

SUPPORTING INFORMATION

associated with the paper

Phenylisoxazole - 3/5 – carbaldehyde isonicotinohydrazide derivatives :

Synthesis Characterization, and antituberculous activity

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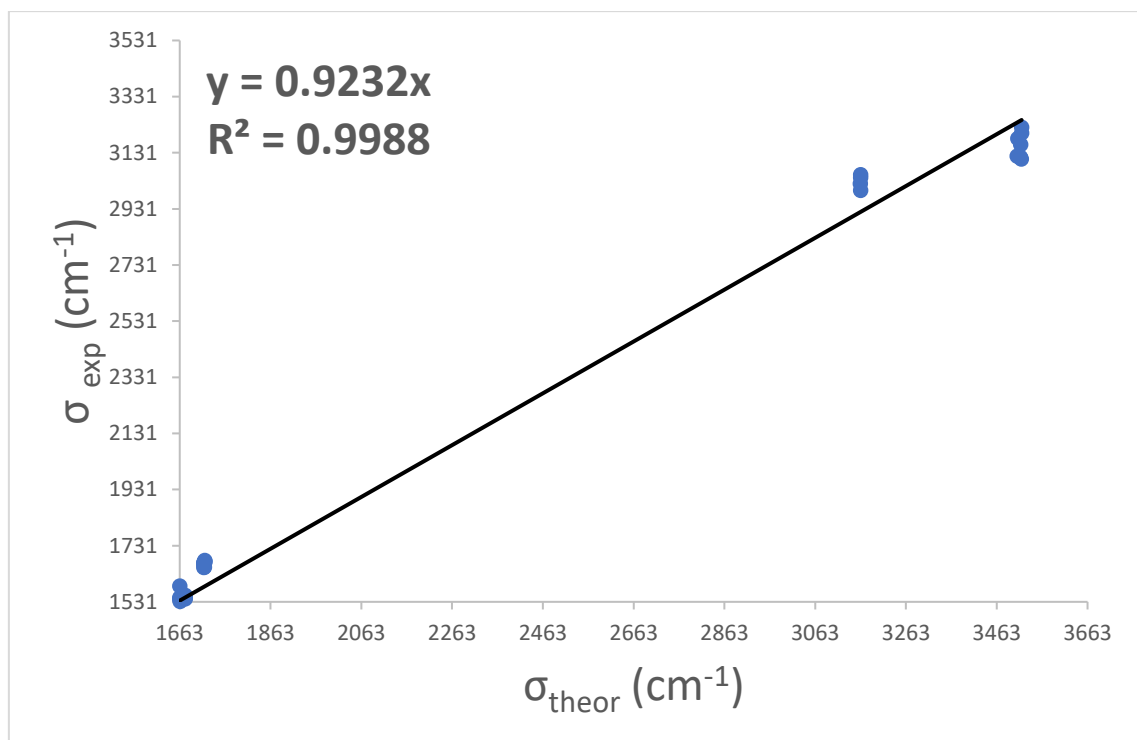
Supplementary table 1. Computational results, at B3LYP/6-311++G(d,p) for **1** to **8** synthesized compounds. Relative enthalpies (ΔH) of stable conformers and their equilibrium molar fractions (populations).

Compound		E_0^a	G_{298}^a	H_{298}^a	ΔH^b	μ^c	Population (%)
Gas phase							
1	<i>cisE</i>	-1085.832	-1085.636	-1085.566	0.0	3.159	90.2
	<i>transE</i>	-1085.830	-1085.634	-1085.563	6.6	2.311	8.8
	<i>cisZ</i>	-1085.828	-1085.632	-1085.561	12.0	4.395	1.0
	<i>transZ</i>	-1085.825	-1085.628	-1085.558	20.5	5.432	< 0.1
2	<i>cisE</i>	-1101.120	-1100.885	-1100.811	0.0	3.074	88.5
	<i>transE</i>	-1101.118	-1100.883	-1100.809	6.3	1.221	9.8
	<i>cisZ</i>	-1101.117	-1100.882	-1100.808	9.2	4.407	1.7
	<i>transZ</i>	-1101.114	-1100.878	-1100.804	18.7	5.788	< 0.1
3	<i>cisE</i>	-1446.183	-1445.989	-1445.917	0.0	3.042	87.1
	<i>transE</i>	-1446.180	-1445.987	-1445.915	6.2	2.285	12.3
	<i>cisZ</i>	-1446.179	-1445.984	-1445.913	11.6	4.460	0.6
	<i>transZ</i>	-1446.175	-1445.981	-1445.909	20.5	5.362	< 0.1
4	<i>cisE</i>	-1446.187	-1445.995	-1445.921	0.0	2.301	92.7
	<i>transE</i>	-1446.185	-1445.992	-1445.919	5.4	2.910	7.2
	<i>cisZ</i>	-1446.182	-1445.988	-1445.916	13.2	3.133	0.1
	<i>transZ</i>	-1446.178	-1445.985	-1445.912	23.9	3.728	< 0.1
5	<i>cisE</i>	-3560.107	-3559.916	-3559.842	0.0	0.862	82.9
	<i>transE</i>	-3560.105	-3559.915	-3559.840	5.2	2.573	16.8

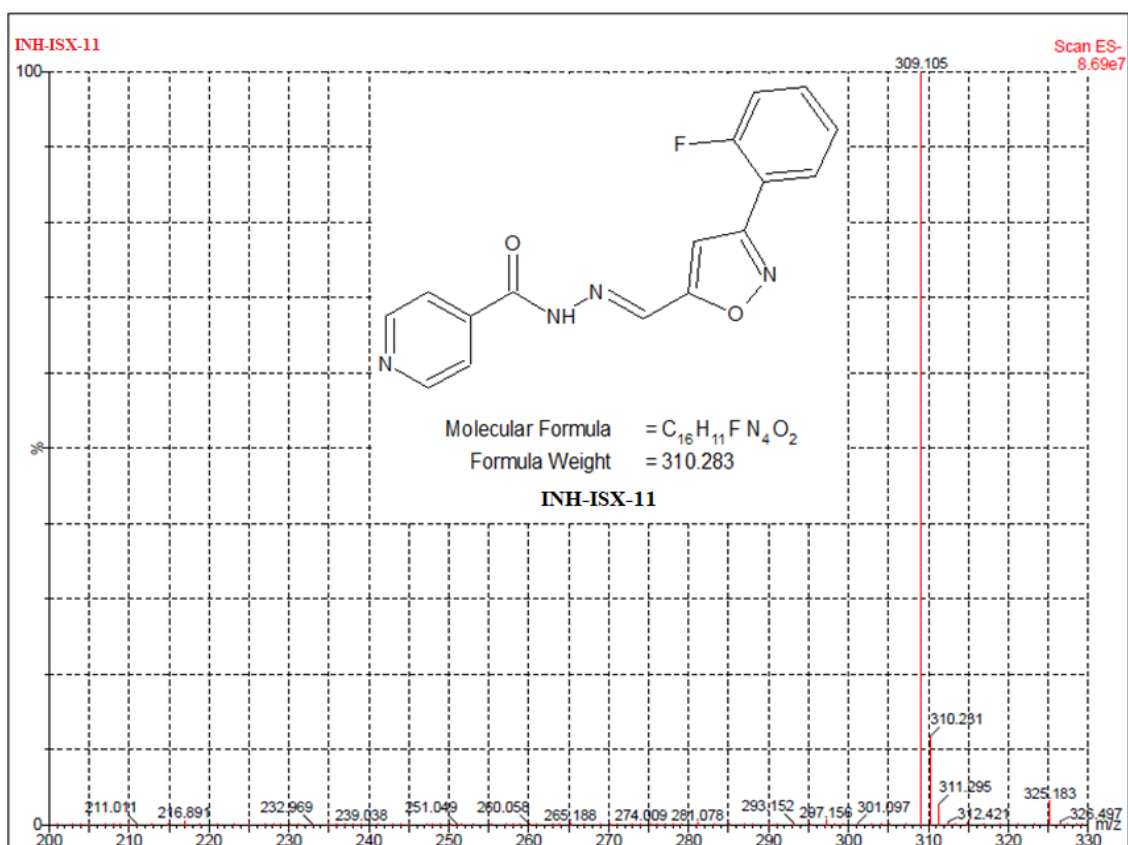
	<i>cisZ</i>	-3560.103	-3559.911	-3559.837	12.9	1.666	0.3
	<i>transZ</i>	-3560.098	-3559.907	-3559.833	24.6	2.677	< 0.1
6	<i>cisE</i>	-1101.126	-1100.892	-1100.818	0.0	5.232	90.8
	<i>transE</i>	-1101.124	-1100.890	-1100.815	5.3	3.712	9.2
	<i>cisZ</i>	-1101.120	-1100.885	-1100.810	19.1	6.879	< 0.1
	<i>transZ</i>	-1101.115	-1100.882	-1100.806	30.2	7.715	< 0.1
7	<i>cisE</i>	-1025.897	-1025.667	-1025.594	0.0	4.128	84.0
	<i>transE</i>	-1025.895	-1025.666	-1025.592	5.2	2.374	15.9
	<i>cisZ</i>	-1025.890	-1025.660	-1025.586	19.5	5.871	0.1
	<i>transZ</i>	-1025.885	-1025.656	-1025.582	30.7	6.881	< 0.1
8	<i>cisE</i>	-1446.191	-1445.997	-1445.925	0.0	1.694	86.0
	<i>transE</i>	-1446.189	-1445.995	-1445.923	4.6	1.475	14.0
	<i>cisZ</i>	-1446.183	-1445.989	-1445.917	20.5	3.393	< 0.1
	<i>transZ</i>	-1446.178	-1445.986	-1445.913	32.1	4.279	< 0.1
Acetone							
1	<i>cisE</i>	-1085.849	-1085.653	-1085.582	2.5	3.925	28.5
	<i>transE</i>	-1085.85	-1085.654	-1085.583	0.0	3.463	71.4
	<i>cisZ</i>	-1085.843	-1085.646	-1085.576	18.2	5.787	< 0.1
	<i>transZ</i>	-1085.843	-1085.646	-1085.576	17.9	7.336	< 0.1
2	<i>cisE</i>	-1101.139	-1100.904	-1100.830	2.7	3.413	4.5
	<i>transE</i>	-1101.14	-1100.906	-1100.831	0.0	1.306	95.4
	<i>cisZ</i>	-1101.133	-1100.898	-1100.824	16.9	5.578	< 0.1
	<i>transZ</i>	-1101.133	-1100.898	-1100.824	17.4	8.012	< 0.1
3	<i>cisE</i>	-1446.2	-1446.006	-1445.934	2.6	3.915	23.6
	<i>transE</i>	-1446.201	-1446.007	-1445.935	0.0	3.466	76.4
	<i>cisZ</i>	-1446.194	-1446.000	-1445.929	18.0	5.748	< 0.1
	<i>transZ</i>	-1446.194	-1445.999	-1445.929	18.2	7.234	< 0.1
4	<i>cisE</i>	-1446.204	-1446.011	-1445.939	2.6	3.287	6.3
	<i>transE</i>	-1446.205	-1446.013	-1445.940	0.0	4.238	93.6
	<i>cisZ</i>	-1446.199	-1446.004	-1445.933	18.4	4.247	< 0.1
	<i>transZ</i>	-1446.198	-1446.005	-1445.932	19.7	5.305	< 0.1
5	<i>cisE</i>	-3560.125	-3559.933	-3559.860	2.5	1.440	34.6
	<i>transE</i>	-3560.126	-3559.934	-3559.860	0.0	3.463	65.3
	<i>cisZ</i>	-3560.119	-3559.927	-3559.853	18.7	2.249	< 0.1
	<i>transZ</i>	-3560.119	-3559.926	-3559.853	19.9	3.893	< 0.1
6	<i>cisE</i>	-1101.145	-1100.911	-1100.836	2.6	6.201	28.1
	<i>transE</i>	-1101.146	-1100.911	-1100.837	0.0	4.920	71.9
	<i>cisZ</i>	-1101.137	-1100.903	-1100.828	23.7	8.330	< 0.1
	<i>transZ</i>	-1101.137	-1100.902	-1100.828	24.0	9.946	< 0.1
7	<i>cisE</i>	-1025.914	-1025.684	-1025.611	2.6	4.824	22.4
	<i>transE</i>	-1025.915	-1025.685	-1025.612	0.0	3.144	77.6
	<i>cisZ</i>	-1025.906	-1025.676	-1025.603	24.1	7.189	< 0.1
	<i>transZ</i>	-1025.906	-1025.675	-1025.602	24.7	9.016	< 0.1

8	<i>cisE</i>	-1446.208	-1446.014	-1445.942	2.4	2.115	45.6
	<i>transE</i>	-1446.209	-1446.014	-1445.943	0.0	2.460	54.4
	<i>cisZ</i>	-1446.2	-1446.006	-1445.934	24.6	4.216	< 0.1
	<i>transZ</i>	-1446.199	-1446.005	-1445.933	25.2	5.905	< 0.1
DMSO							
1	<i>cisE</i>	-1085.850	-1085.654	-1085.583	3.2	3.955	24.0
	<i>transE</i>	-1085.851	-1085.655	-1085.584	0.0	3.539	76.0
	<i>cisZ</i>	-1085.844	-1085.647	-1085.577	19.0	5.856	< 0.1
	<i>transZ</i>	-1085.844	-1085.648	-1085.577	18.1	7.444	< 0.1
2	<i>cisE</i>	-1101.140	-1100.905	-1100.831	3.3	3.418	8.3
	<i>transE</i>	-1101.141	-1100.907	-1100.832	0.0	1.279	91.6
	<i>cisZ</i>	-1101.134	-1100.899	-1100.825	17.8	5.648	< 0.1
	<i>transZ</i>	-1101.135	-1100.899	-1100.825	17.3	8.137	< 0.1
3	<i>cisE</i>	-1446.201	-1446.007	-1445.935	3.2	3.969	19.0
	<i>transE</i>	-1446.202	-1446.008	-1445.937	0.0	3.552	80.9
	<i>cisZ</i>	-1446.195	-1446.001	-1445.929	18.8	5.816	< 0.1
	<i>transZ</i>	-1446.195	-1446.001	-1445.930	18.3	7.341	< 0.1
4	<i>cisE</i>	-1446.205	-1446.012	-1445.940	3.4	3.342	26.4
	<i>transE</i>	-1446.207	-1446.013	-1445.941	0.0	4.272	73.5
	<i>cisZ</i>	-1446.199	-1446.005	-1445.934	19.3	4.300	< 0.1
	<i>transZ</i>	-1446.200	-1446.005	-1445.934	19.0	5.471	< 0.1
5	<i>cisE</i>	-3560.126	-3559.934	-3559.860	3.1	1.474	29.1
	<i>transE</i>	-3560.127	-3559.935	-3559.862	0.0	3.534	70.9
	<i>cisZ</i>	-3560.120	-3559.926	-3559.855	17.2	2.275	< 0.1
	<i>transZ</i>	-3560.120	-3559.928	-3559.854	19.3	4.052	< 0.1
6	<i>cisE</i>	-1101.146	-1100.912	-1100.837	3.2	6.245	21.8
	<i>transE</i>	-1101.148	-1100.913	-1100.838	0.0	4.990	78.2
	<i>cisZ</i>	-1101.138	-1100.904	-1100.829	24.4	8.390	< 0.1
	<i>transZ</i>	-1101.139	-1100.903	-1100.829	24.0	10.129	< 0.1
7	<i>cisE</i>	-1025.915	-1025.685	-1025.612	3.2	4.856	19.0
	<i>transE</i>	-1025.916	-1025.686	-1025.613	0.0	3.188	81.0
	<i>cisZ</i>	-1025.907	-1025.678	-1025.603	24.7	7.302	< 0.1
	<i>transZ</i>	-1025.907	-1025.676	-1025.604	24.4	9.134	< 0.1
8	<i>cisE</i>	-1446.209	-1446.015	-1445.943	3.0	2.139	35.5
	<i>transE</i>	-1446.210	-1446.016	-1445.944	0.0	2.536	64.5
	<i>cisZ</i>	-1446.200	-1446.007	-1445.935	25.2	4.255	< 0.1
	<i>transZ</i>	-1446.201	-1446.006	-1445.935	24.8	5.994	< 0.1

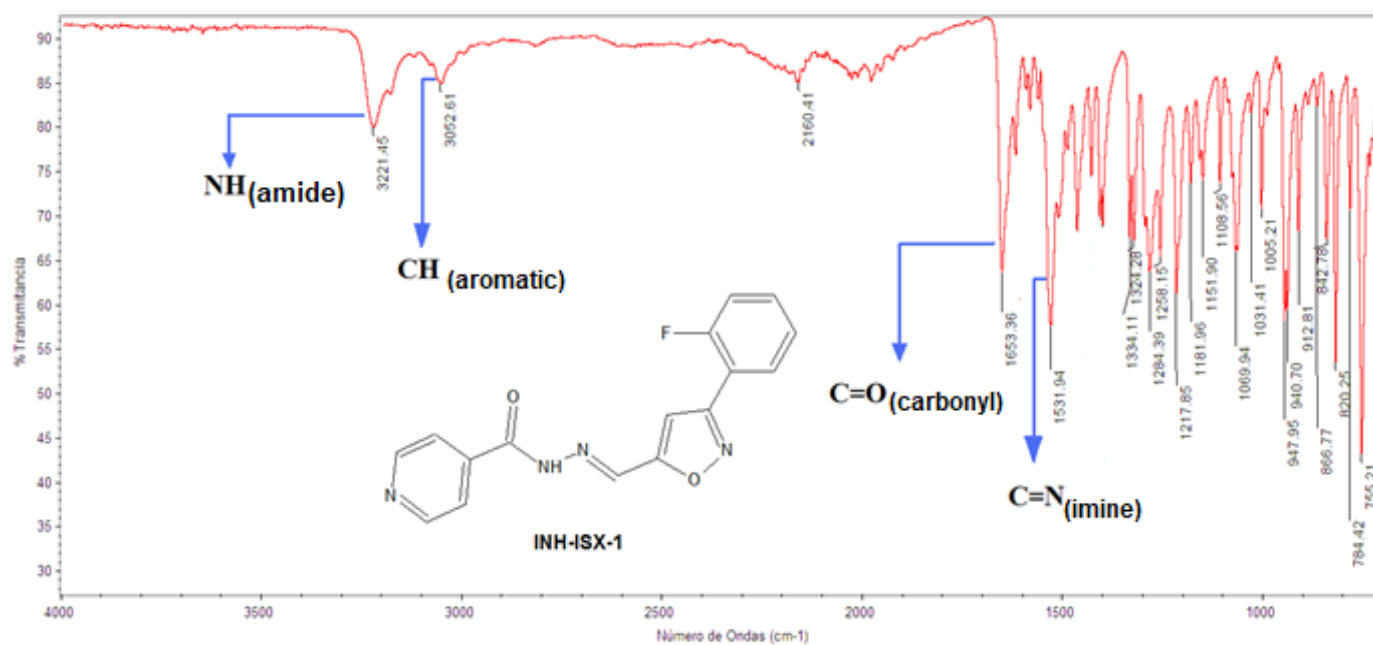
^aAll values in units of Hartree/particle. ^b Values in kJ·mol⁻¹. E_0 = Total Energies at 0 K. H_{298} = Enthalpies and G_{298} = Gibbs Free Energies at 298.15 K. ^c Value in Debye. μ = Dipole Moment.



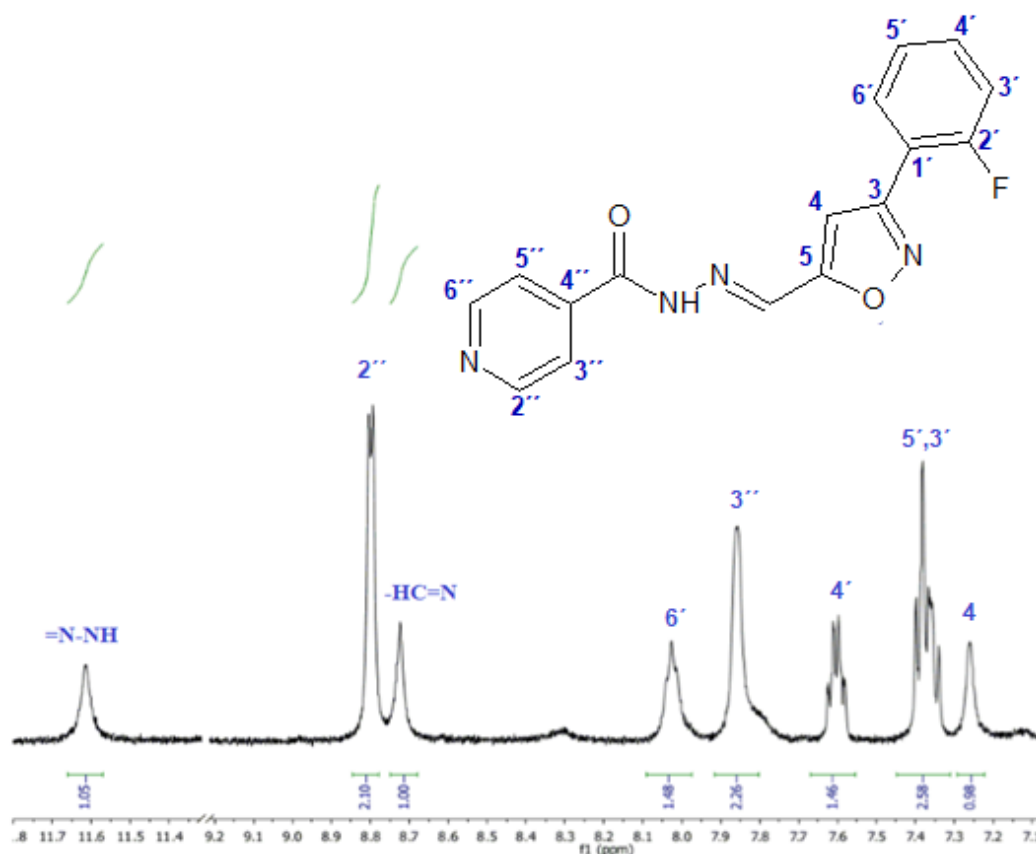
Supplementary figure 1. Linear Correlation of vibrational frequencies (given as wave numbers σ , in cm^{-1}) between experimental IR data and the corresponding to B3LYP/6-311++G(d,p) theoretical values for **1** to **8** synthesized compounds



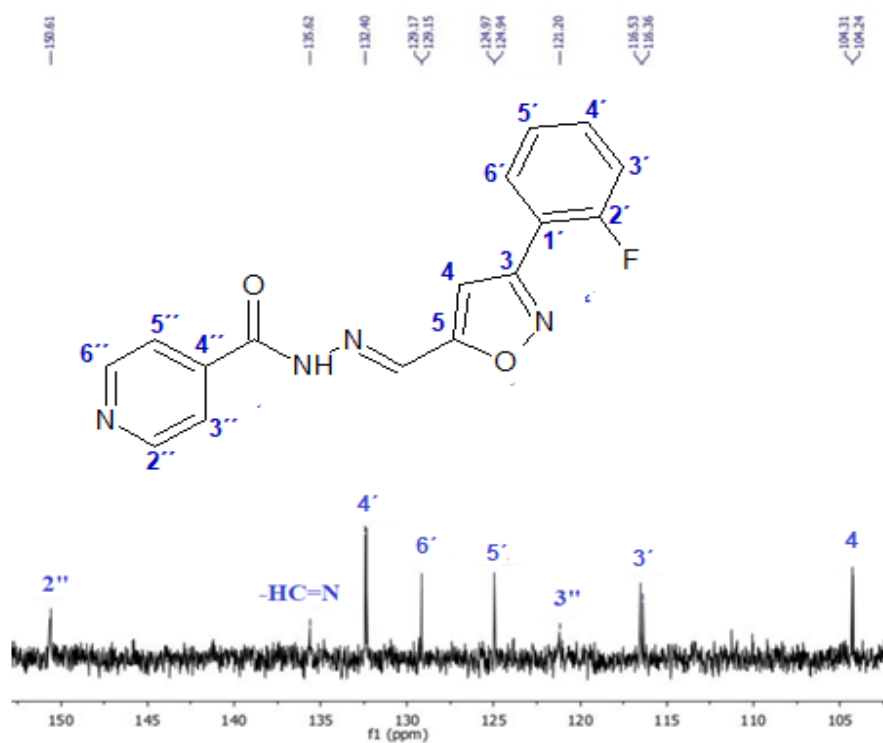
Supplementary figure 2. ESI-mas spectrum of compound 1



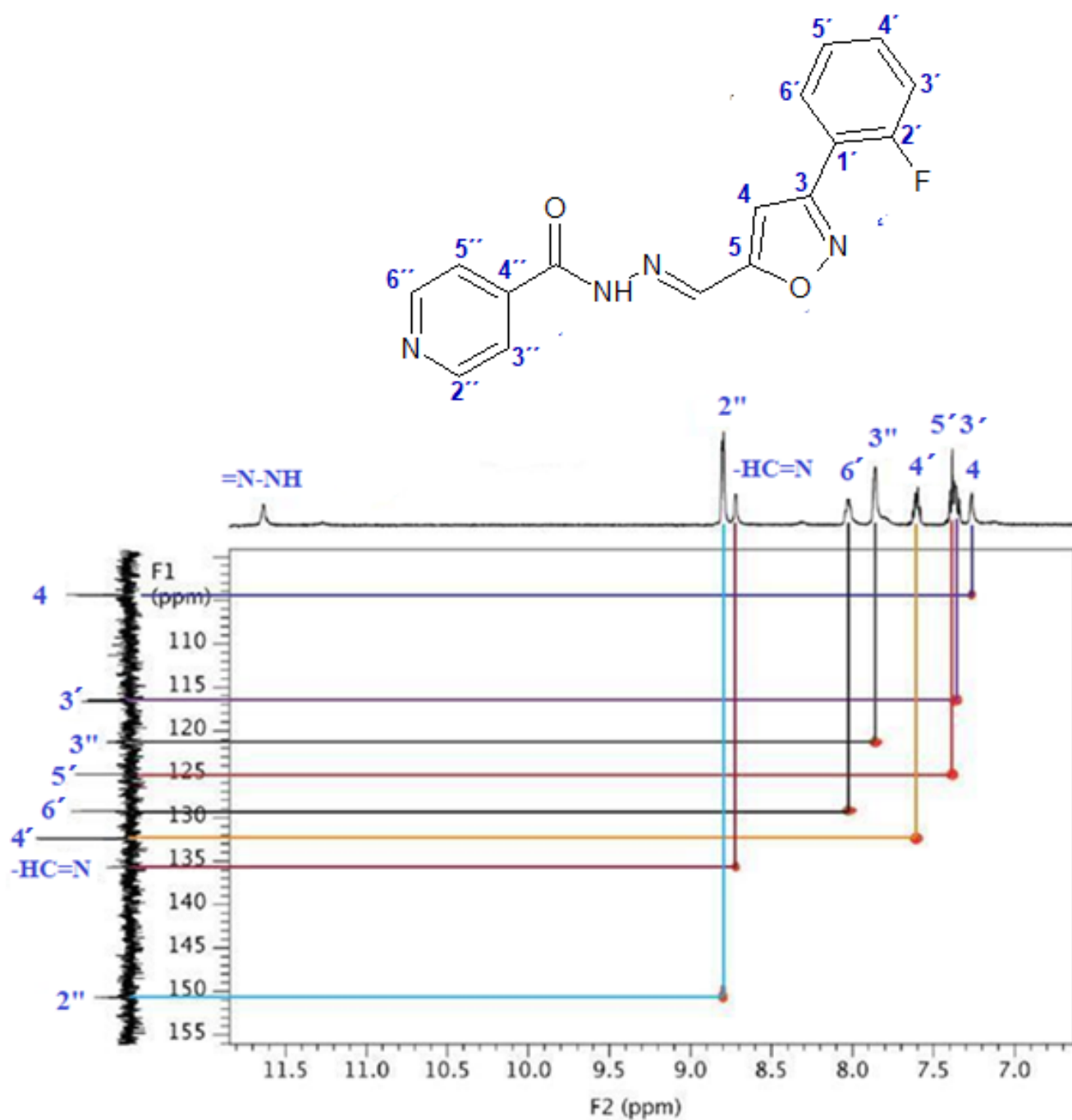
Supplementary figure 3. FT-IR spectrum of compound 1



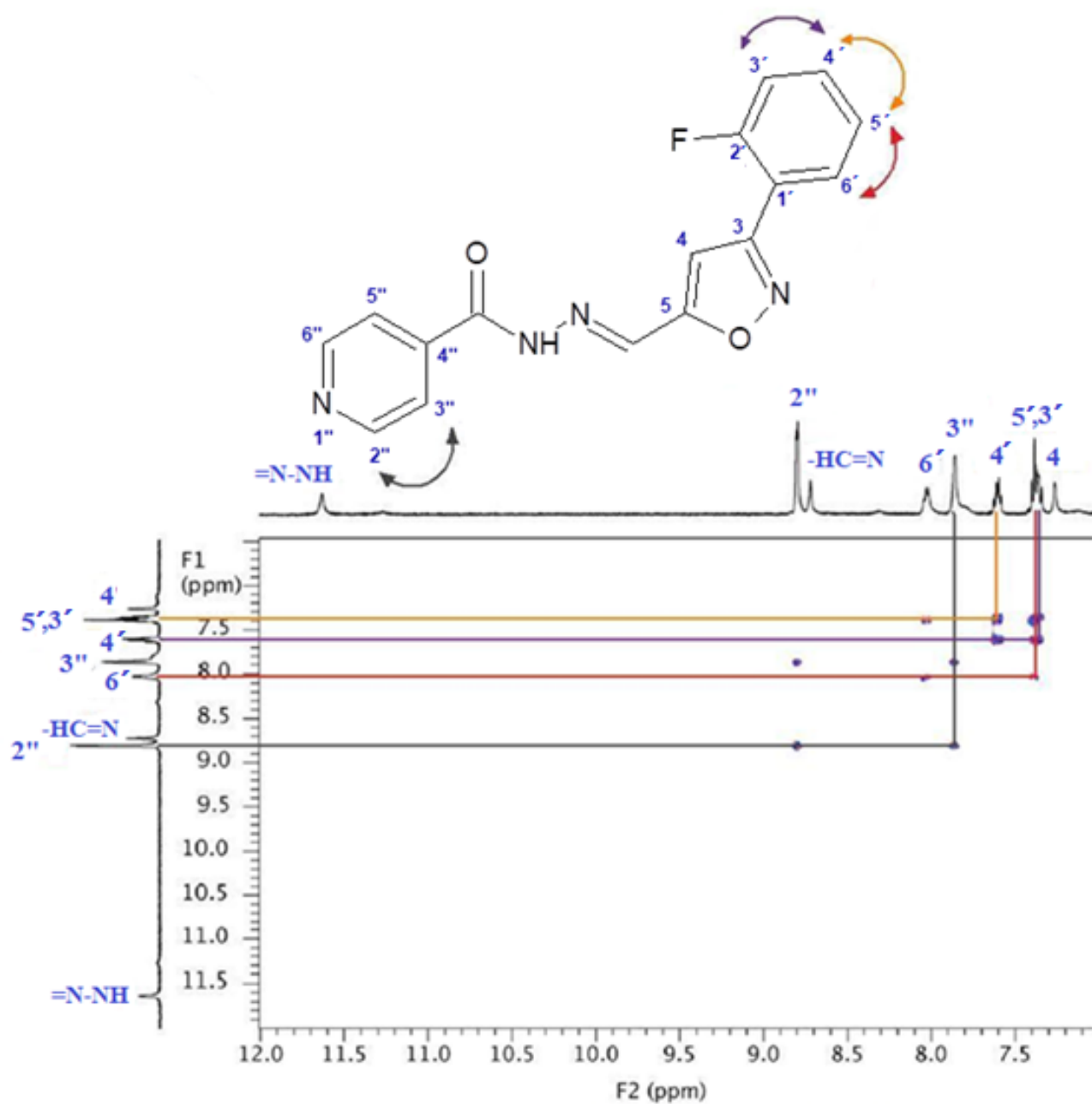
Supplementary figure 4. ^1H NMR spectrum of compound **1** (500 MHz, acetone- d_6)



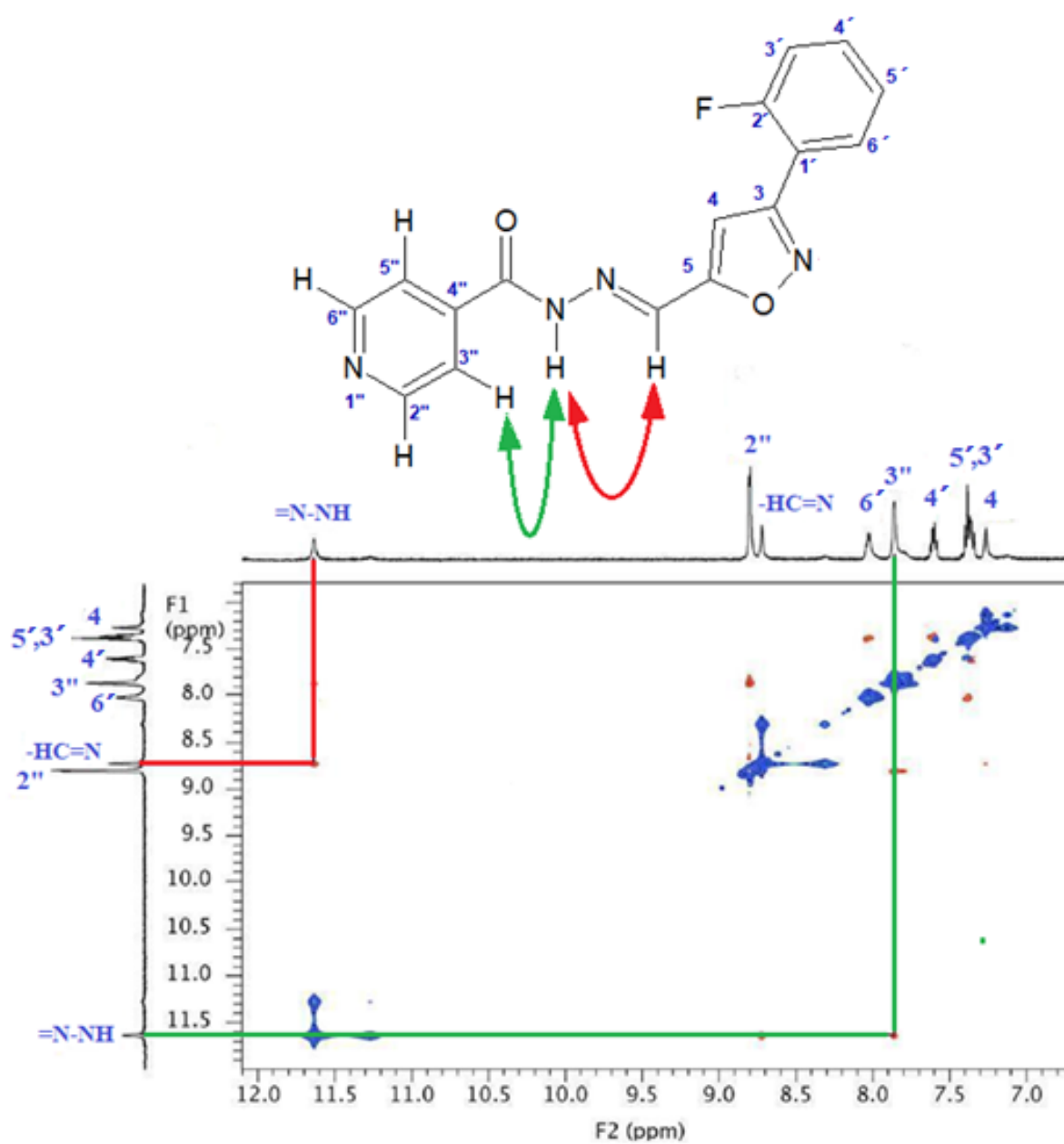
Supplementary figure 5. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of compound **1** (126 MHz, acetone- d_6)



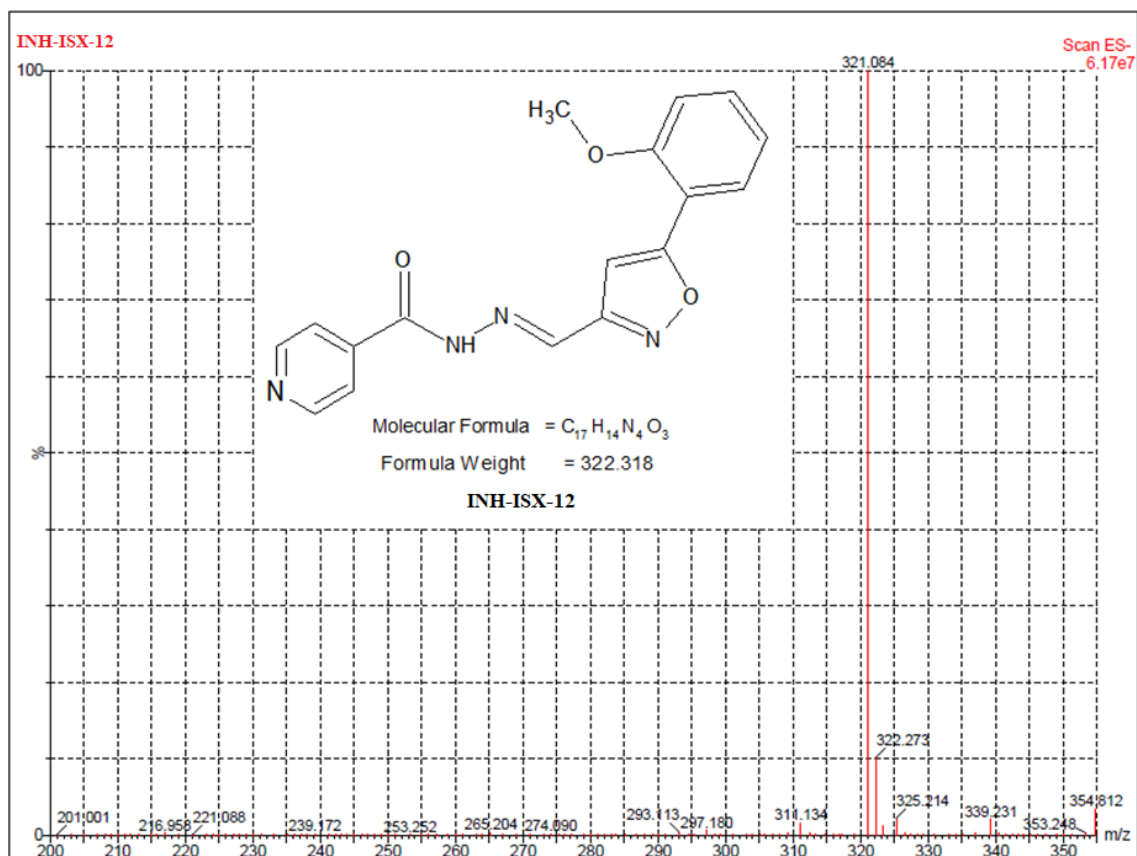
Supplementary figure 6. Two-dimensional ^1H - ^{13}C HSQC NMR spectrum, recorded in acetone- d_6 for **1**



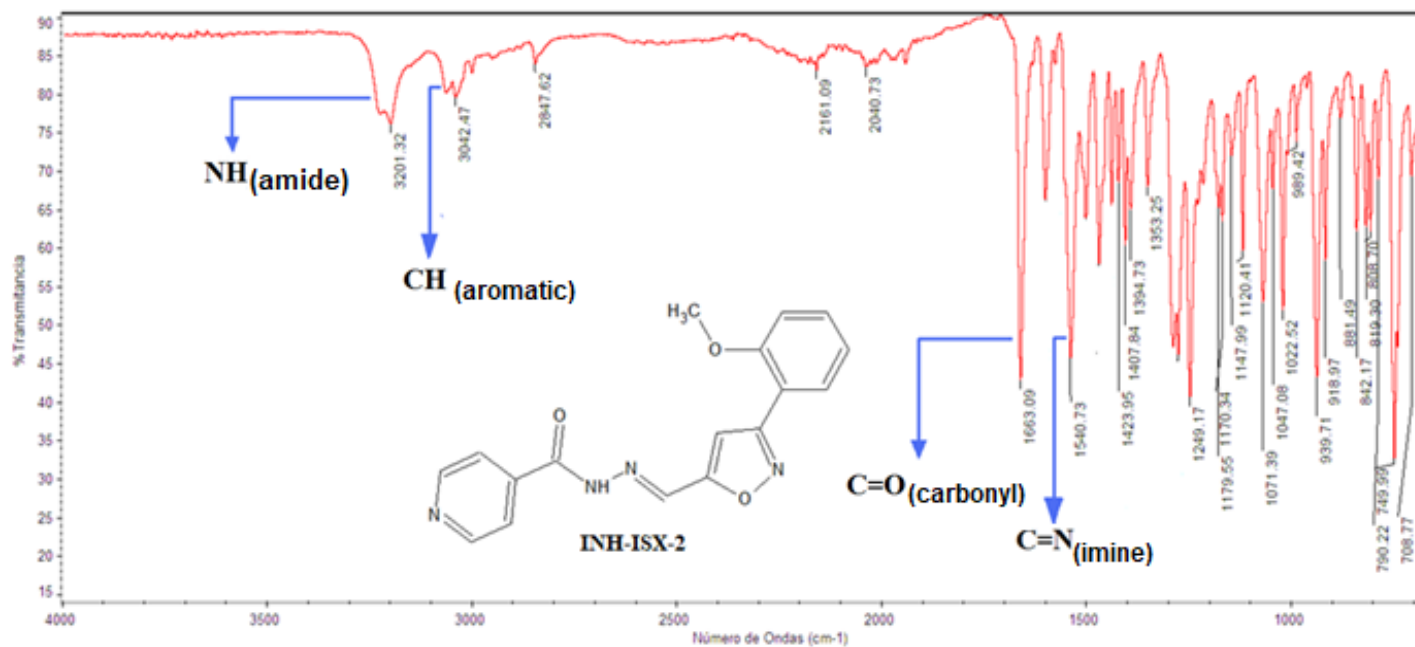
Supplementary figure 7. Two-dimensional ^1H - ^1H DQFCOSY NMR spectrum, recorded in acetone- d_6 for **1**



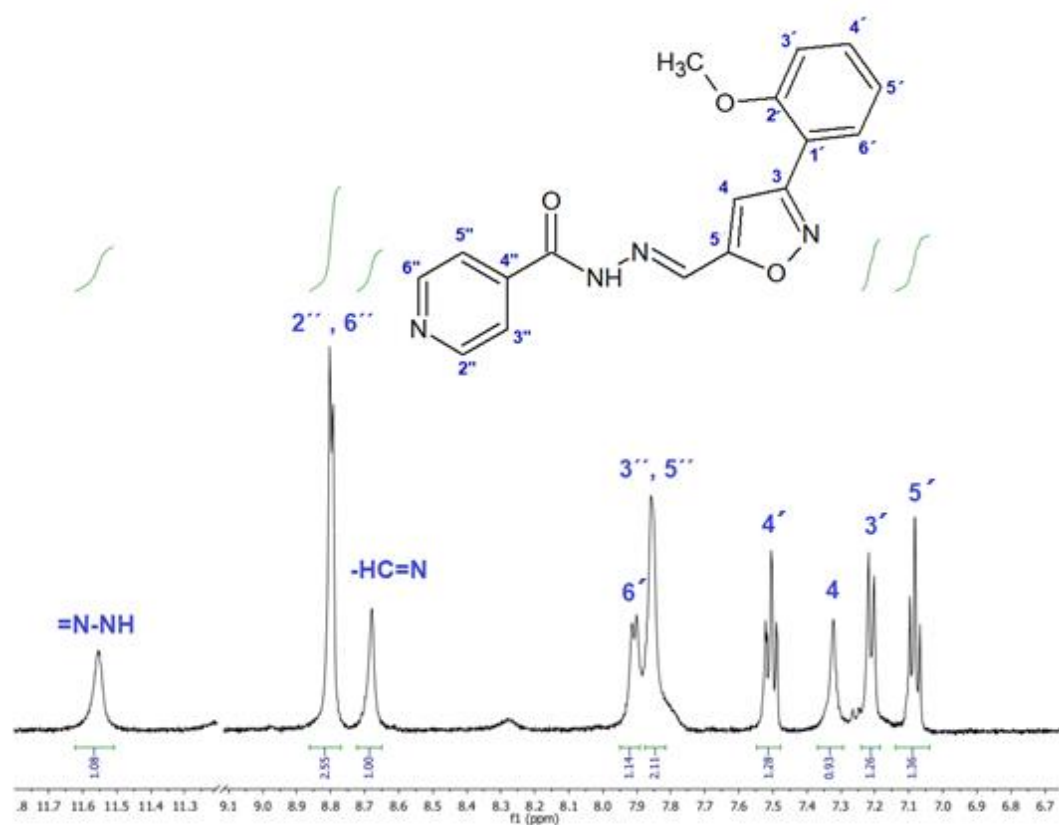
Supplementary figure 8. Two-dimensional ^1H - ^1H NOESY NMR spectrum, recorded in acetone- d_6 for **1**



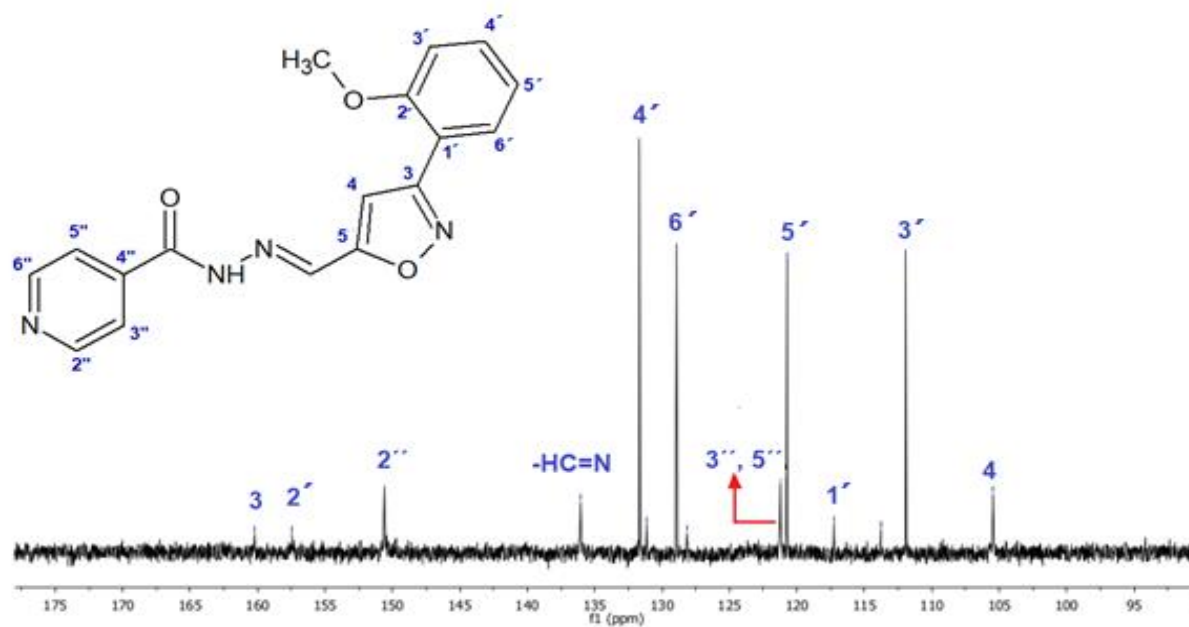
Supplementary figure 9. ESI-mass spectrum of compound 2



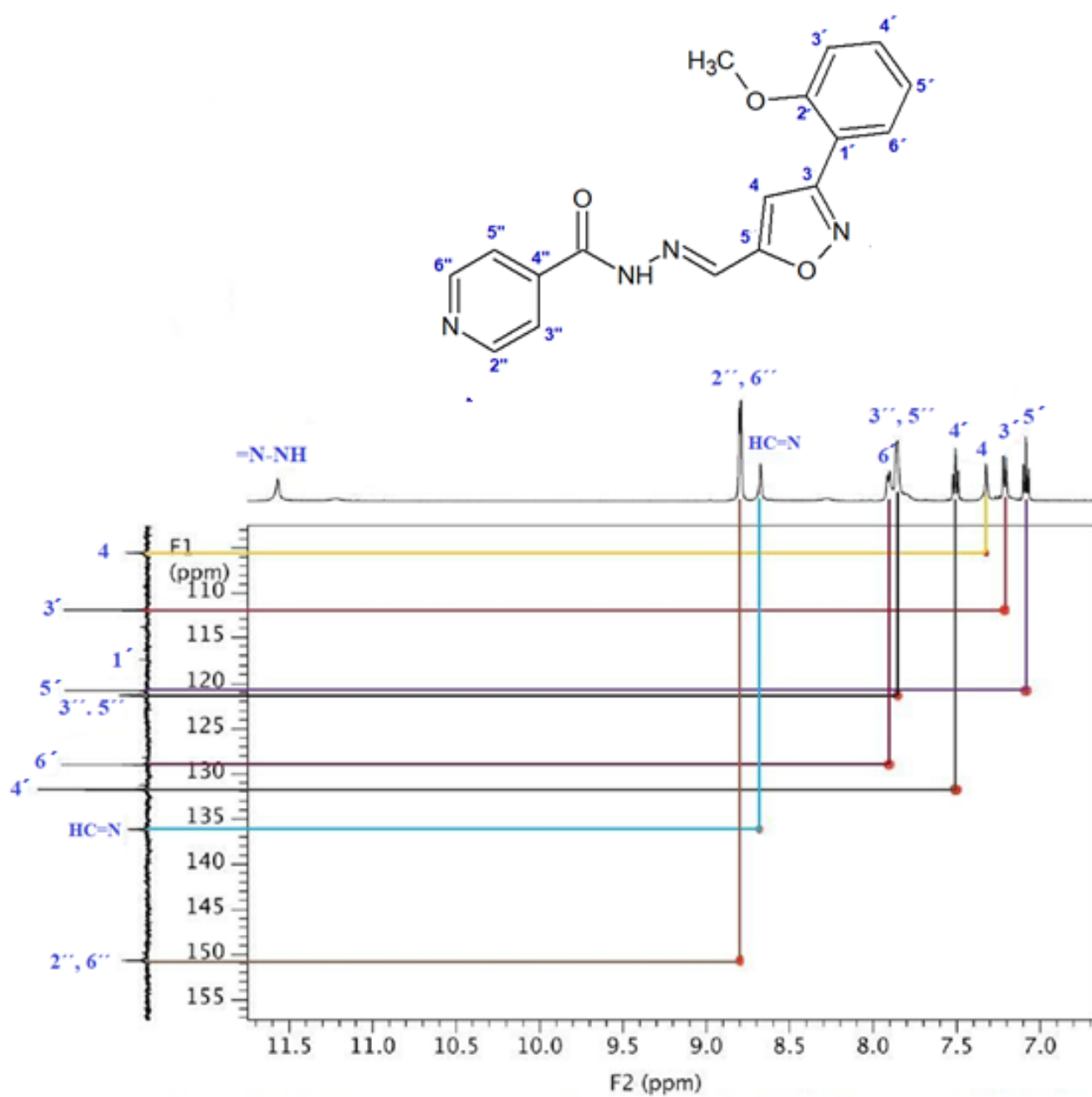
Supplementary figure 10. FT-IR spectrum of compound 2



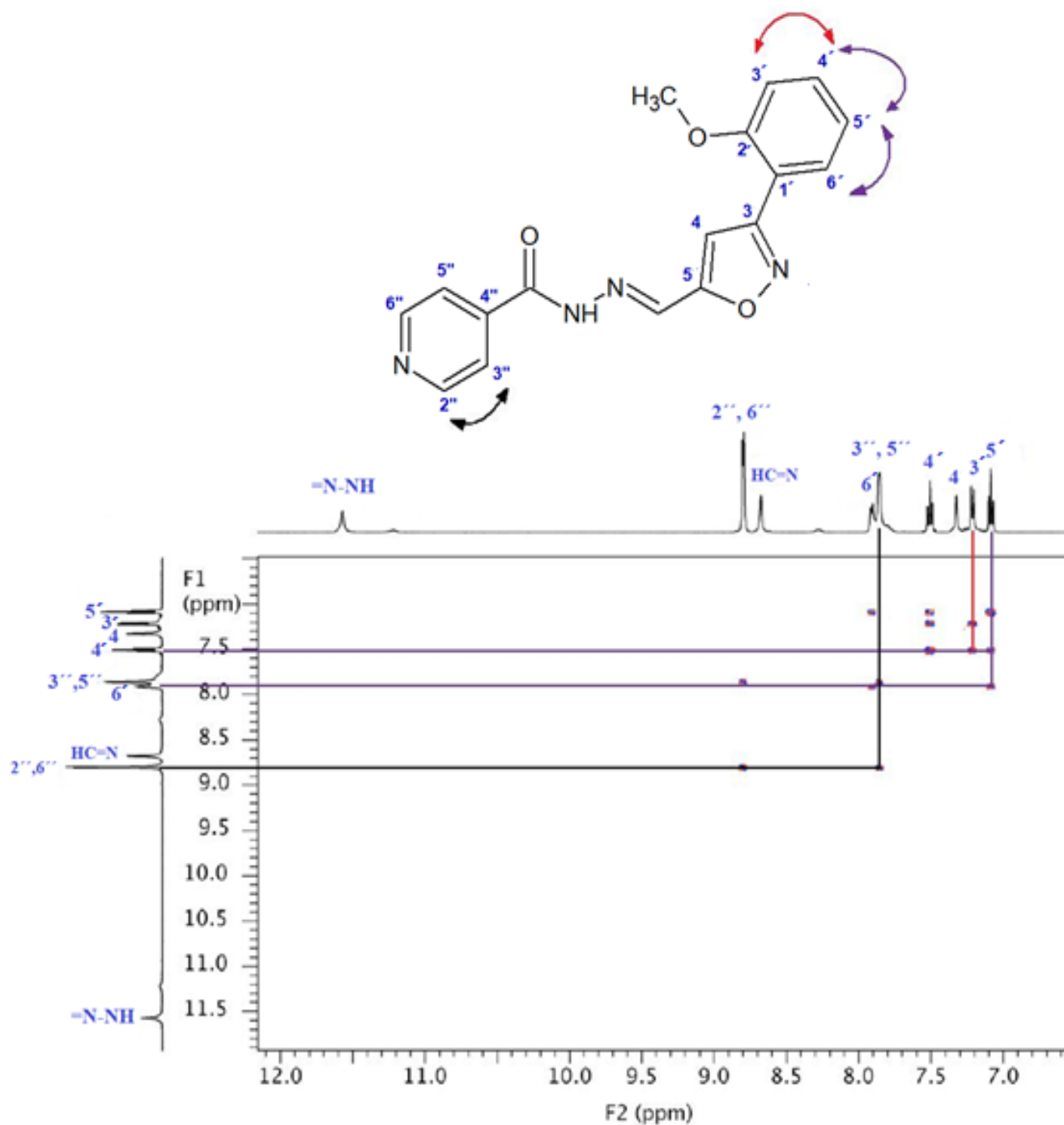
Supplementary figure 11. ^1H NMR spectrum of compound **2** (500 MHz, acetone- d_6)



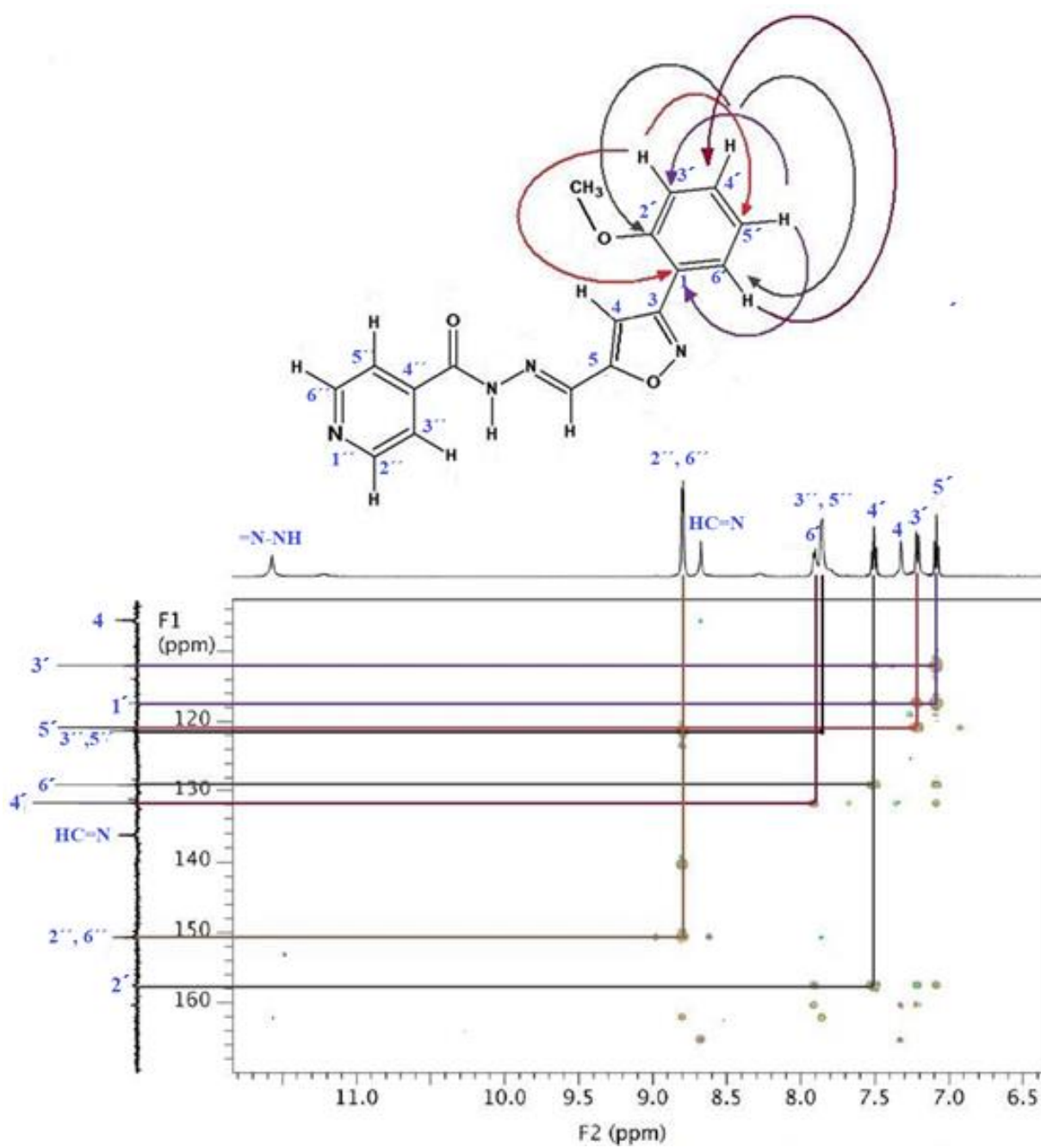
Supplementary figure 12. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of compound **2** (126 MHz, acetone- d_6)



Supplementary figure 13. Two-dimensional ^1H - ^{13}C HSQC NMR spectrum, recorded in acetone- d_6 for **2**

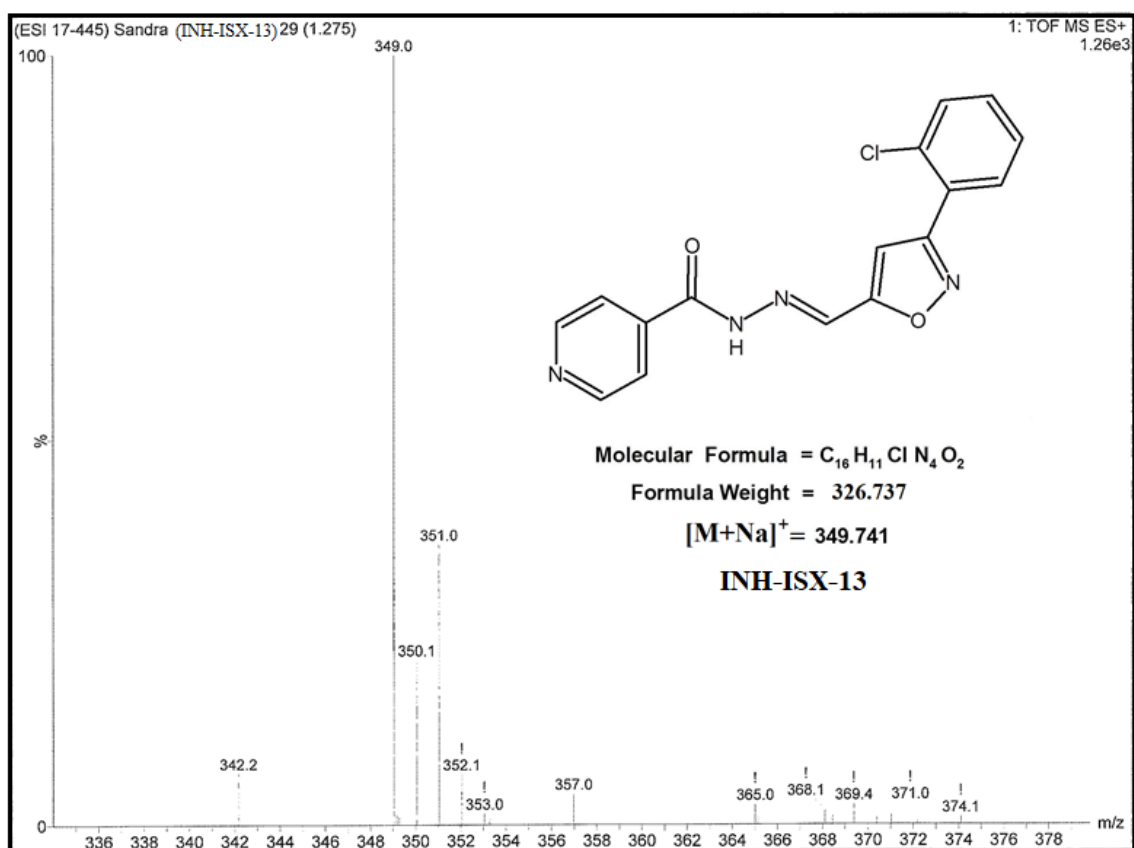


Supplementary figure 14. Two-dimensional ¹H-¹H DQFCOSY NMR spectrum, recorded in acetone-*d*₆ for **2**

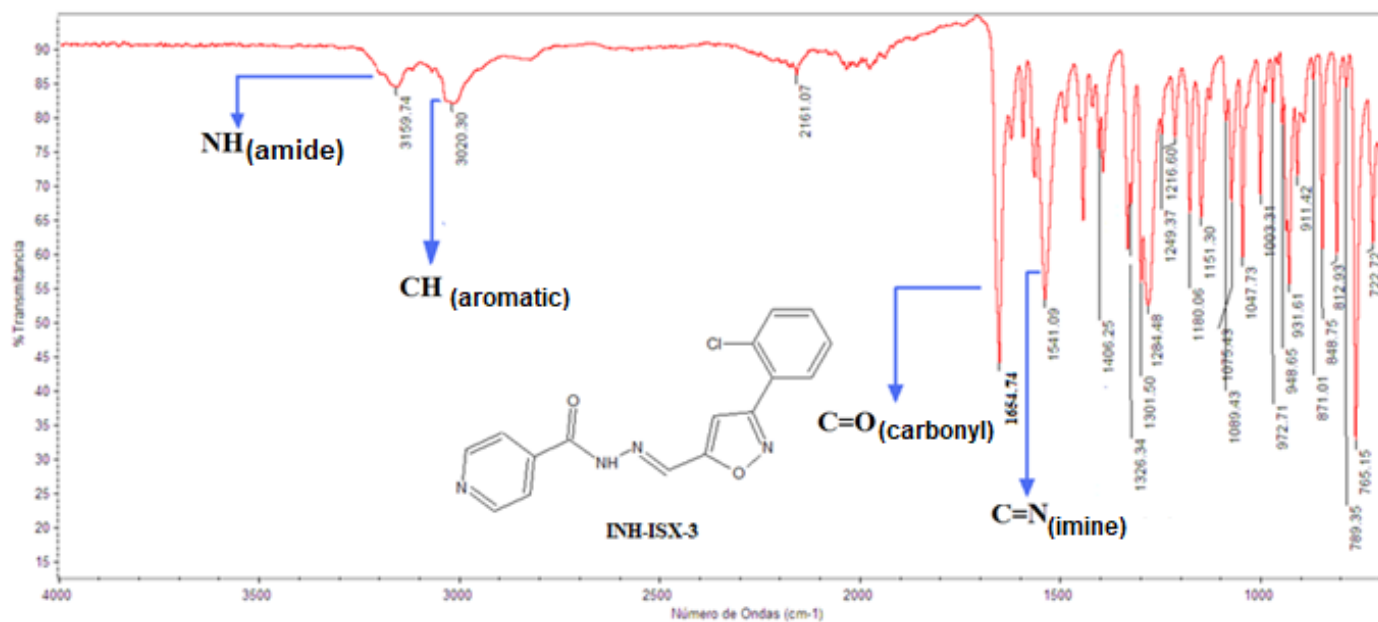


Supplementary figure 15. Two-dimensional ^1H - ^{13}C HMBC NMR spectrum recorded, in acetone- d_6

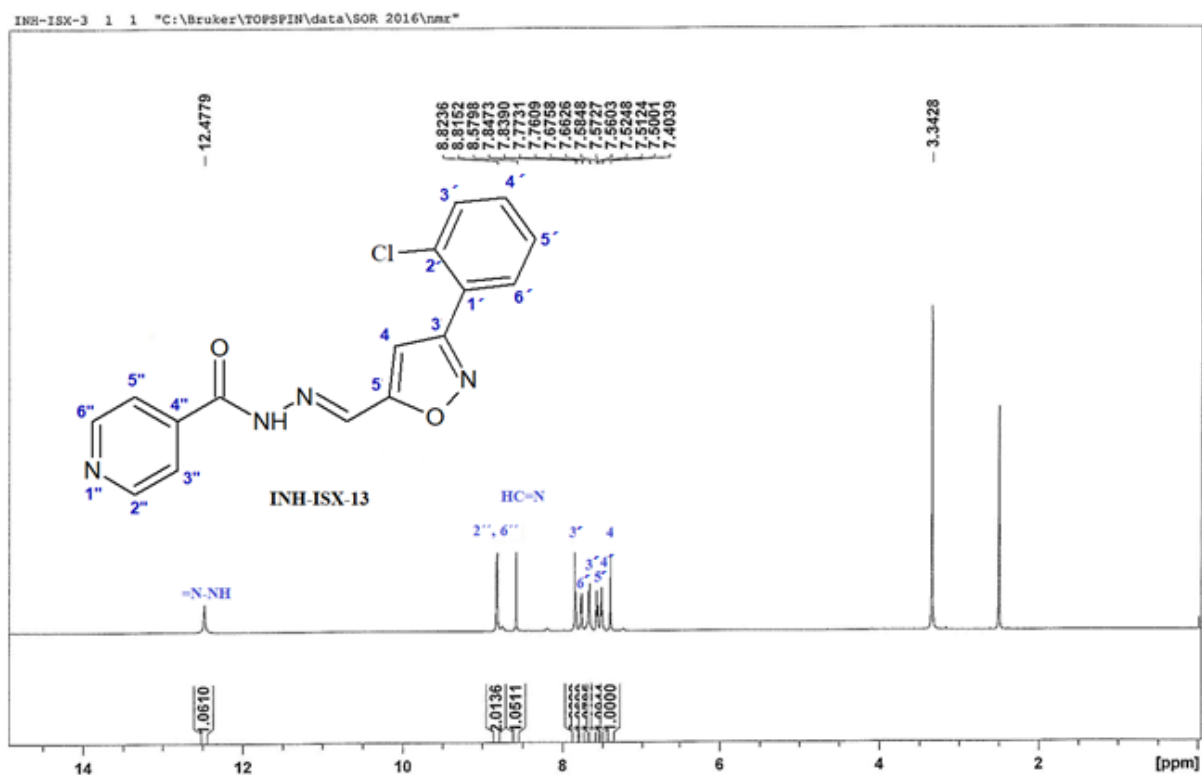
for **2**



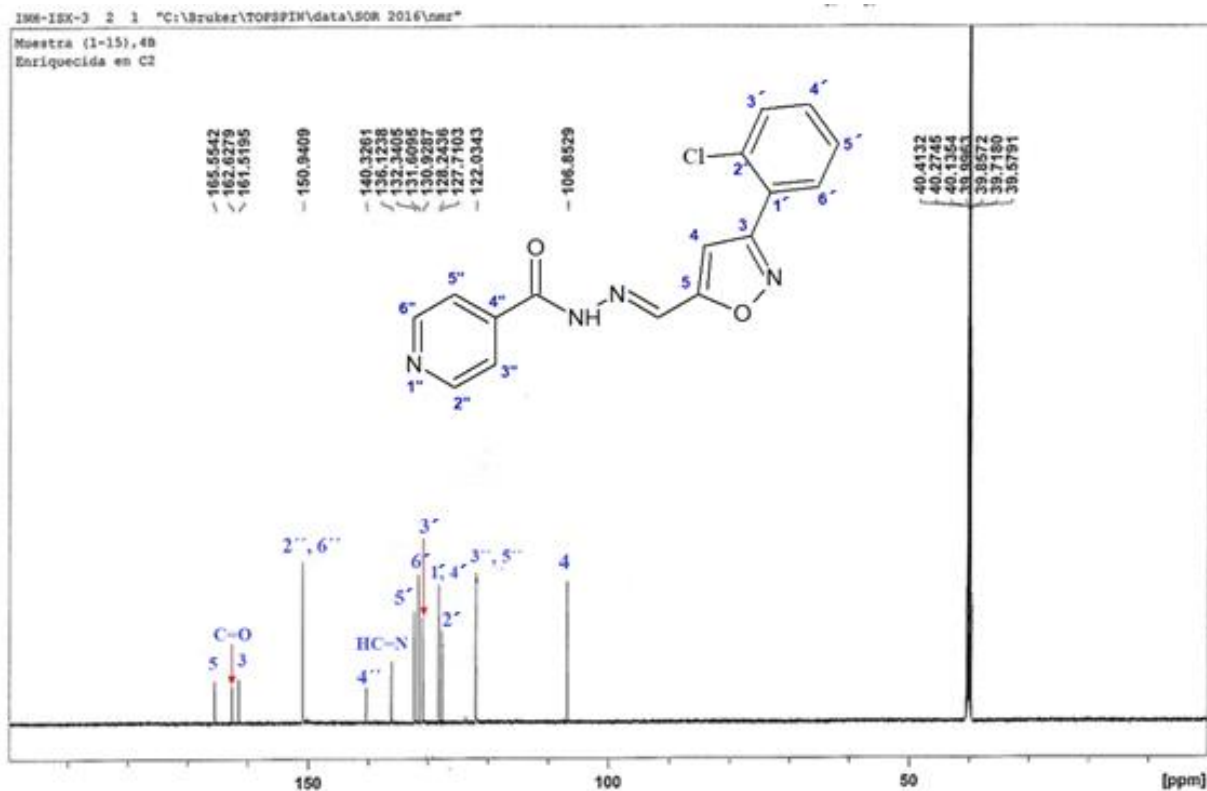
Supplementary figure 16. ESI-mass spectrum of compound **3**



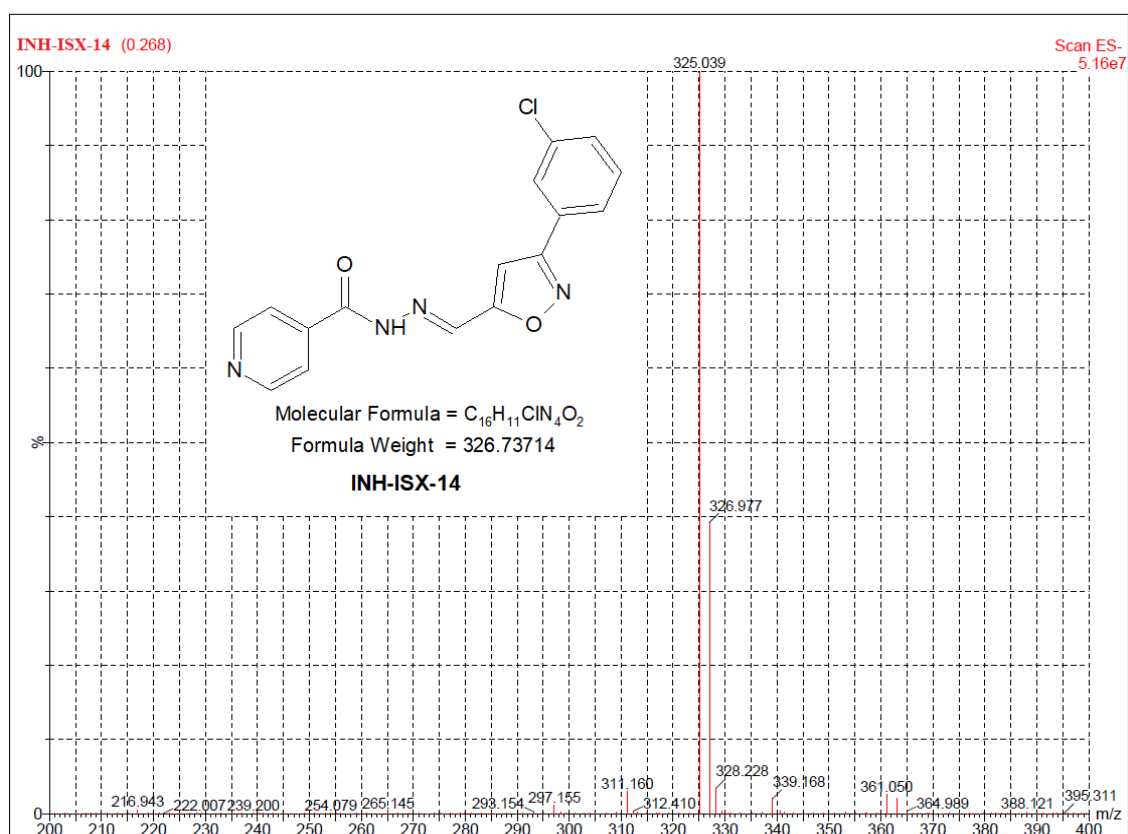
Supplementary figure 17. FT-IR spectrum of compound **3**



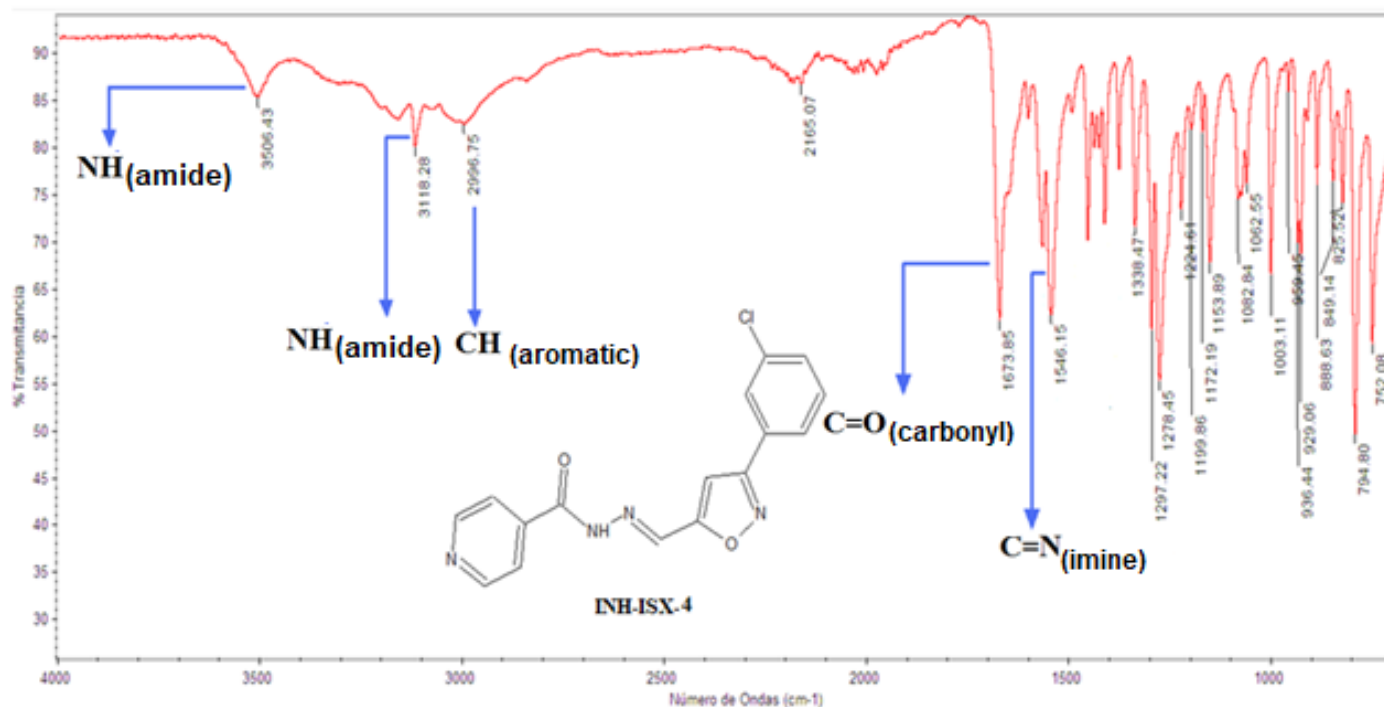
Supplementary figure 18. ^1H NMR spectrum of compound **3** (600 MHz, $\text{DMSO}-d_6$)



Supplementary figure 19. ^{13}C NMR spectrum of compound **3** (150 MHz, $\text{DMSO}-d_6$)

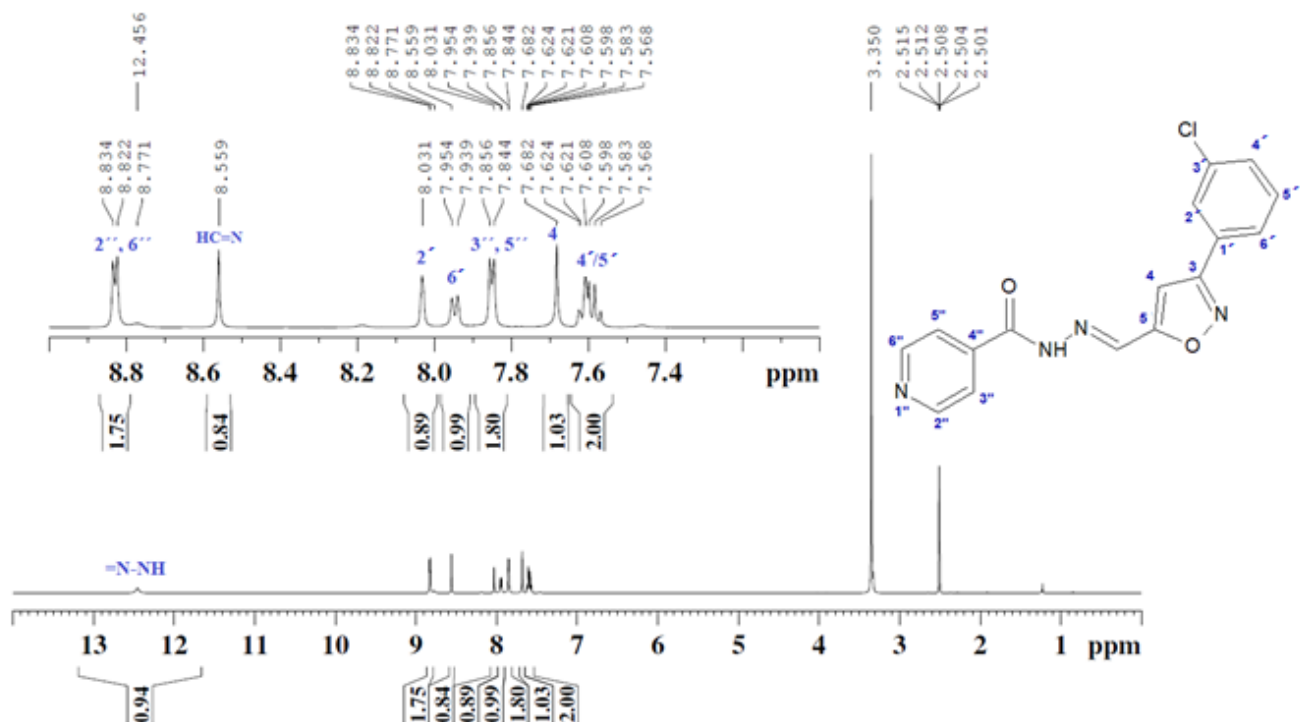


Supplementary figure 20. ESI-mass spectrum of compound **4**

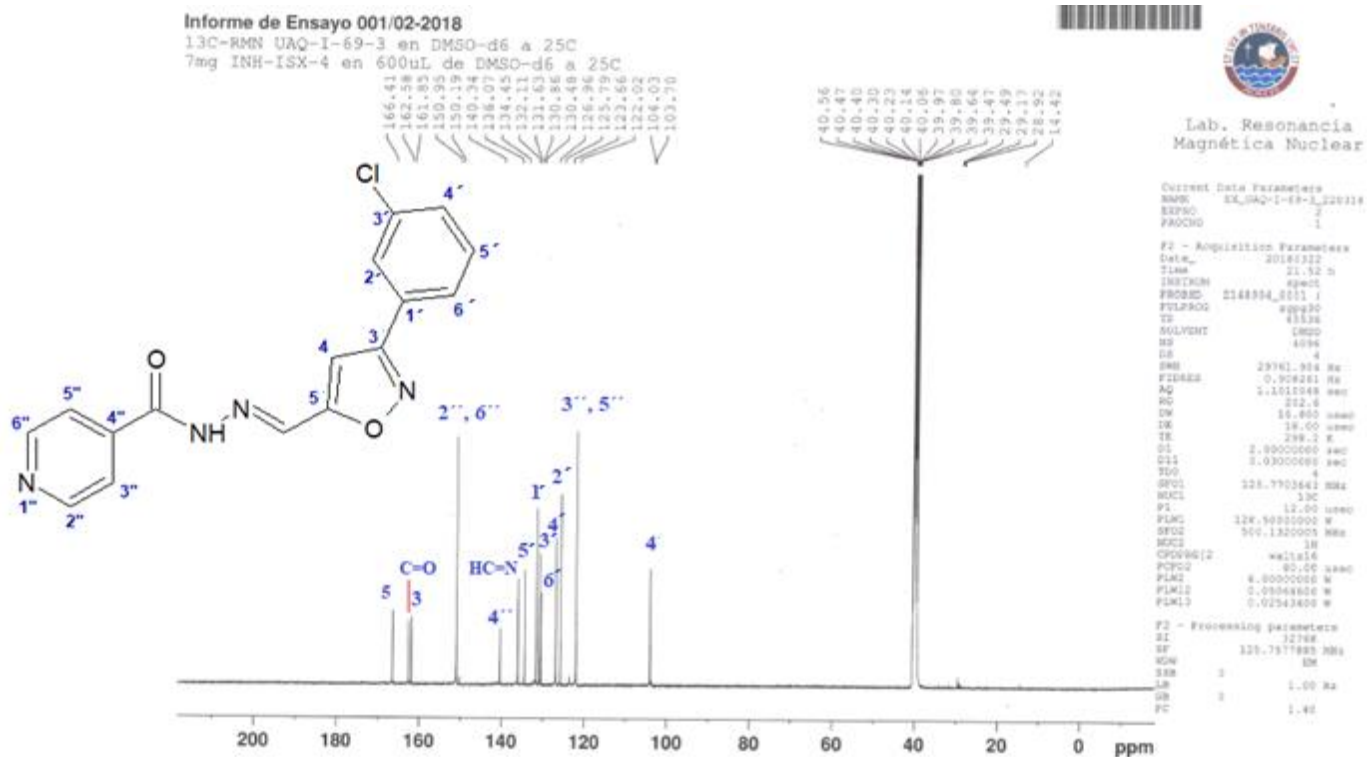


Supplementary figure 21. FT-IR spectrum of compound **4**

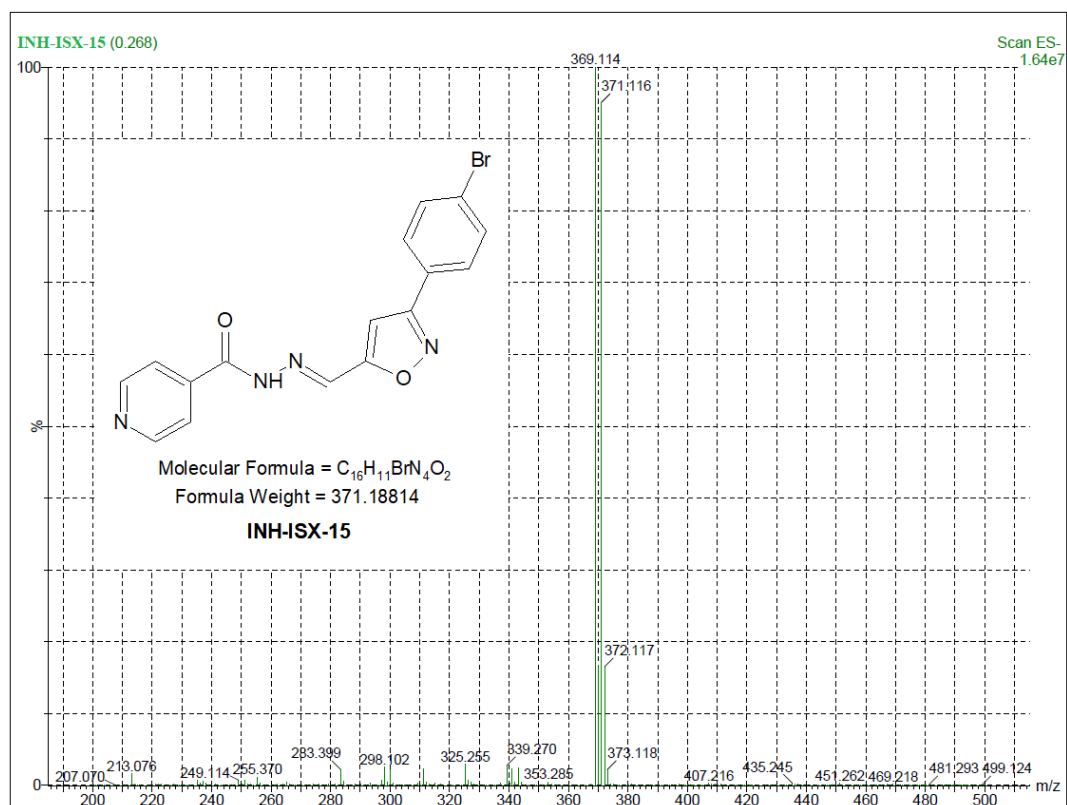
¹H UAQ-I-69-3 en DMSO-d₆ a 25C
7mg de INH-ISX-14 en 600ul de DMSO-d₆



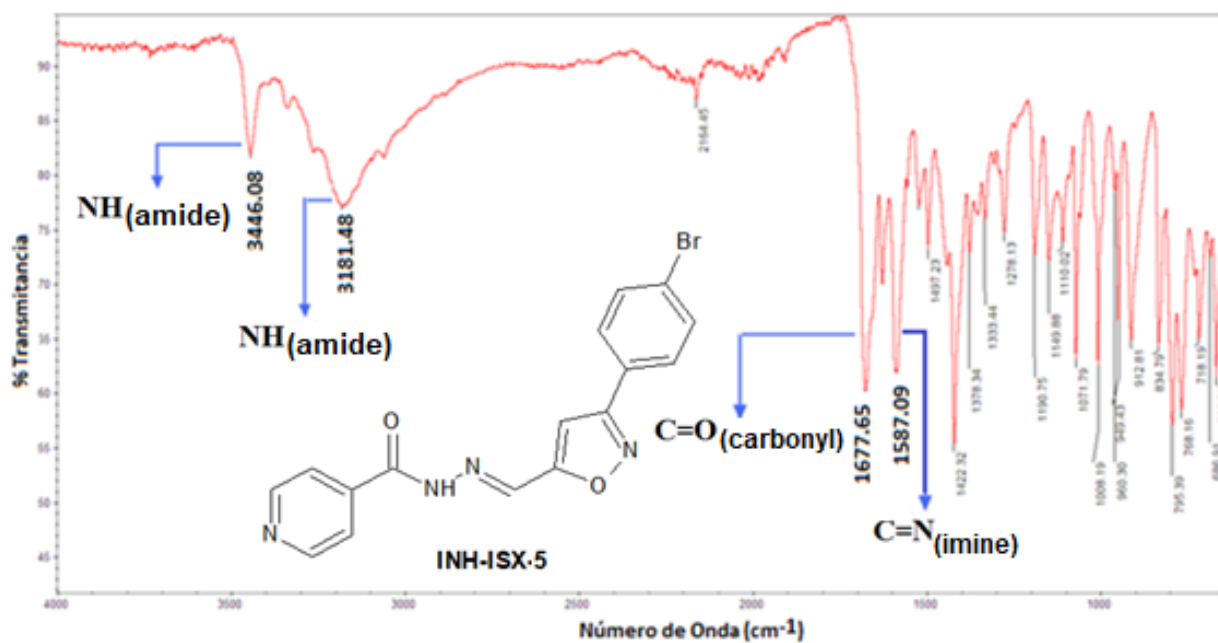
Supplementary figure 22. ¹H NMR spectrum of compound **4** (500 MHz, DMSO-*d*₆)



Supplementary figure 23. ¹³C NMR spectrum of compound **4** (1250 MHz, DMSO-*d*₆)

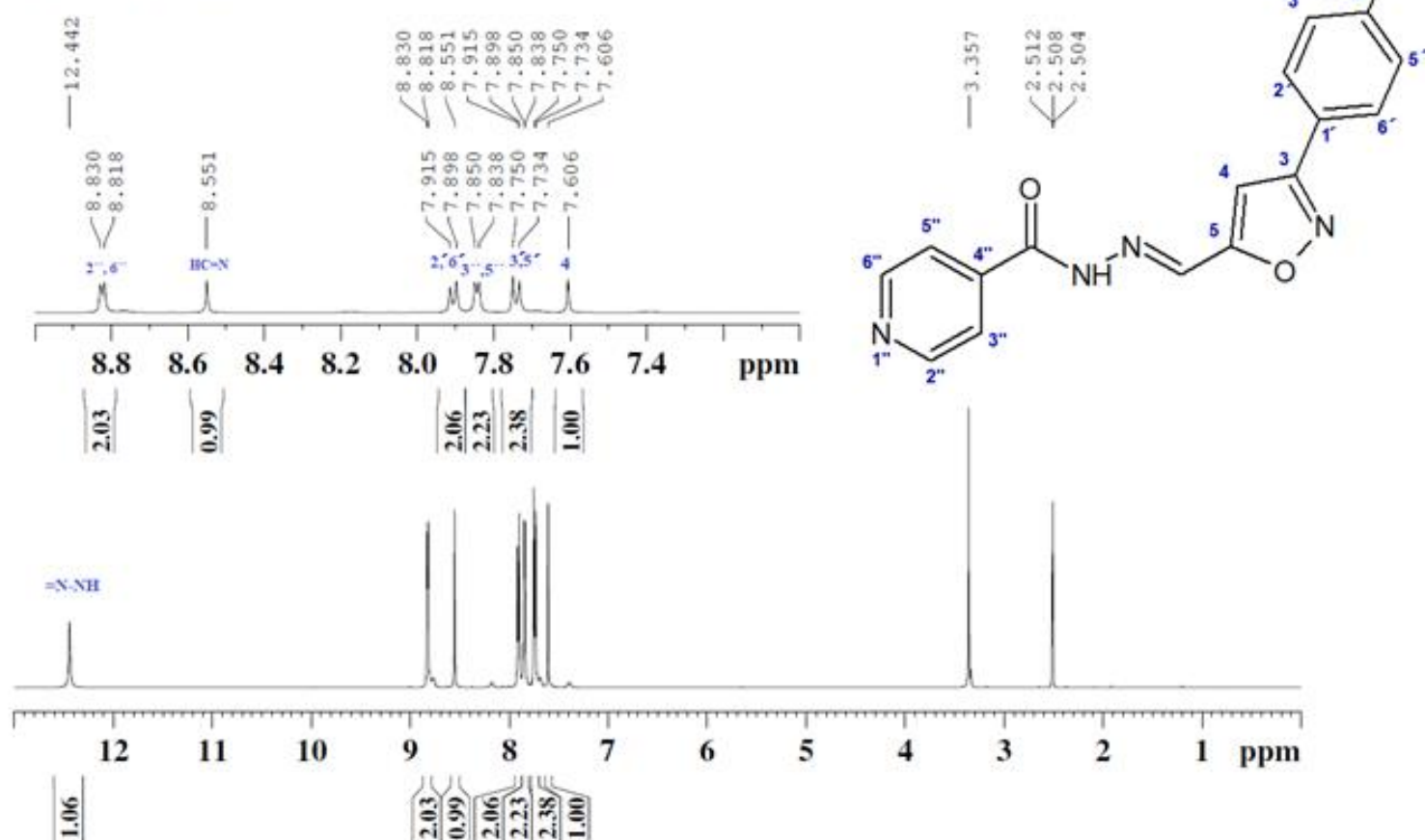


Supplementary figure 24. ESI-mass spectrum of compound **5**

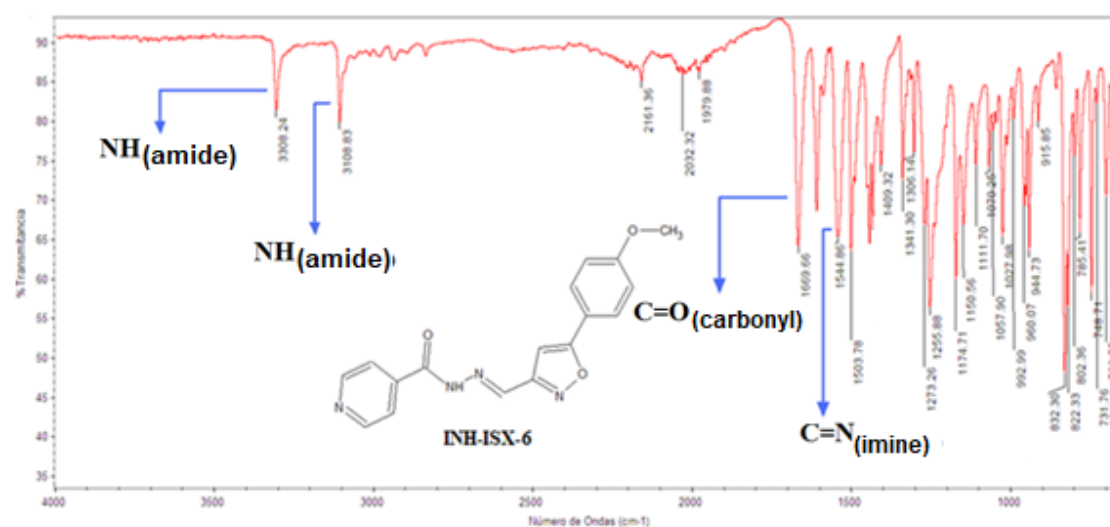


Supplementary figure 25. FT-IR spectrum of compound **5**

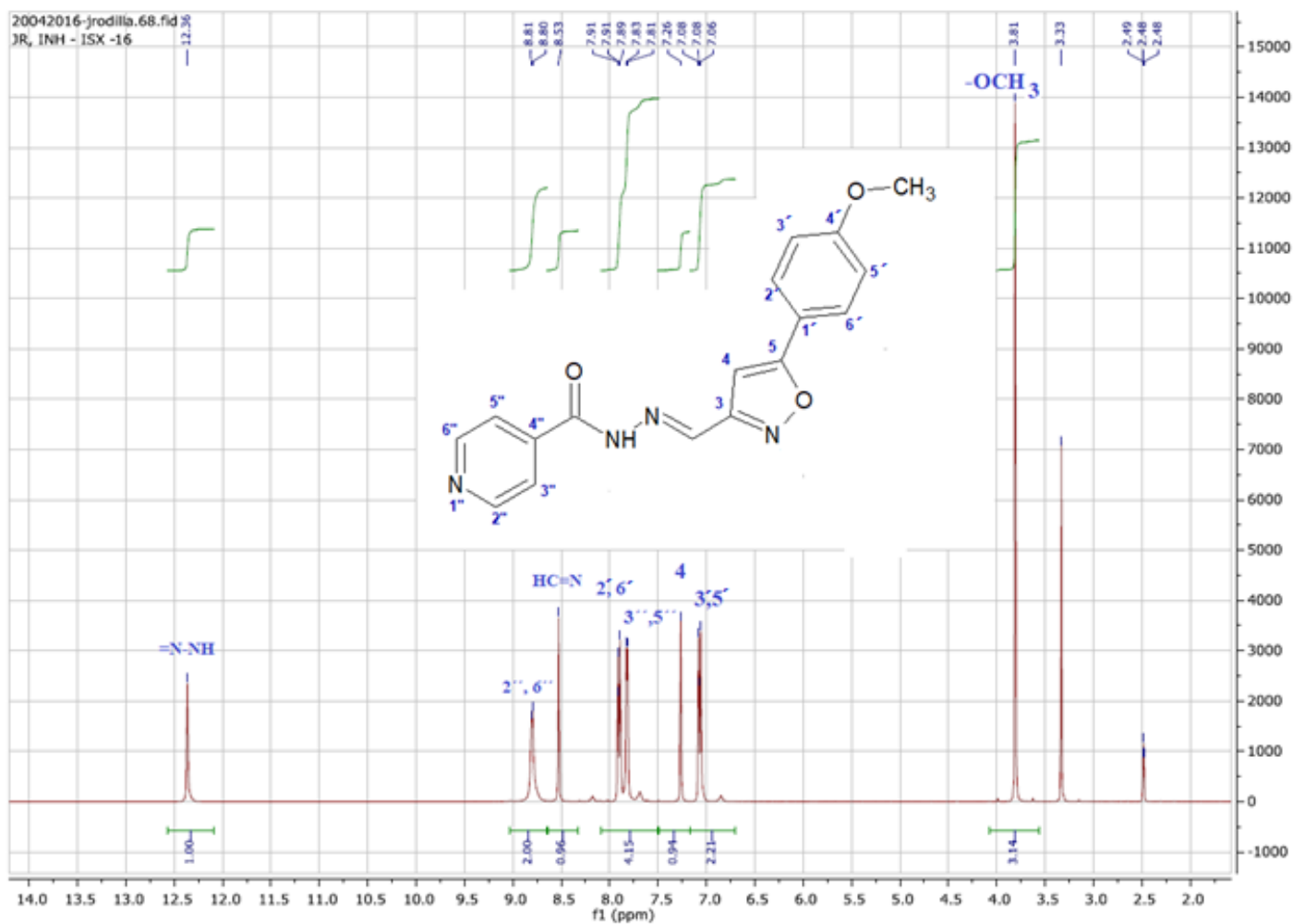
¹H UAQ-I-69-4 en DMSO-d₆ a 25C
7mg de INH-ISX-15 en 600ul de DMSO-d₆



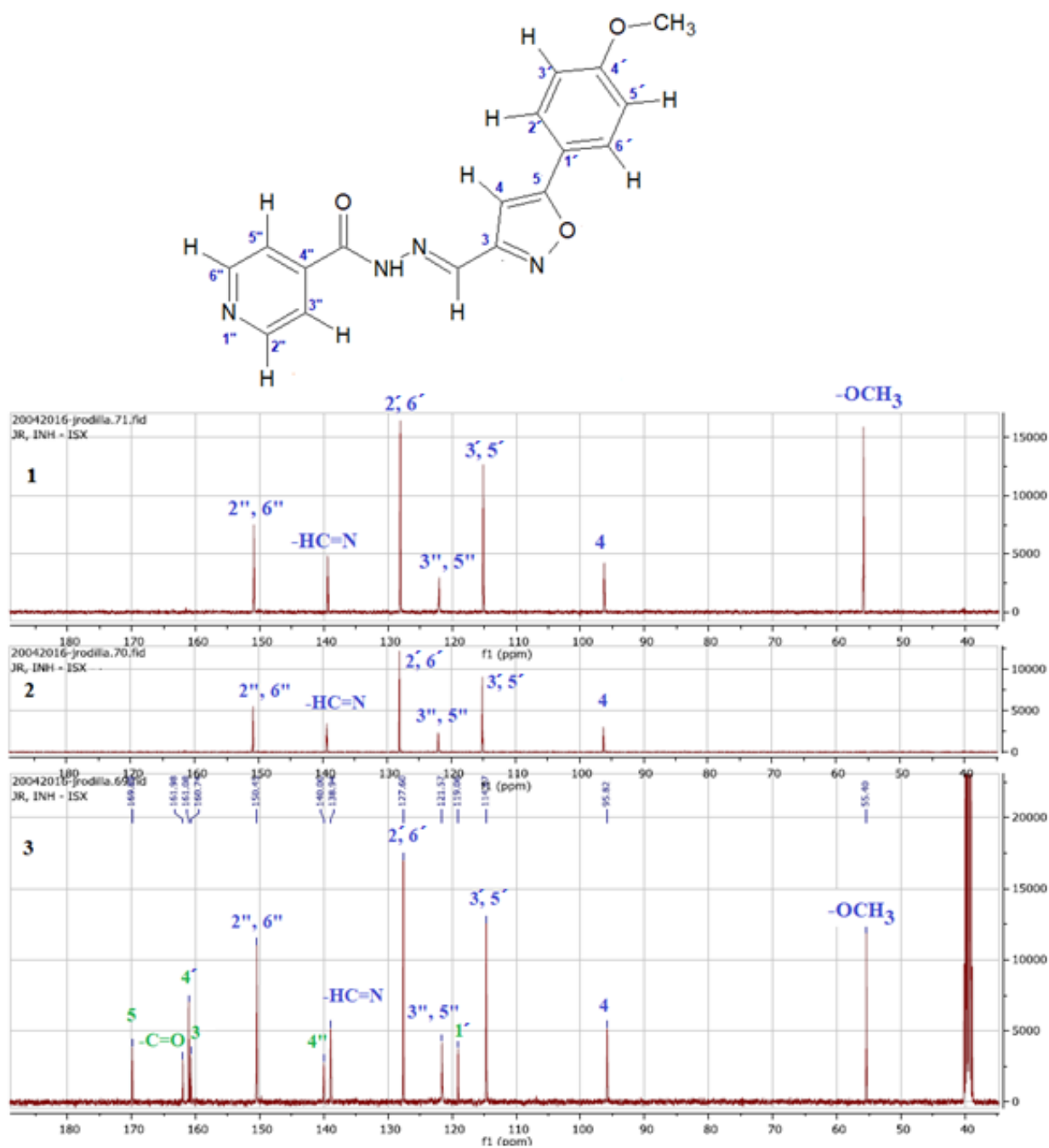
Supplementary figure 26. ¹H NMR spectrum of compound 5 (500 MHz, DMSO-*d*₆)



Supplementary figure 27. FT-IR spectrum of compound 6

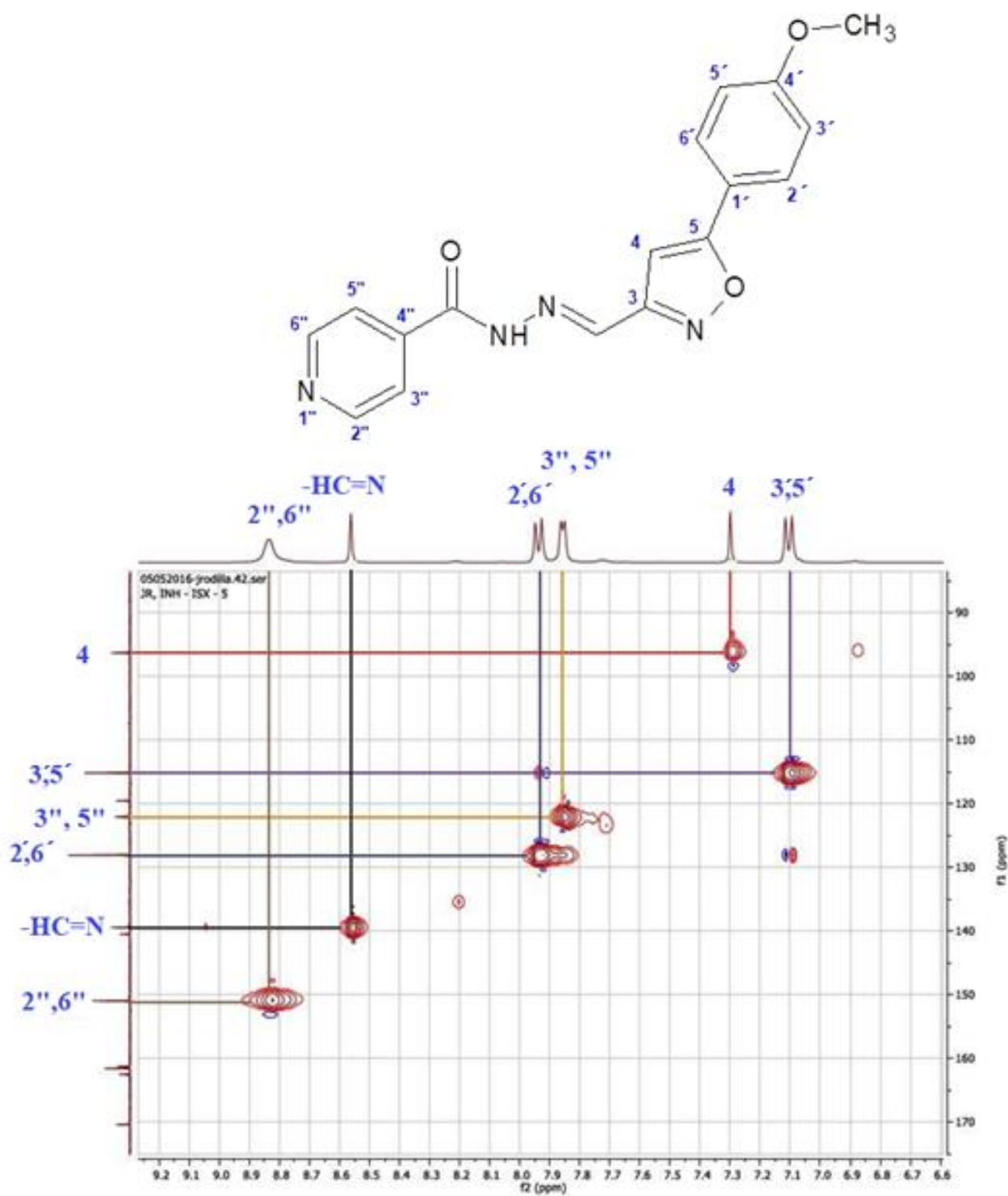


Supplementary figure 28. ¹H NMR spectrum of compound **6** (400 MHz, DMSO-*d*₆)

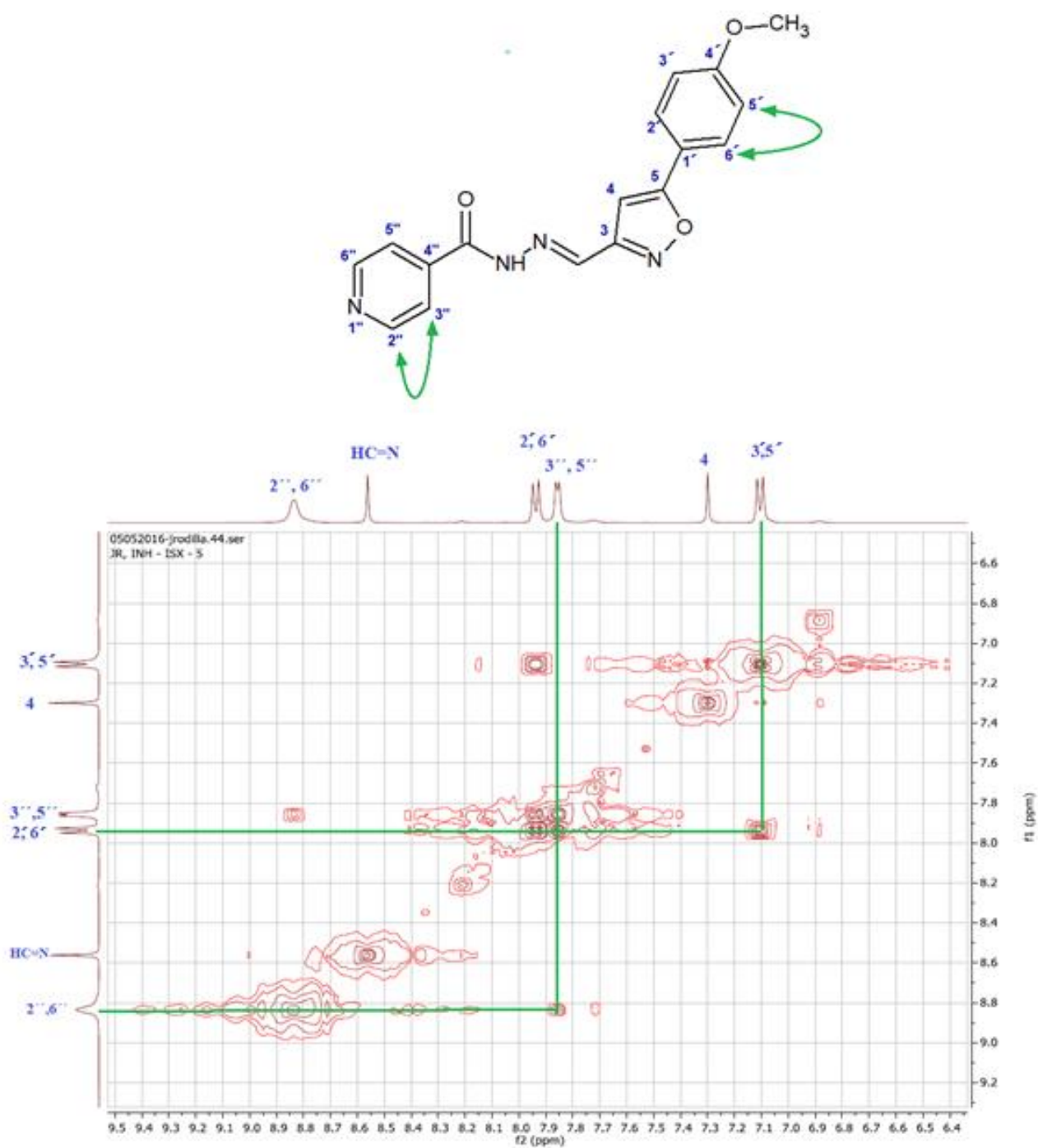


Supplementary figure 29. NMR spectrum of compound **6** (100MHz, DMSO-d₆) 1)

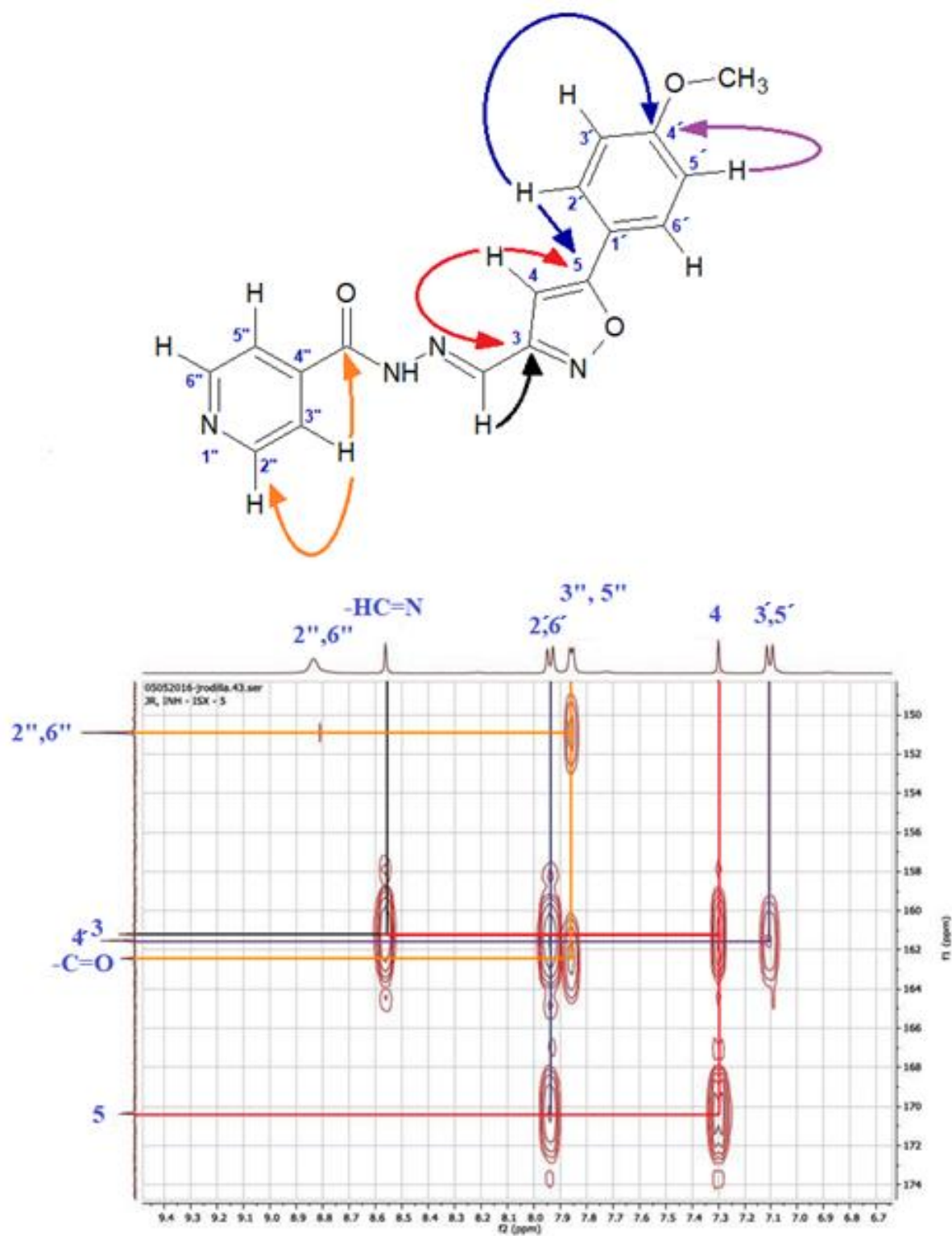
DEPT-45 2) DEPT -90 3) 13C NMR.



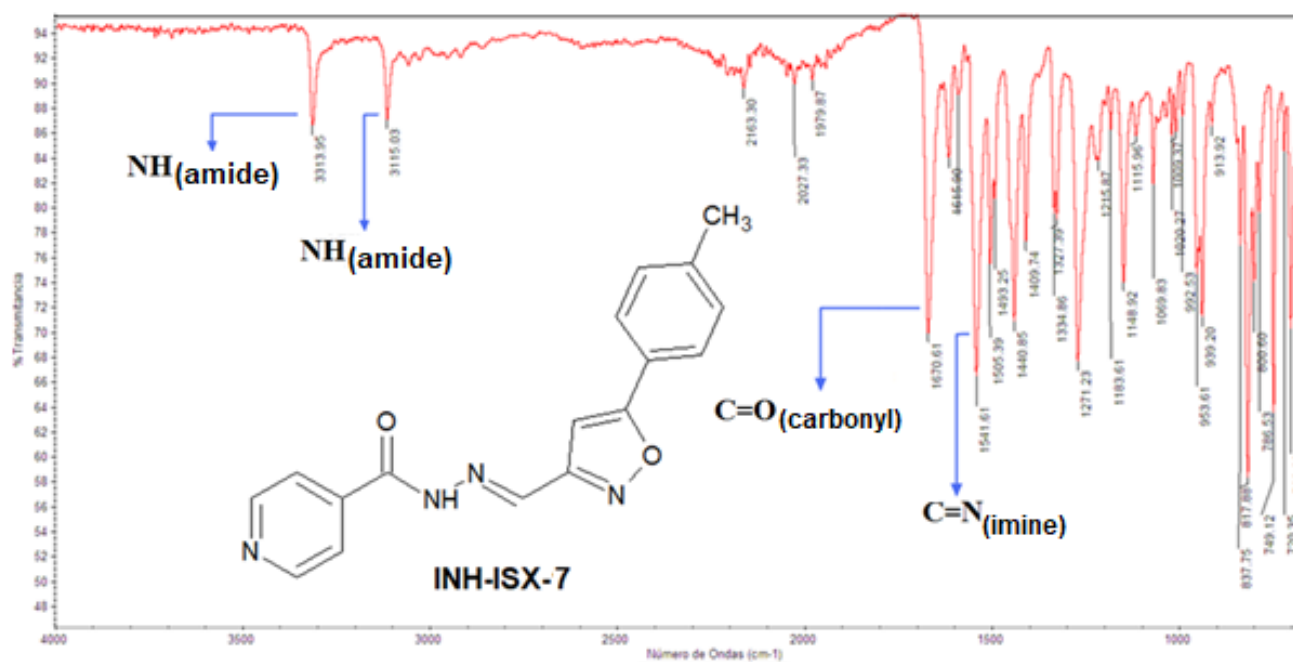
Supplementary figure 30. Two-dimensional ¹H-¹³C HSQC NMR spectrum, recorded in DMSO-*d*₆ for **6**



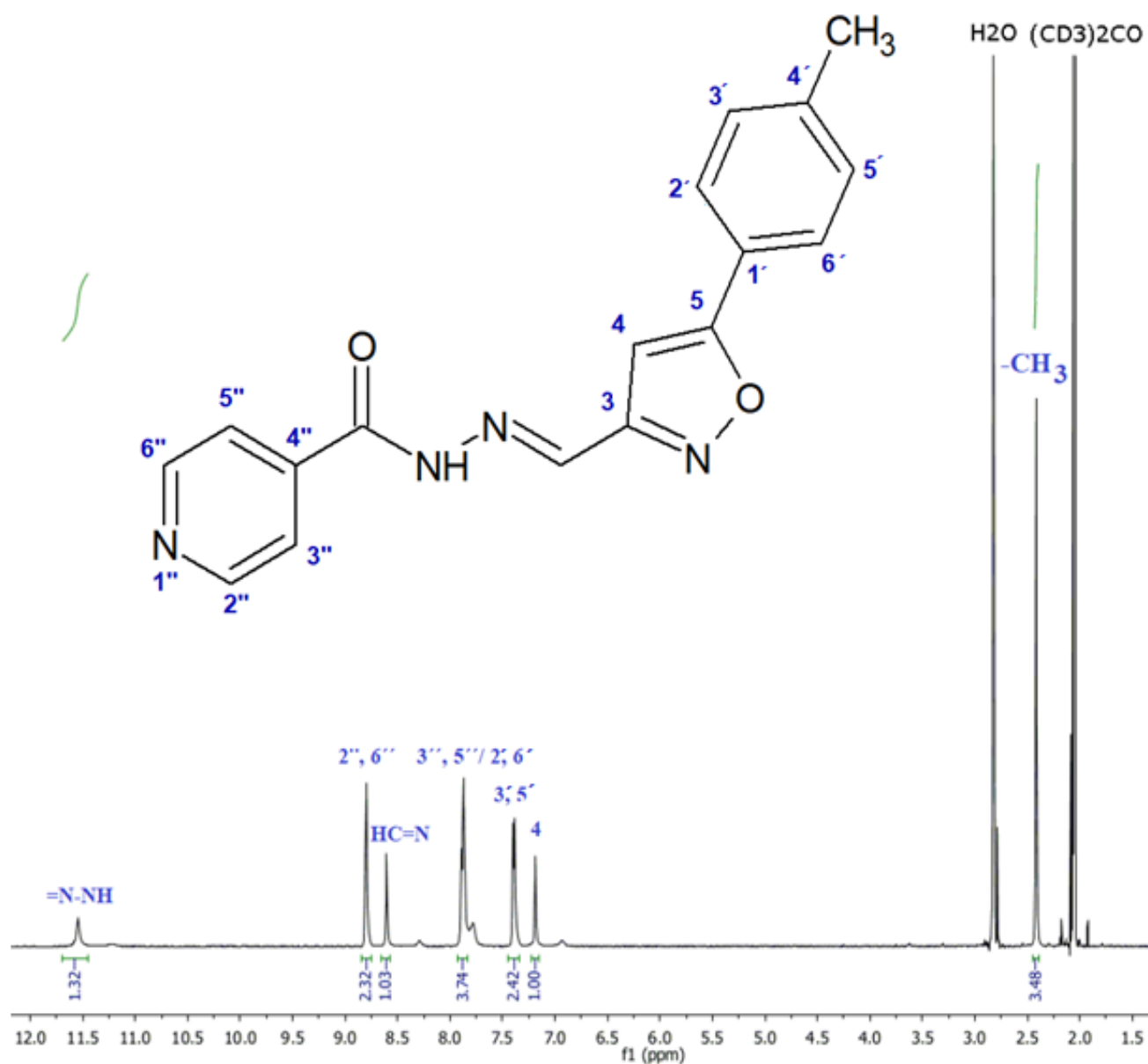
Supplementary figure 31. Two-dimensional ^1H - ^1H COSY NMR spectrum, recorded in $\text{DMSO}-d_6$ for **6**



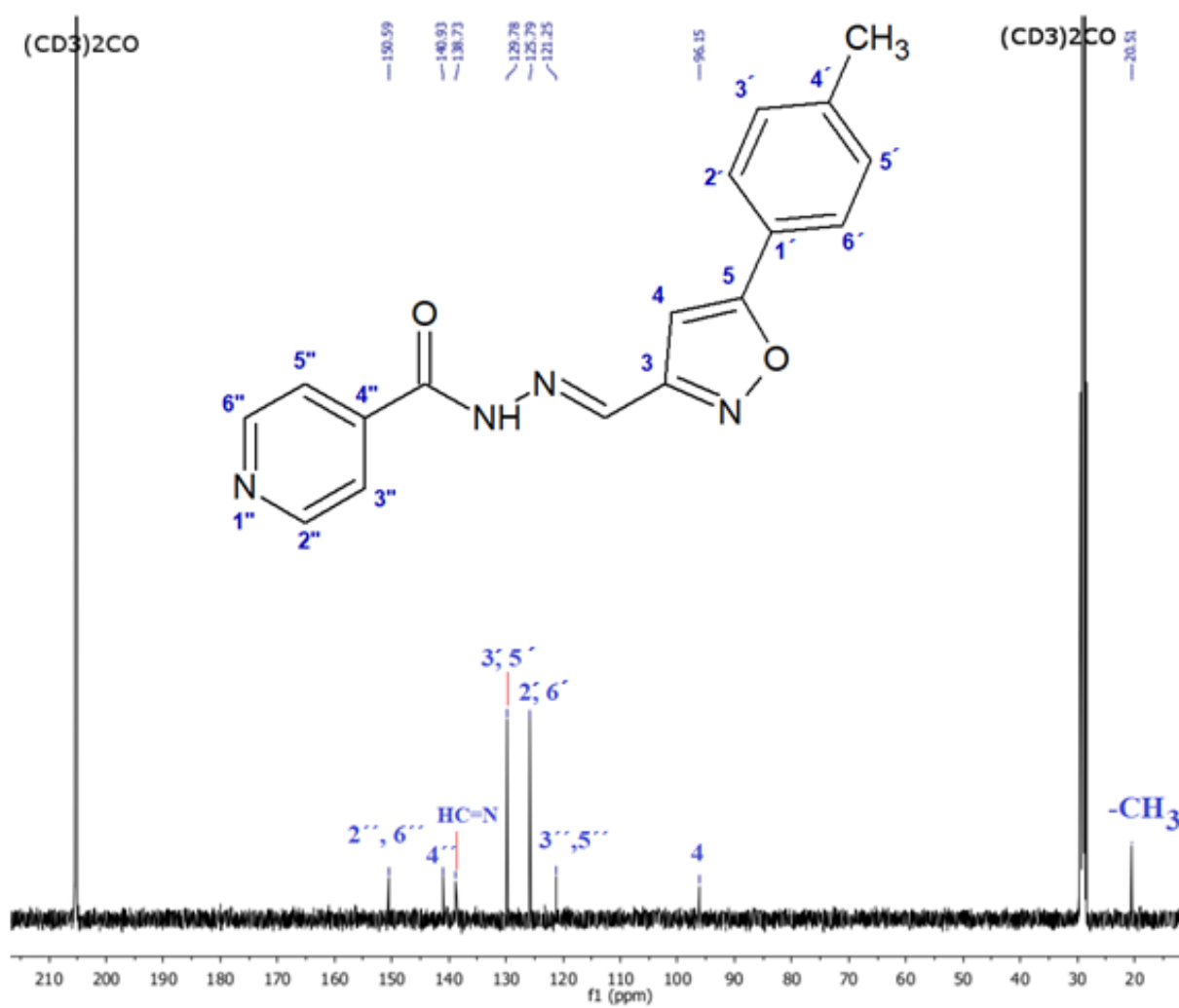
Supplementary figure 32. Two-dimensional ^1H - ^{13}C HMBC NMR spectrum recorded in $\text{DMSO}-d_6$ for **6**



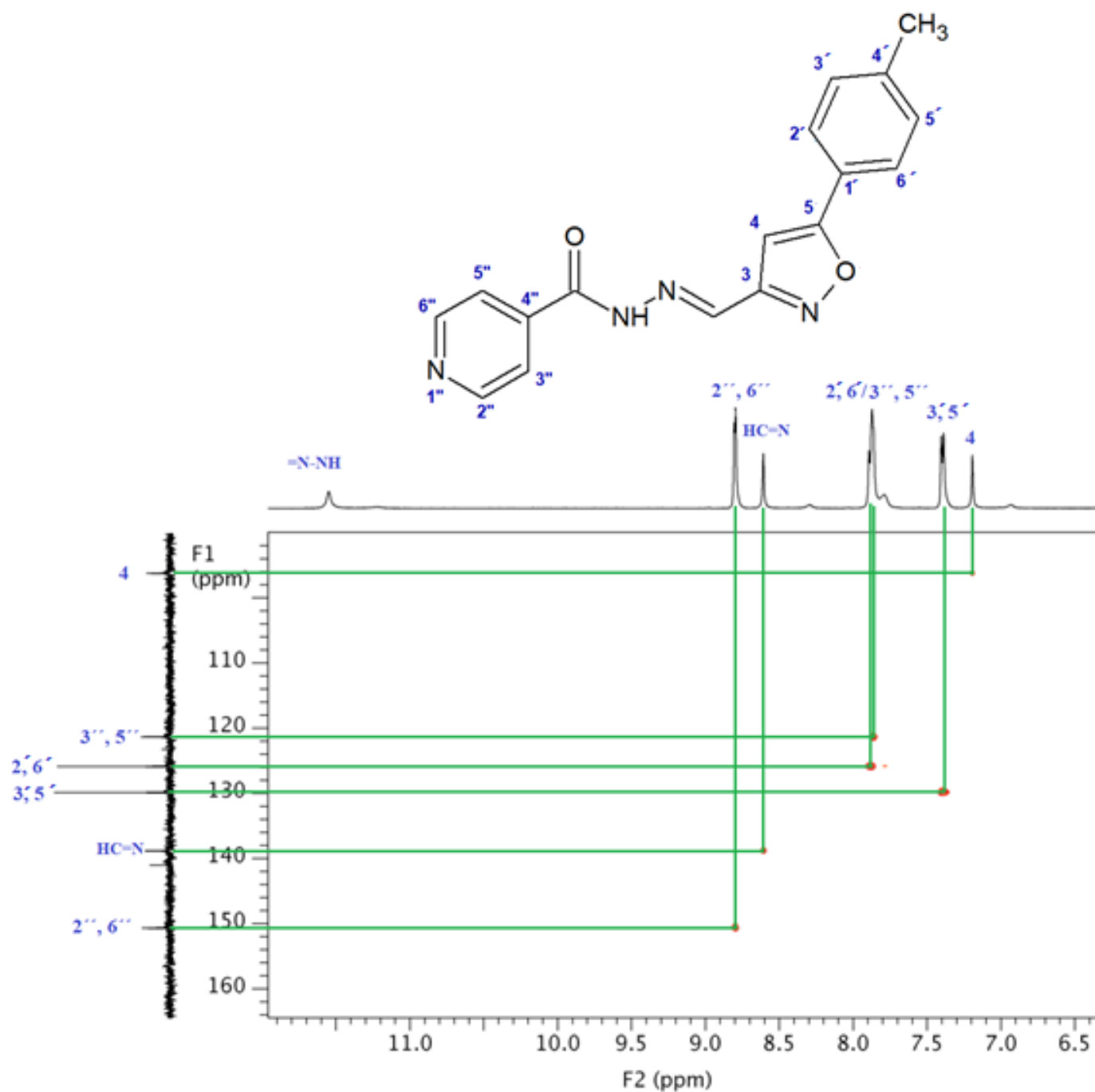
Supplementary figure 33. FT-IR spectrum of compound 7



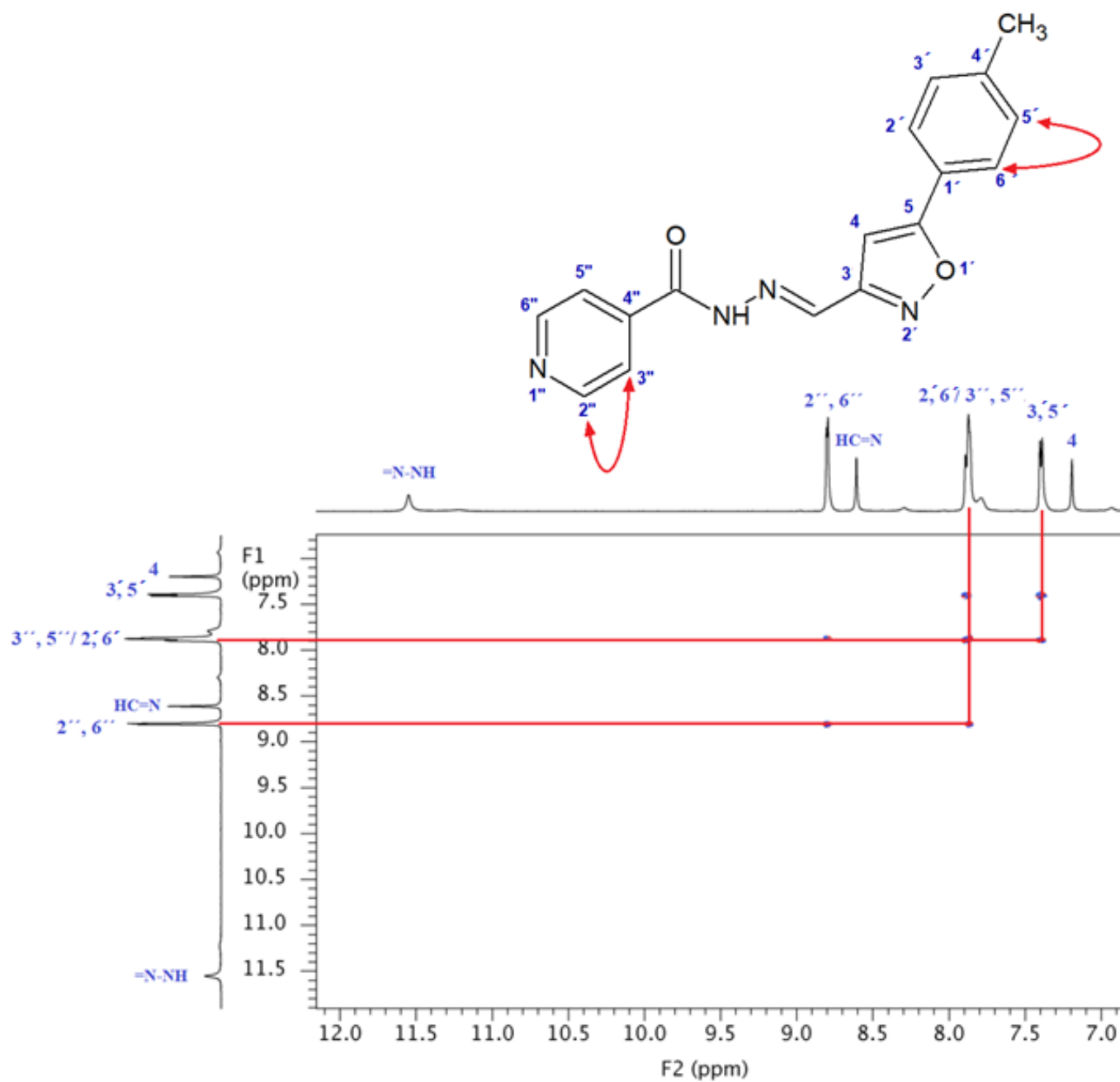
Supplementary figure 34. ^1H NMR spectrum of compound **7** (500 MHz, acetone-*d*₆)



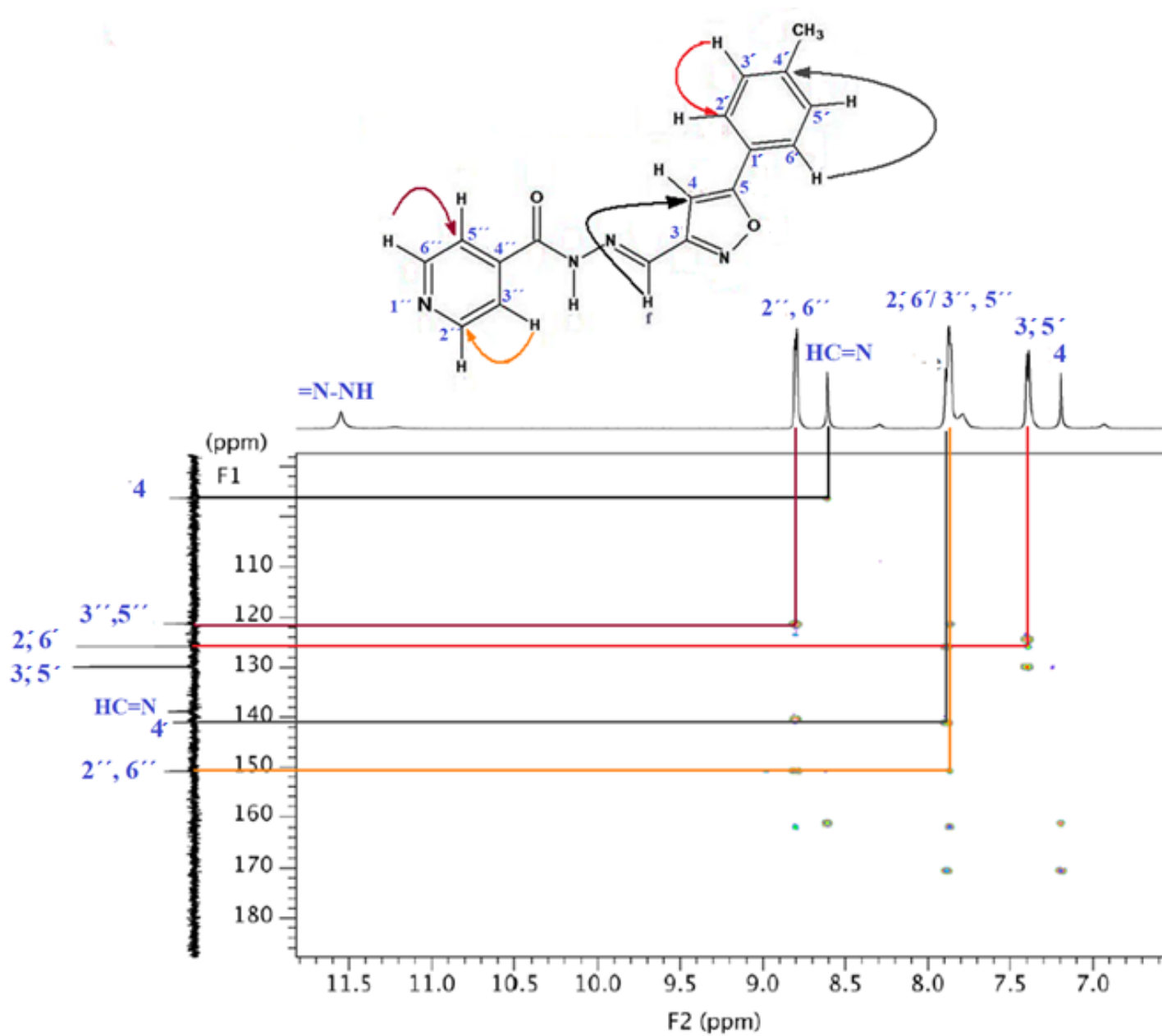
Supplementary figure 35. ¹³C{¹H} NMR spectrum of compound **7** (126 MHz, acetone-*d*₆)



Supplementary figure 36. Two-dimensional ¹H-¹³C HSQC NMR spectrum, recorded in acetone-*d*₆ for **7**

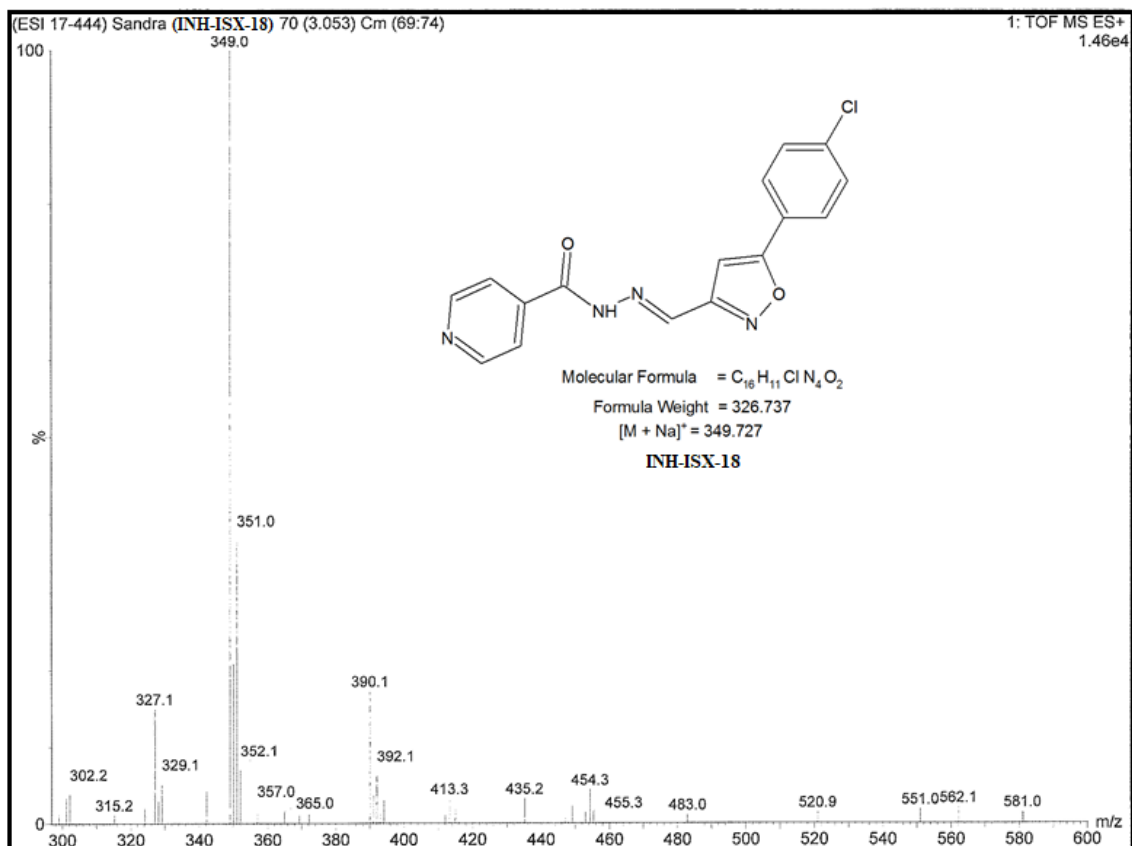


Supplementary figure 37. Two-dimensional ¹H-¹H DQFCOSY NMR spectrum, recorded in acetone-*d*₆ for **7**

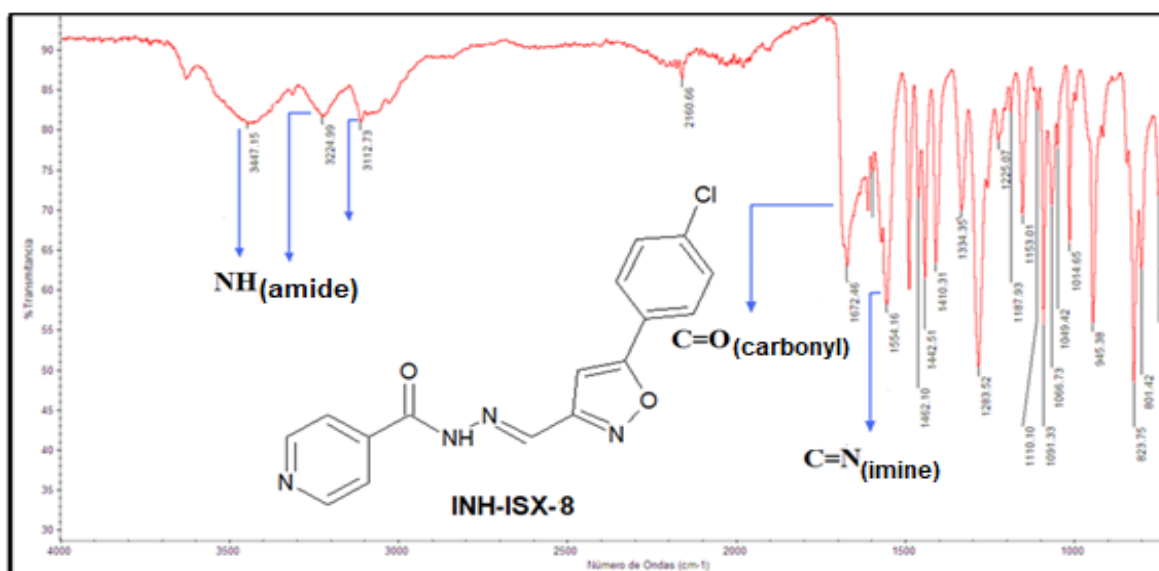


Supplementary figure 38. Two-dimensional ^1H - ^{13}C HMBC NMR spectrum, recorded in acetone- d_6

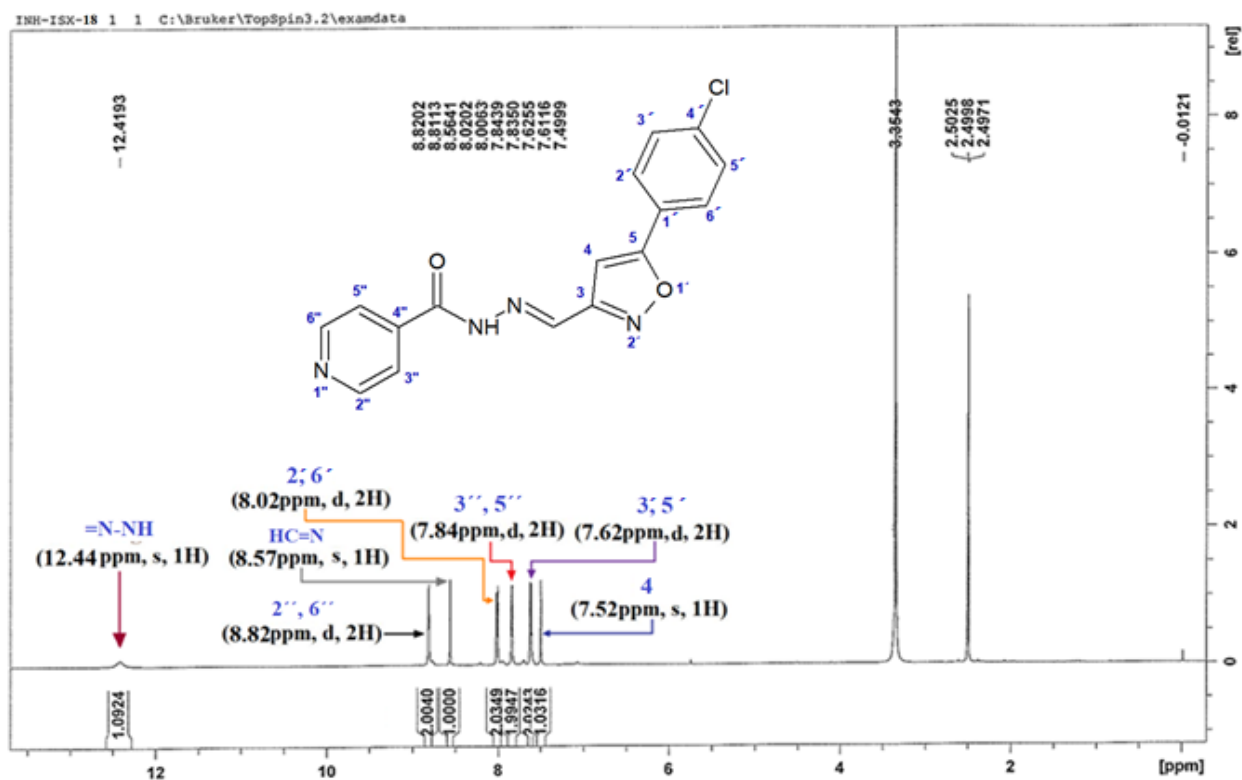
for **7**



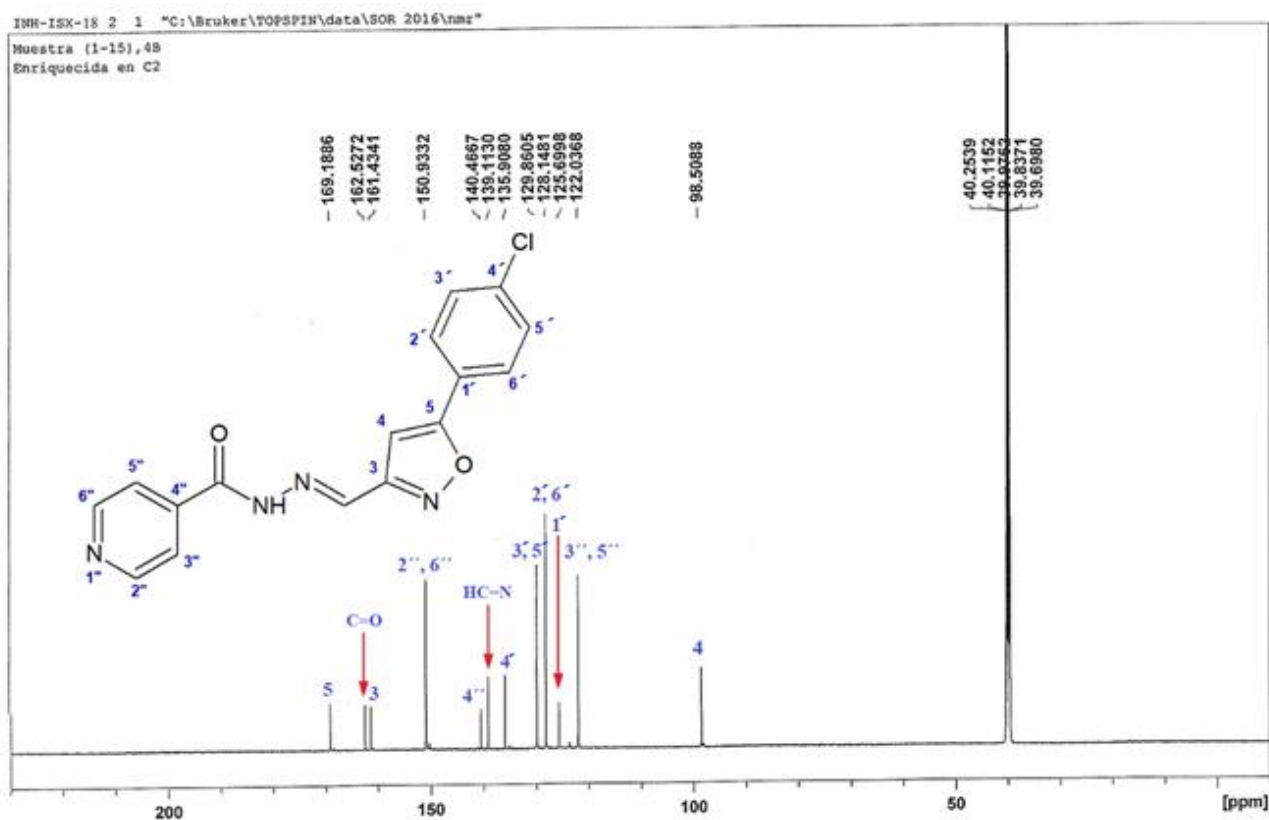
Supplementary figure 39. ESI-mass spectrum of compound **8**



Supplementary figure 40. FT-IR spectrum of compound **8**



Supplementary figure 41. ^1H NMR spectrum of compound **8** (600 MHz, $\text{DMSO-}d_6$)



Supplementary figure 42. ^{13}C NMR spectrum of compound **8** (150 MHz, $\text{DMSO-}d_6$)