Electronic Supplementary Material (ESI) for Photochemical & Photobiological Science

Photochemical isomerisation of aryl hydrazones of 1,2,4-oxadiazole derivatives into the corresponding triazoles.

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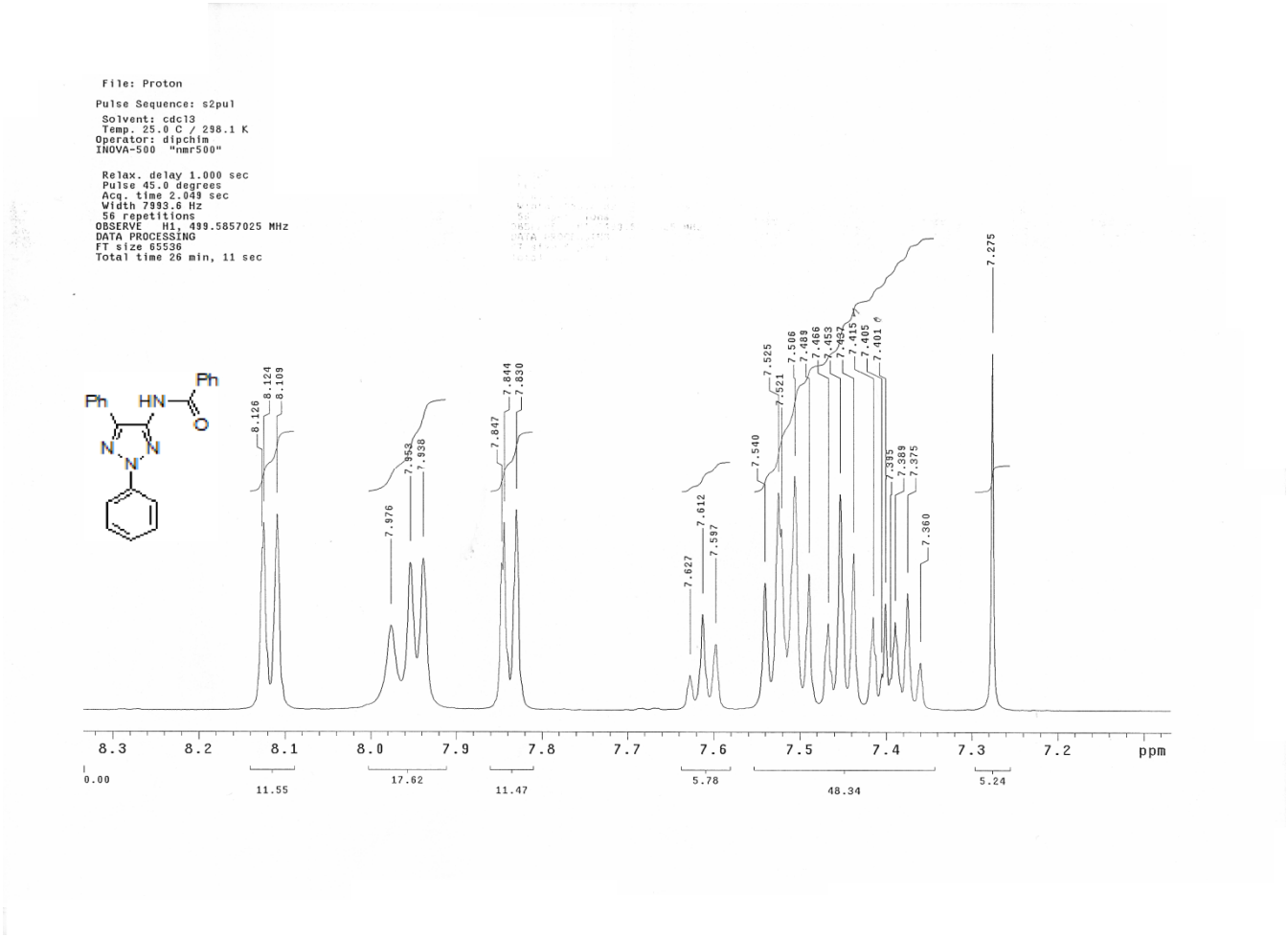
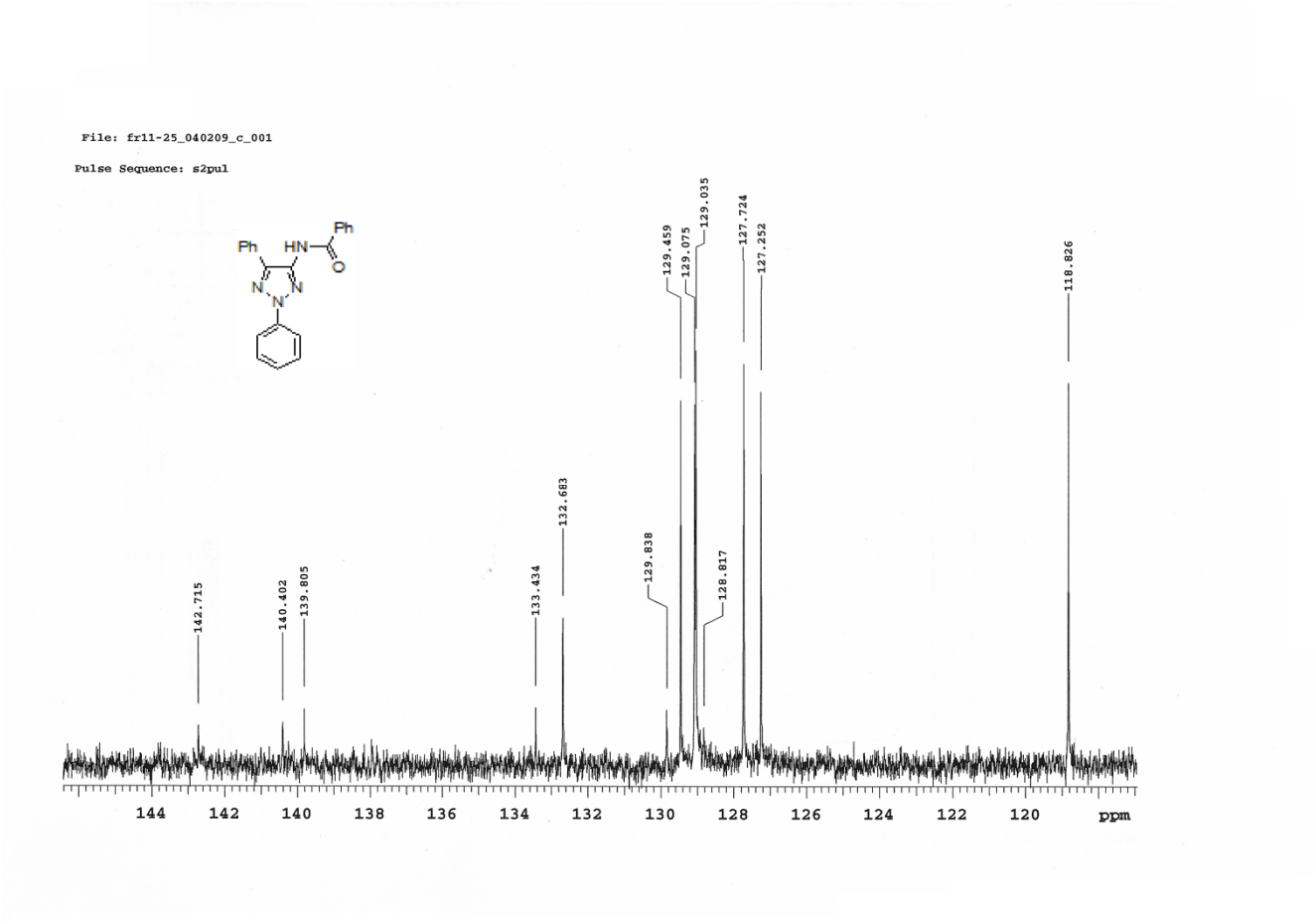
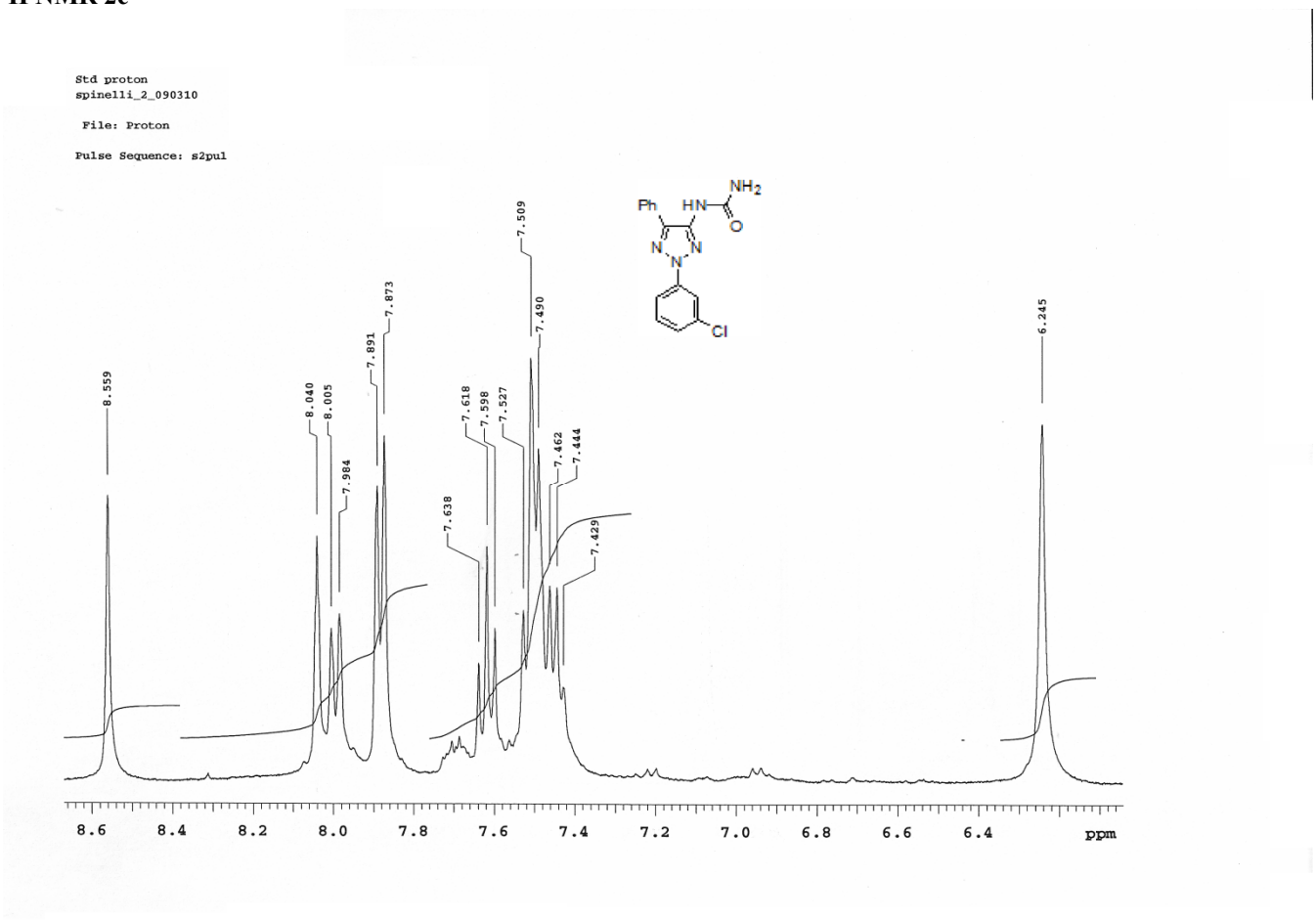
^{1}H NMR 2a



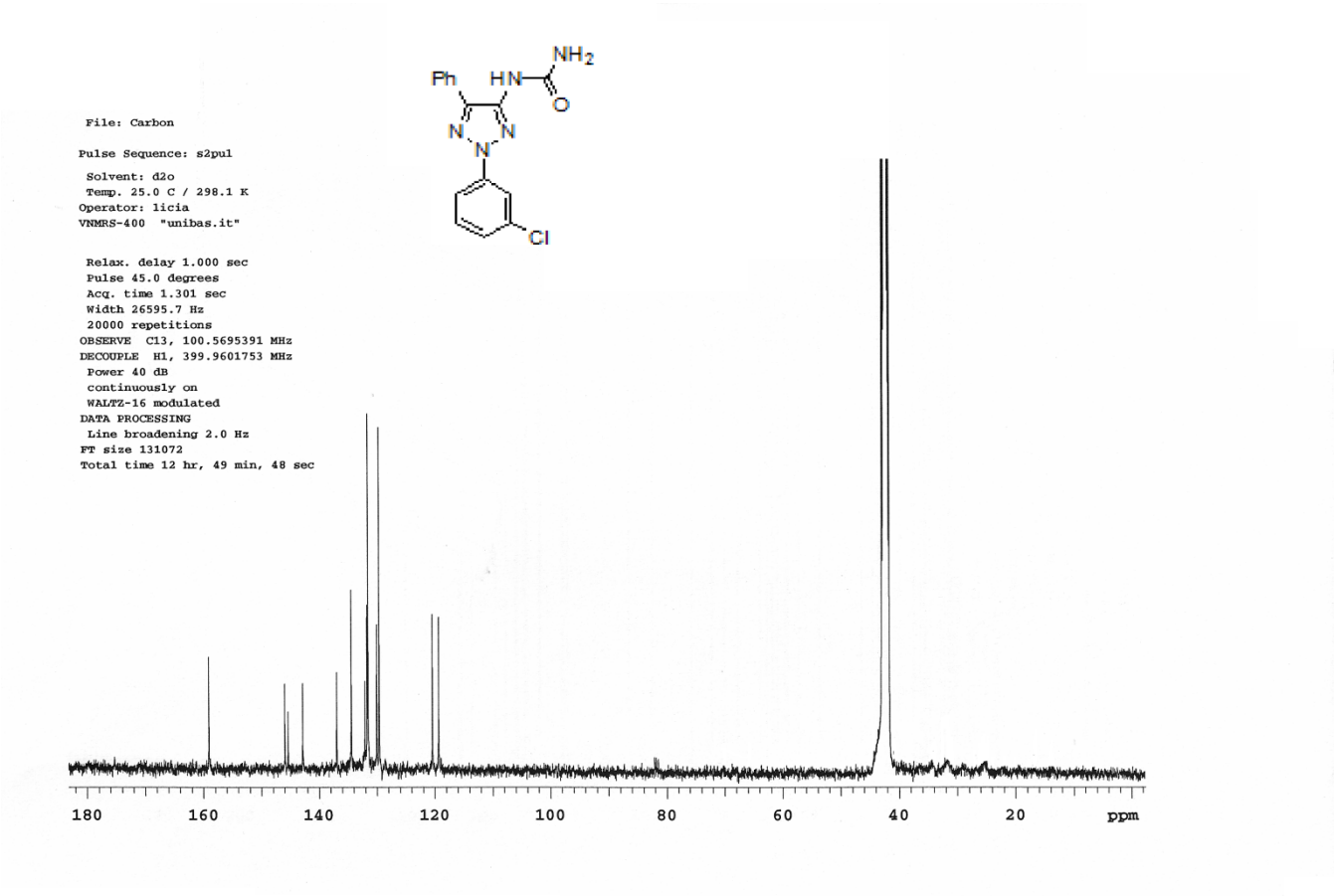
^{13}C NMR 2a



^{1}H NMR 2c



^{13}C NMR 2c



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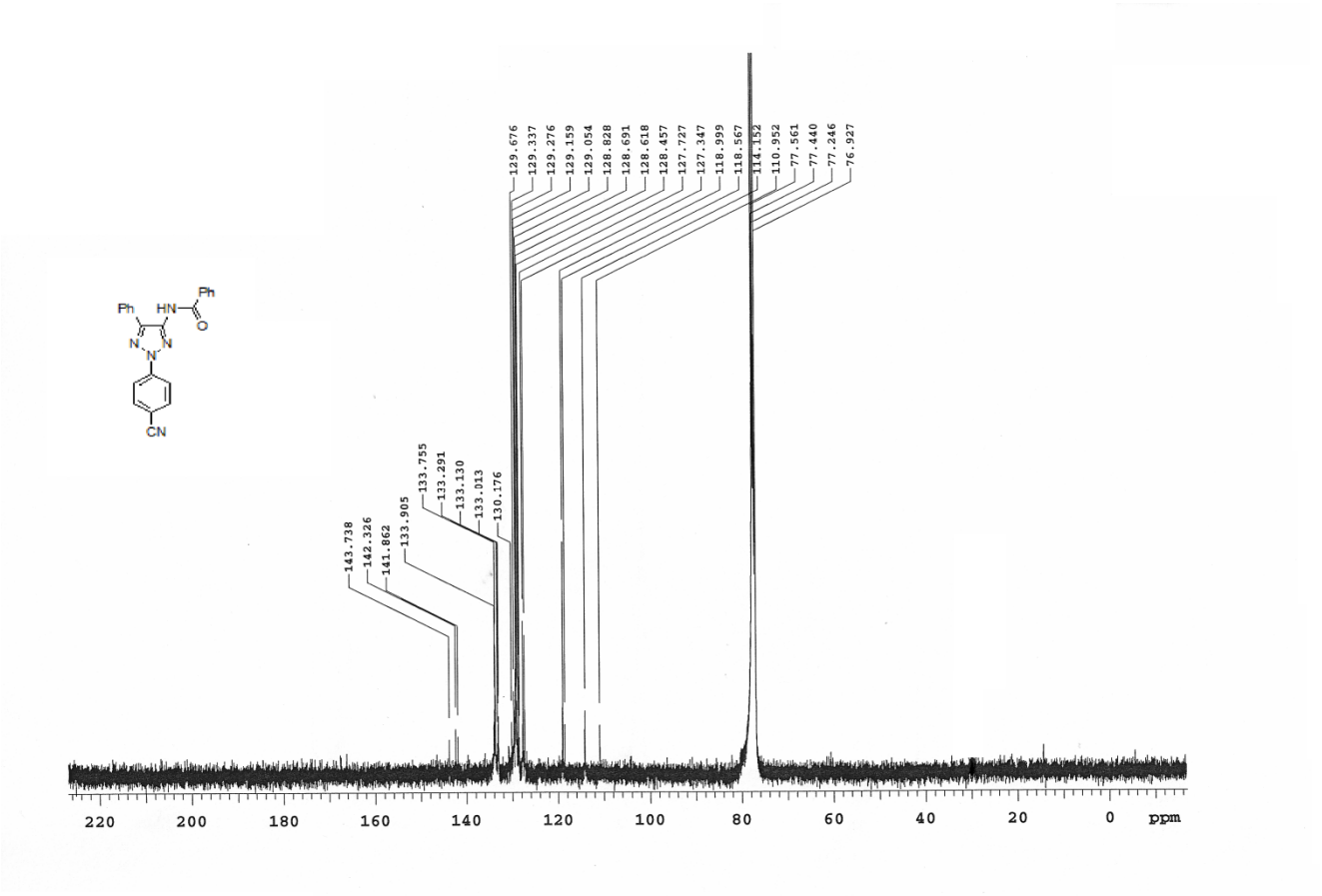
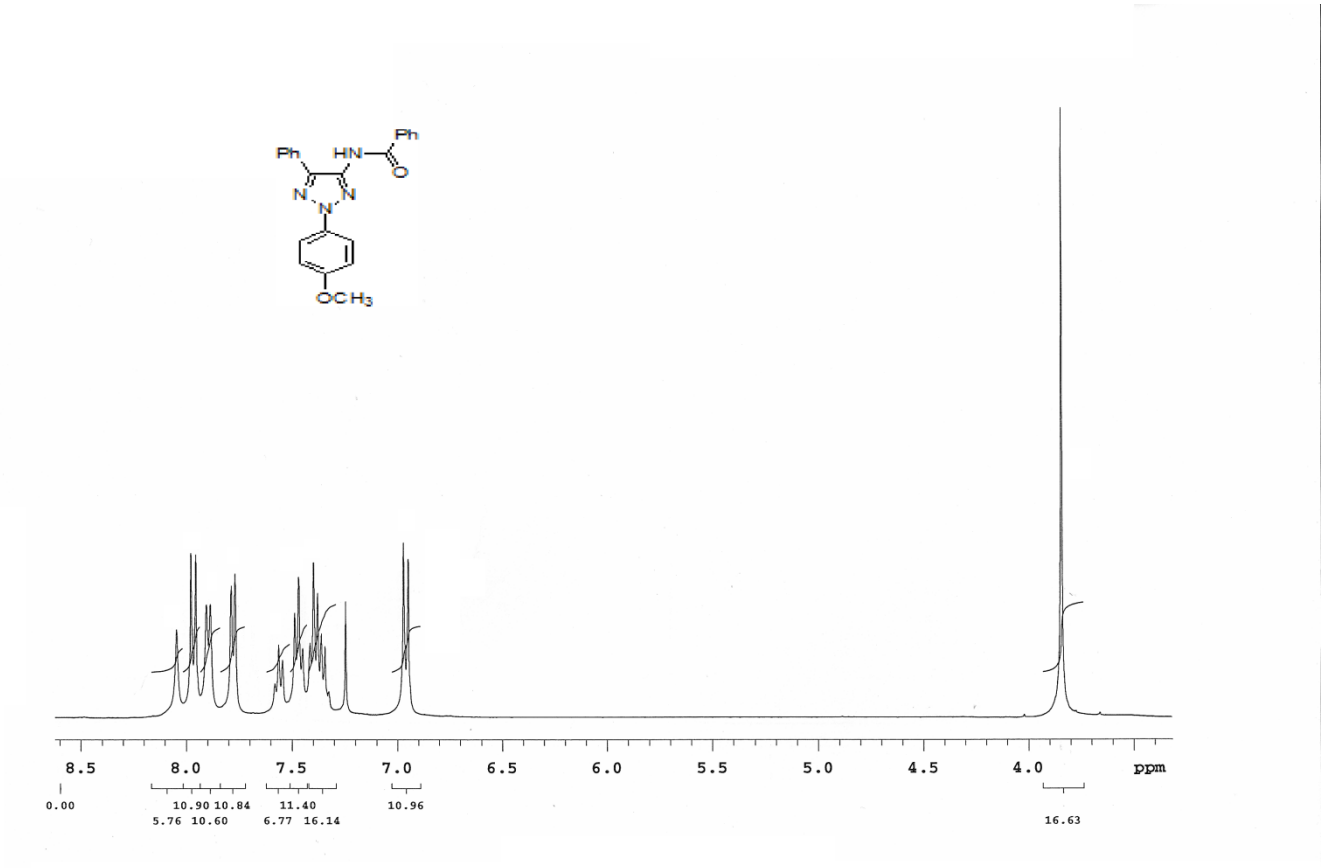
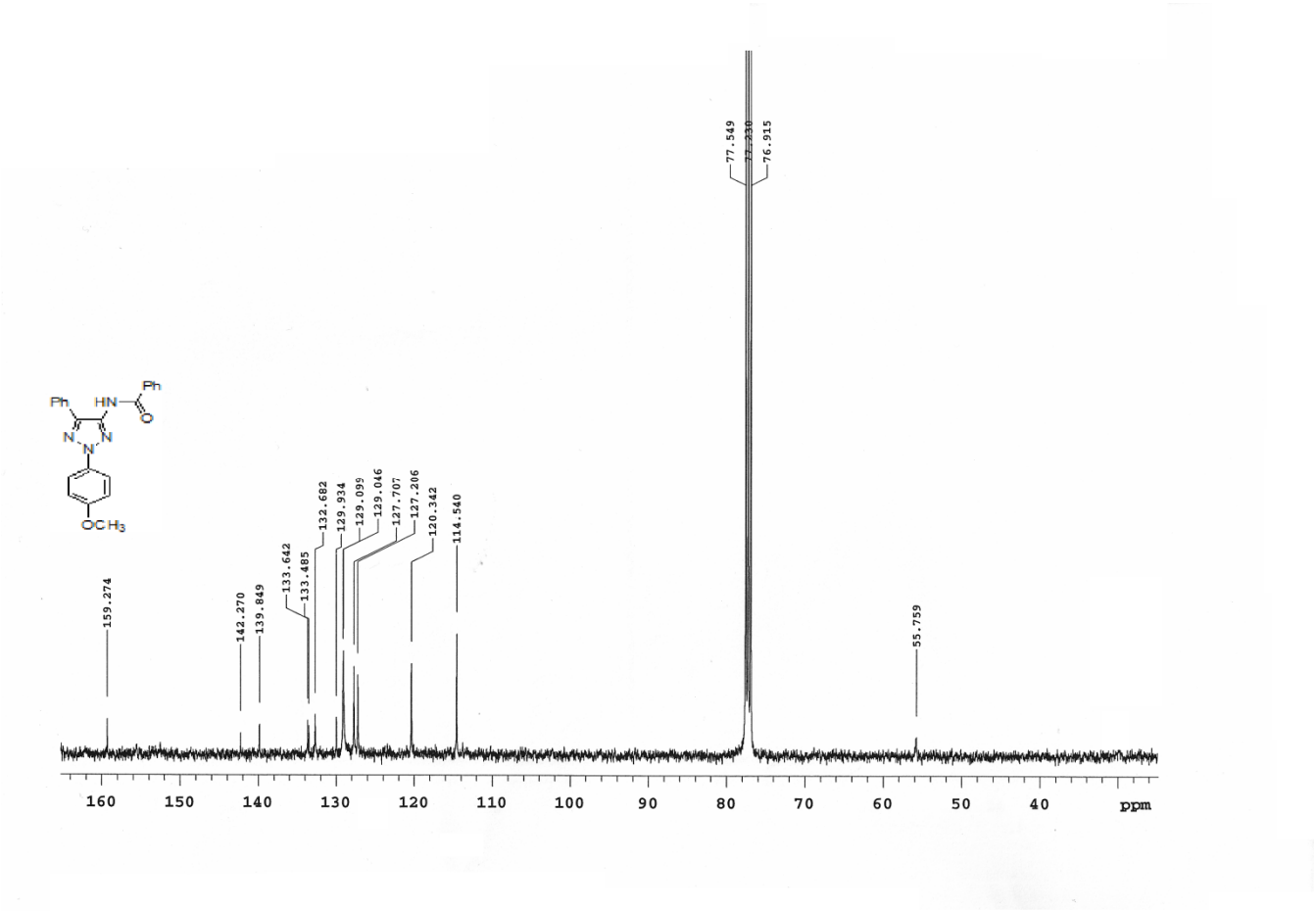


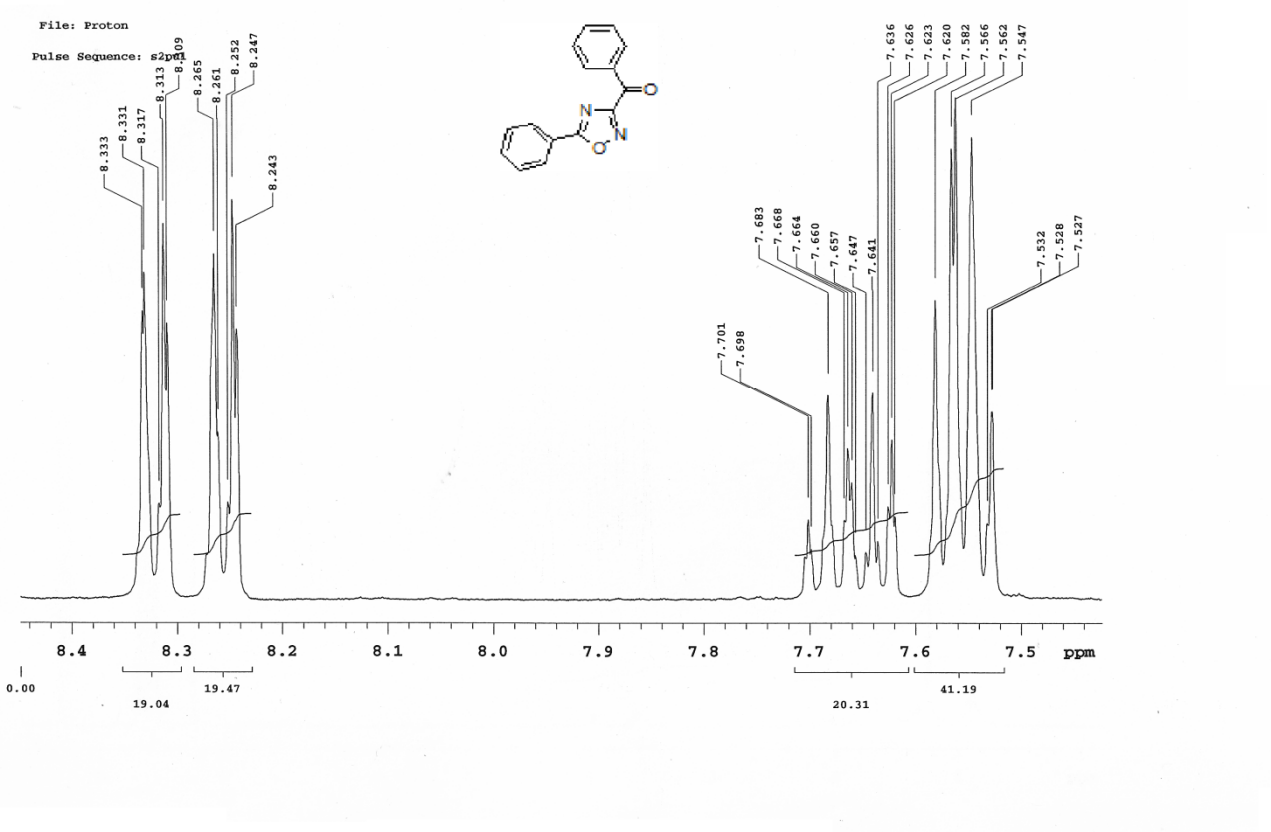
^{1}H NMR 2e



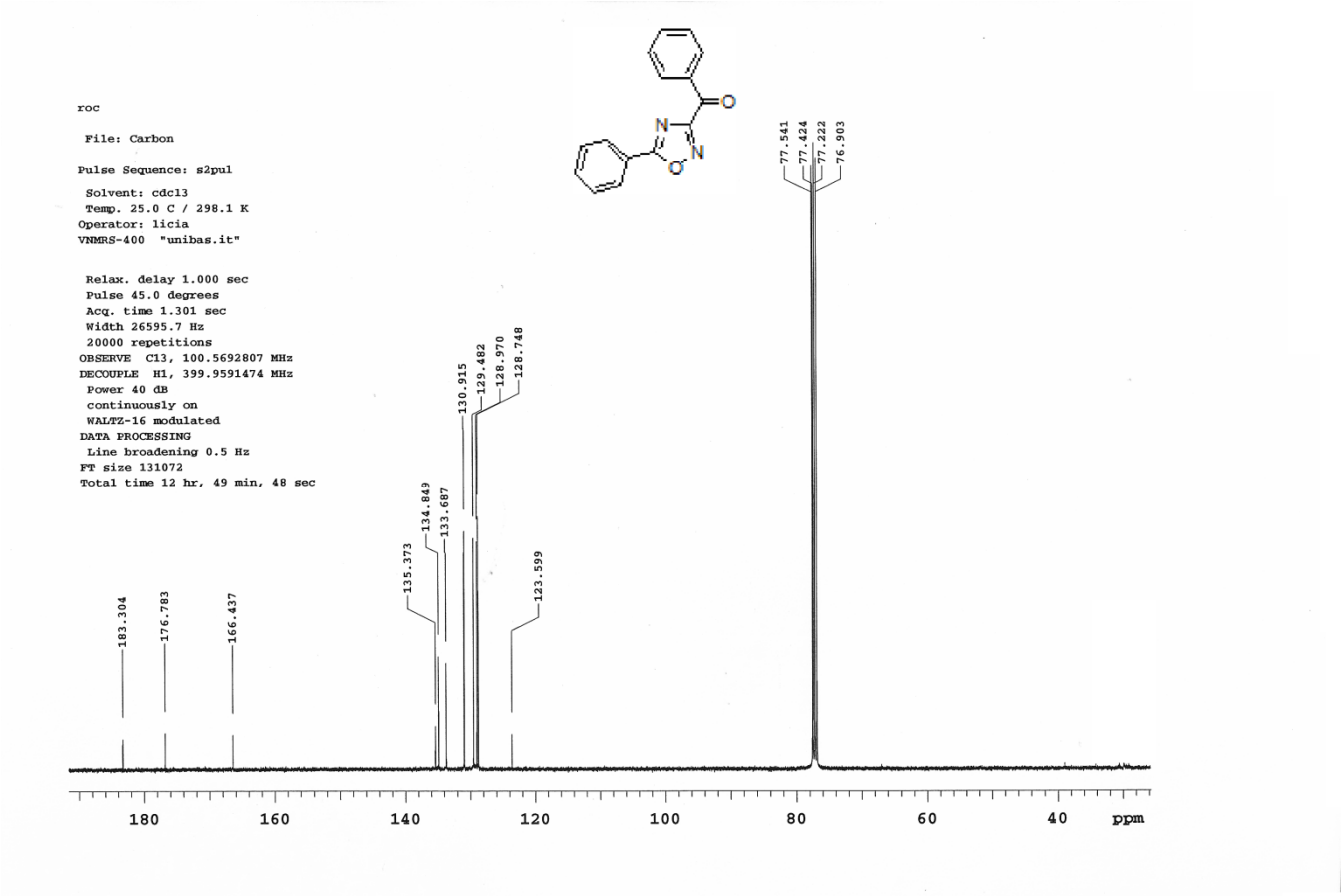
^{13}C NMR 2e



^{1}H NMR 3



^{13}C NMR 3



Compound 1a
Total energy -1104-10439582 H
Atom list:

Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	C							-0.6268090	-0.5396090	0.1697700
2	N	1			1.3798206			-1.8361390	0.0776090	-0.0761320
3	C	2	1		1.3058198	102.9139192		-2.6961740	-0.8922640	0.0815120
4	O	3	2	1	1.3475129	112.6769748	0.2474876	-2.1085430	-2.0592250	0.4111830
5	N	1	2	3	1.3203710	114.2912730	-0.7587914	-0.7233370	-1.8193220	0.4802480
6	C	3	2	1	1.4622811	128.2018589	-179.7737239	-4.1511400	-0.8419290	-0.0556240
7	C	1	5	4	1.4708077	123.8777415	-179.0547403	0.6476510	0.1897230	0.0854980
8	N	7	1	5	1.2994367	116.5039885	15.2669299	1.7265210	-0.5324600	0.0304810
9	C	7	1	5	1.4957346	118.8443915	-163.9462743	0.6246310	1.6852800	0.0866610
10	N	8	7	1	1.3310151	120.2528252	-177.2688089	2.9230290	0.0501560	0.0074930
11	C	10	8	7	1.4008218	121.4143625	179.6668879	4.1018540	-0.7047920	-0.0447260
12	C	11	10	8	1.4035232	121.7701339	1.3141831	4.0794550	-2.1069410	-0.1026380
13	C	12	11	10	1.3945969	119.3464025	179.9101017	5.2838000	-2.8081640	-0.1549830
14	C	13	12	11	1.3989995	121.1289006	-0.1018568	6.5117110	-2.1377690	-0.1528400
15	C	14	13	12	1.3978533	119.1429482	0.0439707	6.5246850	-0.7411240	-0.0961980
16	C	15	14	13	1.3944940	120.4971746	-0.0178835	5.3299780	-0.0238770	-0.0428560
17	C	6	3	2	1.4049618	119.1391379	0.0187821	-4.7642250	0.3746060	-0.3992620
18	C	17	6	3	1.3934328	119.8872992	-179.9032117	-6.1497350	0.4407290	-0.5320960
19	C	18	17	6	1.3990814	120.2001972	-0.0051742	-6.9319070	-0.7005450	-0.3244200
20	C	19	18	17	1.3982337	119.9743672	-0.0261241	-6.3230570	-1.9120760	0.0169770
21	C	20	19	18	1.3945375	120.2138927	0.0251669	-4.9371230	-1.9874400	0.1520400
22	C	9	7	1	1.4052050	120.4597623	-116.1787091	1.0752480	2.4055160	-1.0326270
23	C	22	9	7	1.3971659	120.5620266	-179.2133257	1.0699880	3.8026630	-1.0276040
24	C	23	22	9	1.3974532	120.0980735	0.1041483	0.6164410	4.4977200	0.0967030
25	C	24	23	22	1.3979707	119.7454978	-0.1767373	0.1648030	3.7897090	1.2143190

26	C	25	24	23	1.3959852	120.1884950	0.1155775	0.1685670	2.3937370	1.2095450
27	H	10	8	7	1.0172544	120.0603803	1.8136771	2.9975730	1.0632740	0.0608000
28	H	12	11	10	1.0832643	119.3814976	-0.2892944	3.1274100	-2.6237310	-0.1025390
29	H	13	12	11	1.0863683	118.9551135	179.8873993	5.2590830	-3.8934070	-0.1977940
30	H	14	13	12	1.0854743	120.4604737	-179.9743946	7.4426520	-2.6944410	-0.1943070
31	H	15	14	13	1.0862253	120.2140084	179.9686693	7.4681950	-0.2029190	-0.0930970
32	H	16	15	14	1.0876118	120.1008262	179.9232746	5.3476190	1.0626530	0.0023180
33	H	17	6	3	1.0847411	119.0936719	0.1243581	-4.1450160	1.2510360	-0.5577360
34	H	18	17	6	1.0858657	119.7008629	-179.9962038	-6.6204020	1.3825090	-0.7978540
35	H	19	18	17	1.0860813	120.0246445	179.9941356	-8.0115890	-0.6457520	-0.4286170
36	H	20	19	18	1.0857905	120.1208907	-179.9692645	-6.9277460	-2.7993740	0.1782050
37	H	21	20	19	1.0847855	120.3804986	-179.9837394	-4.4619140	-2.9260400	0.4165510
38	H	22	9	7	1.0867806	119.5261103	2.1205815	1.4097410	1.8682230	-1.9160990
39	H	23	22	9	1.0862062	119.7300131	-179.3946432	1.4120690	4.3457730	-1.9038780
40	H	24	23	22	1.0861129	120.1218861	-179.8971021	0.6106180	5.5838110	0.1003980
41	H	25	24	23	1.0861580	120.0918409	-179.7402510	-0.1928800	4.3242240	2.0895880
42	H	26	25	24	1.0860492	119.9761925	-179.5796352	-0.1894540	1.8471660	2.0770610

Compound 1c

Total energy: -1332.60819518 H

Atom list:

Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	C							1.8508940	1.4966040	-0.1269100
2	N	1			1.3882062			3.1067380	2.0179790	-0.4064460
3	C	2	1		1.2949552	102.0851121		2.8856510	3.2933240	-0.3673990
4	O	3	2	1	1.3378026	114.1871393 0.	2725231	1.6196950	3.6218000	-0.0860190
5	N	1	2	3	1.3190781	114.104639 3	-0.7661113	0.9235870	2.4101680	0.0863260
6	C	1	5	4	1.4702387	124.0681016	-179.0086056	1.6055280	0.0477050	-0.0812050
7	C	6	1	5	1.4953598	119.0199748	-164.3778556	2.7721710	-0.8830030	0.0127510
8	N	6	1	5	1.2994488	116.3040767	14.8627205	0.3616180	-0.3269110	-0.1115010
9	N	8	6	1	1.3314457	120.1572354	-13.9825734	-0.6092330	0.5595700	0.0990870
10	C	9	8	6	1.3991917	121.2262715	179.8937809	-1.9559610	0.1811770	0.0694260
11	C	7	6	1	1.4052491	120.3588304	-115.9615752	3.0482990	-1.7832970	-1.0302970
12	C	11	7	6	1.3970573	120.5209997	-179.1223423	4.1264970	-2.6668990	-0.9380710
13	C	12	11	7	1.3974240	120.0878926	0.0811509	4.9404820	-2.6627560	0.1978010
14	C	13	12	11	1.3978548	119.7797422	-0.1674257	4.6743020	-1.7693560	1.2394260
15	C	14	13	12	1.3960039	120.1831481	0.1308416	3.5976590	-0.8854340	1.1480550
16	C	10	9	8	1.4034049	121.7887441	1.5943841	-2.3454390	-1.1491920	-0.1495960
17	C	16	10	9	1.3935647	119.8180860	179.8089989	-3.6987860	-1.4811140	-0.1669810
18	C	17	16	10	1.3959414	120.0723959	-0.0890918	-4.6639990	-0.4930360	0.0348060
19	C	18	17	16	1.3947805	120.5583249	0.0649056	-4.2874030	0.8319630	0.2538170
20	C	19	18	17	1.3936479	119.4901186	-0.0343289	-2.9346930	1.1668240	0.2710840
21	Cl	18	17	16	1.7600474	119.7753195	-179.9381474	-6.3710200	-0.9212480	0.0128830
22	H	3	2	1	1.0813152	128.4147110	-179.6011863	3.5844650	4.1017370	-0.5328380
23	H	9	8	6	1.0172773	120.0722656	1.8861751	-0.3805910	1.5383390	0.2558900
24	H	11	7	6	1.0868089	119.5482670	2.2436011	2.4297050	-1.7743800	-1.9238380
25	H	12	11	7	1.0861232	119.7295620	-179.3525985	4.3345390	-3.3500560	-1.7564100
26	H	13	12	11	1.0860340	120.1020903	-179.8373107	5.7802880	-3.3477260	0.2685960
27	H	14	13	12	1.0860606	120.0939347	-179.7039216	5.3065040	-1.7584620	2.1224490
28	H	15	14	13	1.0860669	119.9561195	-179.6199851	3.3979180	-0.1886310	1.9568260
29	H	16	10	9	1.0831191	119.5274803	-0.3337694	-1.5886500	-1.9081170	-0.3059620
30	H	17	16	10	1.0845894	119.9139634	179.9306027	-4.0015610	-2.5085750	-0.3372320
31	H	19	18	17	1.0843913	120.2707440	179.9369632	-5.0411470	1.5959560	0.4090240
32	H	20	19	18	1.0871229	119.4543054	179.8951808	-2.6418710	2.2000300	0.4401310