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Supplementary Material

A facile eco–friendly one pot five component syntheses of novel 1,2,3-triazole linked pentasubstituted 1,4-dihydropyridines and their biological and photophysical studies.

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Table S1. Antibacterial activity of compounds (**1a – 1p**).

Entry	Product	Diameter of growth of inhibition zone (mm)[a]			
		Staphylococcus aureus	*Bacillus Subtilis*	*Escherichia coli*	*Pseudomonas aeruginosa*
1	1a	13.6	14.6	-	-
2	1b	15.3	14.3	-	-
3	1c	15.3	16.3	-	-
4	1d	13.6	14.3	-	-
5	1e	14.3	14.0	-	-
6	1f	17.6	19.3	-	-
7	1g	14.6	15.6	-	-
8	1h	14.3	15.3	-	-
9	1i	15.6	17.3		
10	1j	14.6	15.3	-	-
11	1k	15.6	16.3	-	-
12	1l	14.3	15.3	-	-
13	1m	15.3	16.3	-	-
14	1n	13.0	14.6	-	-
15	1o	15.3	14.3	-	-
16	1p	14.3	13.6	-	-
17	Ciprofloxacin	26.6	24.0	25.0	22.0

- No activity, [a]Values, including diameter of the well (8 mm), are means of three replicates

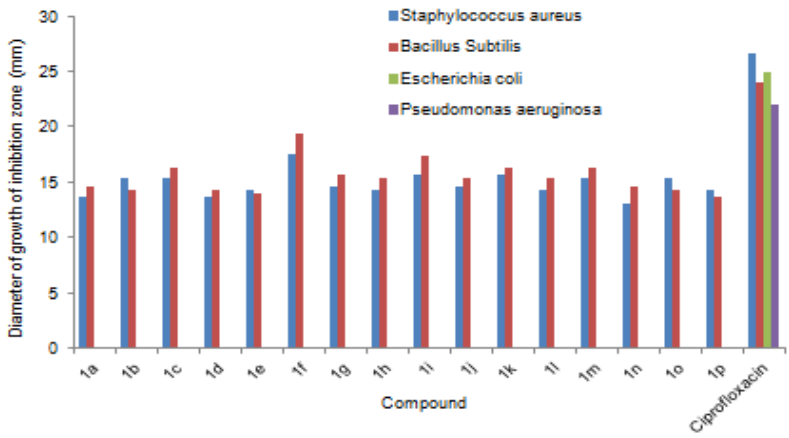


Figure S1. Graphical representation of diameter of growth of inhibition zone (mm) of compounds (**1a -1p**) against Gram positive bacteria.

Table S2. Minimum inhibitory concentration (MIC) (in µg/ml) of compounds **(1a - 1p)** against Gram positive bacteria.

Entry	Product	*Staphylococcus aureus*	*Bacillus Subtilis*
1	1a	256	256
2	1b	128	256
2	1c	128	128
4	1d	512	256
5	1e	256	256
6	1f	64	64
7	1g	256	128
8	1h	512	128
9	1i	128	128
10	1j	256	128
11	1k	128	128
12	1l	256	128
13	1m	128	128
14	1n	512	256
15	1o	128	256
16	1p	256	512
17	Ciprofloxacin	6.25	6.25

Table S3. Antifungal activity of compounds **(1a - 1p)** through poisoned food method.

Entry	Product	Mycelial growth inhibition (%)	
		Aspergillus niger	*Aspergillus flavus*
1	1a	35.5	38.8
2	1b	44.4	51.1
3	1c	43.6	45.5
4	1d	41.4	45.5
5	1e	31.4	41.1
6	1f	51.1	55.8
7	1g	51.1	52.2
8	1h	48.1	51.4
9	1i	43.3	45.3
10	1j	38.8	42.5
11	1k	48.8	45.5
12	1l	37.7	43.3
13	1m	43.6	42.5
14	1n	42.5	46.9
15	1o	48.8	45.8
16	1p	43.3	47.7
17	Fluconazole	81.1	77.7

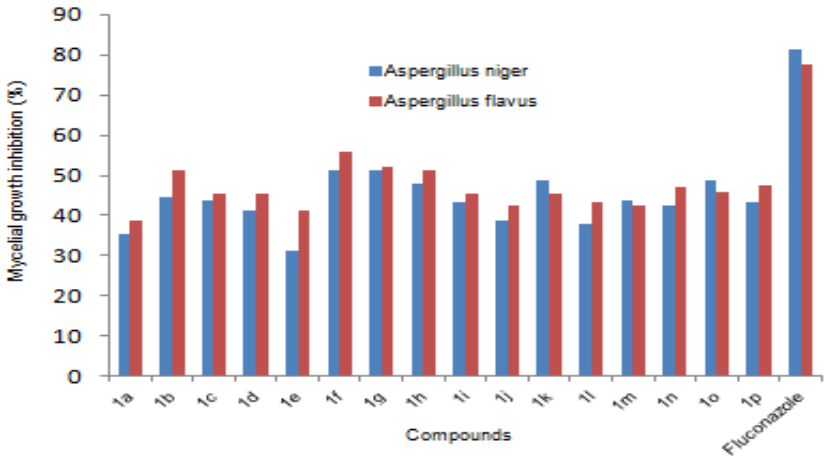


Figure S2. Graphical representation of antifungal activity of compounds (**1a - 1p**) against *Aspergillus niger and Aspergillus flavus.*

Table S4. DPPH[a] radical scavenging activity (%) of 1,2,3 triazole linked multisubstituted 1,4-dihydropyridines.

Product	Scavenging activity (%)	
	0.4 µM/mL[b]	0.8 µM/mL[b]
1a	28.15	39.35
1b	04.25	31.08
1c	22.93	38.88
1d	46.50	85.18
1e	22.00	27.02
1f	21.19	41.00
1g	13.60	27.87
1h	22.08	43.54
1i	20.23	39.25
1j	-[c]	11.20
1k	18.46	21.34
1l	13.88	23.12
1m	16.16	22.08
1n	42.27	79.20
1o	38.88	72.56
1p	52.84	84.12
BHT[d]	83.43	86.01

[a]0.1mM methanolic solution of DPPH was used for all the experiments, [b]Solution of compounds was prepared in methanol, [c]does not show activity. [d]Butylated hydroxyl toluene (BHT) was used as a reference compound.

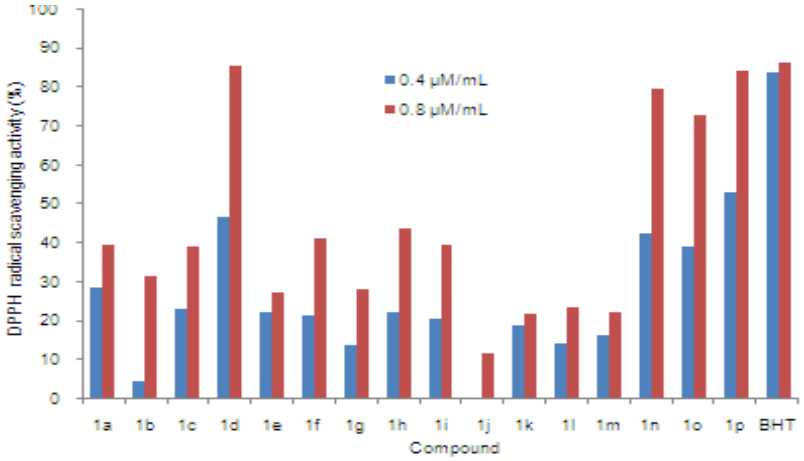


Figure S3. Graphical representation of DPPH radical scavenging activity (%) of 1,2,3-triazole linked pentasubstituted 1,4-dihydropyridines.

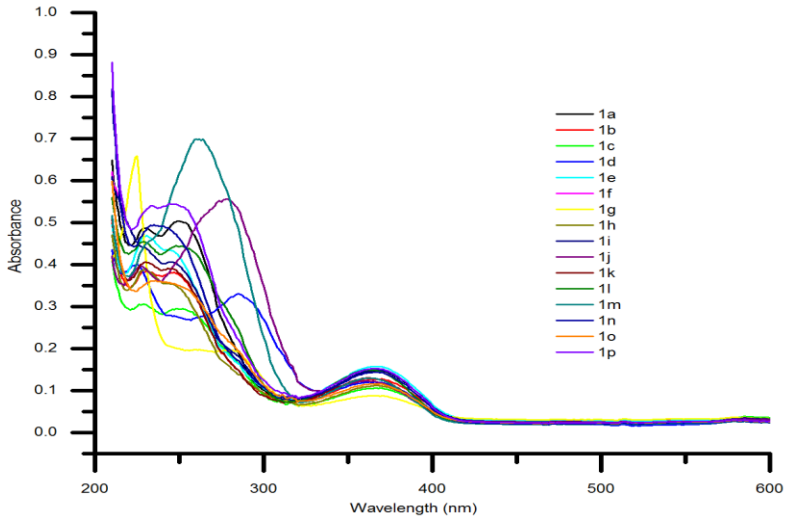


Figure S4. UV – Vis spectra of compounds **1a** – **1p** in methanol solution ($1x10^{-5}$ M).

Table S5. Photophysical data of compounds (**1a – 1p**) in methanol.

Product	λ_{max} (nm)	ε x10^5 ($Lmol^{-1}cm^{-1}$)	λ_{em} (nm)	Stoke shift (Δν) cm^{-1}
1a	229, 250, 366	0.48, 0.50, 0.14	447	4951
1b	229, 248, 368	0.38, 0.37, 0.12	446	4752
1c	228, 251, 367	0.30, 0.29, 0.10	450	5025
1d	225, 285, 367	0.39, 0.32, 0.12	447	4876
1e	230, 248, 368	0.46, 0.43, 0.15	450	4951
1f	229, 247, 367	0.44, 0.40, 0.14	451	5075
1g	225, 278, 368	0.65, 0.19, 0.08	449	4902
1h	225, 246, 369	0.38, 0.35, 0.11	449	4828
1i	228, 245, 366	0.42, 0.40, 0.15	447	4951
1j	229, 274, 364	0.39, 0.55, 0.11	439	4693
1k	229, 247, 362	0.40, 0.38, 0.13	442	4999
1l	227, 249, 365	0.45, 0.43, 0.15	441	4721
1m	230, 262, 363	0.44, 0.70, 0.12	441	4872
1n	234, 242, 367	0.48, 0.47, 0.13	446	4826
1o	232, 246, 367	0.36, 0.34, 0.11	449	4976
1p	232, 252, 365	0.54, 0.52, 0.15	446	4975

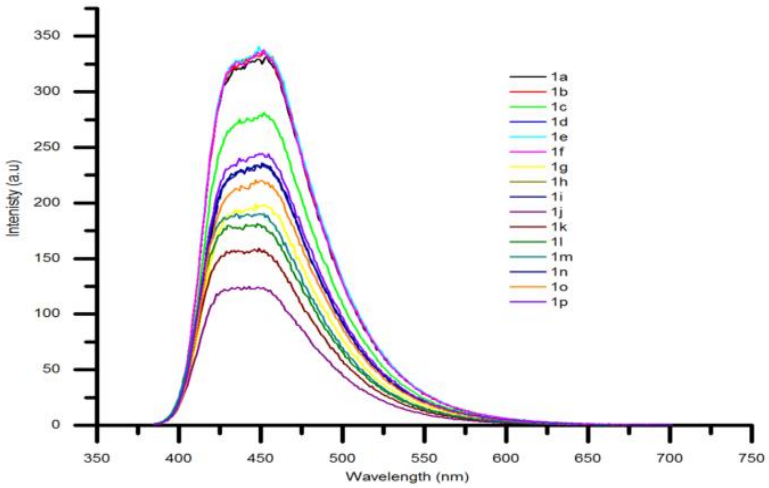


Figure S5. Fluorescence spectra of compounds **1a – 1p** in methanol solution ($1x10^{-5}$ M).

Table S6. Spectral properties of compound **1c** in different solvents.

Entry	Solvent	Orientation polarizaibility (Δf)	λ_{max} (nm)	ε x10^4 ($Lmol^{-1}cm^{-1}$)	λ_{em} (nm)	Stoke shift ($\Delta\nu$) cm^{-1}
1	1,4 Dioxane	0.0203	352	0.54	416	4370
2	Chloroform	0.1491	355	0.46	420	4359
3	Methanol	0.3098	367	0.74	450	5025
4	Acetonitirle	0.3054	353	0.86	418	4405
5	DMSO	0.2637	362	0.66	423	3983

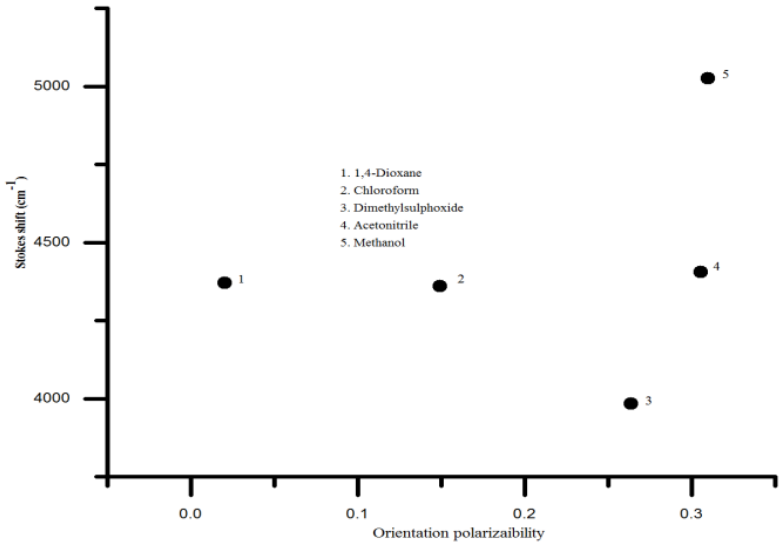


Figure S6. The Lippert – Mataga plot for compound **1c.**

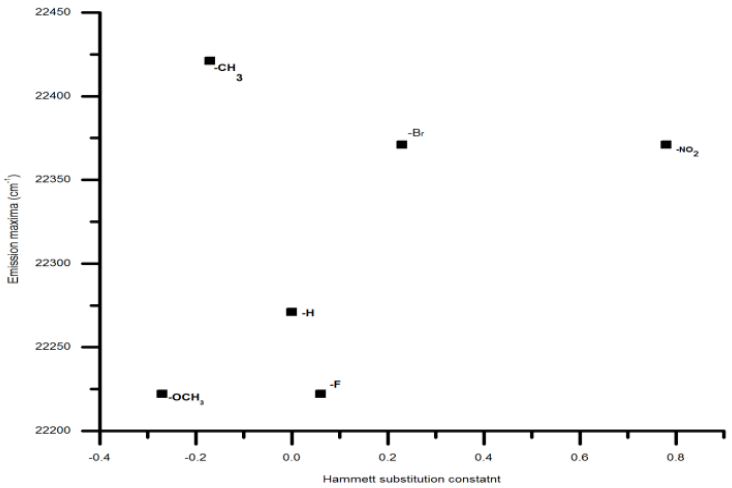


Figure S7. Dependence of fluorescence emission on the *para* hammett substitution constant in phenyl ring of 1,2,3-triazole linked to dihydropyridines

Experimental procedure for antibacterial activity

The antibacterial activity of all compounds was evaluated by the agar well diffusion method (1). All the microbial cultures were adjusted to 0.5 McFarland standard, which is visually comparable to a microbial suspension of approximately 1.5 $\times 10^6$ cfu/mL. 20 mL of Mueller Hinton agar medium was poured into each Petri plate and plates were swabbed with 100 µL inocula of the test microorganisms and kept for 15 min for adsorption. Using sterile cork borer of 8 mm diameter, wells were bored into the seeded agar plates and these were loaded with a 100 µL volume with concentration of 2.0 mg/mL of each compound reconstituted in dimethylsulphoxide (DMSO). All the plates were incubated at 37^0C for 24 h. Antibacterial activity of each compound was evaluated by measuring the zone of growth inhibition against the test organisms with zone reader (HiAntibiotic zone scale). DMSO was used as a negative control whereas Ciprofloxacin was used as positive control. This procedure was performed in

three replicate plates for each organism and the mean values of the diameter of inhibition zones ± standard deviations were calculated.

Determination of Minimum Inhibitory Concentration (MIC) of chemical compounds

MIC of the compounds against bacterial strains was tested through a modified agar well diffusion method (1). In this method, a two fold serial dilution of each chemically synthesized compound was prepared by first reconstituting the compound in DMSO followed by dilution in sterile distilled water to achieve a decreasing concentration range of 512 to 1µg/mL. A 100 µL volume of each dilution was introduced into wells (in triplicate) in the agar plates already seeded with 100 µL of standardized inoculum (10^6 cfu/mL) of the test microbial strain. All test plates were incubated aerobically at 37^oC for 24 h and observed for the inhibition zones. MIC, taken as the lowest concentration of the chemical compound that completely inhibited the growth of the microbe, showed by a clear zone of inhibition, was recorded for each test organism. Ciprofloxacin was used as positive control.

Experimental procedure for antifungal activity

The antifungal activity all compounds was evaluated by poisoned food technique (2). The molds were grown on Sabouraud dextrose agar (SDA) at 25^0C for 7 days and used as inocula. The 15 mL of molten SDA (45^0C) was poisoned by the addition of 100 µL volume of each compound having concentration of 2.0 mg/mL reconstituted in the DMSO, poured into a sterile Petri plate and allowed it to solidify at room temperature. The solidified poisoned agar plates were inoculated at the center with fungal plugs (8 mm diameter) obtained from the colony margins and incubated at 25^0C for 7 days. DMSO was used as the negative control whereas fluconazole was used as the positive control. The experiments were performed in triplicates. Diameter of fungal colonies was measured and expressed as percent mycelial inhibition.

Percent inhibition of myelial growth = (dc-dt) / dc × 100

dc = average diameter of fungal colony in negative control sets; dt = average diameter fungal colony in experimental sets.

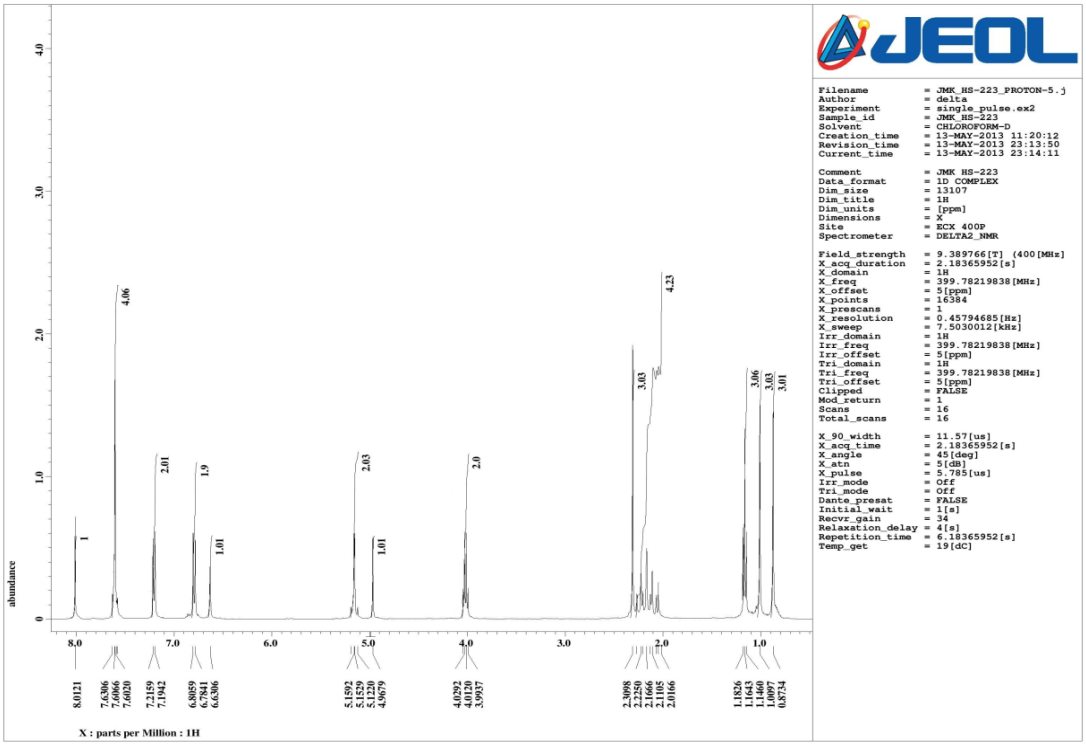
Experimental procedure for DPPH free radical scavenging assay

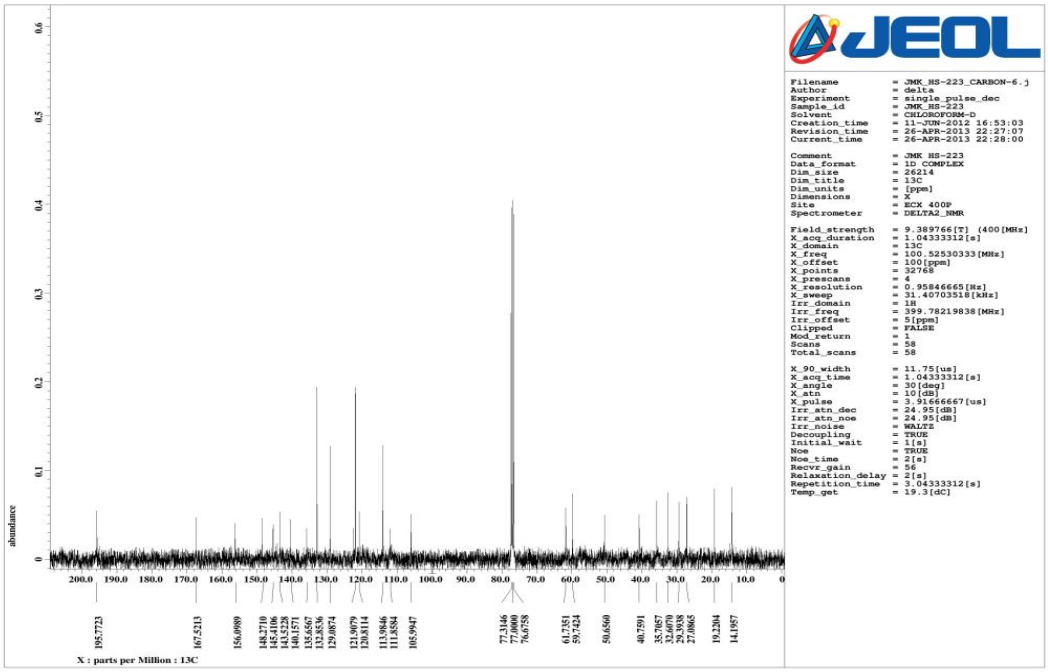
Methanol solution of 2,2-diphenyl-1-picrylhydrazyl (DPPH) was used as a reagent for the spectrophotometric assay (3). Solutions of two different concentration of triazole linked pentasubstituted-1,4-dihydropyridines (**1a -1p**) *i.e.* 0.8 µM/mL and 0.4 µM/mL were prepared using methanol. 1 mL of 0.1 mM methanolic solution of DPPH was added to 3 mL solution of the compounds and the mixture was shaken vigorously using vortex mixer. Absorbance was read against a blank at 517 nm after incubation of the reaction mixtures for 60 min in dark at room temperature. Butylated hydroxyl toluene (BHT) was used as a reference compound. The radical scavenging activities were expressed as the inhibition percentage and were calculated using the formula:

Radical Scavenging activity (%) = $[(A_0 - A_1)/A_0) \times 100]$

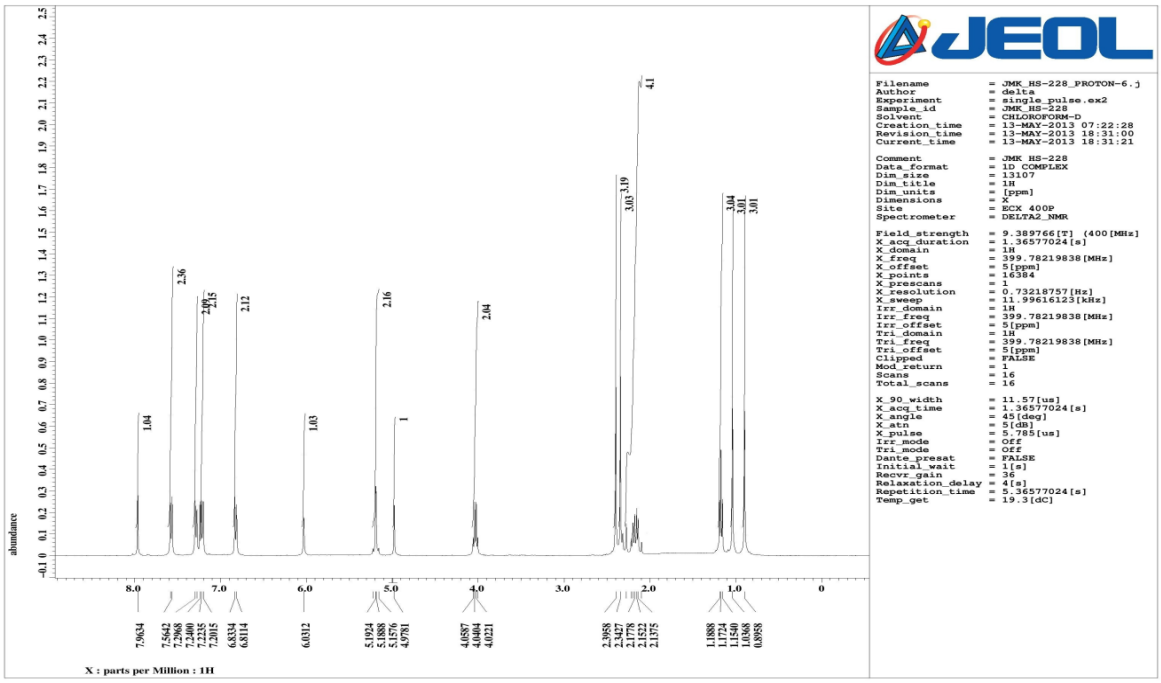
Where A_0 is absorbance of the control (blank, without compound) and A_1 is the absorbance of the compound.

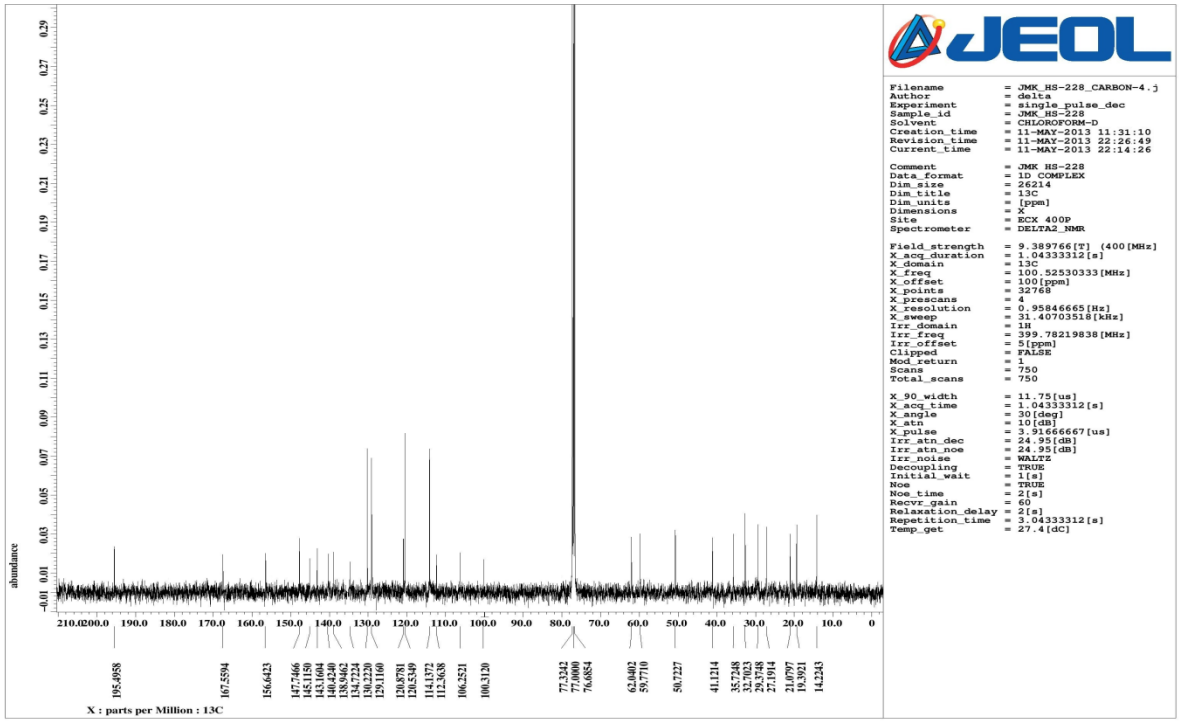
^{1}H and ^{13}C NMR spectra of compound 1a



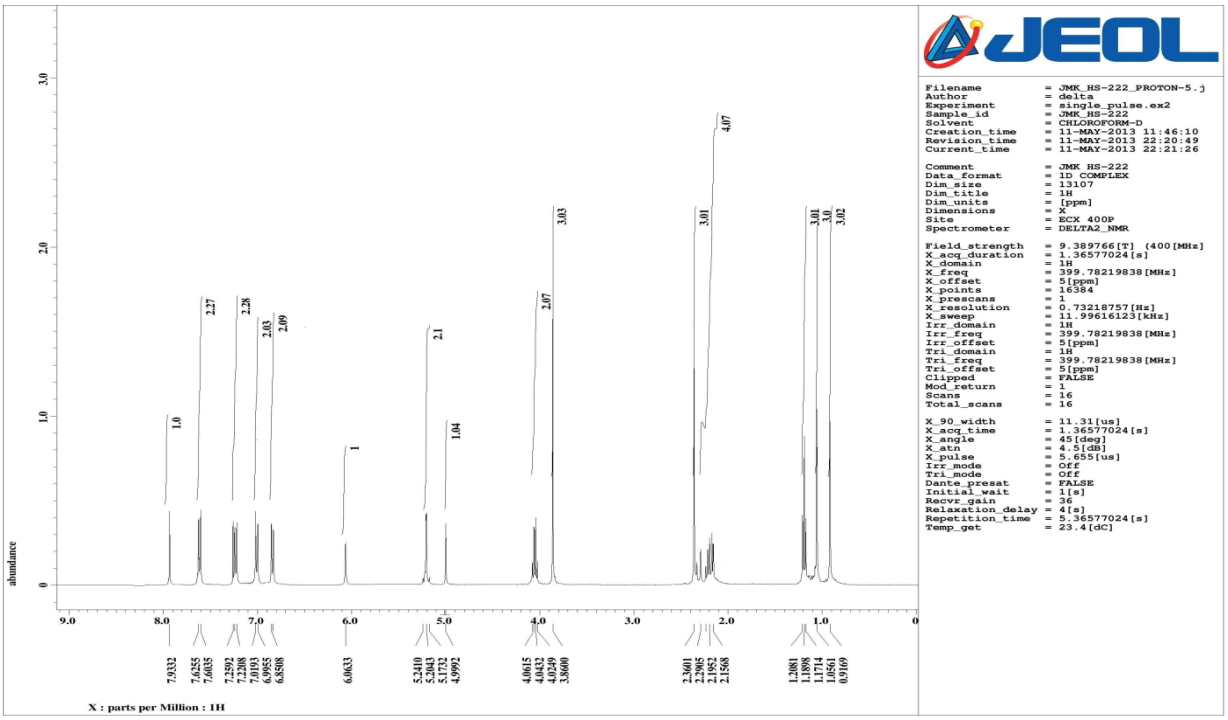


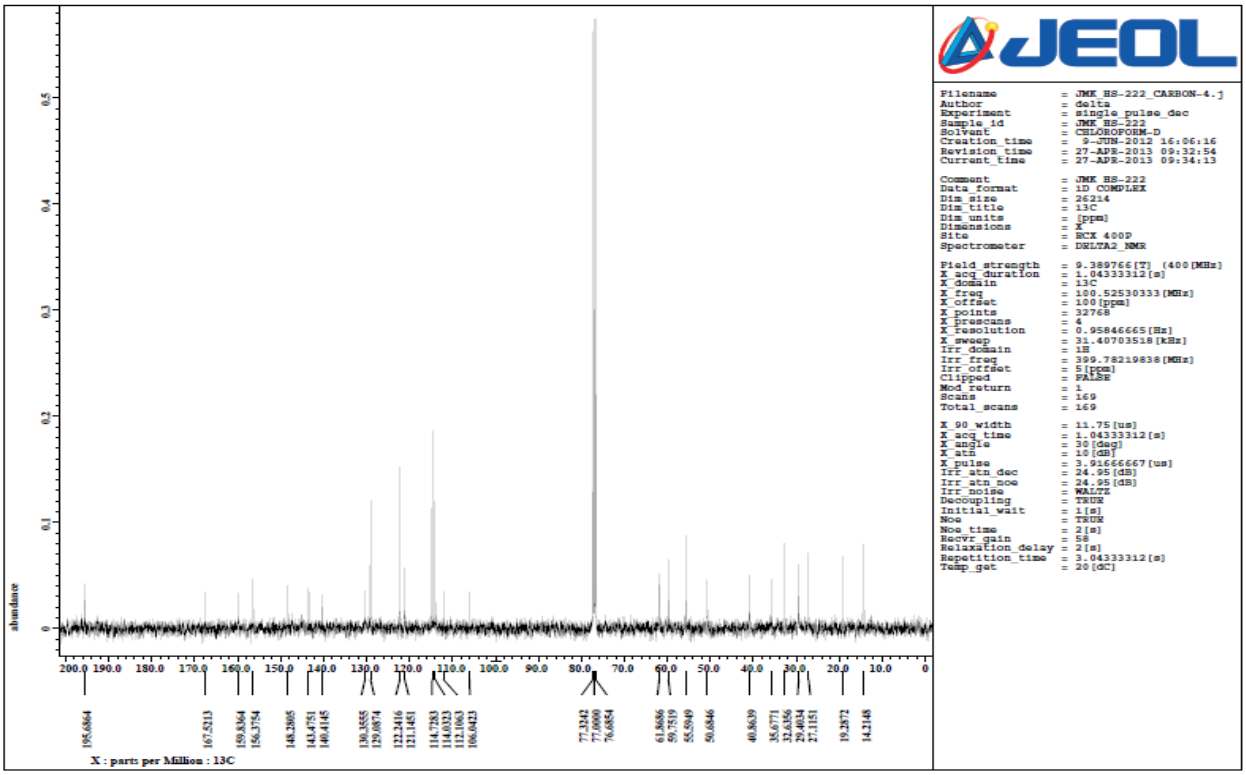
^{1}H and ^{13}C NMR spectra of compound 1b



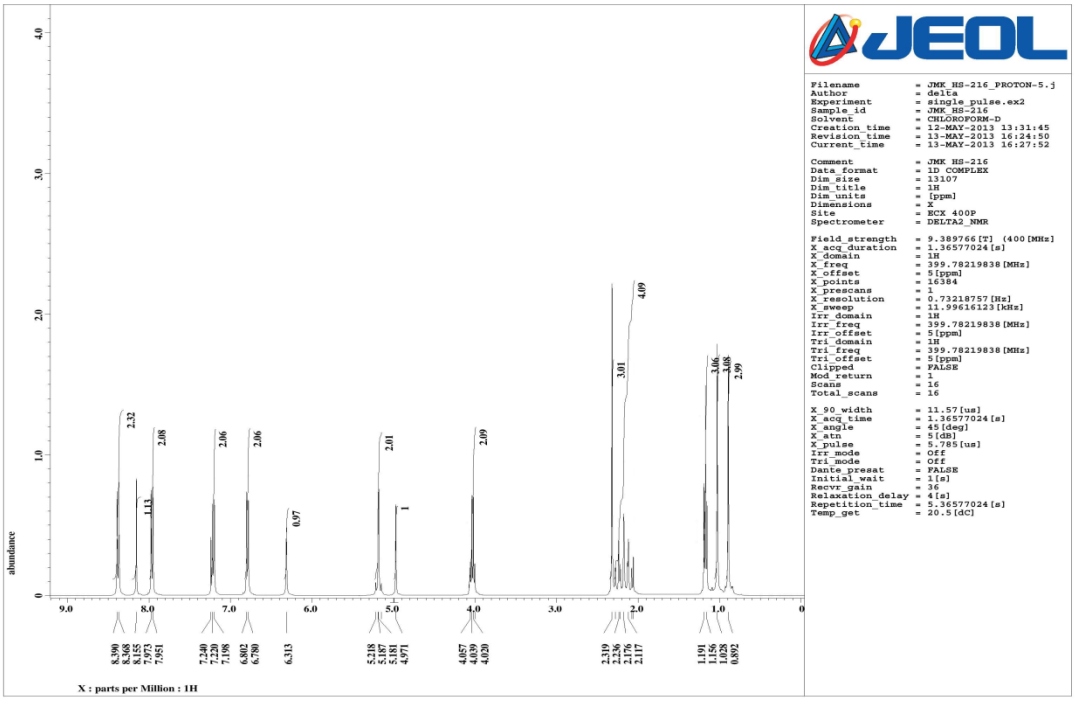


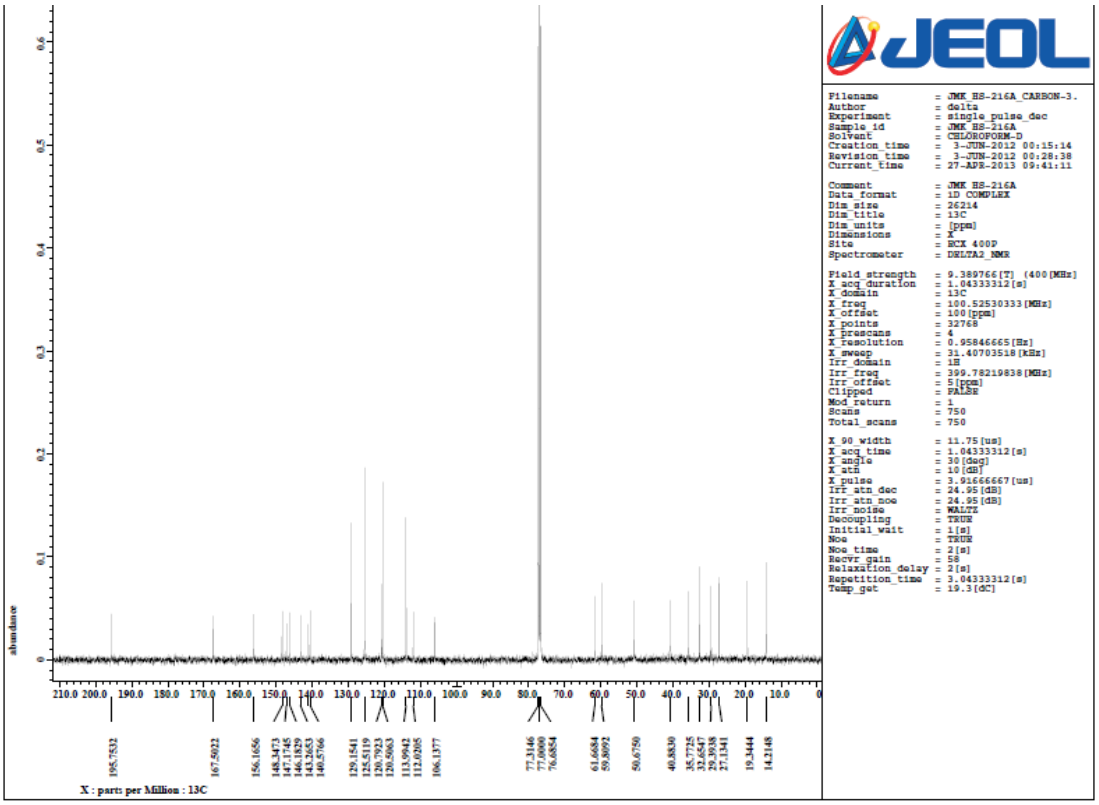
^{1}H and ^{13}C NMR spectra of compound 1c





^{1}H and ^{13}C NMR spectra of compound 1d





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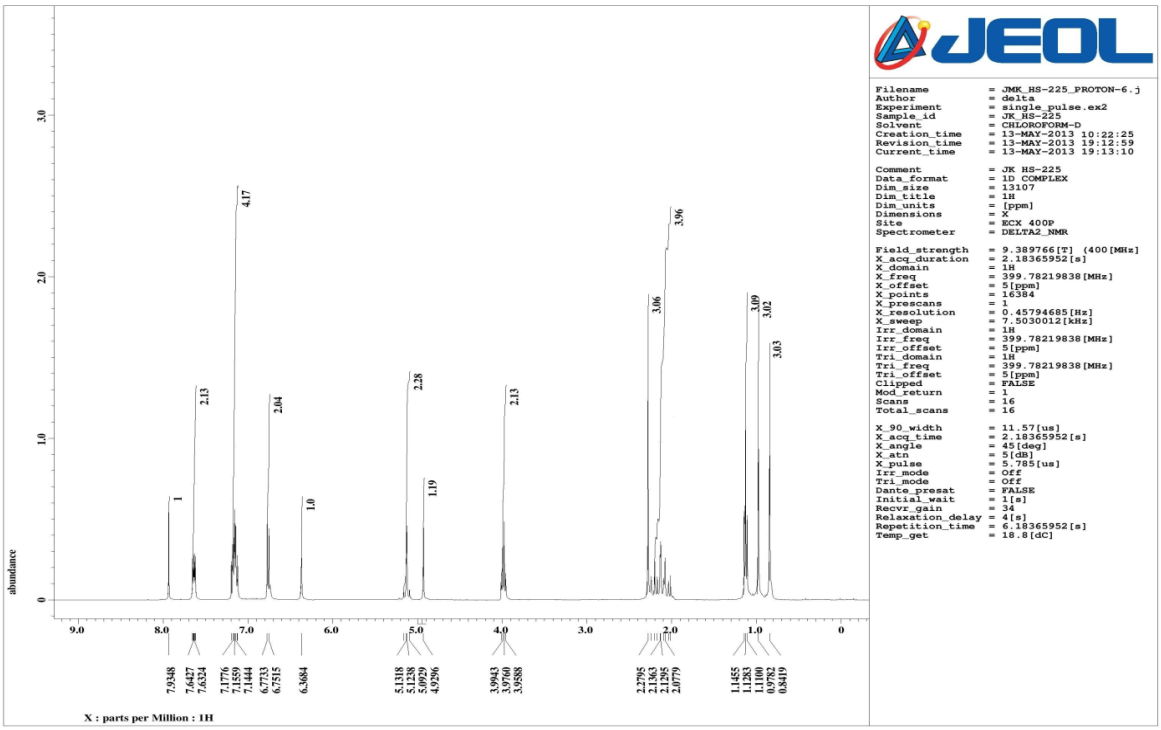

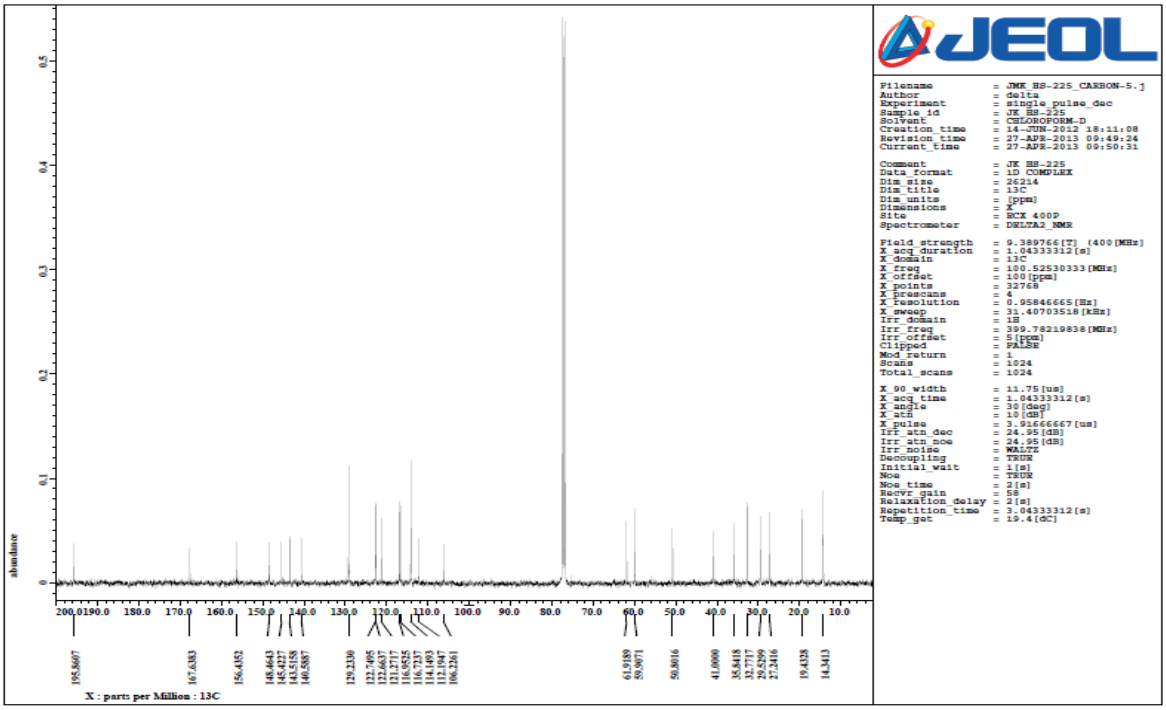

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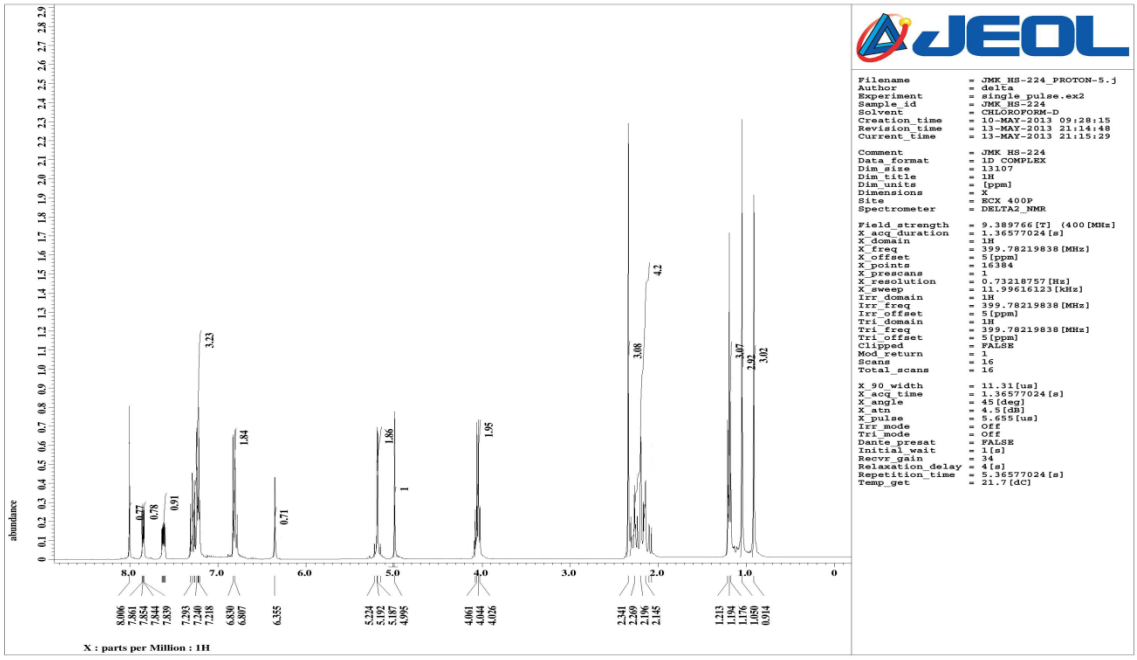

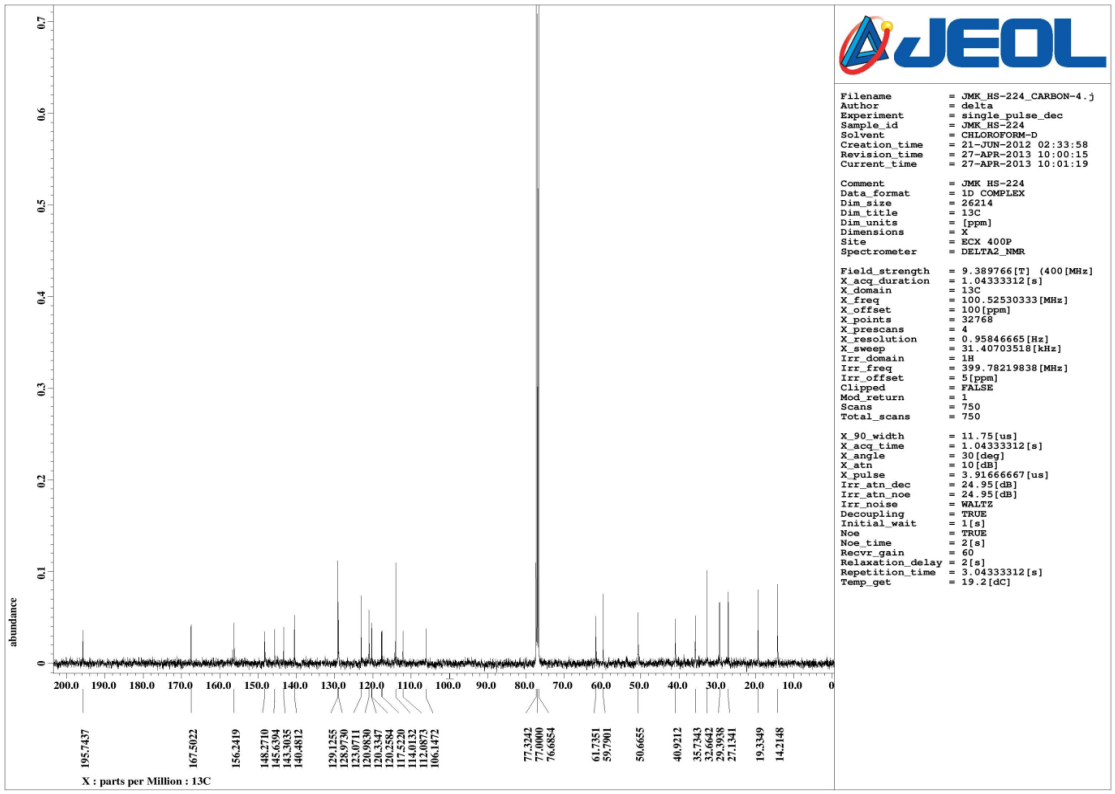

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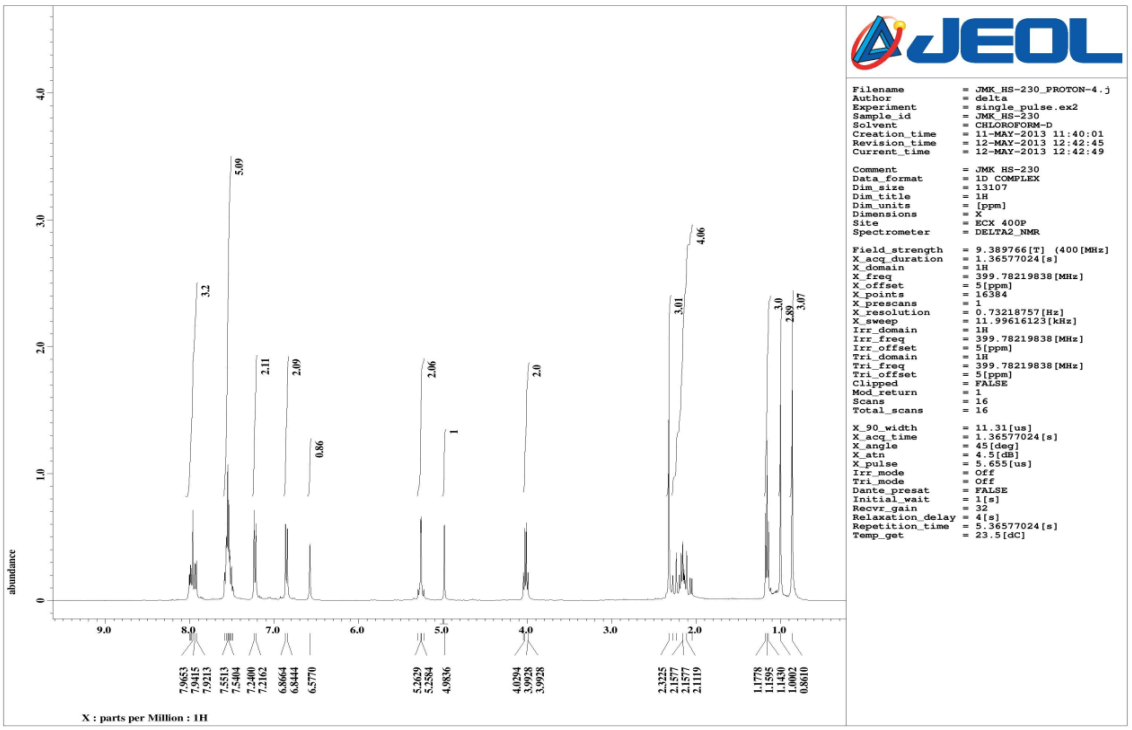
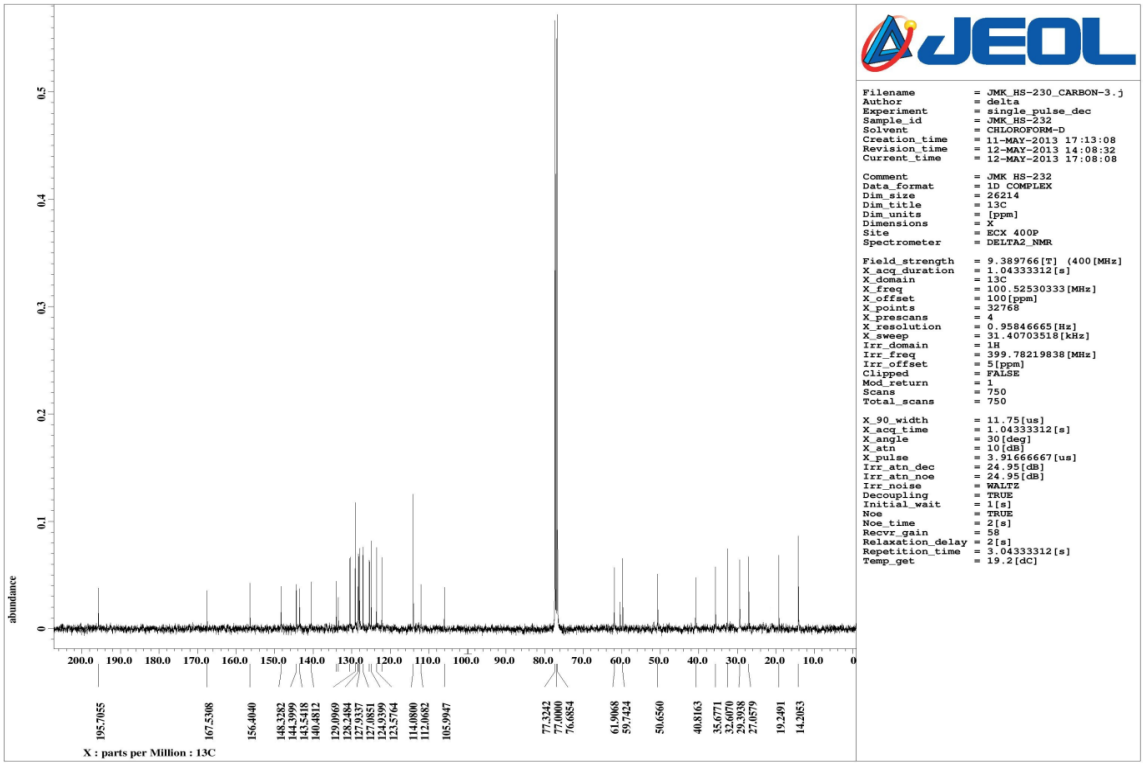
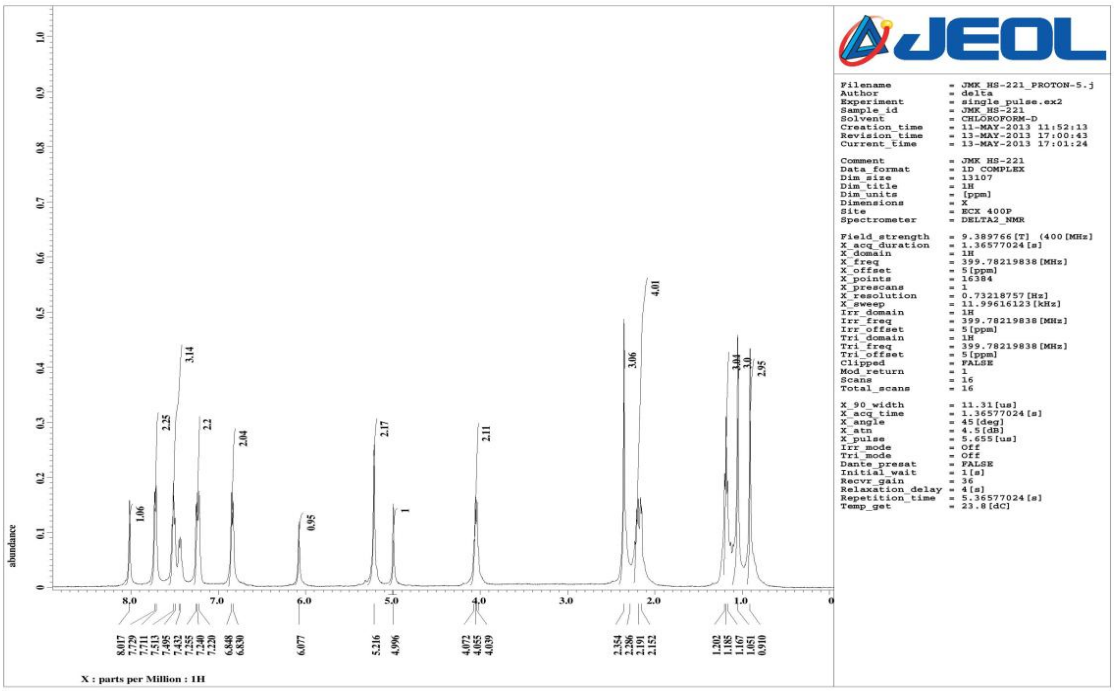
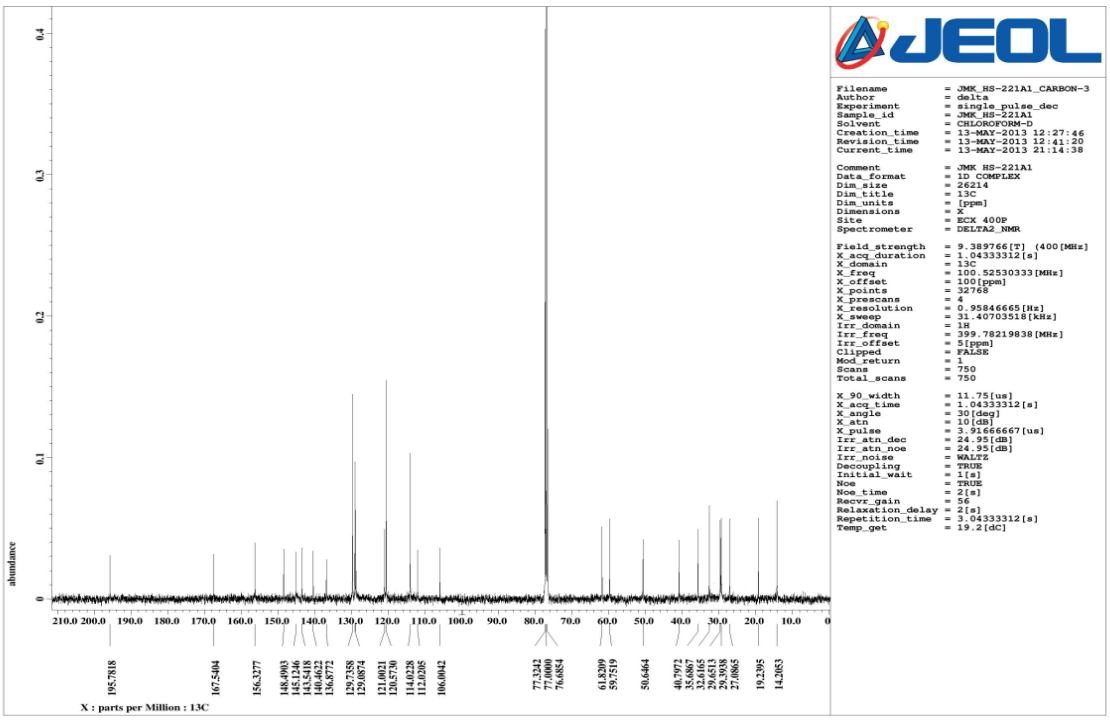


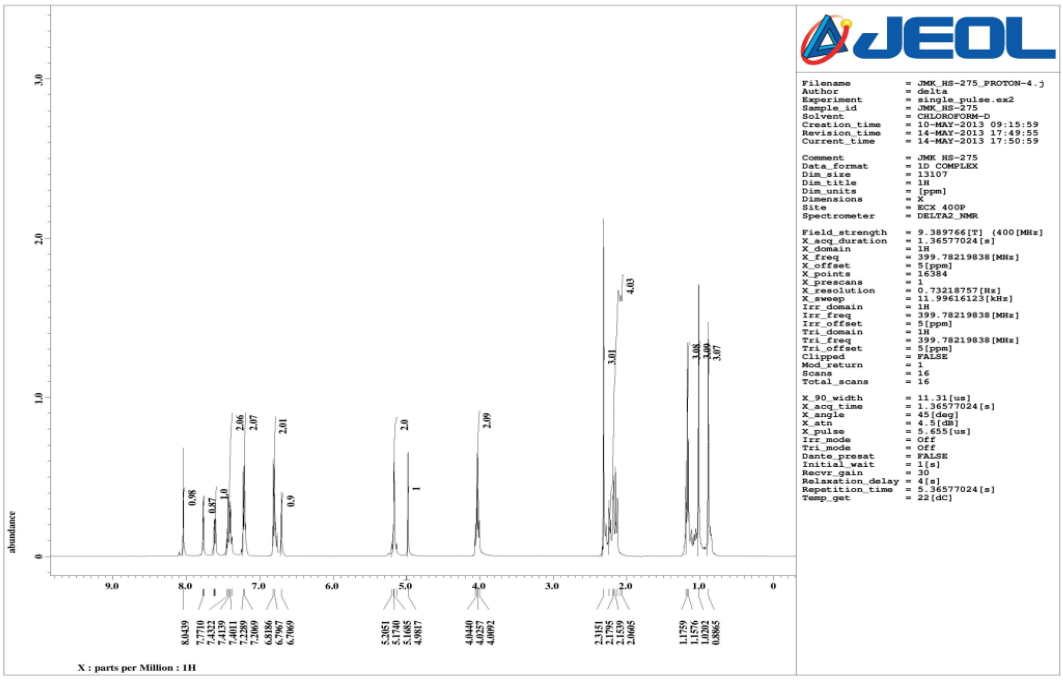


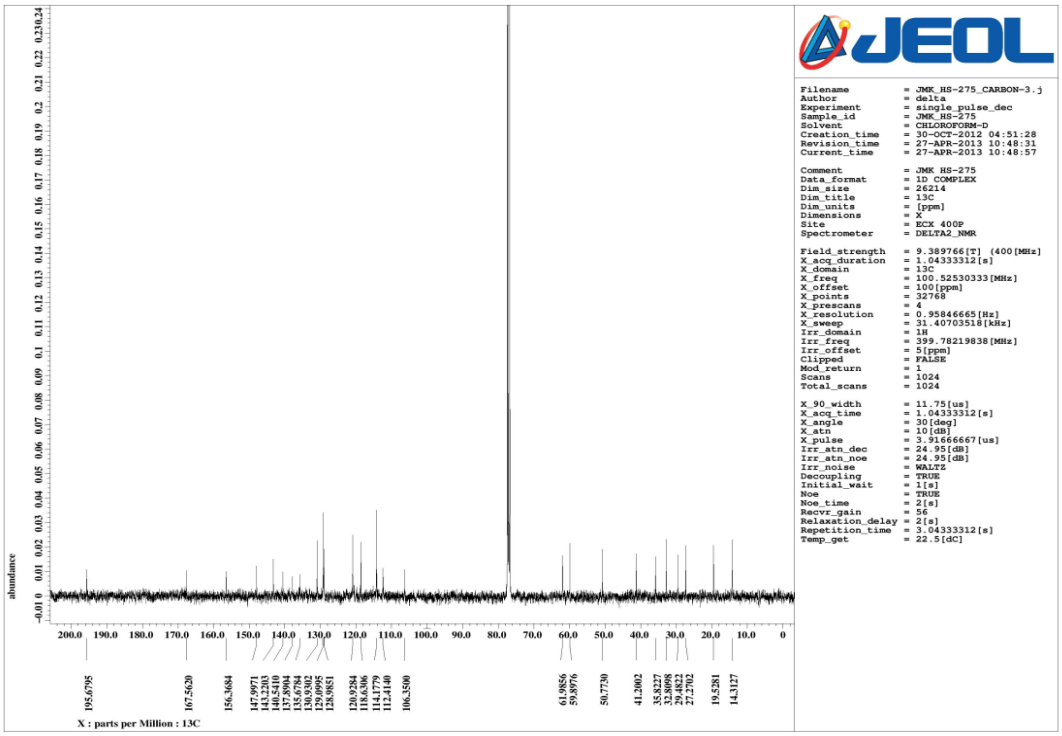
^{1}H and ^{13}C NMR spectra of compound 1h





^{1}H and ^{13}C NMR spectra of compound 1i





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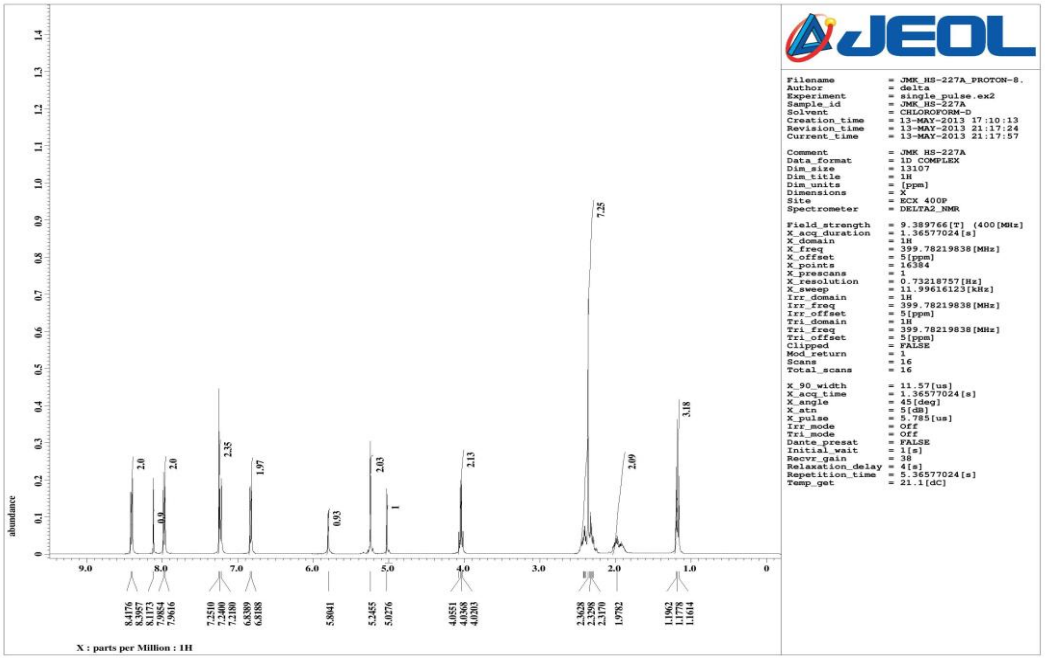

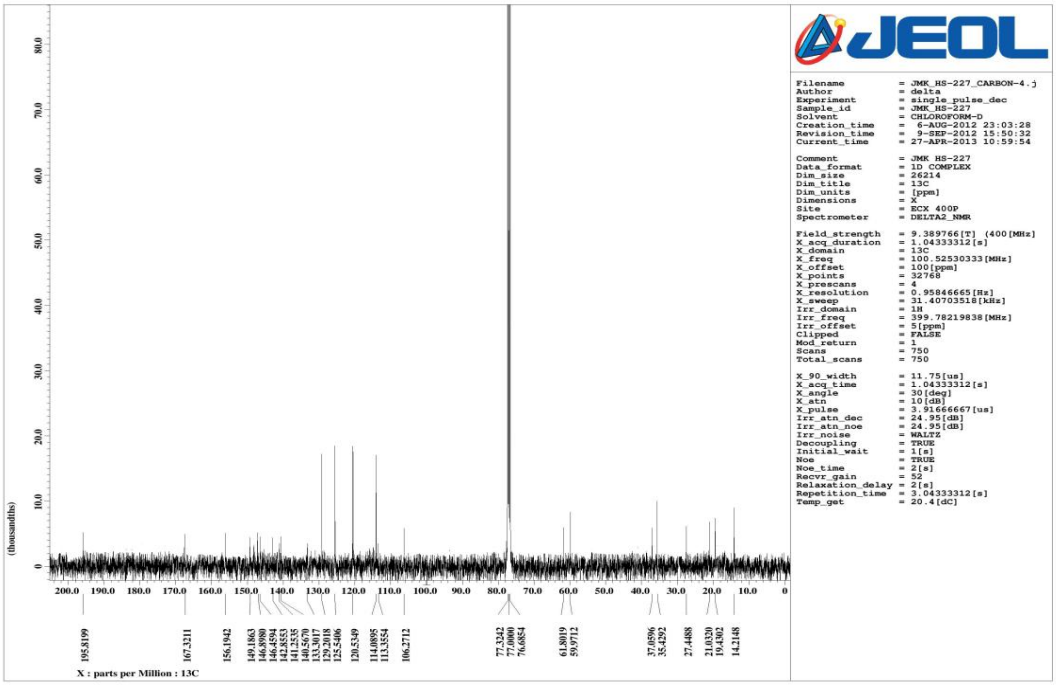

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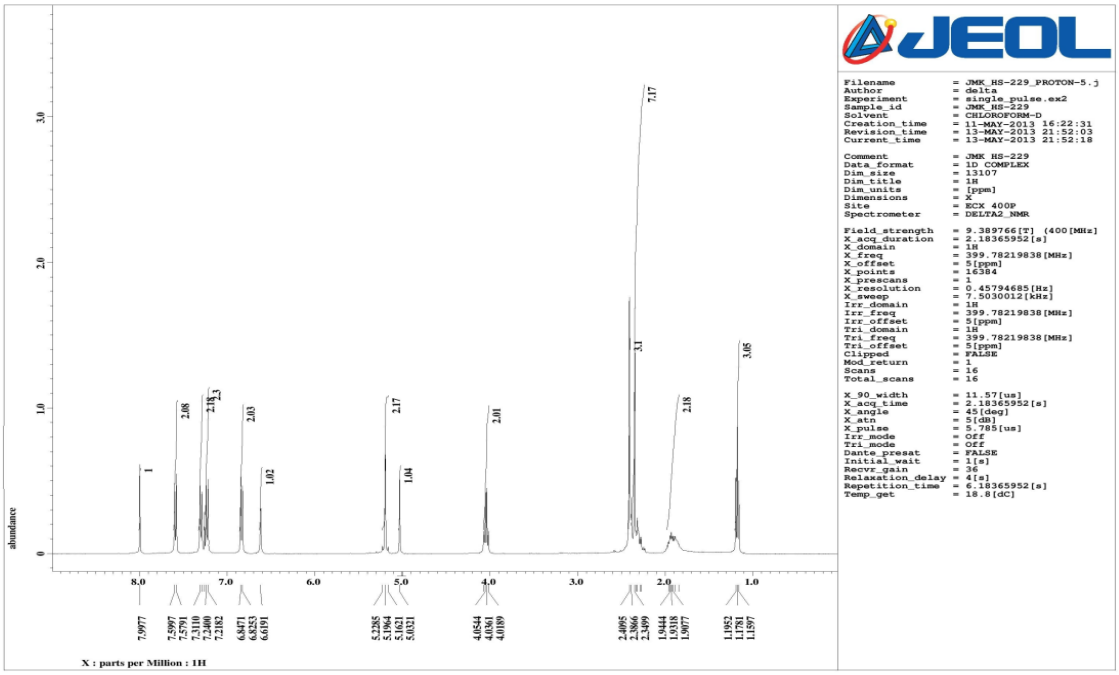

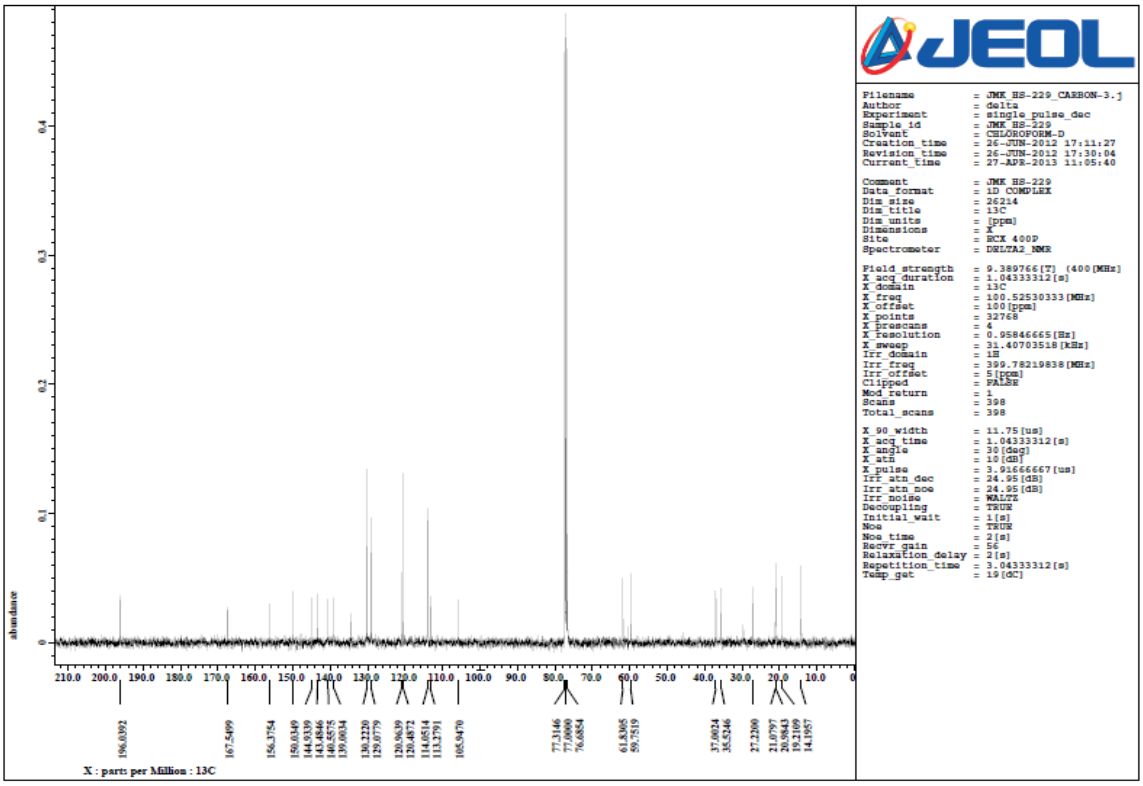

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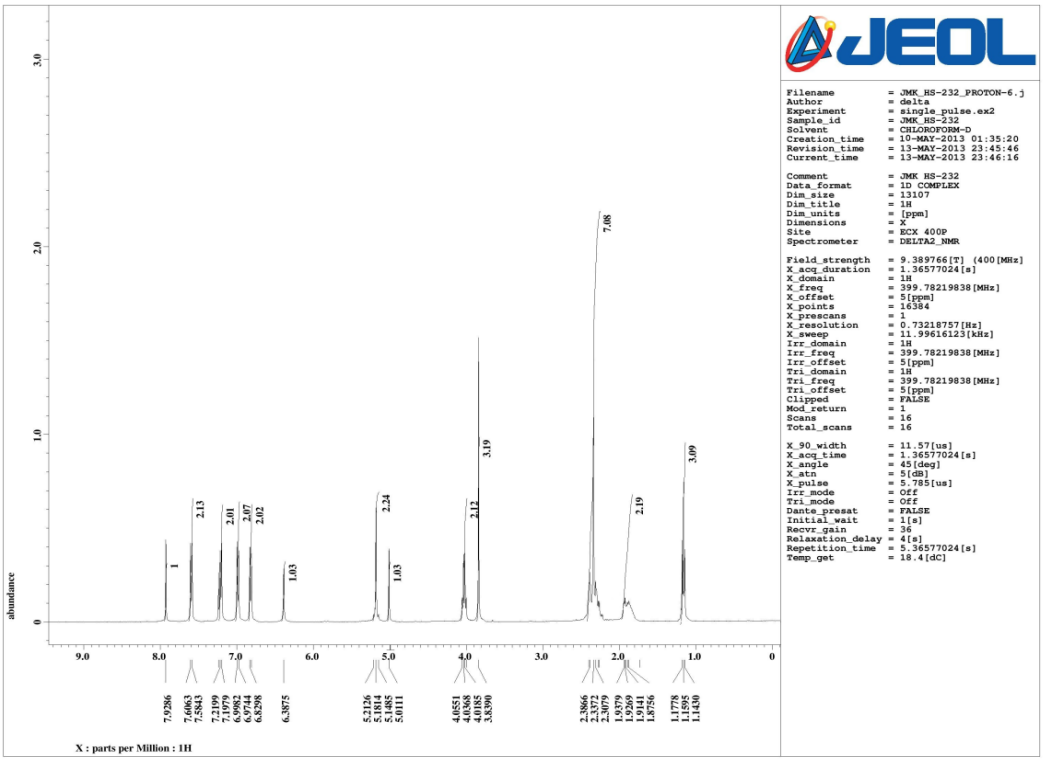
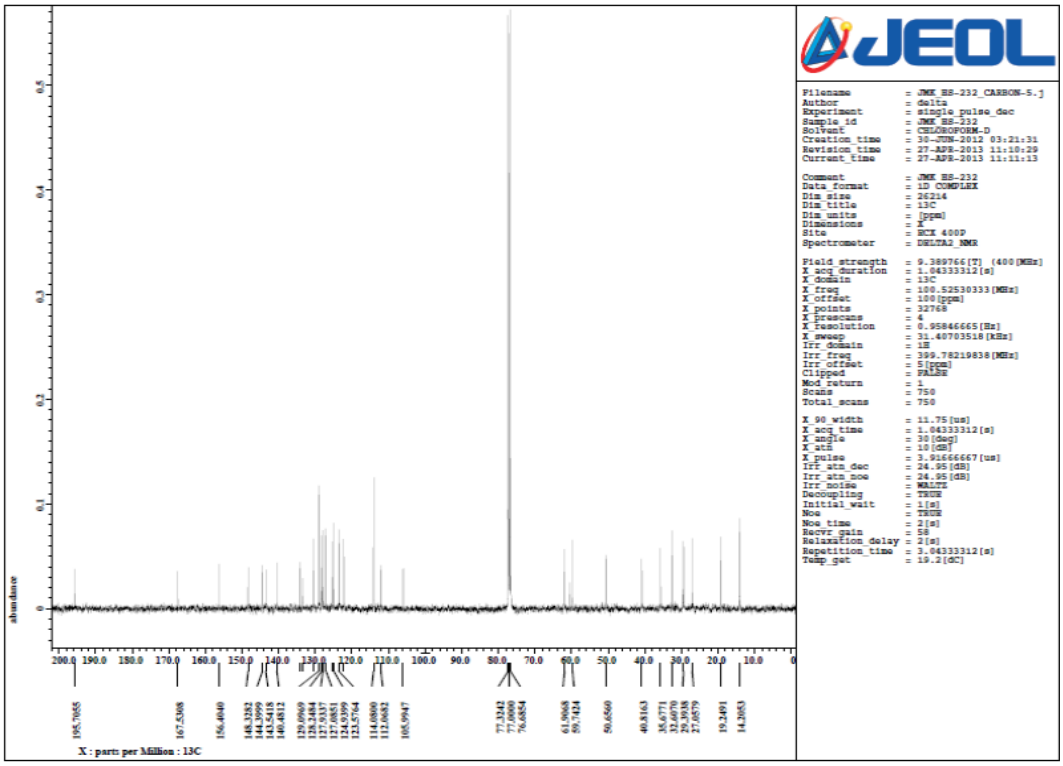
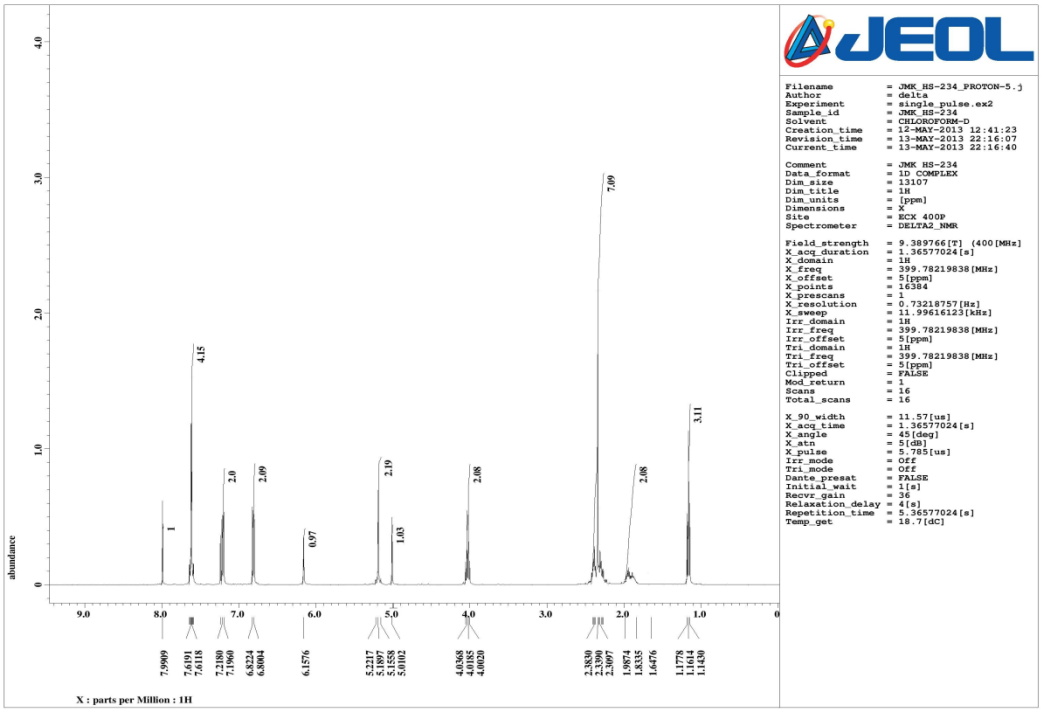
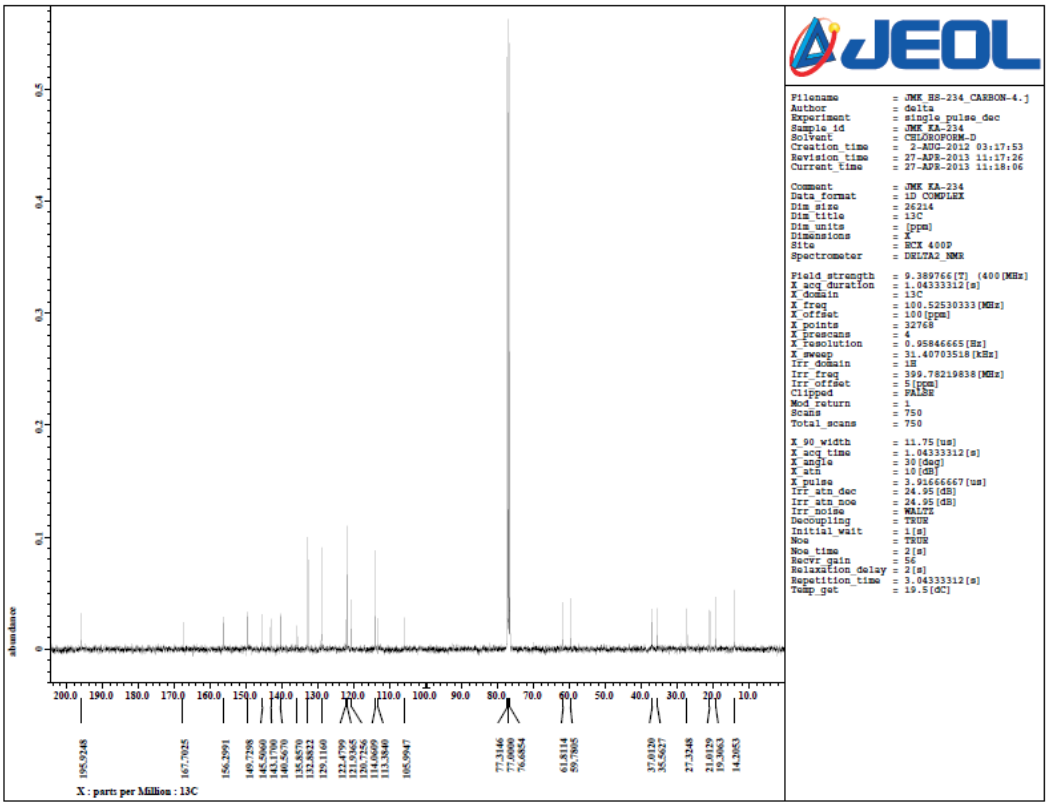


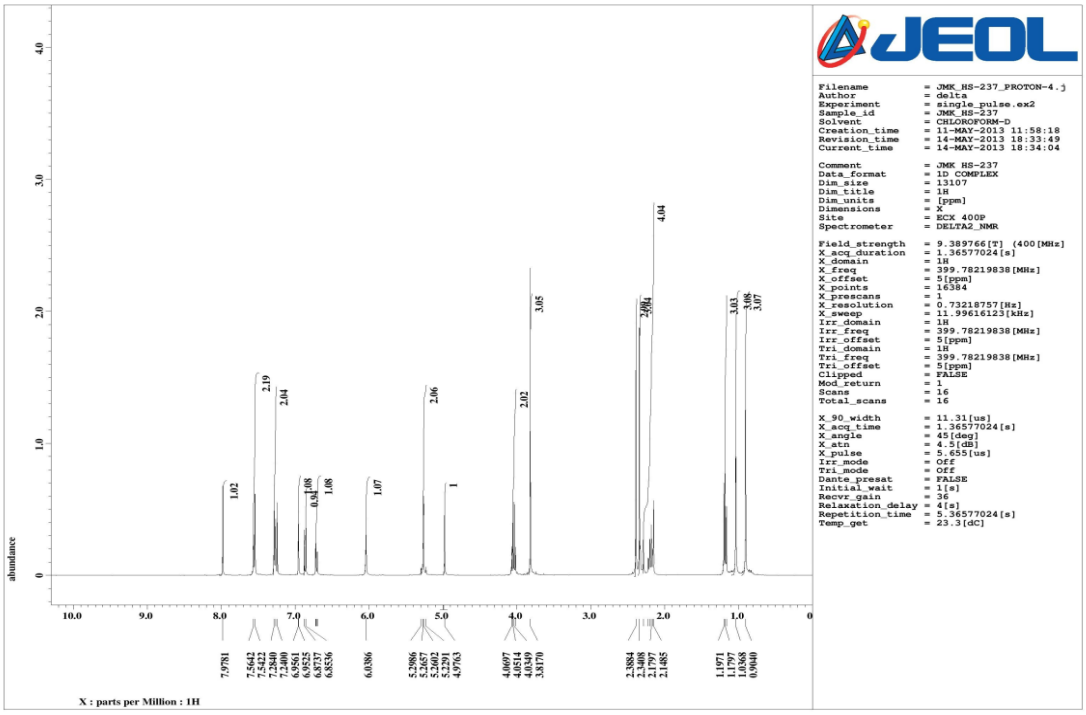


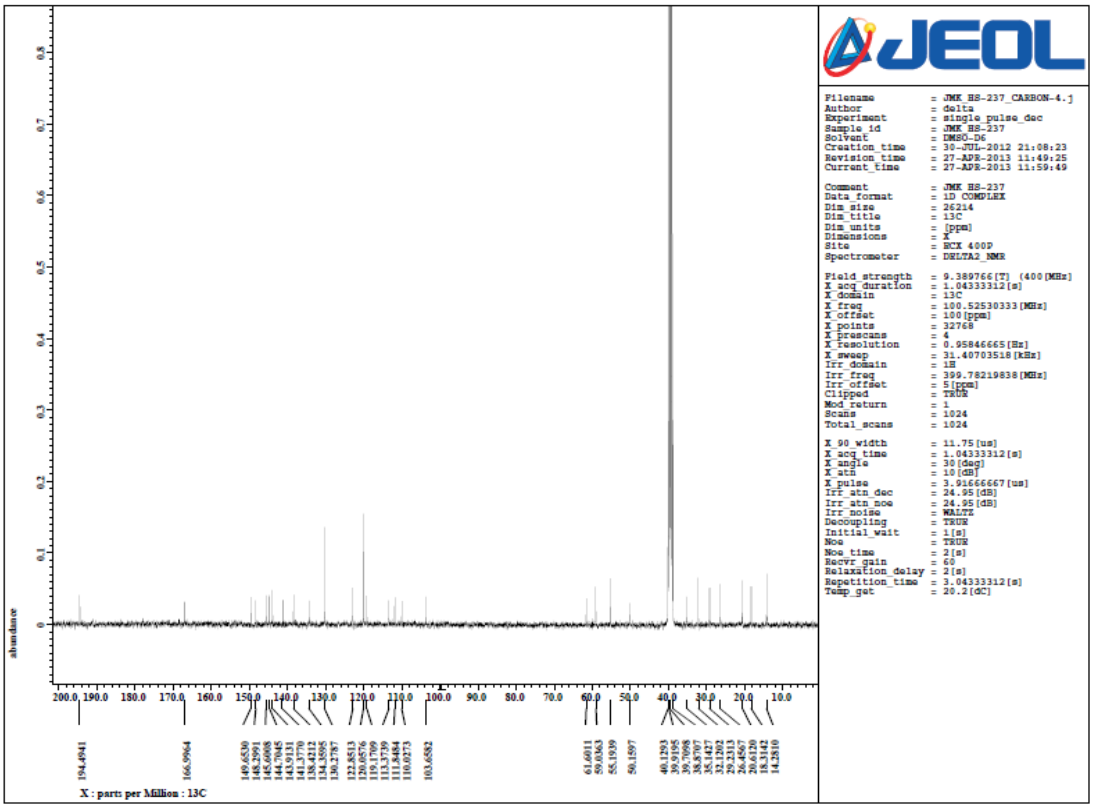
^{1}H and ^{13}C NMR spectra of compound 1m



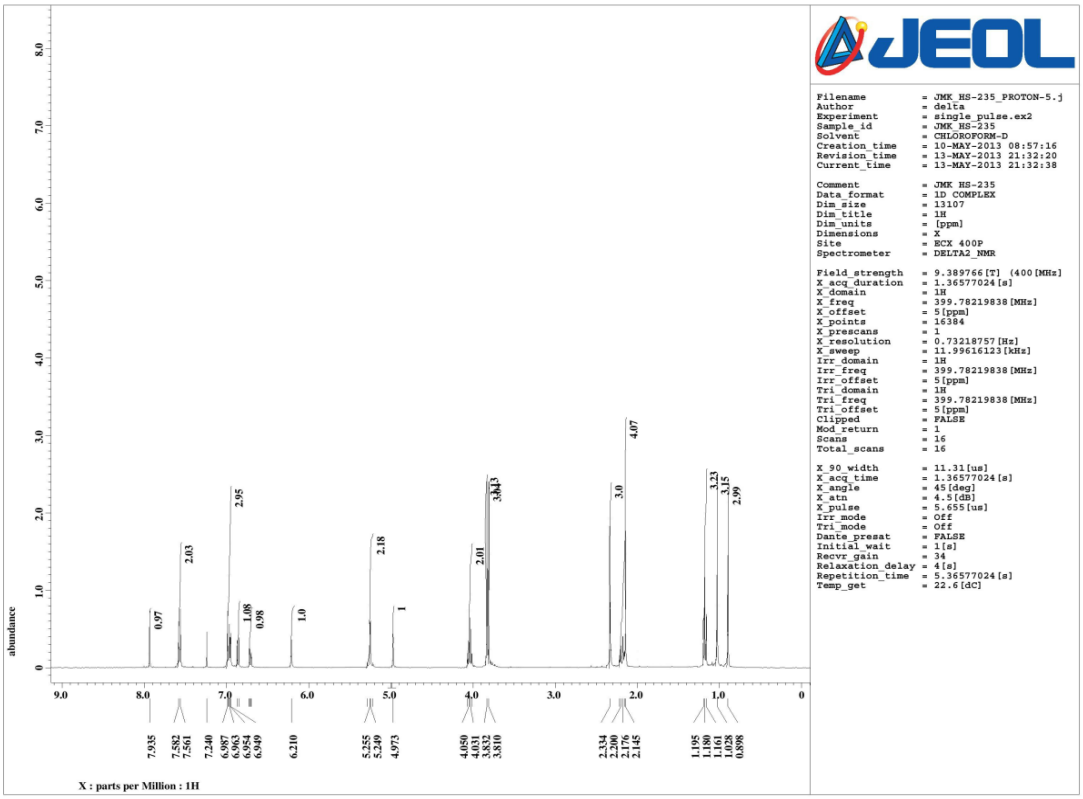


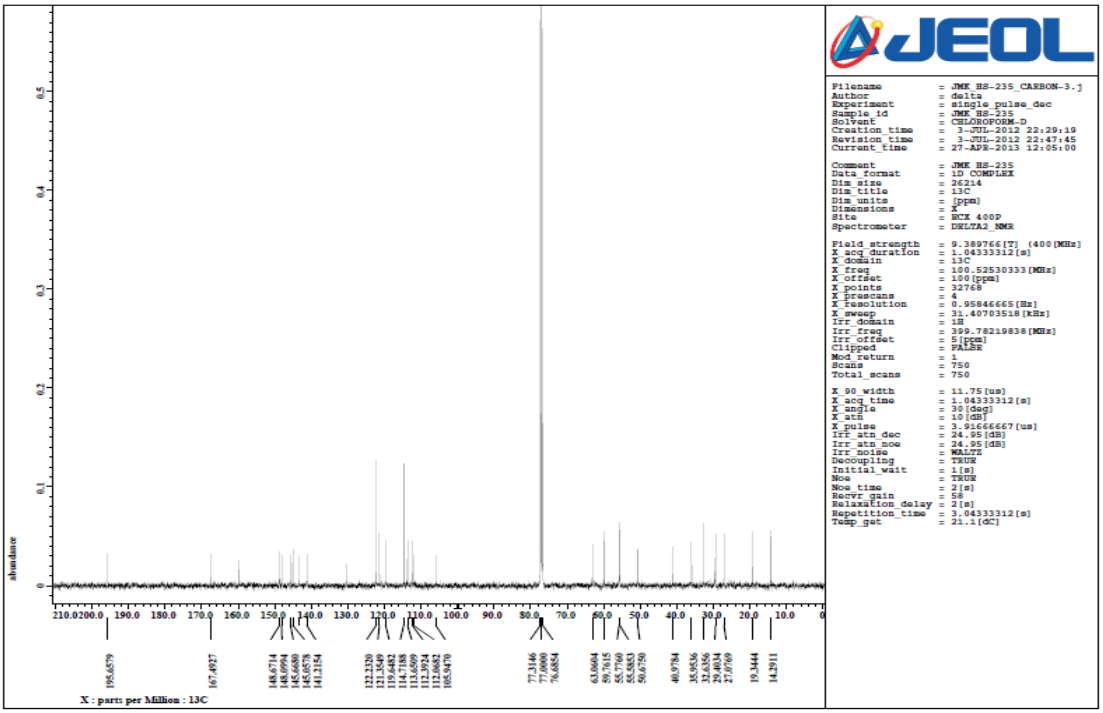
^{1}H and ^{13}C NMR spectra of compound 1n



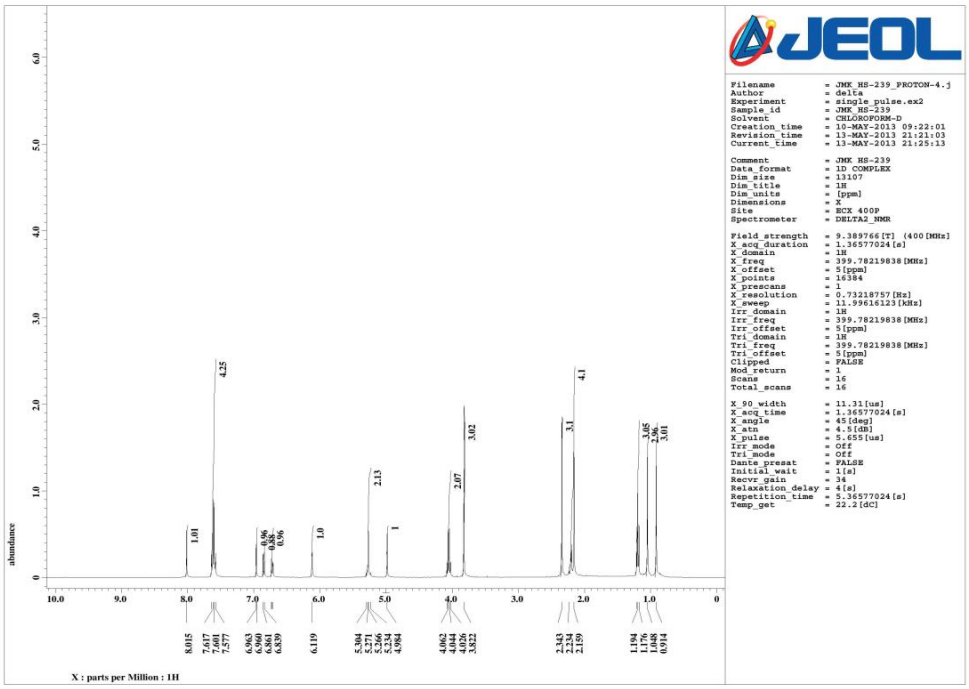


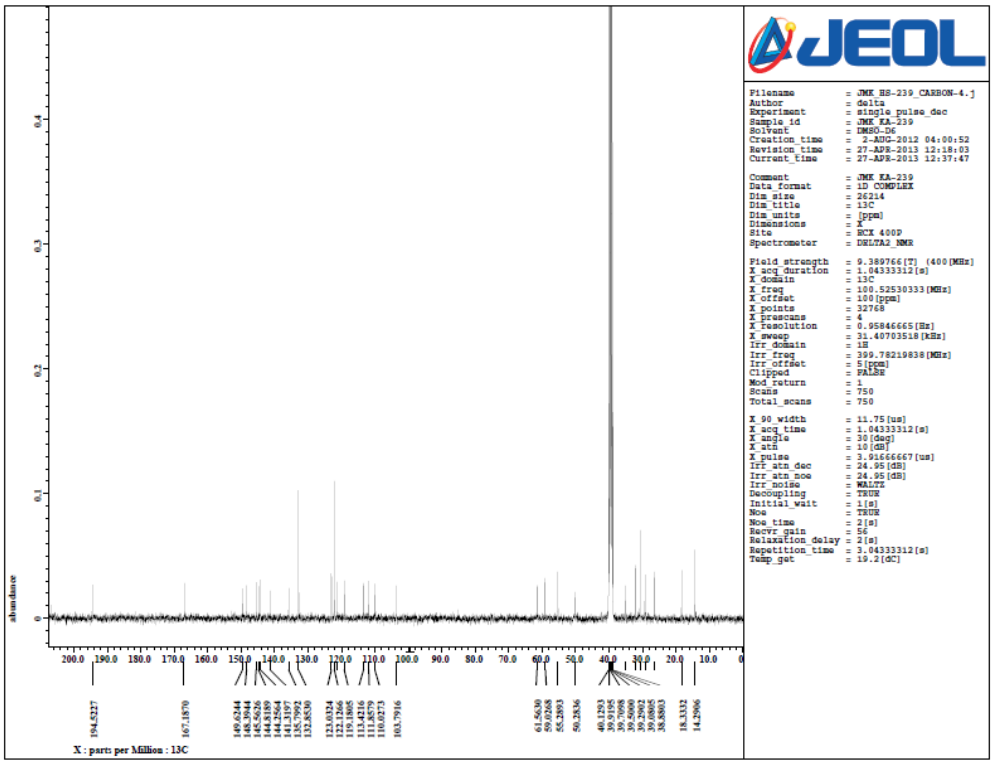
^{1}H and ^{13}C NMR spectra of compound 1o





^{1}H and ^{13}C NMR spectra of compound 1p





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