Supplemental Material

A multi-component reaction (MCR) approach for synthesizing biologically potent tetrazole scaffolds and investigation of their properties using quantum mechanical *ab initio* studies

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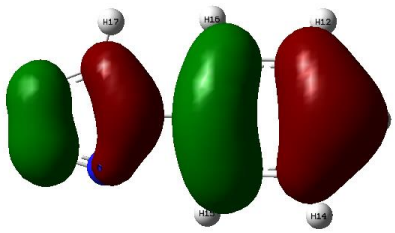
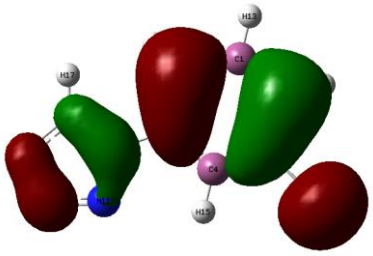
Table 4. Optimized geometrical parameters of fused 1-substituted-1*H*-1,2,3,4-tetrazoles bond length (Å) and bond angles (Å)

S. No.	Bond Length(Å)	DFT B3LYP	Hartree-fock Method	Bond Angle(Å)	DFT B3LYP	Hartree-fock Method
1.	C1-C2	1.3962	1.3932	C2-C1-C6	120.185	120.4376
2.	C1-C6	1.3962	1.3924	C2-C1-H12	119.8751	120.2627
3.	C1-H12	1.0824	1.0812	C6-C1-H12	119.94	119.2997
4.	C2-C3	1.396	1.394	C1-C2-C3	119.9555	119.5682
5.	C2-H13	1.0824	1.081	C1-C2-H13	120.0226	120.1757
6.	C3-C4	1.3981	1.3915	C3-C2-H13	120.0219	120.256
7.	C3-H14	1.0824	1.0813	C2-C3-C4	120.1179	120.6958
8.	C4-C5	1.4079	1.3957	C2-C3-H14	119.9218	120.1247
9.	C4-H15	1.0824	1.0787	C4-C3-H14	119.9603	119.1795
10.	C5-C6	1.4094	1.3956	C3-C4-C5	120.58	119.1958
11.	C5-N7	1.442	1.4277	C3-C4-H15	118.8096	121.2319
12.	C6-H16	1.0803	1.08	C5-C4-H15	120.6104	119.5723
13.	N7-C8	1.3468	1.3536	C4-C5-C6	118.7092	120.6726
14.	N7-N11	1.3226	1.3593	C4-C5-N7	119.9666	119.2554
15.	C8-N9	1.3452	1.3116	C6-C5-N7	121.3241	120.072
16.	C8-H17	1.0807	1.0733	C1-C6-C5	120.4523	119.43
17.	N9-N10	1.3254	1.3605	C1-C6-H16	118.2865	119.5378
18.	N10-N11	1.3241	1.2857	C5-C6-H16	121.2612	121.0323
19.	----	----	----	C5-N7-C8	128.9673	131.2724
20.	----	----	----	C5-N7-N11	124.7391	121.7351
21.	----	----	----	C8-N7-N11	106.2936	106.9925
22.	----	----	----	N7-C8-N9	109.4847	109.2225
23.	----	----	----	N7-C8-H17	126.2926	125.0454
24.	----	----	----	N9-C8-H17	124.2228	125.7321
25.	----	----	----	C8-N9-N10	105.6733	105.6936
26.	----	----	----	N9-N10-N11	109.7166	111.1756
27.	----	----	----	N7-N11-N10	108.8318	106.9159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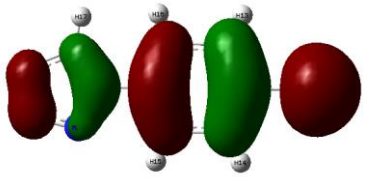	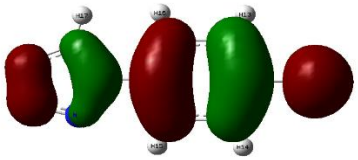
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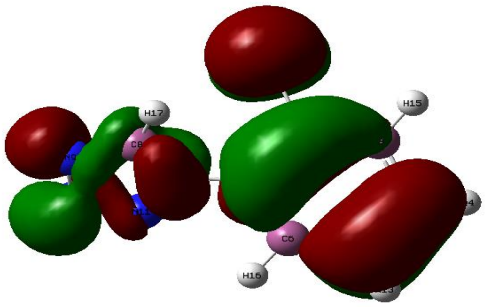	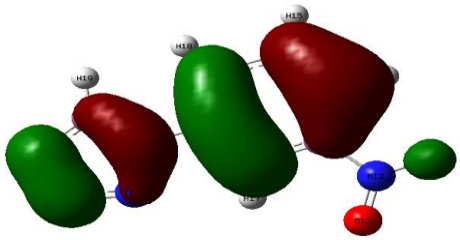
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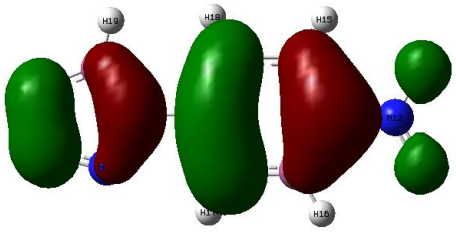	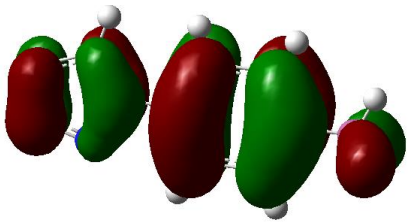

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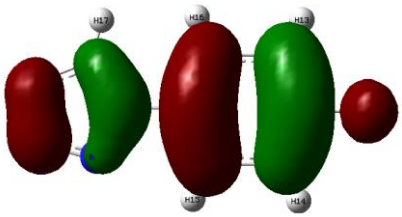
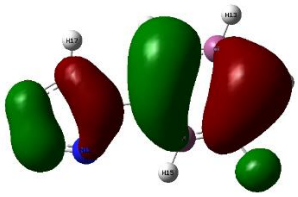
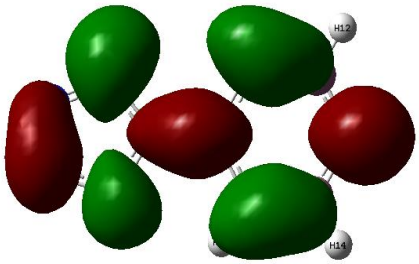
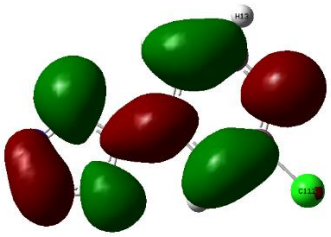
	
4i	4j

Figure 2. HOMO of the synthesized compounds (**4a-j**)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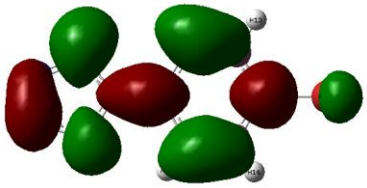
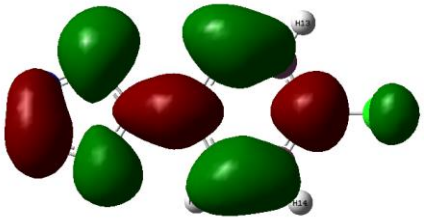
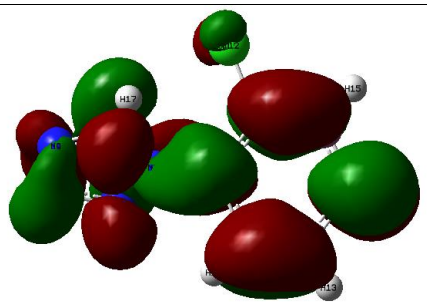
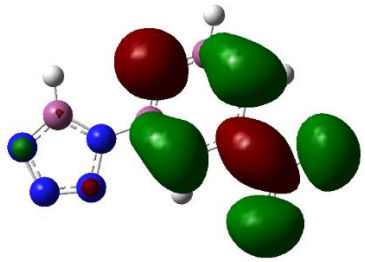
	
4c	4d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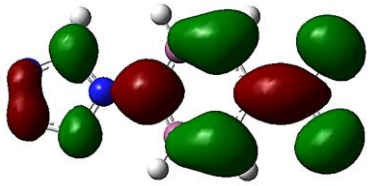	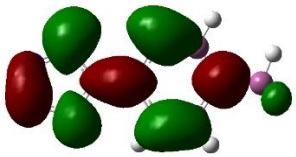
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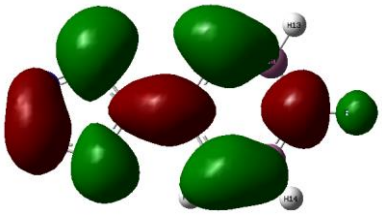
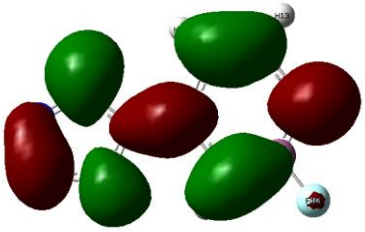
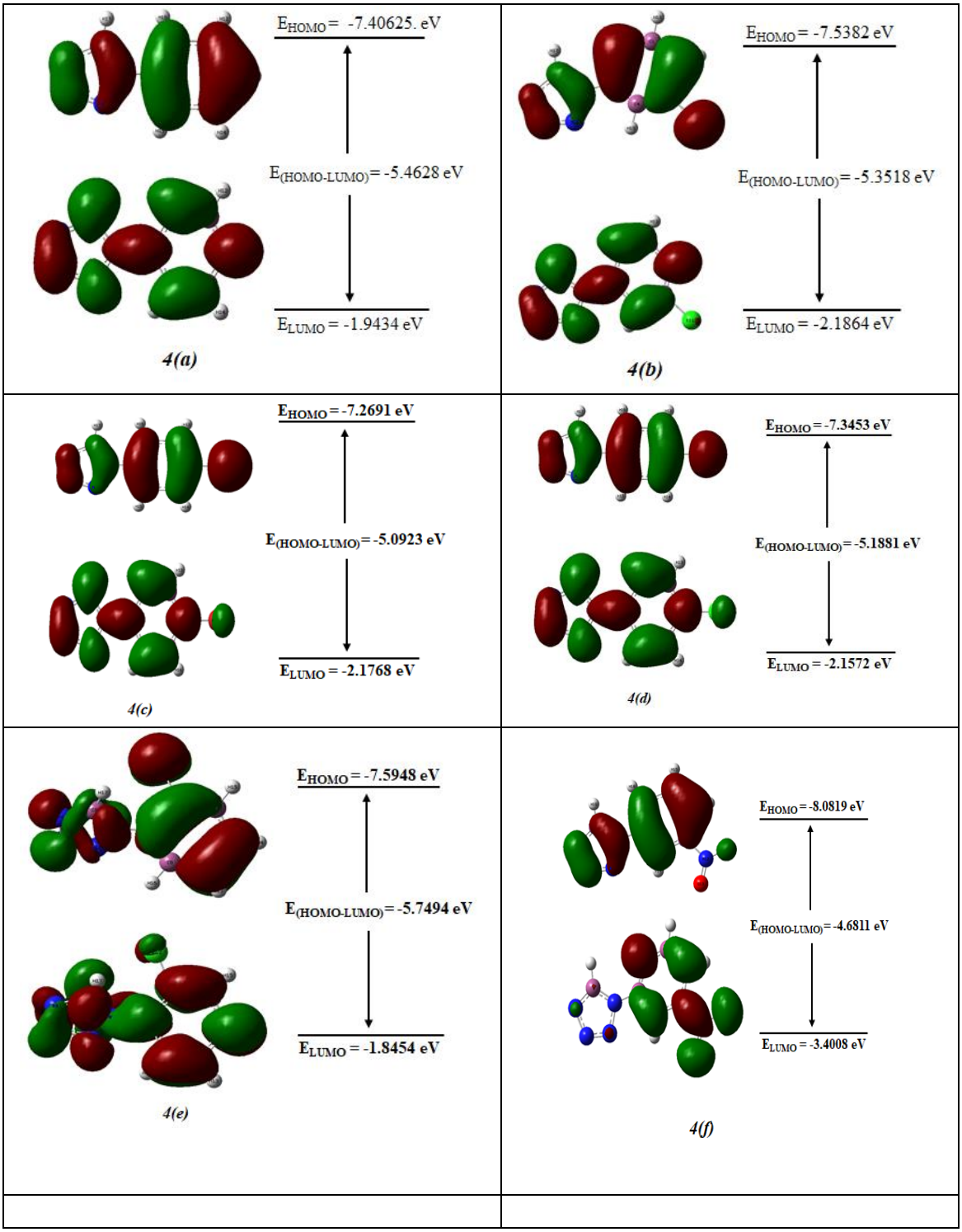
	
4i	4j

Figure 3. LUMO of the synthesized compounds (**4a-j**)


E(HOMO) = -7.40625. eV
E(HOMO-LUMO) = -5.4628 eV
E(LUMO) = -1.9434 eV
4(a)
E(HOMO) = -7.5382 eV
E(HOMO-LUMO) = -5.3518 eV
E(LUMO) = -2.1864 eV
4(b)
E(HOMO) = -7.2691 eV
E(HOMO-LUMO) = -5.0923 eV
E(LUMO) = -2.1768 eV
4(c)
E(HOMO) = -7.3453 eV
E(HOMO-LUMO) = -5.1881 eV
E(LUMO) = -2.1572 eV
4(d)
E(HOMO) = -7.5948 eV
E(HOMO-LUMO) = -5.7494 eV
E(LUMO) = -1.8454 eV
4(e)
E(HOMO) = -8.0819 eV
E(HOMO-LUMO) = -4.6811 eV
E(LUMO) = -3.4008 eV
4(f)

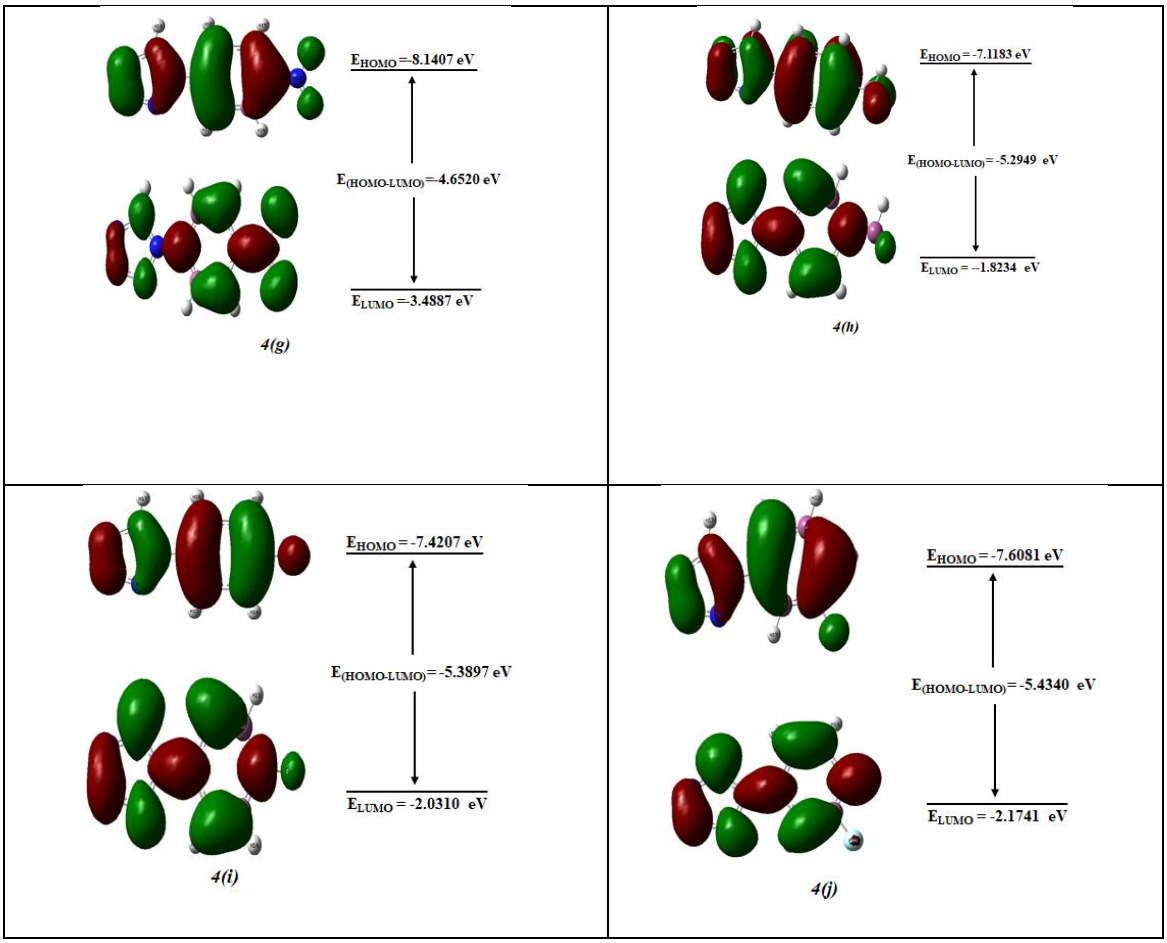
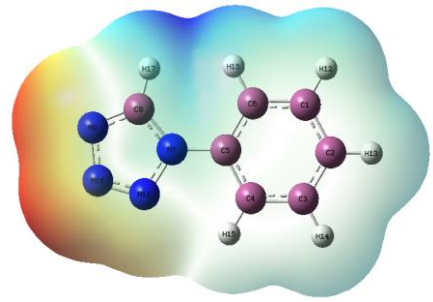
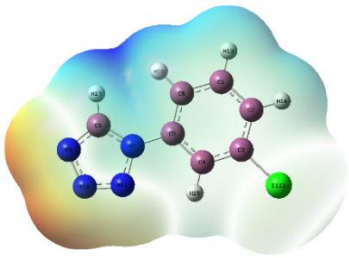
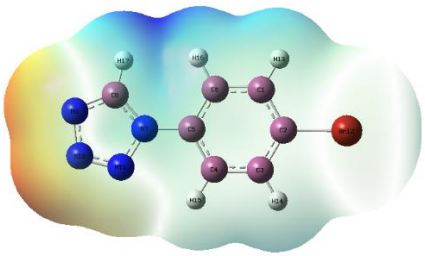
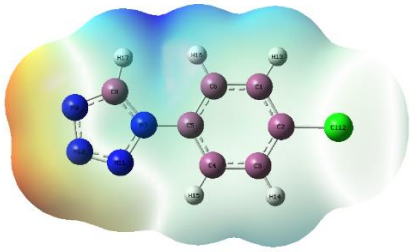


Figure 4. HOMO-LUMO energy gap of the synthesized compound (**4a-j**)

	
4a	**4b**
	
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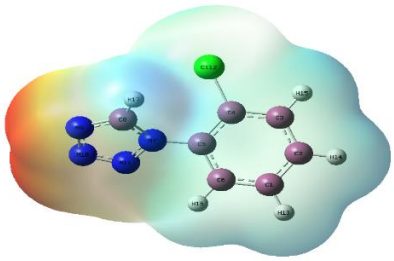	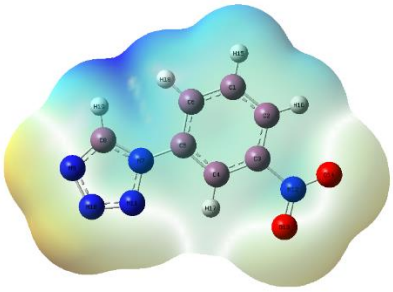
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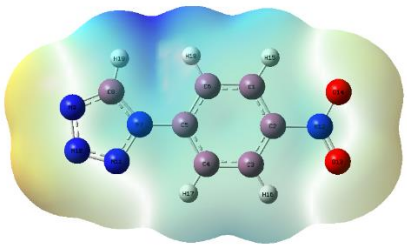
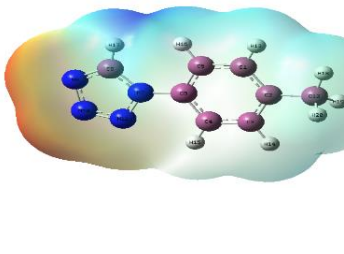
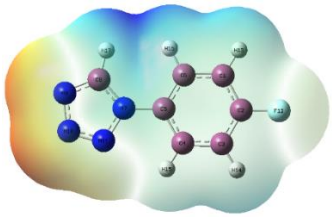
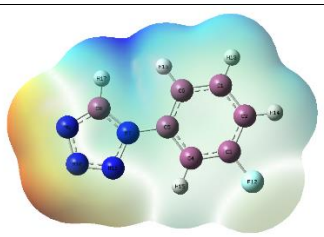
	
4g	**4h**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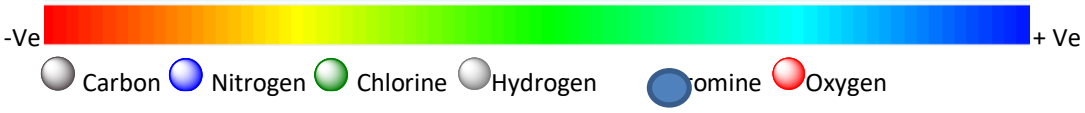

Figure 5. Molecular electrostatic potential (MEP) for the synthesized compounds (**4a-J**)

Spectra of the synthesized compounds

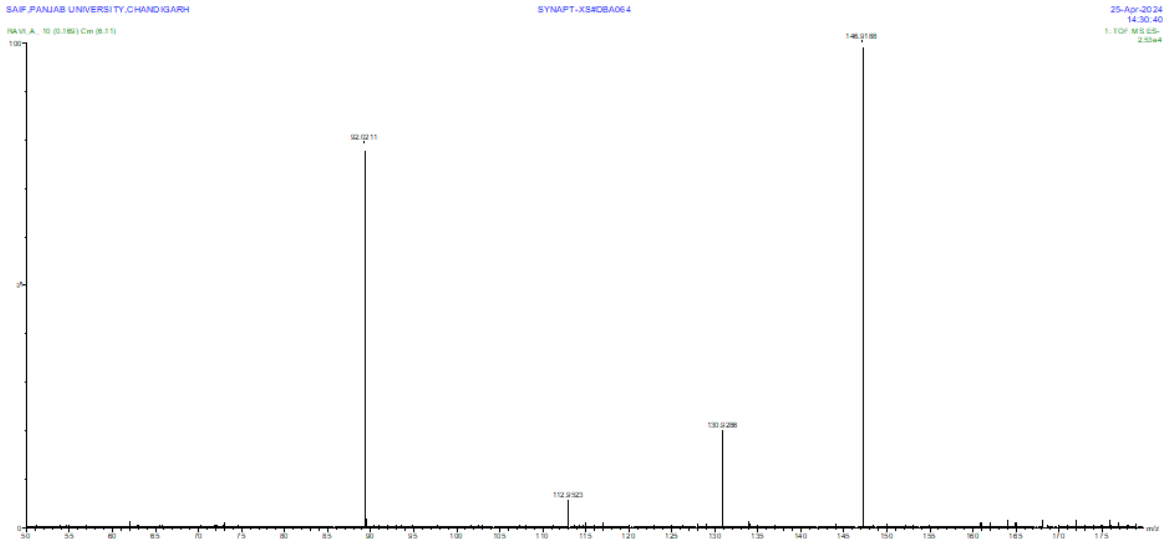

Figure 12. Mass Spectra of 1-phenyl-1*H*-tetrazole **(4a)**

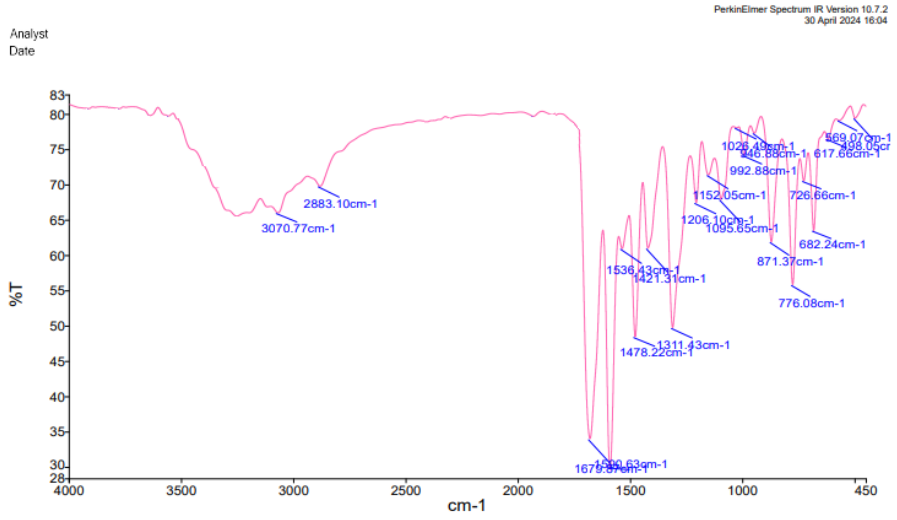

Figure 13. FTIR spectra of 1-phenyl-1H-tetrazole (**4a**)

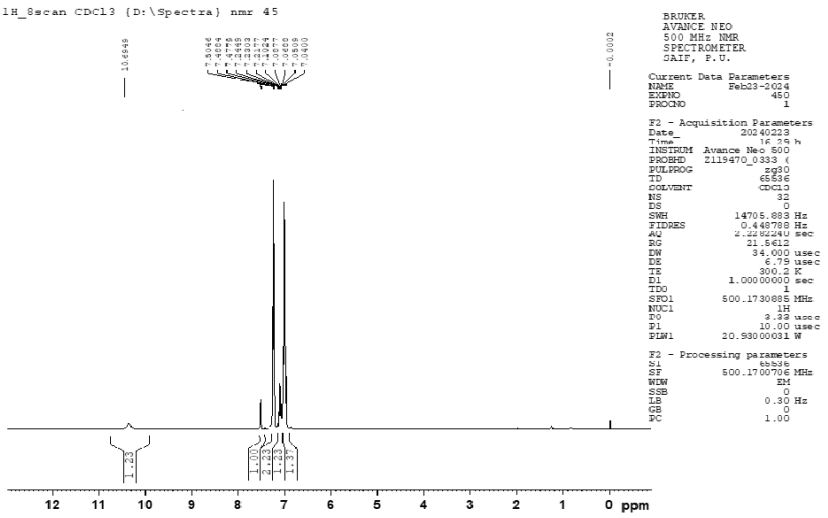

Figure 14. ^{1}H-NMR spectra of 1-phenyl-1*H*-tetrazole **(4a)**

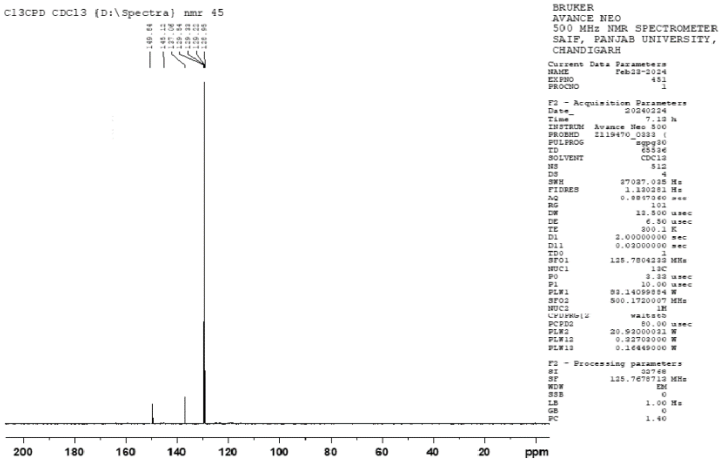

Figure 15. ^{13}C-NMR spectra of 1-phenyl-1*H*-tetrazole **(4a)**

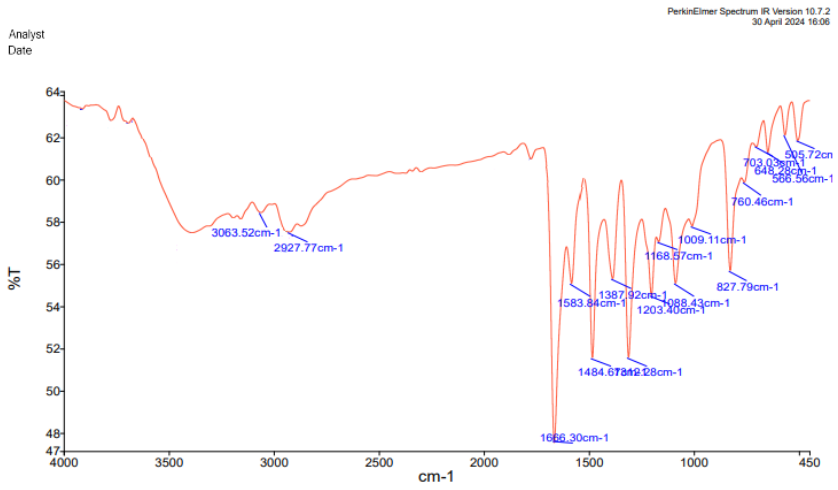

Figure 16 FT-IR spectra of 1-(3-chlorophenyl)-1*H*-tetrazole **(4b)**

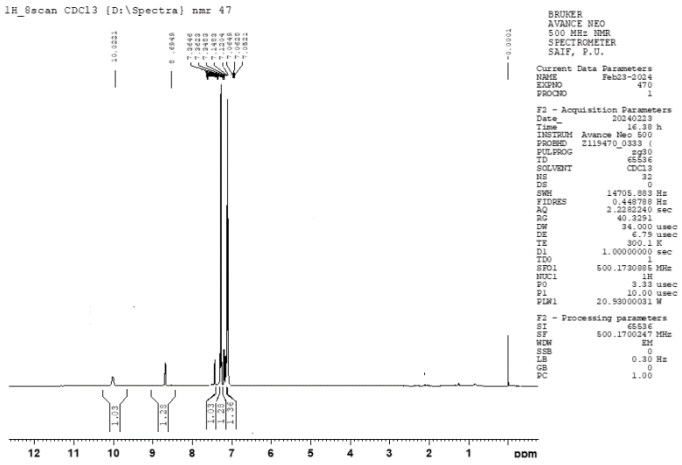

Figure 17. ^{1}H-NMR spectra of 1-(3-chlorophenyl)-1*H*-tetrazole **(4b)**

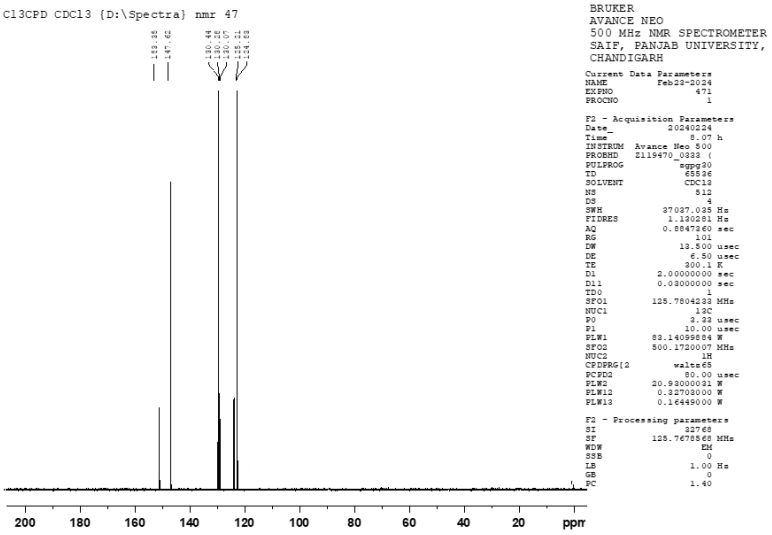

Figure 18. ^{13}C-MNR, 3 spectra of 1-(3-chlorophenyl)-1*H*-tetrazole **(4b)**

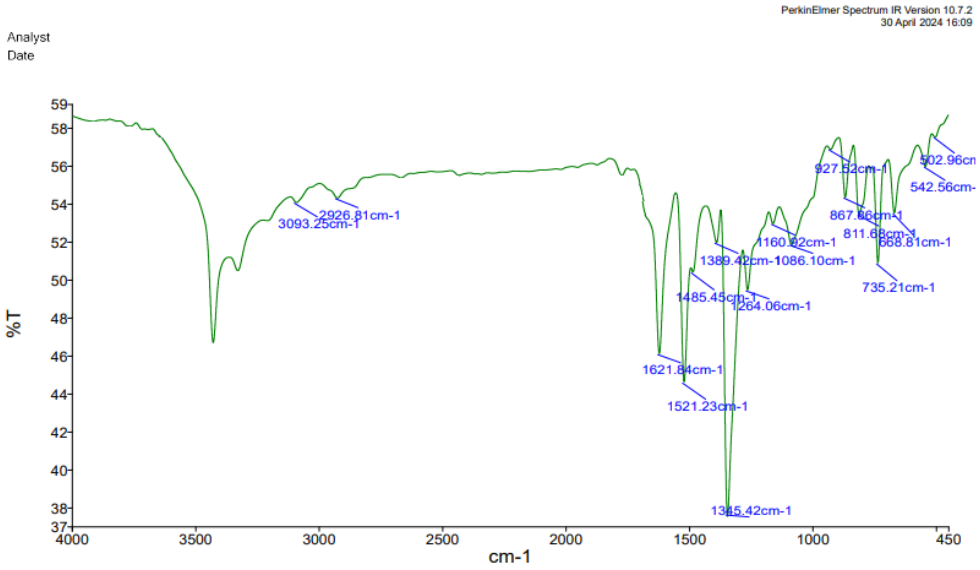

Figure 19. FT-IR spectra of 1-(4-bromophenyl)-1*H*-tetrazole **(4c)**

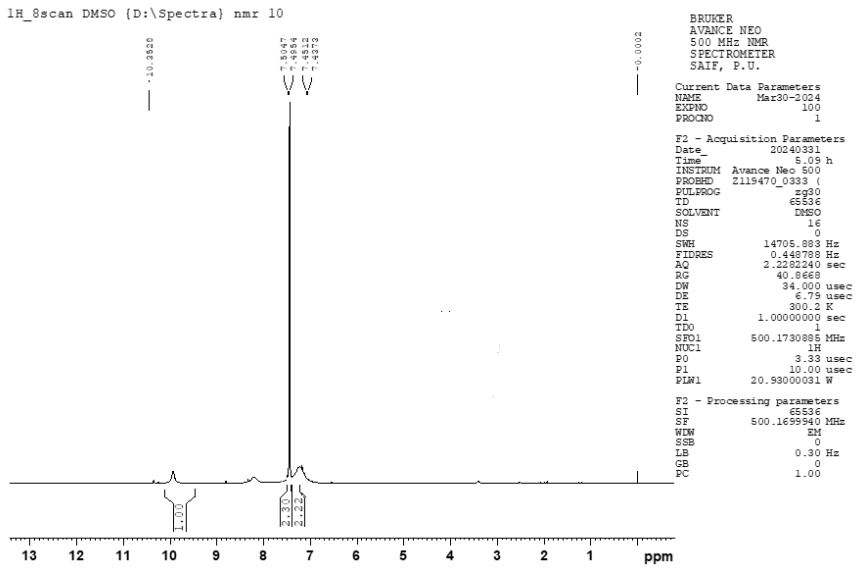

Figure 20. ^{1}H-NMR spectra of 1-(4-bromophenyl)-1*H*-tetrazole **(4c)**

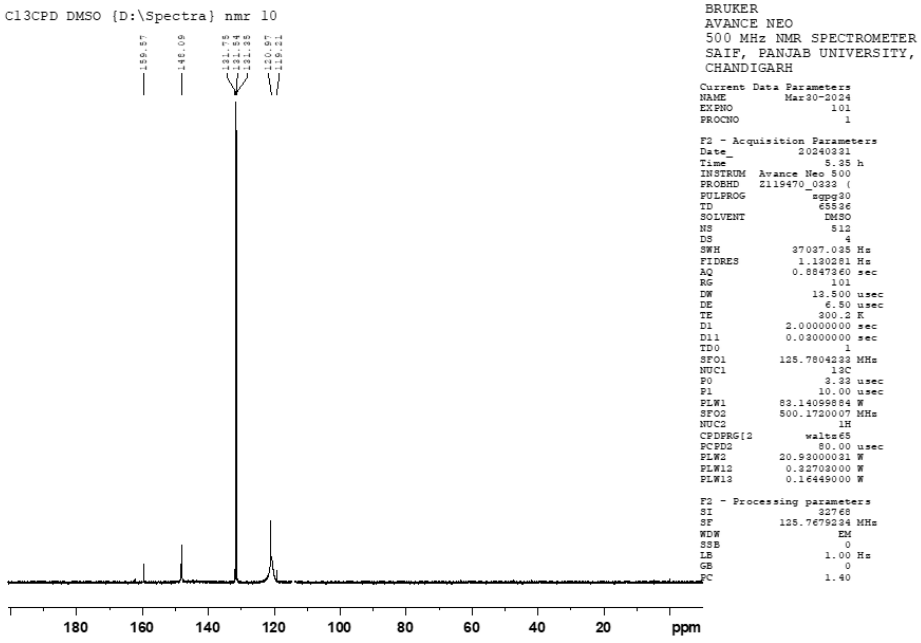

Figure 21. ^{13}C-NMR spectra of 1-(4-bromophenyl)-1*H*-tetrazole **(4c)**

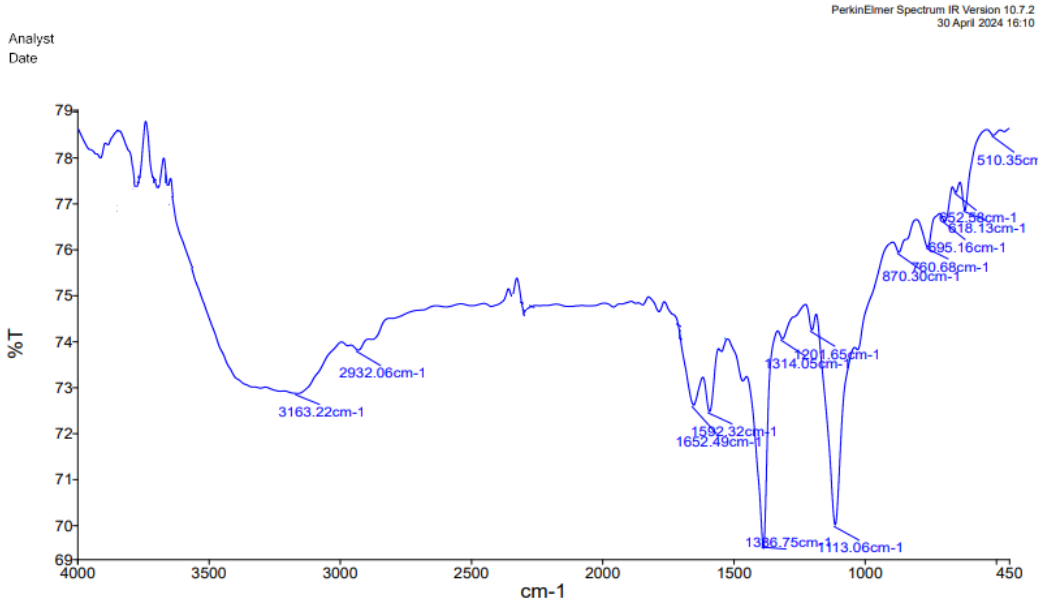

Figure 22. FT-IR spectra of 1-(4-chlorophenyl)-1*H*-tetrazole **(4d)**

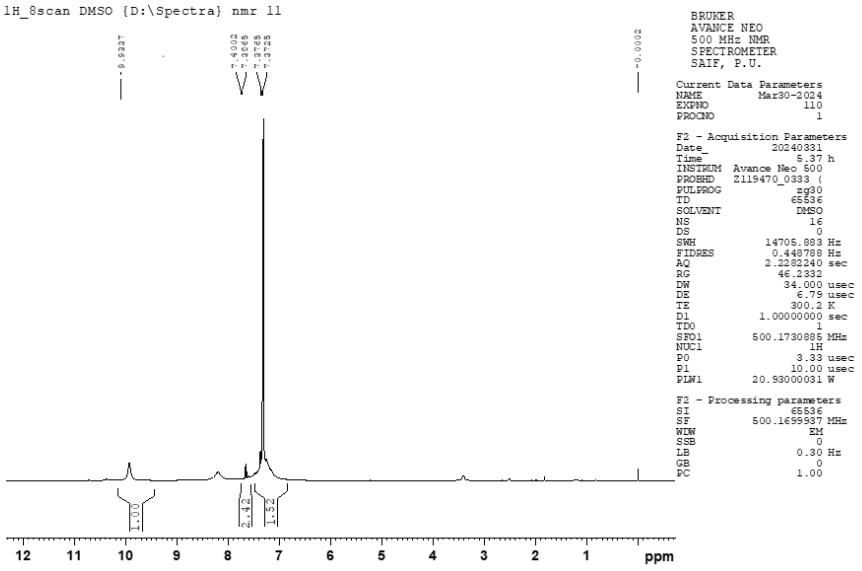

Figure 23. ^{1}H-NMR spectra of 1-(4-chlorophenyl)-1*H*-tetrazole **(4d)**

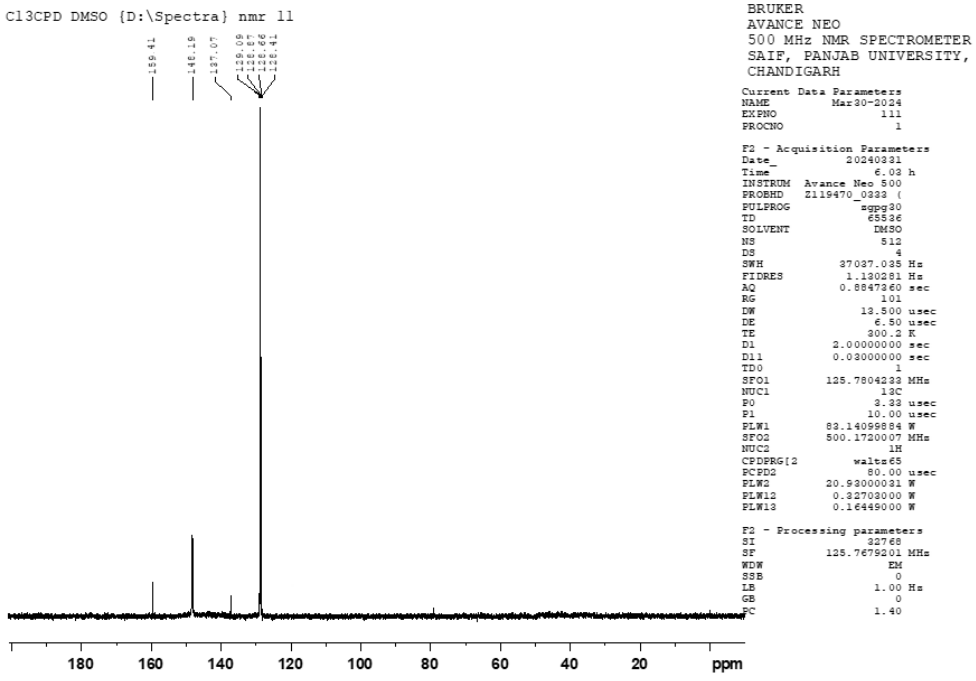

Figure 24. ^{13}C-NMR spectra of 1-(4-chlorophenyl)-1*H*-tetrazole **(4d):**

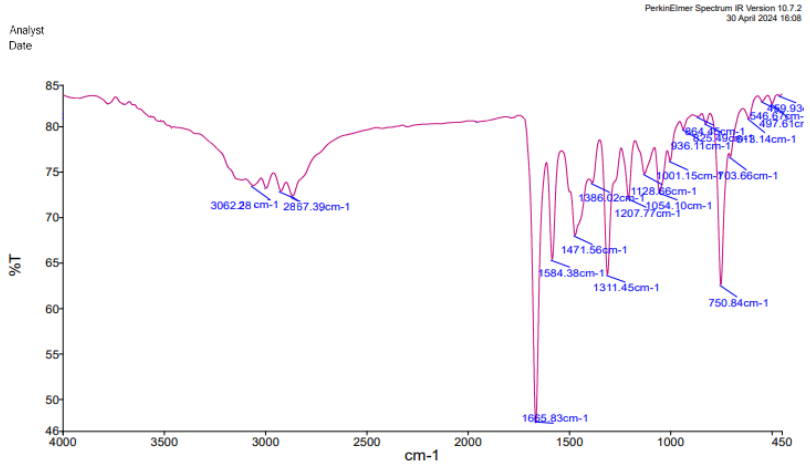

Figure 25. FT-IR spectra of 1-(2-chlorophenyl)-1*H*-tetrazole **(4e)**

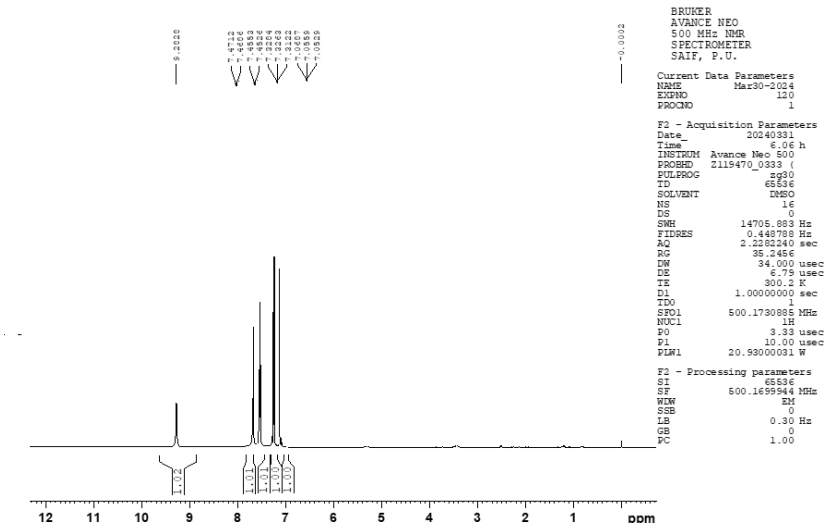

Figure 26. ^{1}H-NMR spectra of 1-(2-chlorophenyl)-1*H*-tetrazole **(4e)**

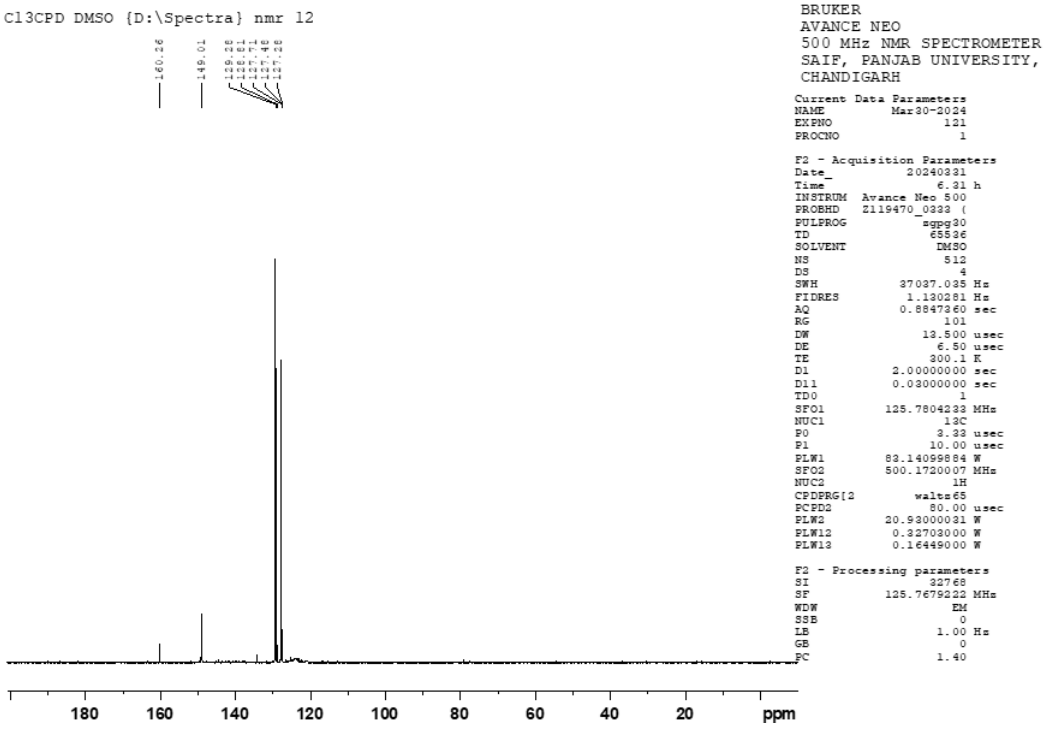

Figure 27. ^{13}C-NMR spectra of 1-(2-chlorophenyl)-1*H*-tetrazole **(4e)**

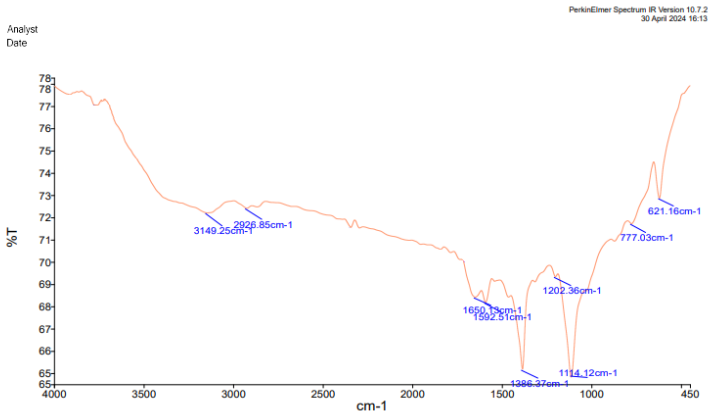

Figure 28. FT-IR spectra of 1-(3-nitrohenyl)-1*H*-tetrazole **(4f)**

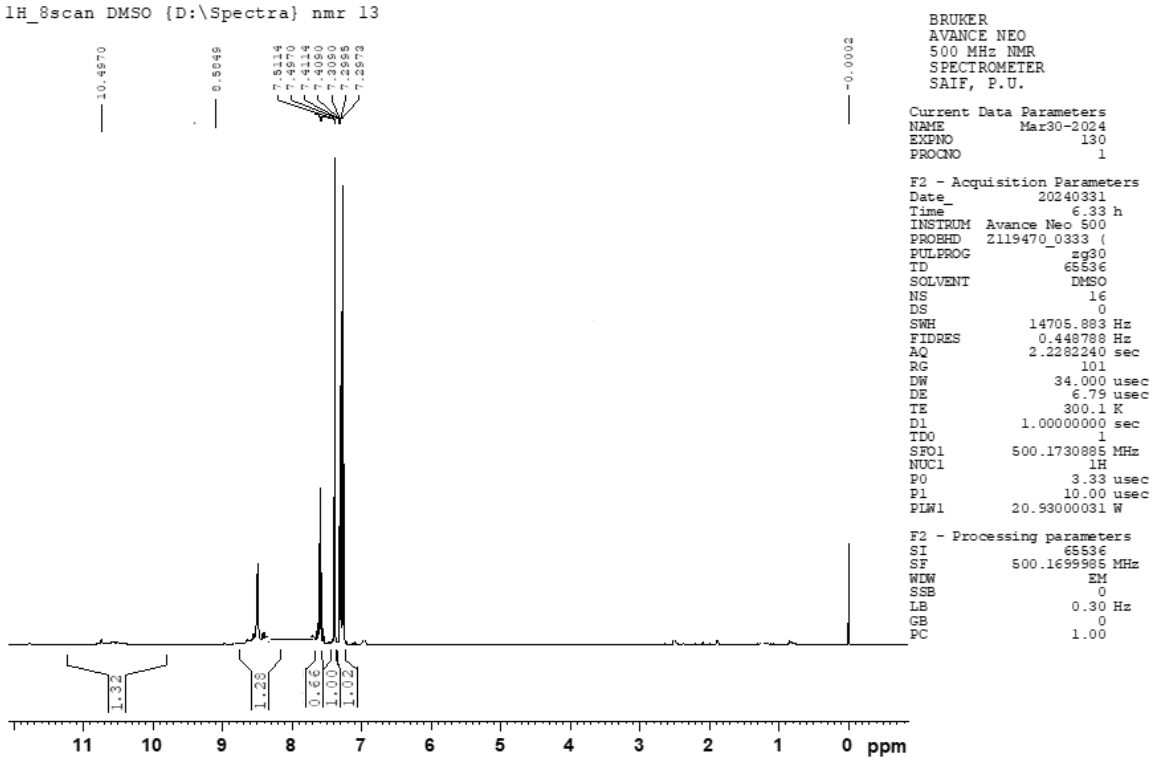

Figure 29. ^{1}H-NMR spectra of 1-(3-nitrohenyl)-1*H*-tetrazole **(4f)**

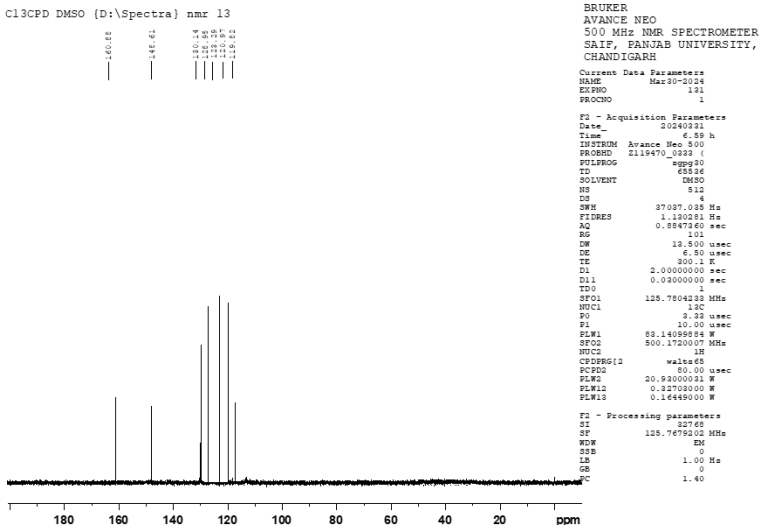

Figure 30. ^{13}C-NMR spectra of 1-(3-nitrohenyl)-1*H*-tetrazole **(4f)**

