SUPPORTING INFORMATION

associated with the paper

Indole-3-carbaldehyde semicarbazone derivatives: synthesis, characterization and antibacterial activities

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Table S1. Computational results, at B3LYP/6-311++G(d,p) for the synthesized compounds **1**-**4,** indicating the relative enthalpies (Δ*H*) of stable conformers and their equilibrium molar fractions (populations).

Compound		E_0 [a]	G_{298} [a]	H_{298} [a]	ΔH [b]	μ[c]	Population (%)
Gas phase							
1	***cisE***	-3255.050809	-3254.911800	-3254.851474	0.0	6.6	98.4
	transE	-3255.040251	-3254.900459	-3254.840973	27.6	1.3	< 0.1
	cisZ	-3255.049470	-3254.907928	-3254.849459	5.3	3.2	1.6
	transZ	-3255.034754	-3254.894224	-3254.835092	43.0	8.6	< 0.1
2	***cisE***	-1141.131072	-1140.990312	-1140.931390	0.0	6.6	98.3
	transE	-1141.120482	-1140.979122	-1140.920872	27.6	1.3	< 0.1
	cisZ	-1141.129728	-1140.986502	-1140.929365	5.3	3.2	1.7
	transZ	-1141.115249	-1140.972923	-1140.915190	42.5	7.8	< 0.1
3	***cisE***	-796.063614	-795.882397	-795.820764	0.0	5.0	97.1
	transE	-796.052321	-795.870550	-795.809559	29.4	3.5	< 0.1
	cisZ	-796.062800	-795.879095	-795.819238	4.0	3.7	2.9
	transZ	-796.048584	-795.865752	-795.805313	40.6	6.4	< 0.1
4	***cisE***	-886.067000	-885.914670	-885.853751	0.0	9.8	99.3
	transE	-886.057790	-885.905898	-885.844689	23.8	3.5	< 0.1
	cisZ	-886.063201	-885.909912	-885.849531	11.1	6.7	0.6

	transZ	-886.048547	-885.896563	-885.835265	48.5	10.6	< 0.1
DMSO							
1	***cisE***	-3255.071545	-3254.932256	-3254.872302	0.0	8.9	99.0
	transE	-3255.065972	-3254.926233	-3254.866717	14.7	2.5	0.2
	cisZ	-3255.068655	-3254.927791	-3254.868932	8.8	4.4	0.9
	transZ	-3255.062547	-3254.921449	-3254.862782	25.0	12.4	< 0.1
2	***cisE***	-1141.151749	-1141.010544	-1140.952116	0.0	9.0	99.1
	transE	-1141.146194	-1141.004357	-1140.946454	14.9	2.4	0.1
	cisZ	-1141.148867	-1141.005914	-1140.948695	9.0	4.4	0.7
	transZ	-1141.142547	-1141.000303	-1140.942509	25.2	11.8	< 0.1
3	***cisE***	-796.085256	-795.903600	-795.842489	0.0	6.6	98.8
	transE	-796.079589	-795.897464	-795.836751	15.1	5.4	0.1
	cisZ	-796.082821	-795.899337	-795.839470	7.9	4.6	1.1
	transZ	-796.076475	-795.893690	-795.833279	24.2	9.4	< 0.1
4	***cisE***	-886.091918	-885.941255	-885.878999	0.0	13.9	99.5
	transE	-886.086453	-885.935397	-885.873509	14.4	5.2	0.2
	cisZ	-886.088371	-885.935785	-885.875106	10.2	9.7	0.3
	transZ	-886.082251	-885.929722	-885.868982	26.3	16.2	< 0.1
Acetone							
1	***cisE***	-3255.070572	-3254.931303	-3254.871323	0.0	8.8	99.0
	transE	-3255.064633	-3254.924875	-3254.865411	15.5	2.4	0.1
	cisZ	-3255.067789	-3254.926894	-3254.868050	8.6	4.4	0.9
	transZ	-3255.061059	-3254.919791	-3254.861288	26.3	12.2	< 0.1
2	***cisE***	-1141.150780	-1141.009575	-1140.951127	0.0	8.9	99.1
	transE	-1141.144868	-1141.002958	-1140.945101	15.8	2.3	0.1
	cisZ	-1141.148005	-1141.005007	-1140.947811	8.7	4.4	0.8
	transZ	-1141.141101	-1140.998529	-1140.941015	26.5	11.6	< 0.1
3	***cisE***	-796.084220	-795.902582	-795.841433	0.0	6.6	98.8
	transE	-796.078141	-795.895937	-795.835275	16.2	5.3	0.1
	cisZ	-796.081904	-795.898369	-795.838530	7.6	4.5	1.1
	transZ	-796.075004	-795.892006	-795.831779	25.3	9.2	< 0.1
4	***cisE***	-886.090707	-885.939664	-885.877745	0.0	13.8	99.4
	transE	-886.085030	-885.933621	-885.872072	14.9	5.1	0.2
	cisZ	-886.087206	-885.934617	-885.873907	10.1	9.5	0.5
	transZ	-886.080458	-885.927848	-885.867158	27.8	15.8	< 0.1

[a]All values in units of Hartree/particle. [b] Values in in kJ·mol^{-1}. [c]Values in Debye. E_0 = Total Energies at 0 K. H_{298}= Enthalpies and G_{298} = Gibbs Free Energies at 298.15 K. μ = Dipole Moment.

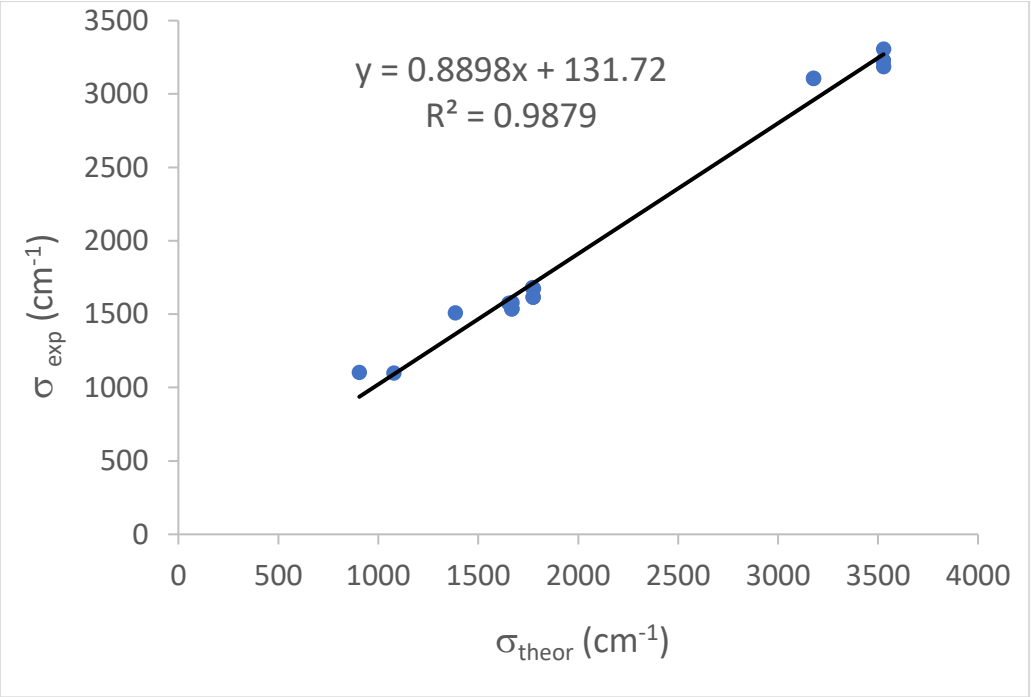


Figure 1. Linear Correlation of vibrational frequencies (given as wave numbers σ, in cm^{-1}) between experimental IR data and the corresponding to B3LYP/6-311++G(d,p) theoretical values for the synthesized compounds **1**-**4**.

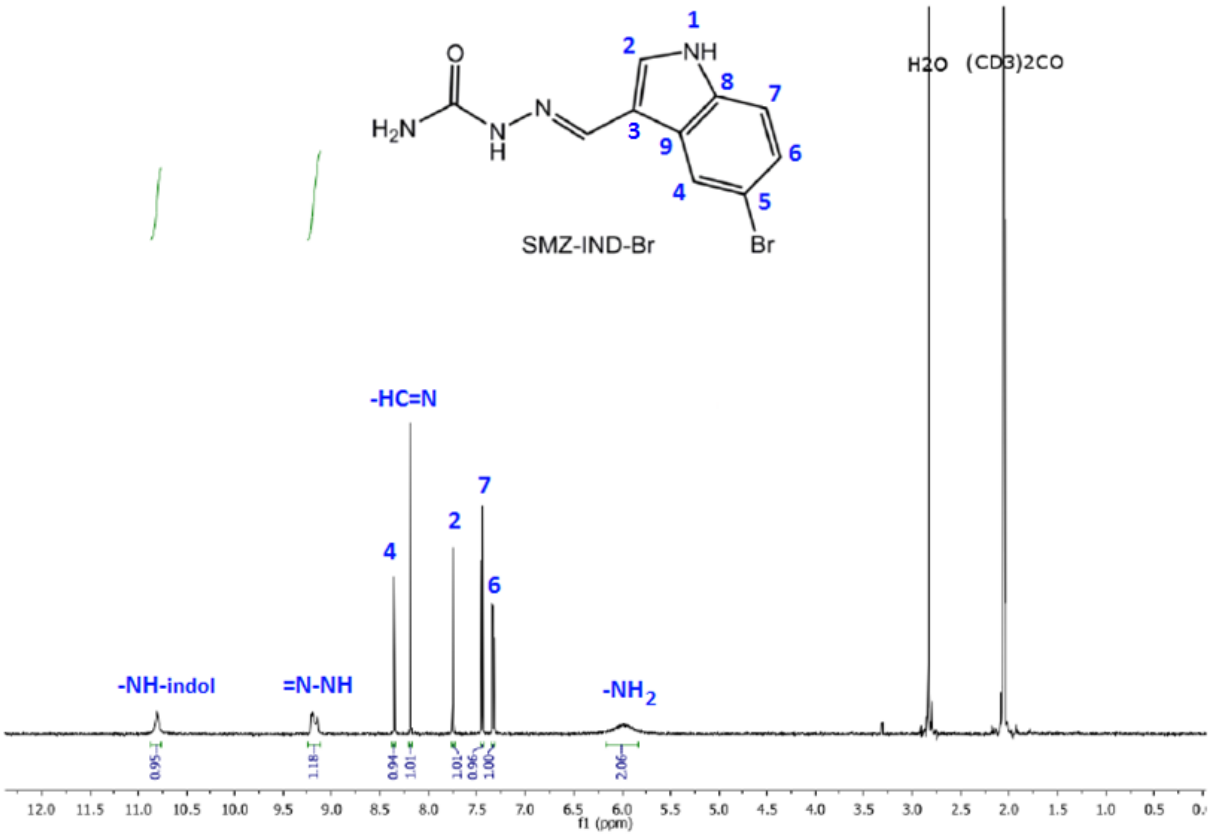


Figure 2. ^{1}H NMR spectrum of compound 1 (500 MHz, acetone-d_6)

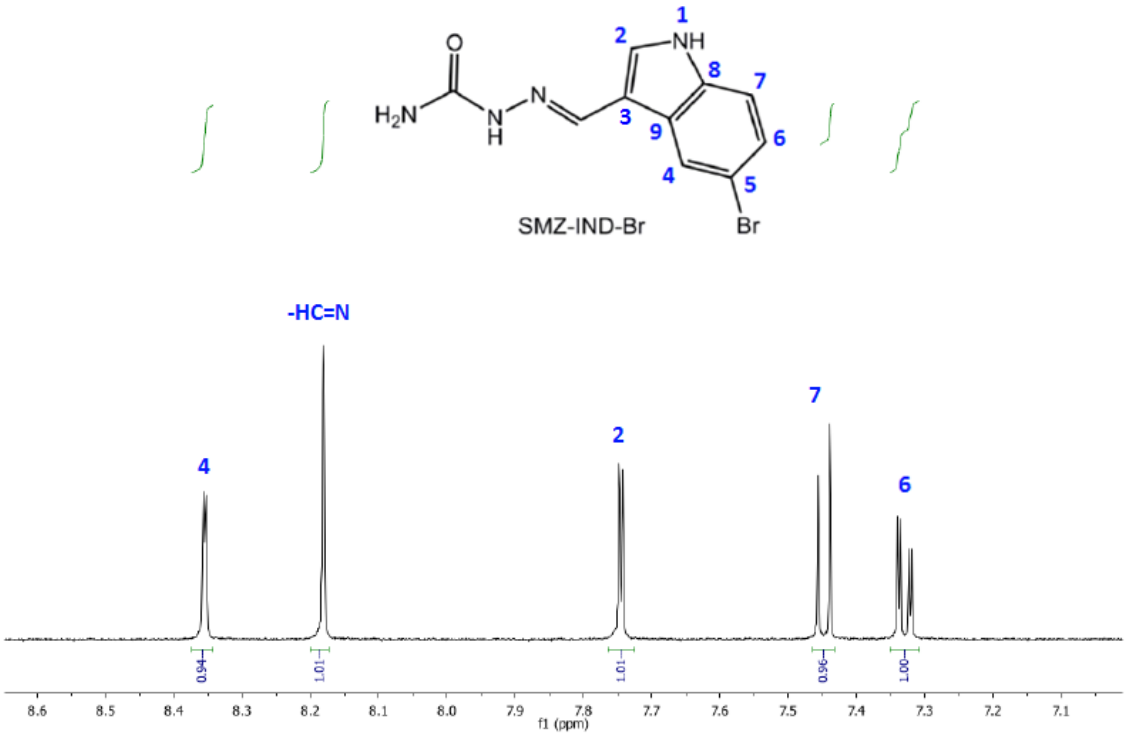


Figure 3. ^{1}H NMR spectrum showing the aromatic zone of compound 1 (500 MHz, acetone-d_6)

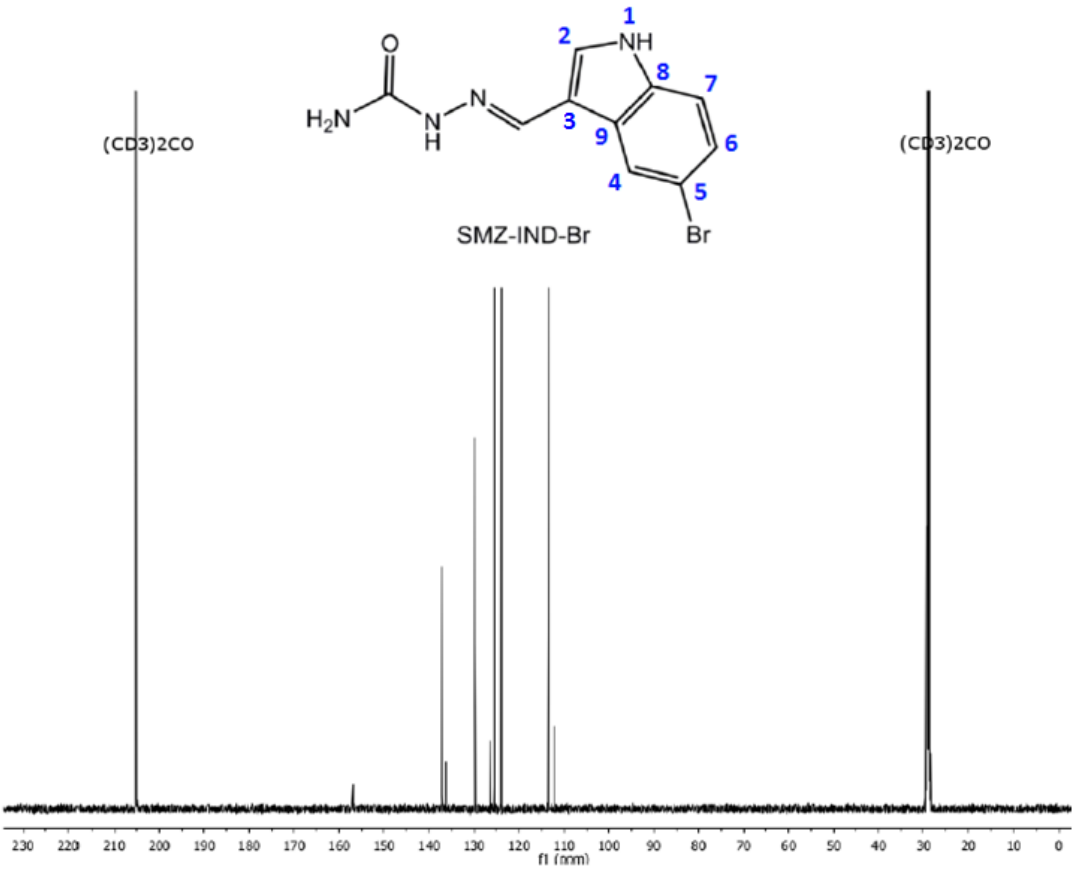


Figure 4. $^{13}C\{^{1}H\}$NMR spectrum of compound 1 (126 MHz, acetone-d_6)

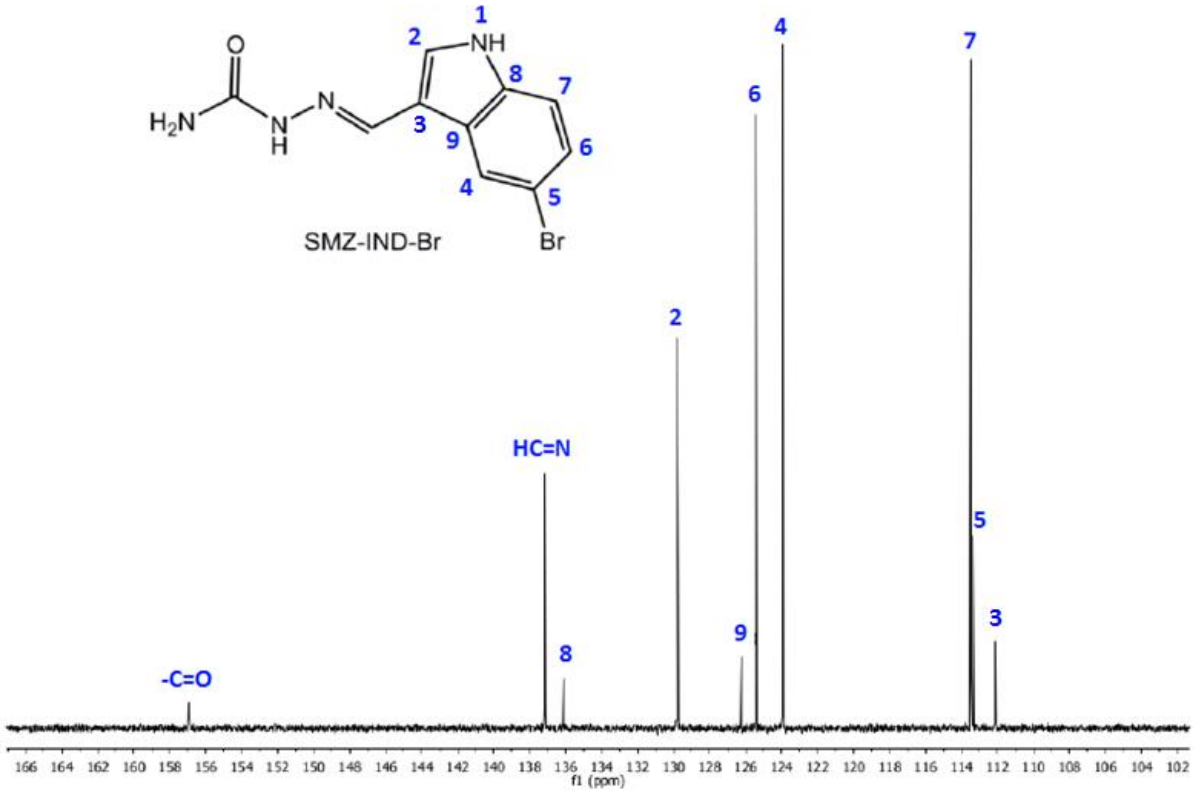


Figure 5. $^{13}C\{^{1}H\}$NMR spectrum showing the aromatic zone of compound **1** (126 MHz, acetone-d_6)

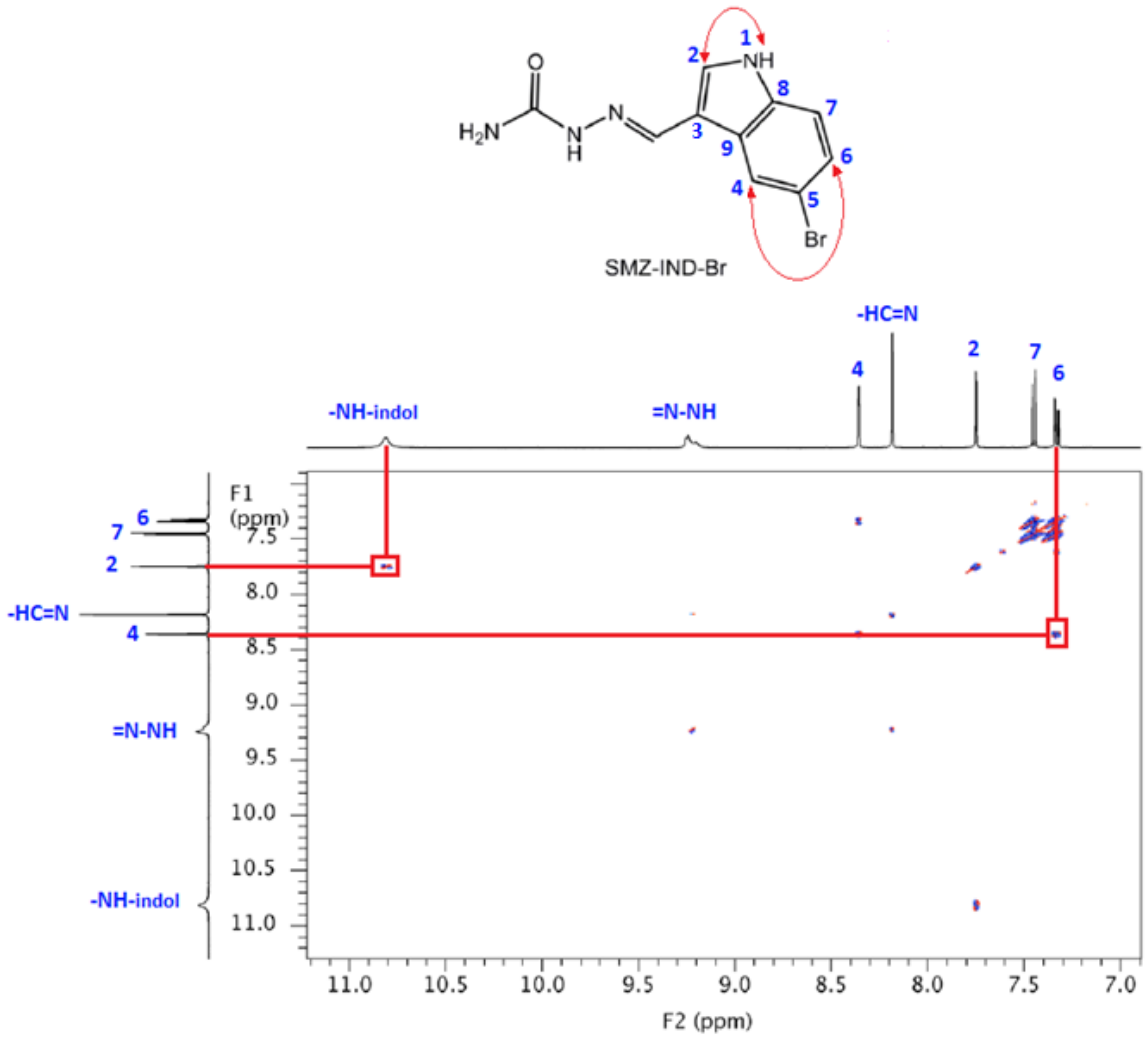


Figure 6. Two-dimensional ^{1}H-^{1}H DQFCOSY NMR spectrum recorded in acetone-d_6 for the compound **1**

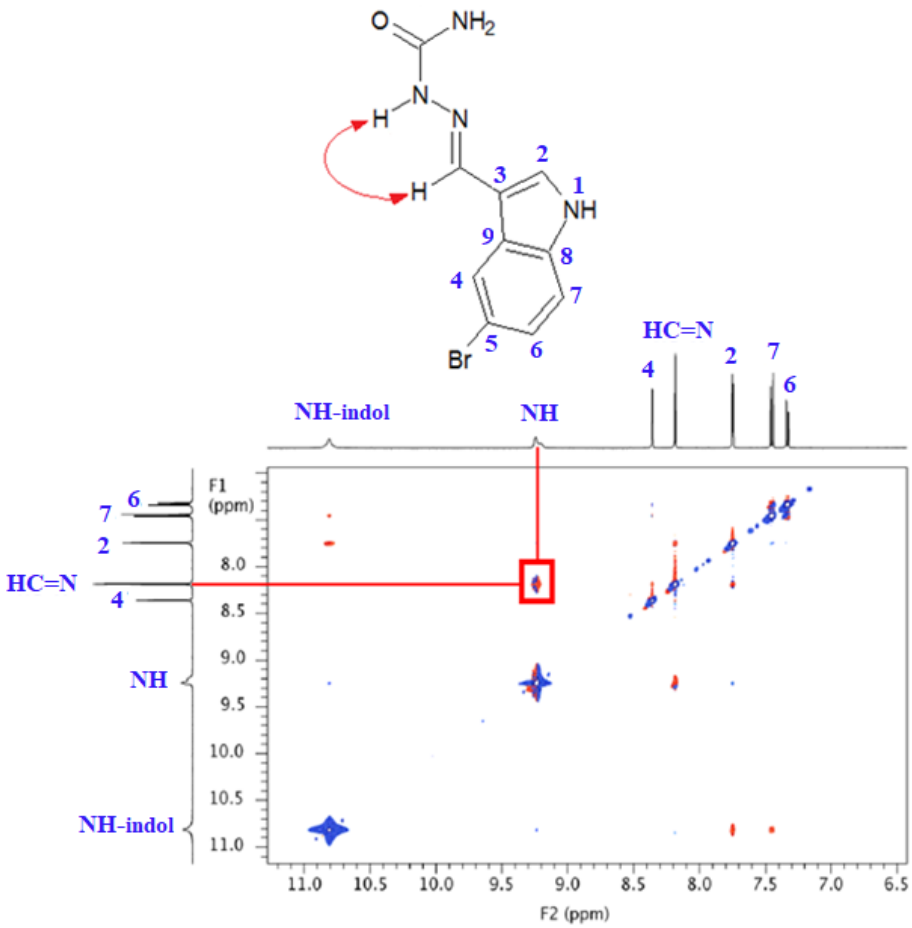


Figure 7. Two-dimensional ^{1}H-^{1}H NOESY NMR spectrum, recorded in acetone-d_6 for the compound **1**

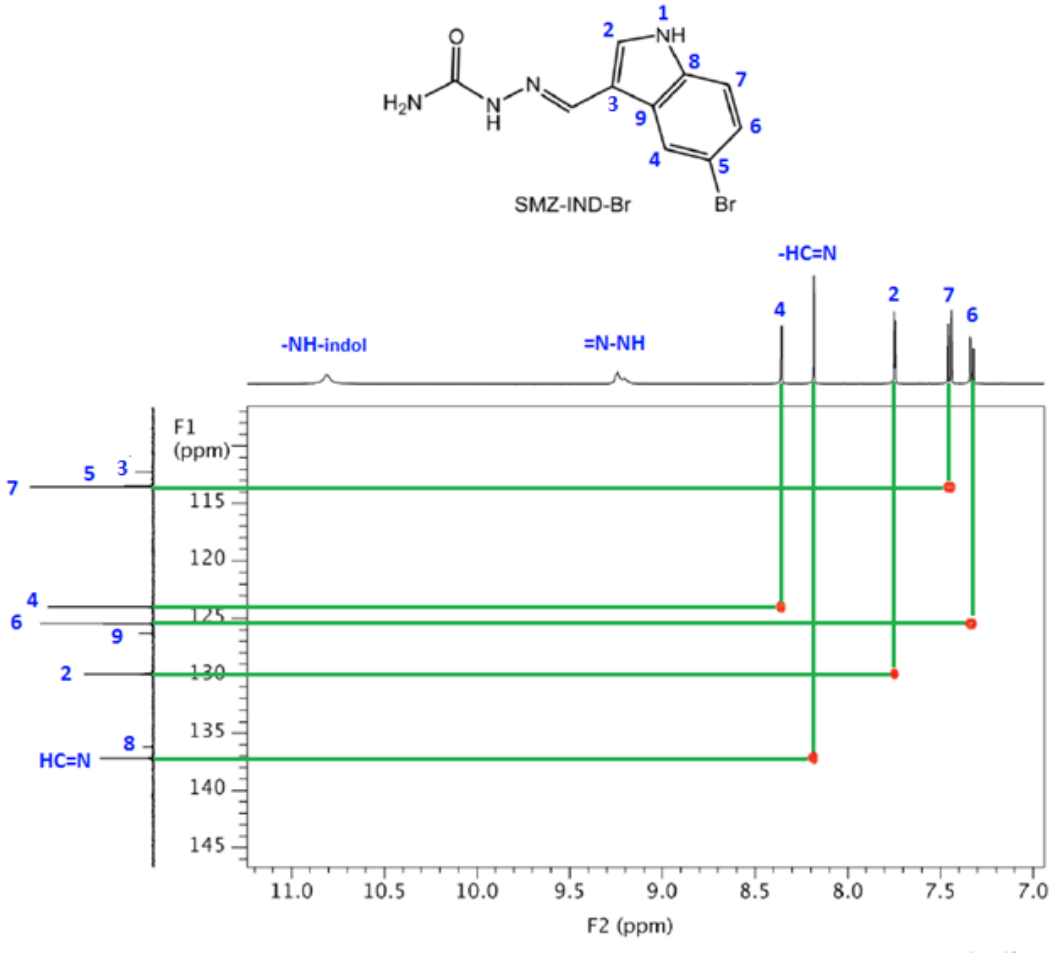


Figure 8. Two-dimensional ^{1}H-^{13}C HSQC NMR spectrum showing the aromatic zone for the compound **1** recorded in acetone-d_6

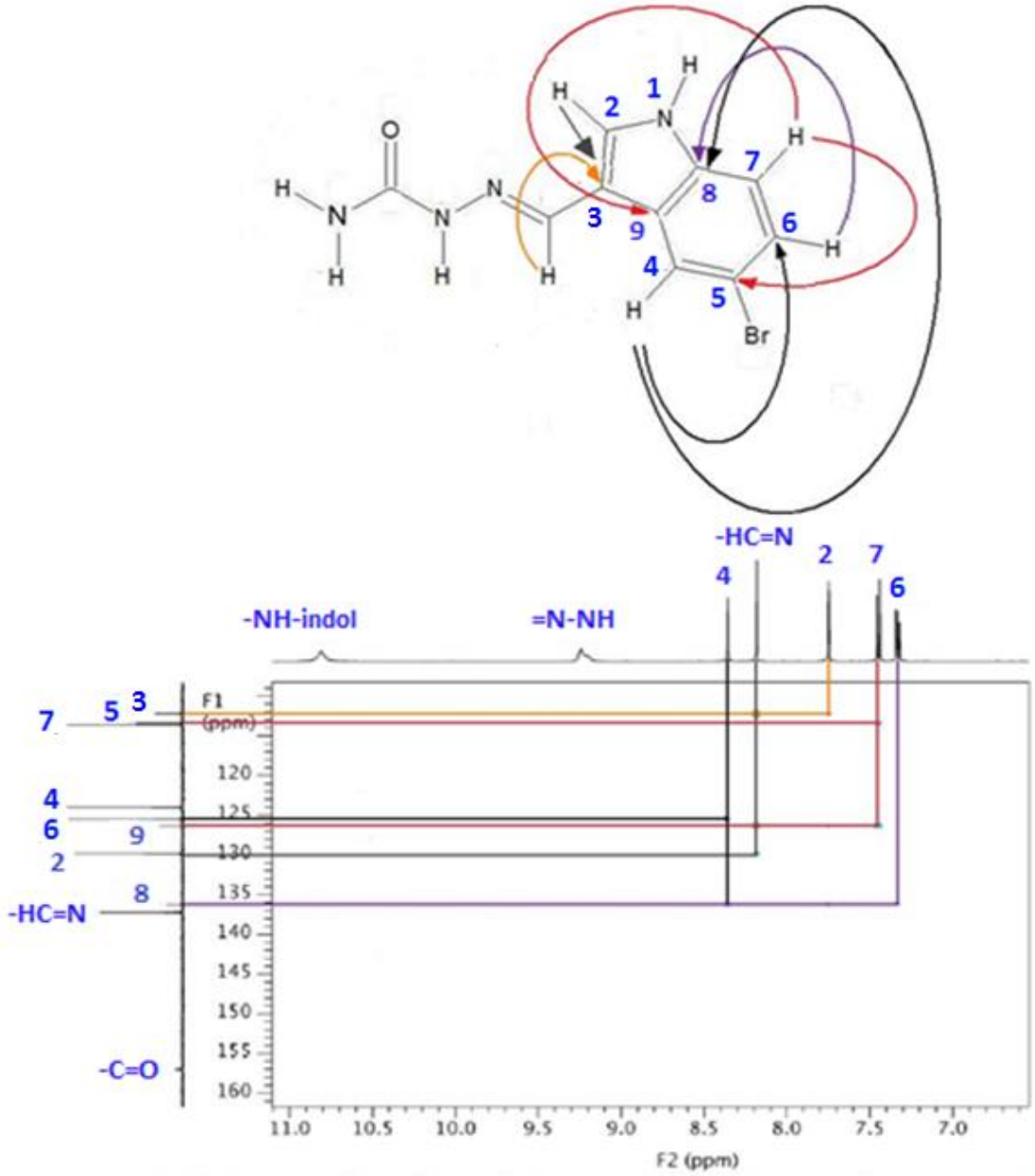


Figure 9. Two-dimensional ^{1}H-^{13}C HMBC NMR spectrum showing the aromatic zone for the compound **1** recorded in acetone-d_6

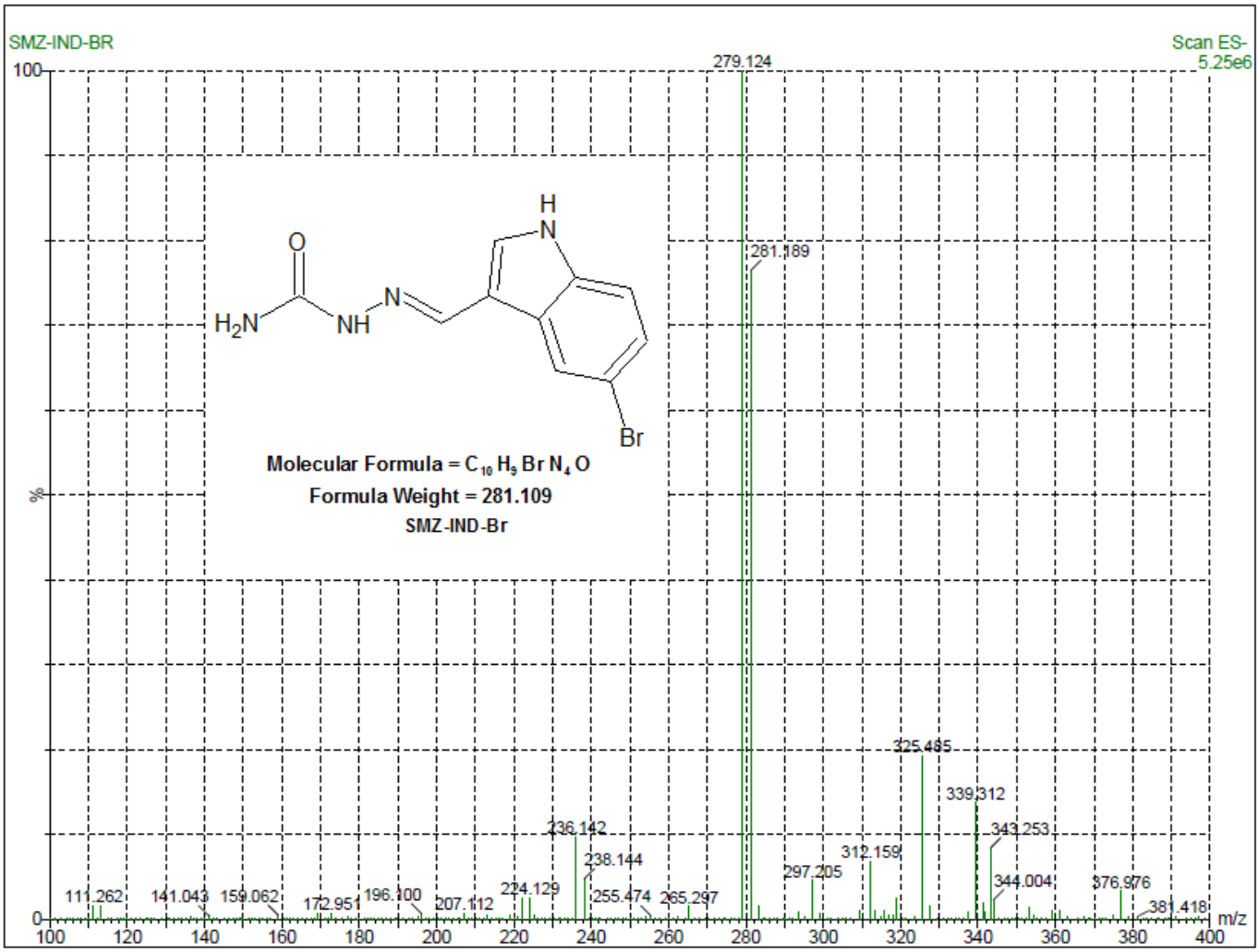


Figure 10. ESI-mass spectrum of the compound **1**

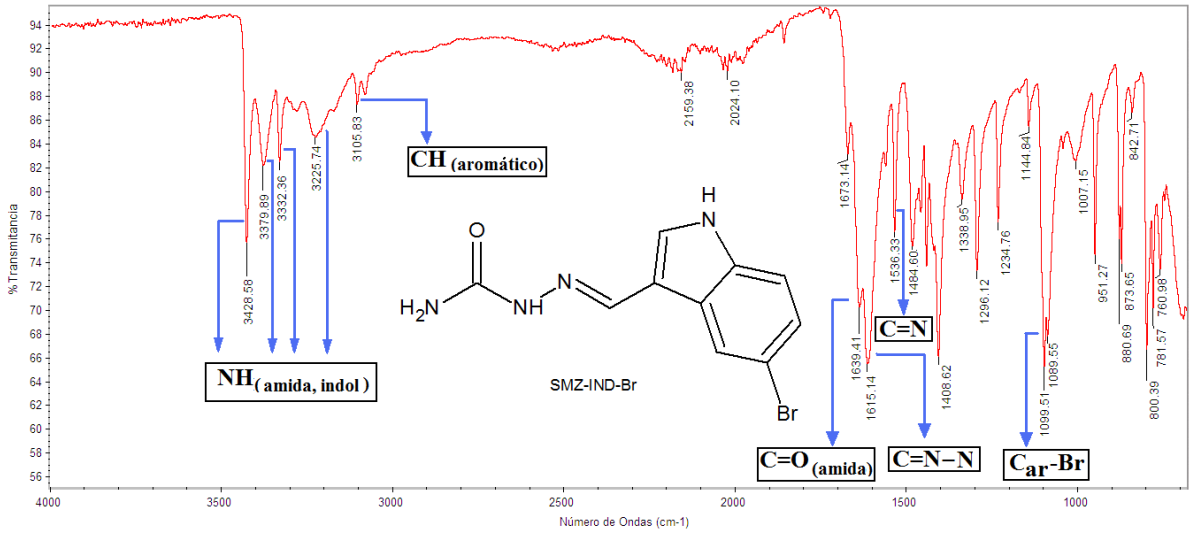


Figure 11. FT-IR spectrum of the compound **1**

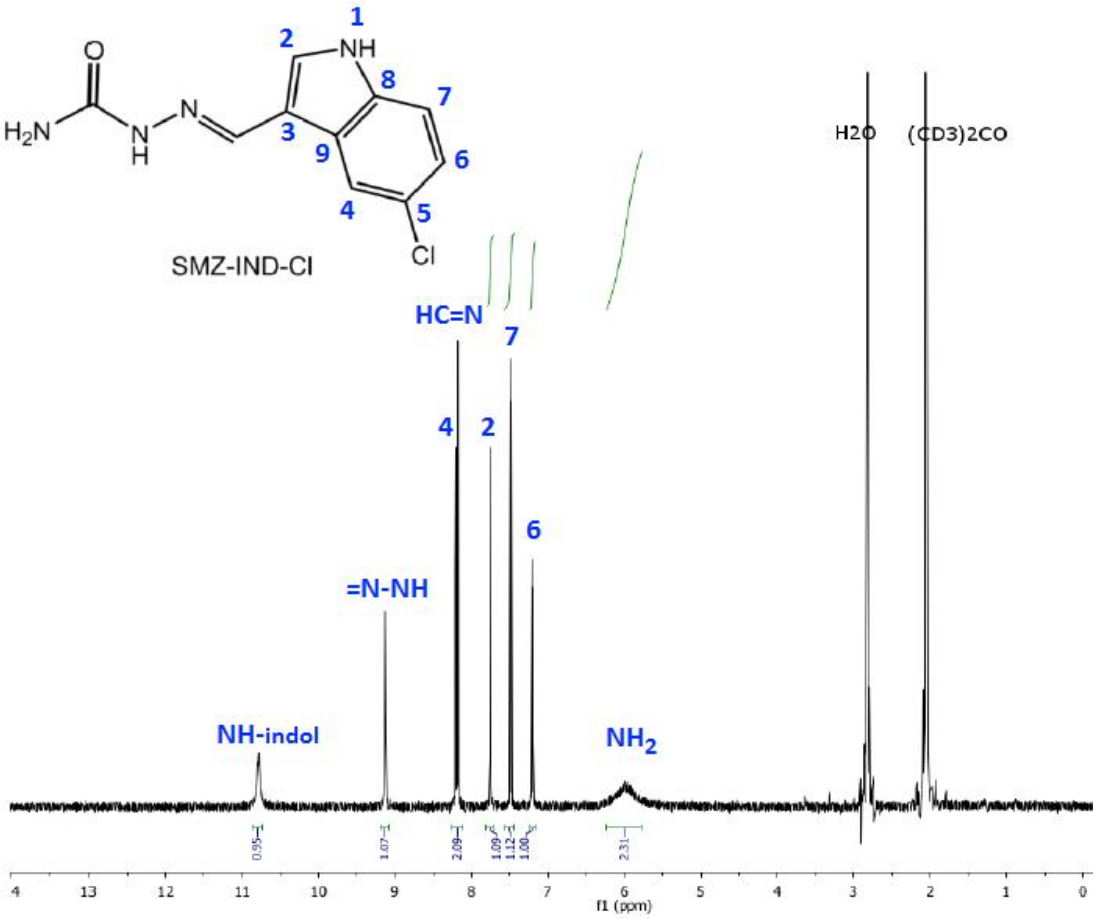


Figure 12. ^{1}H NMR spectrum of compound 2 (500 MHz, acetone-d_6)

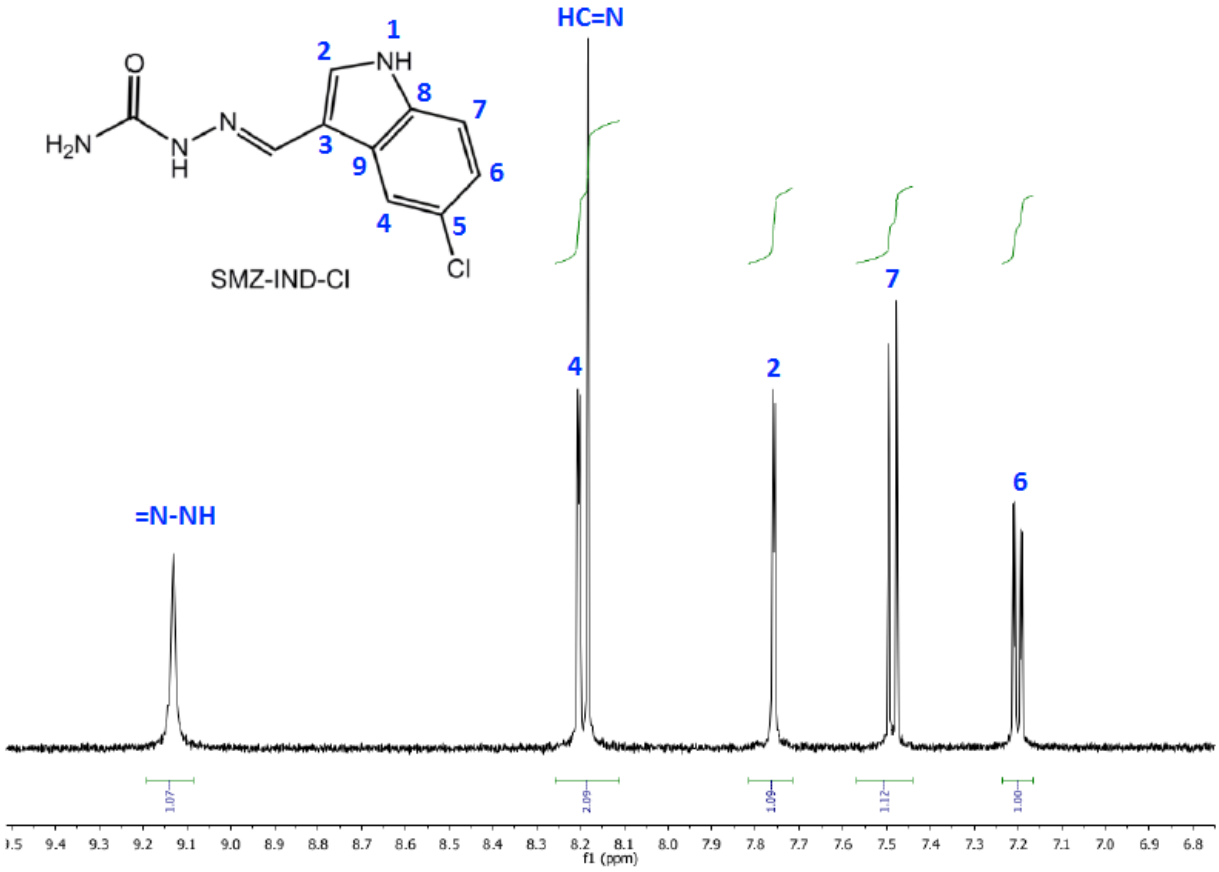


Figure 13. ^{1}H NMR spectrum showing the aromatic zone of compound 2 (500 MHz, acetone-d_6)

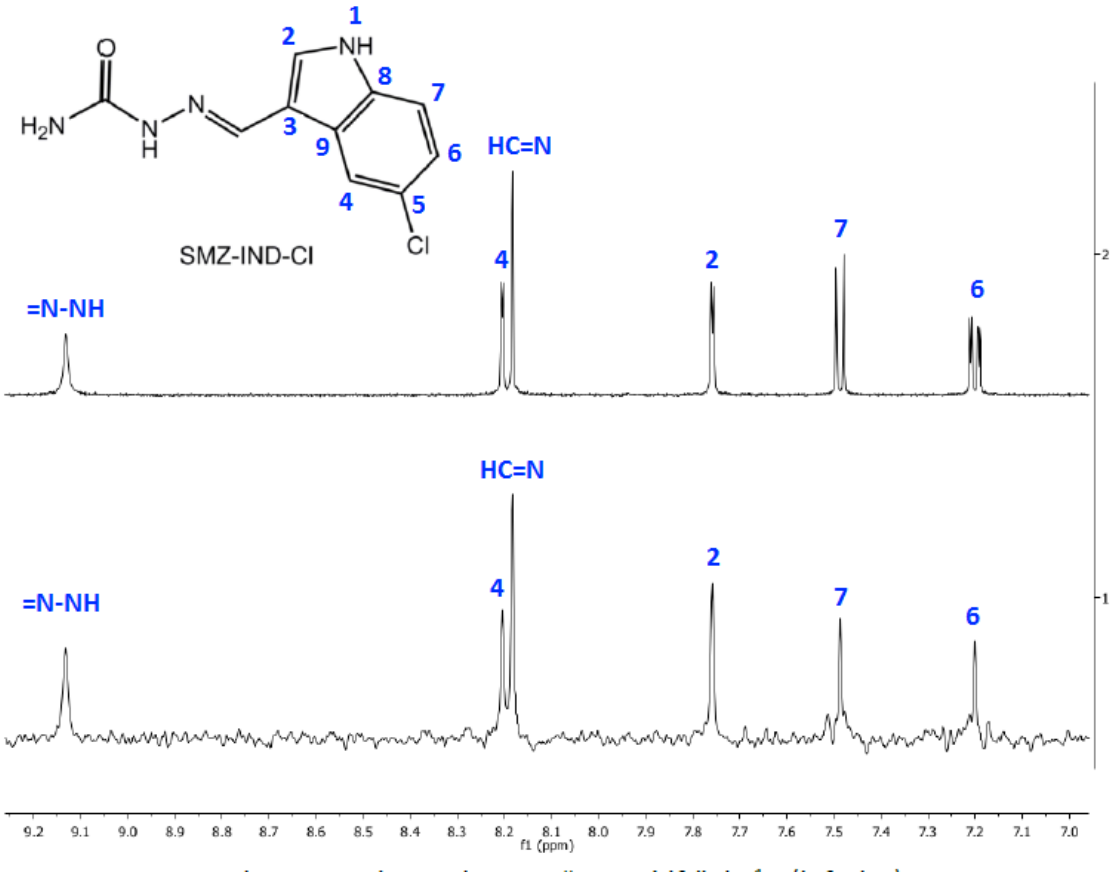


Figure 14. comparison between the experiment "pure shift" of ^{1}H (lower) with the NMR spectrum of ^{1}H (upper) (500 MHz, acetone-d_6)

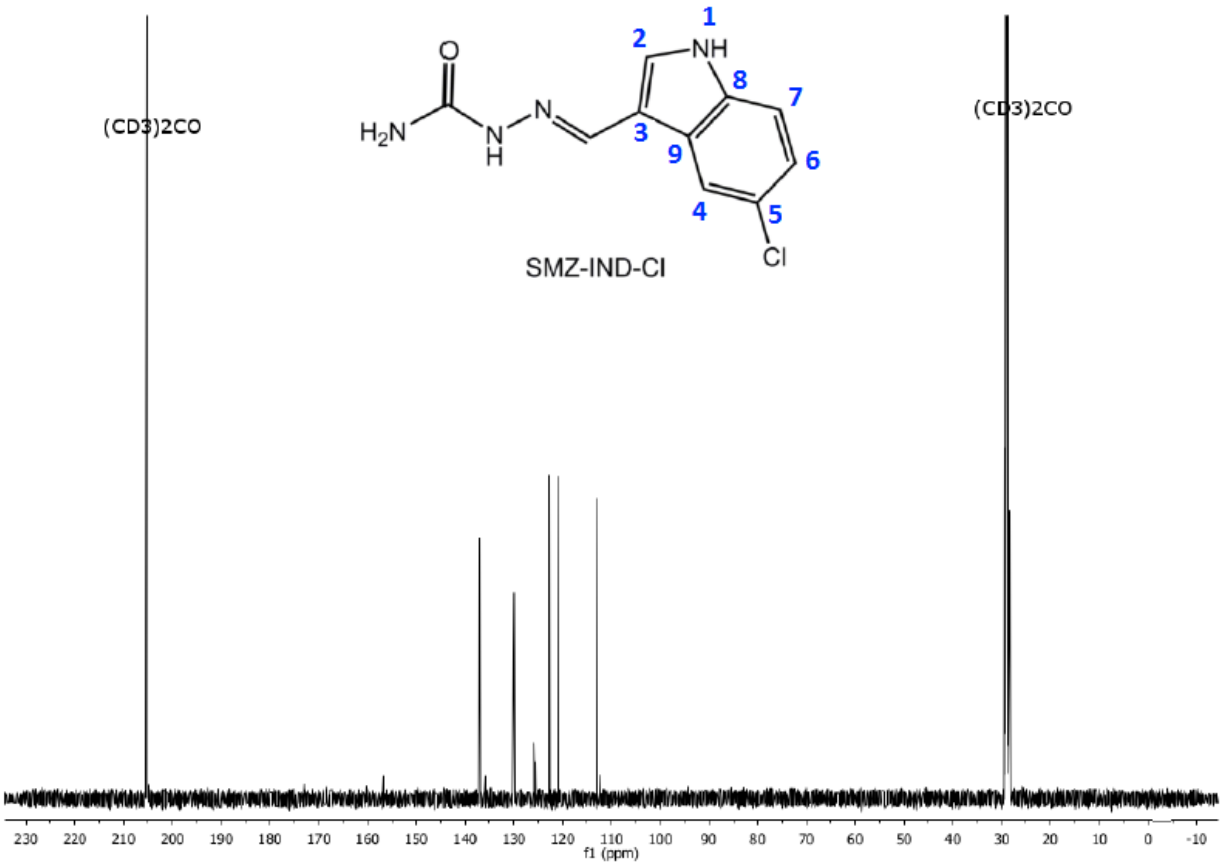


Figure 15. $^{13}C\{^{1}H\}$NMR spectrum of compound 2 (126 MHz, acetone-d_6)

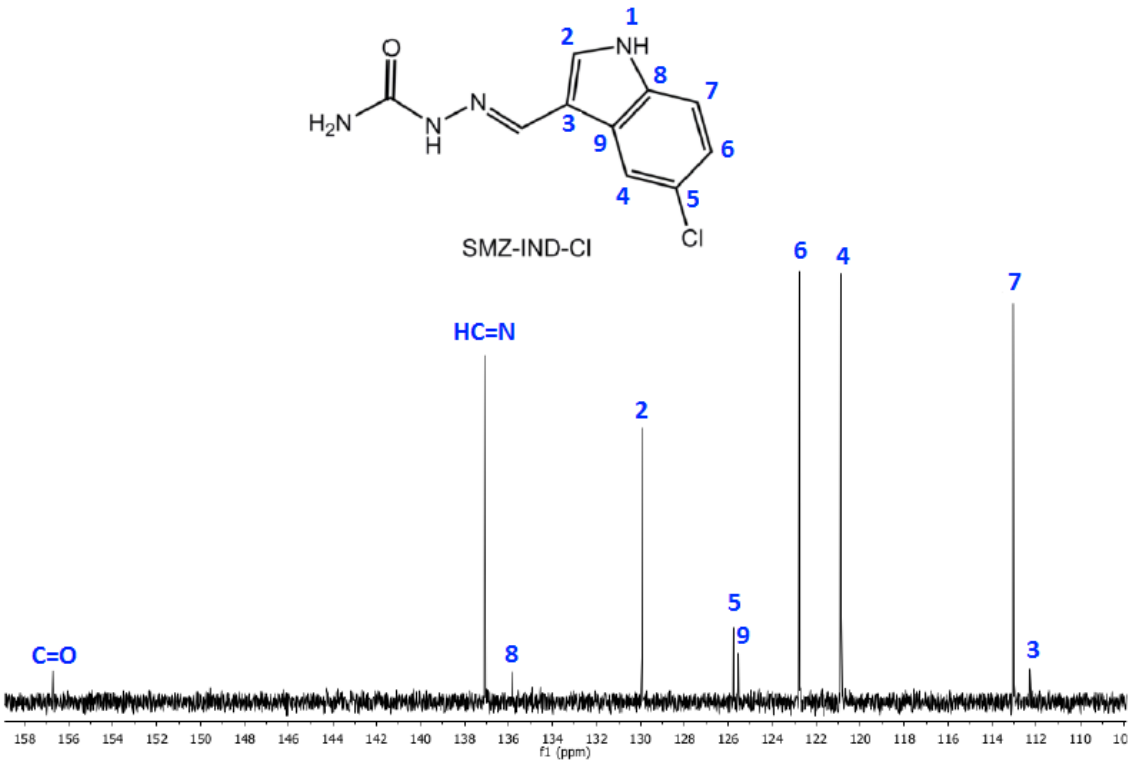


Figure 16. $^{13}C\{^{1}H\}$NMR spectrum showing the aromatic zone of compound **2** (126 MHz, acetone-d_6)

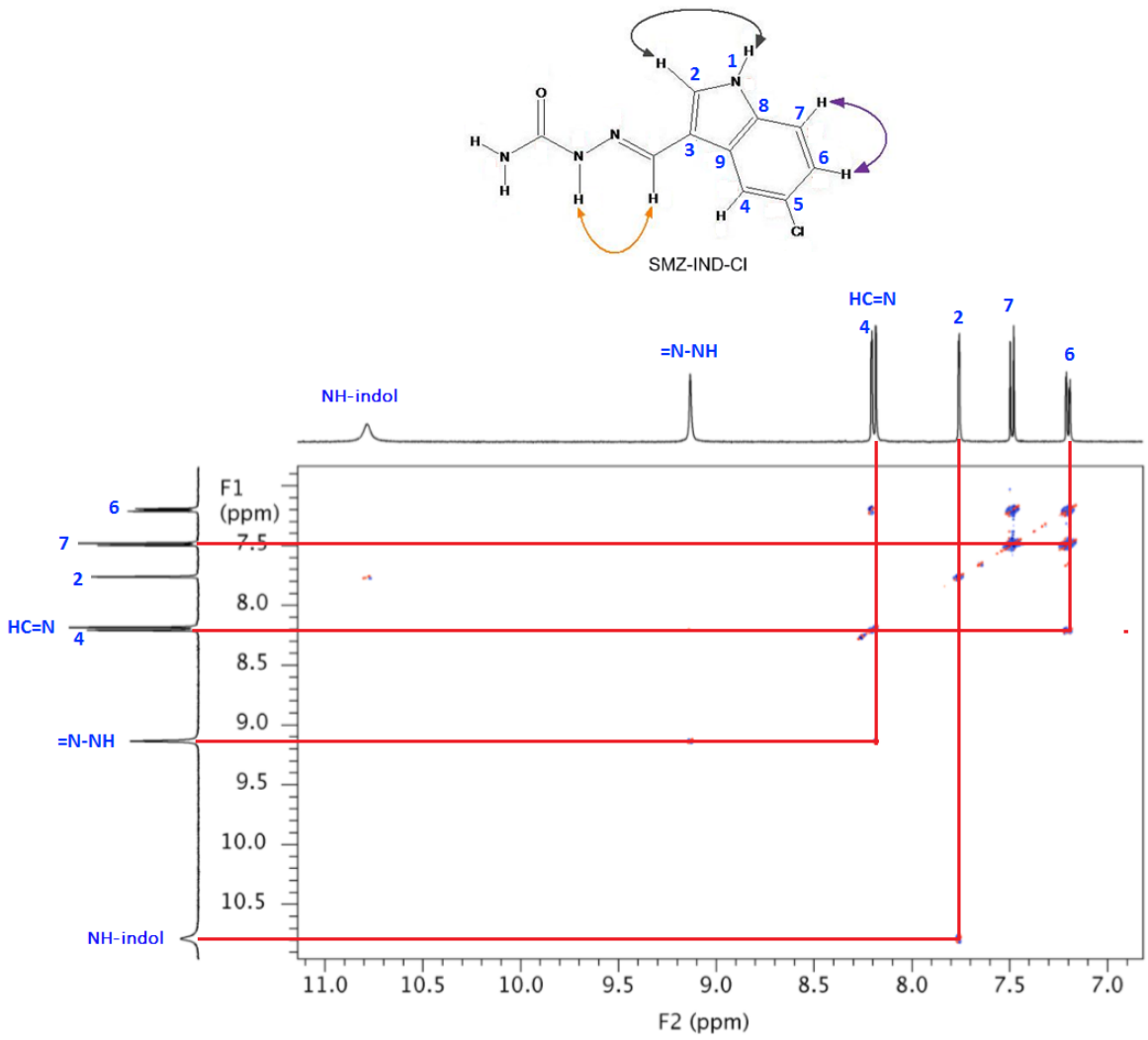
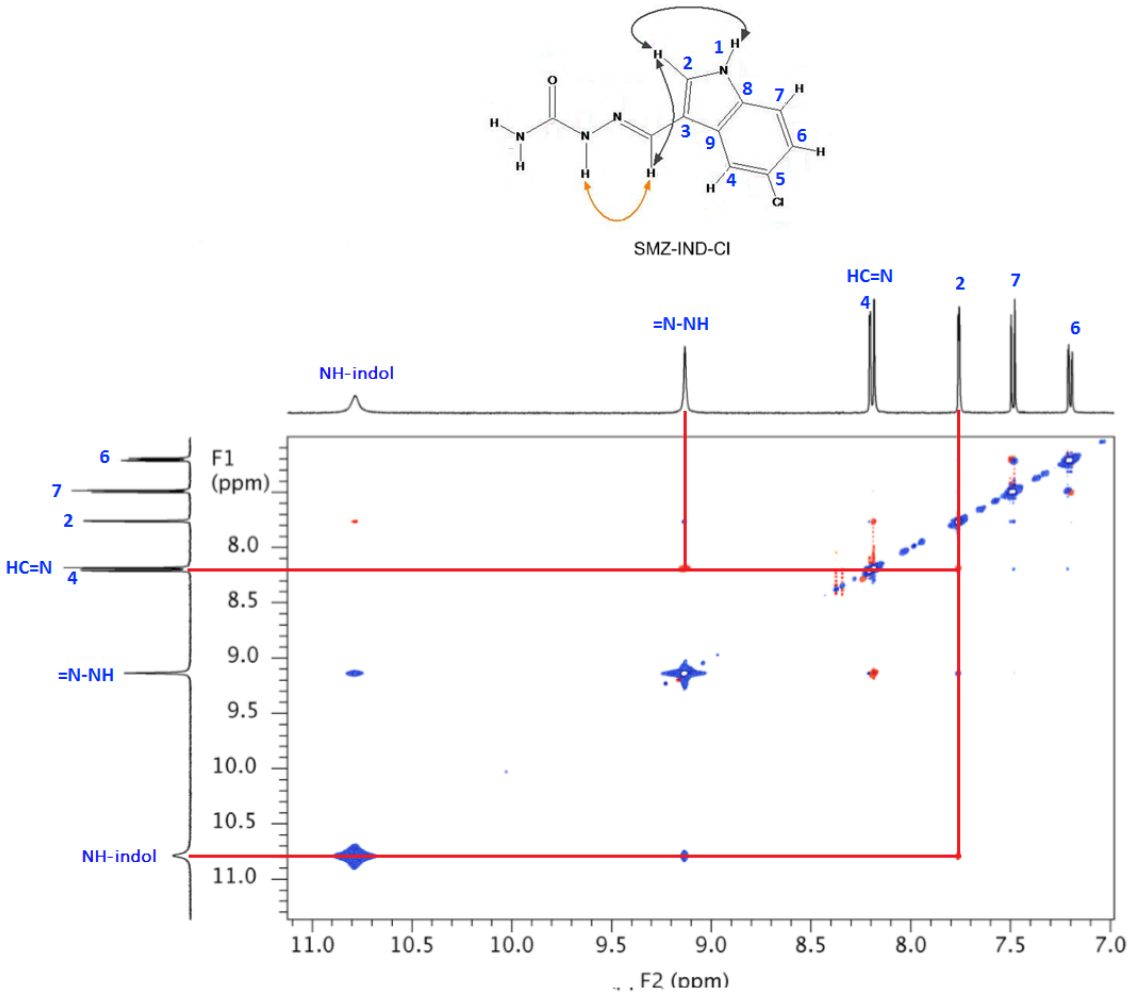


Figure 17. Two-dimensional ^{1}H-^{1}H DQFCOSY NMR spectrum recorded in acetone-d_6 for the compound **2**



Expansión de la zona aromática del experimento de RMN bidimensional ^{1}H-^{1}H NOESY

Figure 18. Two-dimensional ^{1}H-^{1}H NOESY NMR spectrum, recorded in acetone-d_6 for the compound **2**

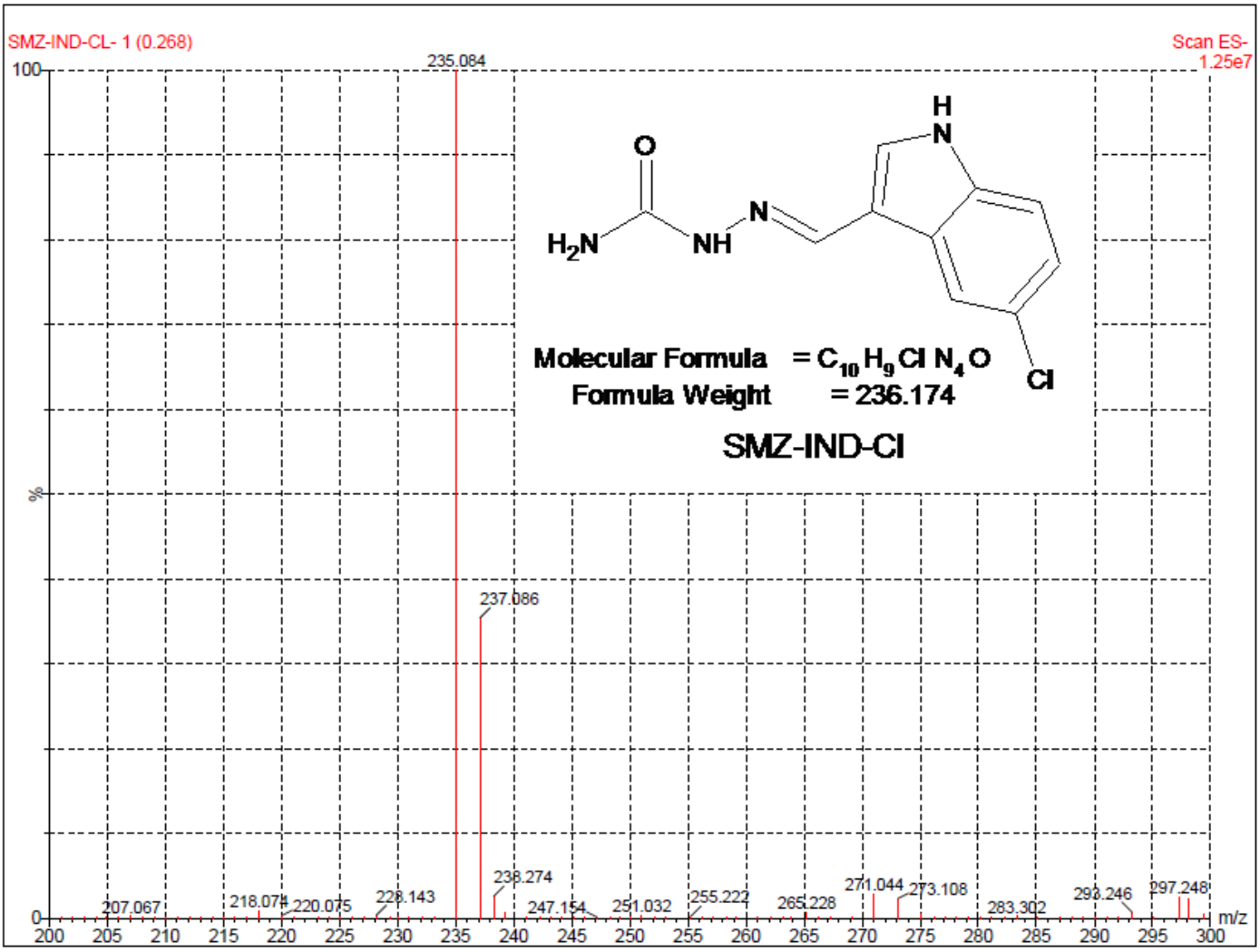


Figure 19. ESI-mass spectrum of the compound **2**

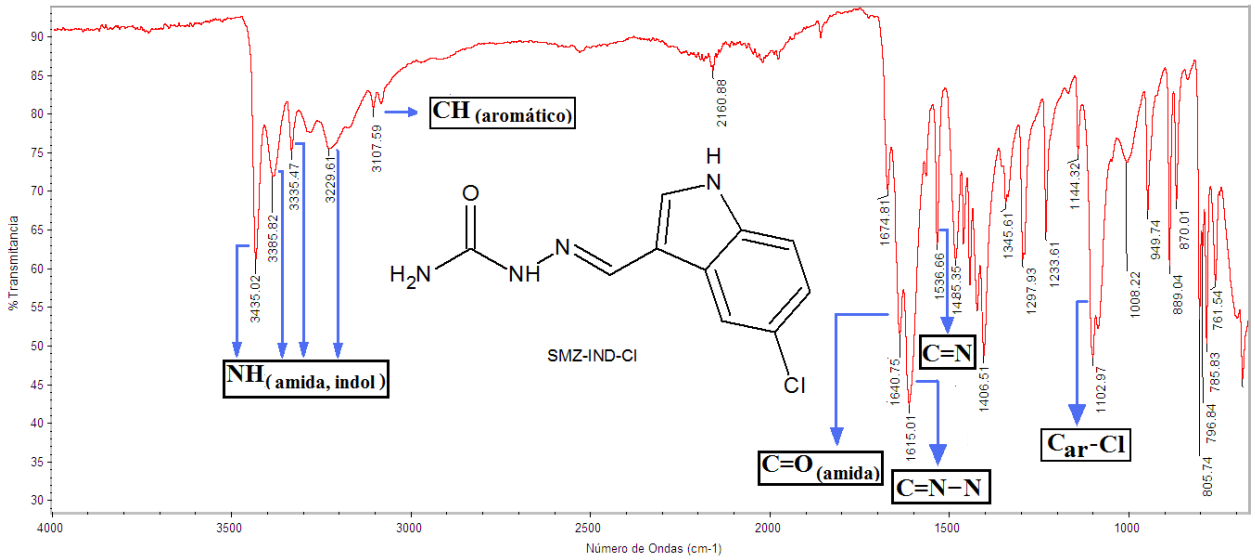


Figure 20. FT-IR spectrum of the compound **2**

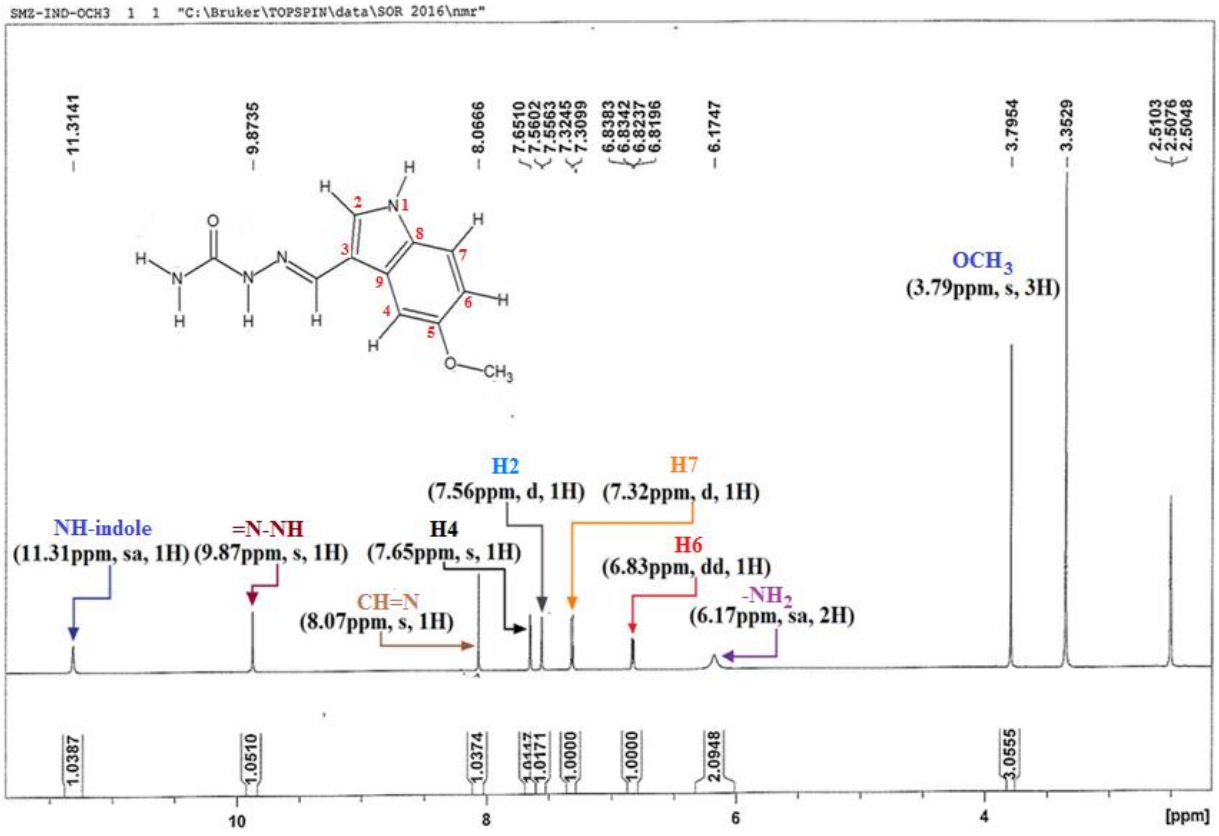


Figure 21. ^{1}H NMR spectrum of compound 3 (600 MHz, DMSO-d_6)

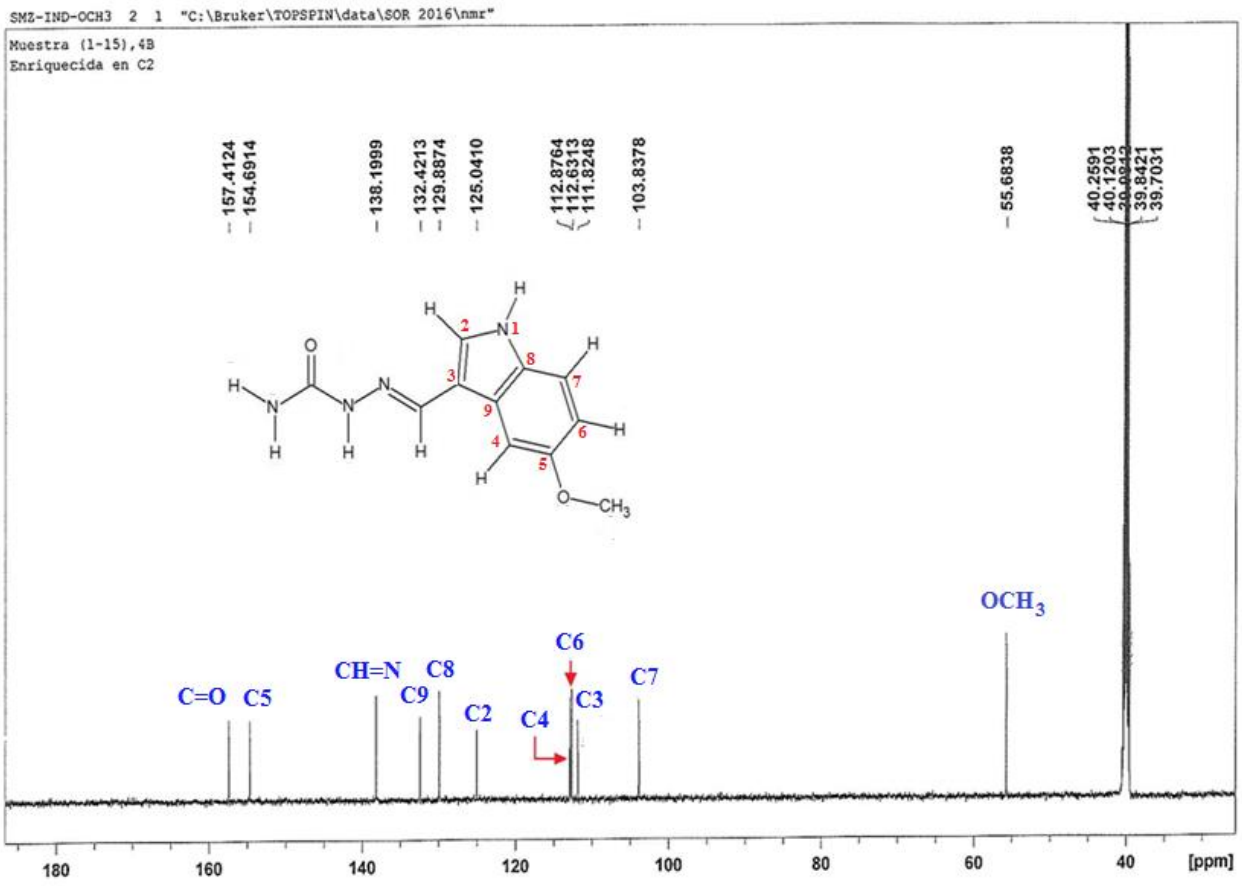


Figure 22. ^{13}C NMR spectrum of compound 3 (150 MHz, DMSO-d_6)

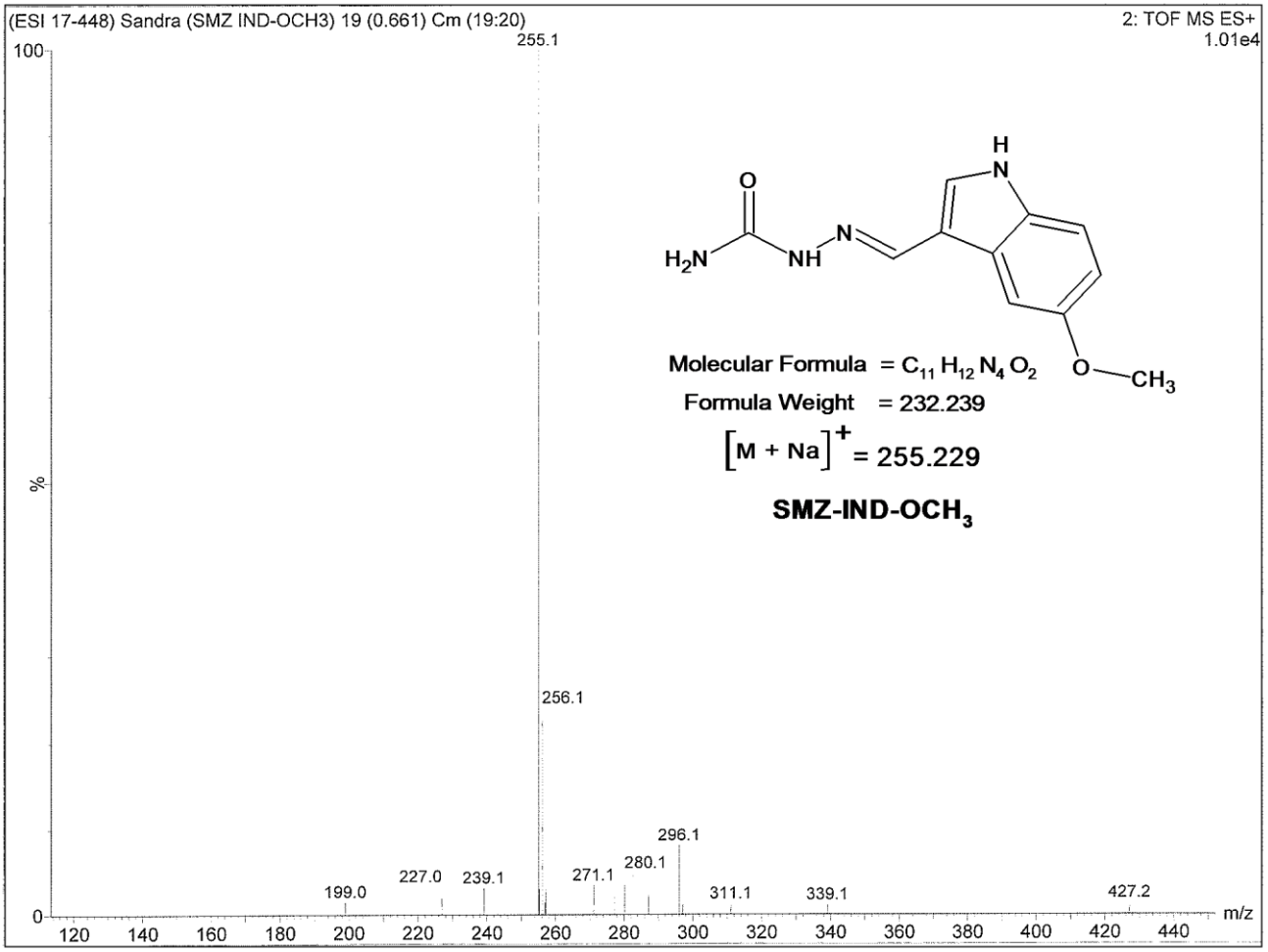


Figure 23. ESI-mass spectrum of the compound **3**

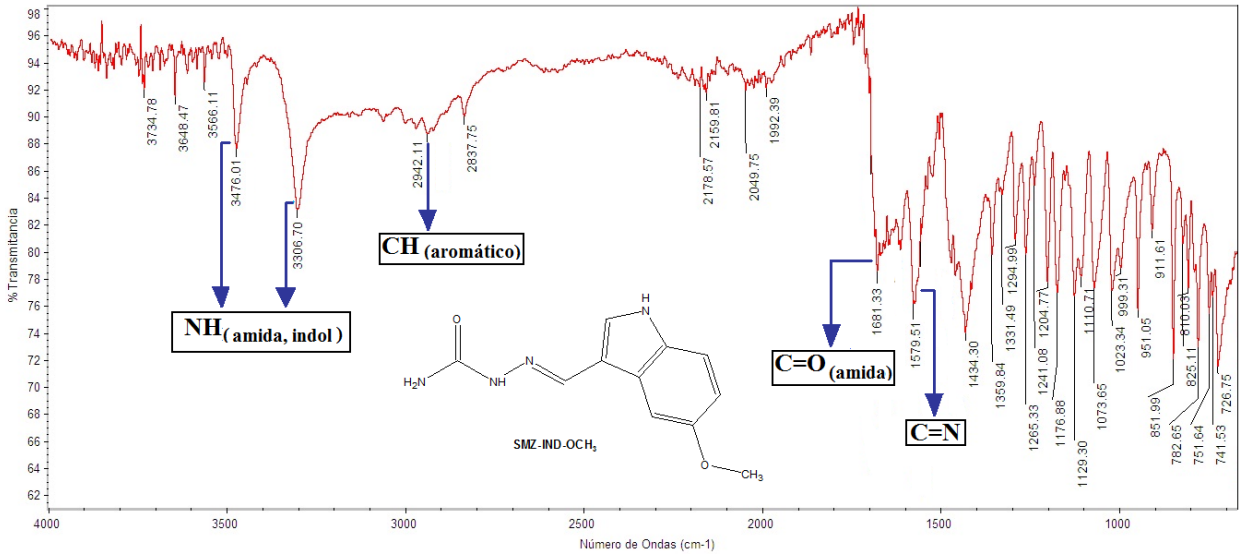


Figure 24. FT-IR spectrum of the compound **3**

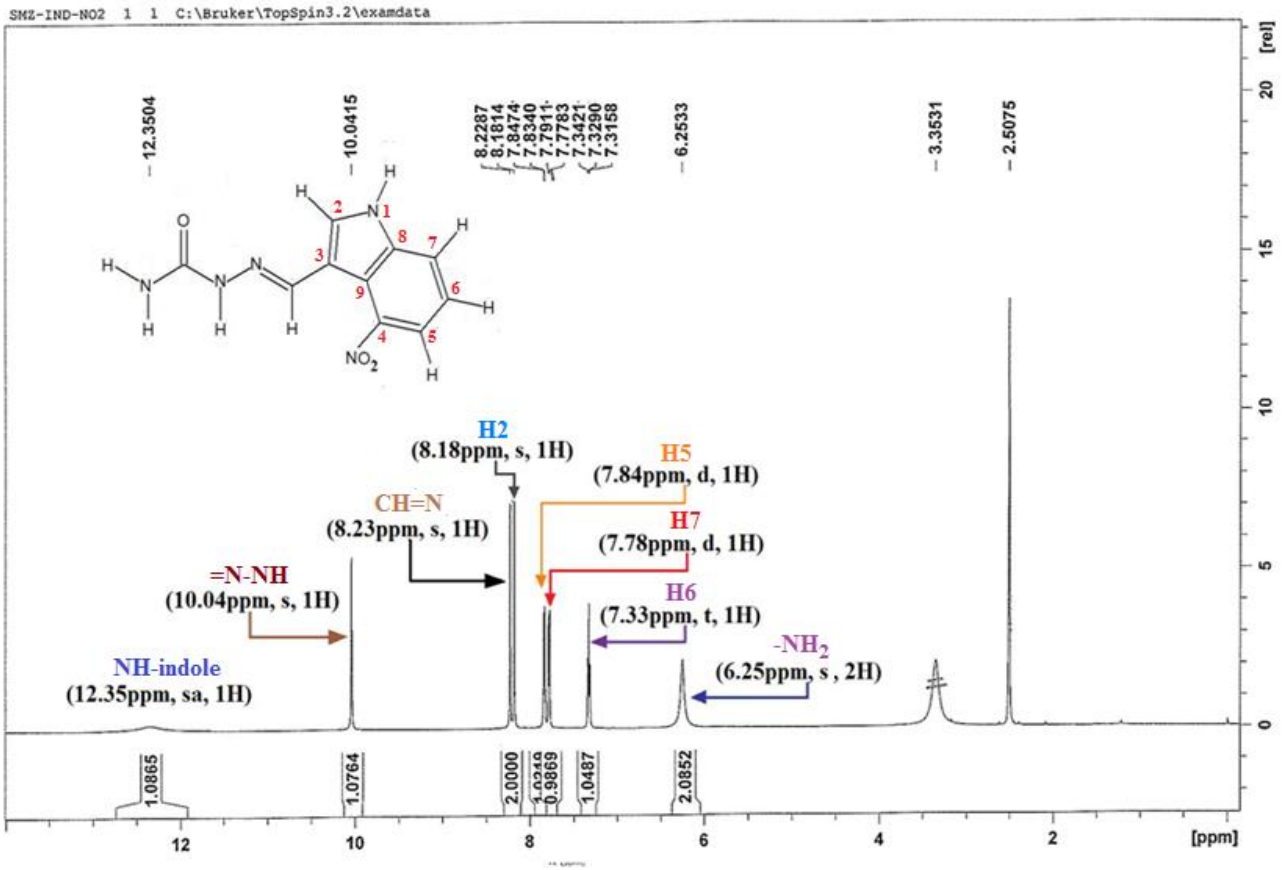


Figure 25. ^{1}H NMR spectrum of compound 4 (600 MHz, DMSO-d_6)

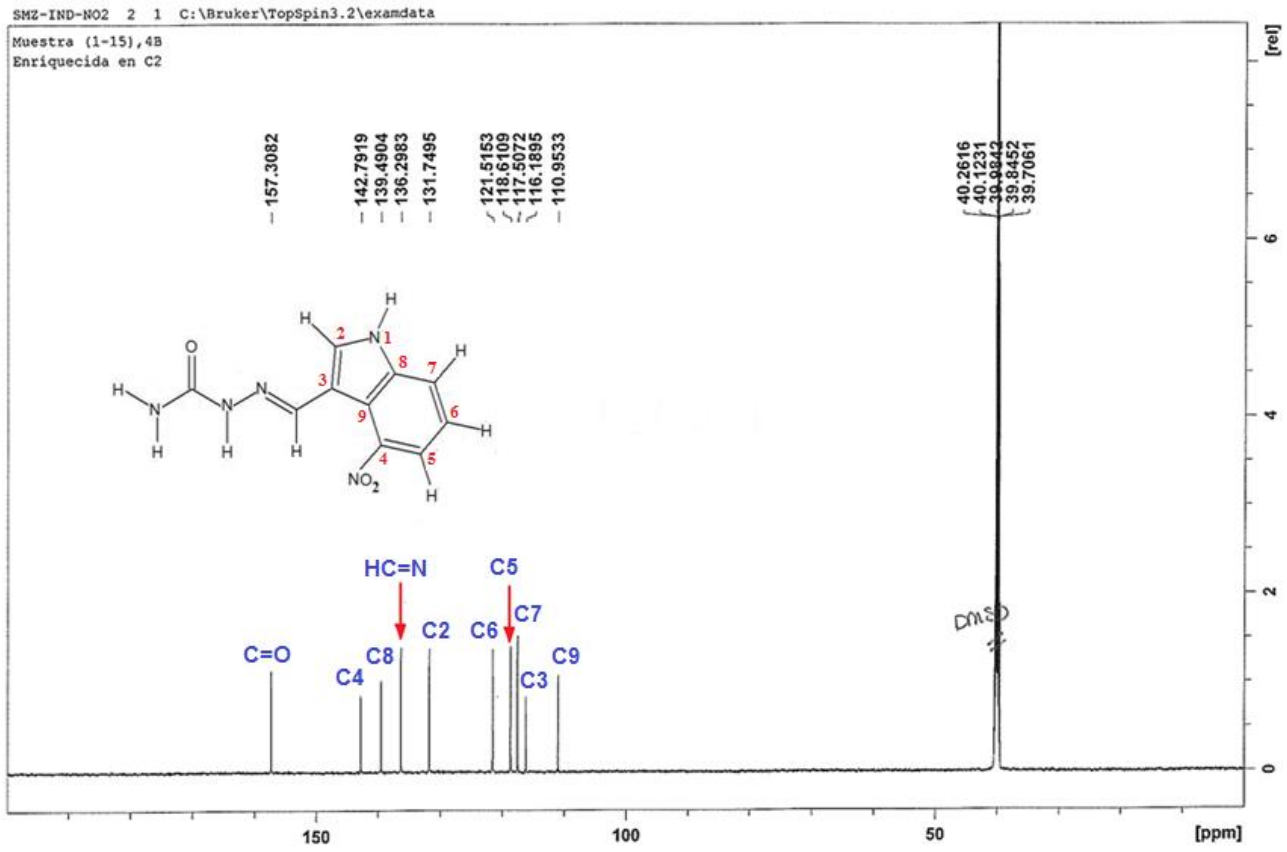


Figure 26. ^{13}C NMR spectrum of compound 4 (150 MHz, DMSO-d_6)

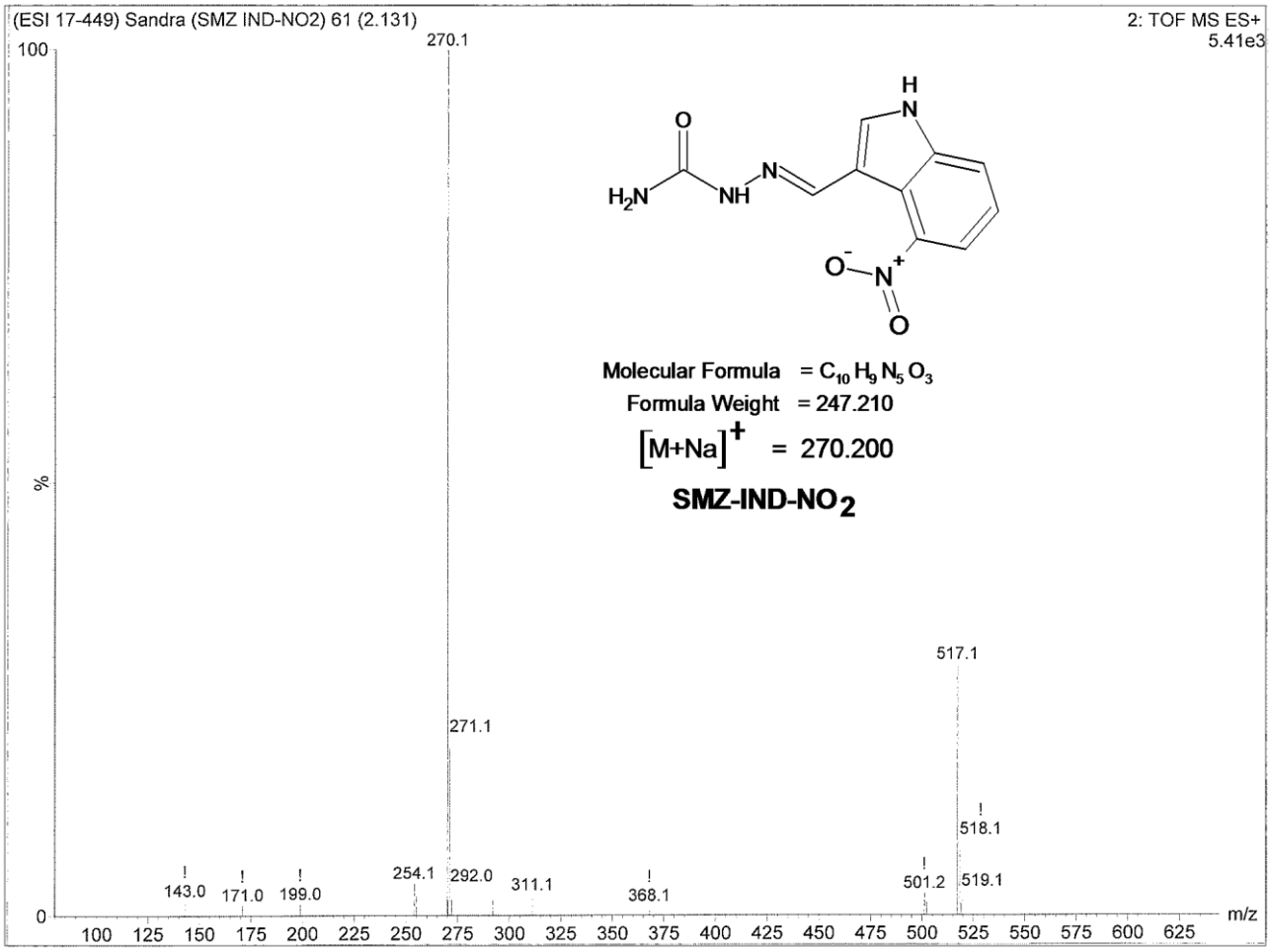


Figure 27. ESI-mass spectrum of the compound **4**

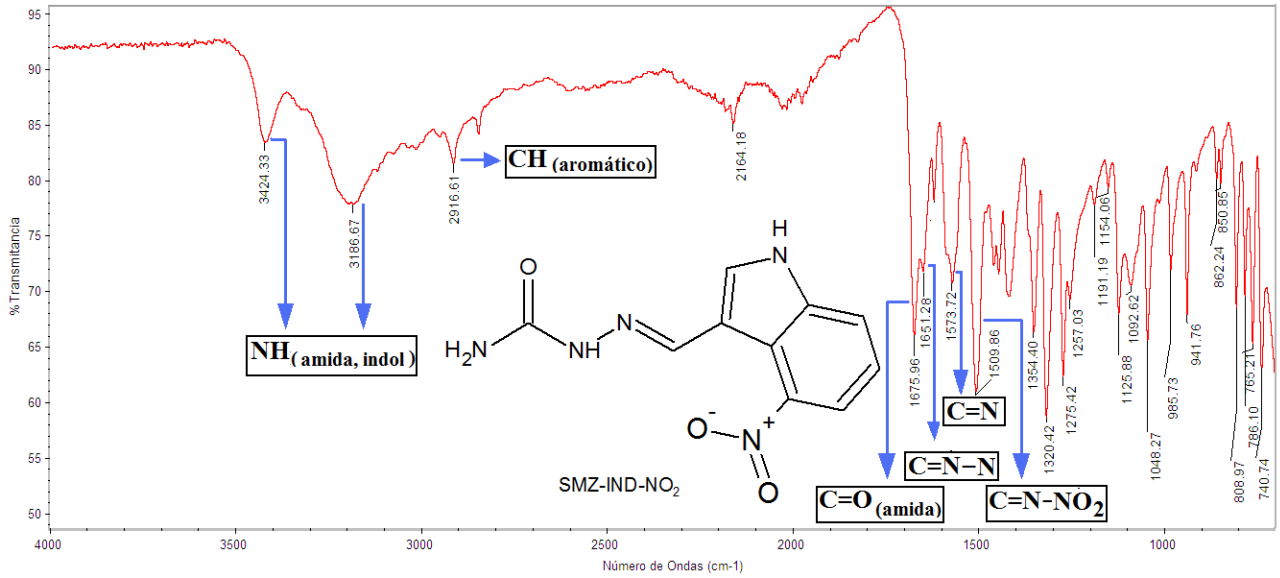


Figure 28. FT-IR spectrum of the compound **4**