

One-Pot Synthesis, Computational Chemical Study, Molecular Docking, Biological Study, and *in Silico* Prediction ADME/Pharmacokinetics Properties of 5-Substituted 1*H*-Tetrazole Derivatives

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Supporting information:

Cont. Table 3. Cytotoxic activity of compound **4c** against the tested cell lines.

		<i>In-vitro</i> cytotoxicity											
Cell lines		<i>BJ-1</i>				<i>A431</i>				<i>HCT116</i>			
Concn.		100	50	25	12.5	100	50	25	12.5	100	50	25	12.5
Antitumor effect	1 st test	42.9	39.02	29	0	70.5	63.2	60.7	2.53	21	11.2	0	0
	2 nd test	50.2	41.03	41.03	6.41	65.8	71.4	66.4	4.11	22	9.6	0	0
	3 rd test	52.9	38.02	42.6	14.1	89.1	54.06	37.3	25.3	19.7	10.4	0	0
	Average	48.667	39.357	37.543	6.837	75.133	62.887	54.8	10.647	20.9	10.4	0	0
	IC ₅₀ (µg/mL)	92.045				44.77				201.45			

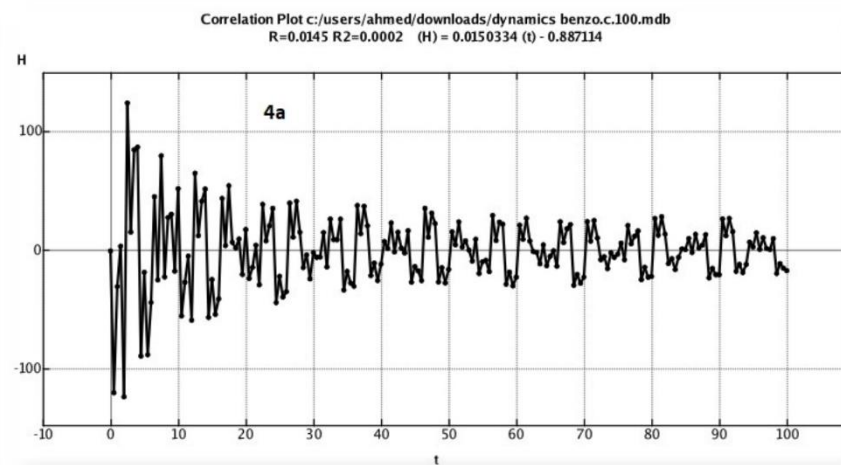
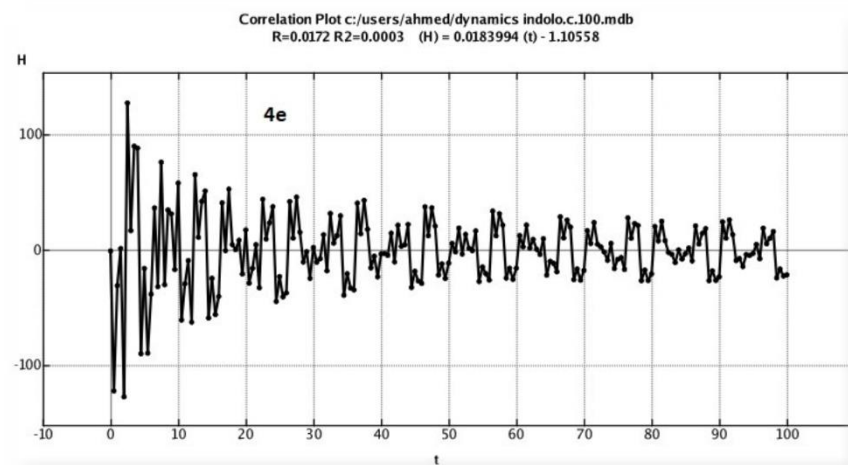
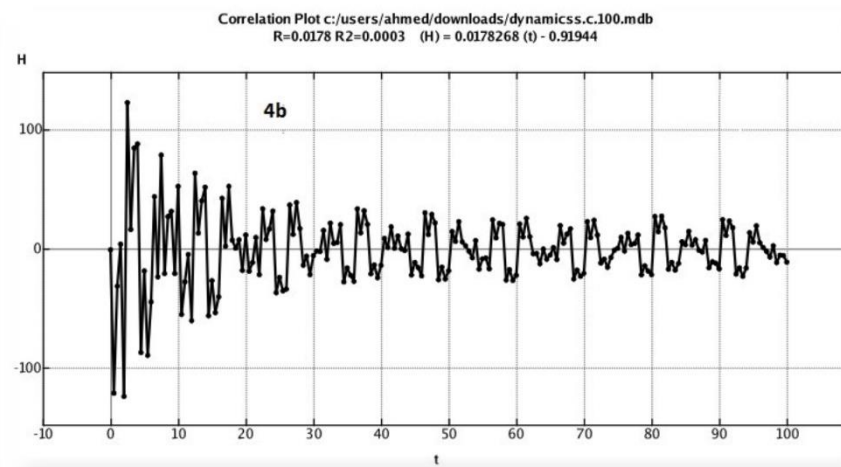
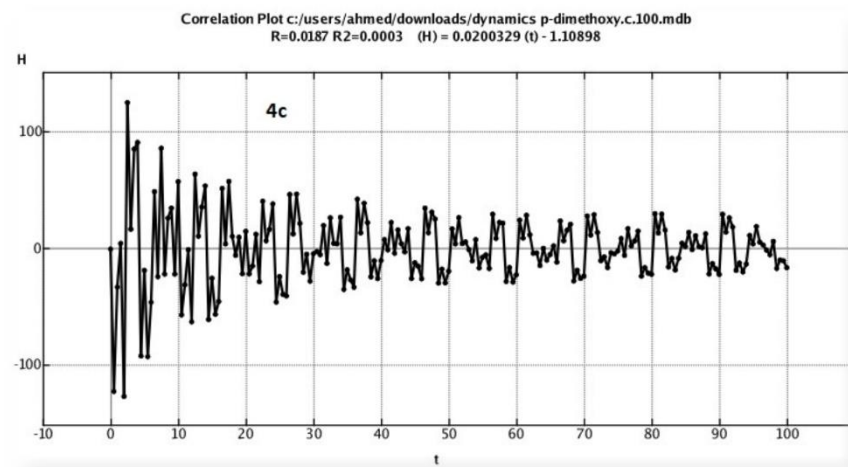


Fig. 17. MD simulation of the synthesized compounds **4a-e**.

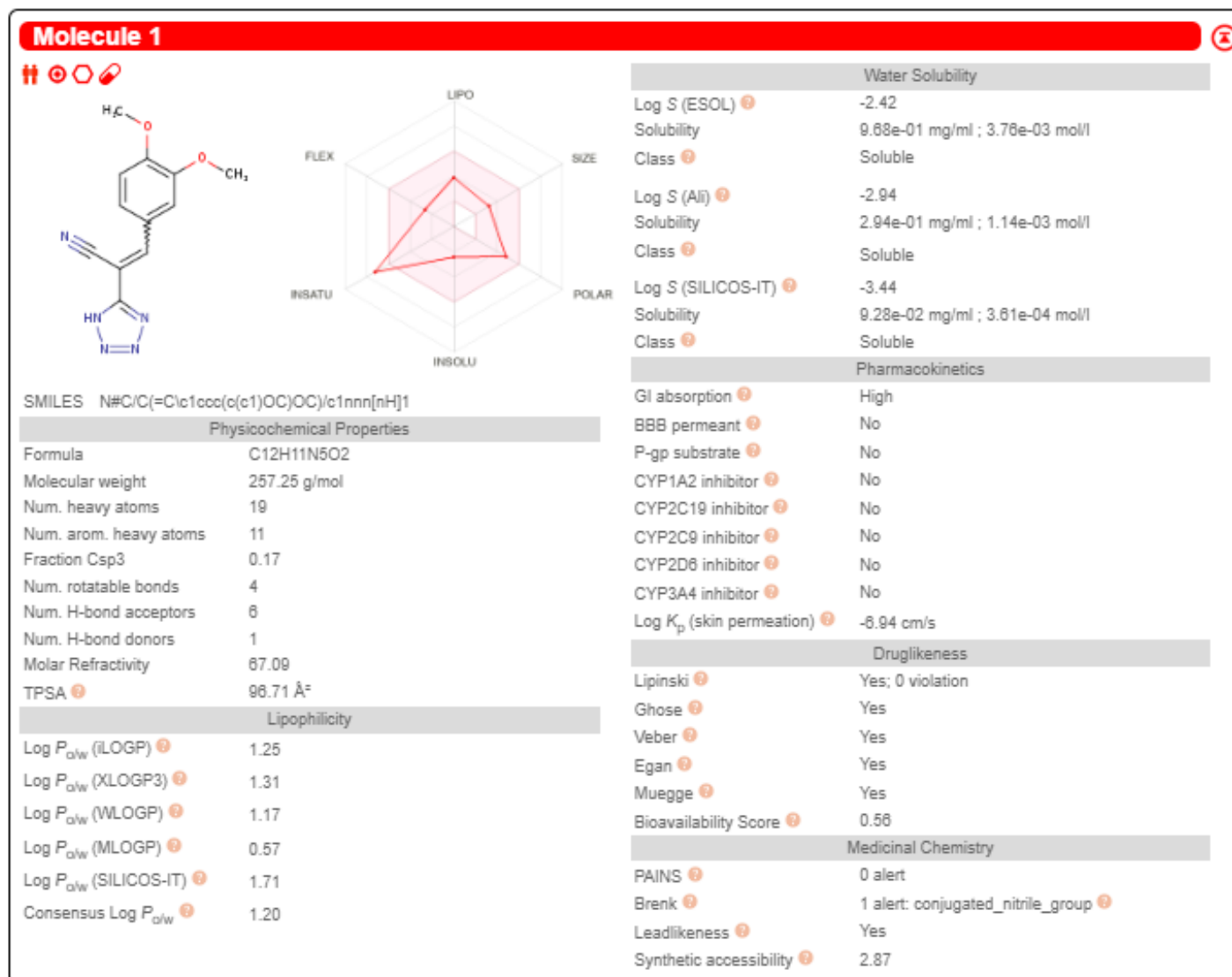


Fig. 18. ADME prediction of compound **4c**.

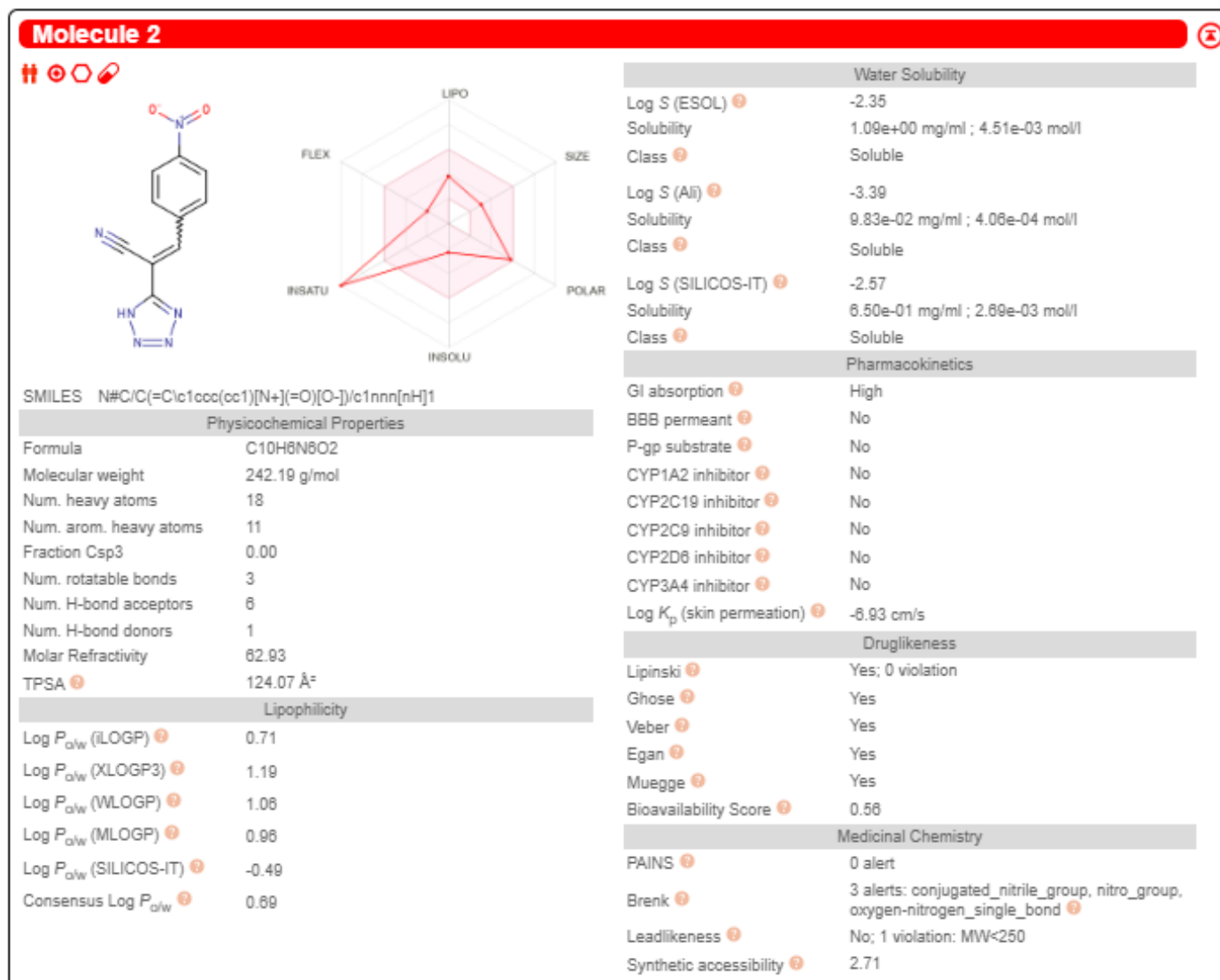


Fig. 19. ADME prediction of compound **4d**.

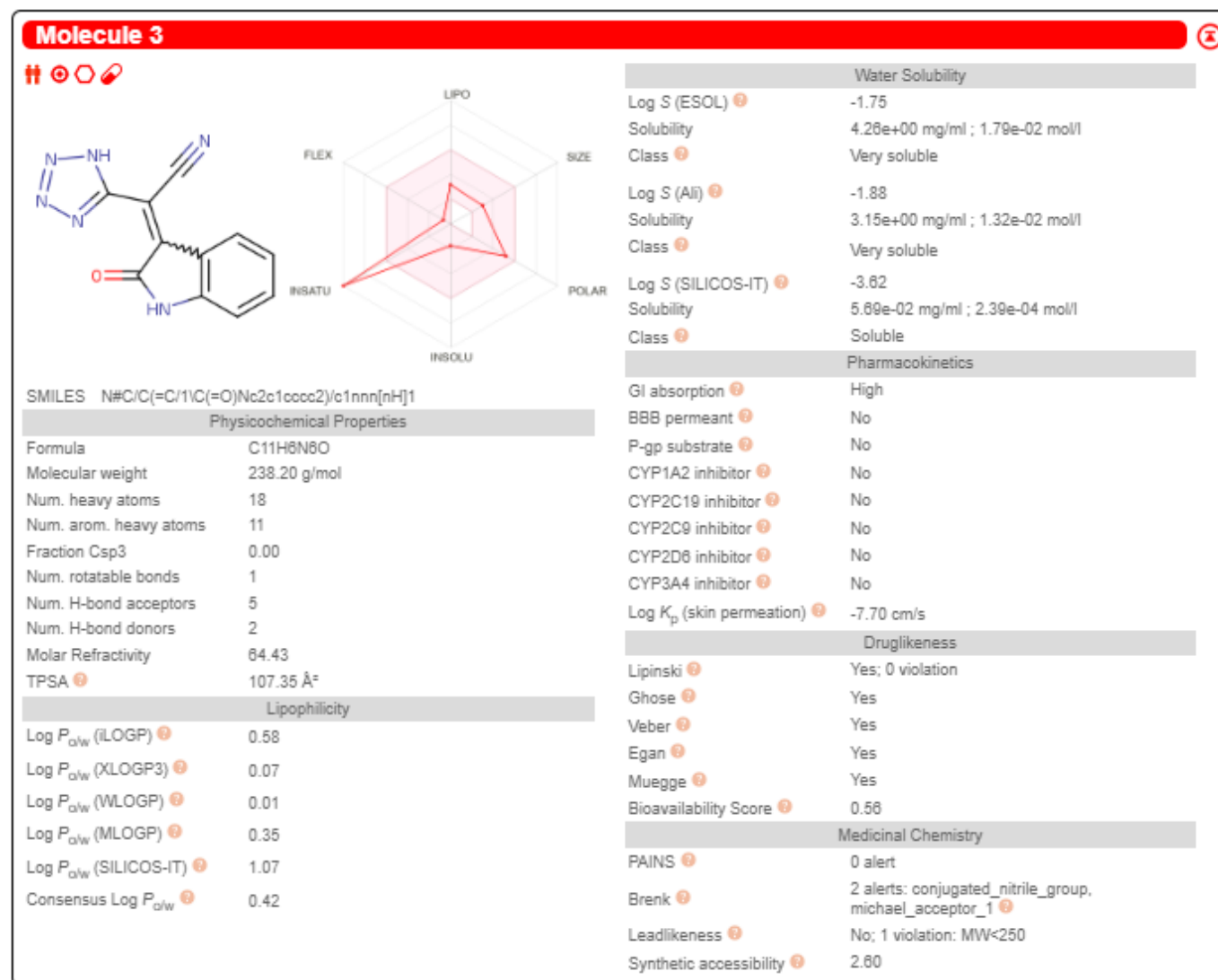


Fig. 20. ADME prediction of compound 4e.

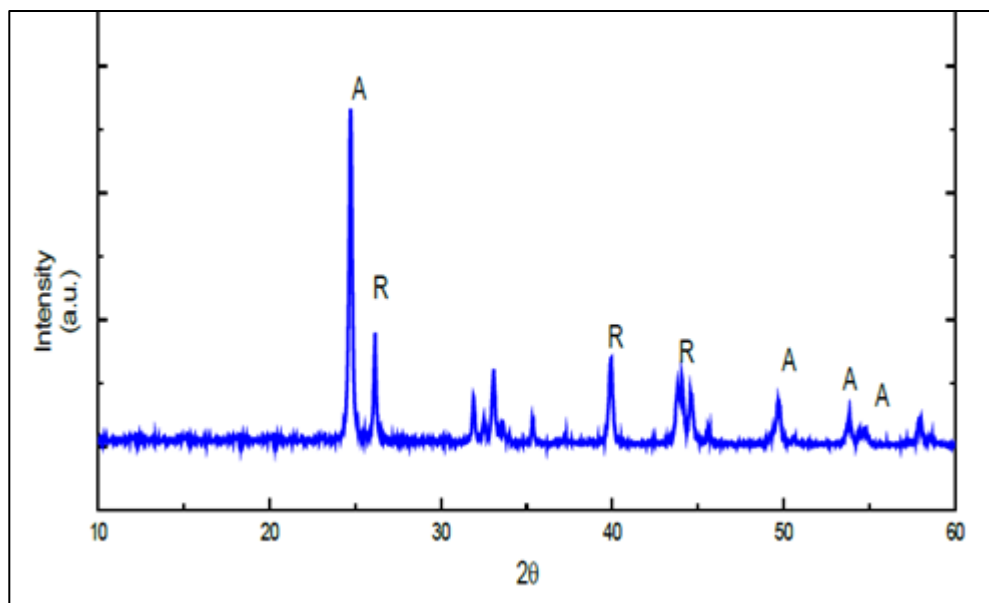


Fig. 21. XRD pattern of TiO₂ nanoparticles.

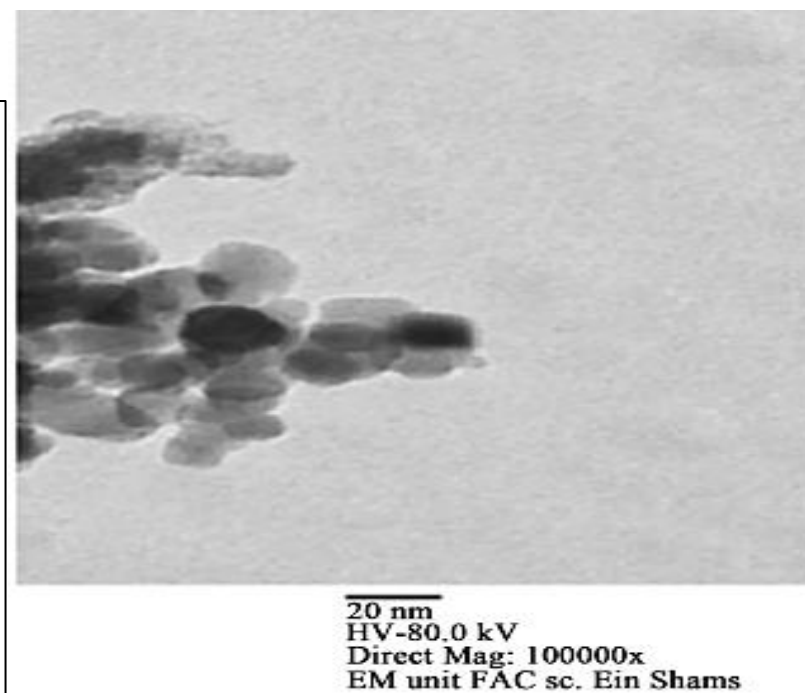


Fig. 22. TEM micrographs of TiO₂ nanoparticles.

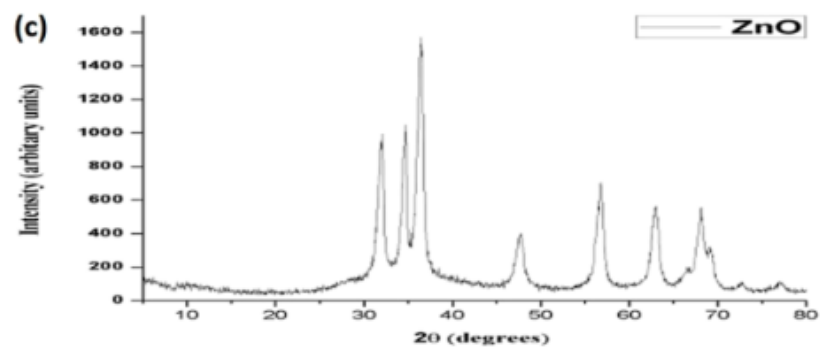


Fig. 23. XRD pattern of ZnO nanoparticles.

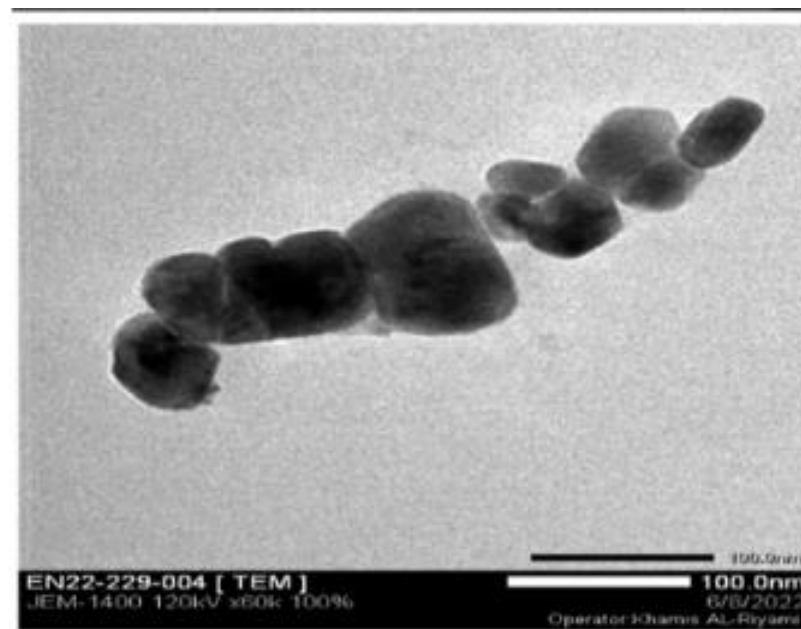
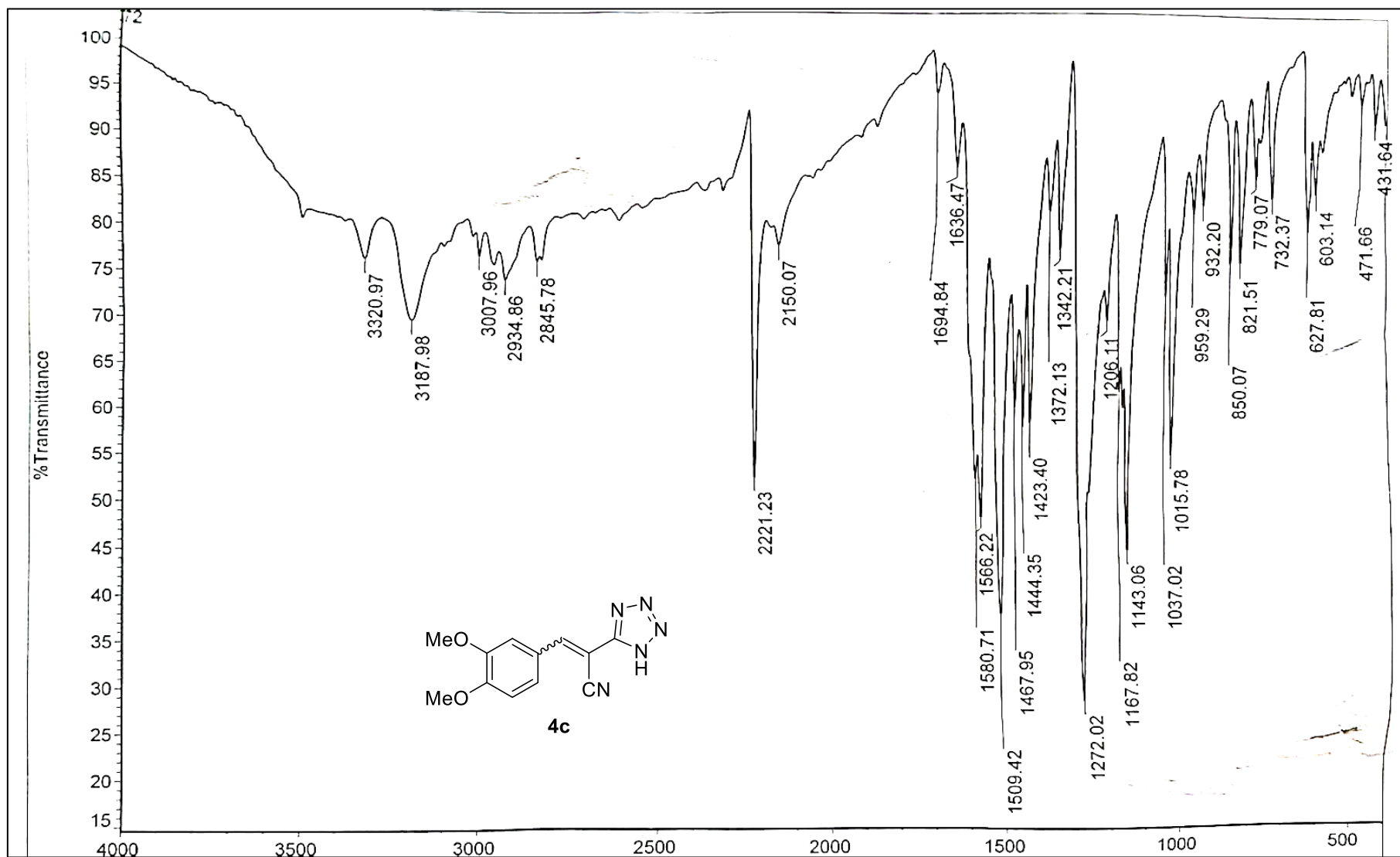
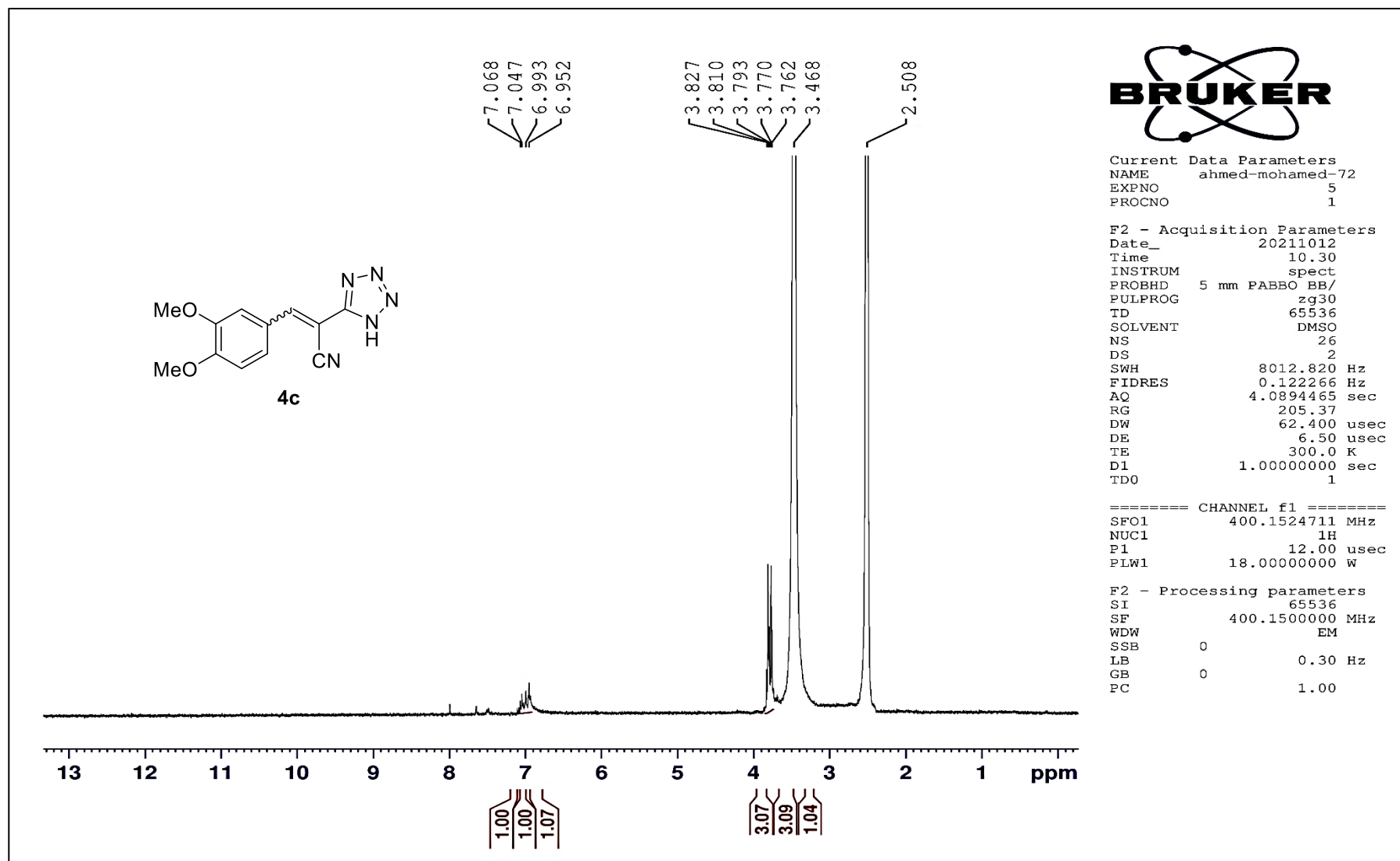


Fig. 24. TEM micrographs of ZnO nanoparticles.

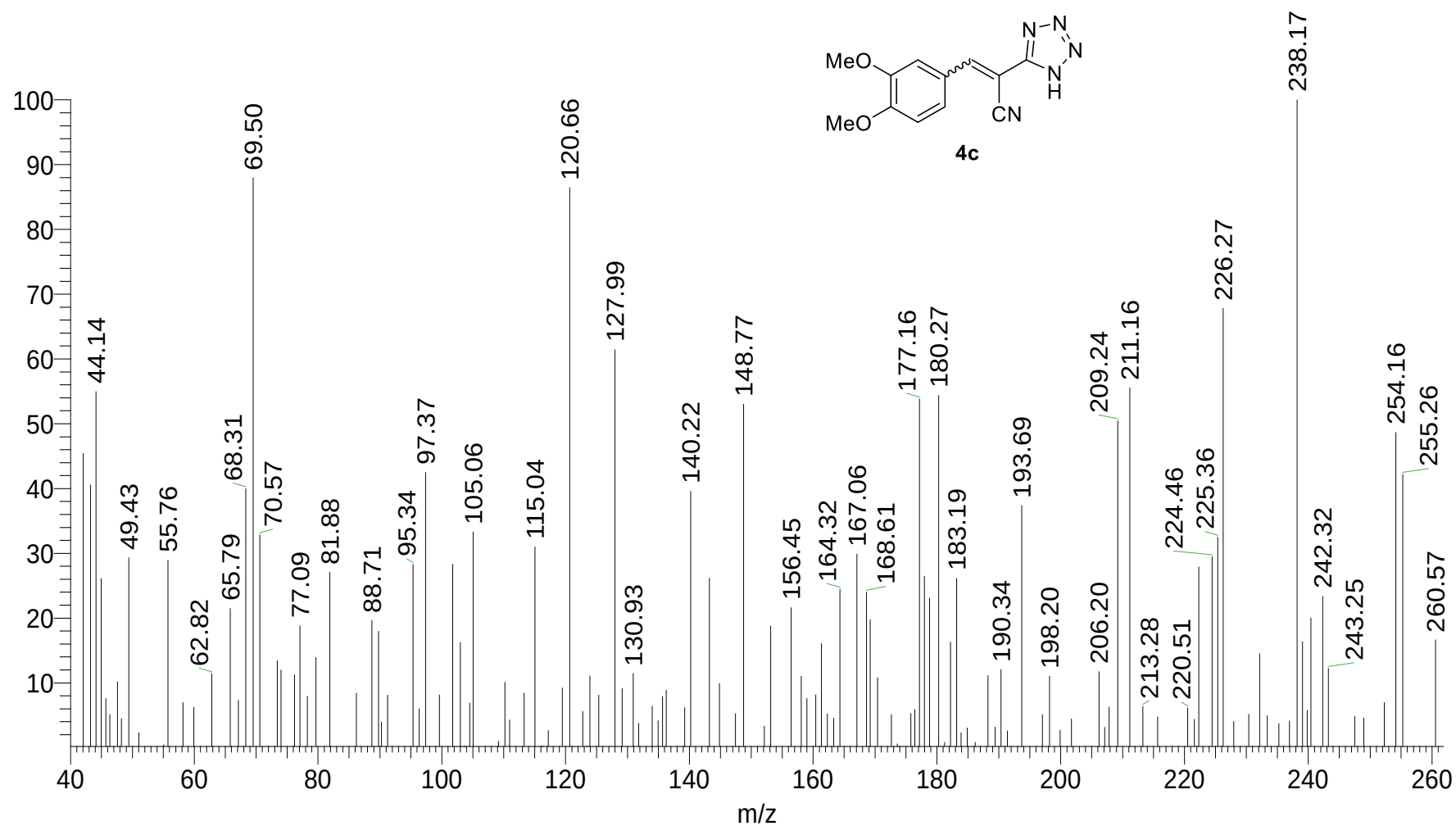


IR spectrum of compound **4c**.

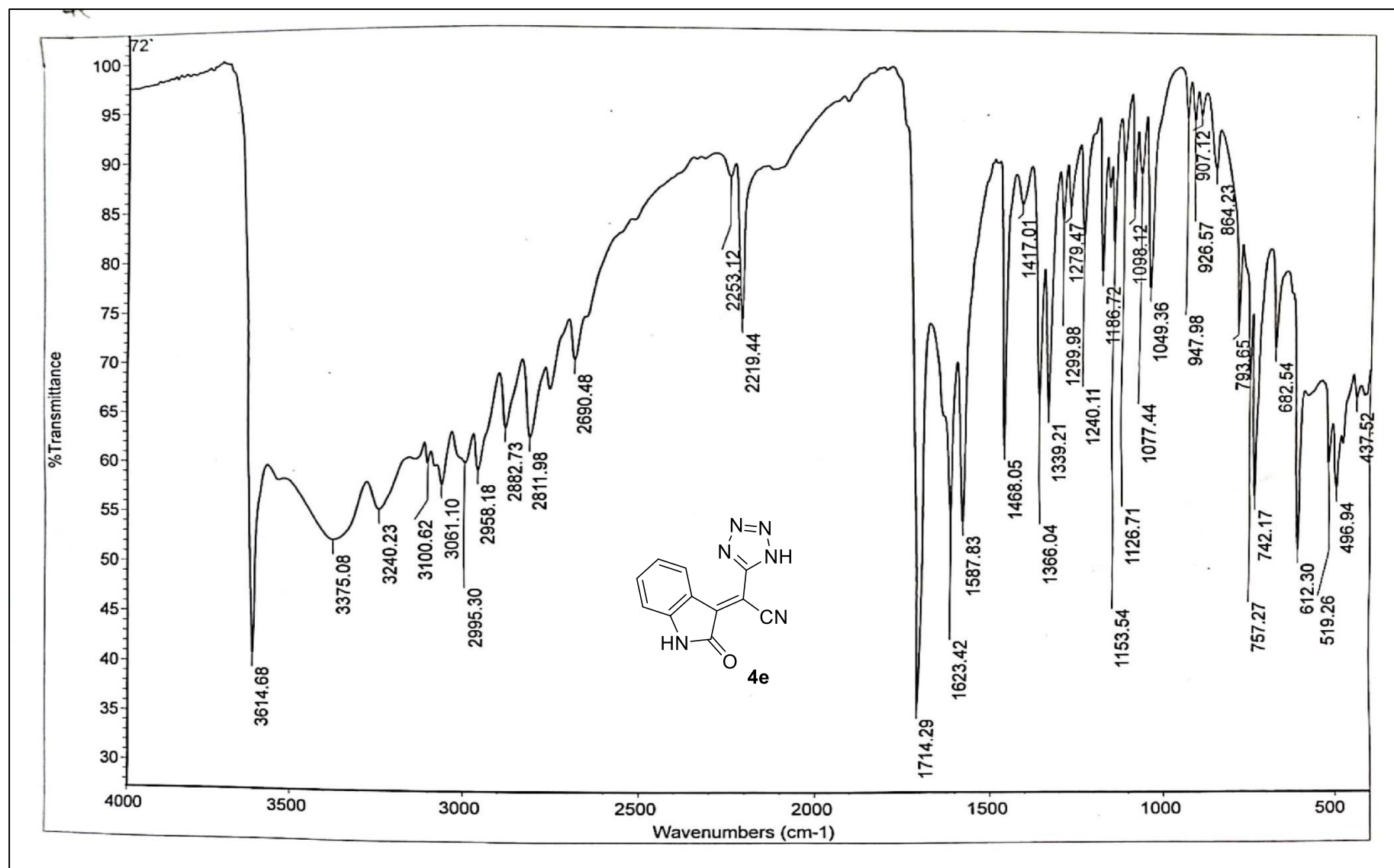


¹H NMR spectrum (DMSO-*d*₆) of compound **4c**.

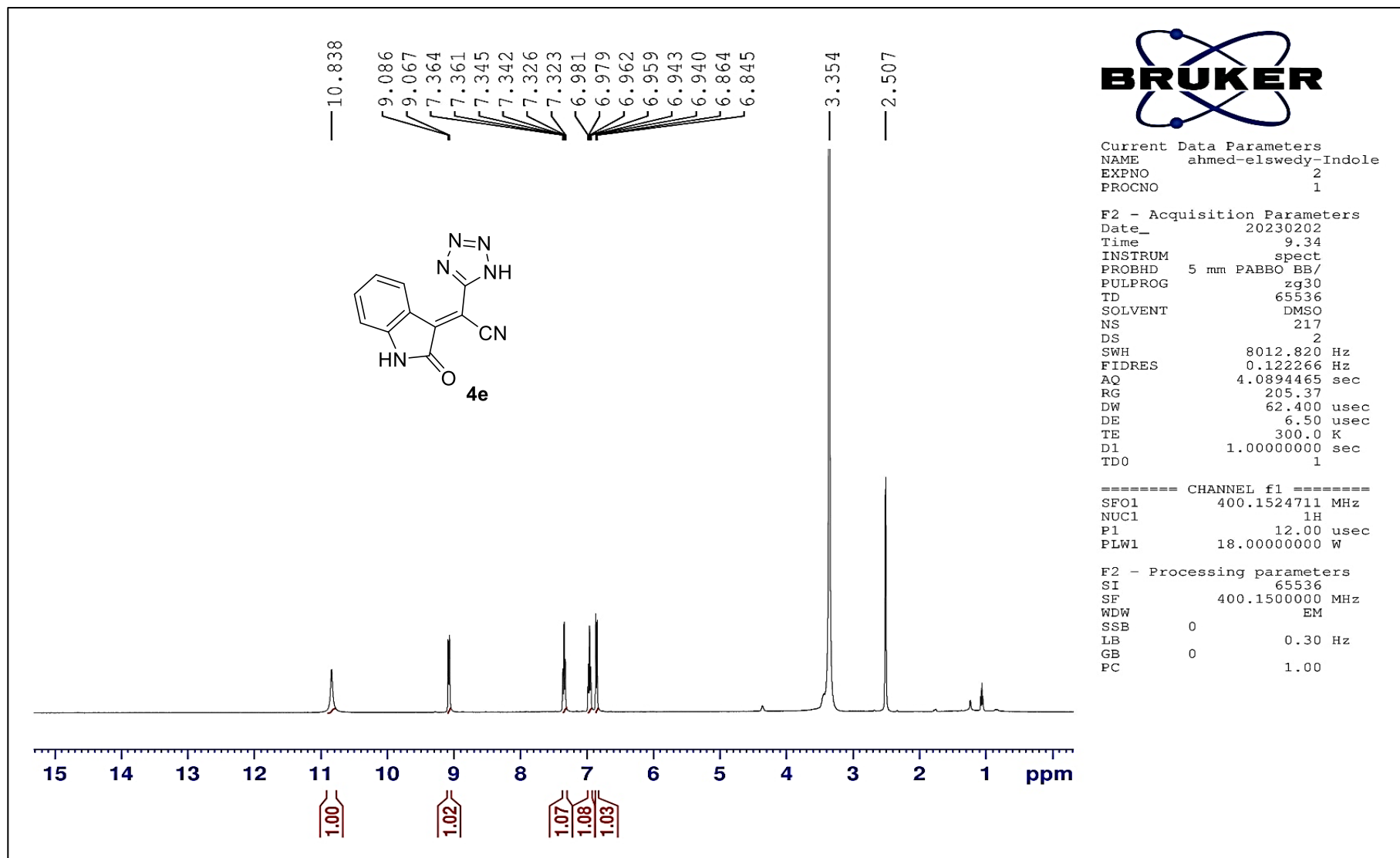
ahmed-4c #230 RT: 3.87 AV: 1 SB: 2 3.82 , 3.53 NL: 2.39E3
T: {0,0} + c EI Full ms [40.00-1000.00]



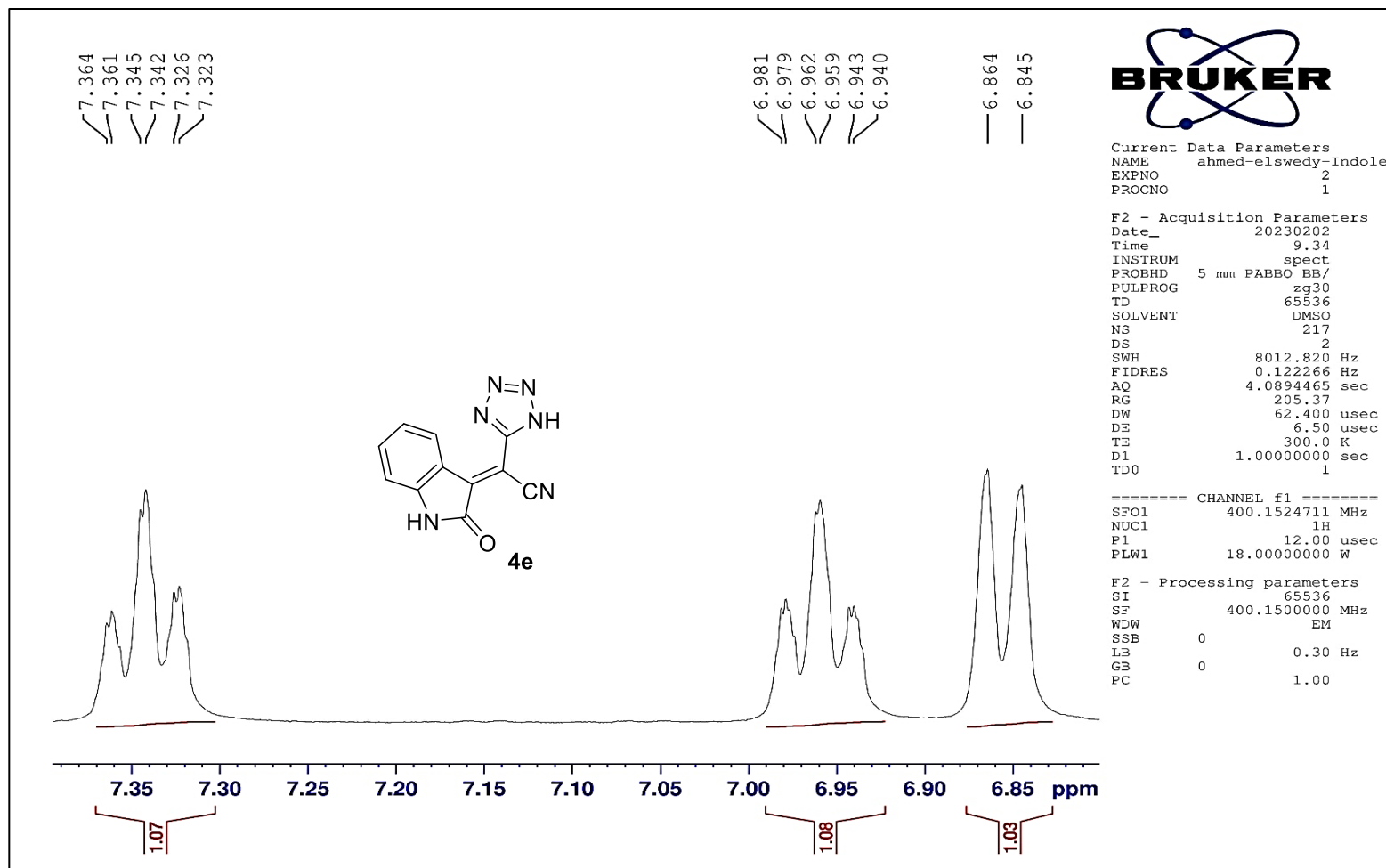
Mass spectrum of compound **4c**.



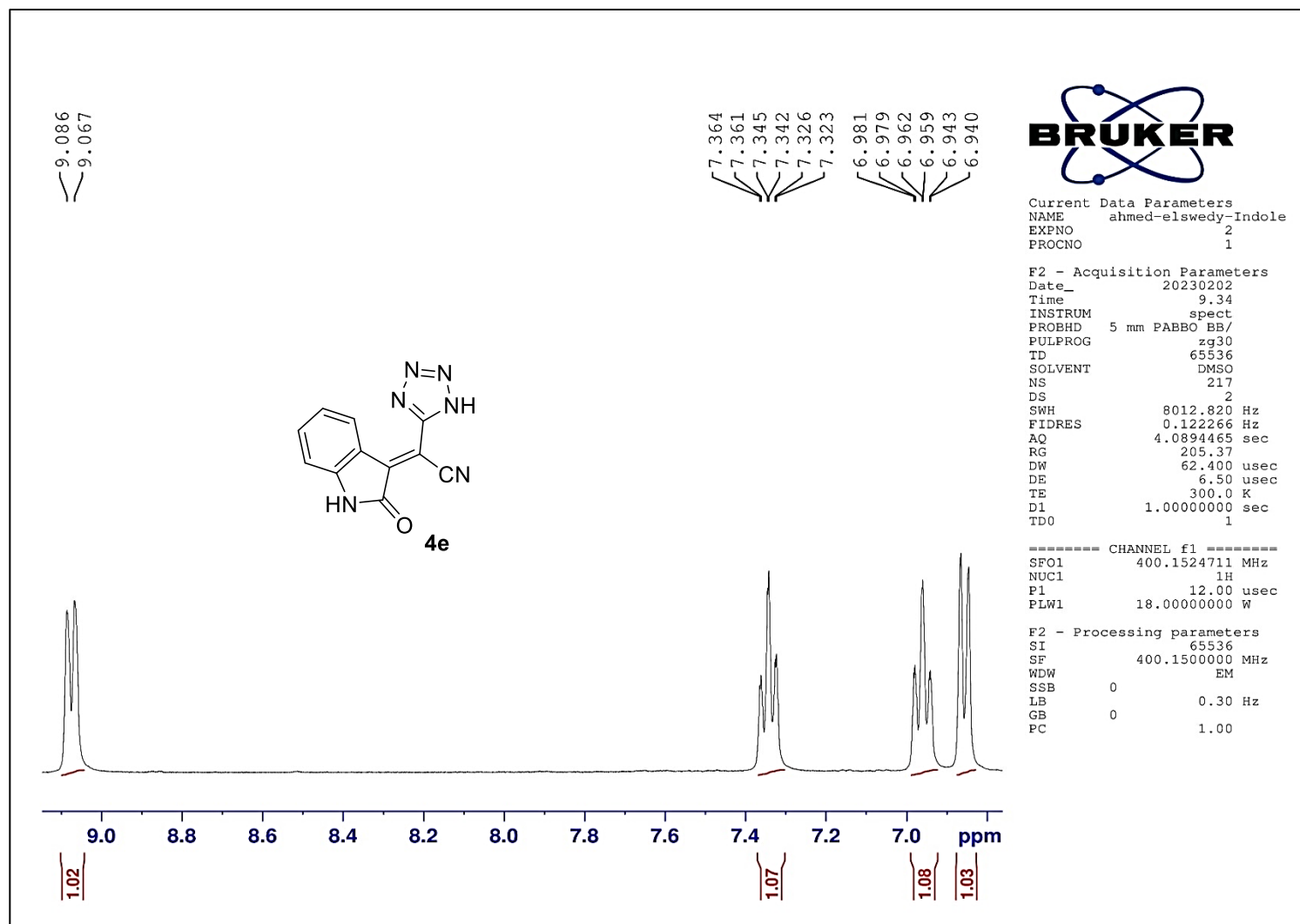
IR spectrum of compound 4e.



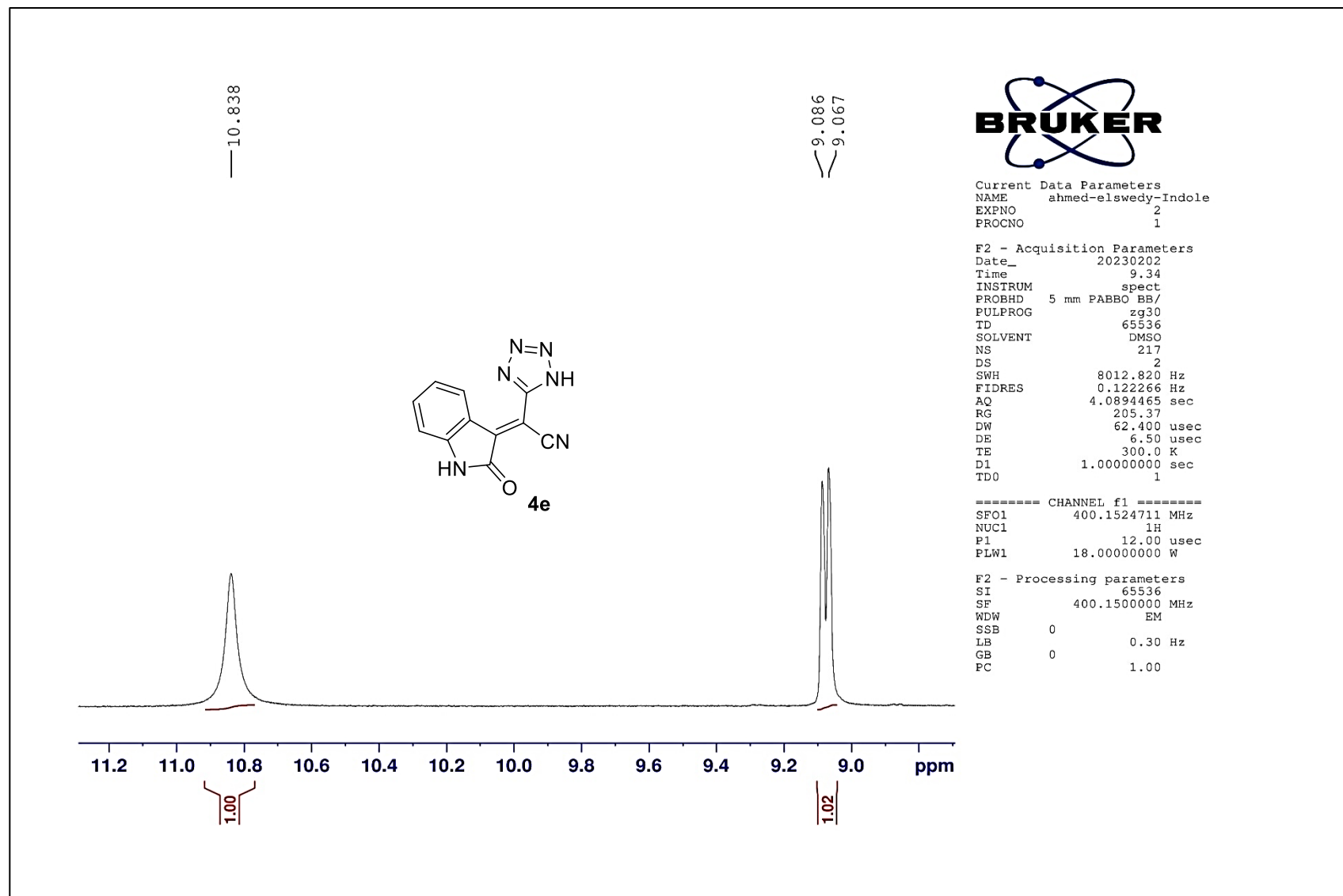
¹H NMR spectrum (DMSO-*d*₆) of compound **4e**.



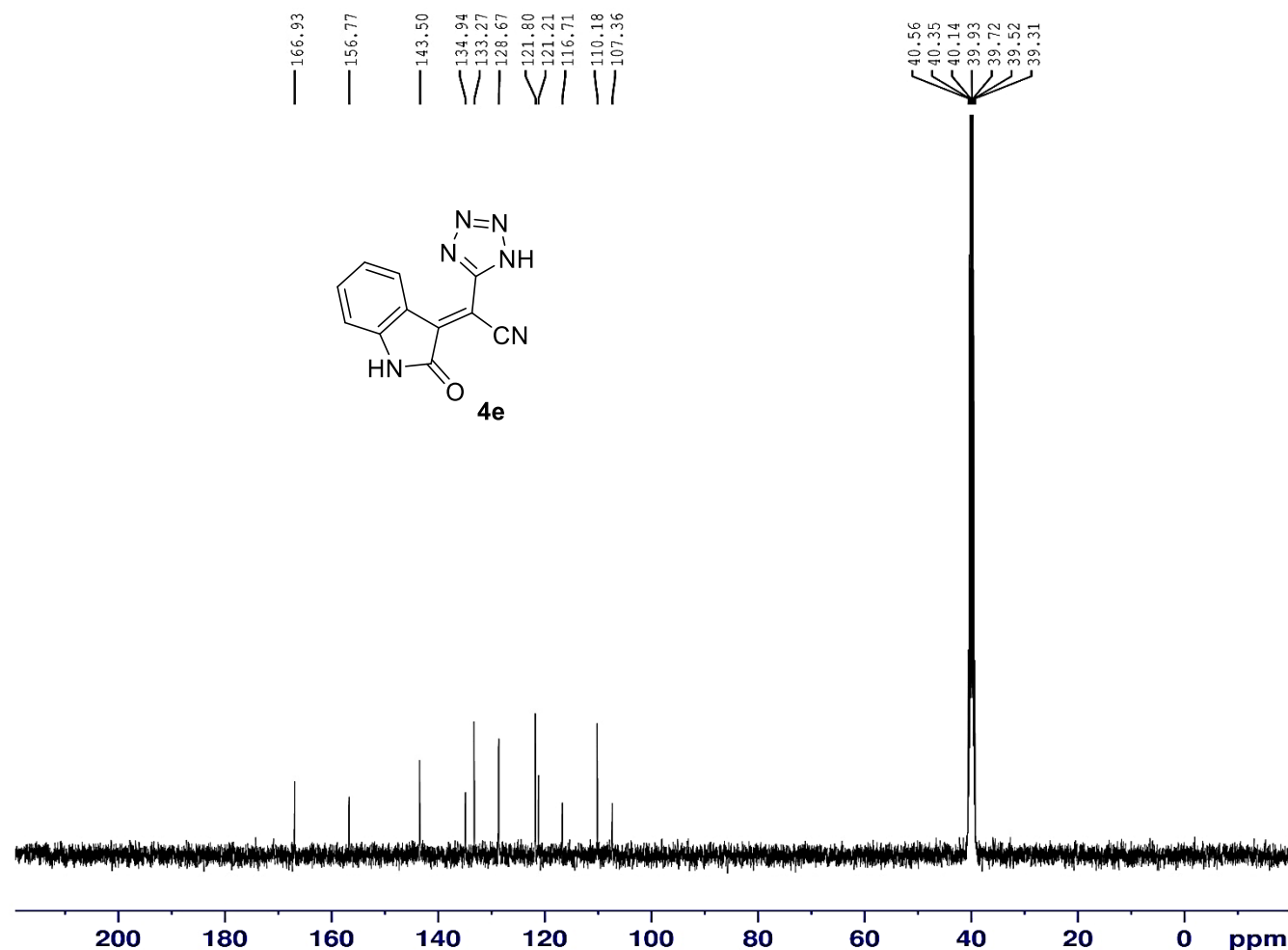
Cont. ^1H NMR spectrum (DMSO- d_6) of compound **4e**.



Cont. ^1H NMR spectrum ($\text{DMSO}-d_6$) of compound **4e**.



Cont. ¹H NMR spectrum (DMSO-*d*₆) of compound **4e**.



Current Data Parameters
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 PROCNO 1

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 PULPROG zgpg30
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 SOLVENT DMSO
 NS 2000
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 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
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 DE 6.50 usec
 TE 300.0 K
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 D11 0.03000000 sec
 TD0 1

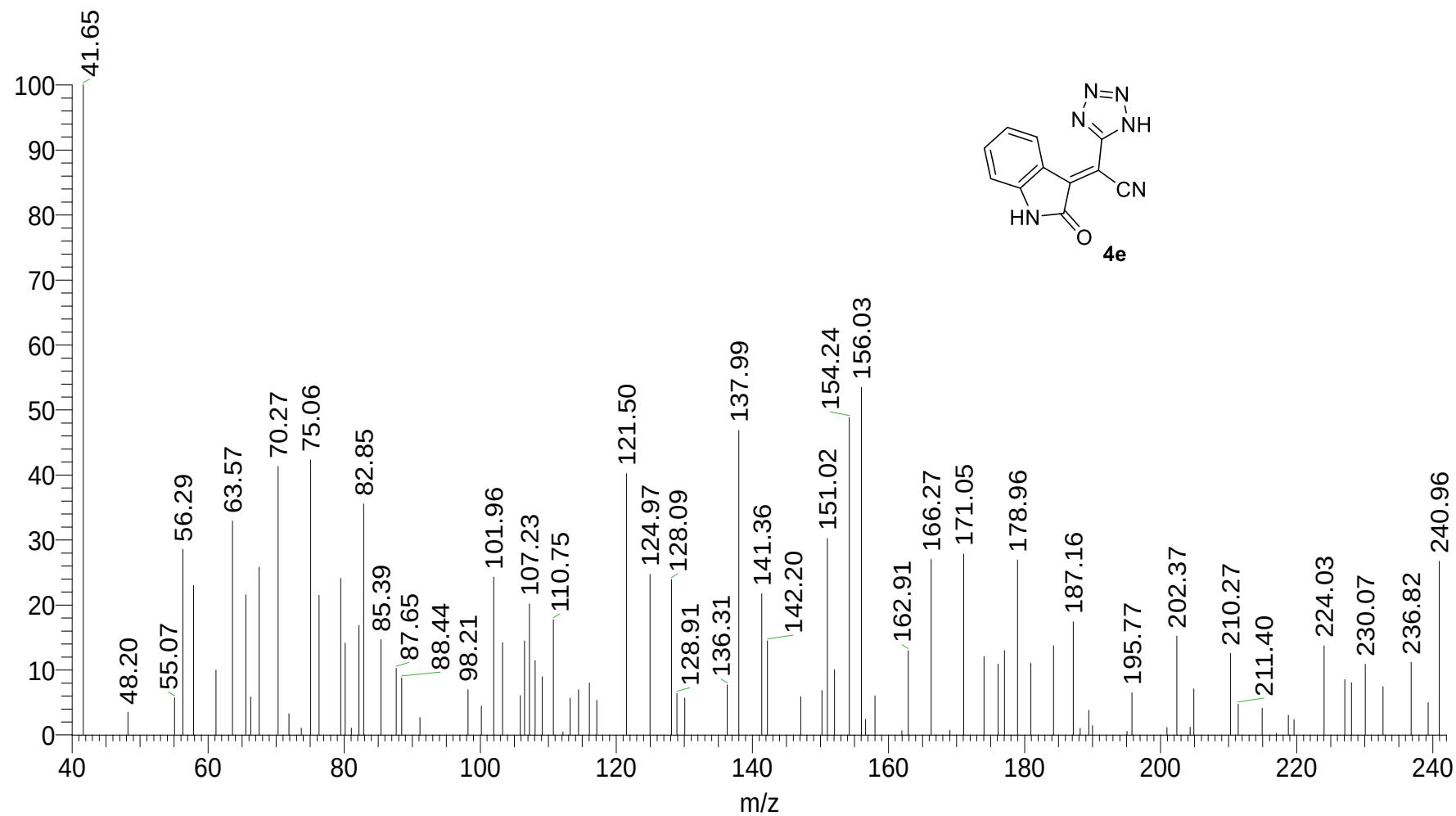
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 NUC2 1H
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 FCPD2 90.00 usec
 PLW2 18.00000000 W
 PLW12 0.34722000 W
 PLW13 0.28125000 W

F2 - Processing parameters
 SI 32768
 SF 100.6177975 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 FC 1.40

¹³C NMR spectrum (DMSO-*d*₆) of compound **4e**.

ahmed-4e #236 RT: 3.97 AV: 1 SB: 2 3.82 , 3.53 NL: 2.71E3
T: {0,0} + c EI Full ms [40.00-1000.00]



Mass spectrum of compound **4e**.