.77, 122.94, 124.70, 129.01, 131.07, 146.72, 152.76, 159.01, 165.57, 196.33.	
1.4d	2-amino-4-(4-hydroxyphenyl)-5-oxo-5,6,7,8-tetrahydro-4H-chromene-3-carbonitrile	
Molecular Formula	C ₁₆ H ₁₄ N ₂ O ₃	
Molecular Weight (g/mol)	282.29	
Colour	Light white solid	
Melting point (°C)	242-244	
FT-IR, ν/cm ⁻¹	3175, 1700, 1549, 1327, 1169, 1091, 1004, 818.	
¹ H-NMR (400 MHz, CDCl ₃ , Me ₄ Si) (ppm): δ	1.83-1.95 (m, 2H), 2.24-2.30 (m, 2H), 2.58-2.61 (t, 2H), 4.08 (s, 1H), 6.64-6.66 (d, 2H), 6.90 (s, 2H), 6.93-6.95 (d, 2H), 9.23 (s, 1H).	
¹³ C-NMR (100 MHz, CDCl ₃ , Me ₄ Si) (ppm): δ	26.92, 35.03, 36.85, 59.16, 114.76, 115.46, 120.38, 128.58, 135.69, 156.46, 158.85, 164.44, 196.31.	
1.4e	2-amino-4-(4-fluorophenyl)-5-oxo-5,6,7,8-tetrahydro-4H-chromene-3-carbonitrile	
Molecular Formula	C ₁₆ H ₁₃ FN ₂ O ₂	
Molecular Weight (g/mol)	285.09	
Colour	Yellow solid	
Melting point (°C)	250-252	
FT-IR, ν/cm ⁻¹	3175, 1700, 1549, 1327, 1169, 1091, 1004, 818.	
¹ H-NMR (400 MHz, CDCl ₃ , Me ₄ Si) (ppm): δ	1.94-1.97 (m, 2H), 2.22-2.36 (t, 2H), 2.50-2.56 (t, 2H), 4.31 (s, 1H), 4.47 (s, 2H), 6.74-6.76 (d, 2H), 7.08-7.10 (d, 2H).	
¹³ C-NMR (100 MHz, CDCl ₃ , Me ₄ Si) (ppm): δ	20.24, 26.94, 35.27, 58.51, 114.13, 115.35, 120.13, 129.45, 129.53, 141.44, 158.92, 160.17, 162.58, 164.95, 196.31.	
1.4f	2-amino-4-(2-chlorophenyl)-5-oxo-5,6,7,8-tetrahydro-4H-chromene-3-carbonitrile	
Molecular Formula	C ₁₆ H ₁₃ ClN ₂ O ₂	
Molecular Weight (g/mol)	300.74	
Colour	Light white solid	
Melting point (°C)	222-224	
FT-IR, ν/cm ⁻¹	3069, 1677, 1420, 1283, 1083, 854, 747.	
¹ H-NMR (400 MHz, CDCl ₃ , Me ₄ Si) (ppm): δ	1.91-1.98 (m, 2H), 2.22-2.30 (t, 2H), 2.60-2.63 (t, 2H), 4.70 (s, 1H), 7.01 (s, 3H), 6.72-6.78 (d, 2H), 7.09-7.21 (d, 3H).	

1.4g	2-amino-4-(naphthalen-1-yl)-5-oxo-5,6,7,8-tetrahydro-4H-chromene-3-carbonitrile
Molecular Formula	$C_{20}H_{16}N_2O_2$
Molecular Weight (g/mol)	316.12
Colour	Light white solid
Melting point (°C)	264-266
FT-IR, ν/cm^{-1}	3326, 1677, 1574, 1441, 1161, 1105, 697.
1H-NMR (400 MHz, $CDCl_3$, Me_4Si) (ppm): δ	1.85-1.98 (m, 2H), 2.08-2.31 (m, 2H), 2.53-2.66 (m, 2H), 4.45 (s, 1H), 4.52 (s, 2H), 7.14-7.16 (d, 1H), 7.29-7.33 (t, 1H), 7.39-7.42 (t, 1H), 7.48-7.52 (d, 1H), 7.63-7.65 (t, 1H), 7.73-7.74 (d, 1H), 8.32-8.34 (d, 1H).
^{13}C-NMR (100 MHz, $CDCl_3$, Me_4Si) (ppm): δ	20.23, 27.07, 36.75, 115.85, 123.34, 125.35, 126.31, 127.95, 128.67, 157.30, 163.66, 196.0.
^{13}C-NMR (100 MHz, $CDCl_3$, Me_4Si) (ppm): δ	20.16, 27.60, 34.35, 37.12, 40.11, 111.61, 112.58, 112.66, 128.25, 128.56, 133.81, 148.52, 158.15.



Signature SIF VIT VELLORE
PD-benz



BRUKER

Current Data Parameters
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EXPNO 10
PROCNO 1

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Time_ 17.05 h
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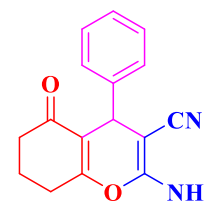


Figure S2. 1H NMR spectrum of 1.4a.

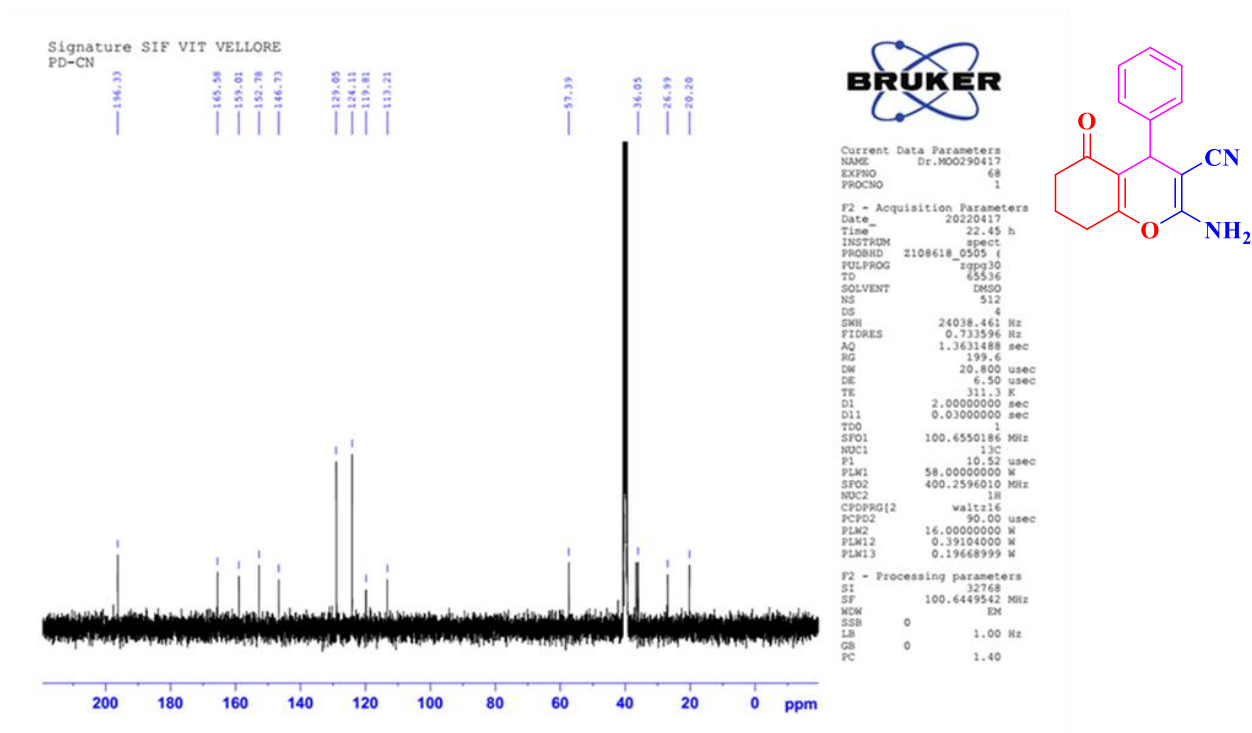
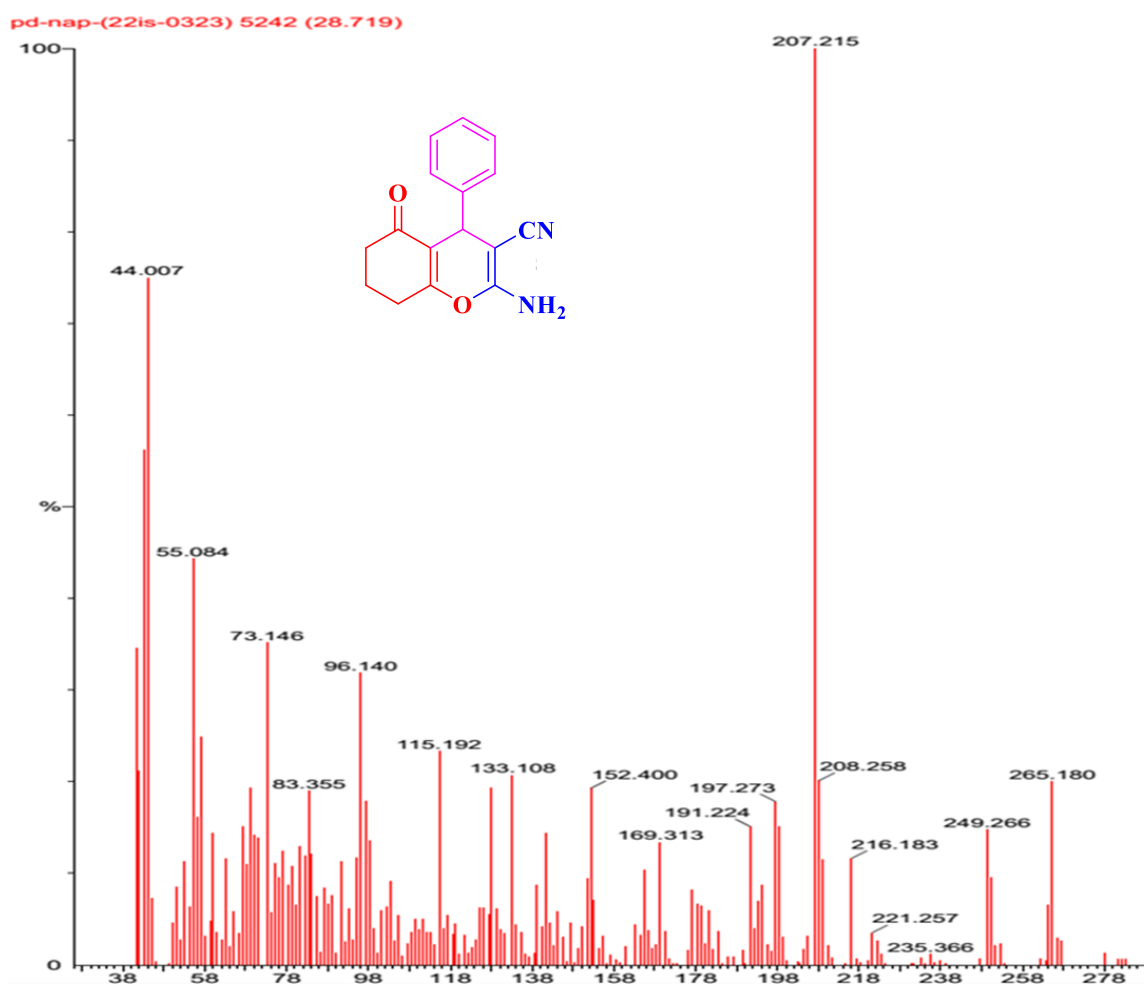
Figure S3. ^{13}C NMR spectrum of 1.4a.

Figure S4. GC-MS spectrum of 1.4a.

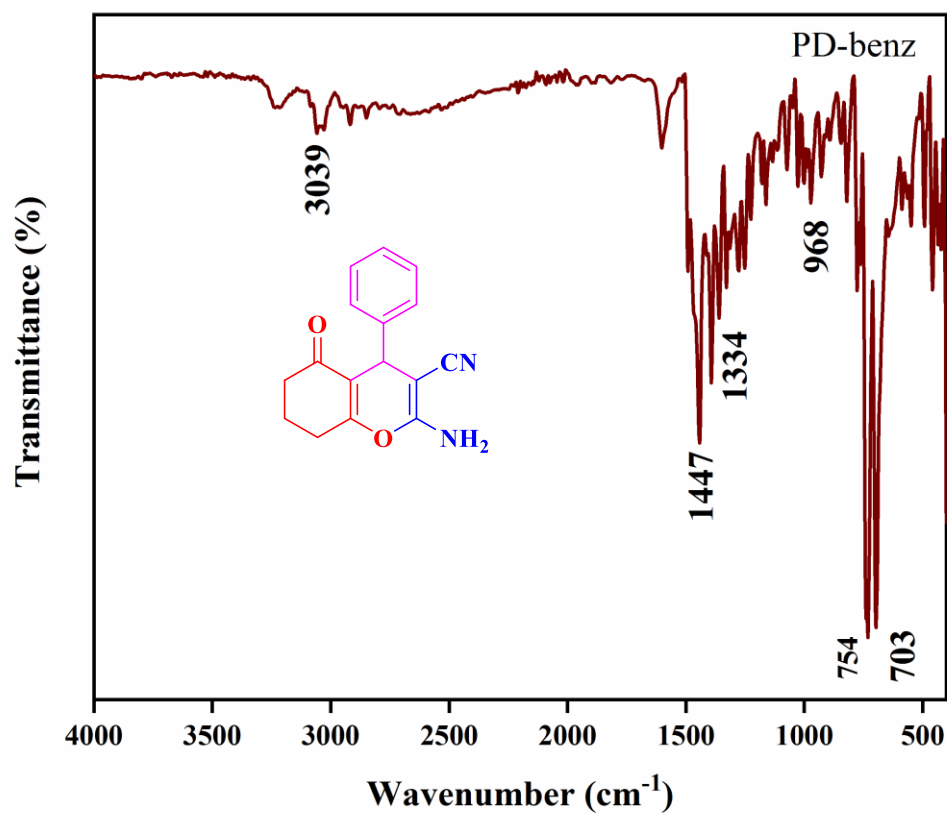
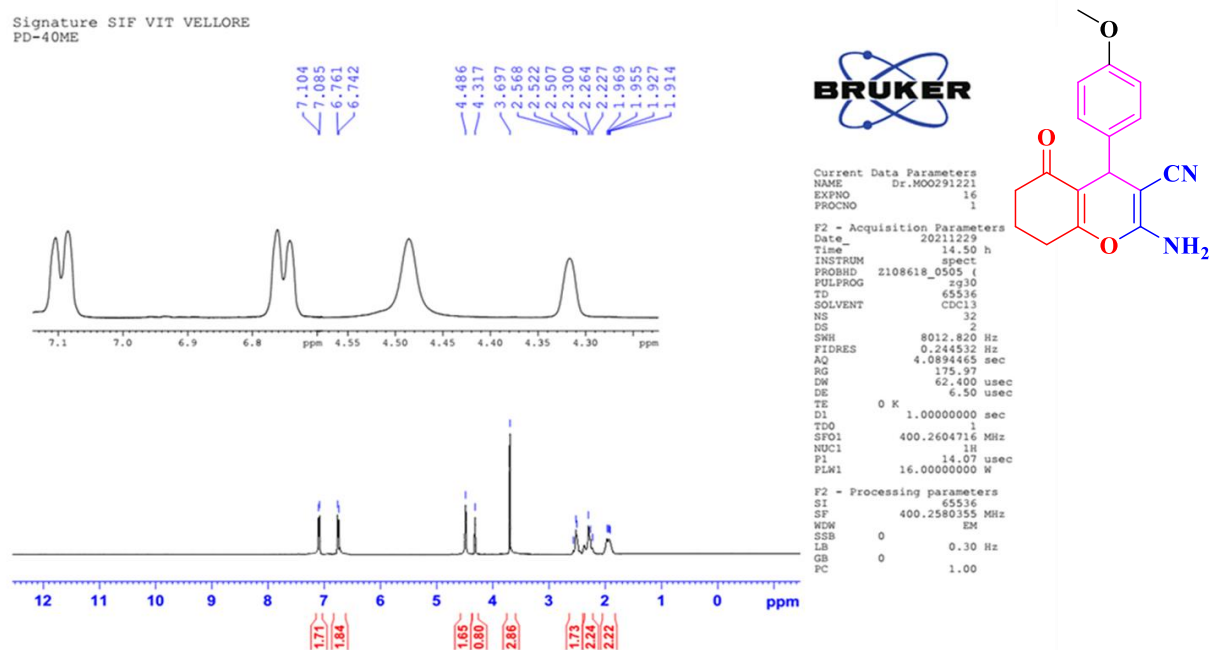
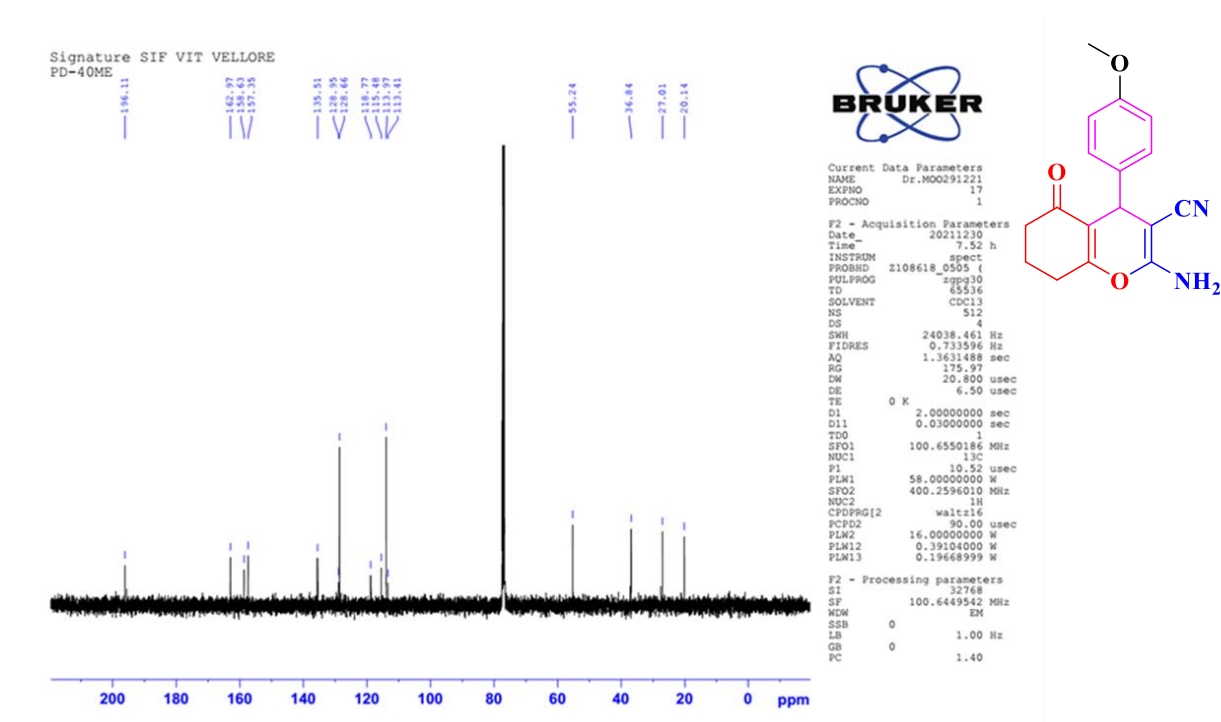


Figure S5. IR spectrum of 1.4a.

Figure S6. ¹H NMR spectrum of 1.4b.

Figure S7. ^{13}C NMR spectrum of 1.4b.

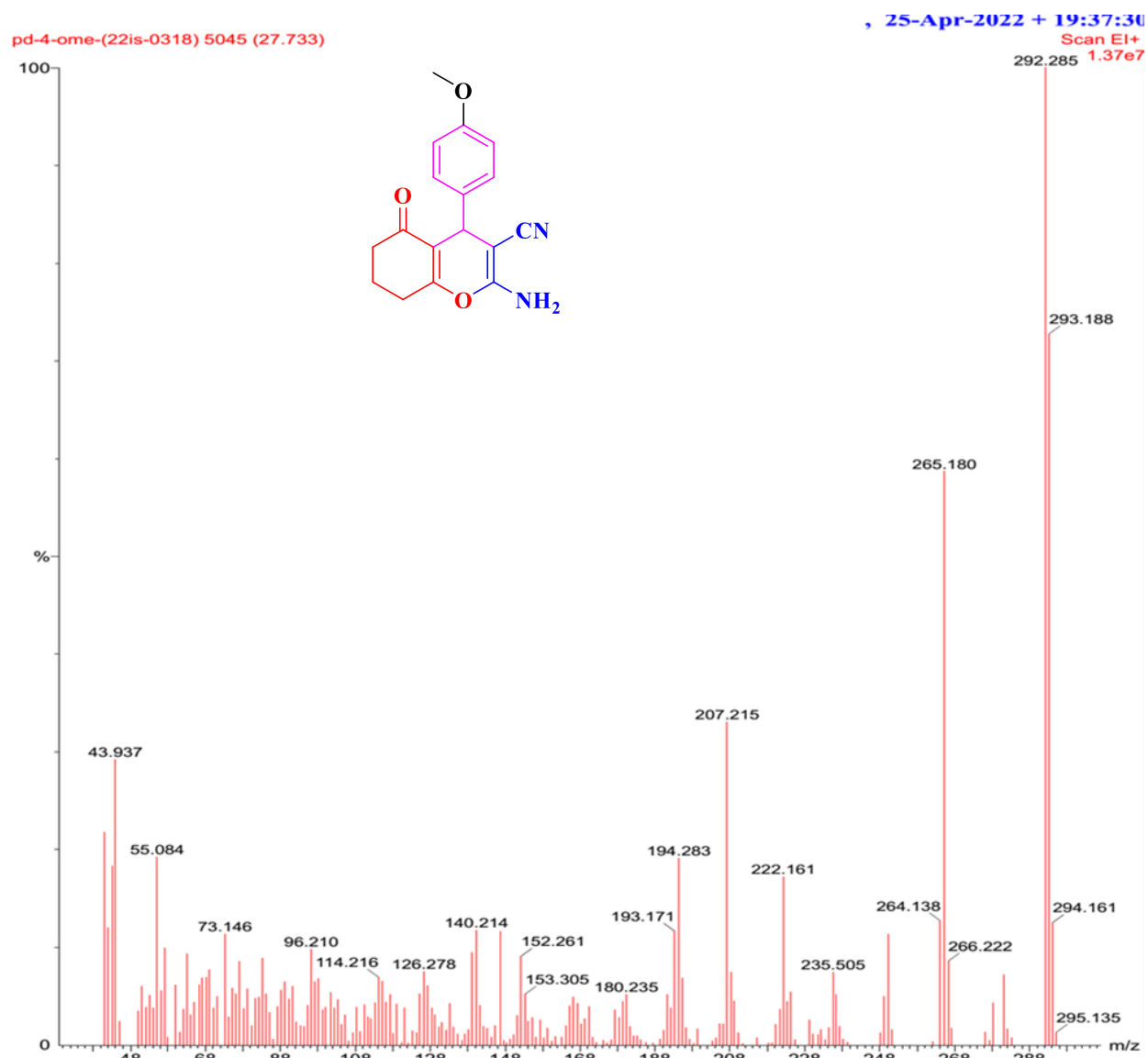


Figure S8. GC-MS spectrum of 1.4b.

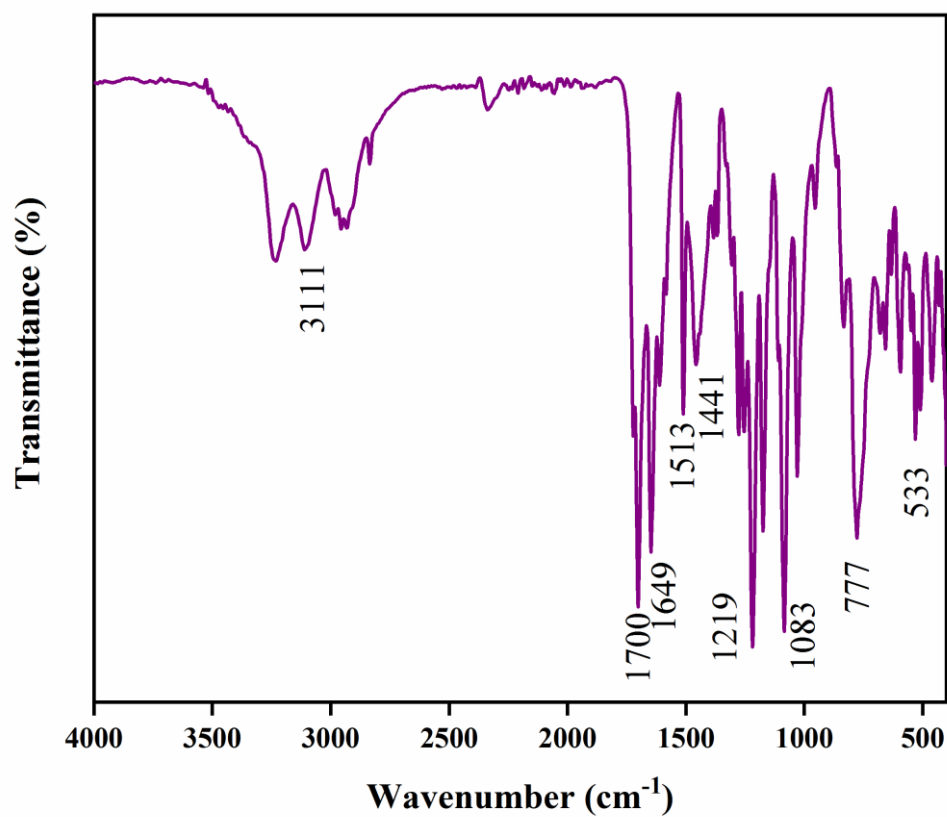
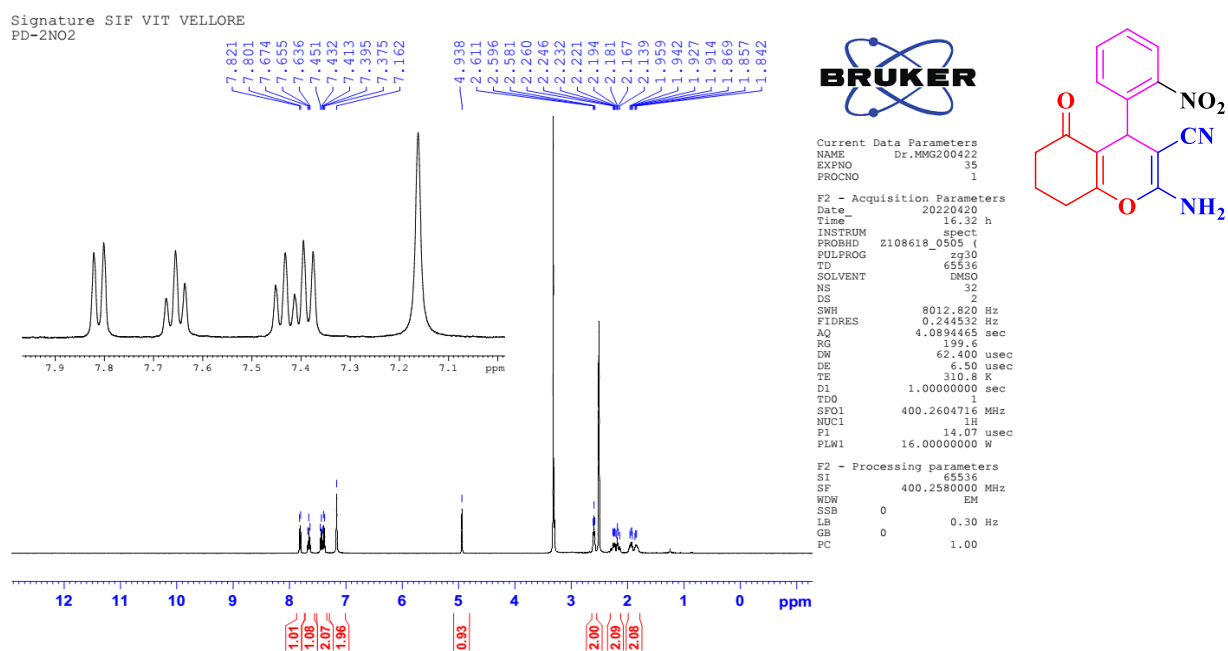


Figure S9. IR spectrum of 1.4b.

Figure S10. ¹H NMR spectrum of 1.4c.

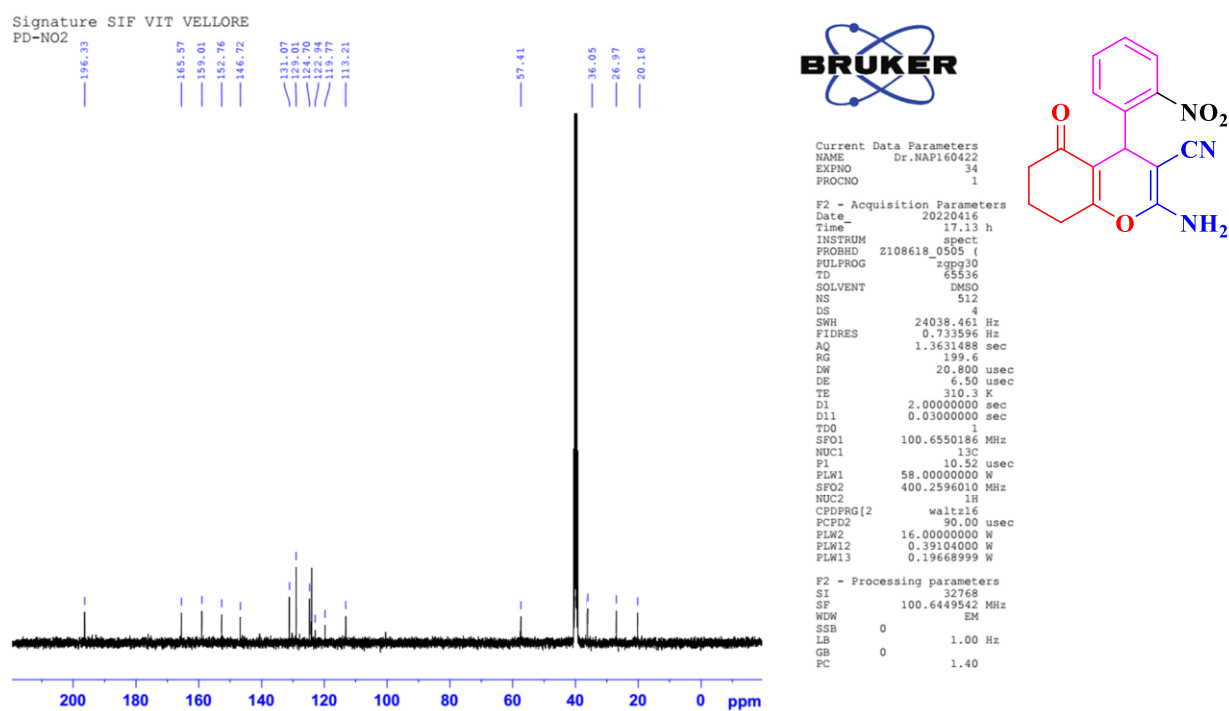
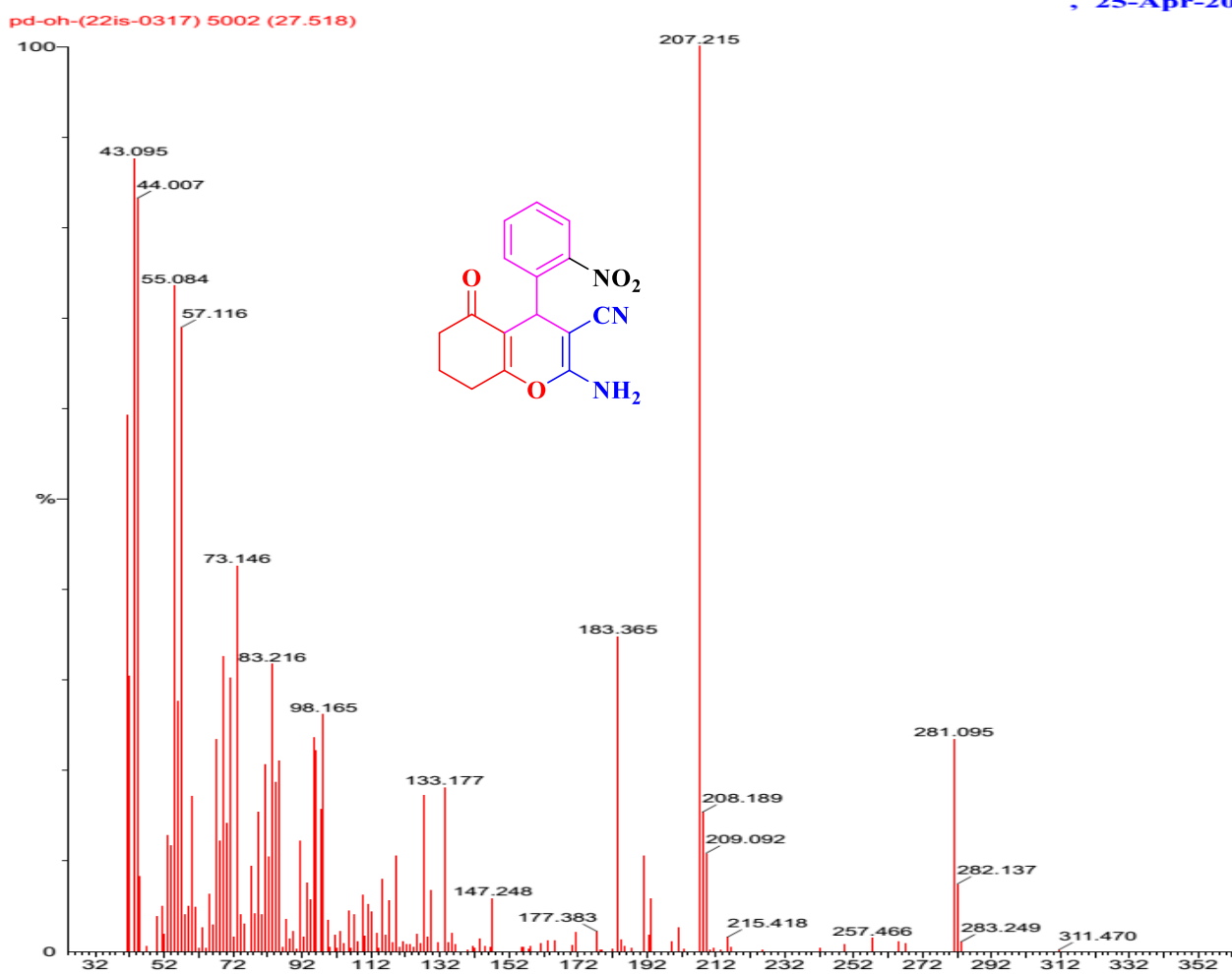
Figure S11. ¹³C NMR spectrum of 1.4c.

Figure S12. GC-MS spectrum of 1.4c.

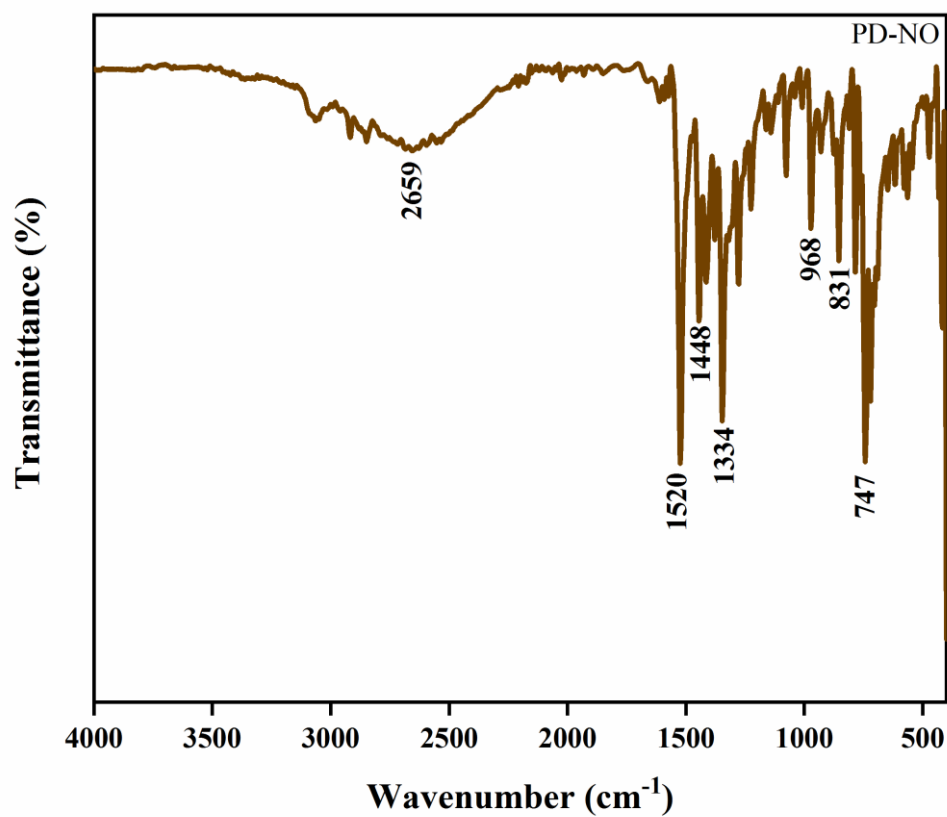
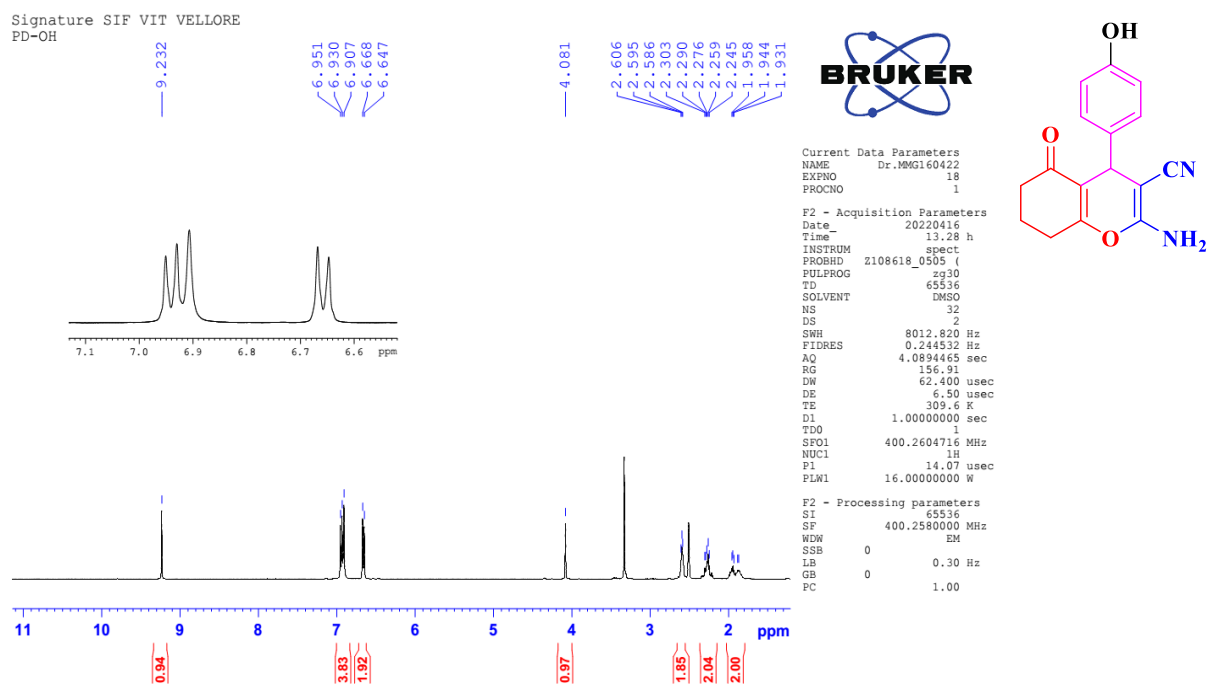
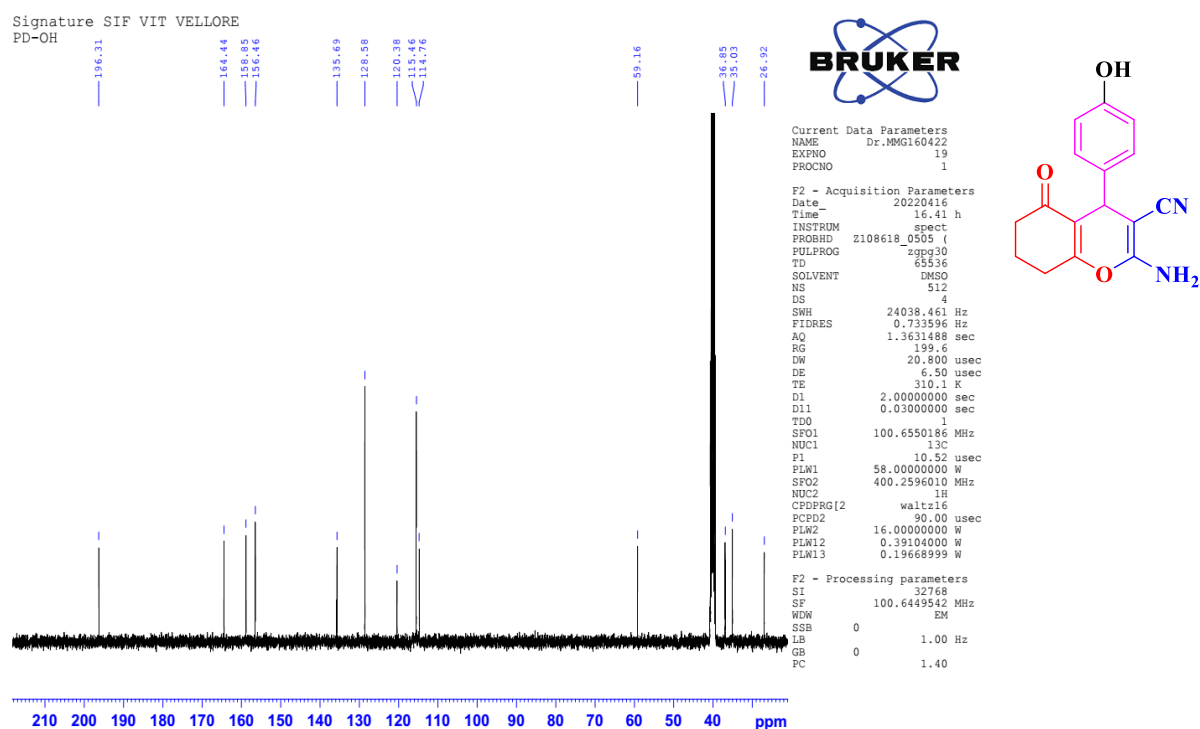


Figure S13. IR spectrum of 1.4c.

Figure S14. ¹H NMR spectrum of 1.4d.

Figure S15. ¹³C NMR spectrum of 1.4d.

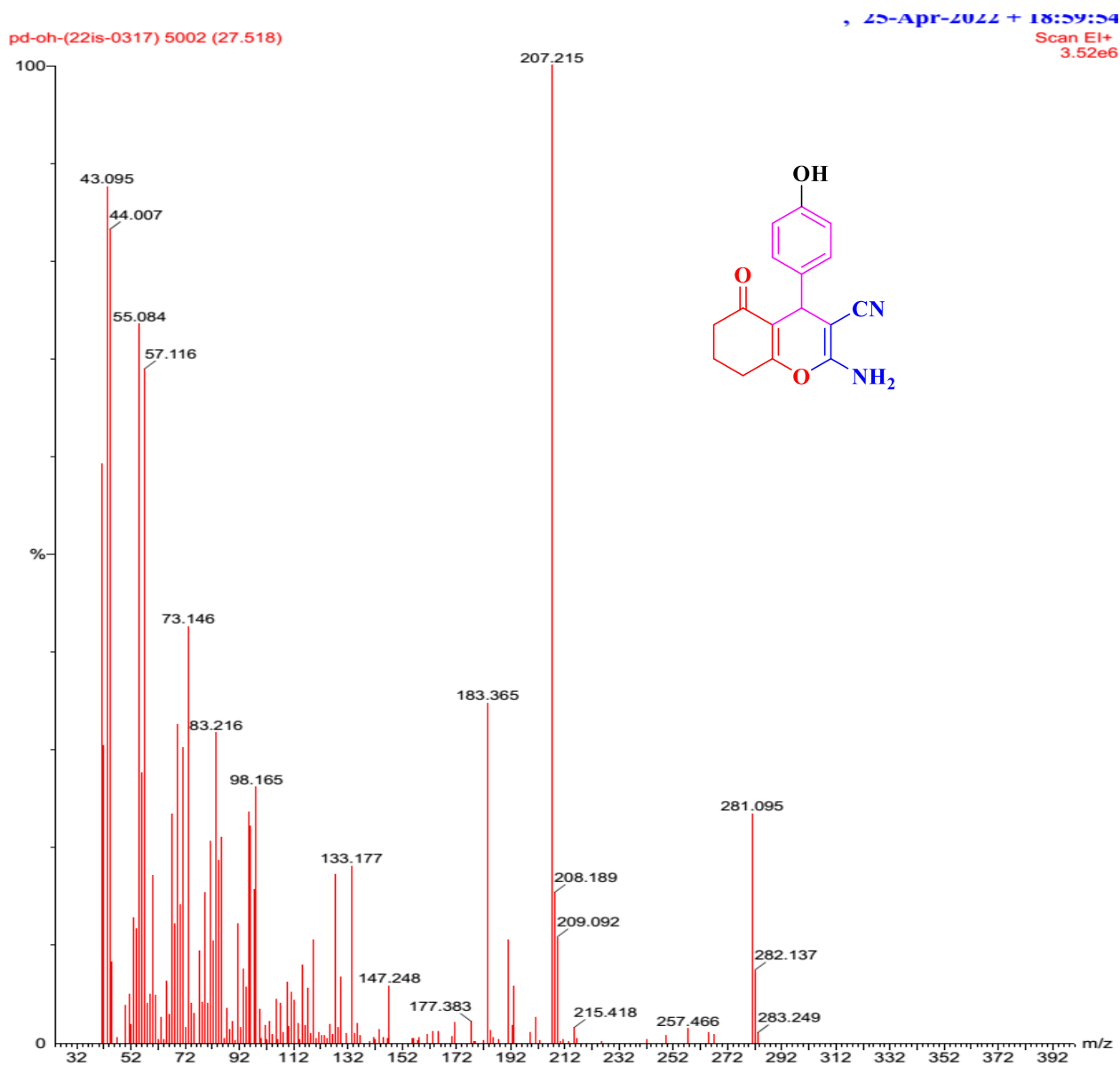


Figure S16. GC-MS spectrum of 1.4d.

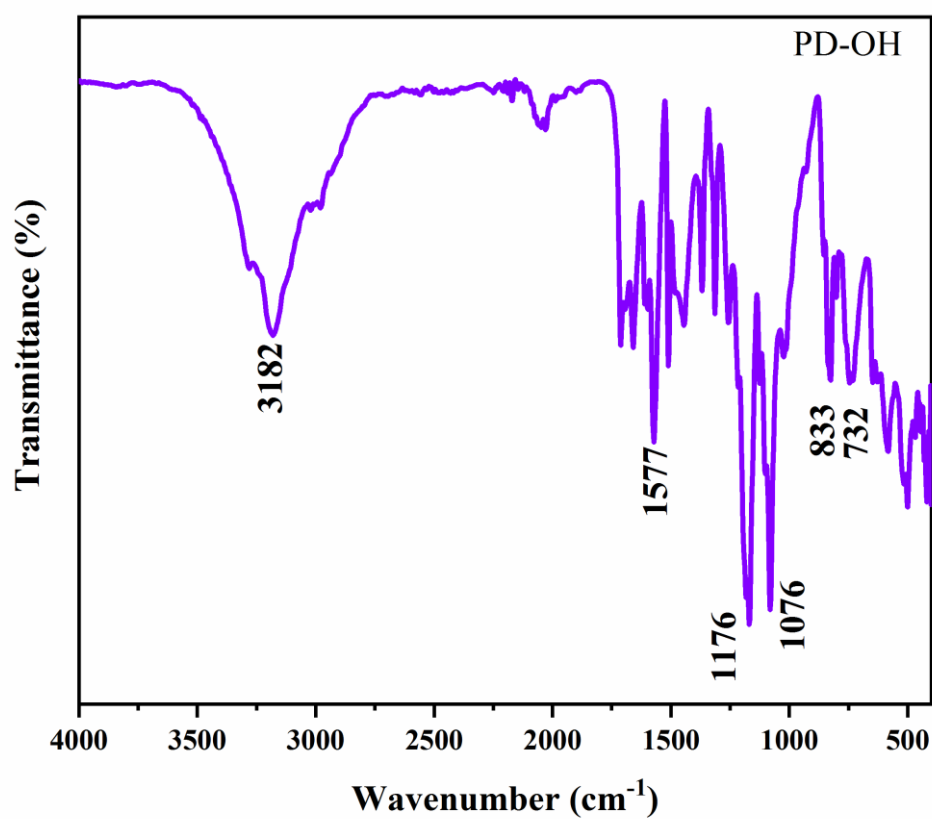
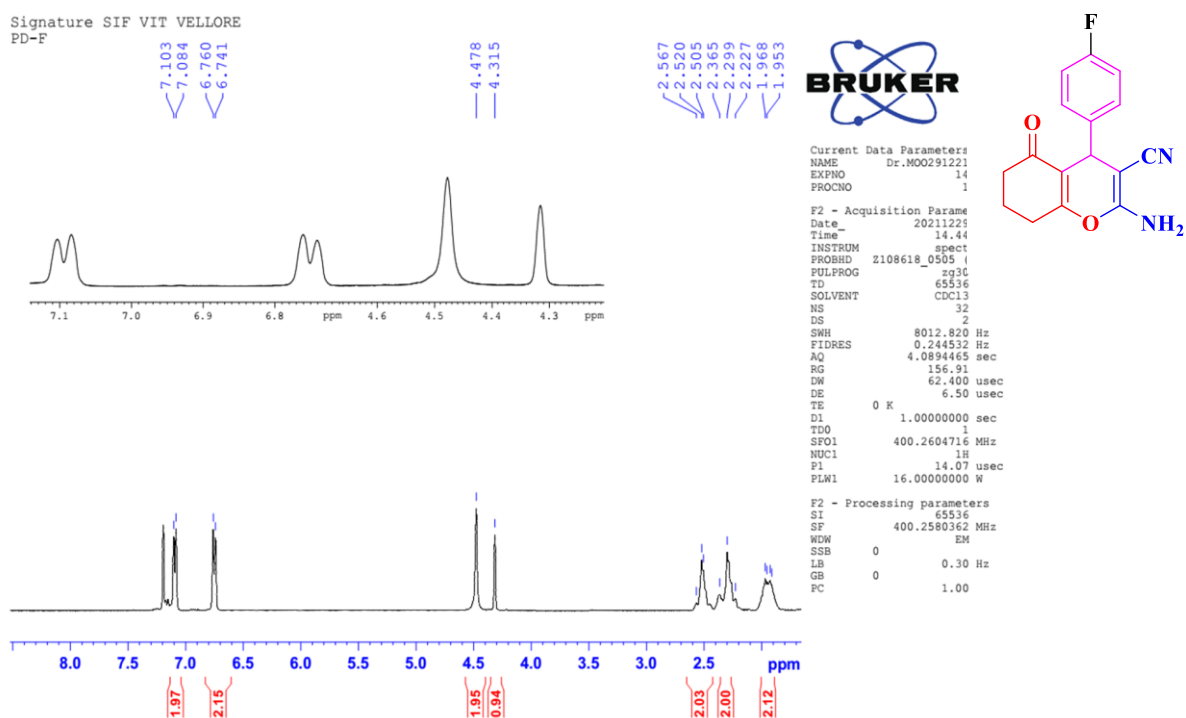
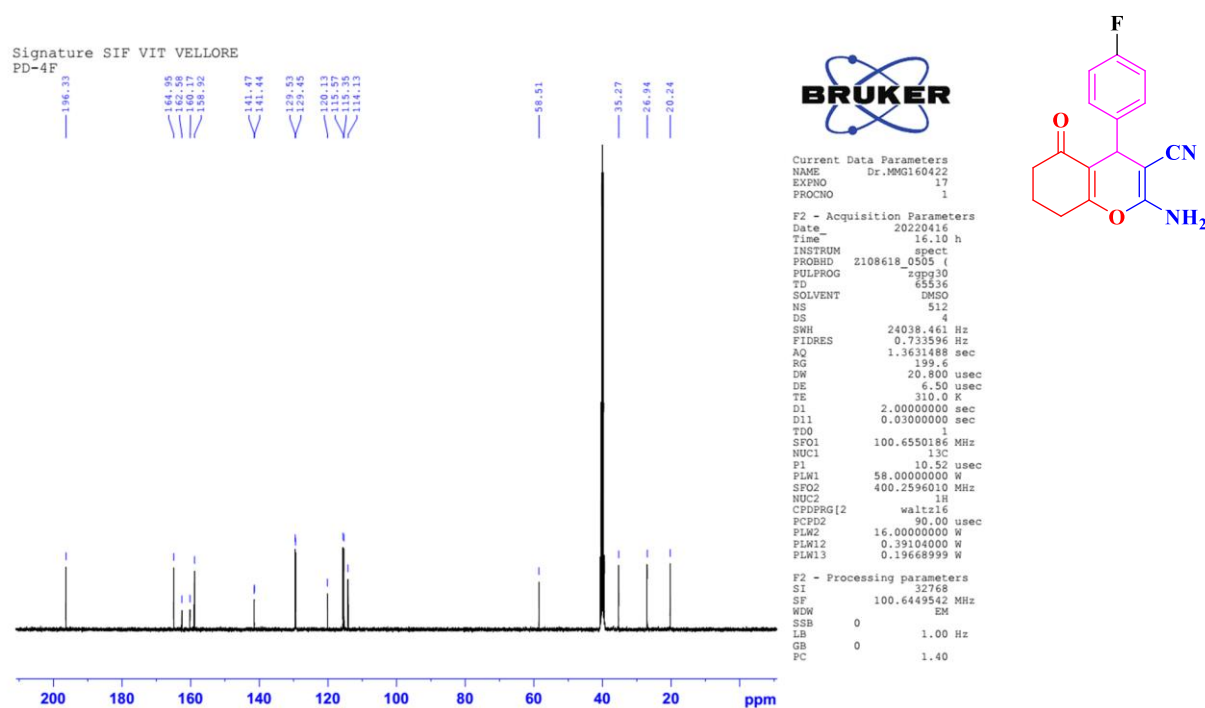


Figure S17. IR spectrum of 1.4d.

Figure S18. ¹H NMR spectrum of 1.4e.

Figure S19. ^{13}C NMR spectrum of 1.4e.

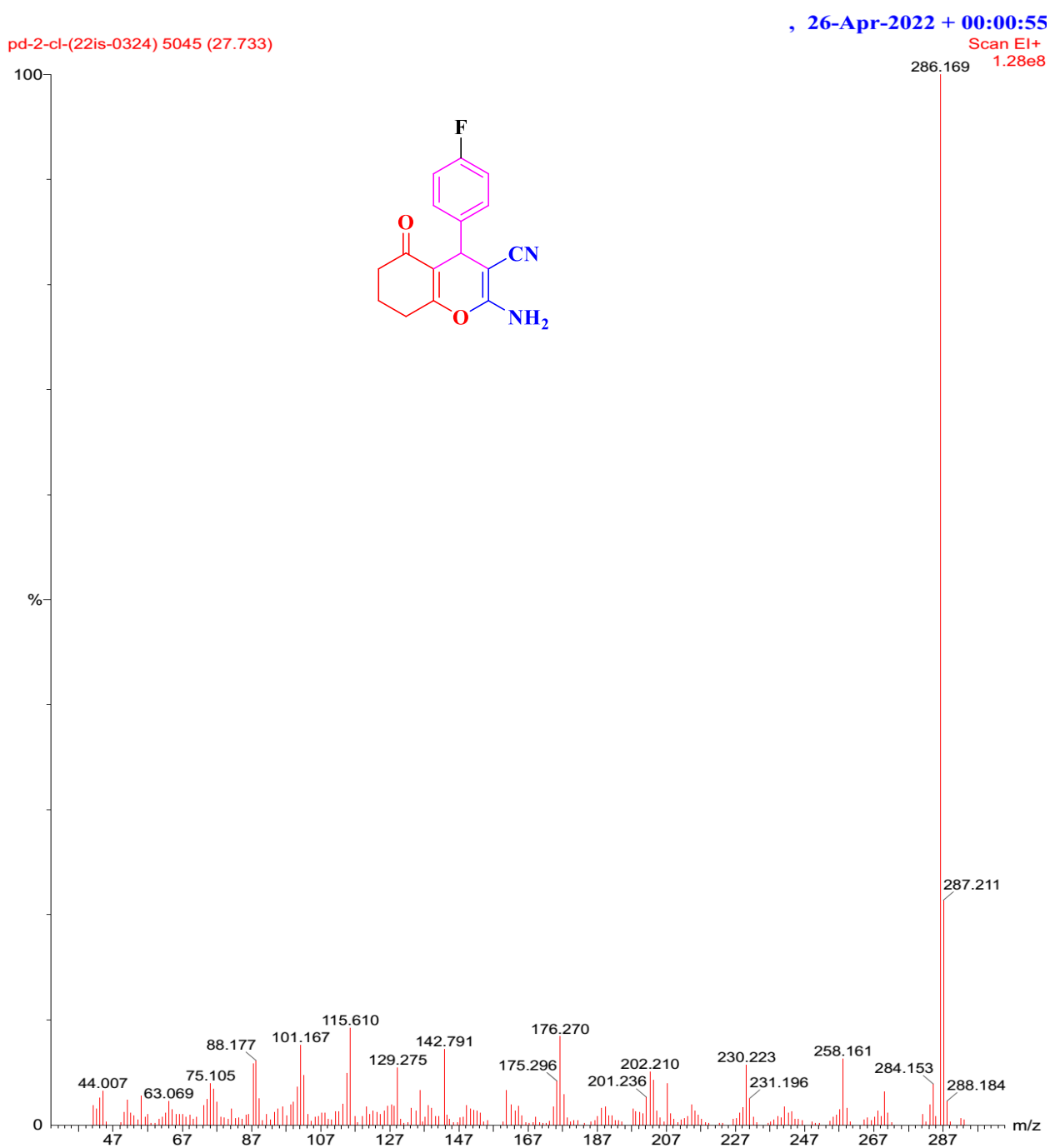


Figure S20. GC-MS spectrum of 1.4e.

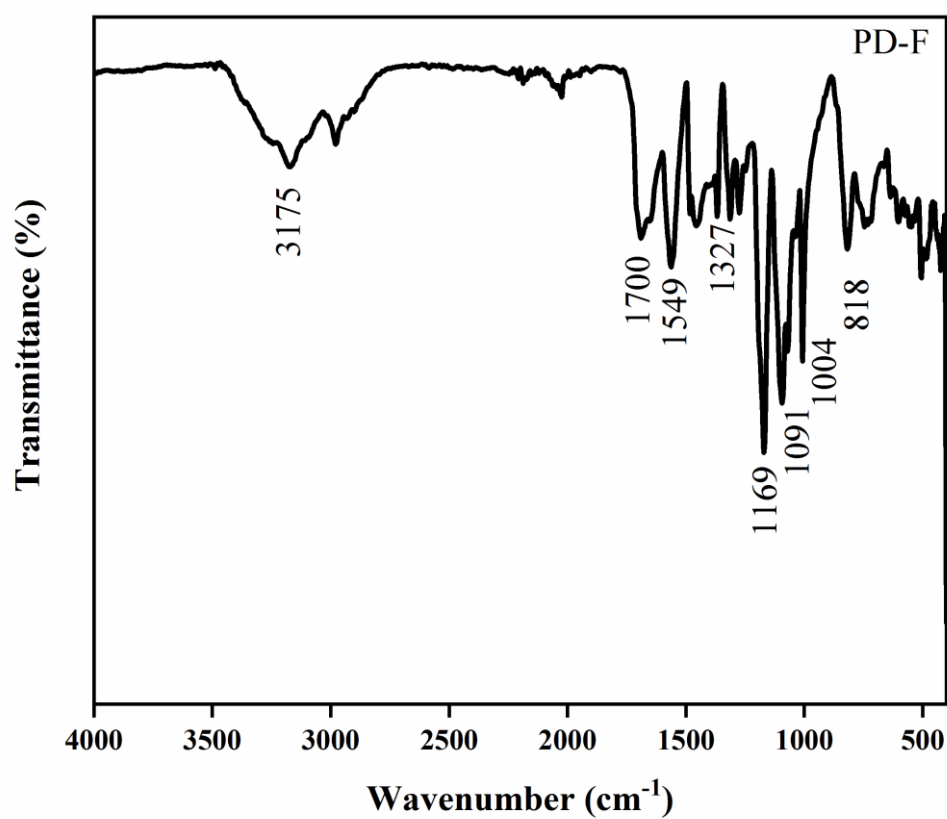
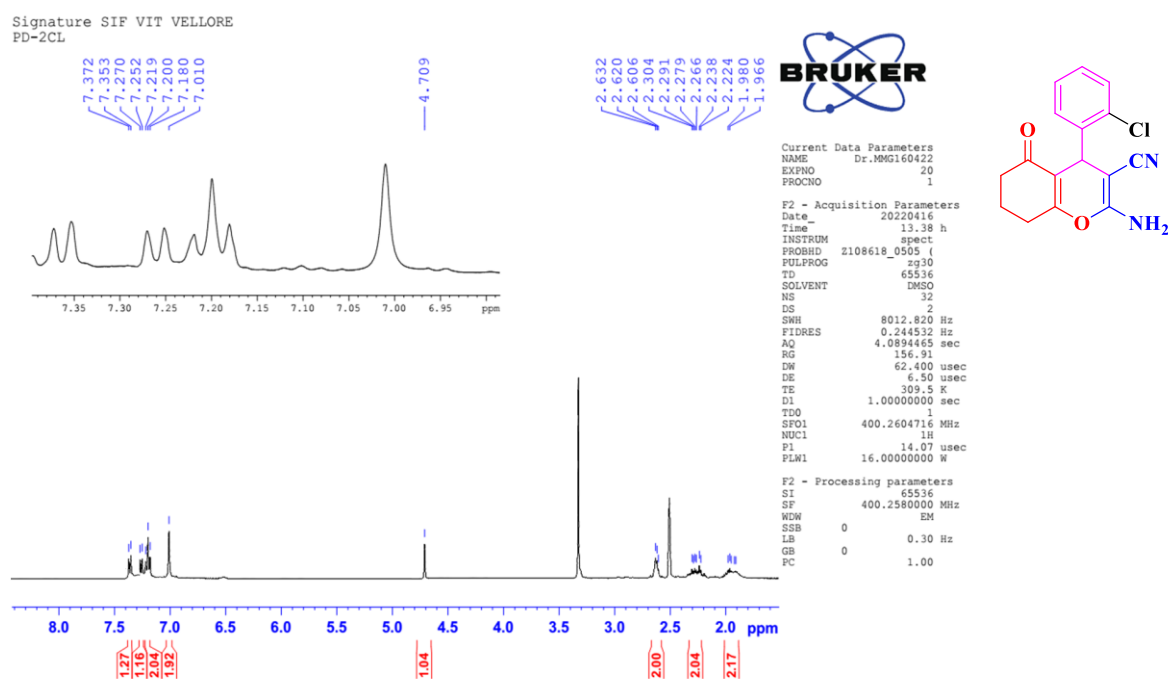


Figure S21. IR spectrum of 1.4e.

Figure S22. ¹H NMR spectrum of 1.4f.

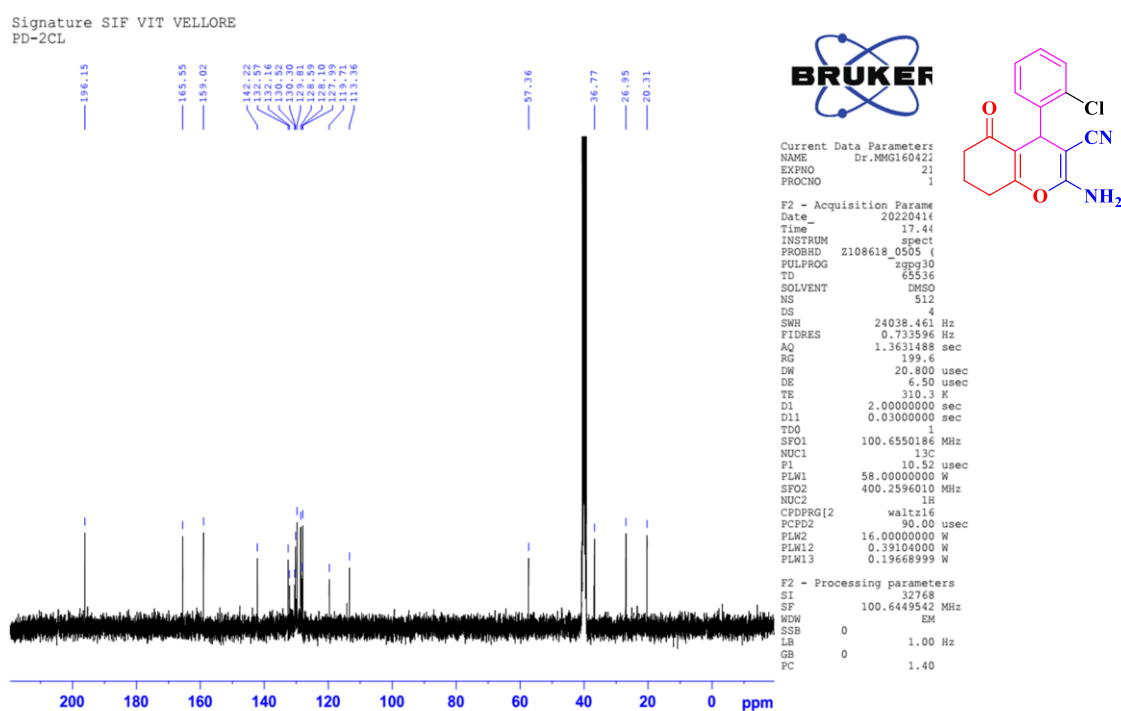
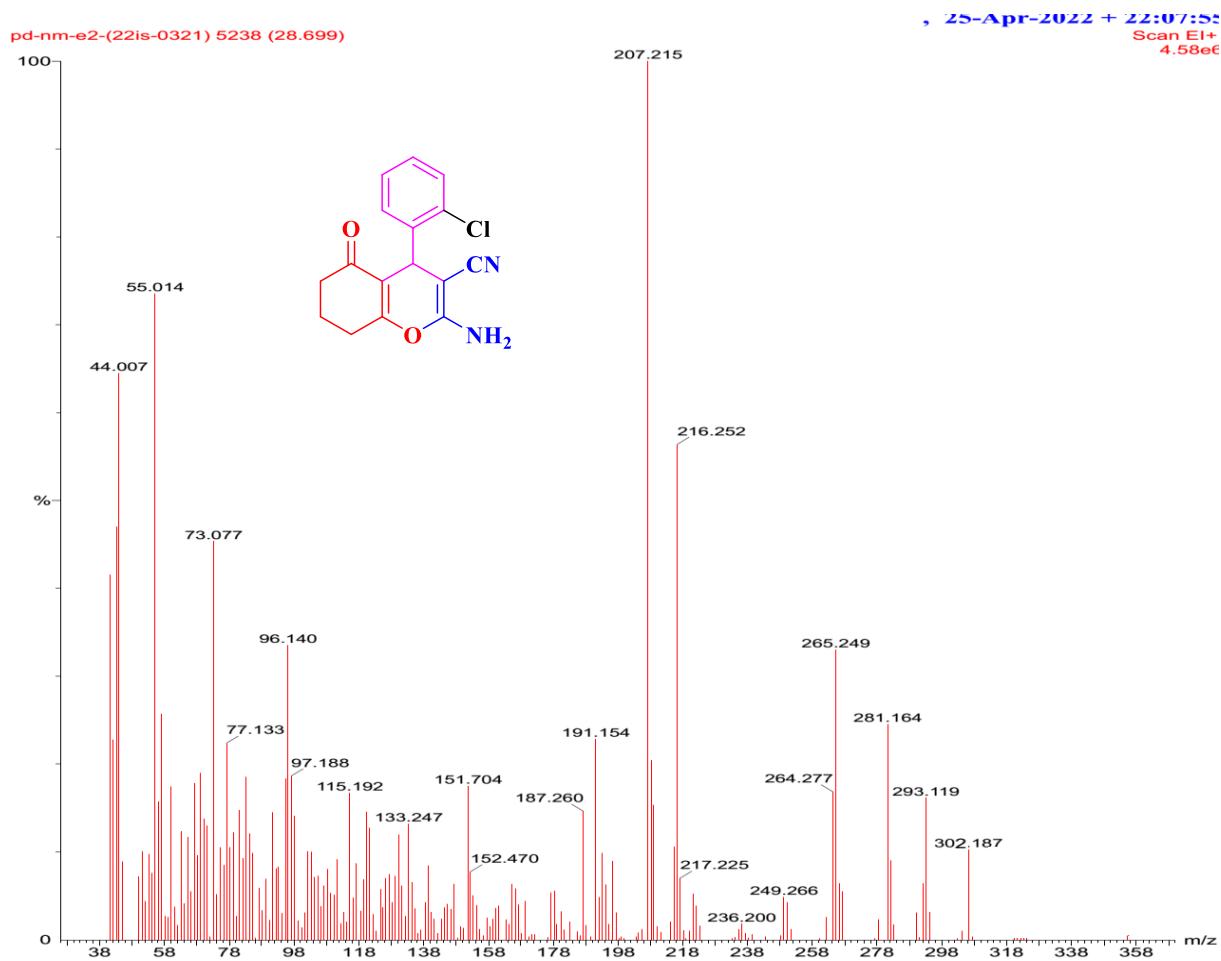
Figure S23. ^{13}C NMR spectrum of 1.4f.

Figure S24. GC-MS spectrum of 1.4f.

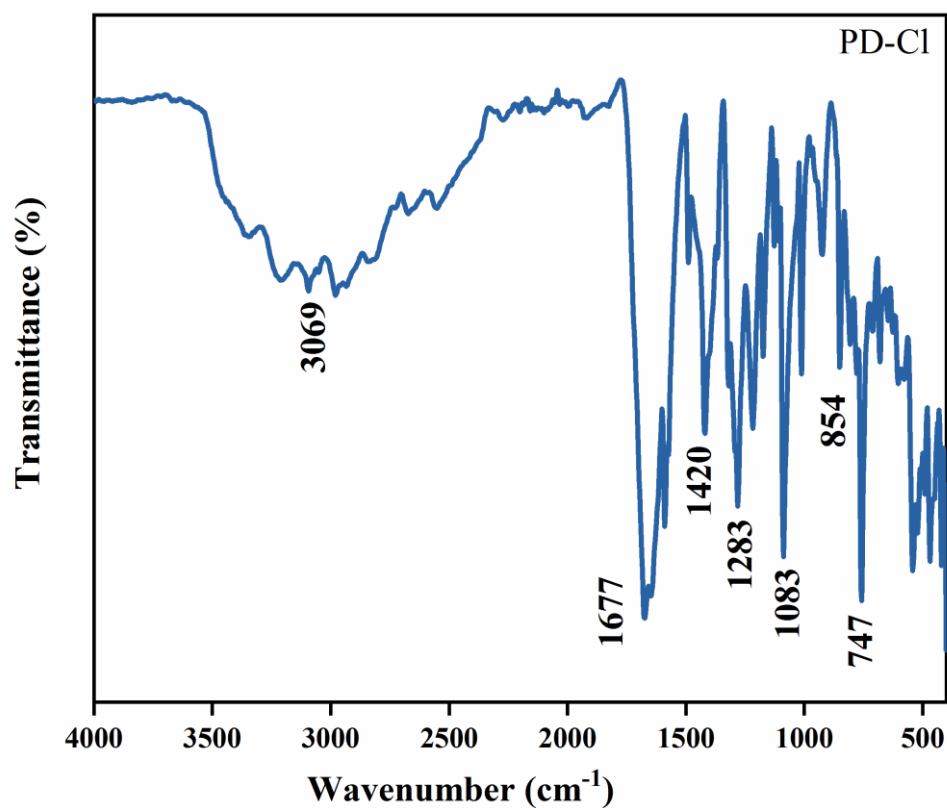
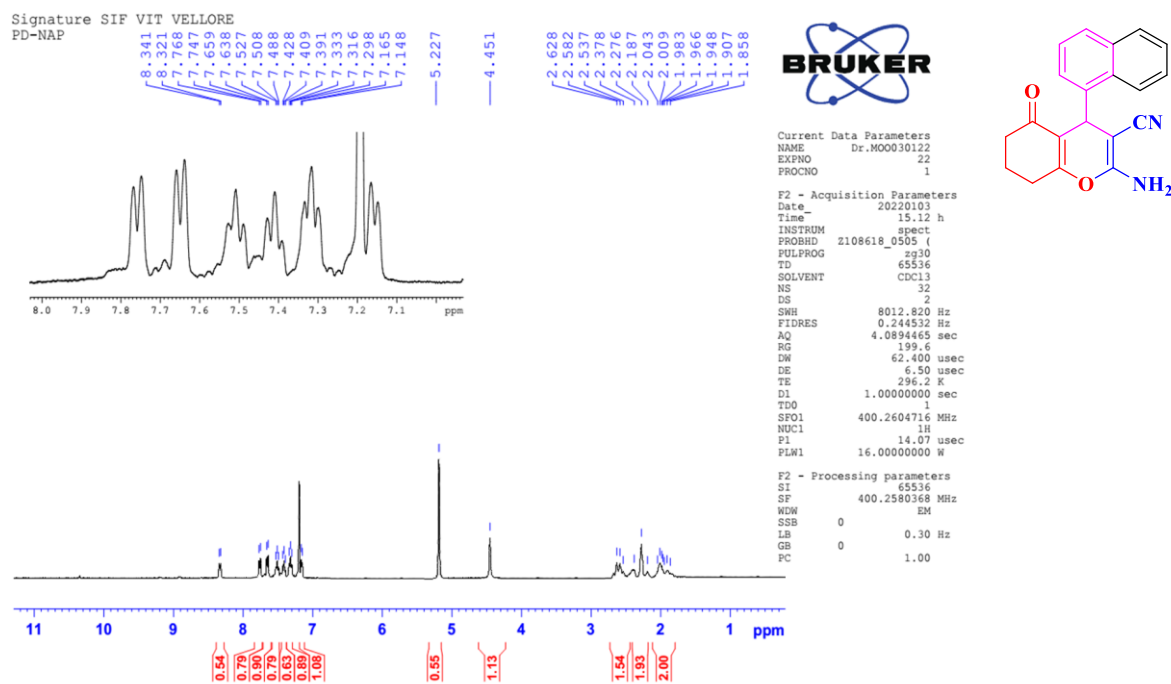
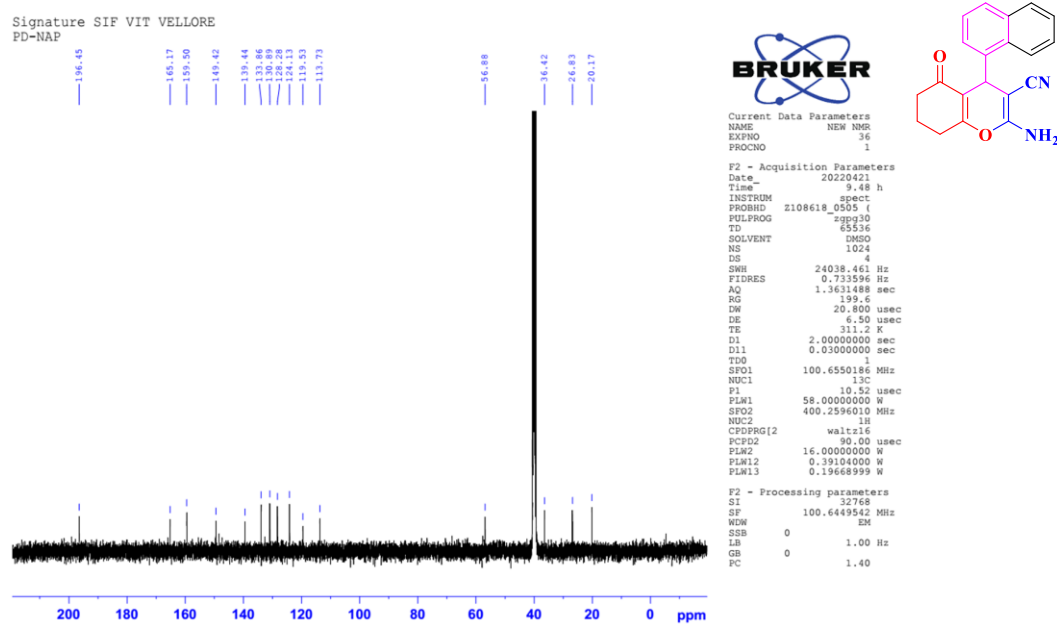


Figure S25. IR spectrum of 1.4f.

Figure S26. ¹H NMR spectrum of 1.4g.

Figure S27. ^{13}C NMR spectrum of 1.4g.

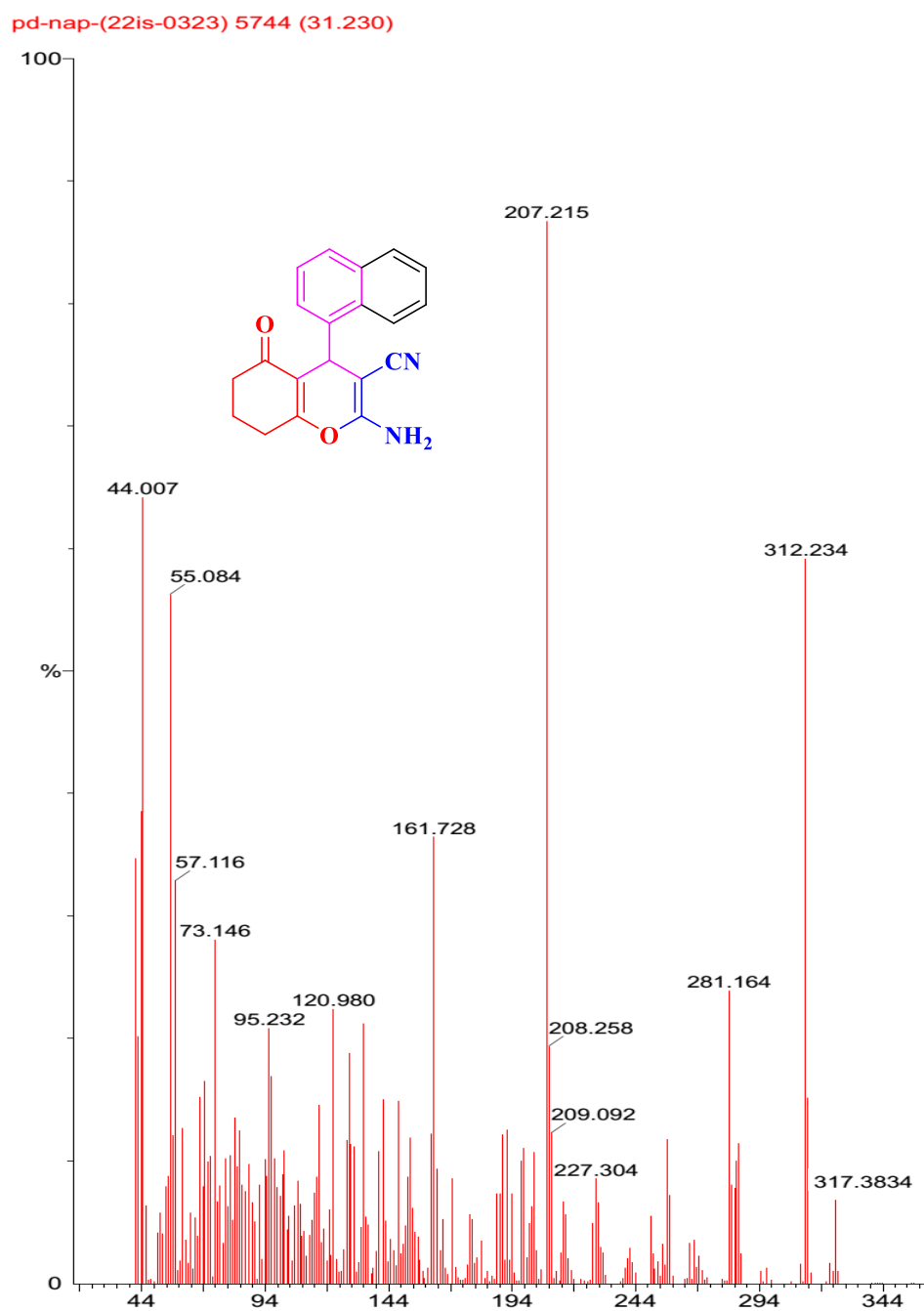


Figure S28. GC-MS spectrum of 1.4g.

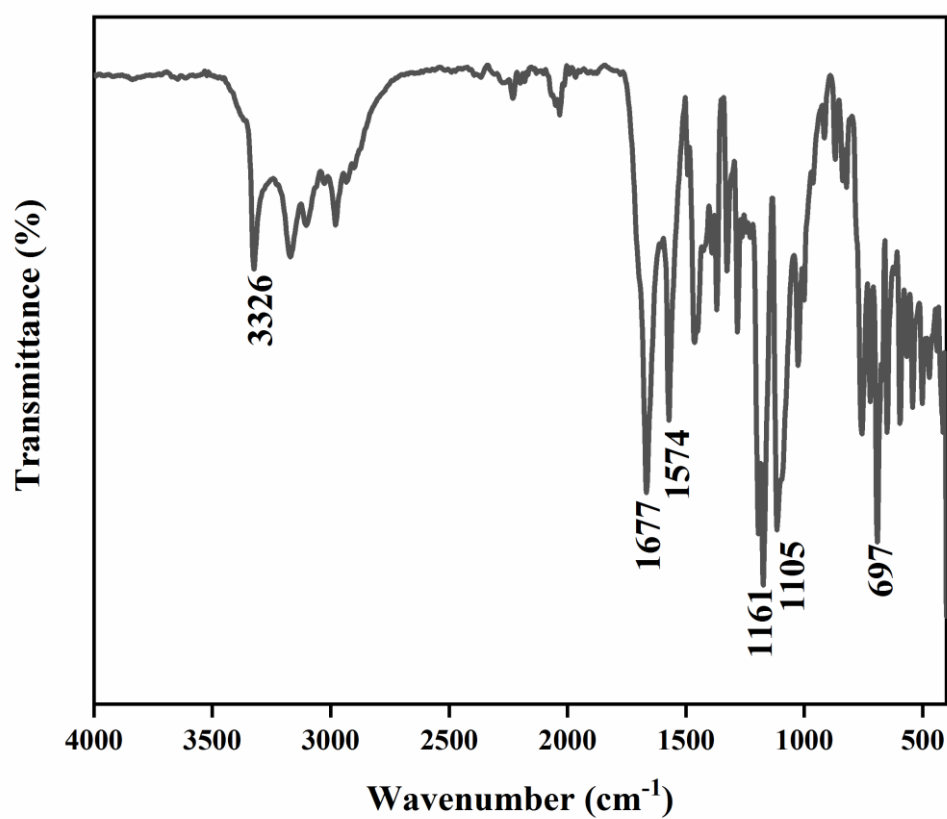


Figure S29. IR spectrum of 1.4g.

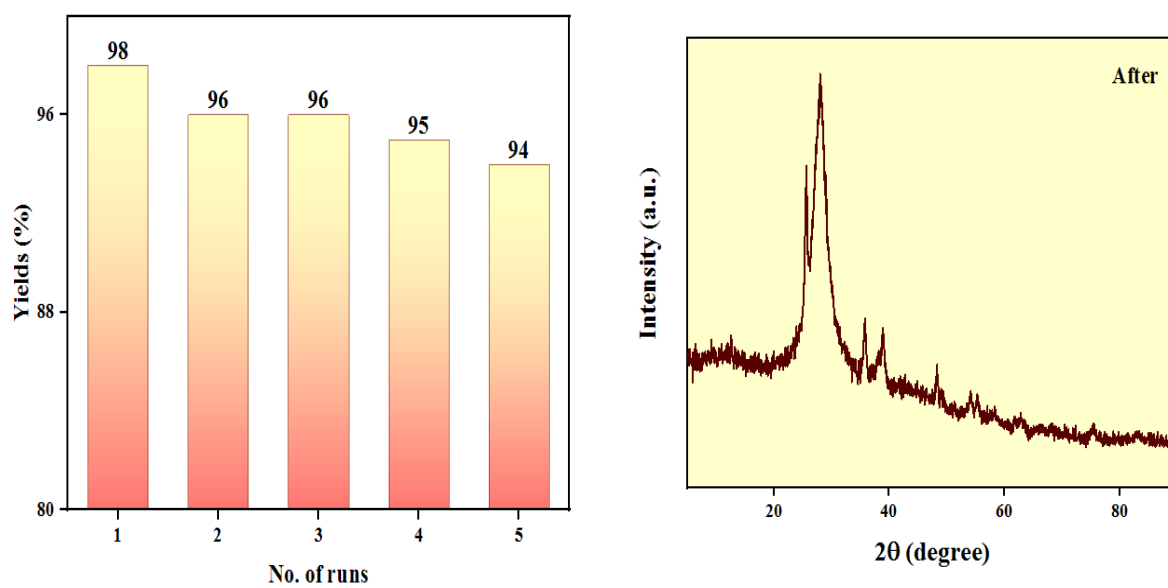


Figure S30. Reusability and reused XRD of 10% CN5CT nanocomposites.