

Supporting Information

**Thiolate-assisted Copper(I) Catalyzed C–S Cross Coupling of Thiols with
Aryl Iodides: Scope and Mechanism**

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Table of Contents	Page No.
1 Optimization chart	S3
2 Determination of Reaction Order in iodobenzene	S4
3 Determination of Reaction Order in 4-methylbenzenethiol	S5
4 Kinetics Analysis Set-I: Initial rates for C-S coupling reaction between 4-methylbenzenethiol with substituted aryl iodides.	S6
5 Kinetics data for Hammett plot with the variation of aryl iodides	S7
6 Kinetics Analysis Set-II: Initial rates for C-S coupling reaction between substituted thiophenols with iodobenzene	S8
7 Kinetics data for Hammett plot with the variation of thiophenols	S10
8 NMR spectra	S11
9 Figure S1: Optimized geometries of Cu complexes shown in Scheme 9	S53
10 Scheme S1: Reaction Profile diagram for pathway-I initiated by Cu(SPh)	S54
11 Scheme S2: Reaction Profile diagram for pathway-II initiated by [Cu(SPh) ₂]K	S54
12 Scheme S3: Reaction Profile diagram for pathway-III initiated by [Cu(SPh)(O ^t Bu)]K	S55
13 Scheme S4: Reaction Profile diagram for pathway-IV initiated by Cu ₂ [μ-(^t BuO) ₂]	S55
14 Scheme S5: Reaction Profile diagram for pathway-V (Solvent Assisted).	S56
15 Scheme S6: Reaction Profile diagram for pathway-VI (Solvent Assisted).	S56
16 Optimized geometries (M062X, Cartesian coordinates in Å) and energies of reactants transition state and intermediates.	S57

1. Optimization chart

Table S1: Screening of solvents and optimization of reaction conditions.

Entry	Solvent	Base	Time (hrs)	Yield (%) (3a)
1	H ₂ O	KOH	16	66
2	H ₂ O	K ₃ PO ₄	16	6
3	H ₂ O	K ₂ CO ₃	16	11
4	H ₂ O	KO ^t Bu	16	44
5	DME	KO ^t Bu	16	61
6	H ₂ O+DME (1:9)	KO ^t Bu	16	77
7	H₂O+DME (1:4)	KO^tBu	16	83
8	H ₂ O+DME (3:7)	KO ^t Bu	16	78
9	H ₂ O+DME (2:3)	KO ^t Bu	16	69
10	H ₂ O+DME (1:1)	KO ^t Bu	16	62
11	H ₂ O+DME (1:4)	KO ^t Bu	4	77
12	Ethanol	KO ^t Bu	4	77
13	Ethanol	KO^tBu	8	78
14	Methanol	KO ^t Bu	4	68
15	Butanol	KO ^t Bu	4	48
16	H ₂ O/Ethanol (1:4)	KO ^t Bu	4	66
17	H ₂ O/Butanol (1:4)	KO ^t Bu	4	59
18	DME/Ethanol (1:4)	KO ^t Bu	4	64
19	THF/Ethanol (1:4)	KO ^t Bu	4	20
20	DMSO	KO ^t Bu	4	54
21	DMF	KO ^t Bu	4	62
22	CH ₃ CN	KO ^t Bu	4	60

Reaction conditions: **1** (0.5 mmol), **2** (0.62 mmol), CuI (0.025 mmol= 5 mol%), base (1 mmol), solvent (250 μ L), 100 $^{\circ}$ C, N₂ atm.

2. Kinetic study

Table S2: Yield of **3a** (%) in 20% H₂O/DME and ethanol

Entry	Time (hrs)	Yield (%)	Yield (%)
		(3a) (20% H ₂ O/DME)	(3a) (Ethanol)
1	1	17	65
2	2	47	73
3	3	72	76
4	4	77	77
5	5	78	78
6	6	78	78

Reaction conditions: **1** (0.5 mmol), **2** (0.62 mmol), CuI (0.025 mmol= 5 mol%), base (1 mmol), solvent (250 μ L), 100 $^{\circ}$ C, N₂ atm.

3. Determination of Reaction Order in iodobenzene: Coupling of 4-methylbenzenethiol with iodobenzene using different concentrations.

Table S3. Yield of **4a** (%) with variation in concentration of iodobenzene (**2**).

4-methylthiophenol (mmol)	2 (mmol)	[2] / M	Yield 4a (%) ^a	Rate (mM/min)
0.5	0.375	1.5	42	6.95
0.5	0.5	2	48	7.95
0.5	0.62	2.48	54	9.00
0.5	0.75	3	56	9.22

^a Yield (%) is calculated with respect to the 4-methylthiophenol.

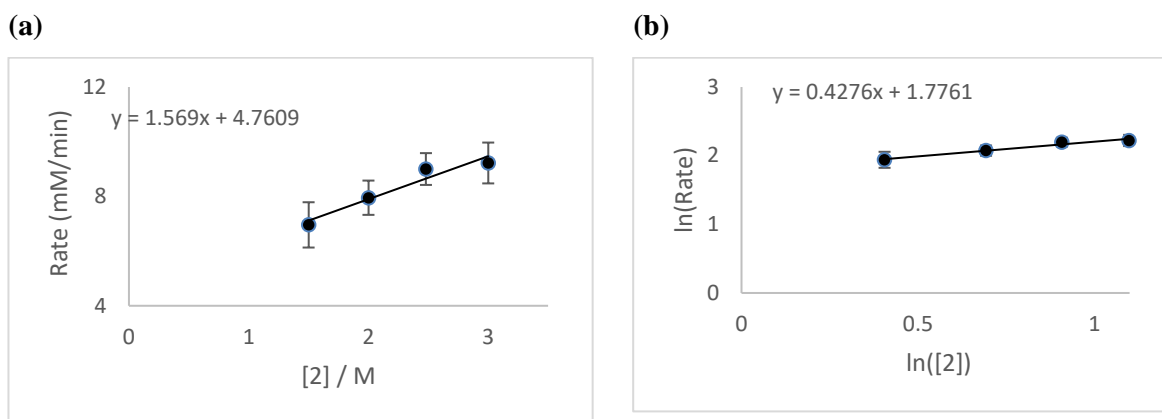


Figure S1: The plot of (a) Rate (M/s) vs concentration of iodobenzene [2], (b) ln(Rate) vs ln[2].

4. Determination of Reaction Order in 4-methylbenzenethiol: Coupling of different concentrations of 4-methylbenzenethiol with iodobenzene.

Table S4. Yield of **4a** (%) with variation in concentration of 4-methylbenzenethiol.

4-methylthiophenol (mmol)	2 (mmol)	[4-methylbenzenethiol] / M	Yield ^a 4a (%)	Rate (mM/min)
0.5	0.62	2	54	8.94
0.62	0.62	2.48	48	9.93
0.75	0.62	3	44	11.32

^a Yield (%) is calculated with respect to the 4-methylthiophenol.

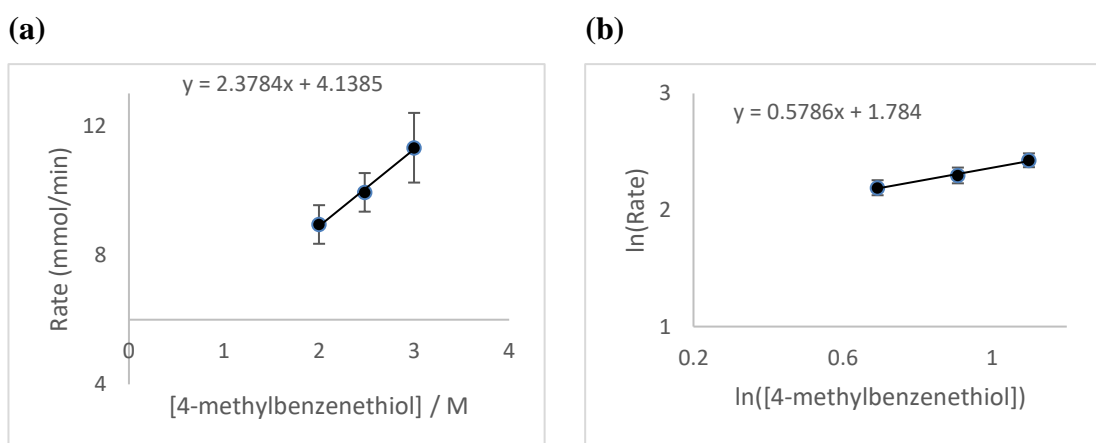
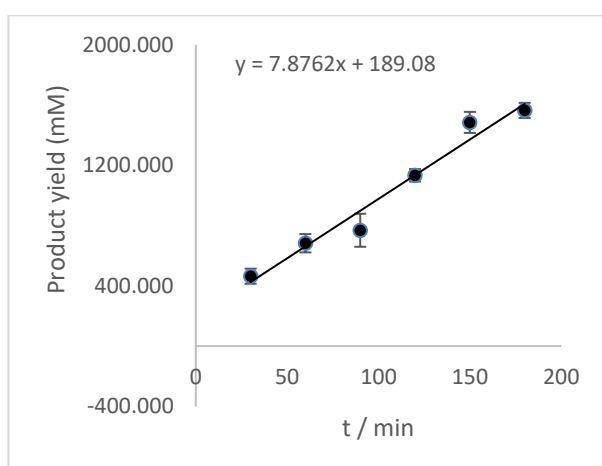


Figure S2: The plot of (a) Rate (M/s) vs concentration of 4-methylbenzenethiol, (b) ln(Rate) vs ln[4-methylbenzenethiol].

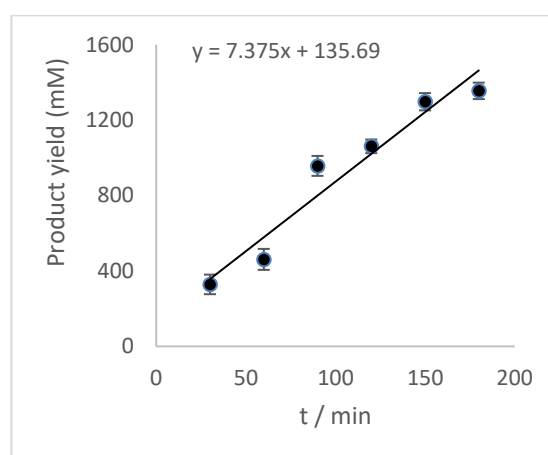
5. Kinetics Analysis Set-I: Initial rates for C-S coupling reaction between 4-methylbenzenethiol with substituted aryl iodides.

Reactions of 4-methylbenzenethiol with substituted aryl iodides were carried out in ethanol under standard reaction conditions. In each set of experiments, reactions were terminated at the interval of 30 min. for three hours duration and product yields were determined. It was difficult to determine the concentration of thiols because of salt formation in basic medium. Similarly, significant variations in concentration of aryl iodides were observed in these coupling reactions. Hence, initial rates were determined using product concentrations at stipulated time interval. Each reaction was repeated thrice to get reliable value of product concentration. Initial rates (mM/min) were determined using plot of product yield (mM) versus time (min). Simple linear regression graphs were obtained in Microsoft Excel. Hammett plot was generated by plotting logarithms of initial rates of coupling constant versus substituents constant. Initial rate of coupling reactions has often used in Hammett analysis.¹

(a) Iodobenzene



(b) 4-iodoanisole



¹ (a) T. Ljungdahl, T. Bennur, A. Dallas, H. Emtenas, J. Martensson, *Organometallics*. 2008, **27**, 2490; (b) K. L. Hull, M. S. Sanford, *J. Am. Chem. Soc.* 2009, **131**, 9651; (c) A. M. Suess, M. Z. Ertem, C. J. Cramer, S. S. Stahl, *J. Am. Chem. Soc.* 2013, **135**, 9797; (d) J. M. Dennis, N. A. White, R. Y. Liu, S. L. Buchwald, *ACS Catal.* 2019, **9**, 3822.

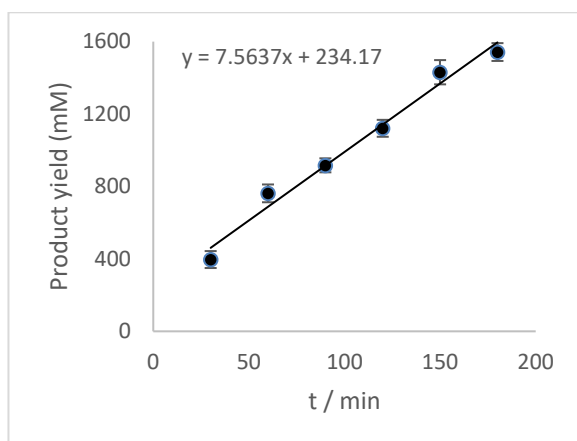
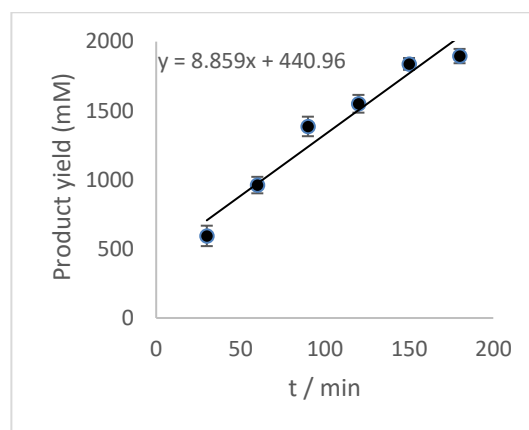
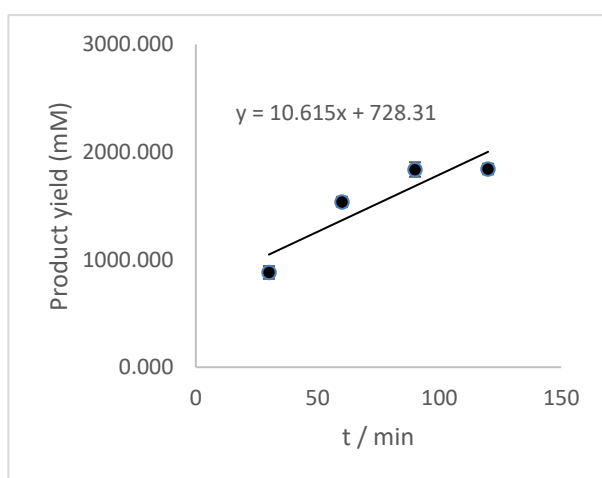
(c) 4-iodotoluene**(d) 1-chloro-4-iodobenzene****(e) 1-bromo-4-iodobenzene**

Figure S3: Initial rate for the reactions between 4-methylbenzenethiol with (a) Iodobenzene, (b) 4-iodoanisole, (c) 4-iodotoluene, (d) 1-chloro-4-iodobenzene, (e) 1-bromo-4-iodobenzene.

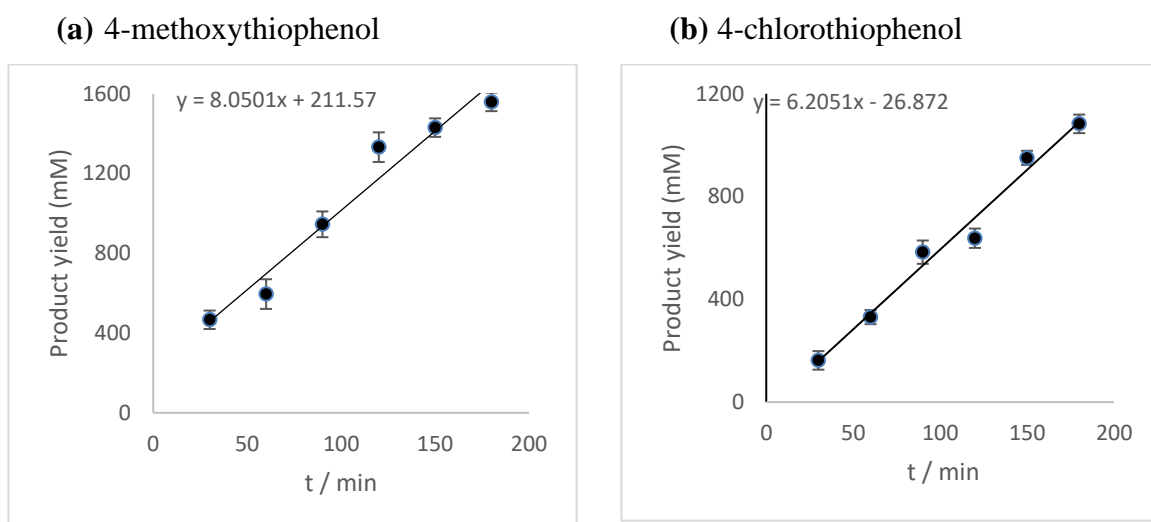
6. Kinetics data for the Hammett plot with the variation of Aryl iodides

Table S4. Hammett parameter, initial rate, and relevant calculated data for C-S coupling reaction between 4-methylbenzenethiol with substituted aryl iodides.

Substrate	Hammett Parameter, σ_p	Initial rate (mM/min)	r_x/r_H	$\log(r_x/r_H)$
Iodobenzene	0	7.87	1	0
4-iodoanisole	-0.37	7.37	0.936365252	-0.02855
4-iodotoluene	-0.17	7.56	0.960234631	-0.01762
1-chloro-4-iodobenzene	0.23	8.85	1.124780986	0.051068
1-bromo-4-iodobenzene	0.25	10.61	1.347731139	0.129603

7. Kinetics Analysis Set-II: Initial rates for C-S coupling reaction between substituted thiophenols with iodobenzene.

Reactions of substituted thiophenols with iodobenzene were carried out in ethanol under standard reaction conditions. In each set of experiments, reactions were terminated at the interval of 30 min. for three hours duration and product yields were determined. It was difficult to determine the concentration of thiols because of salt formation in basic medium. Similarly, significant variations in concentration of iodobenzene were observed in these coupling reactions. Hence, initial rates were determined using product concentrations at stipulated time interval. Each reaction was repeated thrice to get reliable value of product concentration. Initial rates (mM/min) were determined using plot of product yield (mM) versus time (min). Simple linear regression graphs were obtained in Microsoft Excel. Because of unavailability of unsubstituted benzenethiol, we could not determine kinetics data for reactions involving unsubstituted benzenethiol. Initial rate for the reaction of unsubstituted benzenethiol with iodobenzene was determined from plot of initial rates of derivatives of thiophenols versus substituent constant (Figure S5). From this graph, initial rate value corresponds to substituent constant value ($\sigma = 0$) is considered as initial rate for the unsubstituted benzenethiol. Further, Hammett plot was generated by plotting logarithms of initial rates of coupling constant versus substituents constant. Initial rate of coupling reactions has often used in Hammett analysis.¹



(c) 4-fluorothiophenol

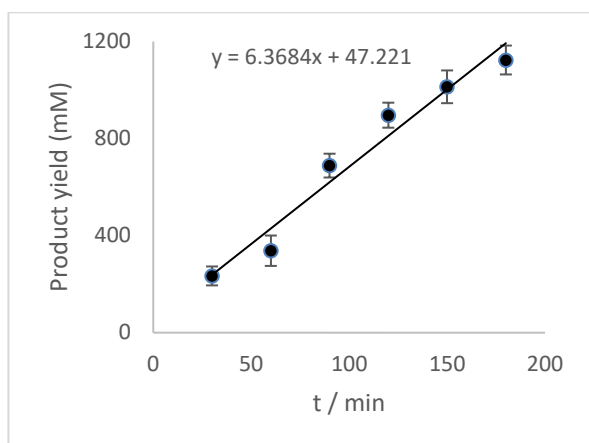


Figure S4: Initial rate for the reactions between (a) 4-methoxythiophenol, (b) 4-chlorothiophenol, (c) 4-fluorothiophenol with iodobenzene.

Table S5: Initial rate for the C–S coupling of substituted thiophenols with iodobenzene

Substrate	Initial Rate (mM/min)
Thiophenol	6.97 (From Figure S5)
4-methoxythiophenol	8.05
4-methylthiophenol	7.87
4-chlorothiophenol	6.20
4-fluorothiophenol	6.36

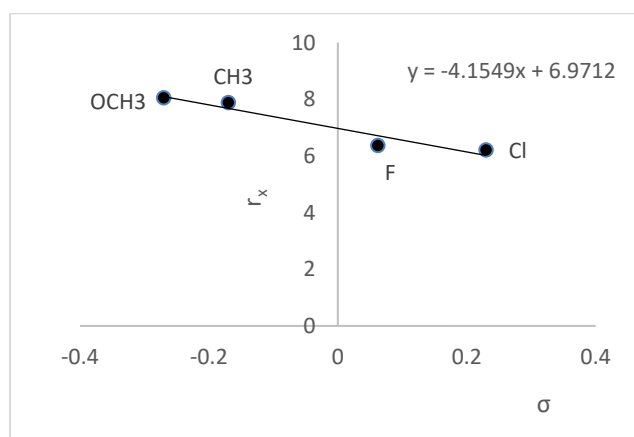


Figure S5: Plot of Initial rate (r_x) versus substituent constant (σ).

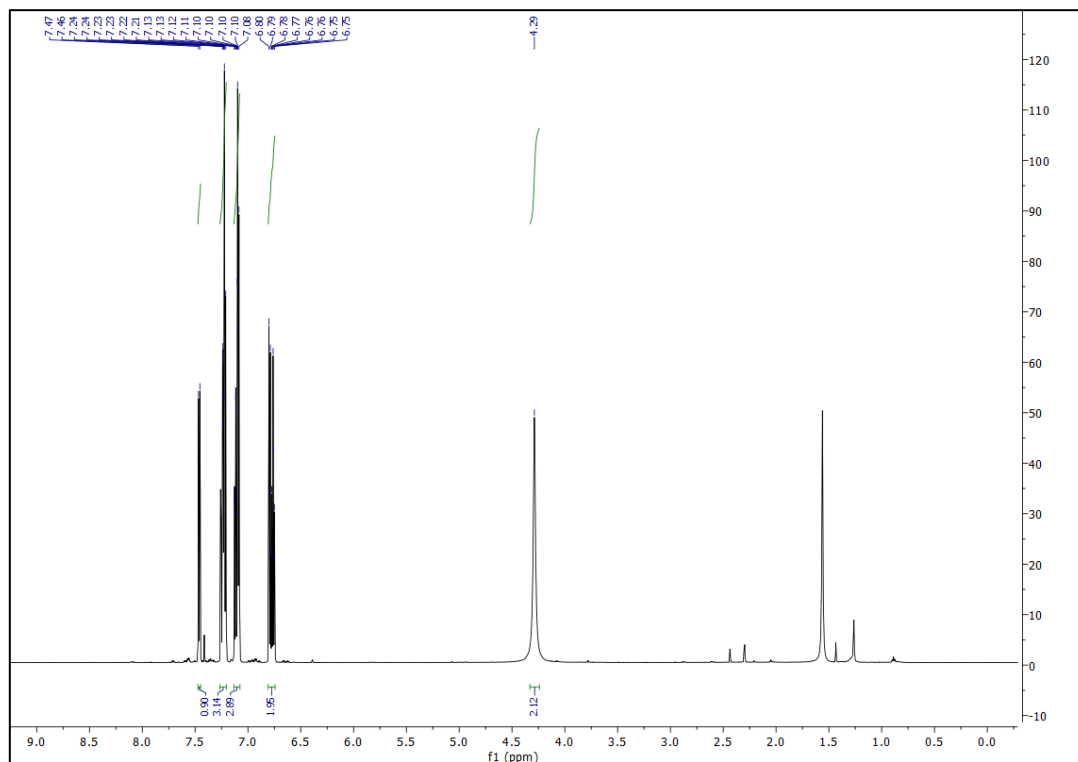
8. Kinetics data for the Hammett plot with the variation of thiophenols

Table S6: Hammett parameter, initial rate, and relevant calculated data for C-S coupling reaction between substituted thiophenols with iodobenzene.

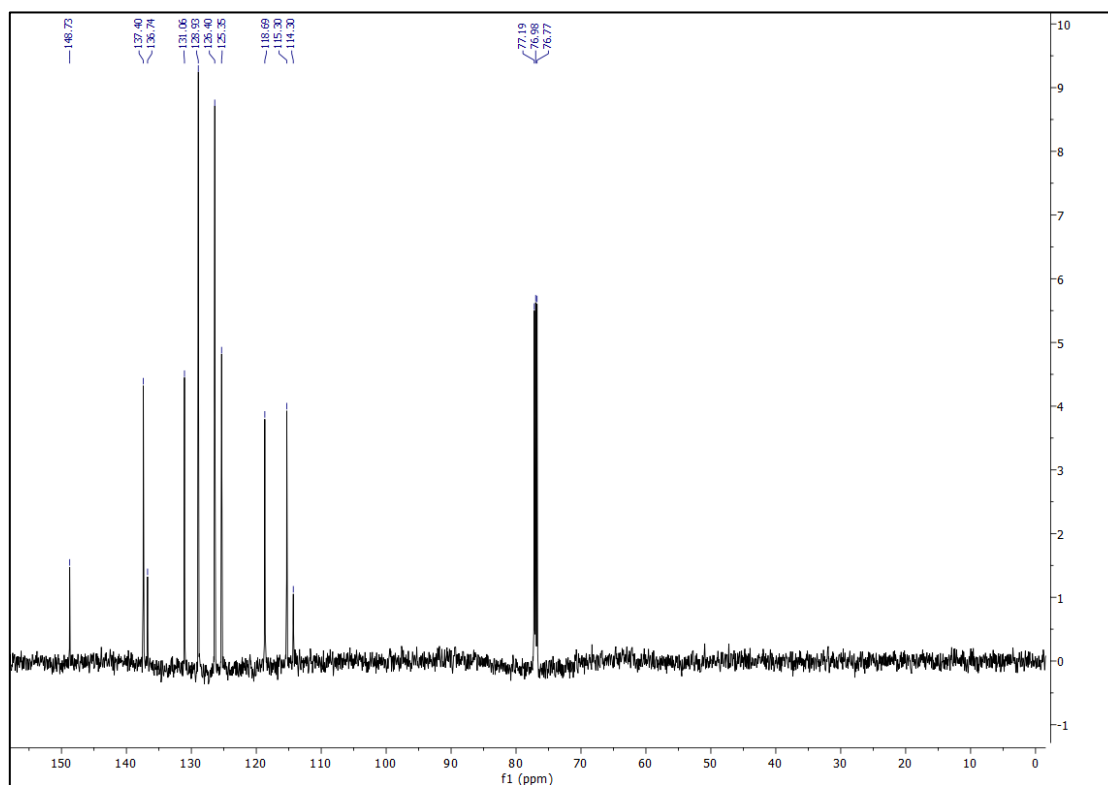
Substrate	Hammett σ_p parameter	Initial rate (mM/min)	r_x/r_H	$\log(r_x/r_H)$
Thiophenol	0	6.97	1	0
4-methoxythiophenol	-0.27	8.05	1.154765	0.062494
4-methylthiophenol	-0.17	7.87	1.12982	0.053009
4-chlorothiophenol	0.23	6.20	0.890105	-0.05056
4-fluorothiophenol	0.25	6.36	0.91353	-0.03928

9. NMR spectra

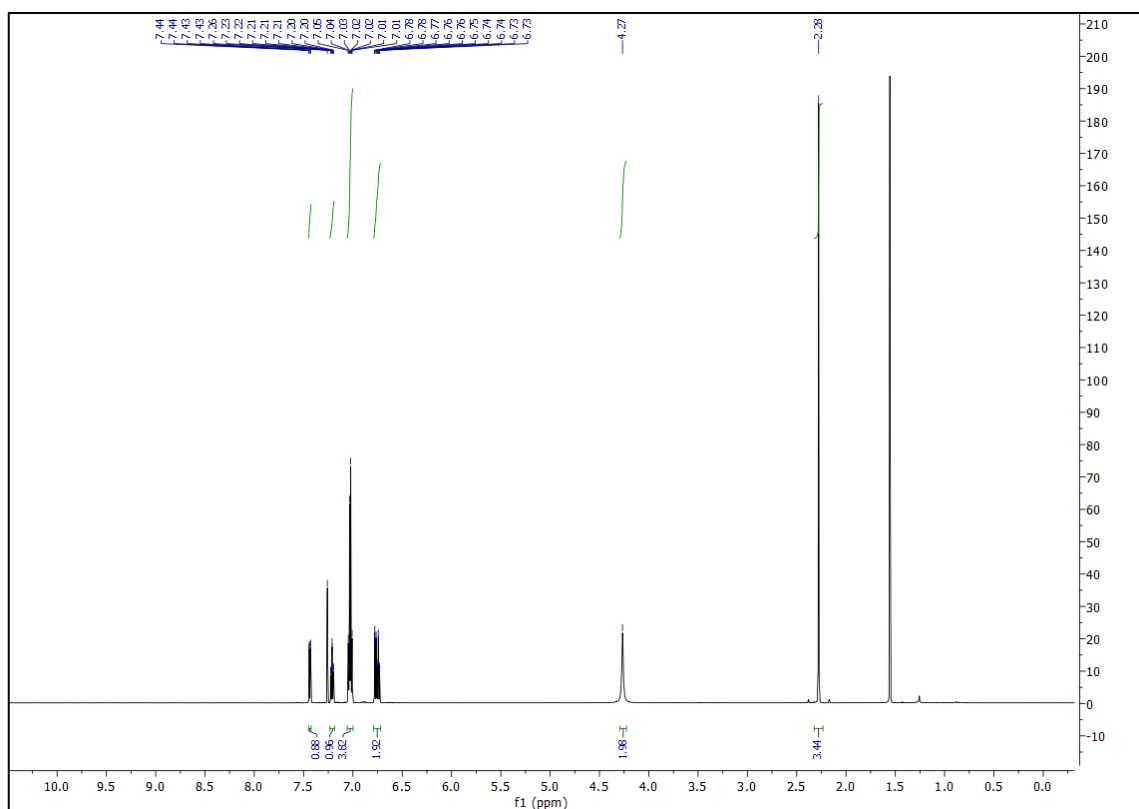
^1H NMR of (3a)



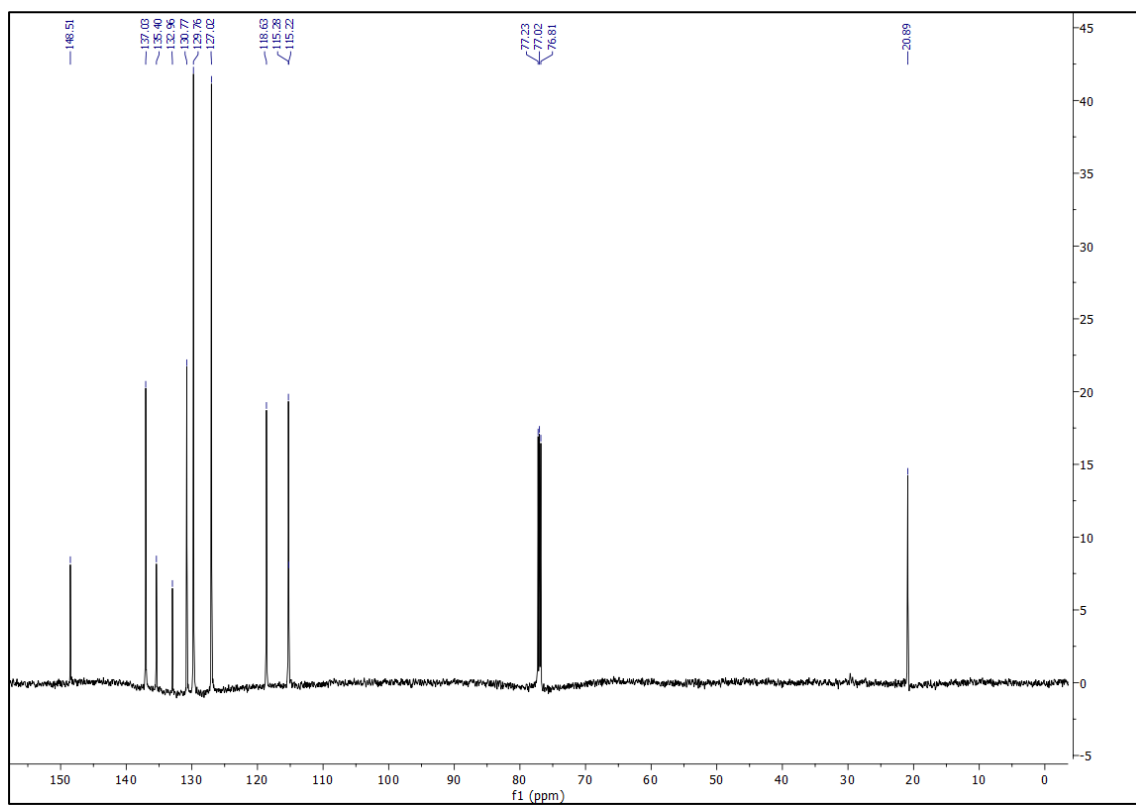
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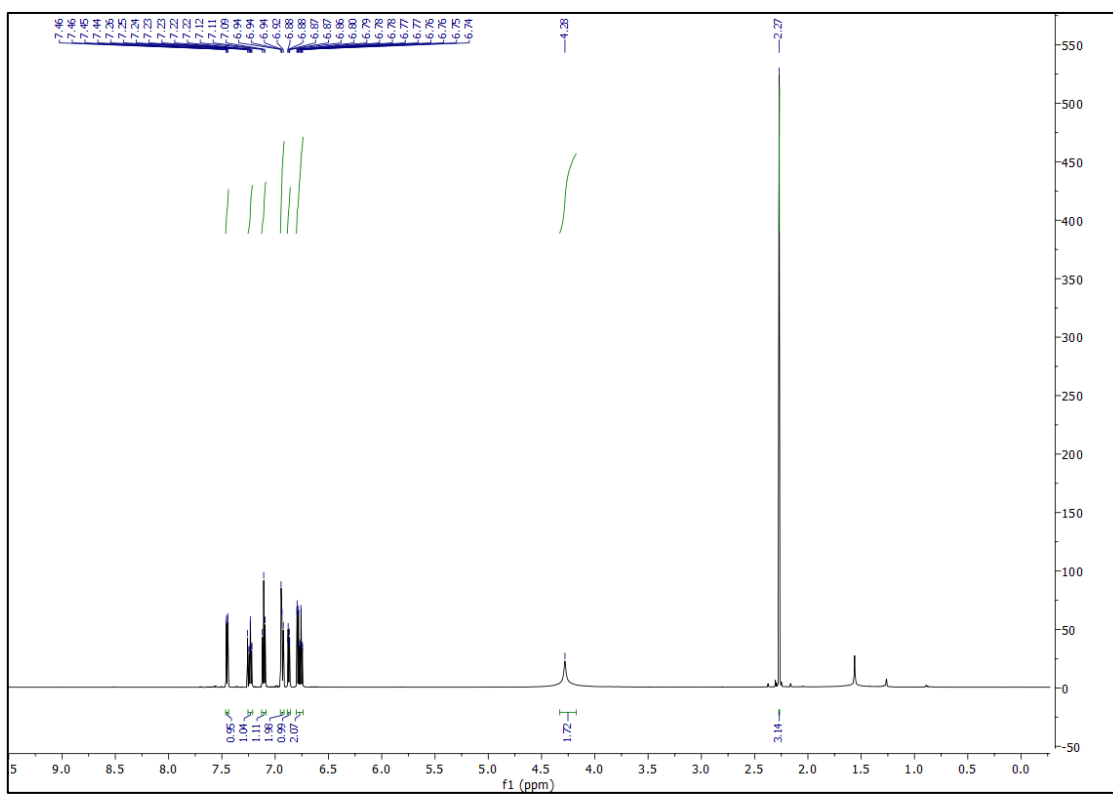
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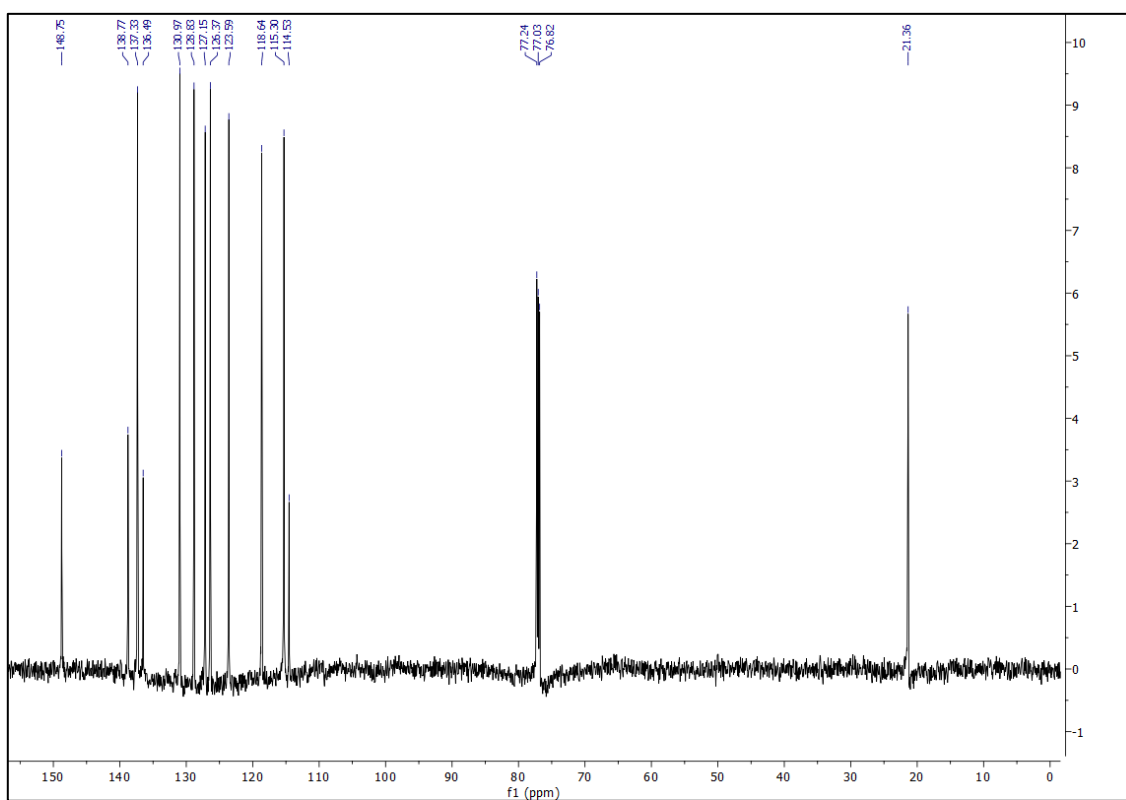
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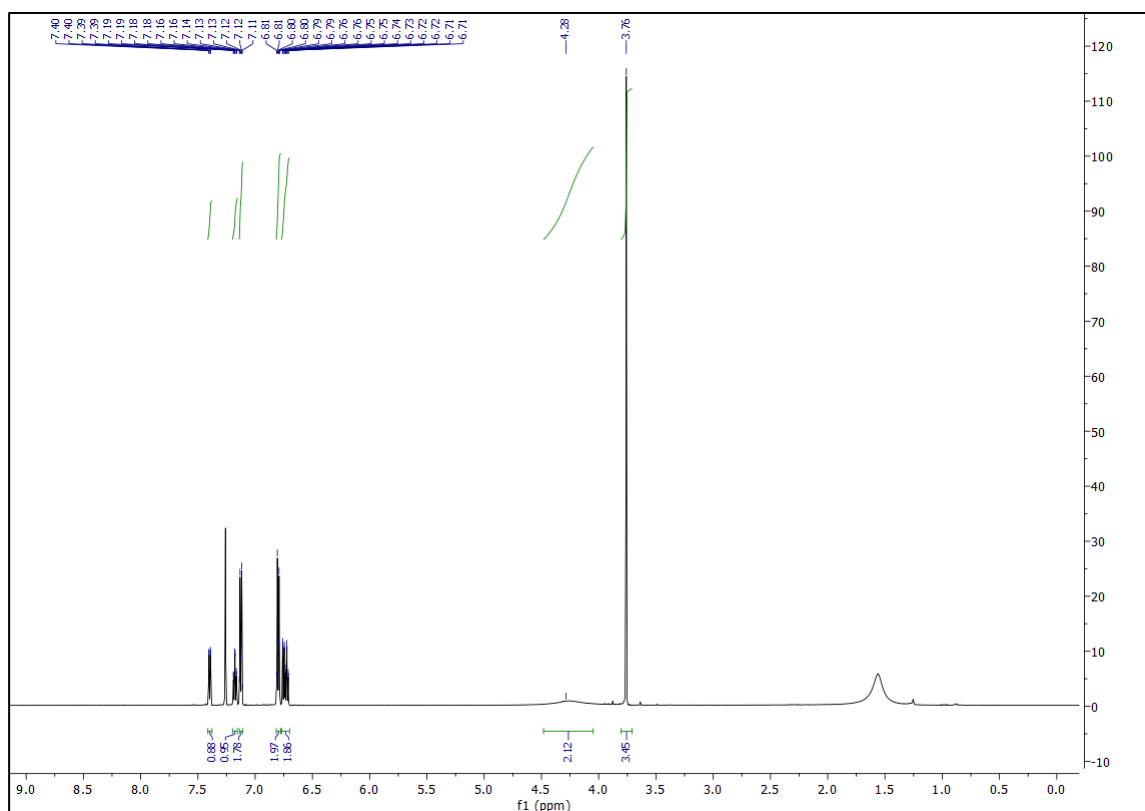
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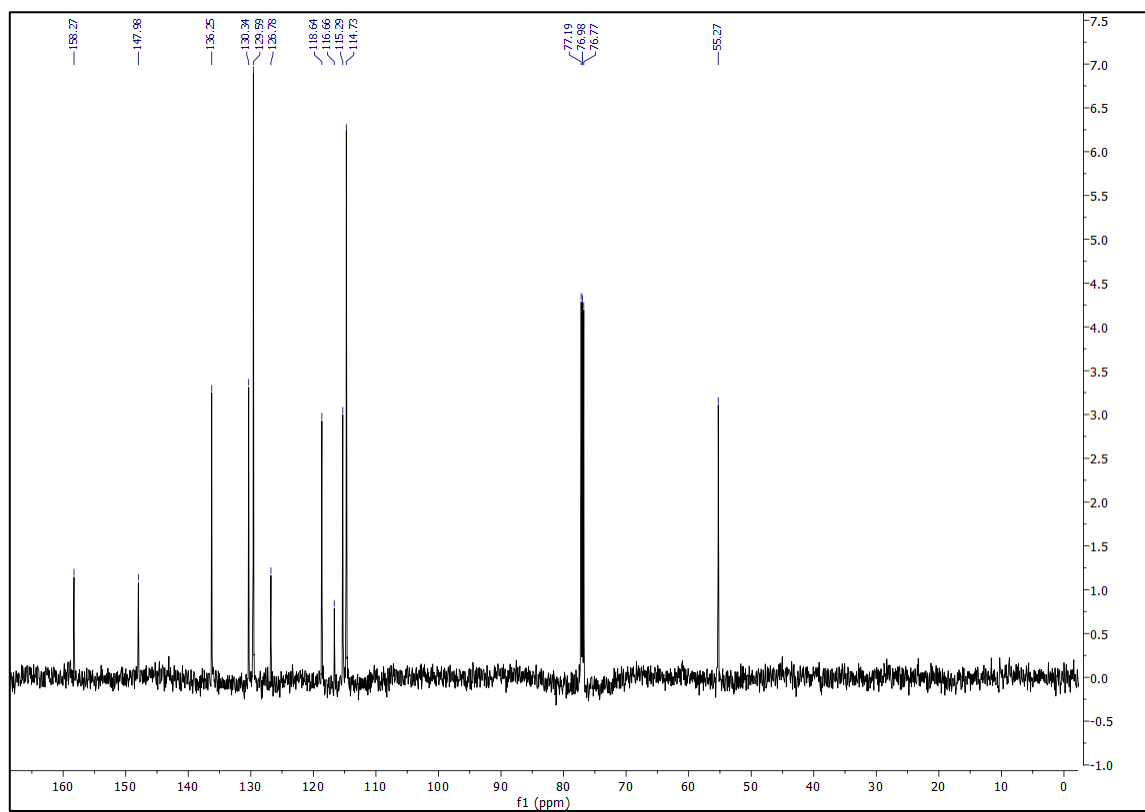
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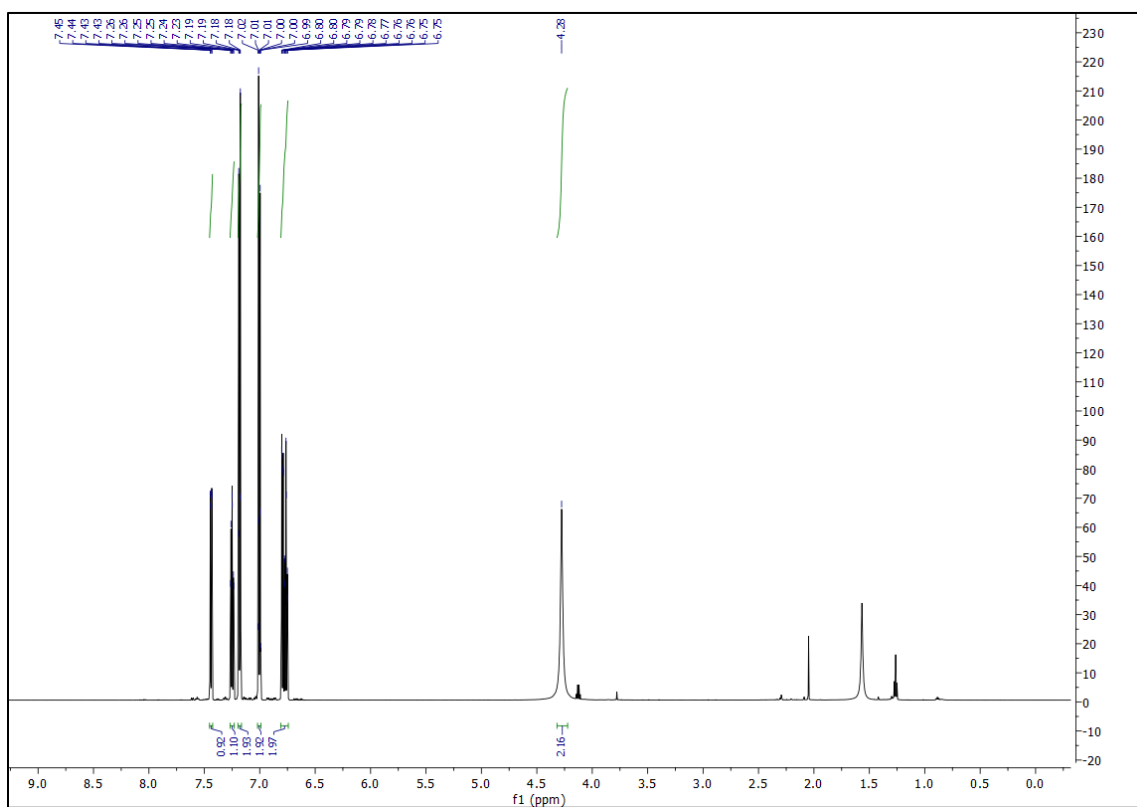
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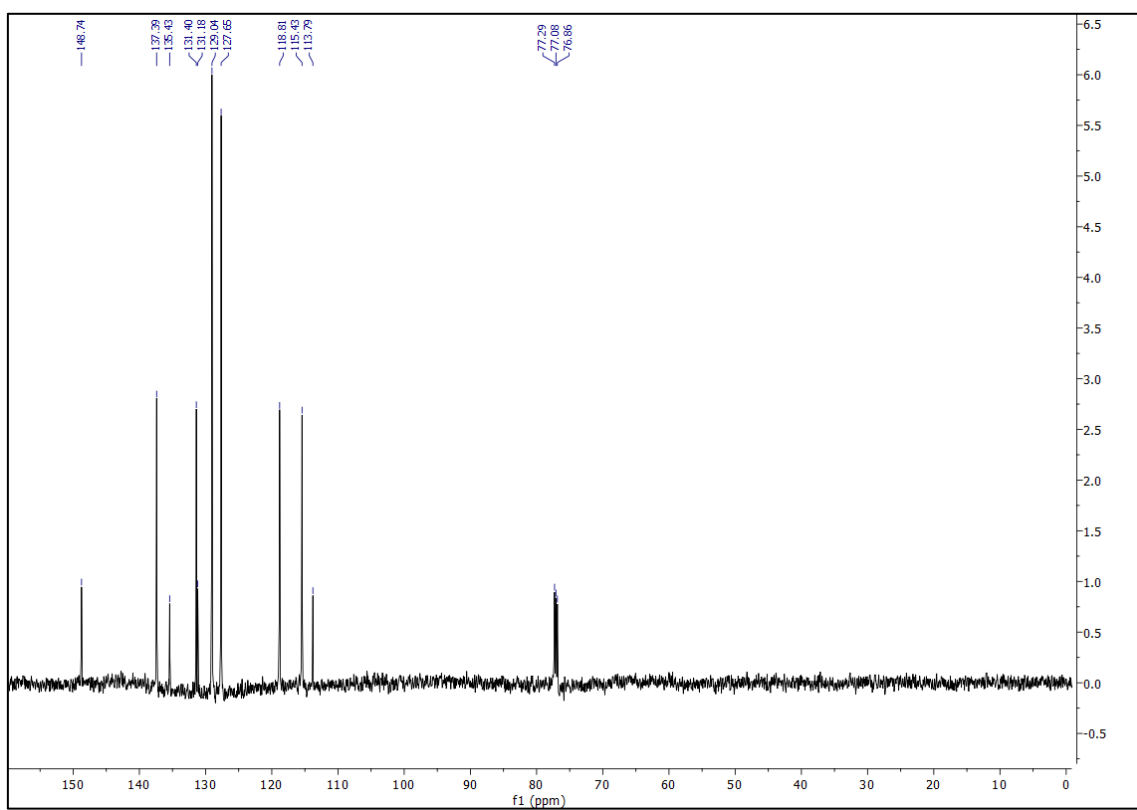
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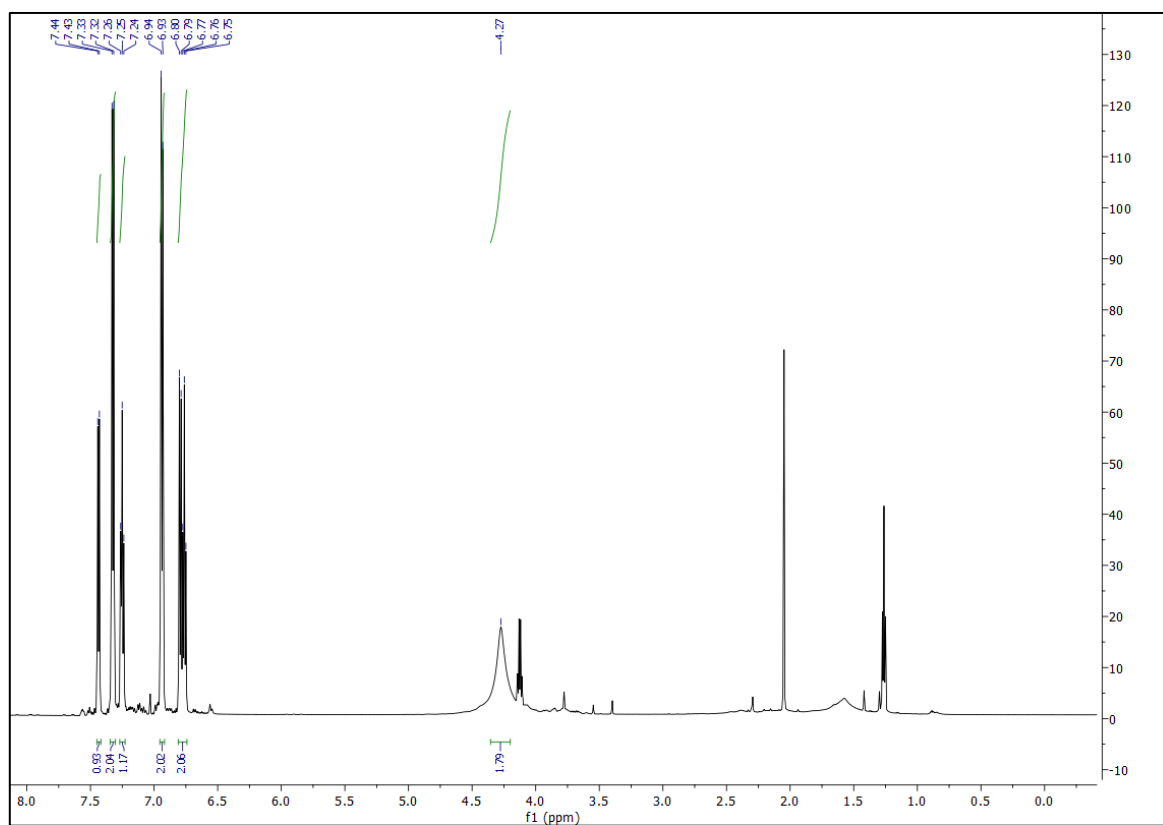
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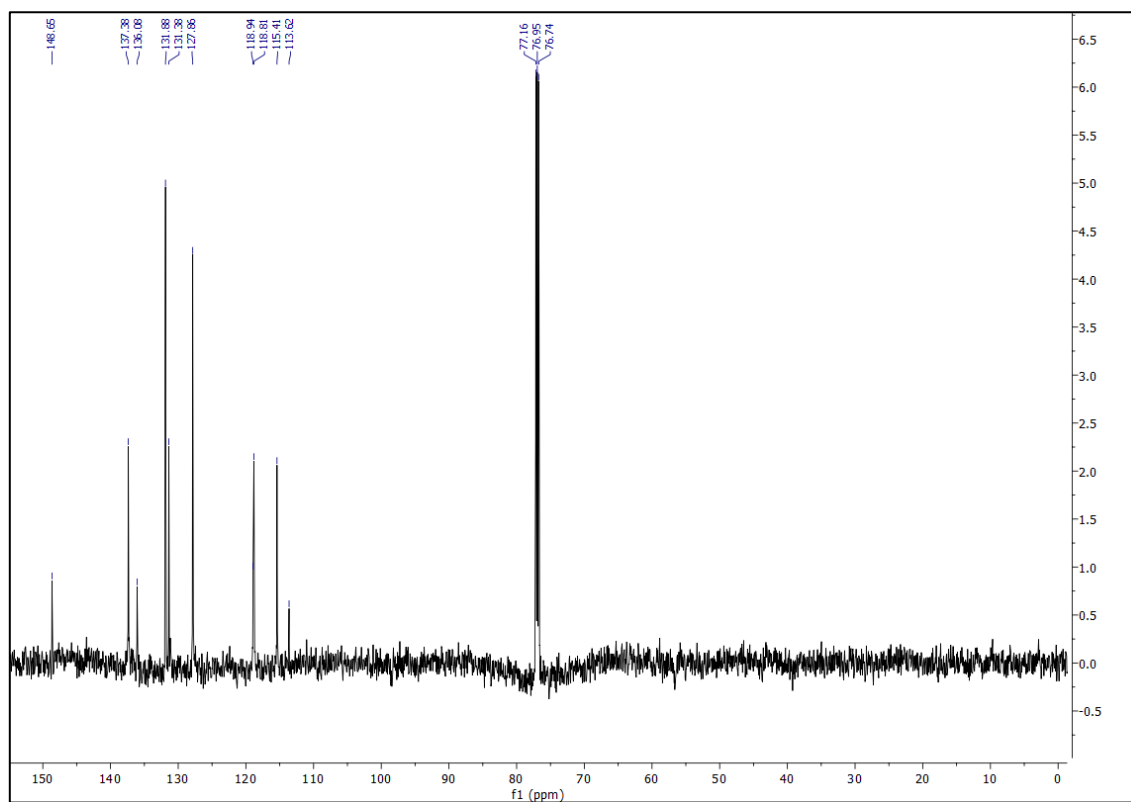
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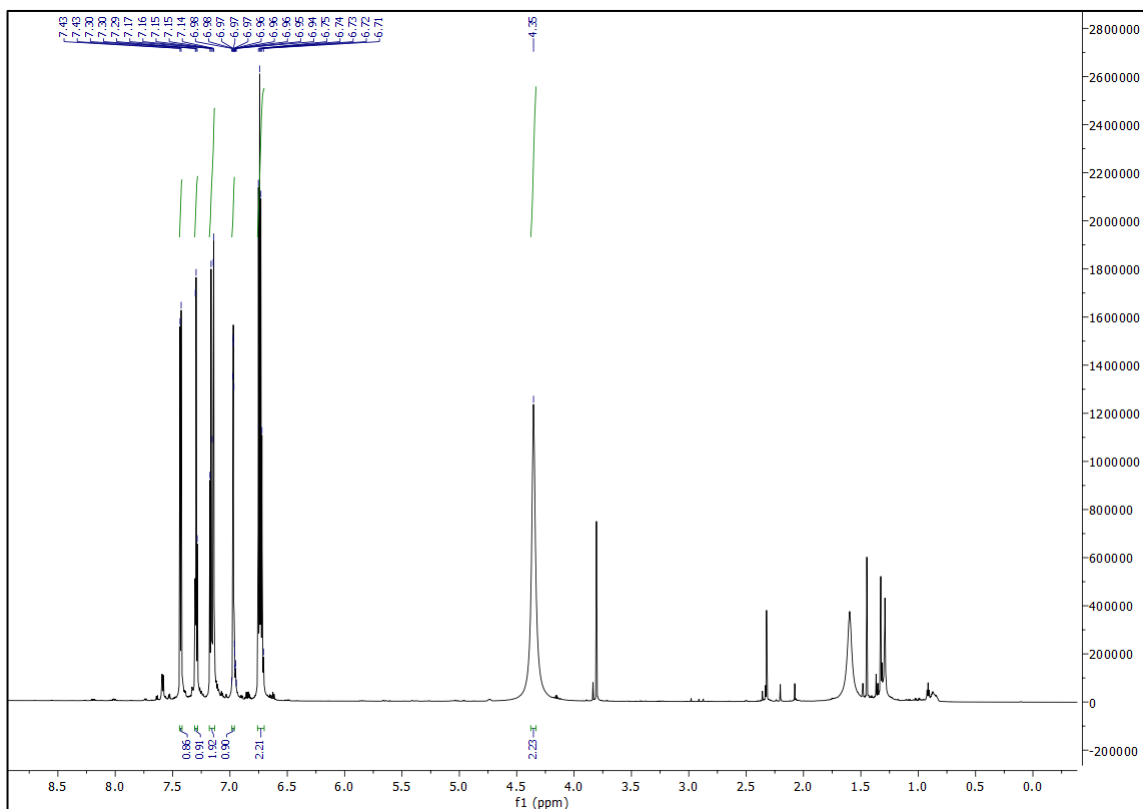
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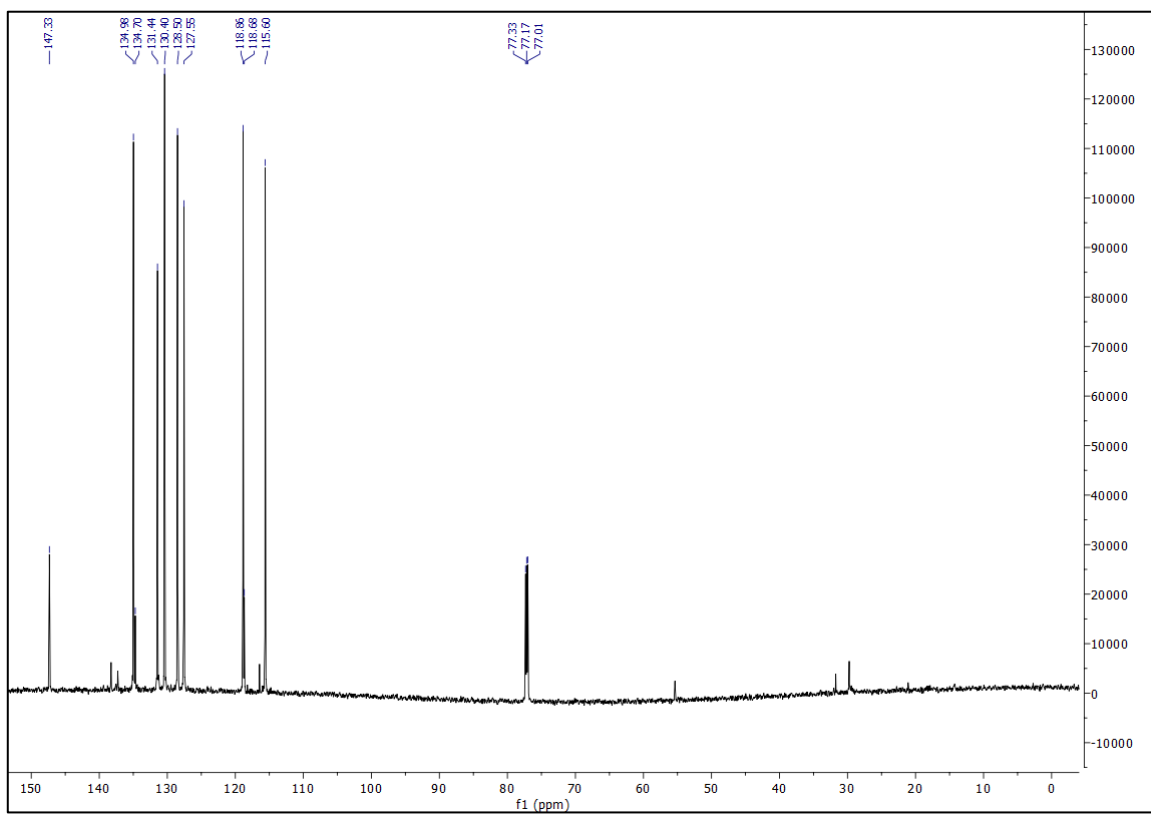
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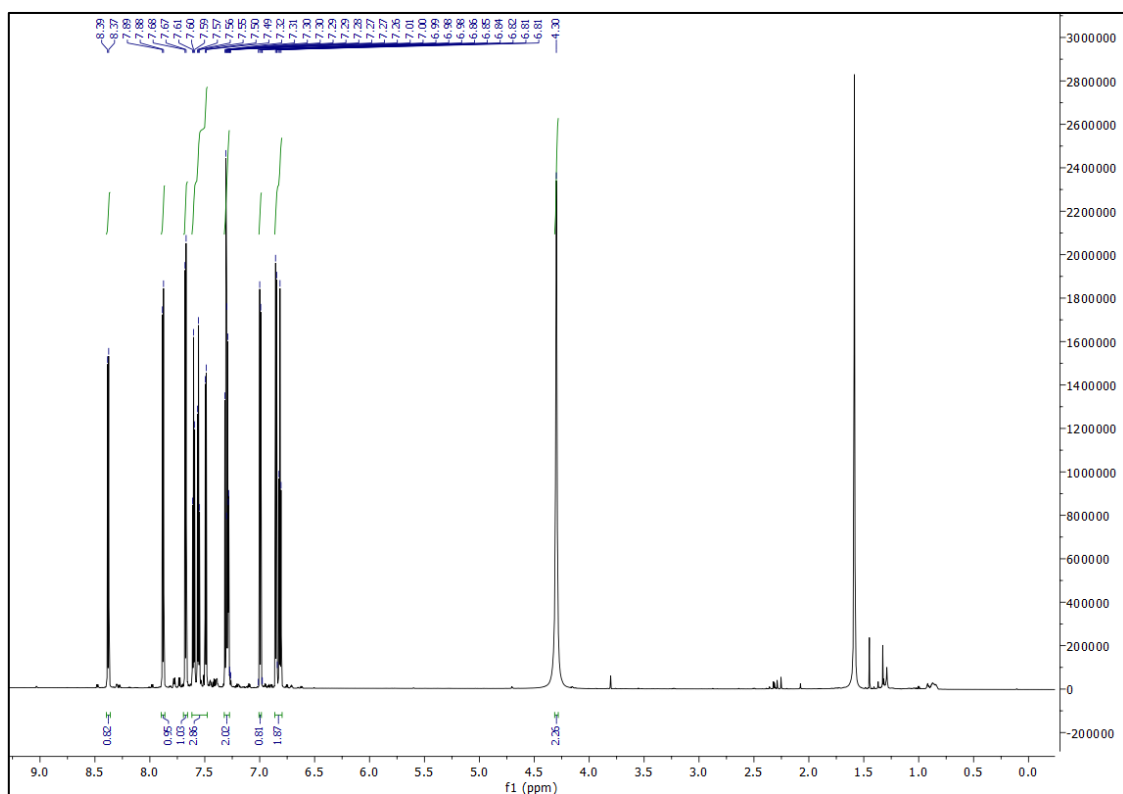
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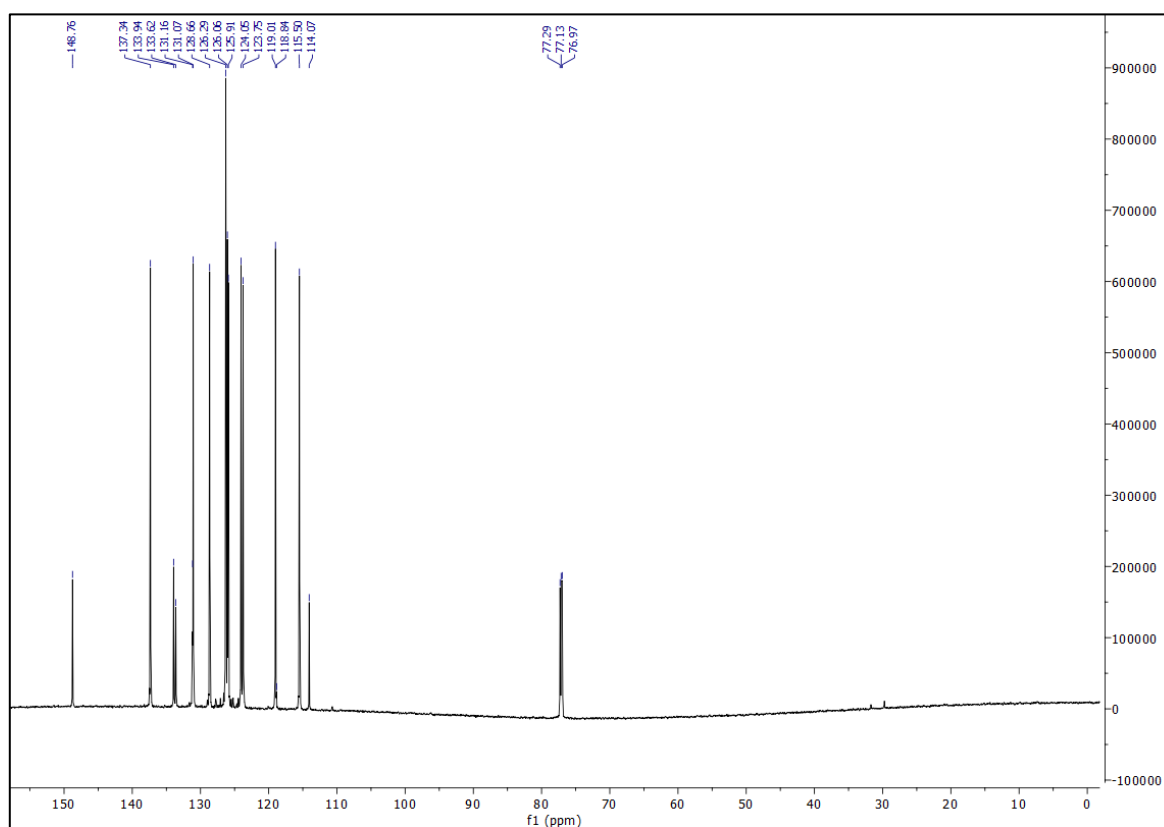
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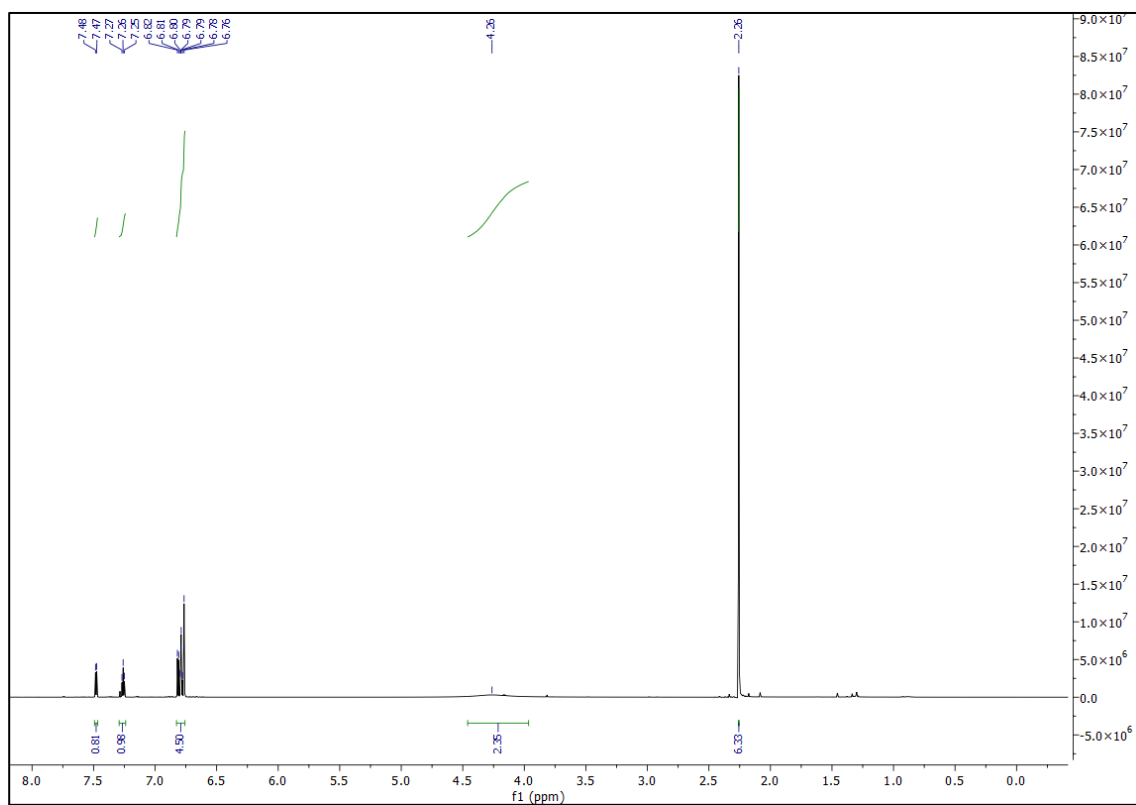
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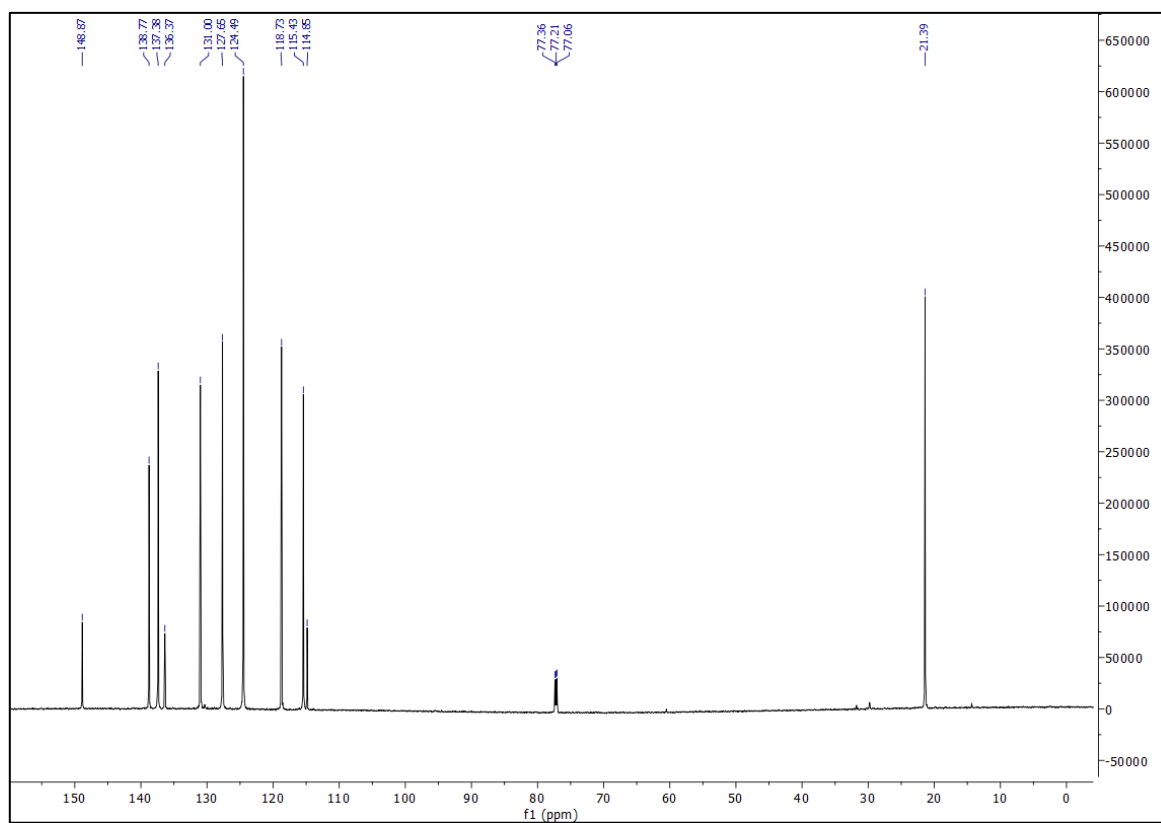
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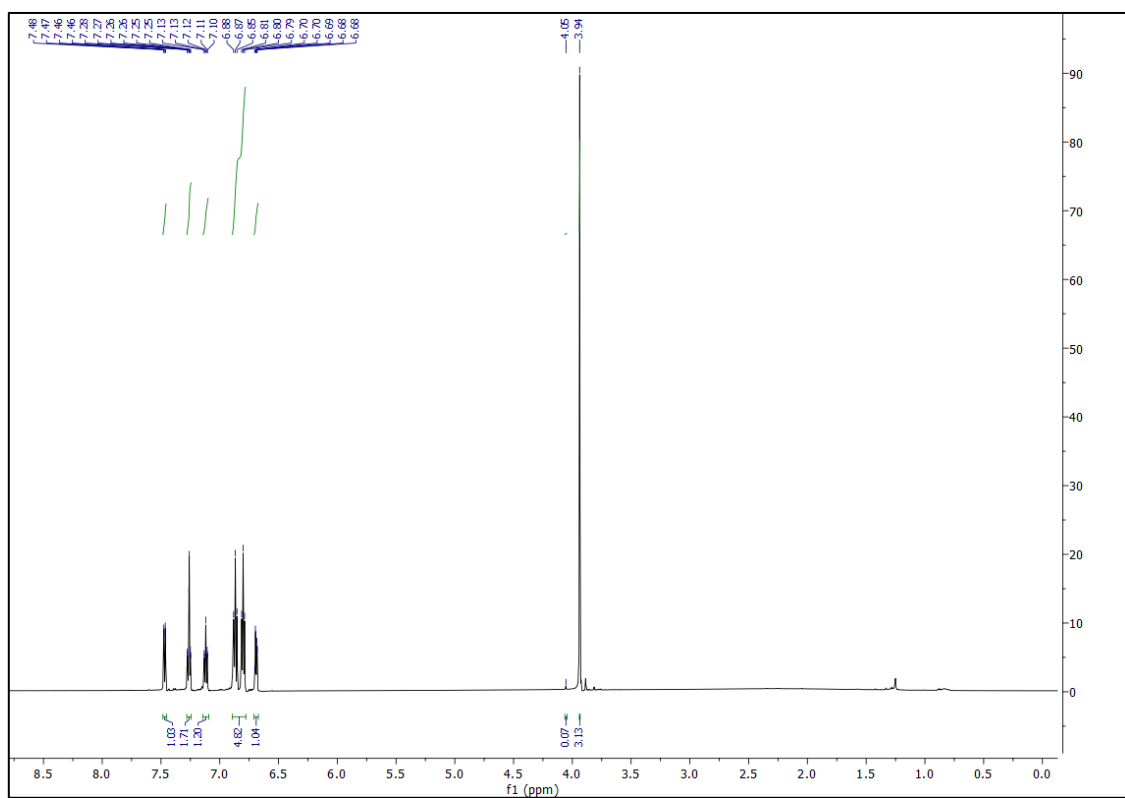
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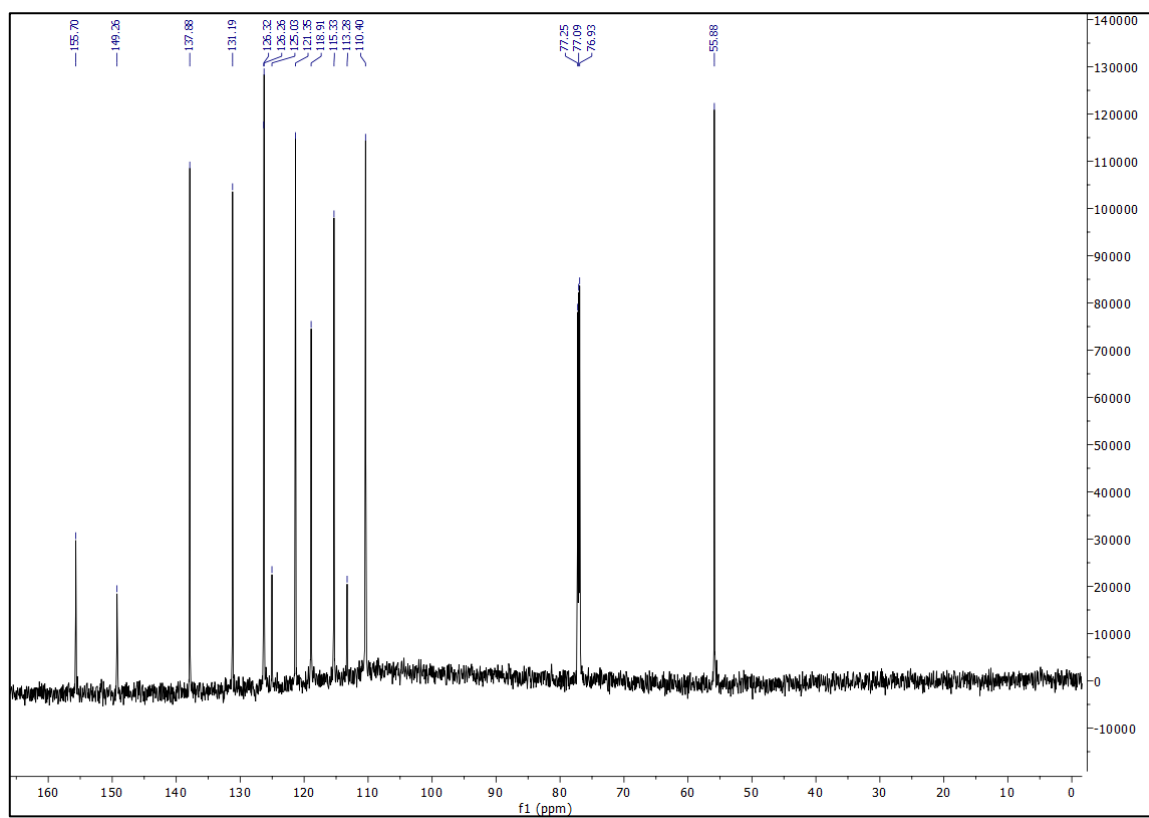
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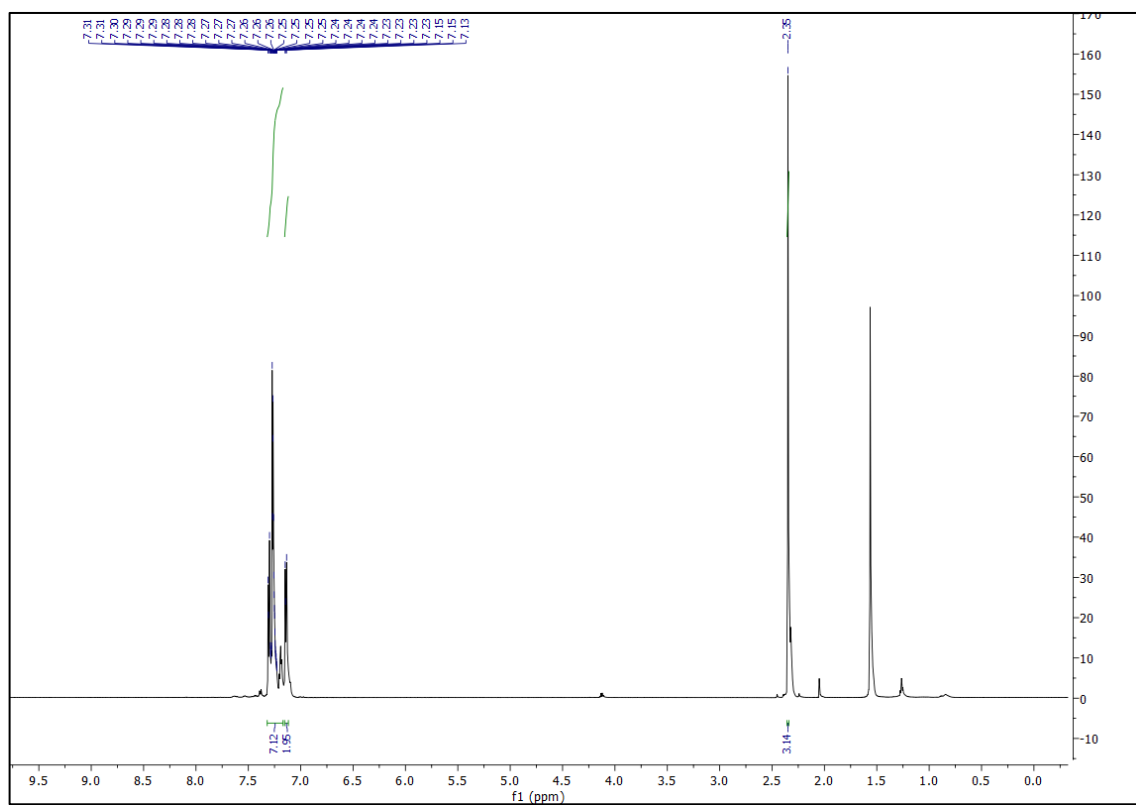
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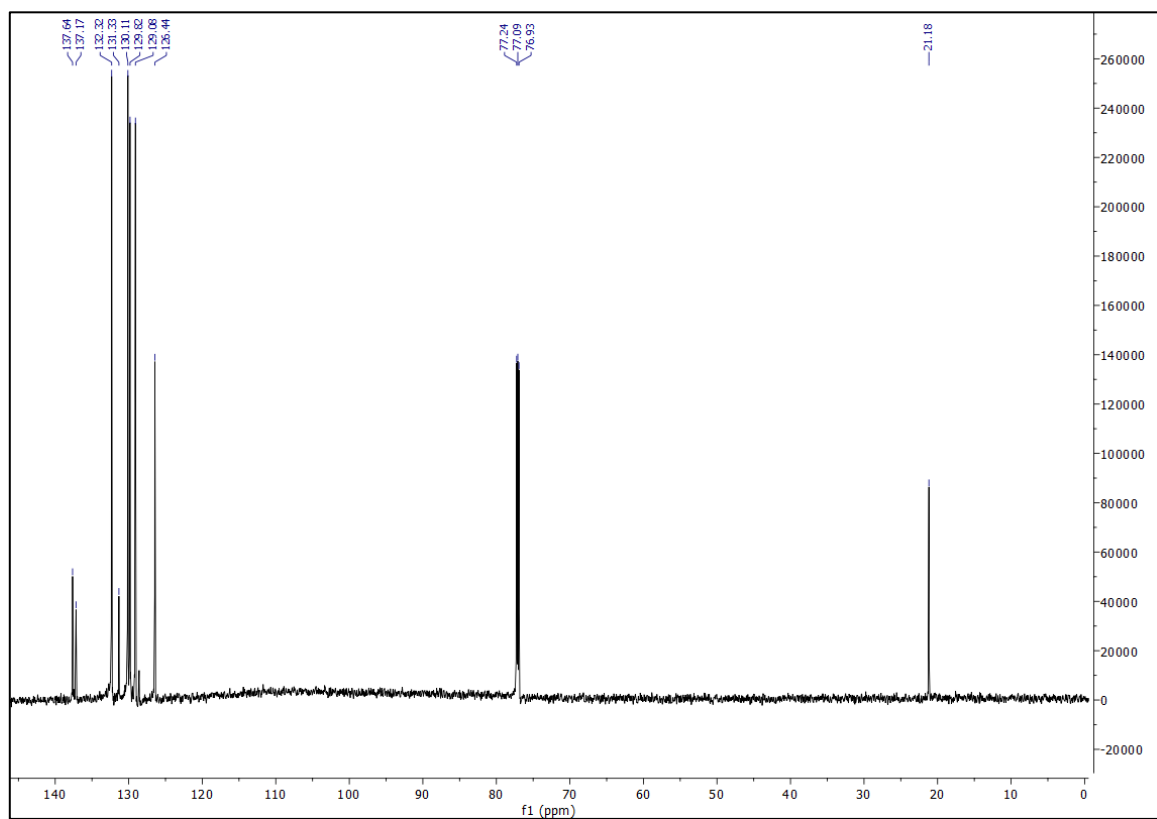
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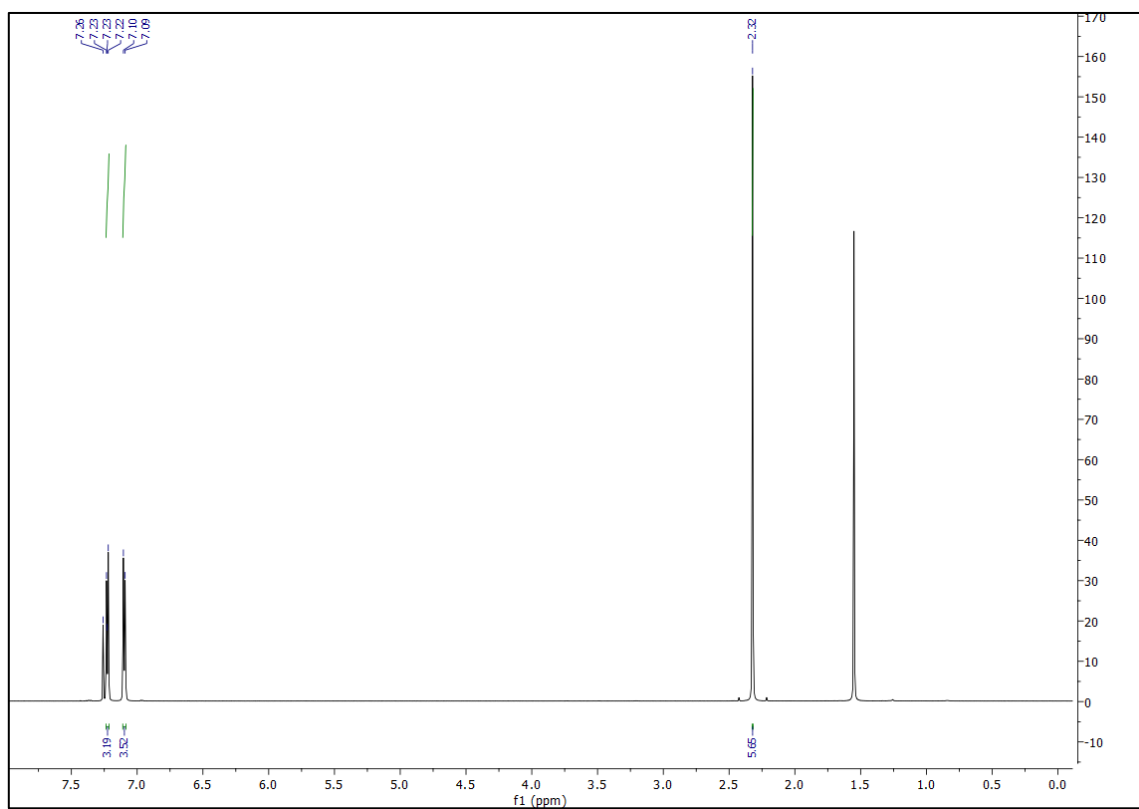
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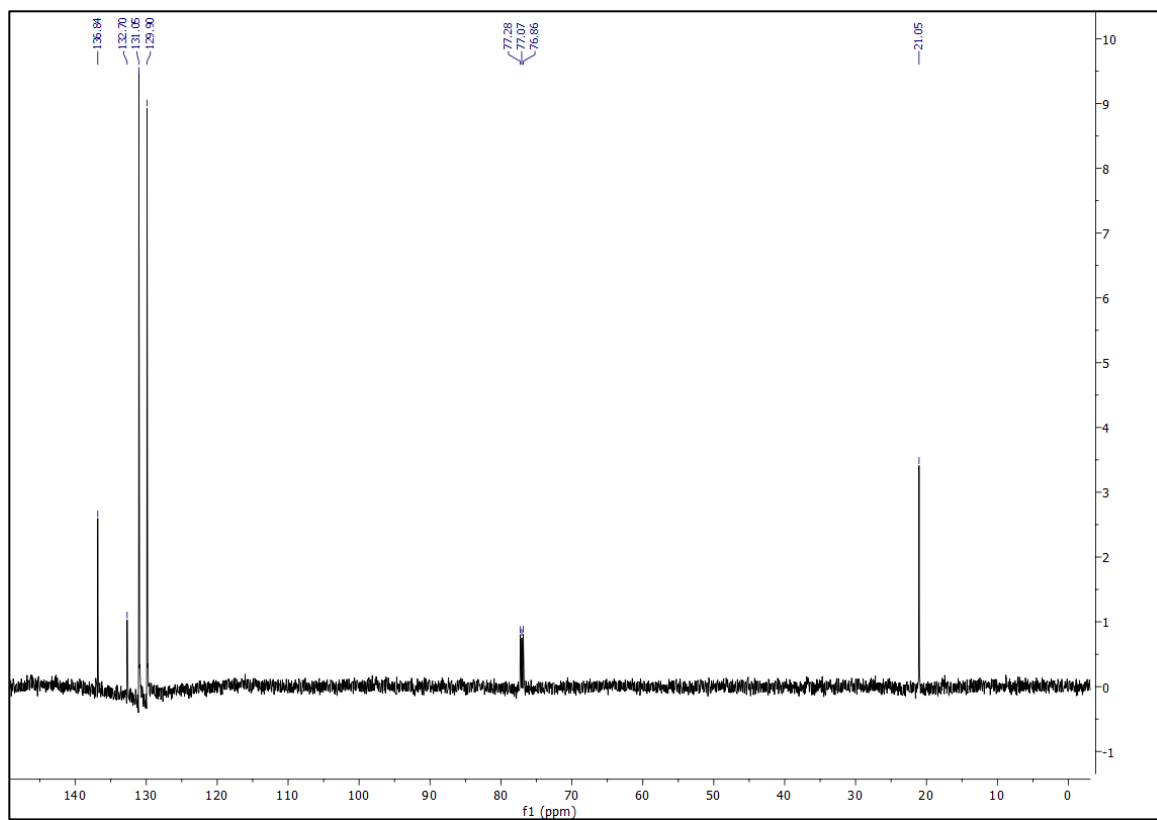
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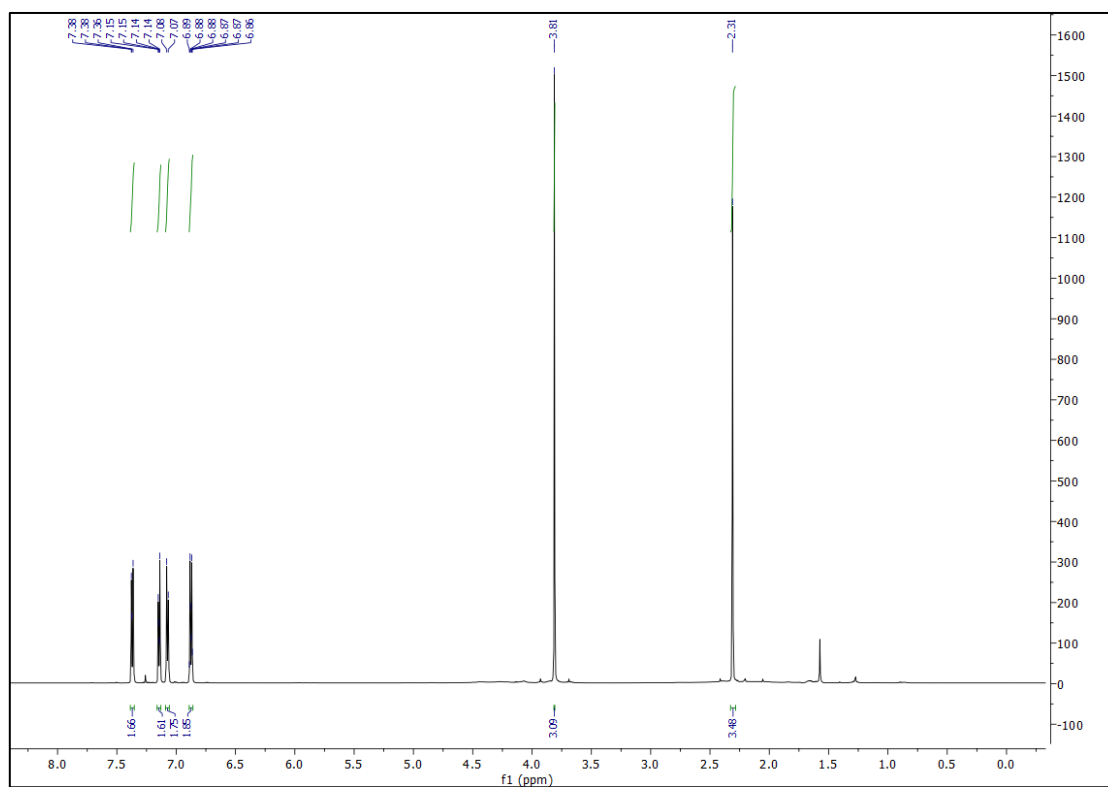
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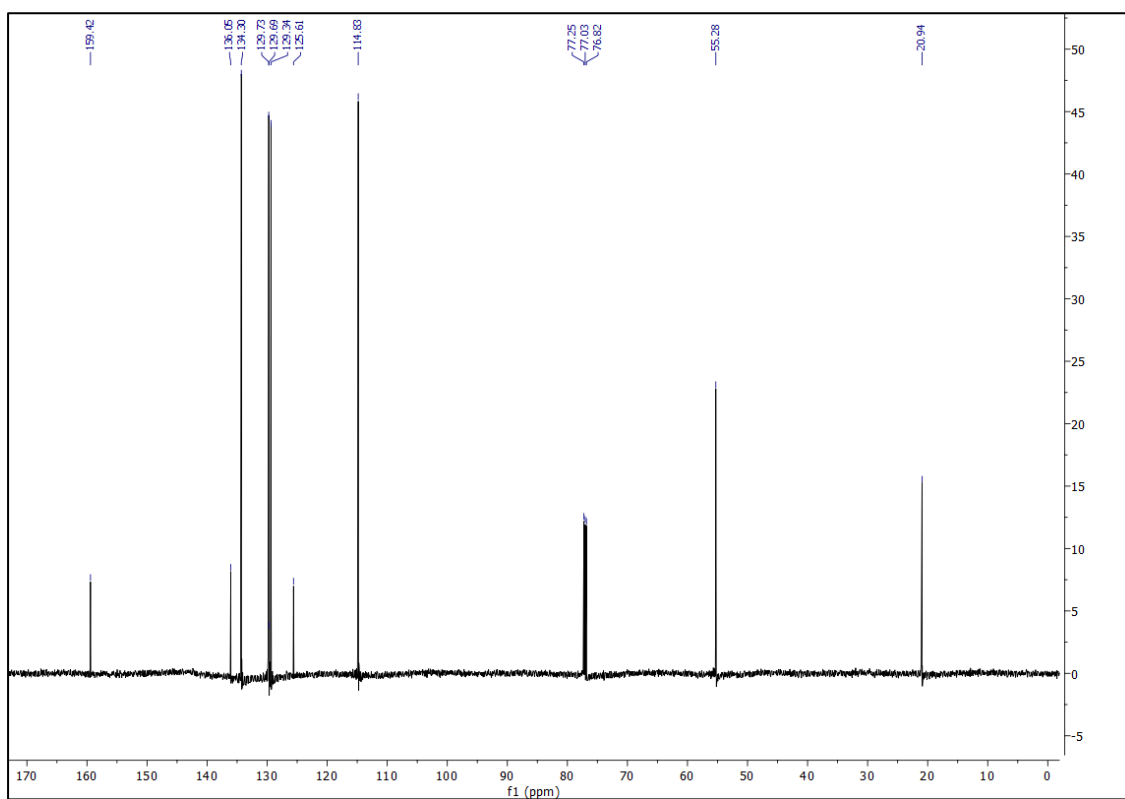
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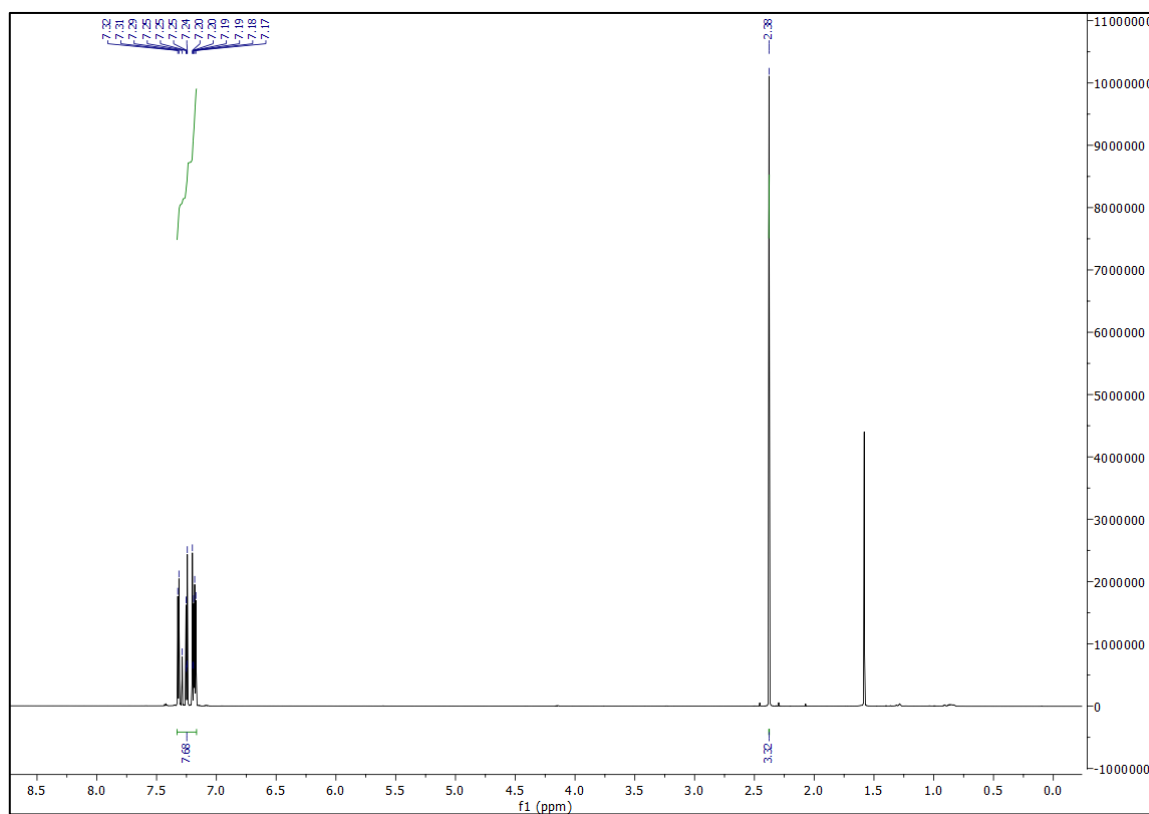
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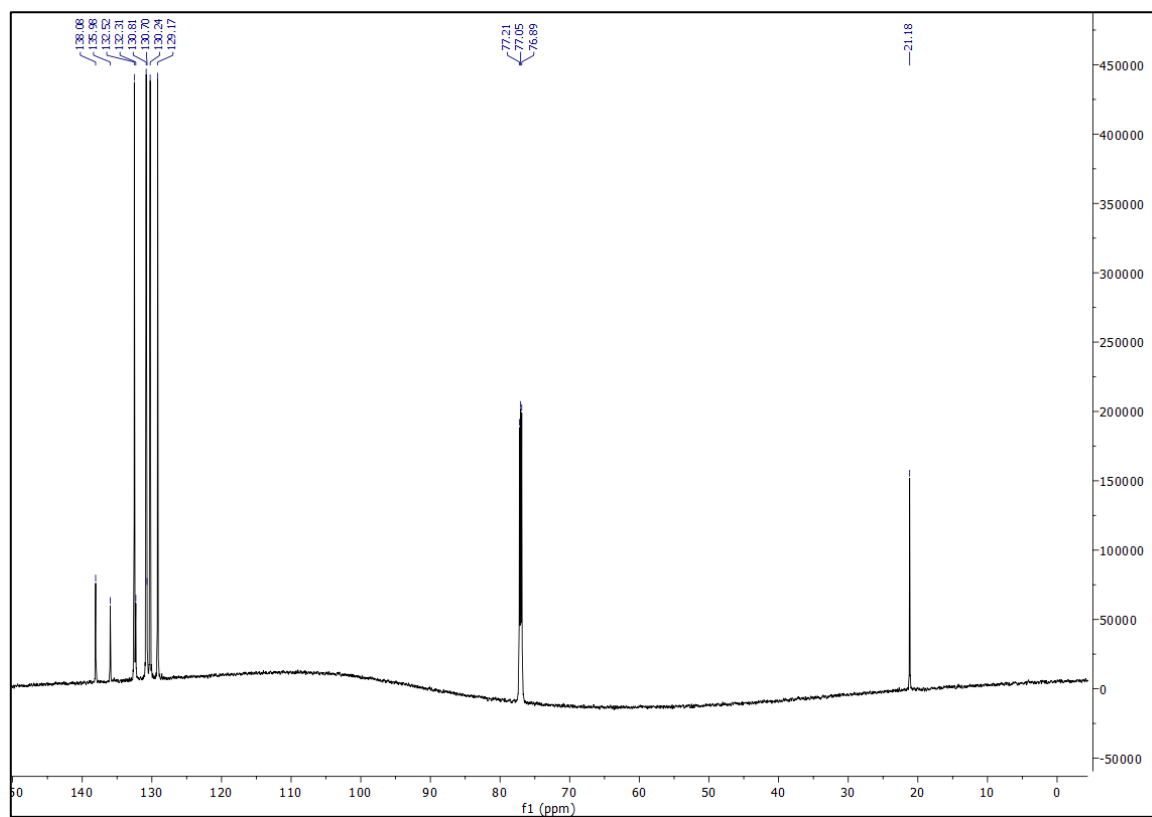
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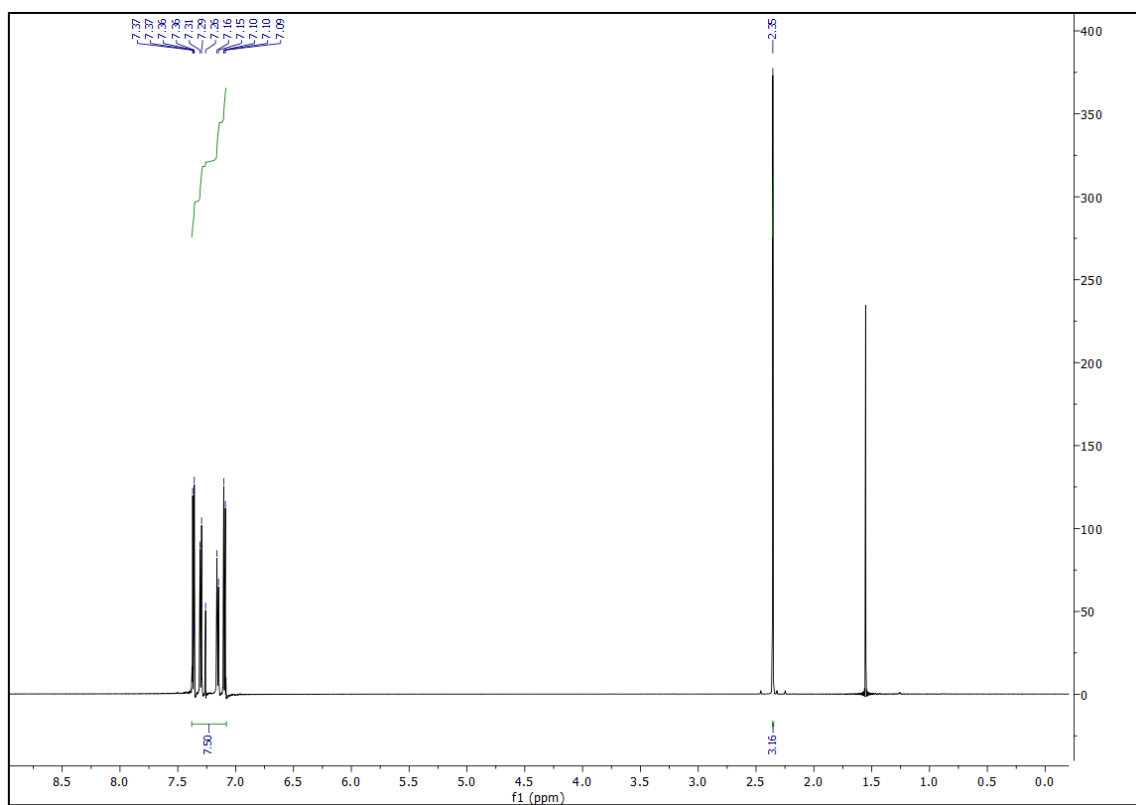
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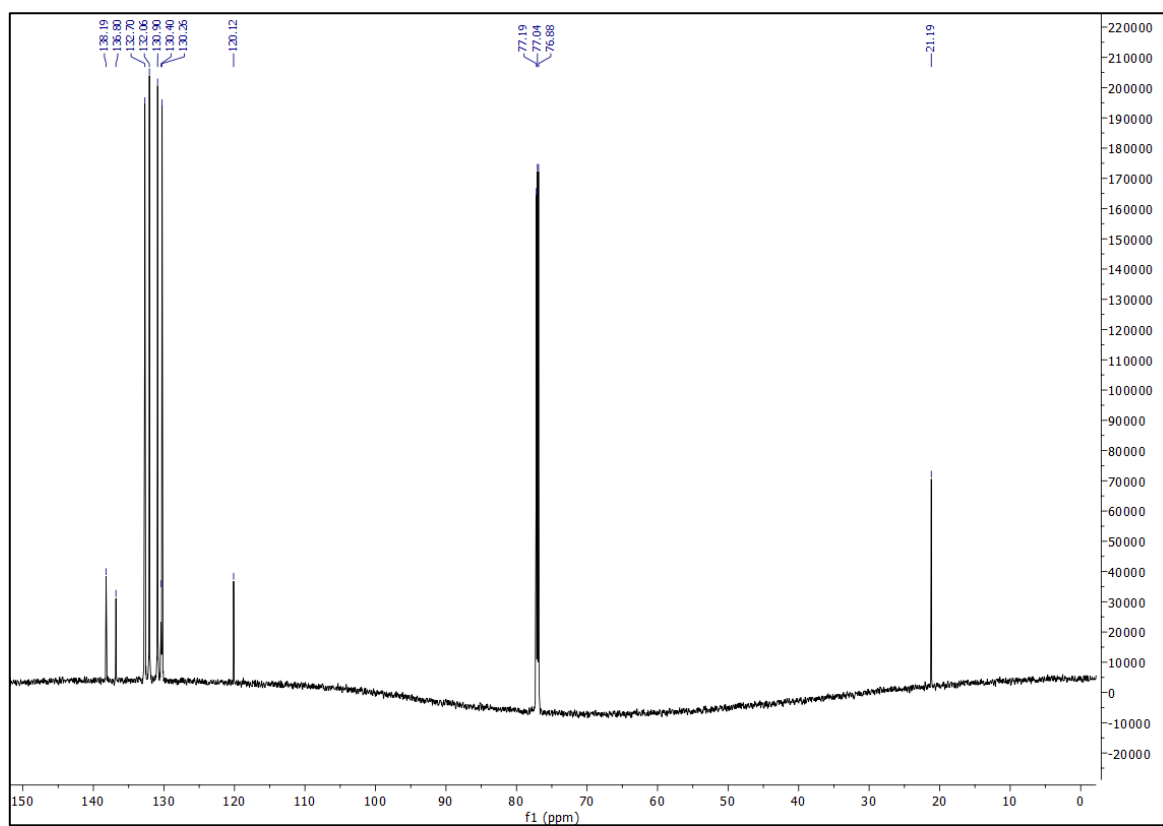
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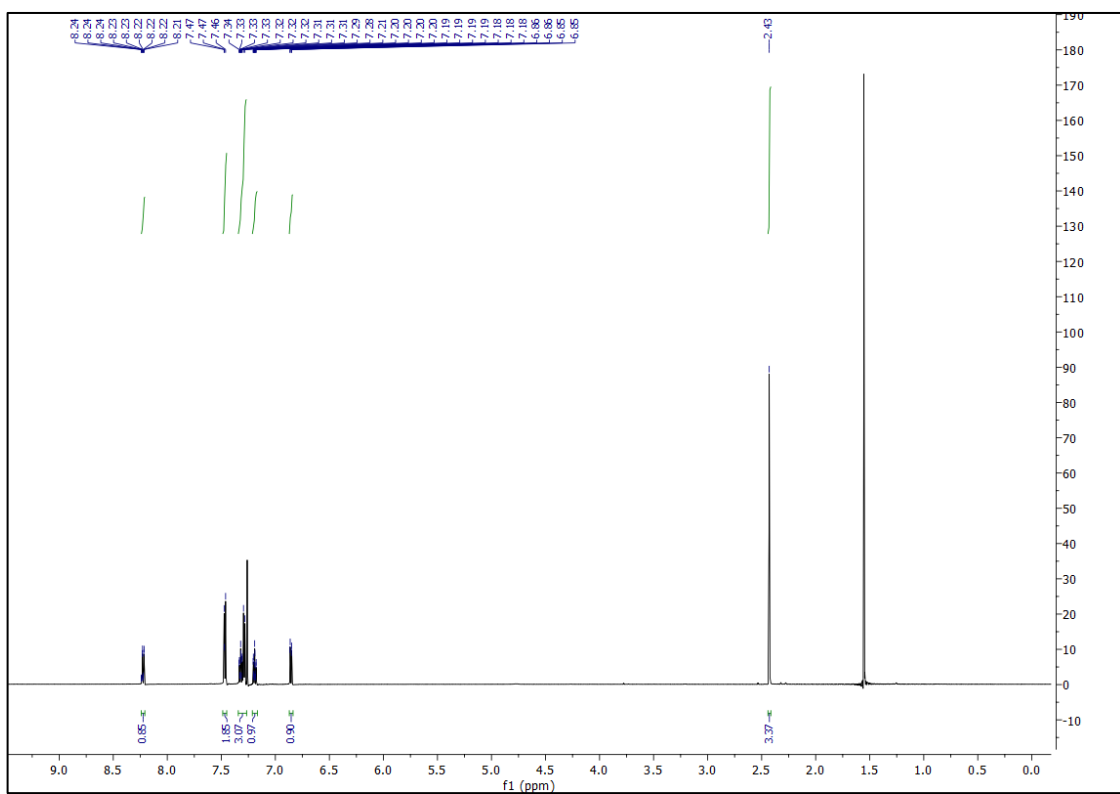
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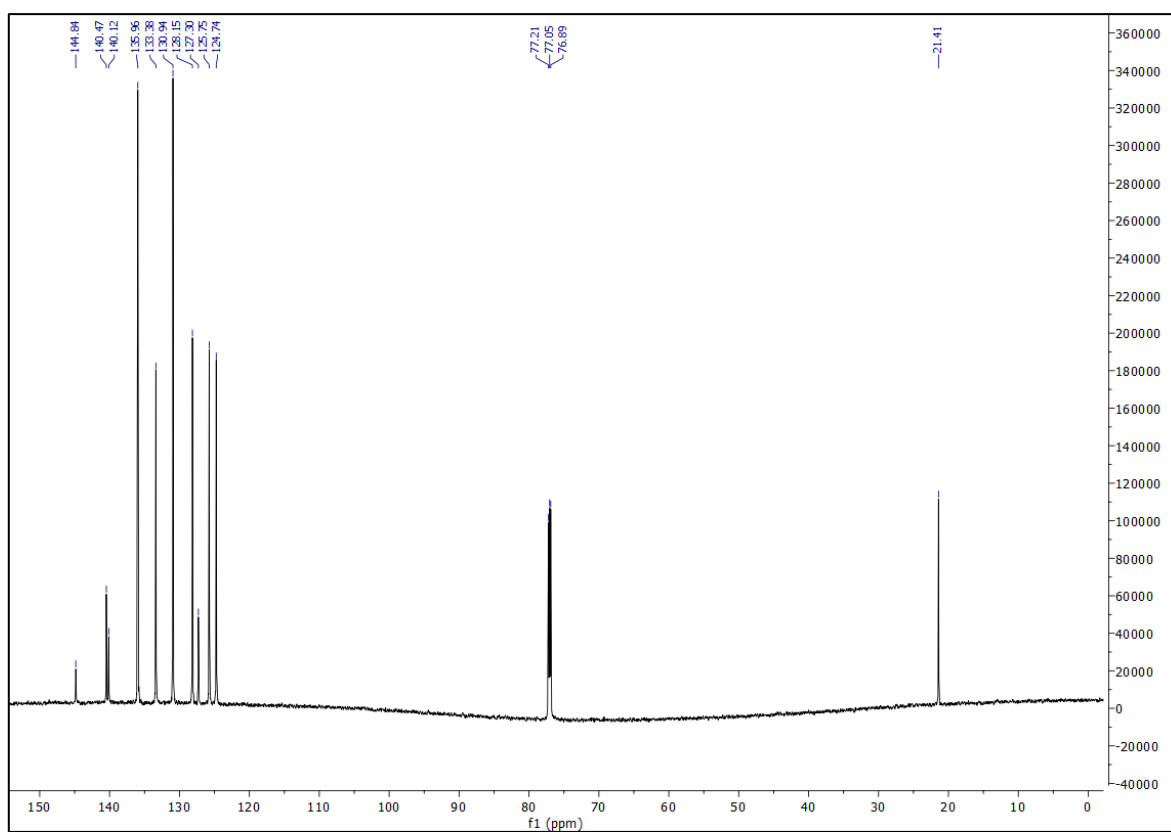
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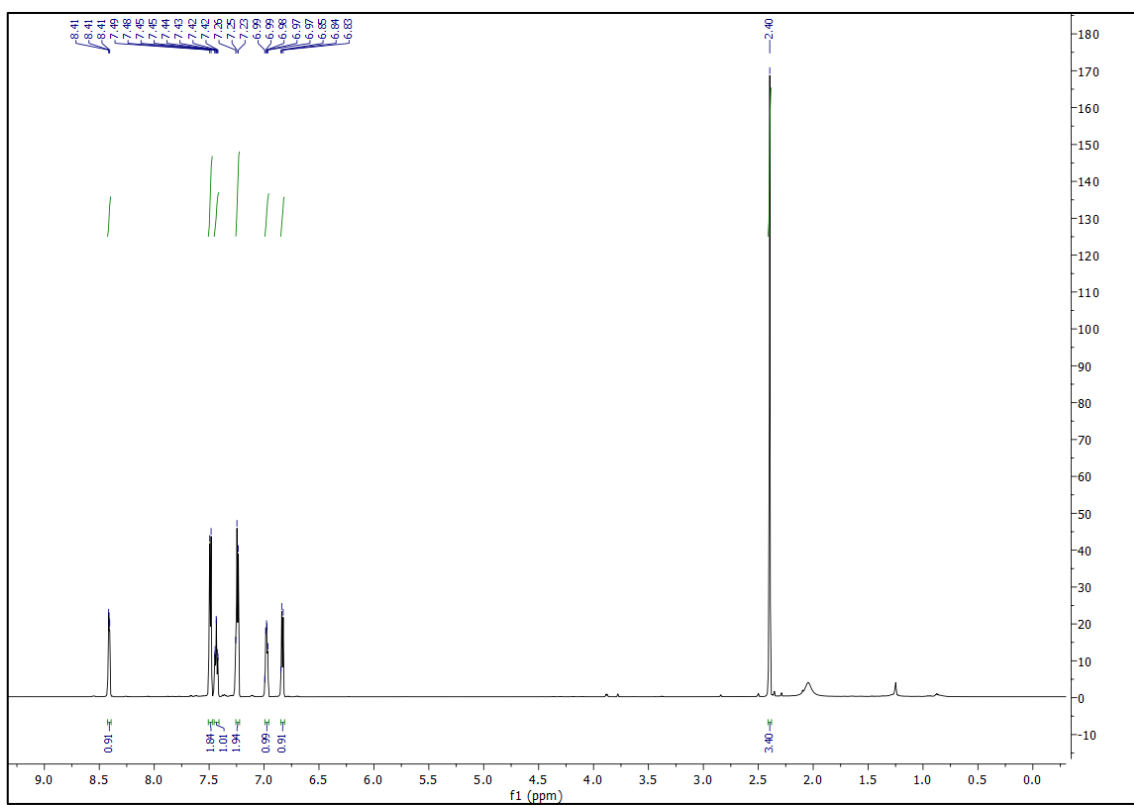
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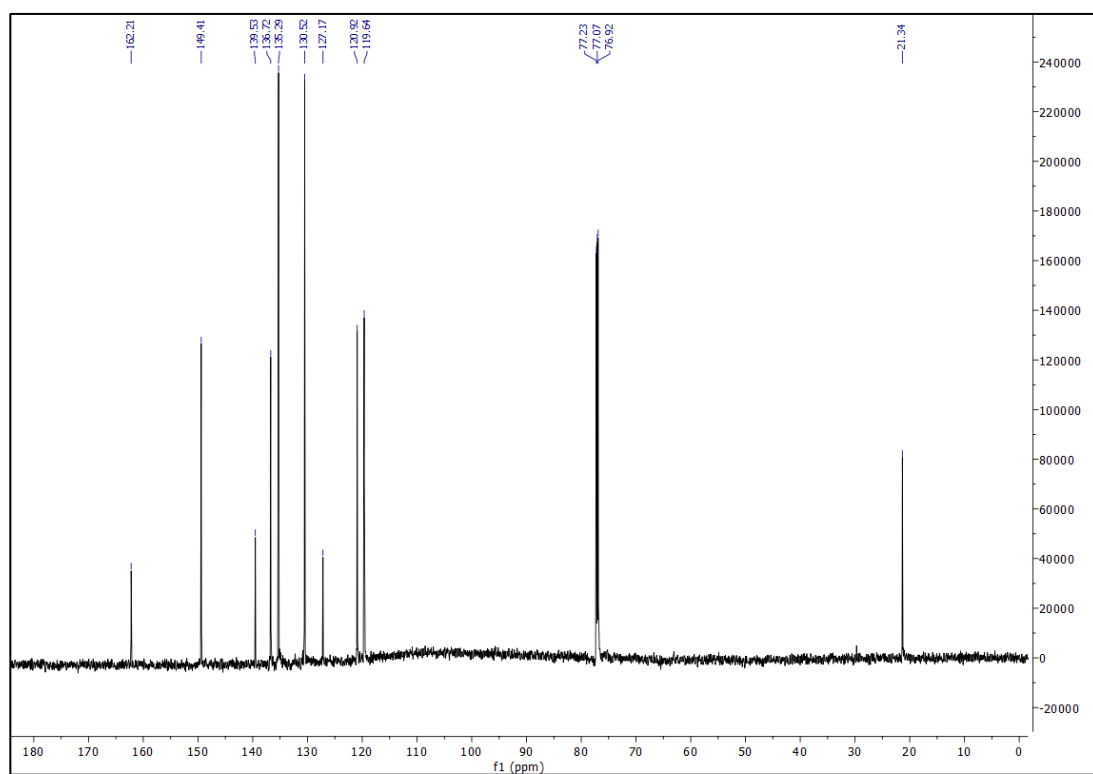
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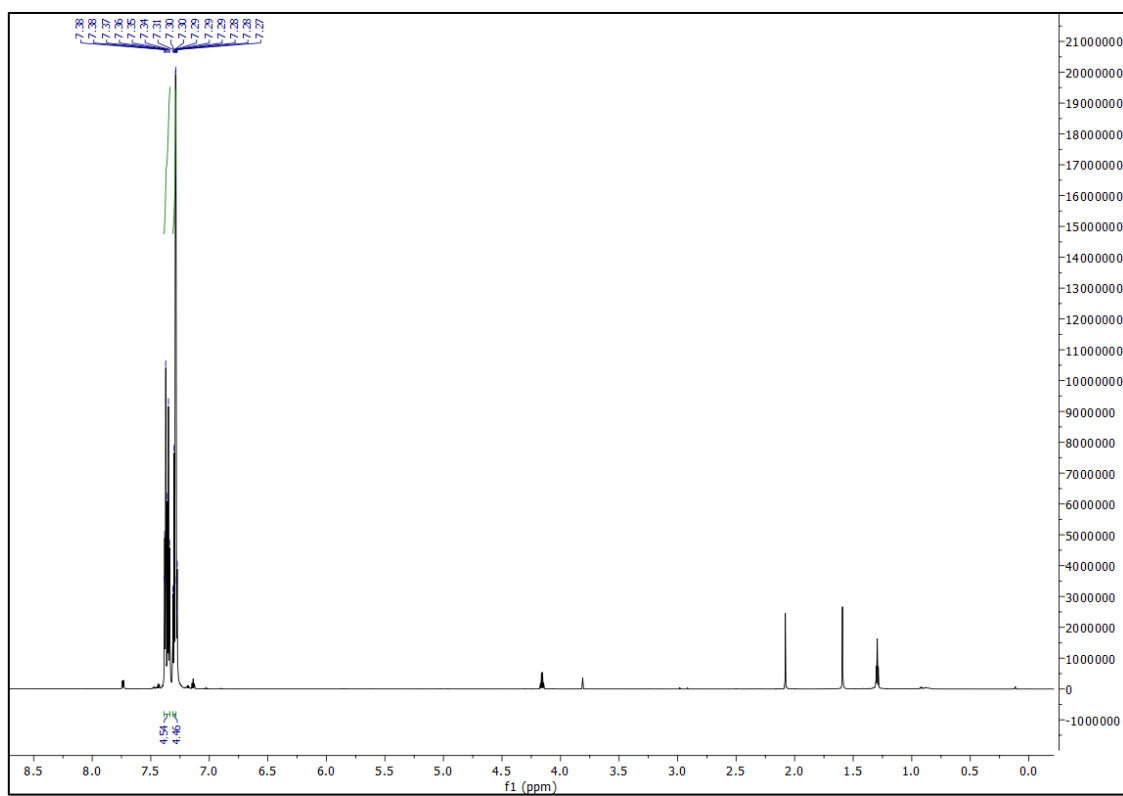
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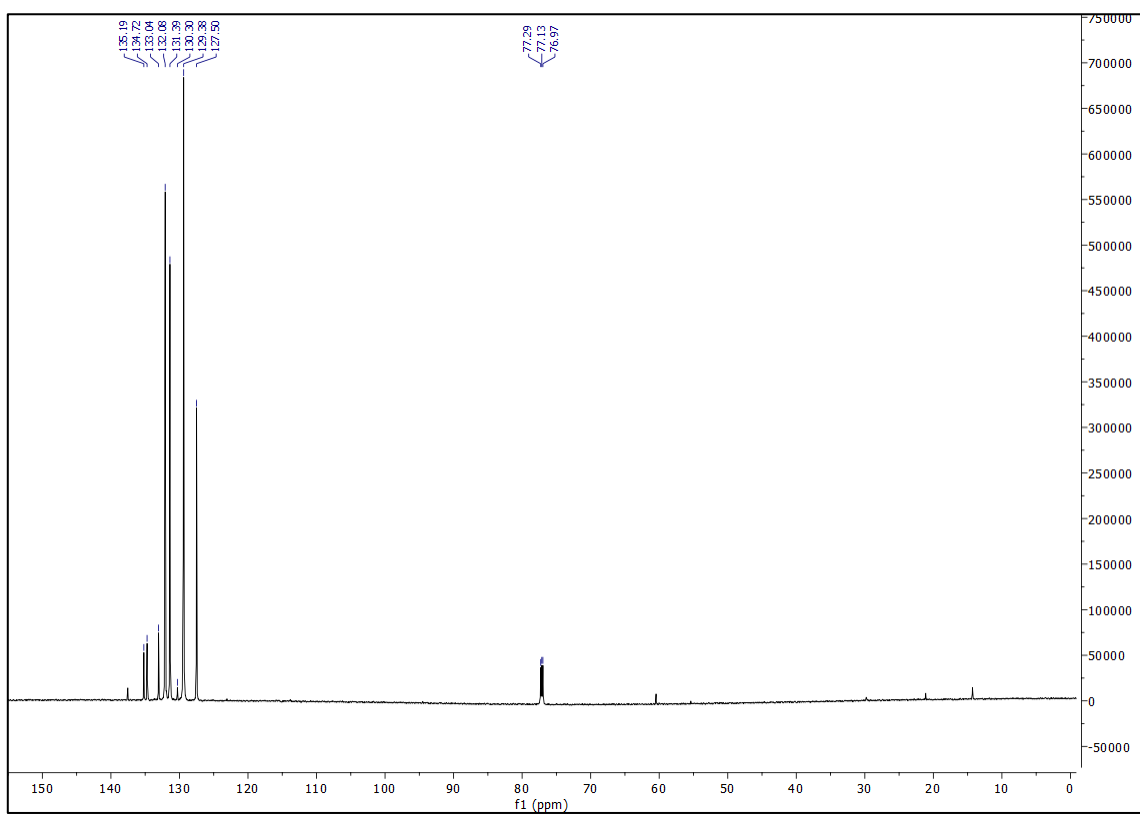
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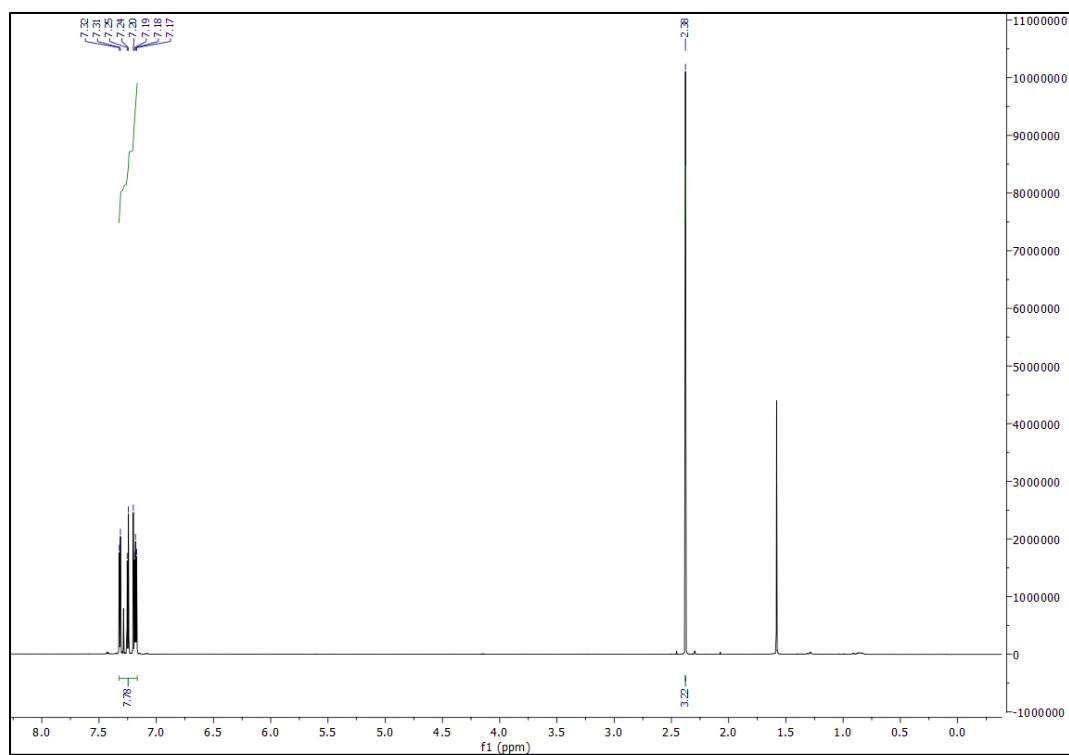
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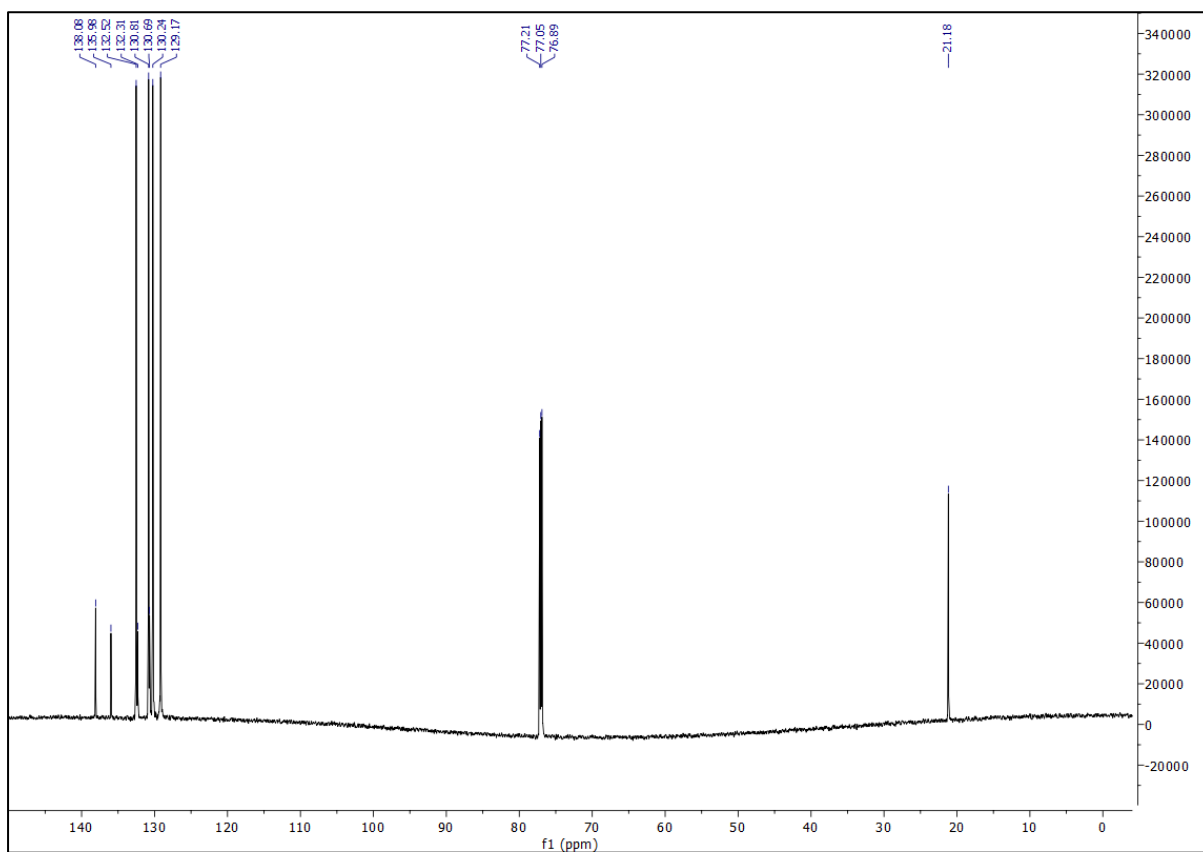
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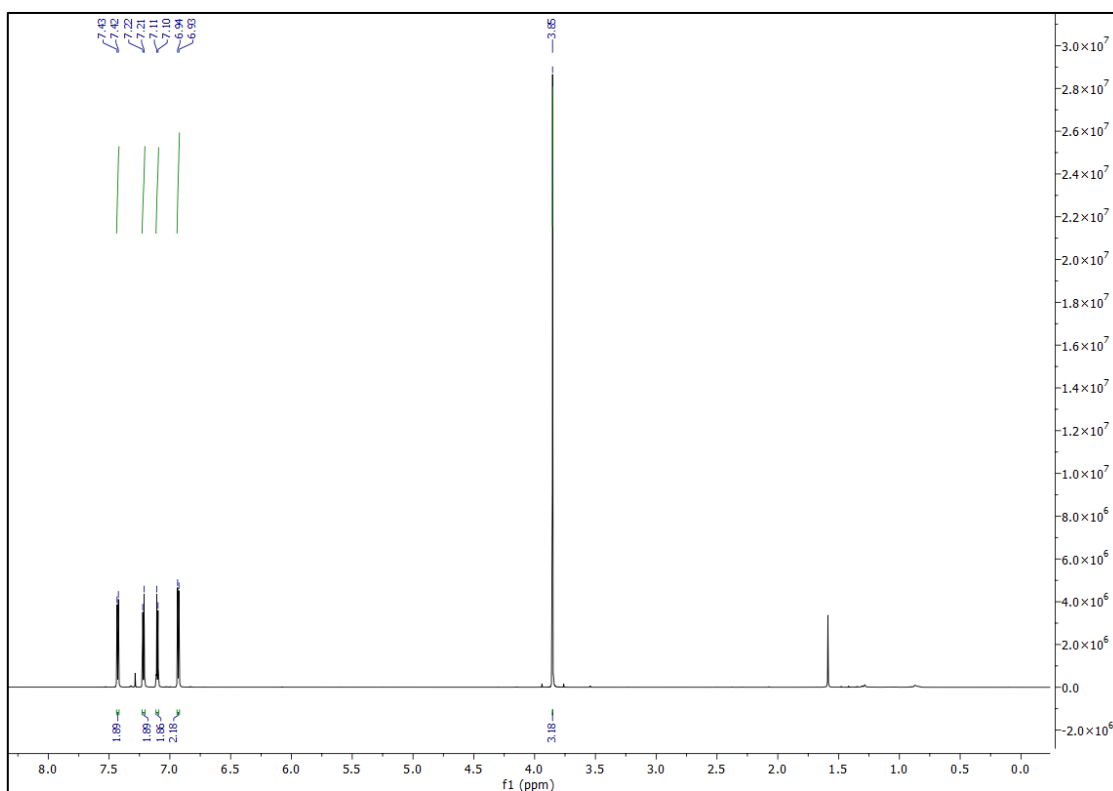
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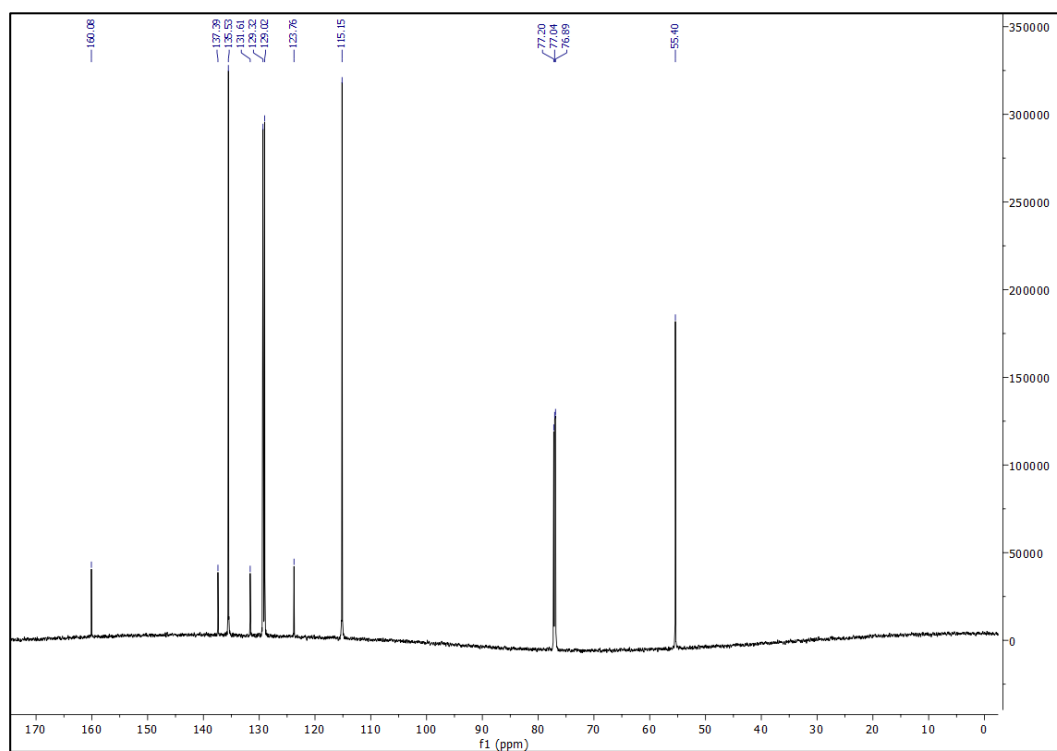
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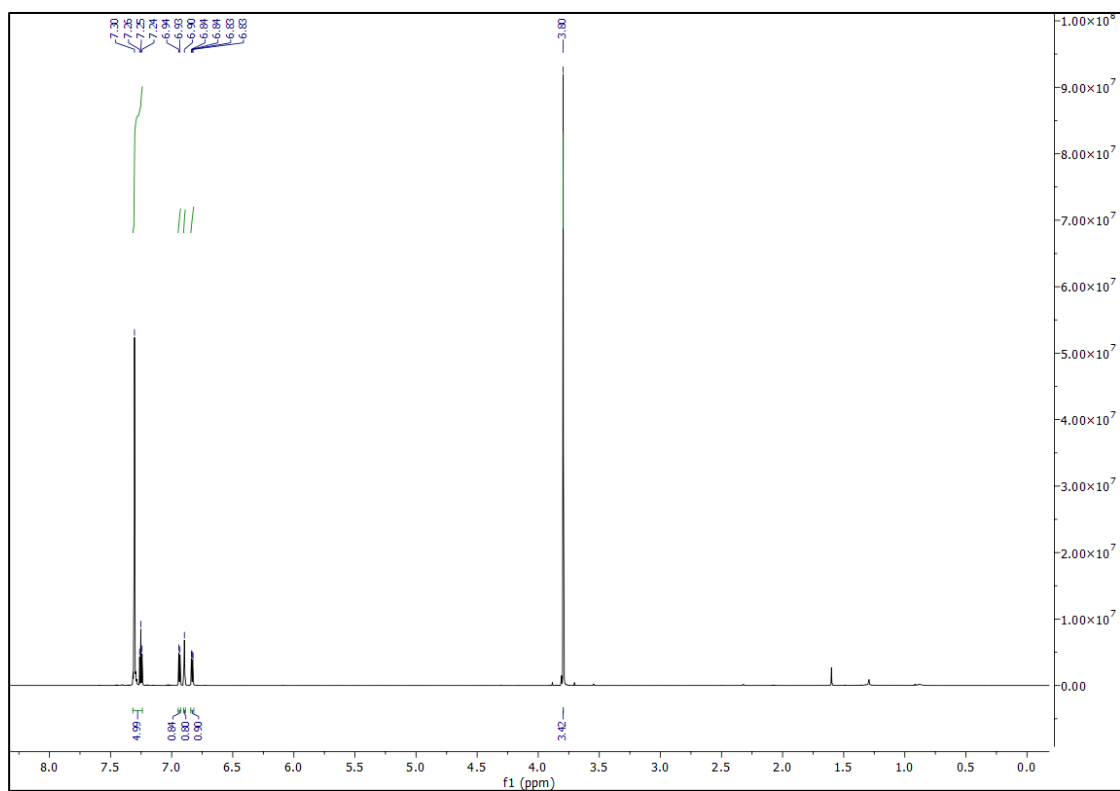
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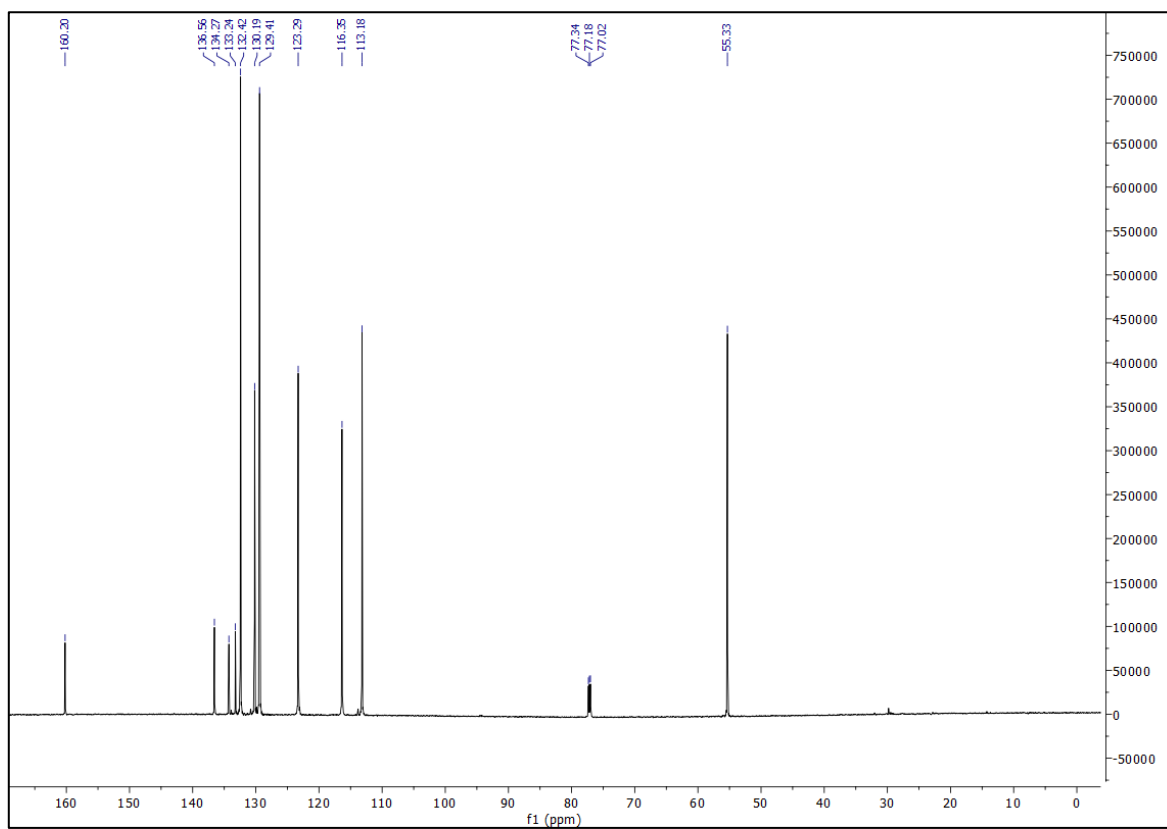
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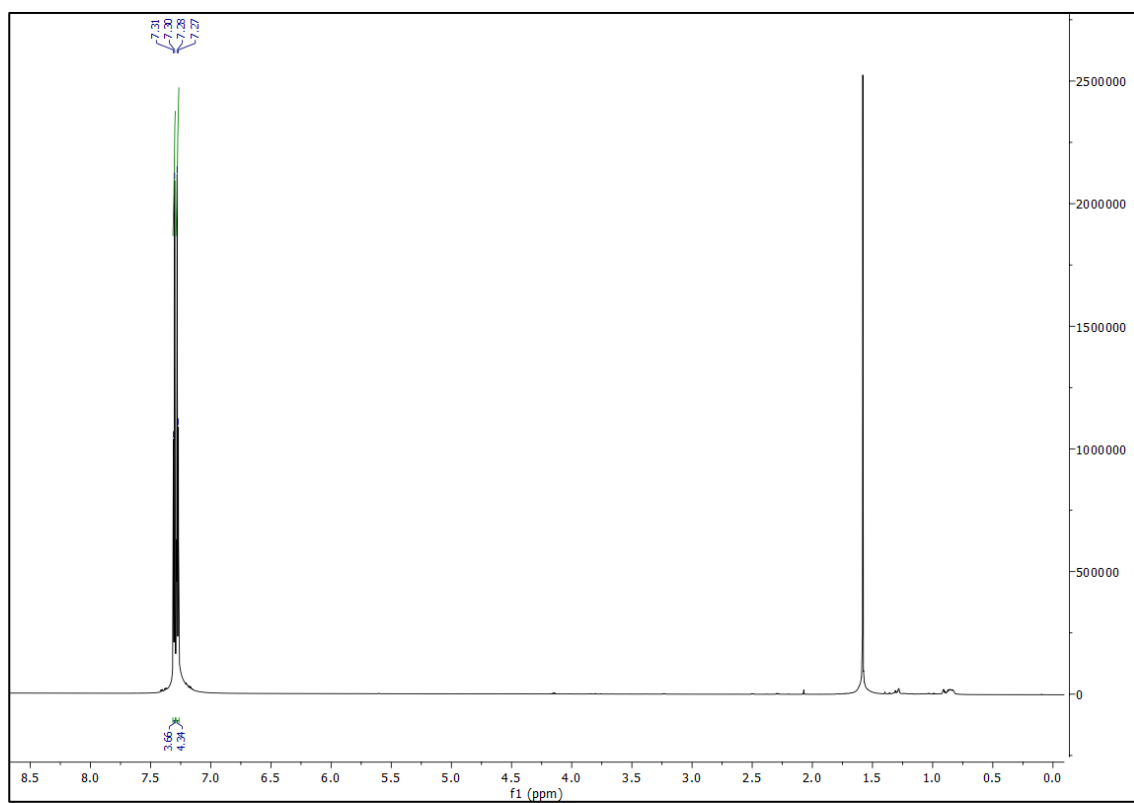
^1H NMR of (**4k**)



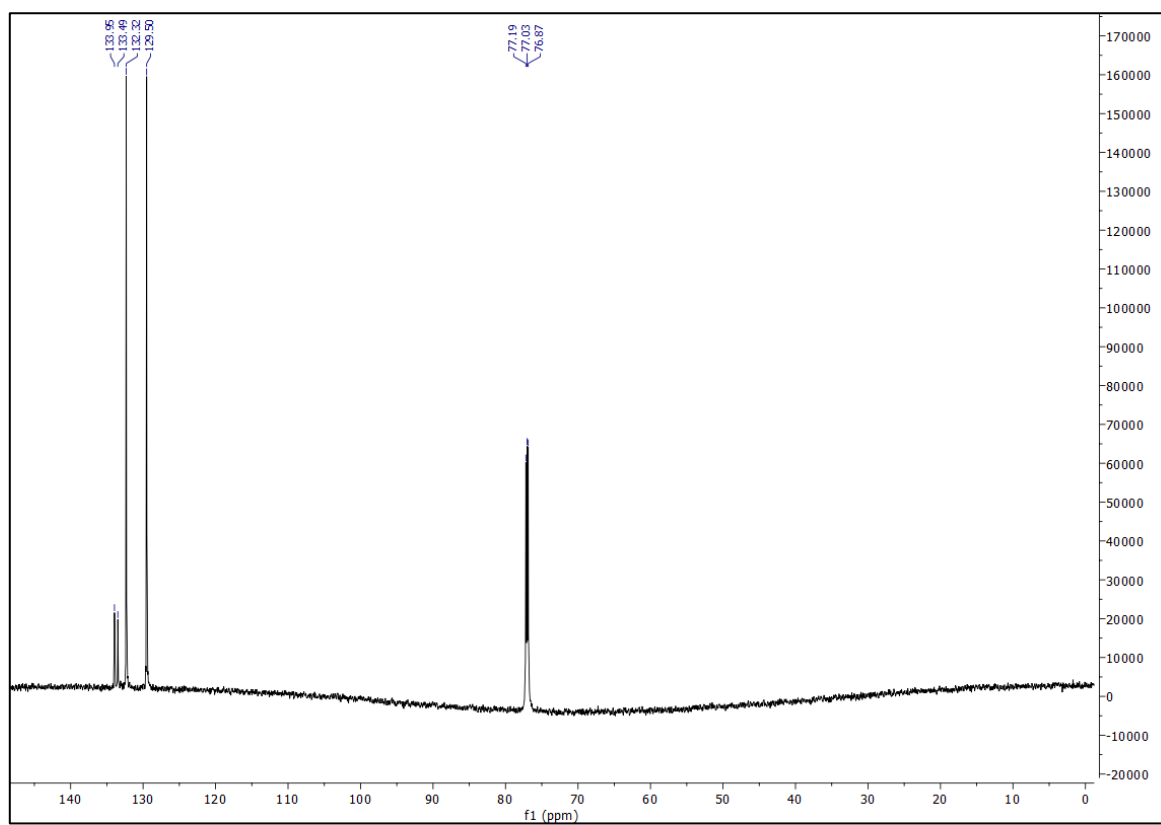
^{13}C NMR of (**4k**)



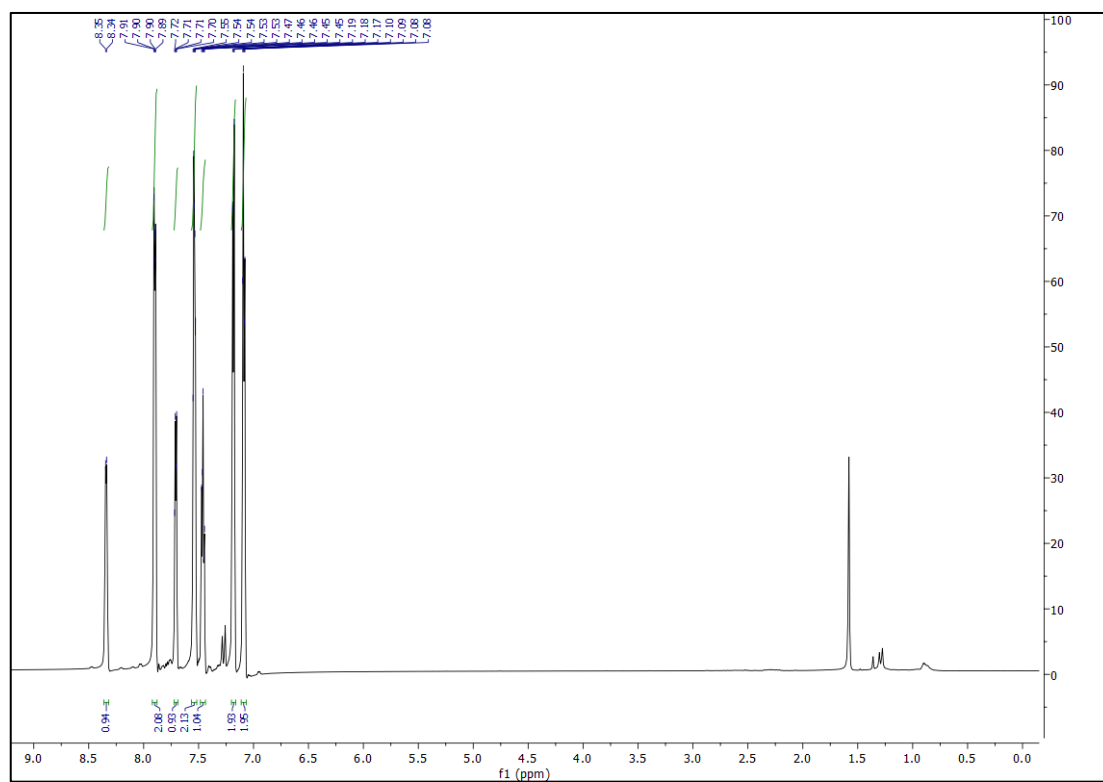
^1H NMR of (4I)



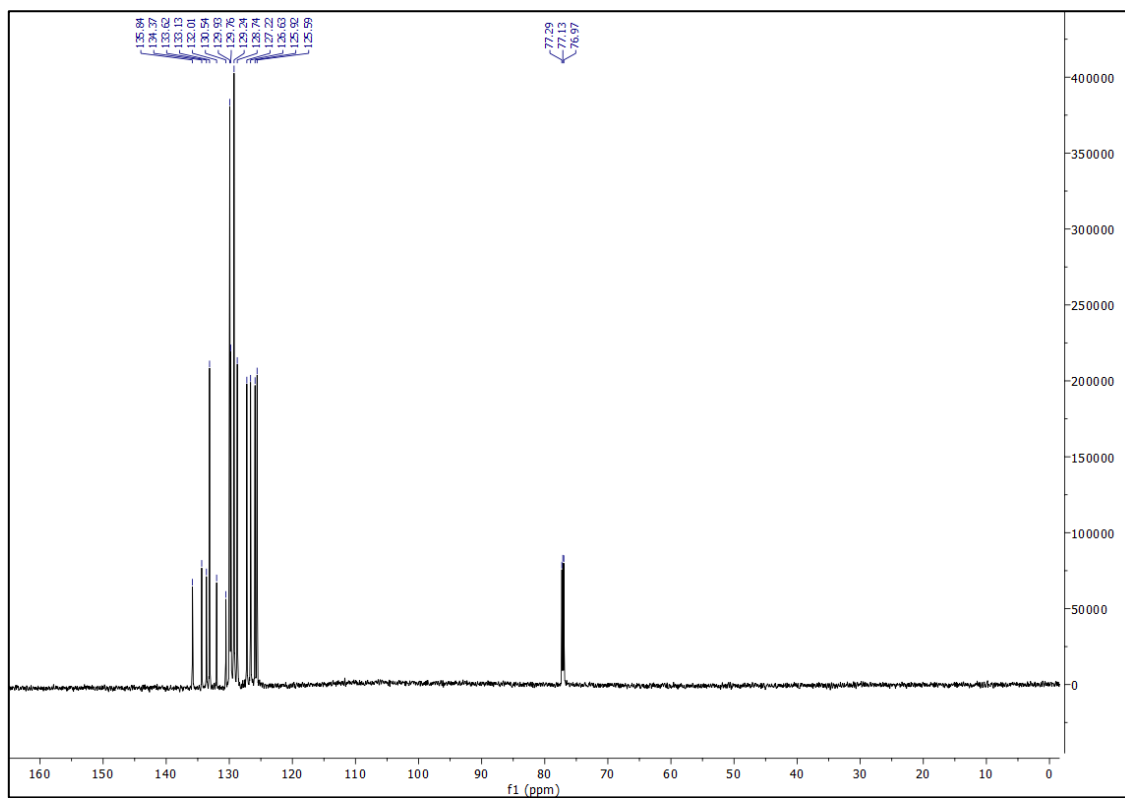
^{13}C NMR of (4I)



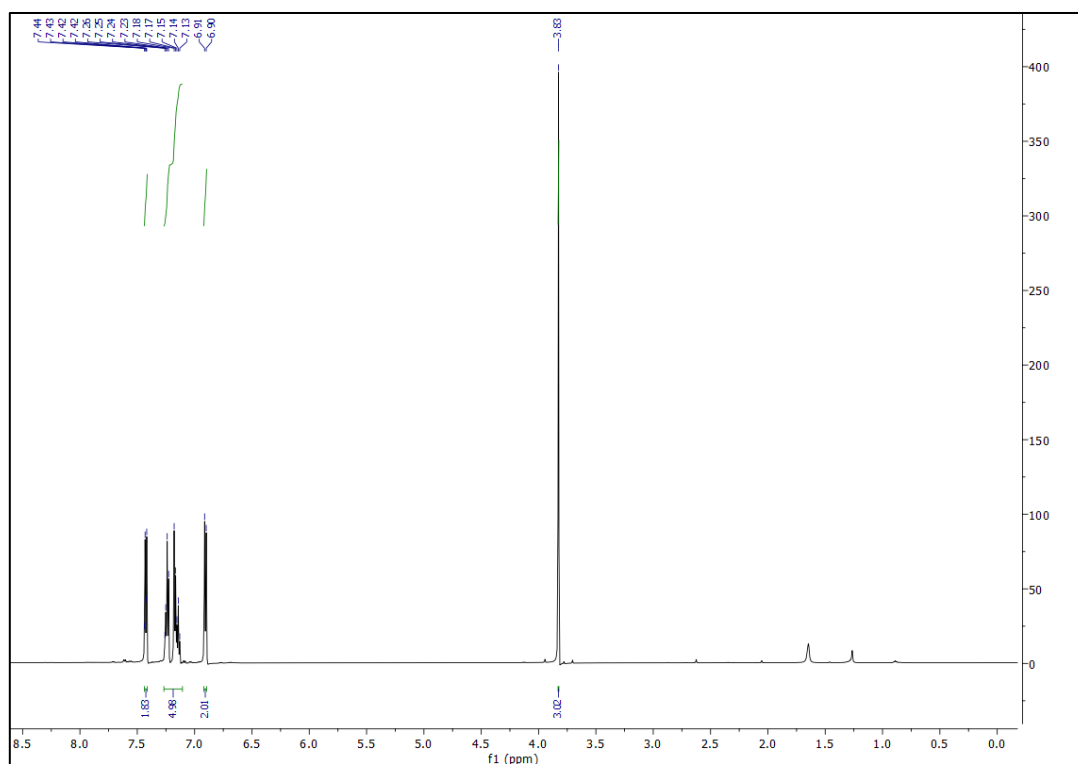
^1H NMR of (4m)



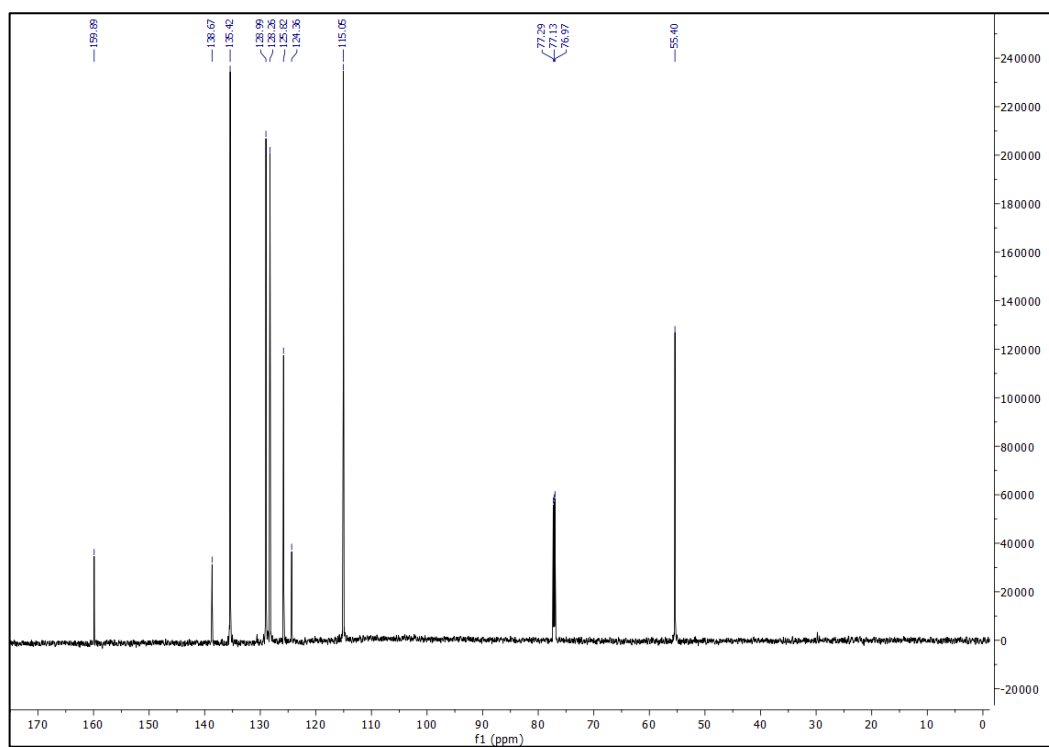
^{13}C NMR of (4m)



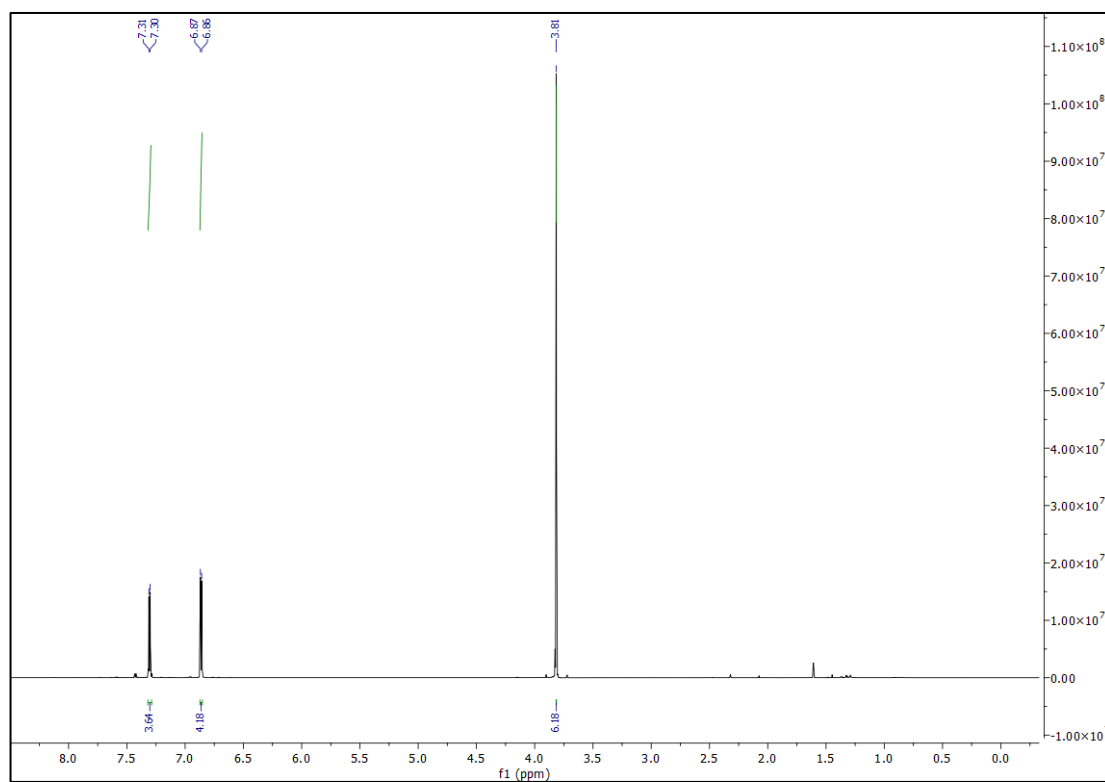
^1H NMR of (4n)



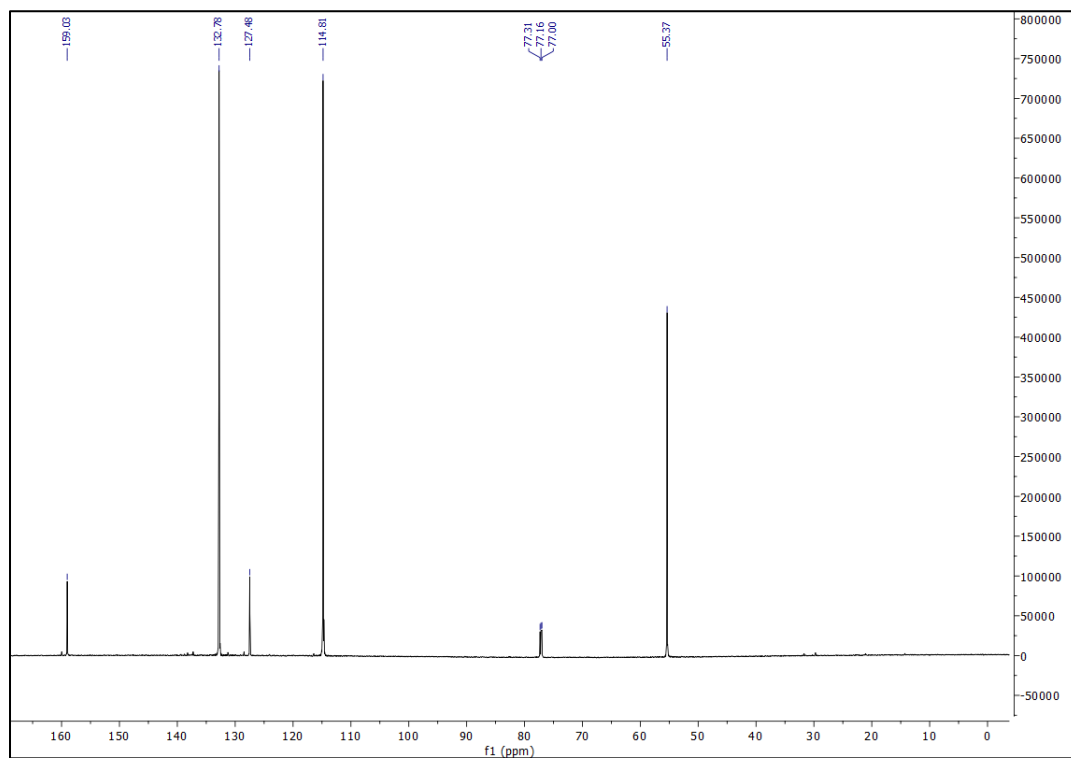
^{13}C NMR of (4n)



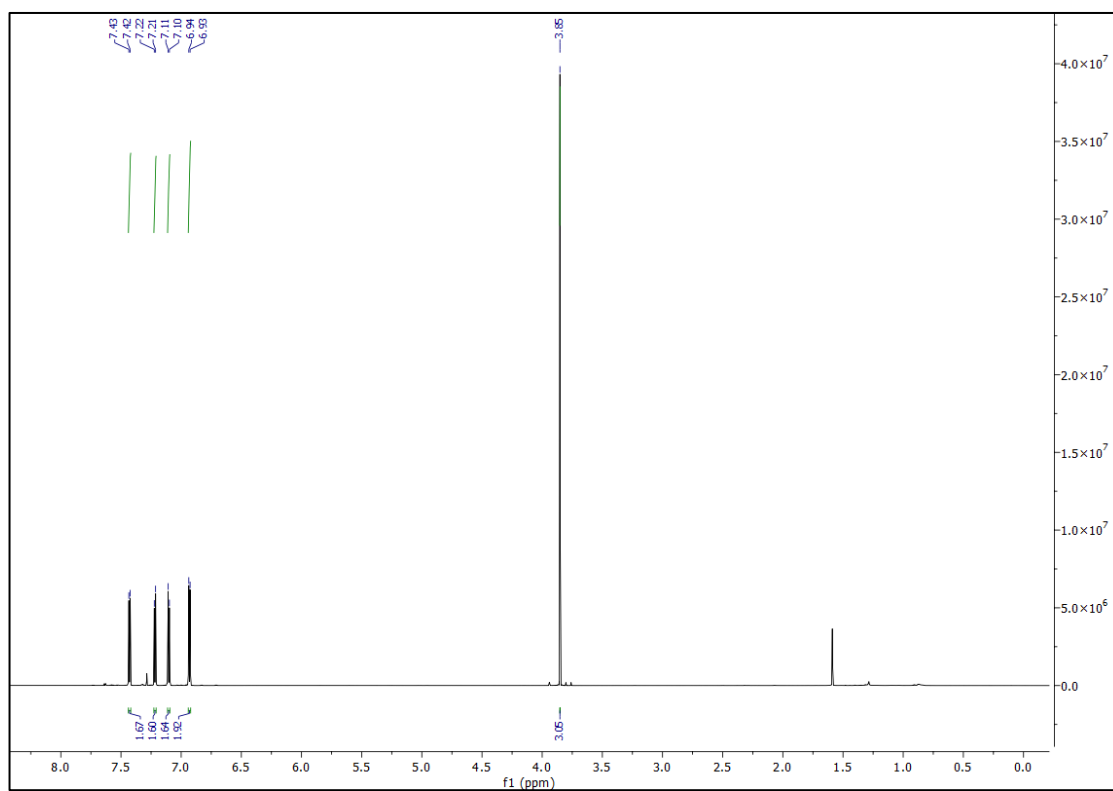
^1H NMR of (4o)



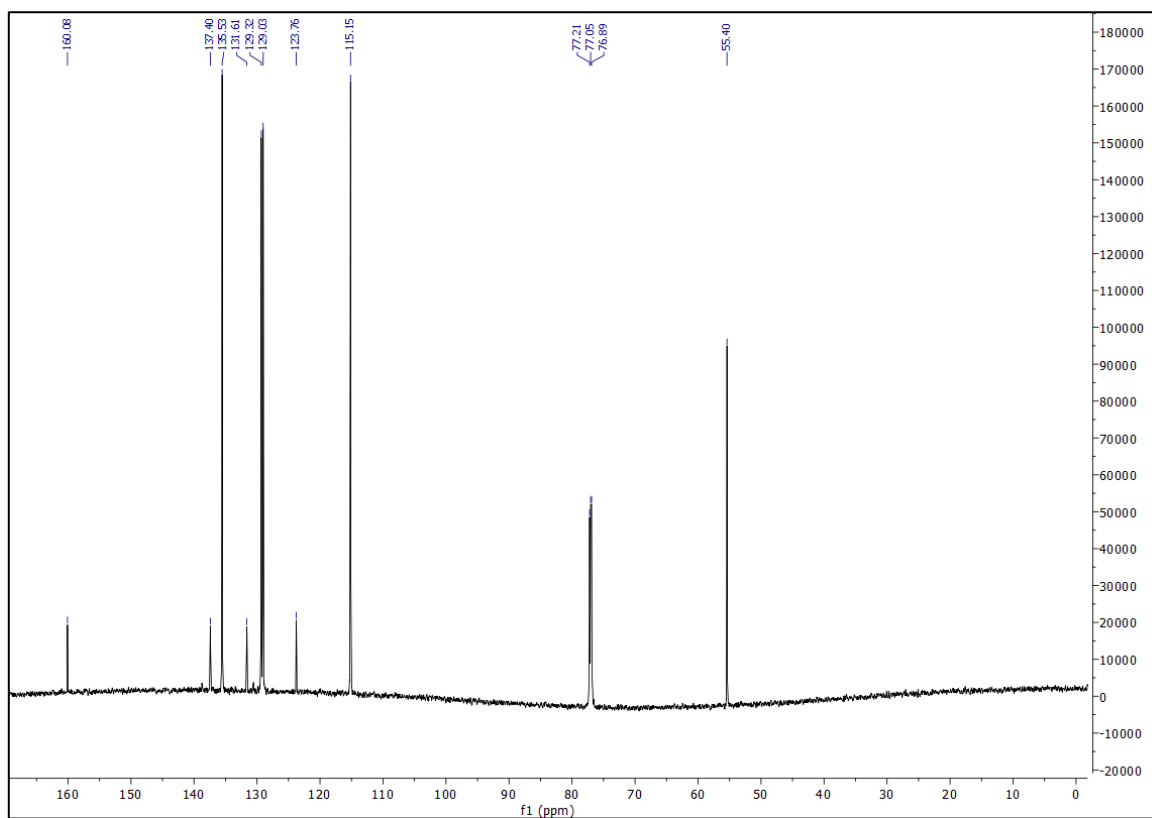
^{13}C NMR of (4o)



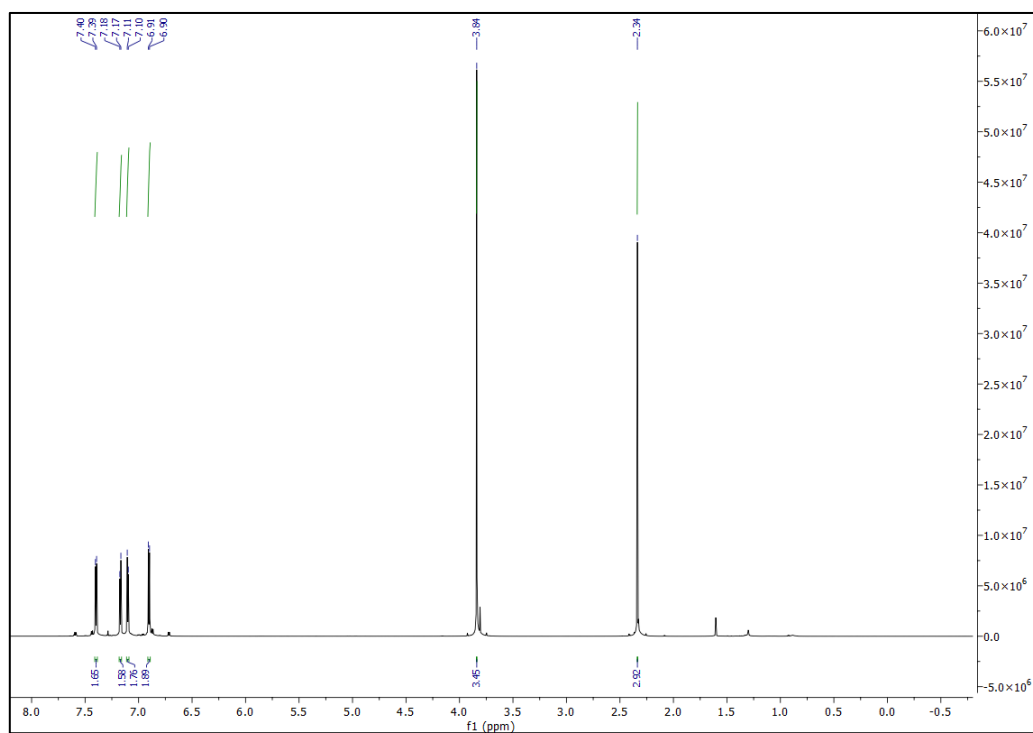
^1H NMR of (4p)



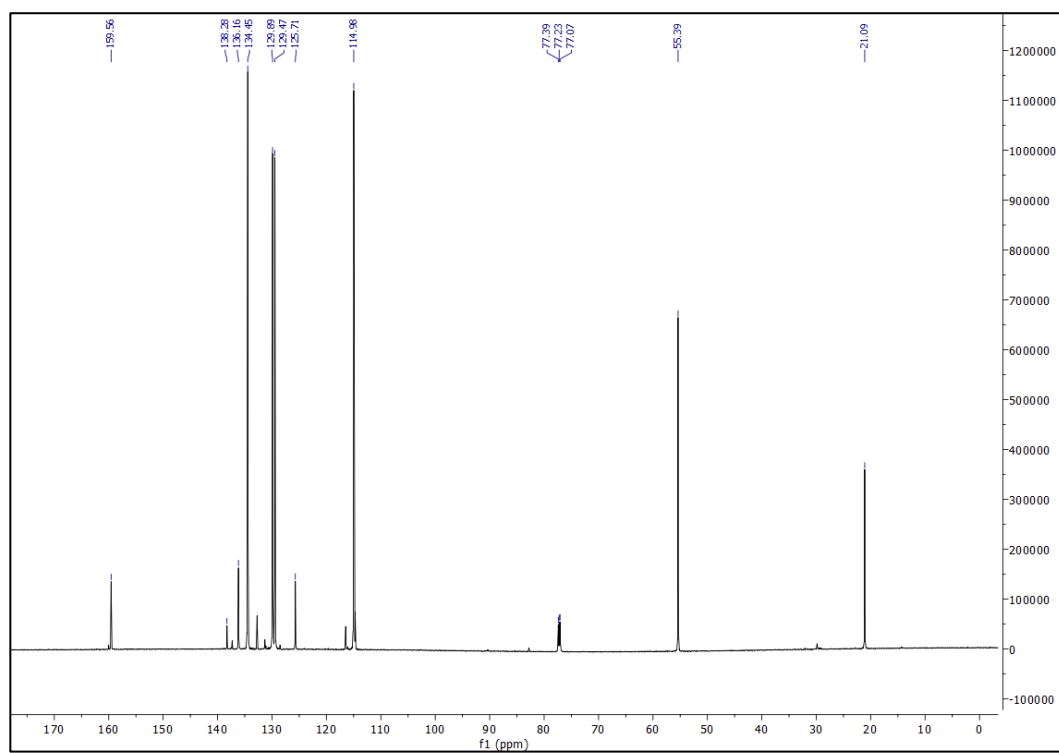
^{13}C NMR of (4p)



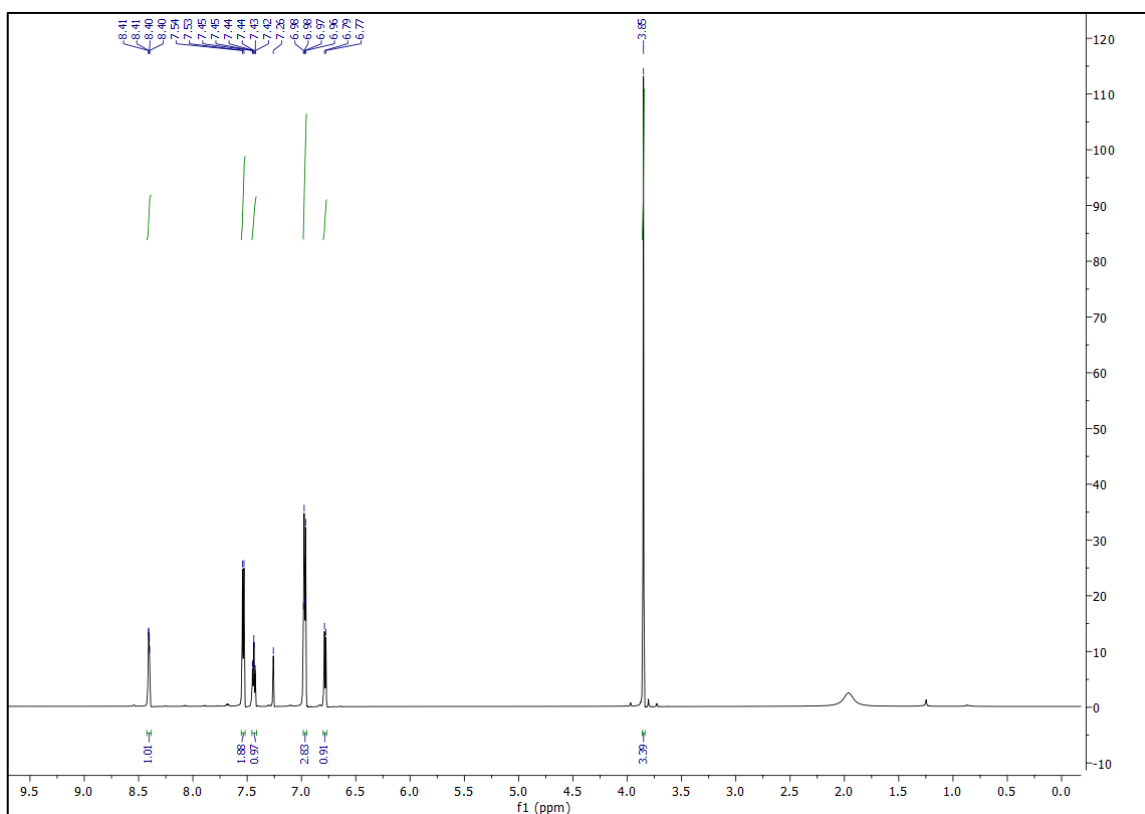
¹H NMR of (4q)



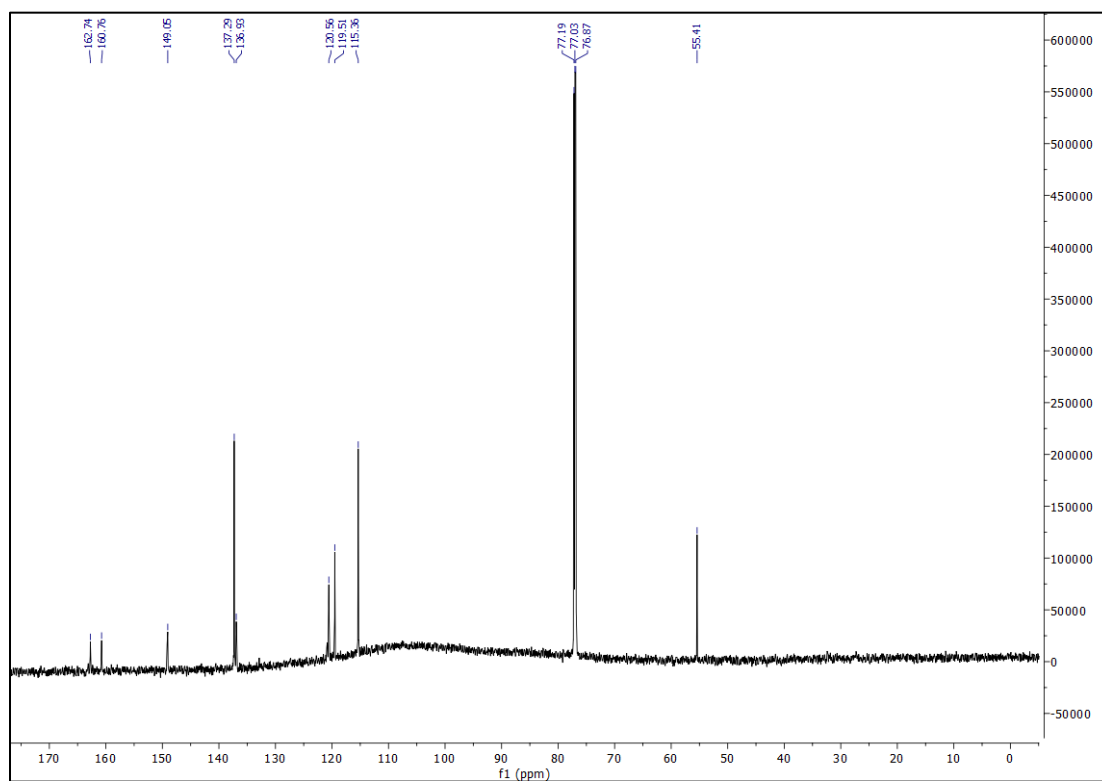
¹³C NMR of (4q)



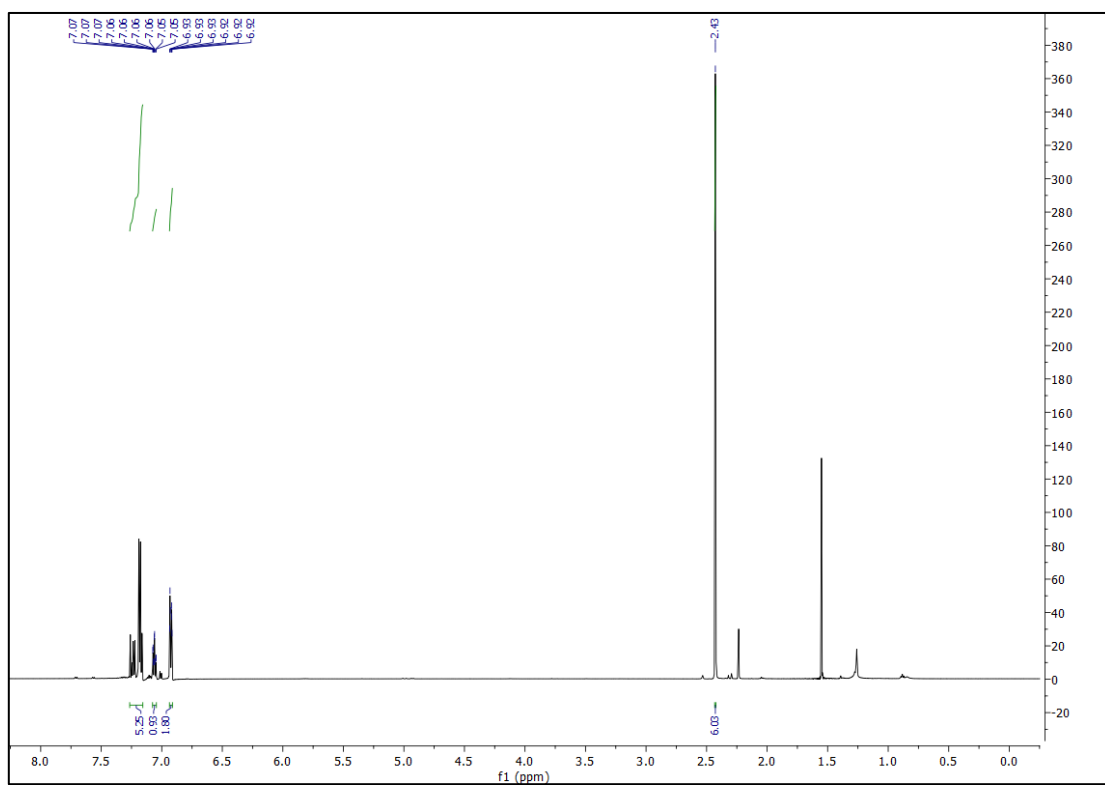
^1H NMR of (**4r**)



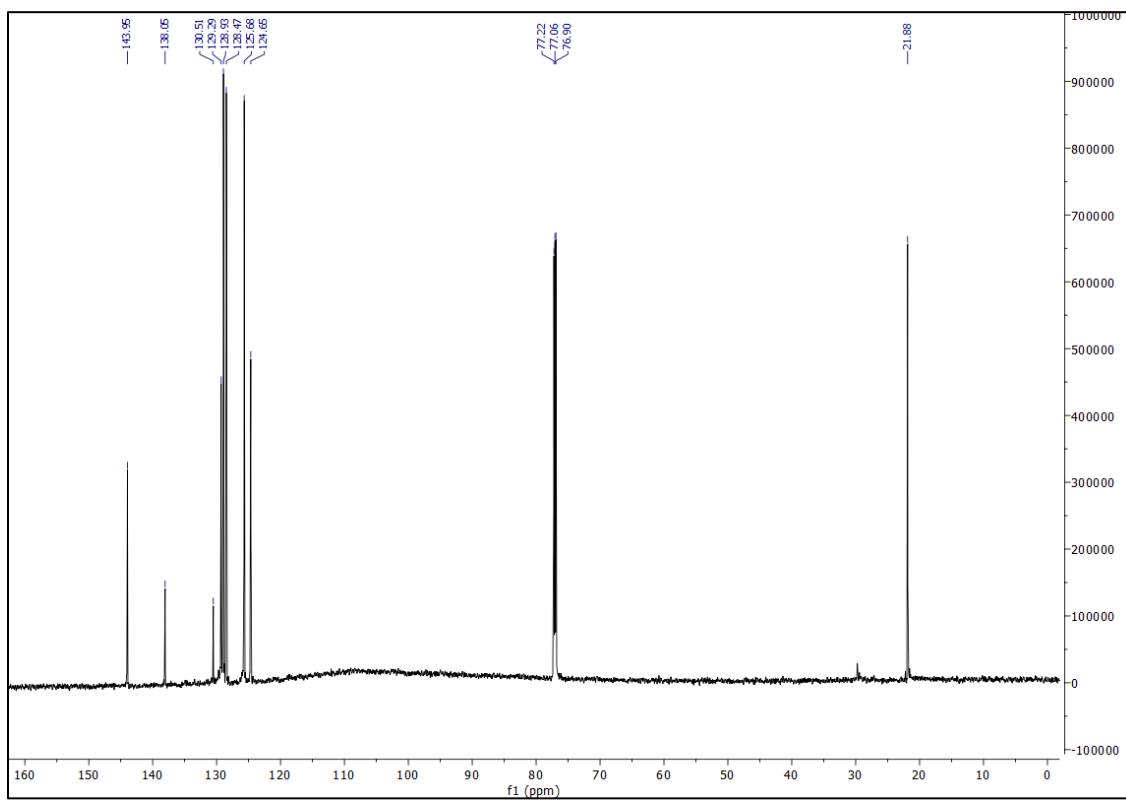
^{13}C NMR of (**4r**)



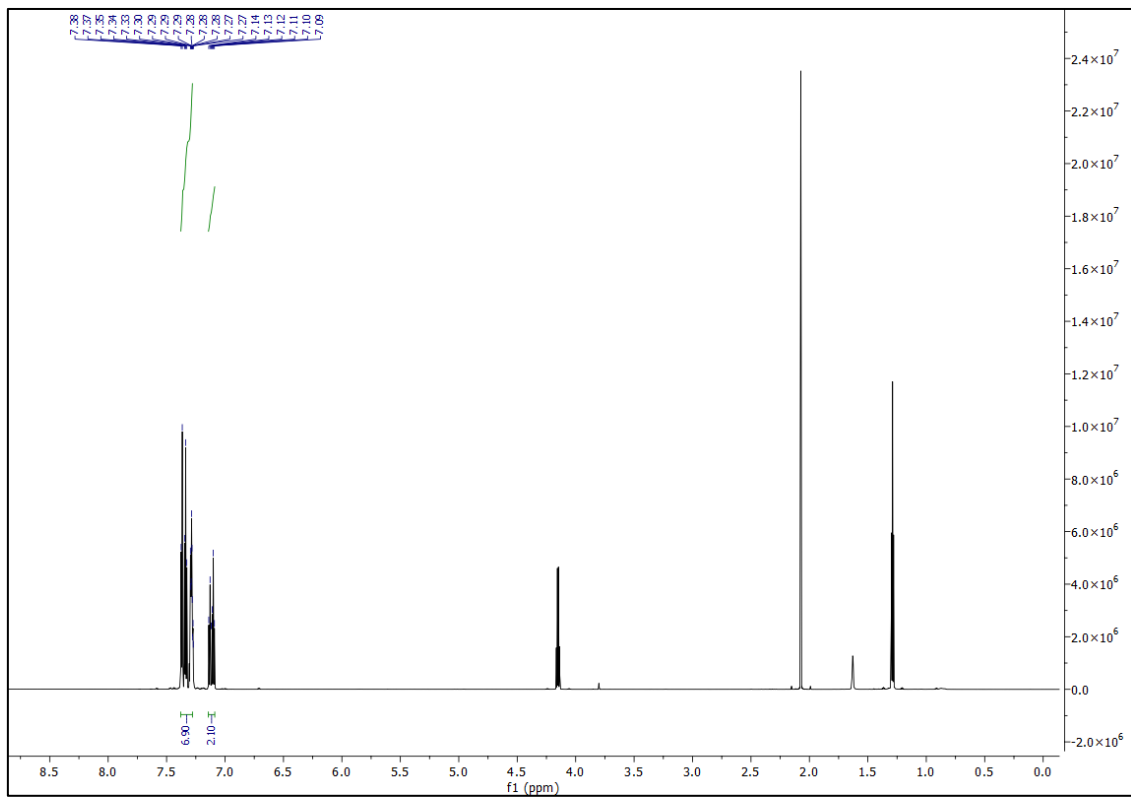
^1H NMR of (4s)



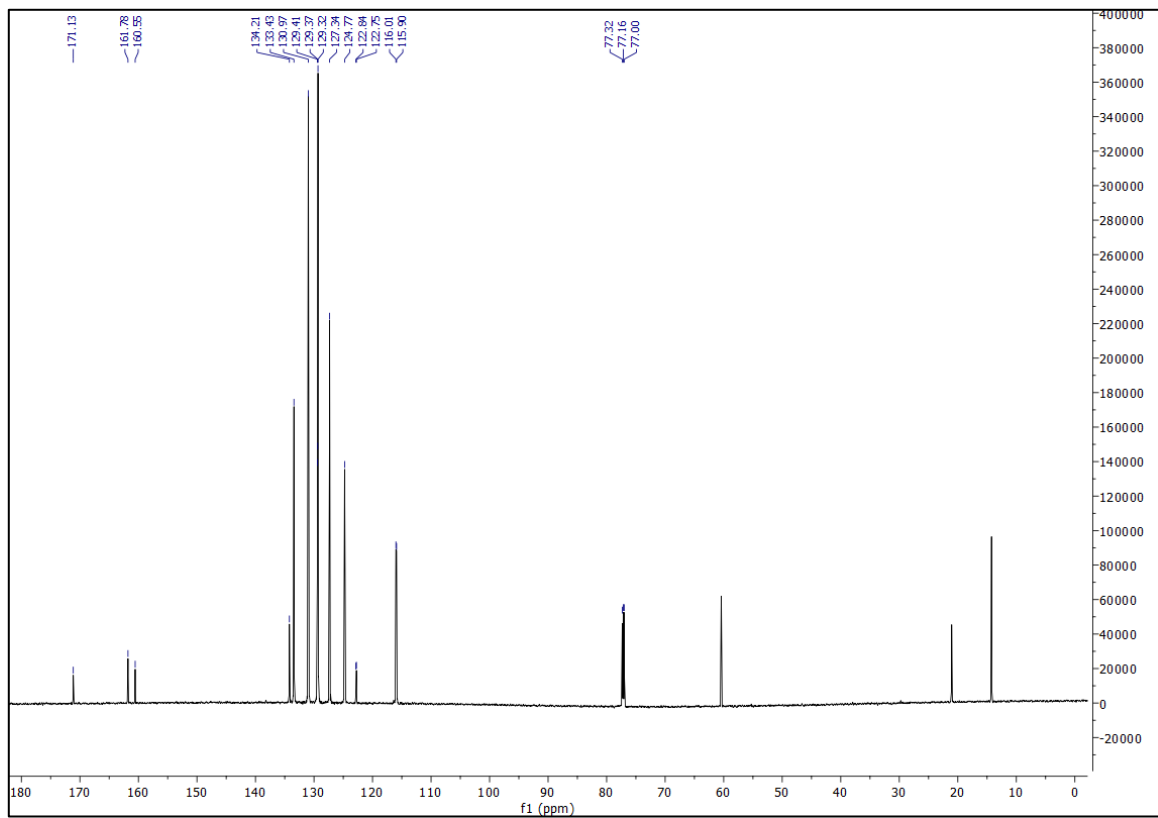
^{13}C NMR spectrum of (4s)



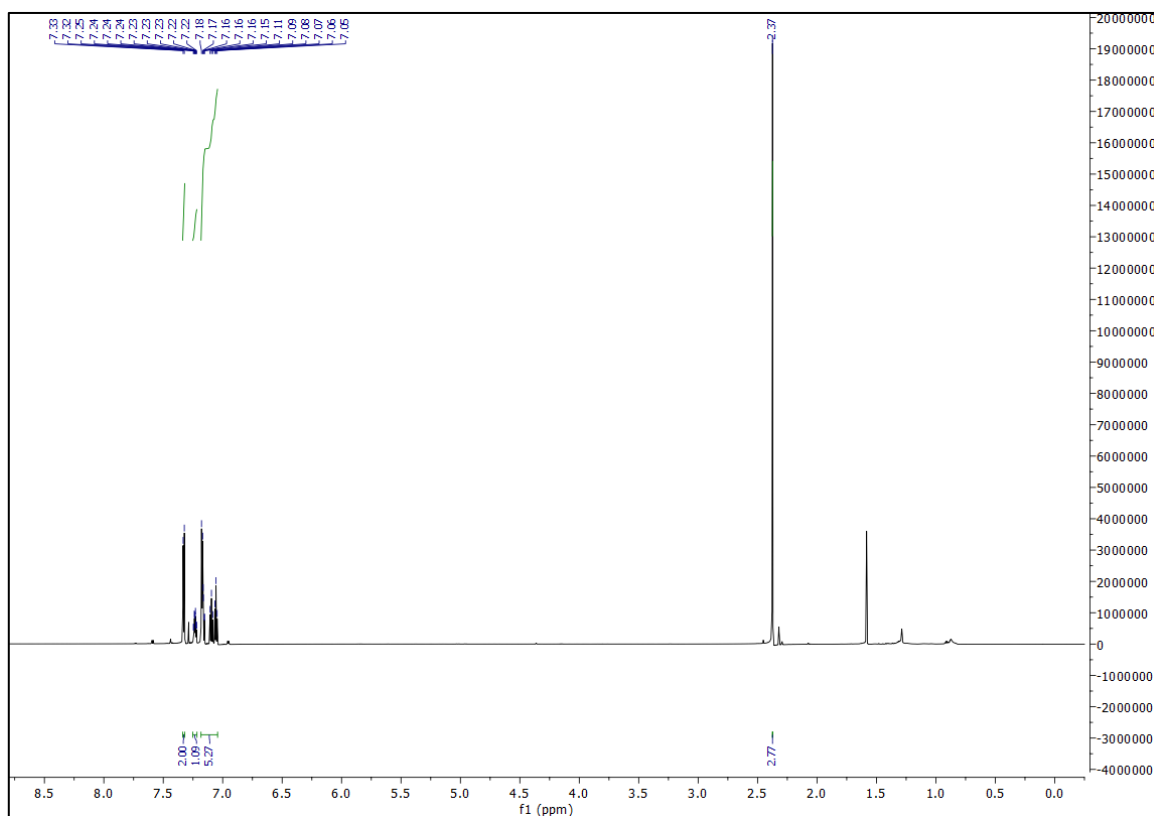
^1H NMR of (4t)



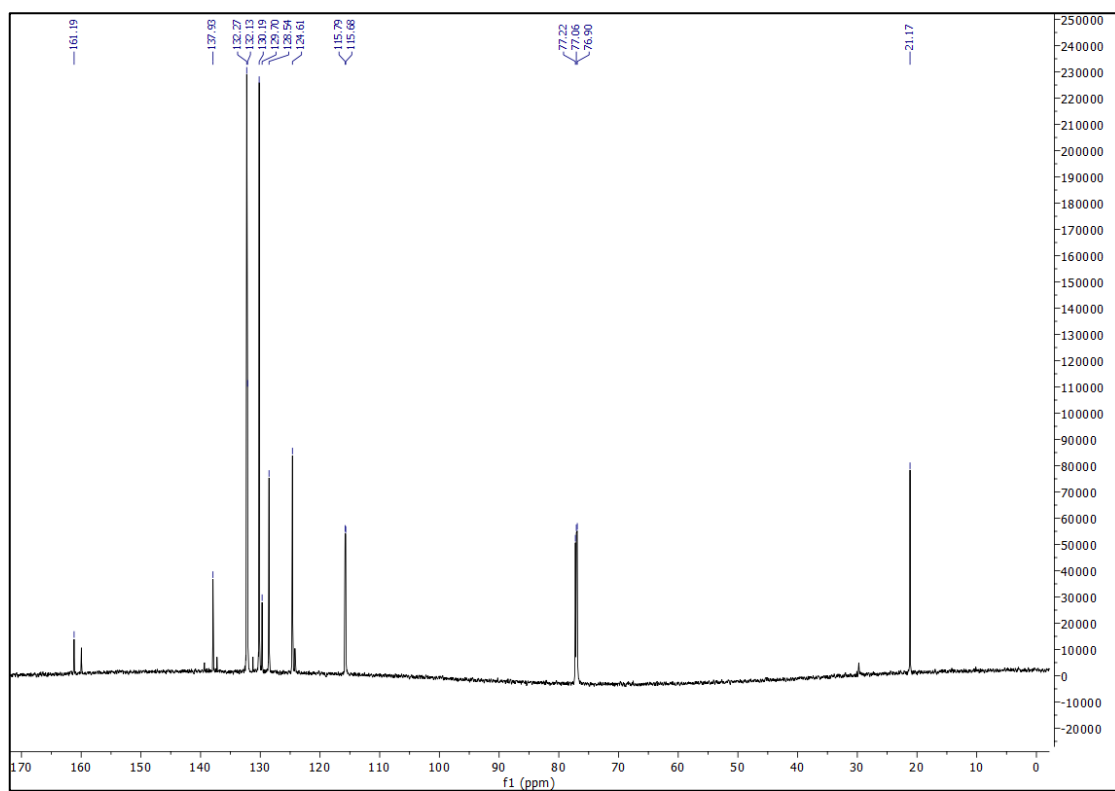
^{13}C NMR of (4t)



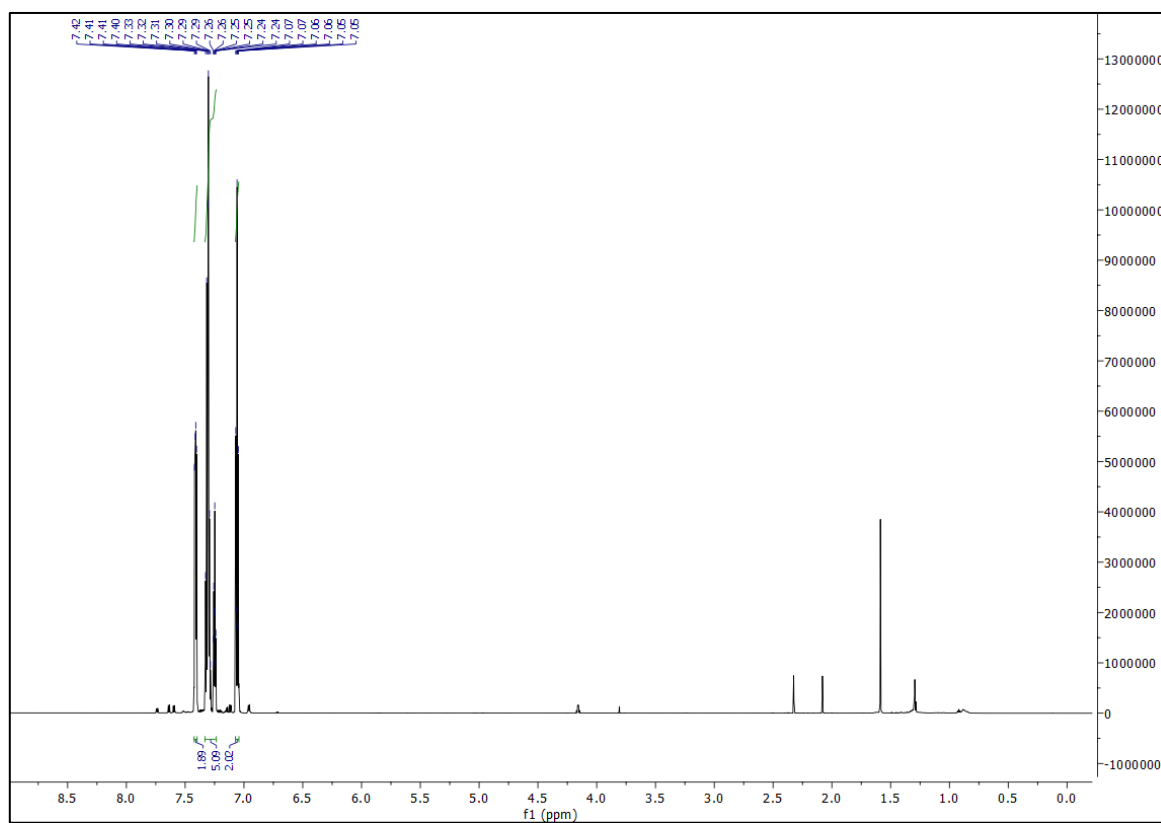
^1H NMR of (**4u**)



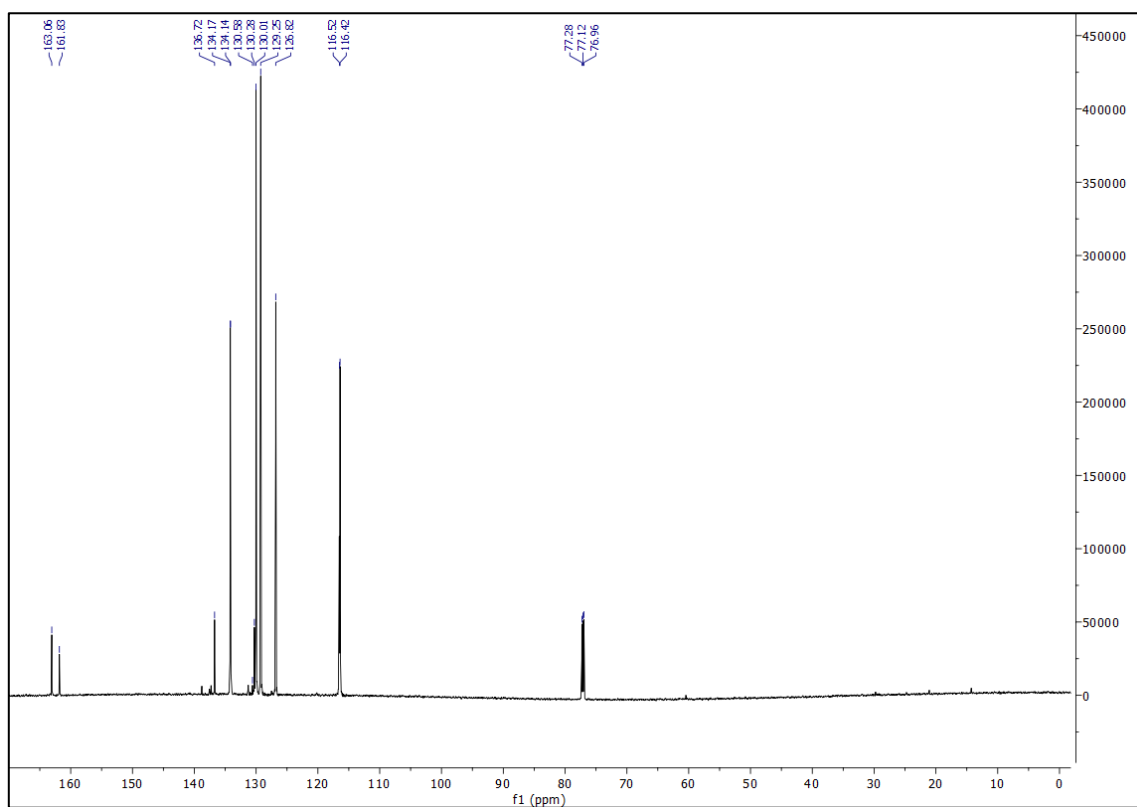
^{13}C NMR of (**4u**)



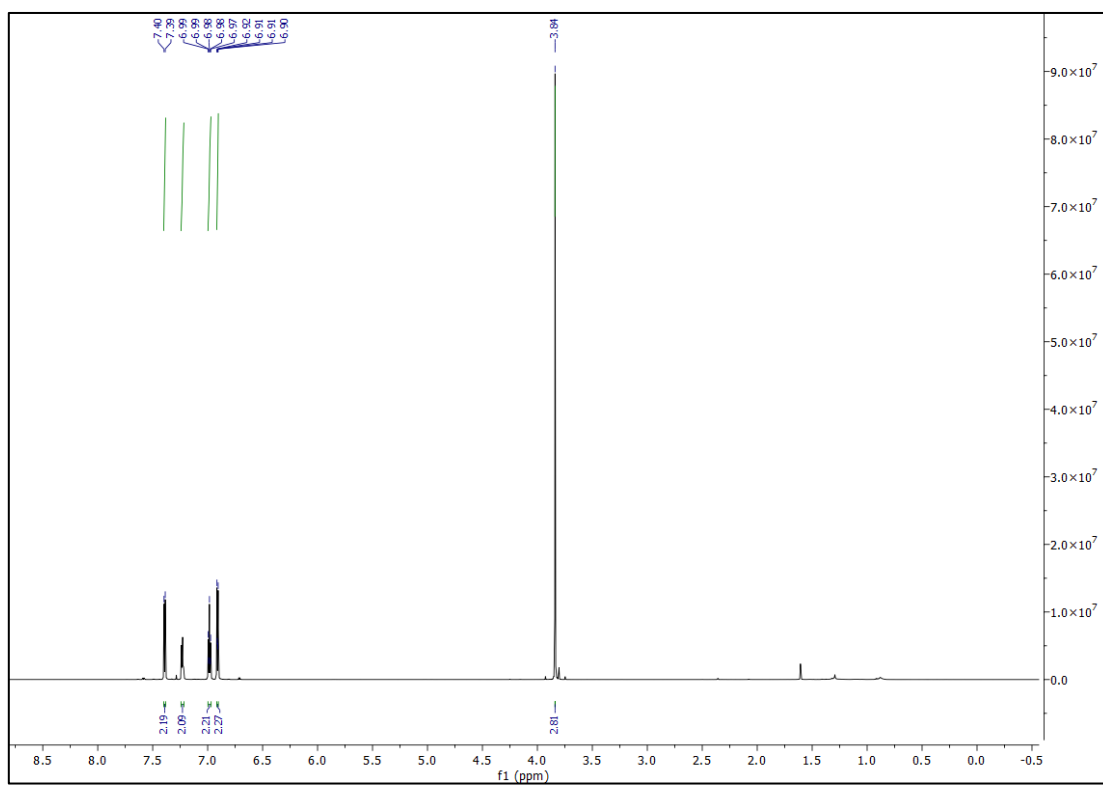
^1H NMR of (4v)



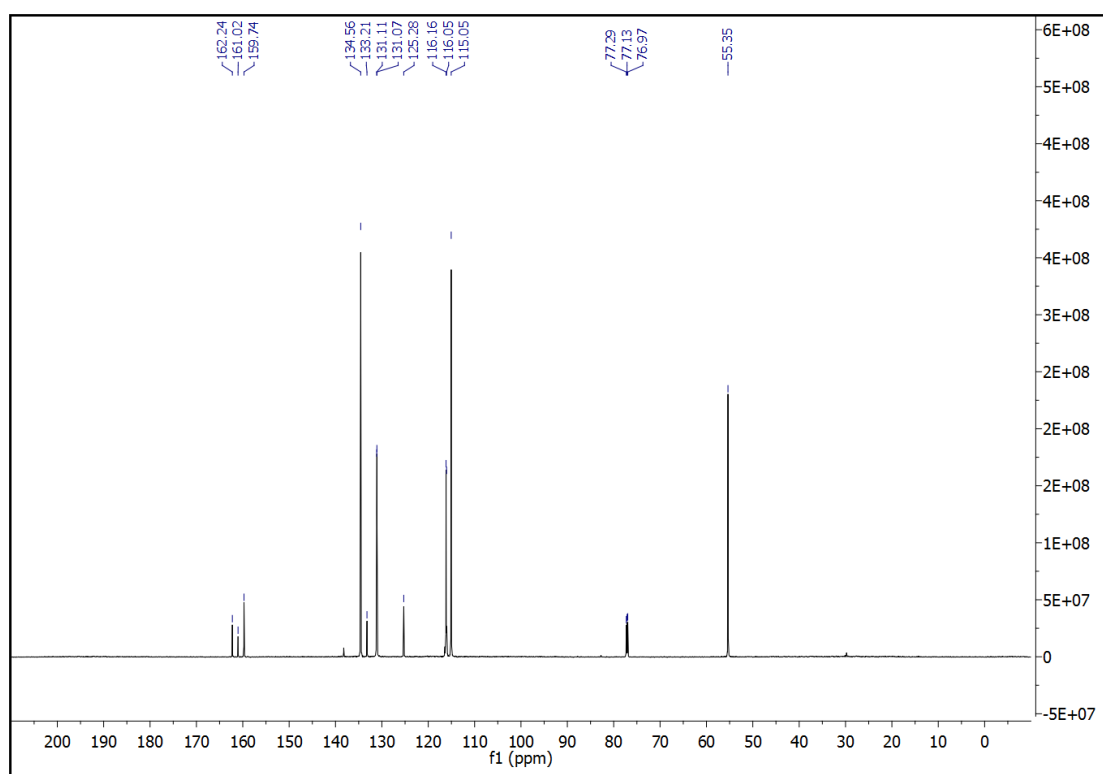
^{13}C NMR of (4v)



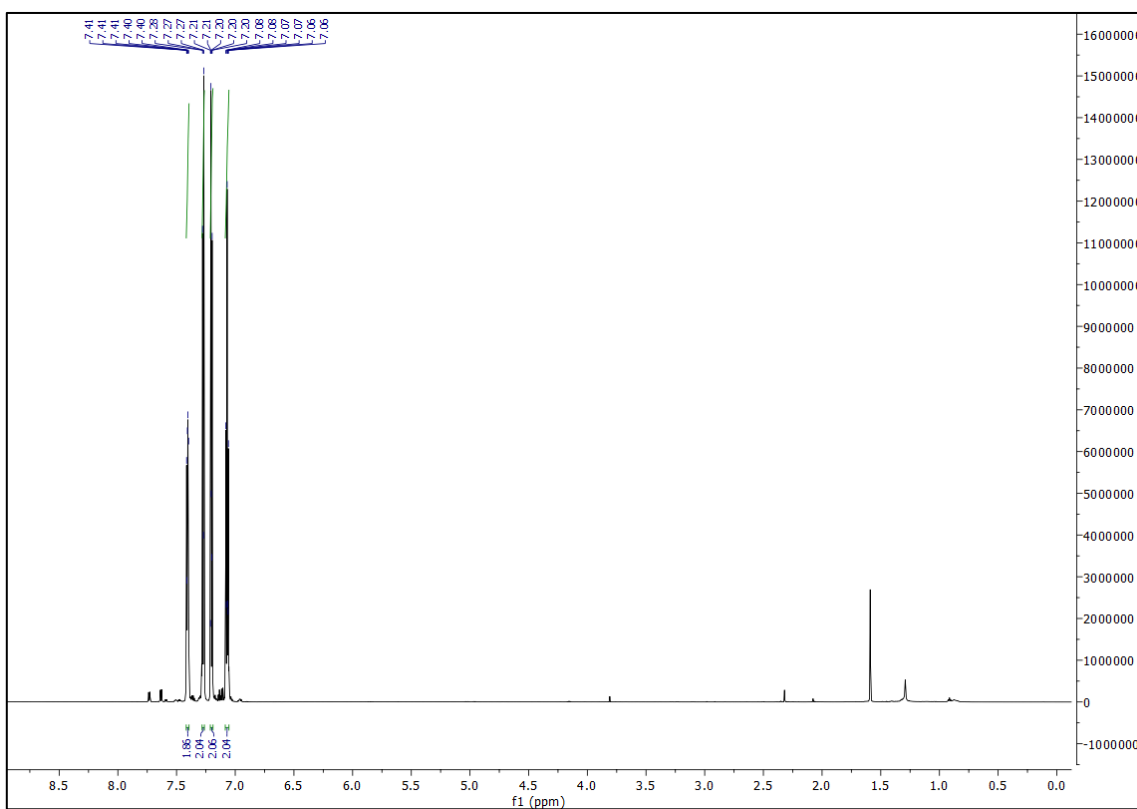
^1H NMR of (4w)



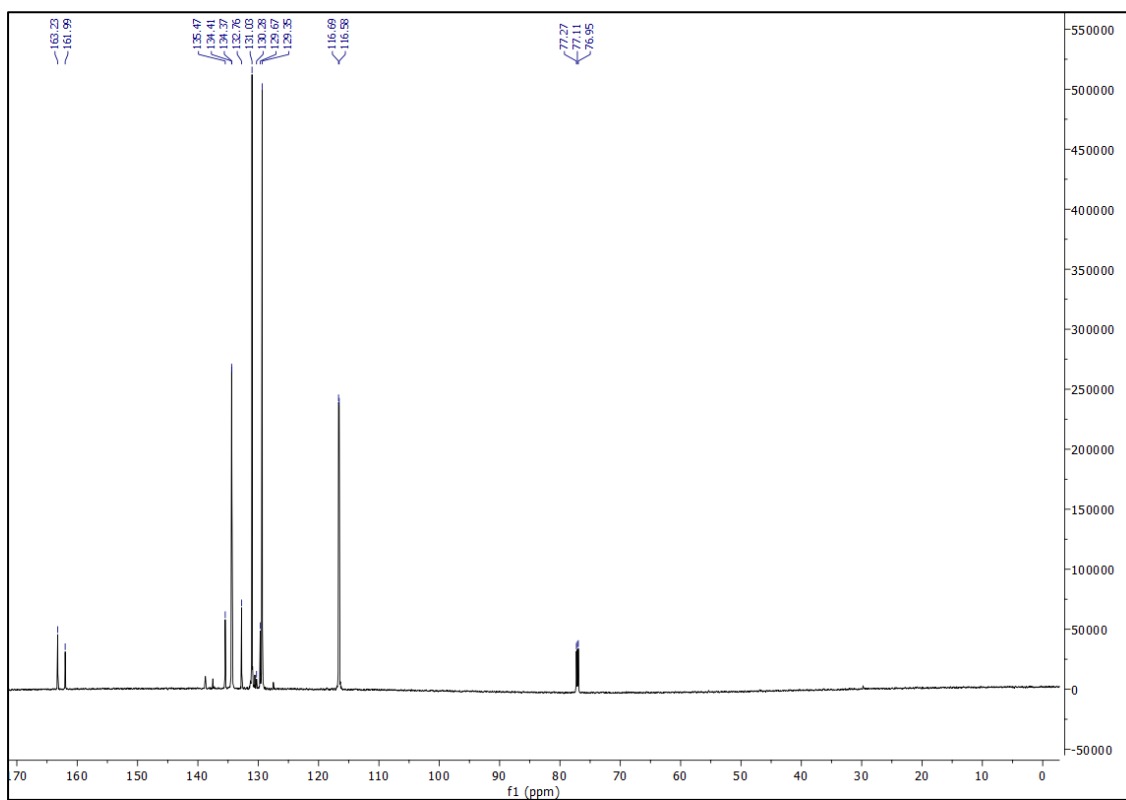
^{13}C NMR of (4w)



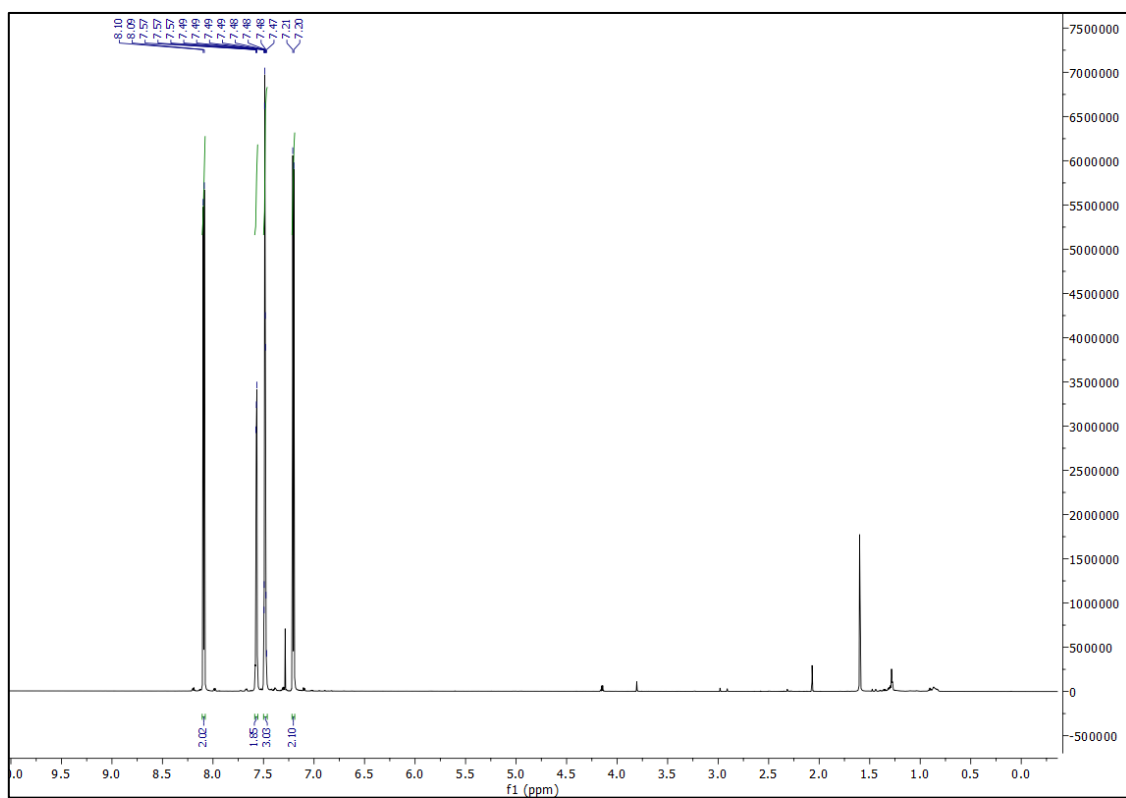
^1H NMR of (4x)



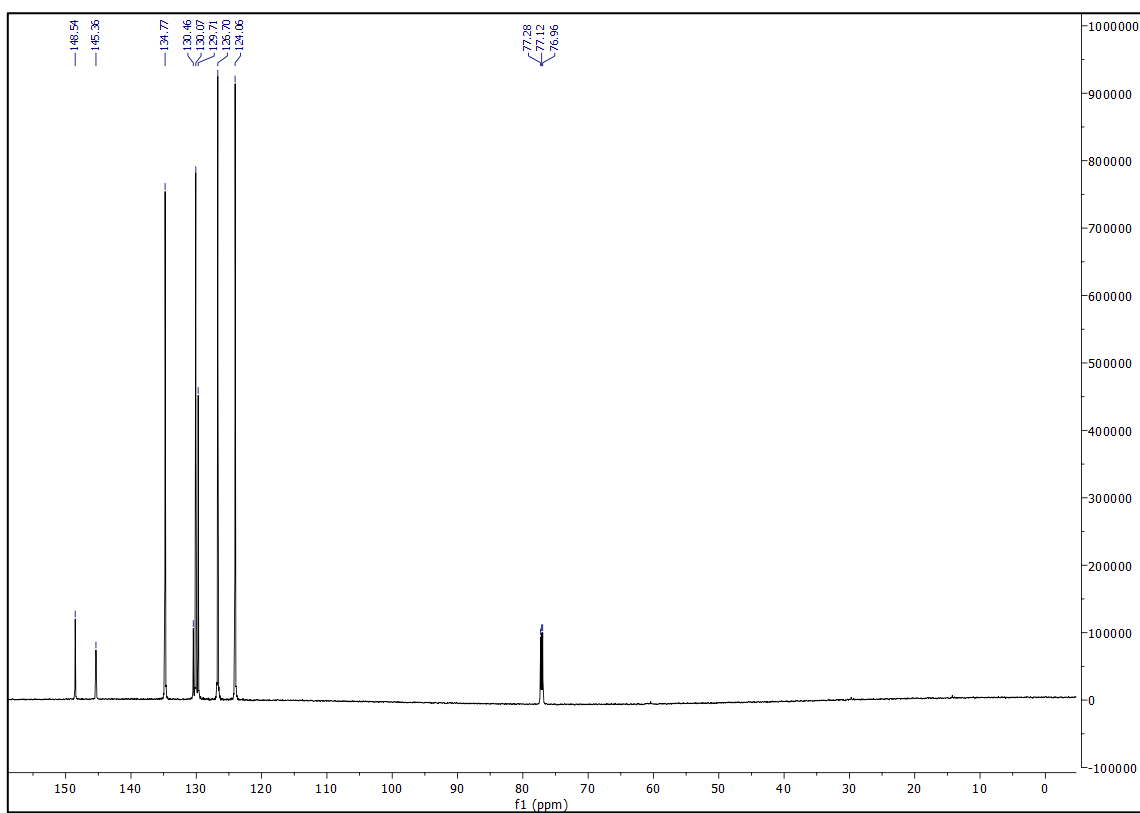
^{13}C NMR of (4x)



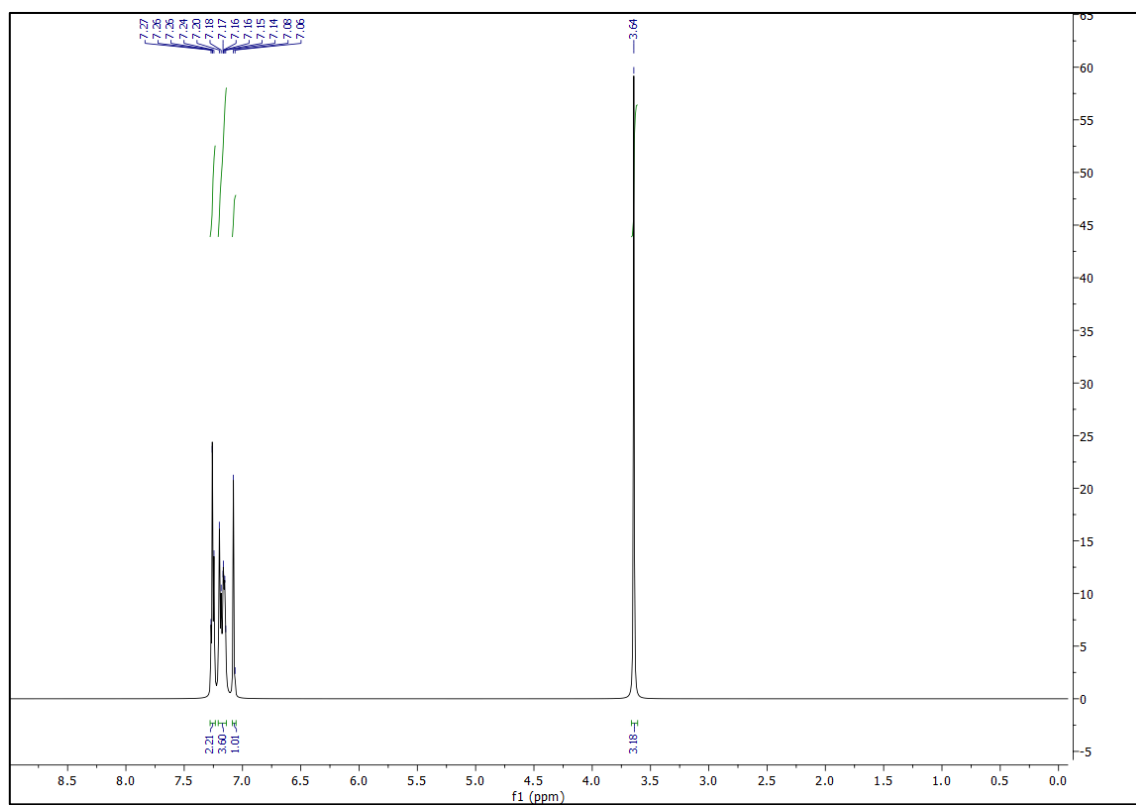
¹H NMR of (4y)



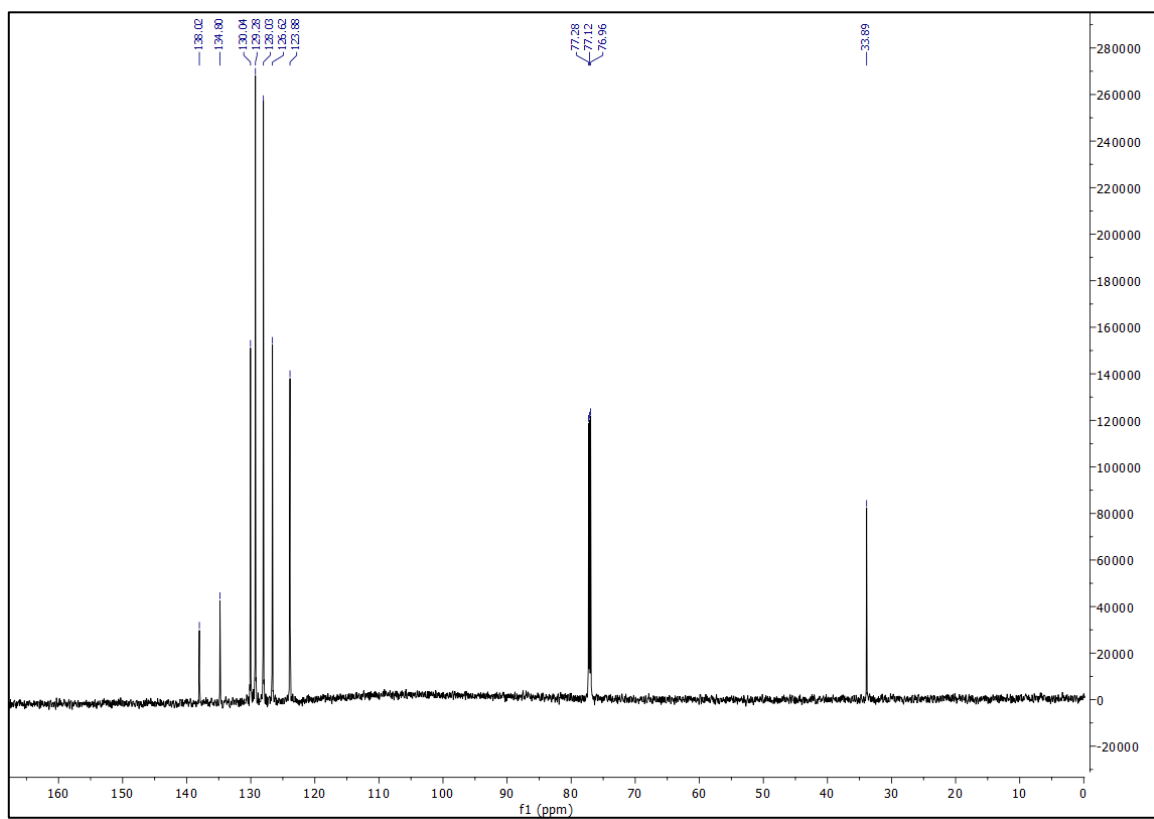
¹³C NMR of (4y)



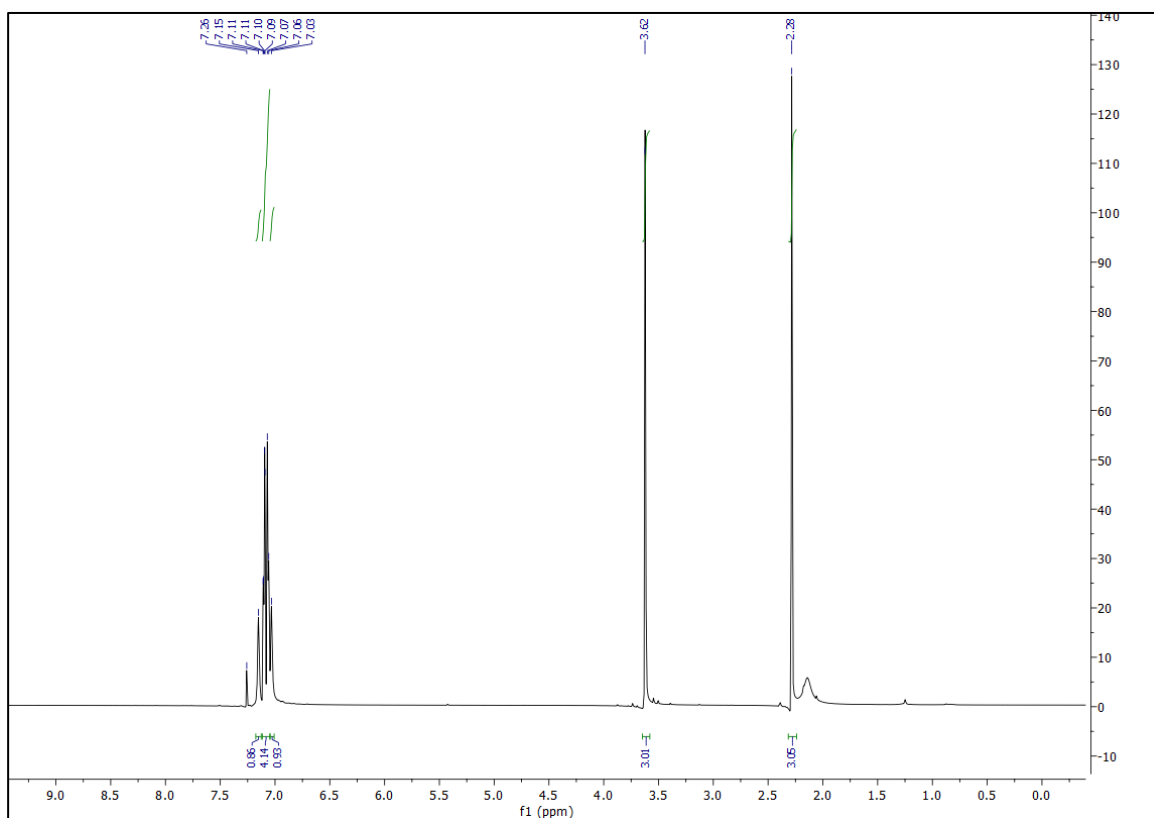
^1H NMR of (5a)



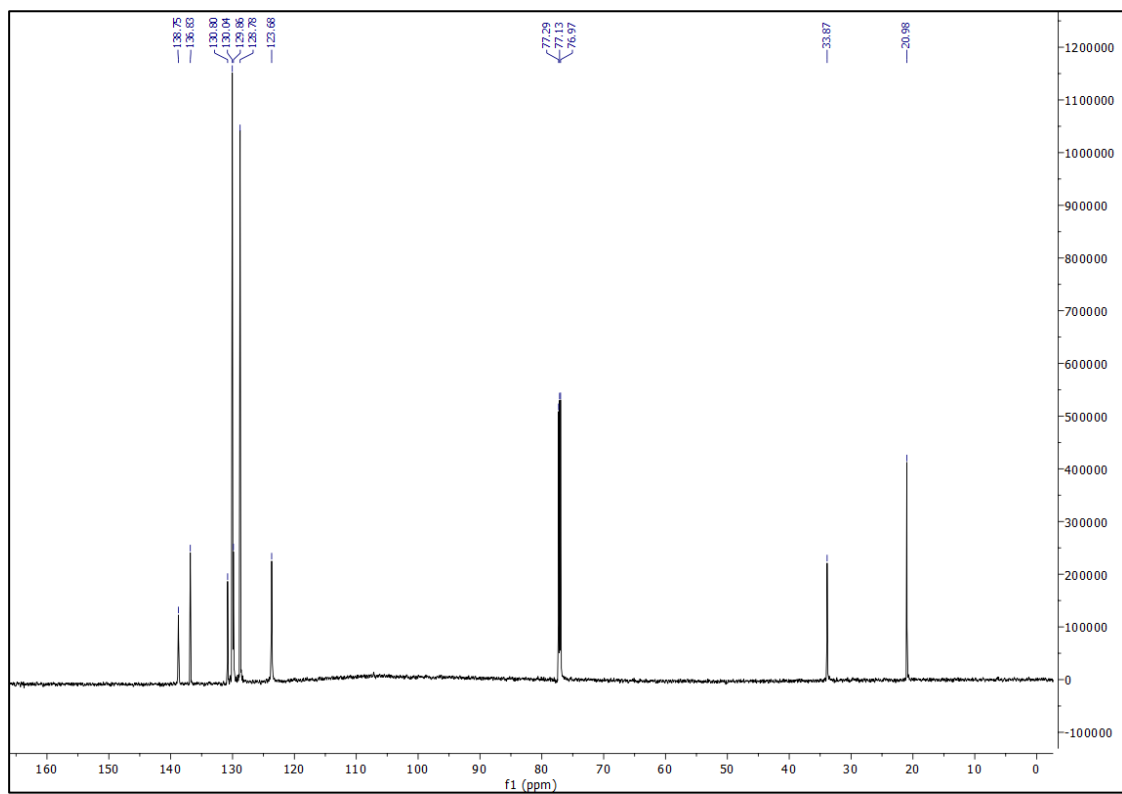
^{13}C NMR of (5a)



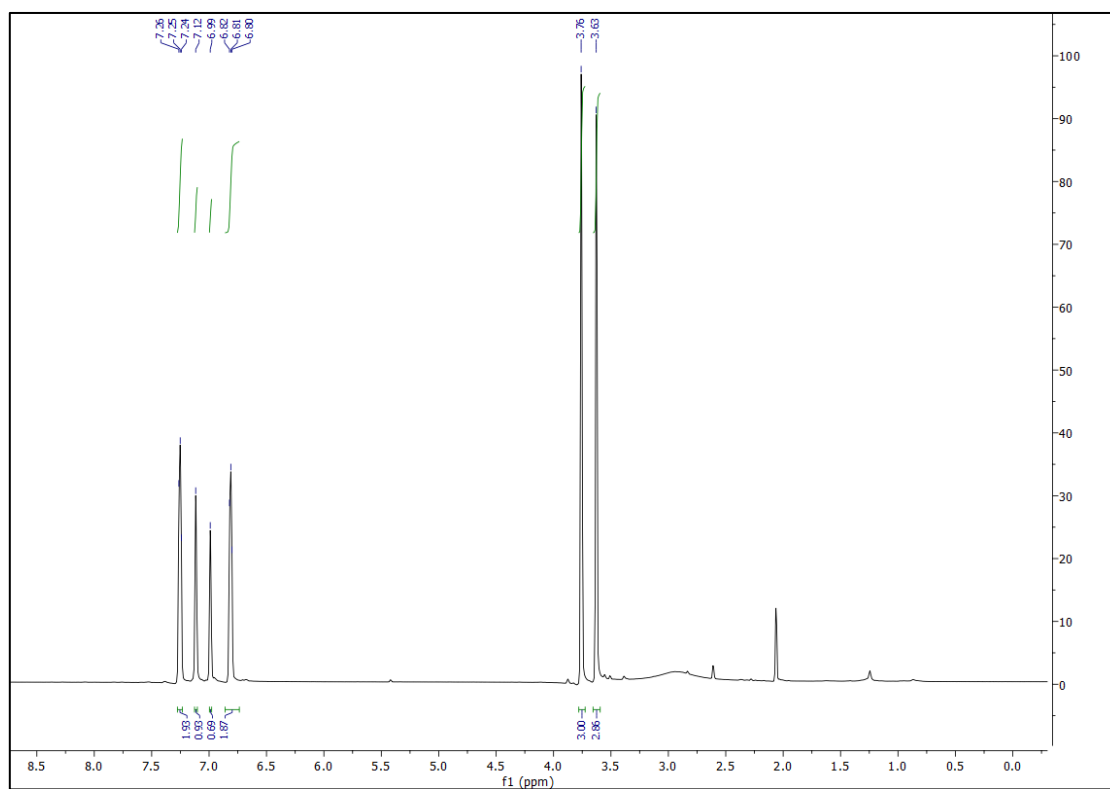
^1H NMR of (5b)



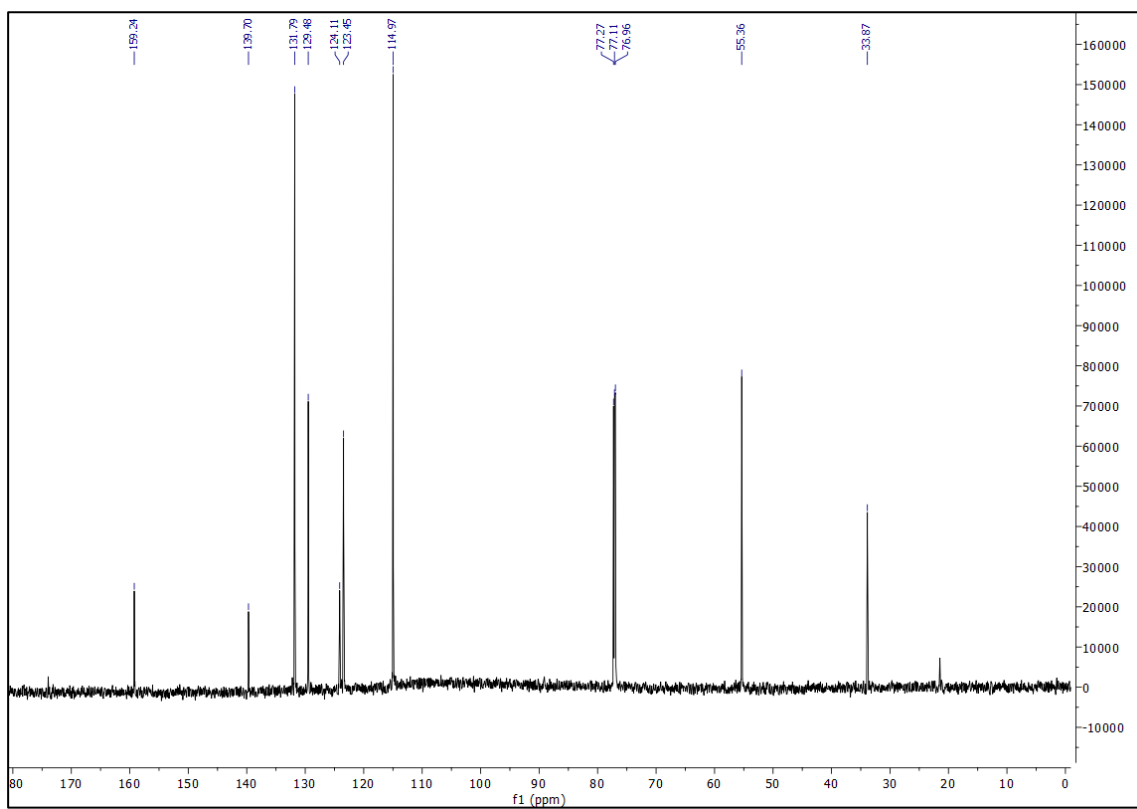
^{13}C NMR of (5b)



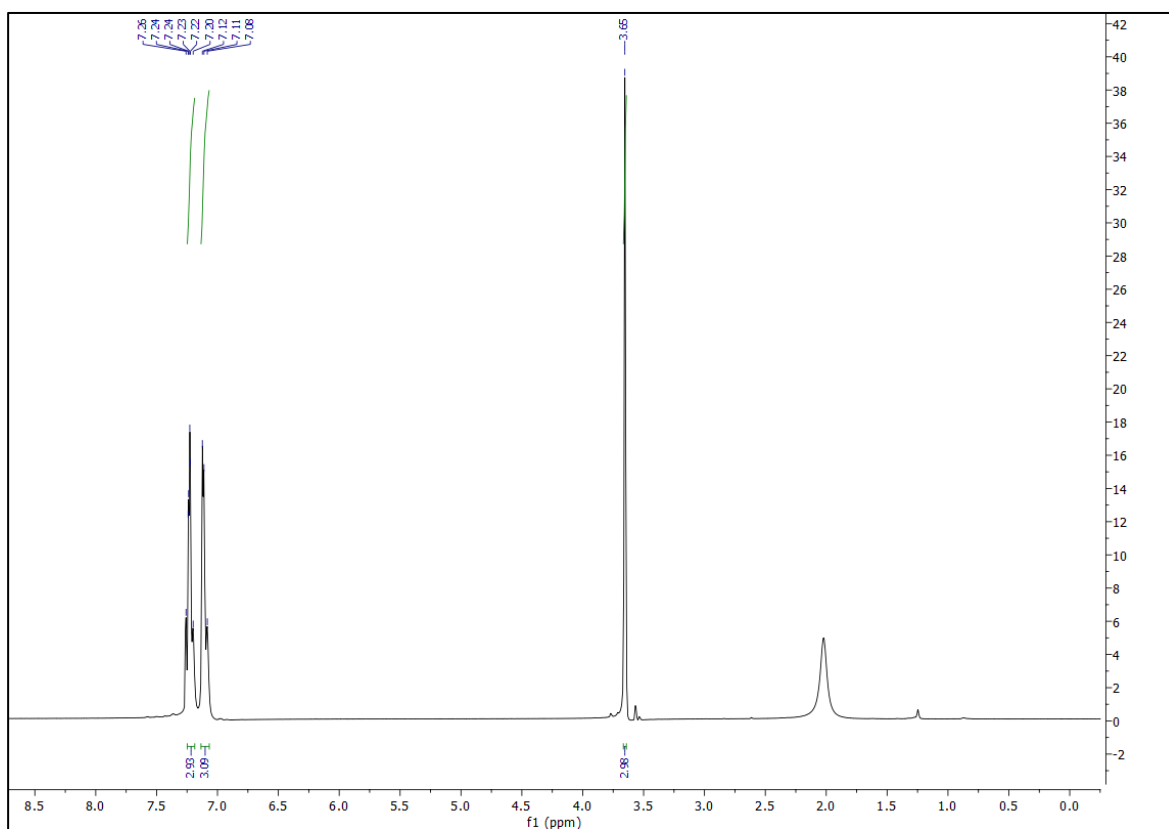
^1H NMR of (5c)



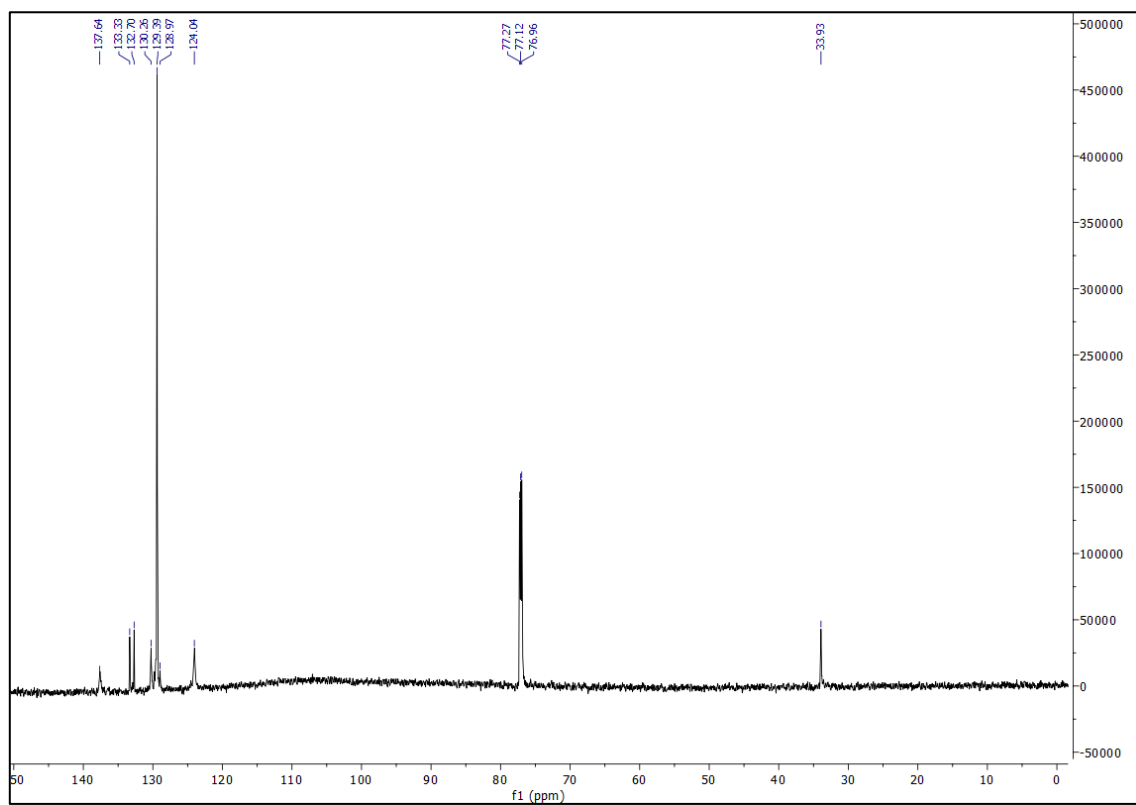
^{13}C NMR of (5c)



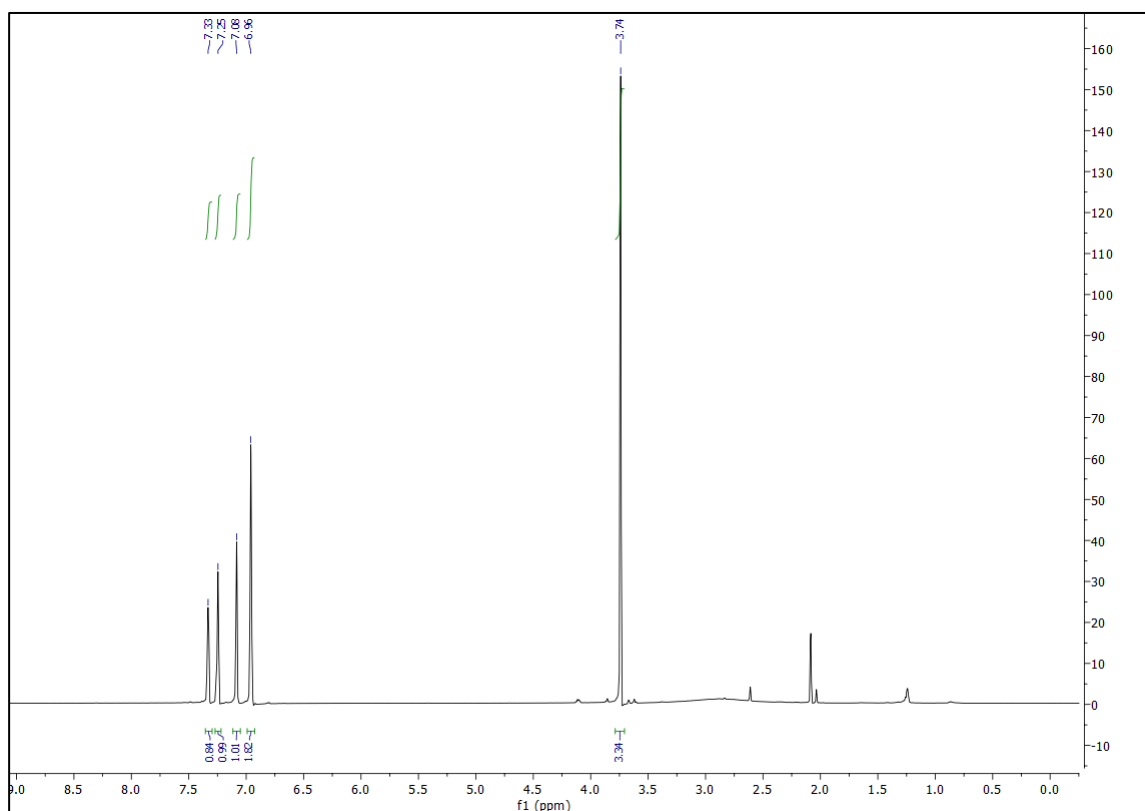
^1H NMR of (5d)



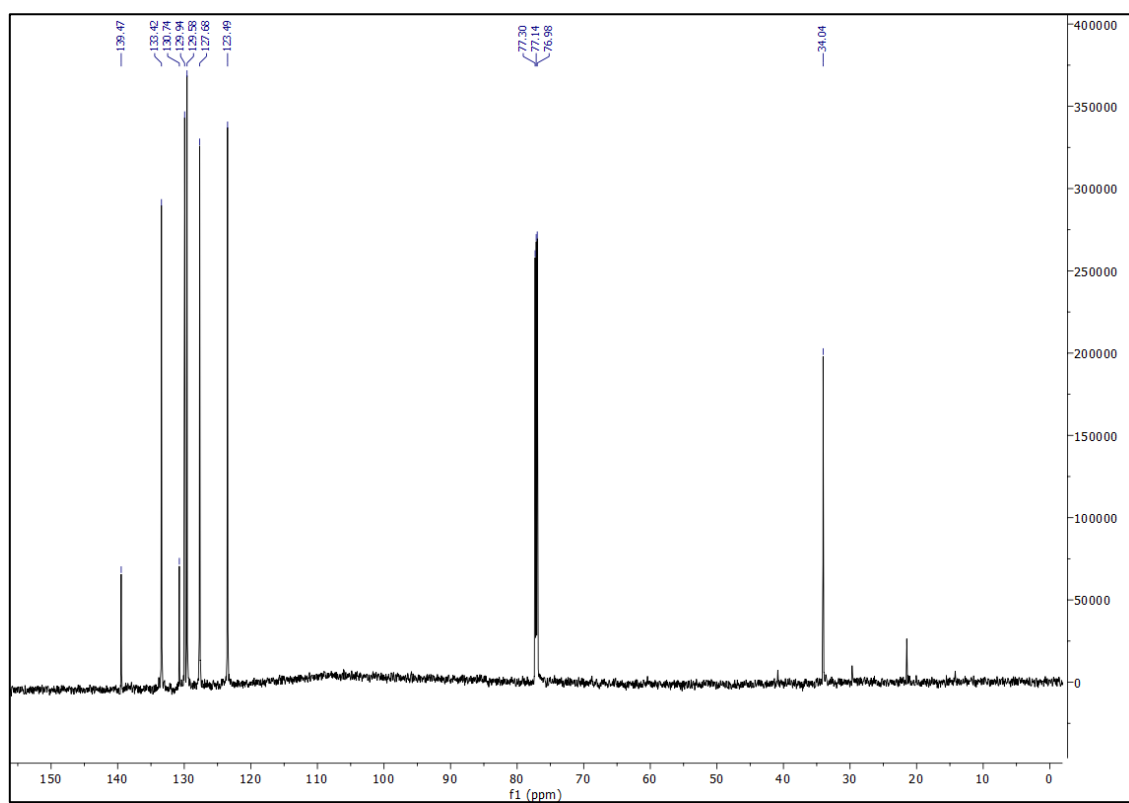
^{13}C NMR of (5d)



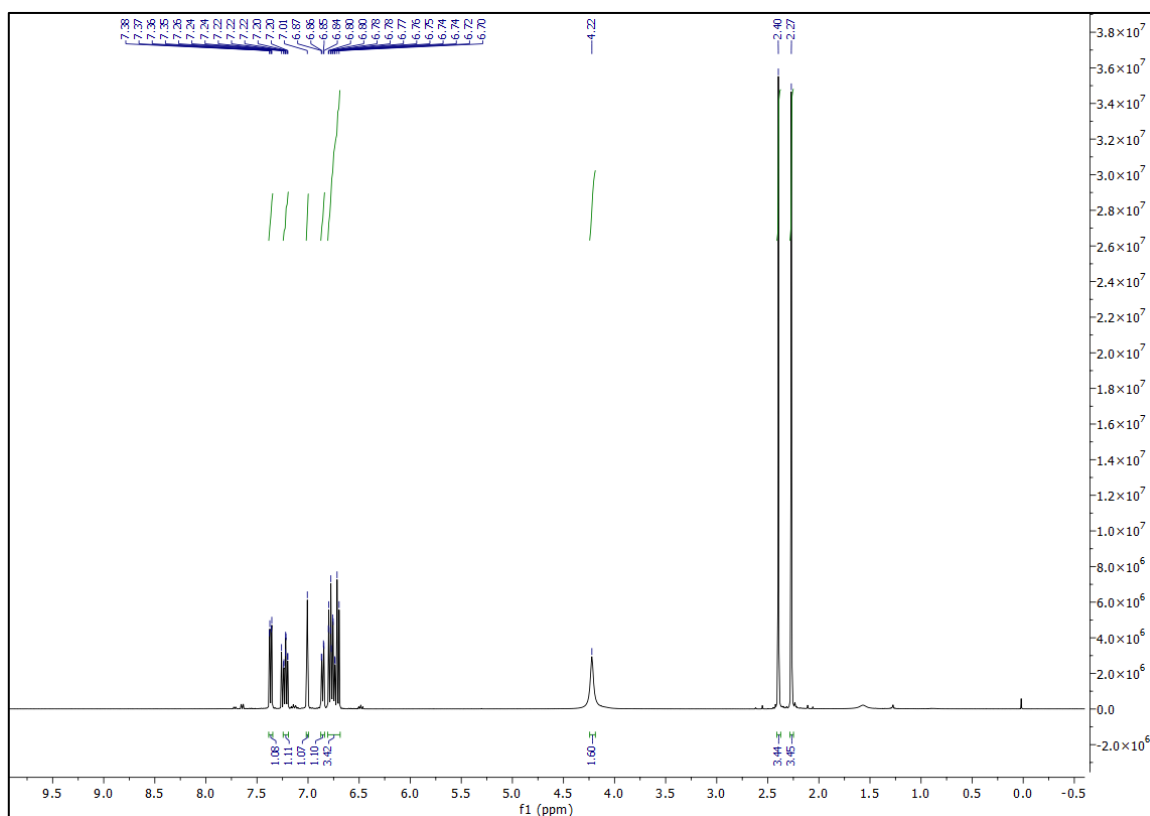
^1H NMR of (5e)



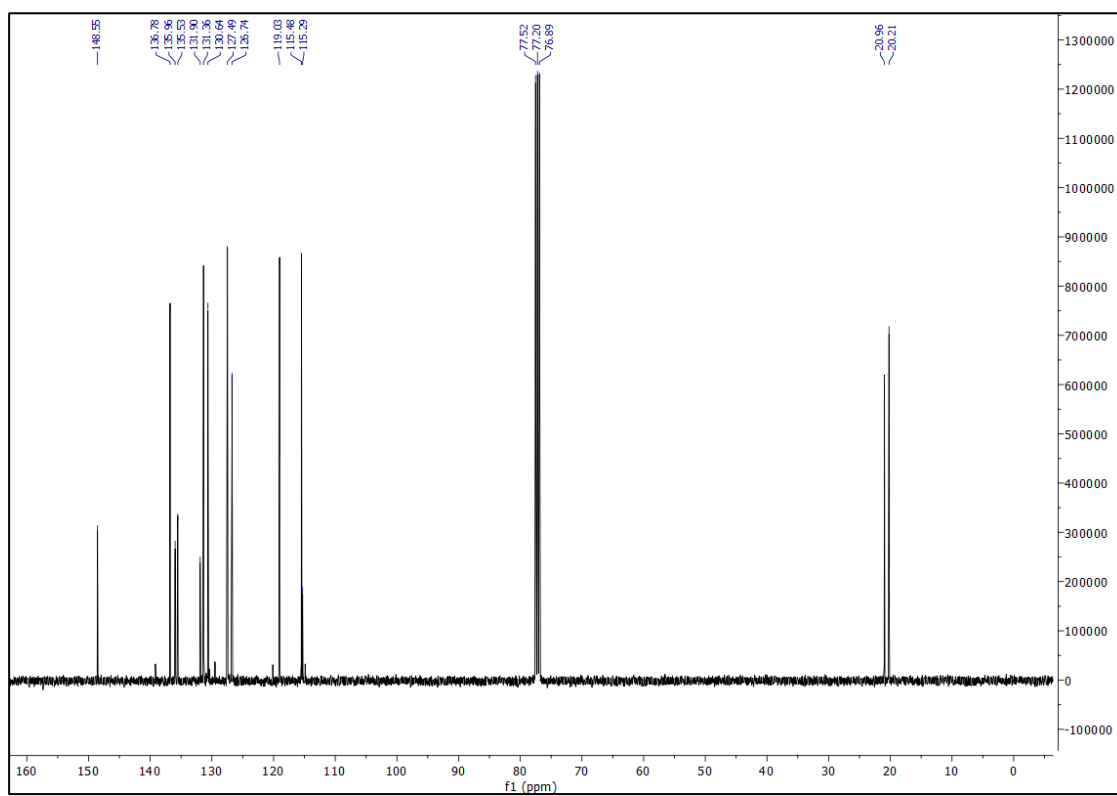
^{13}C NMR of (5e)



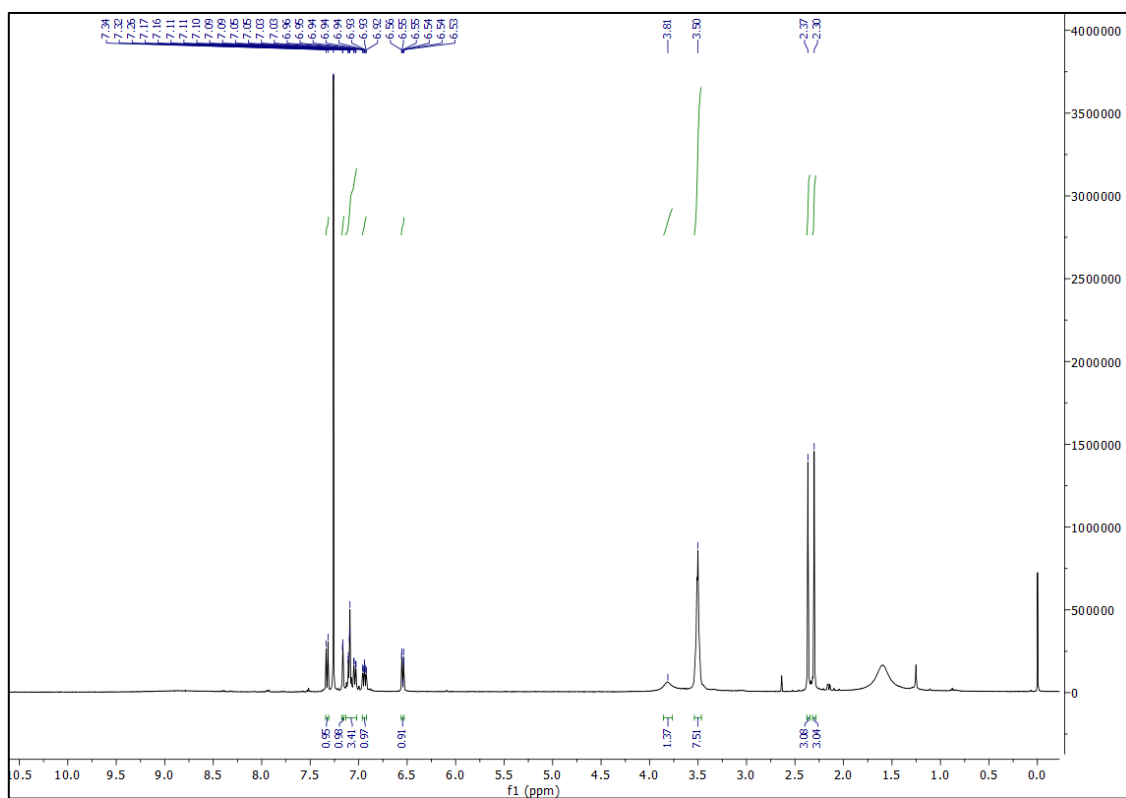
^1H NMR of (3k)



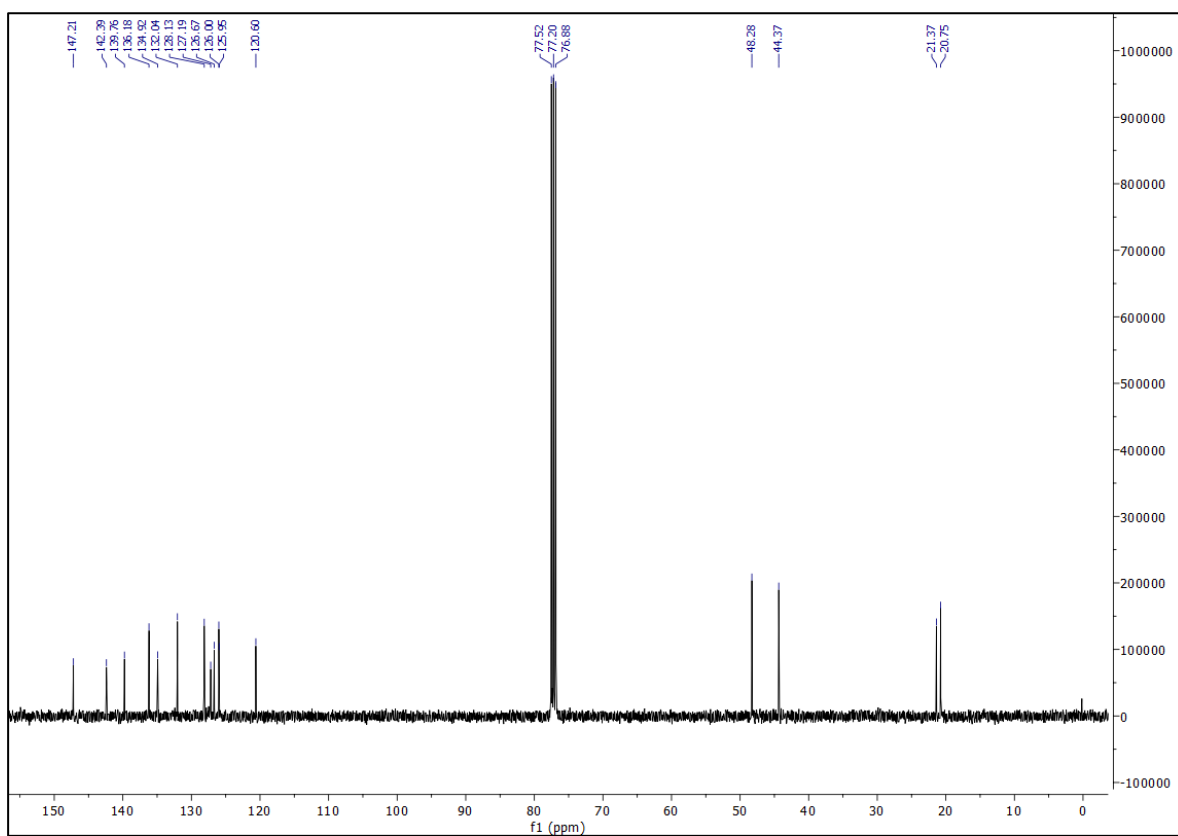
^{13}C NMR of (3k)



^1H NMR of (9)



^{13}C NMR of (9)



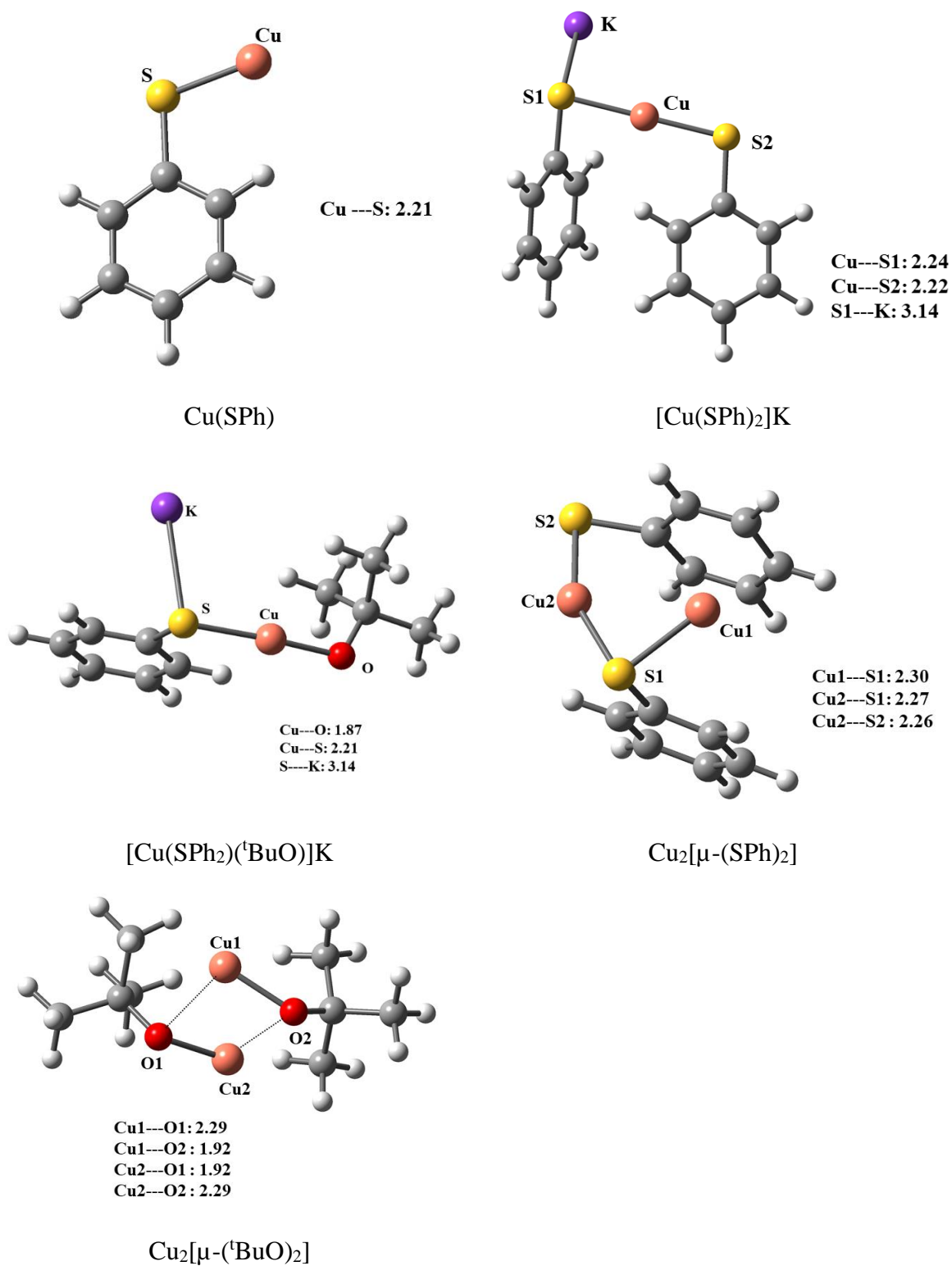
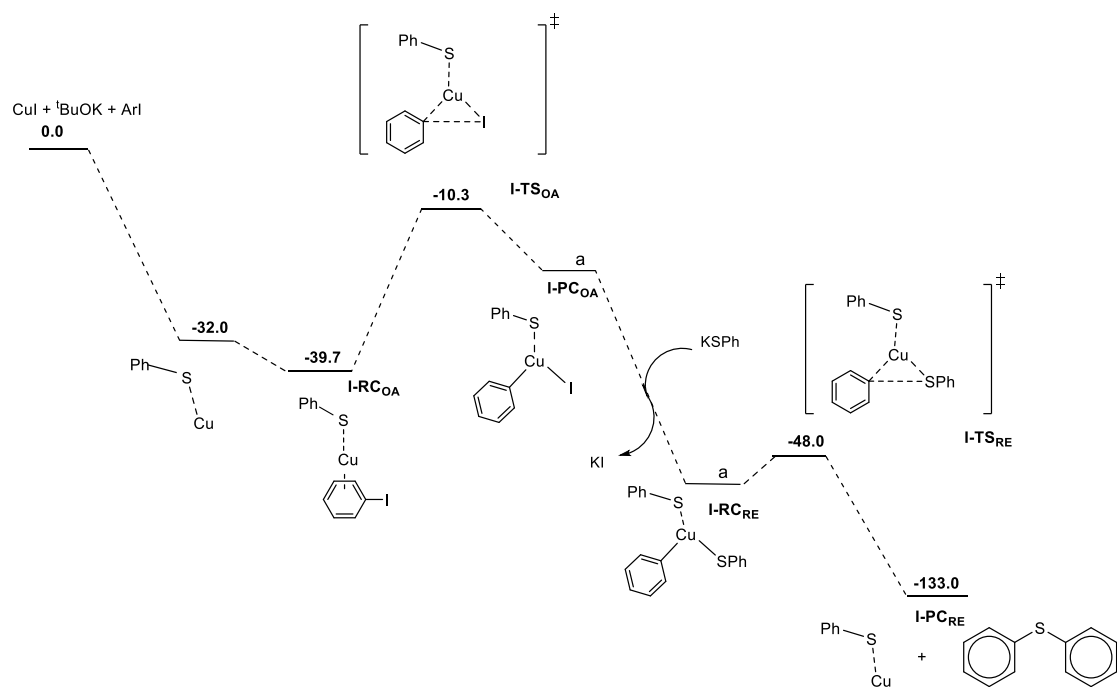
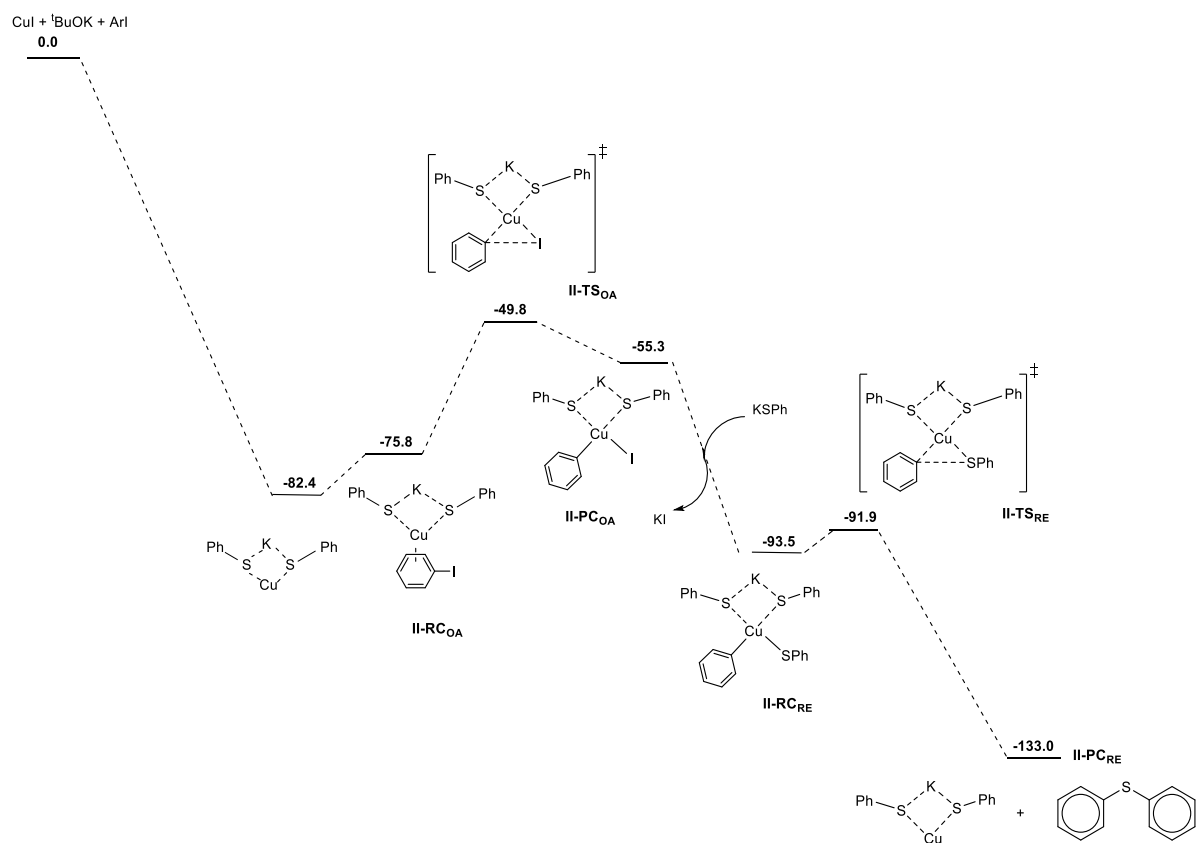


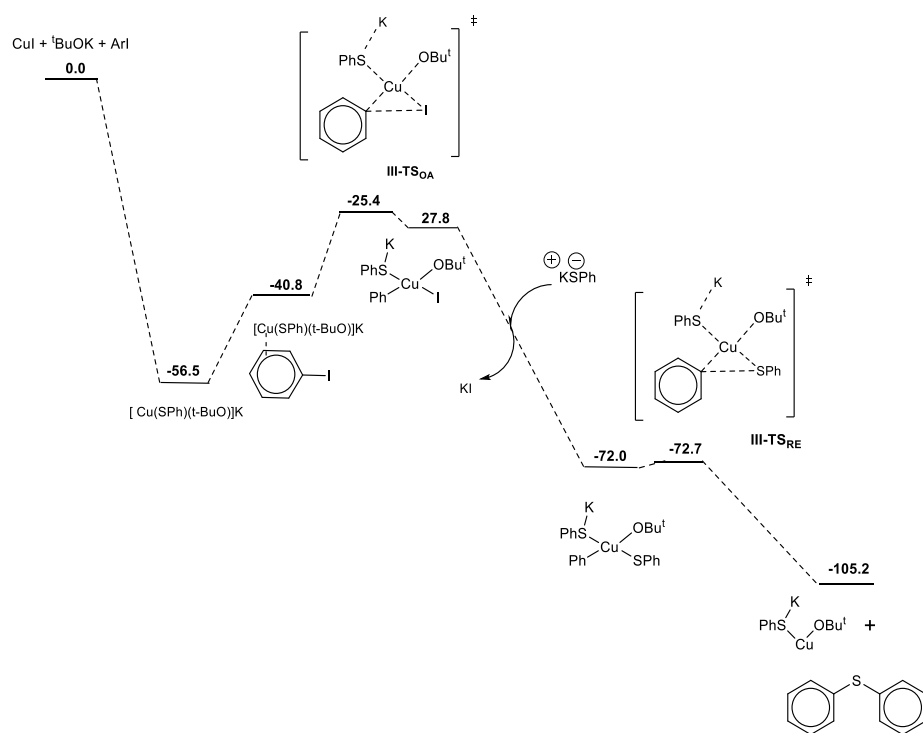
Figure S1. Optimized geometries of Cu complexes shown in Scheme 8



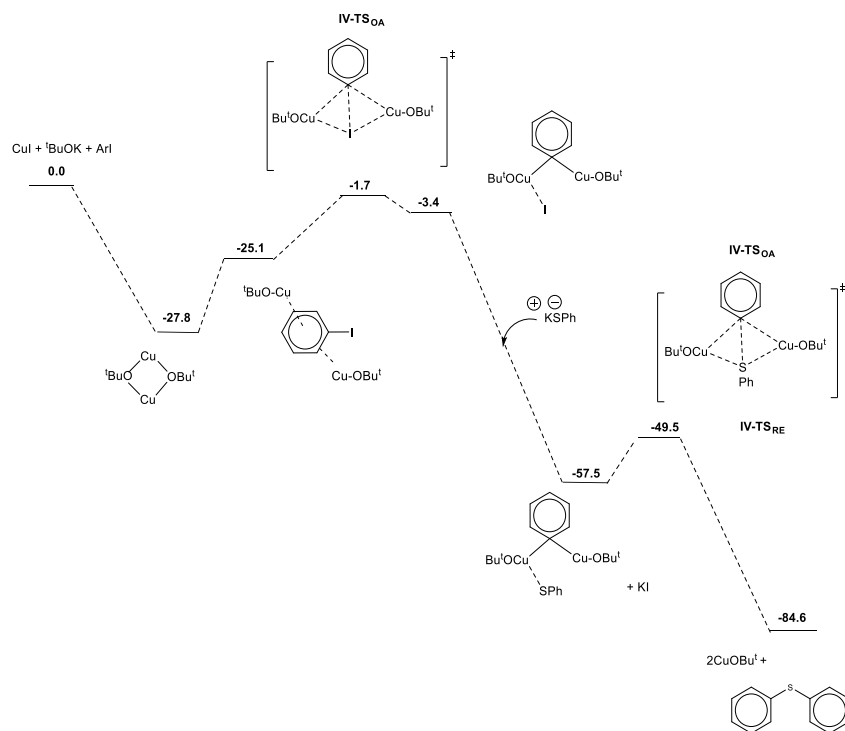
Scheme S1. Reaction Profile diagram for pathway **I** initiated by $\text{Cu}(\text{SPh})_3$. Optimization of I-PC_{0A} and I-RC_{RE} failed to locate a desired intermediate.



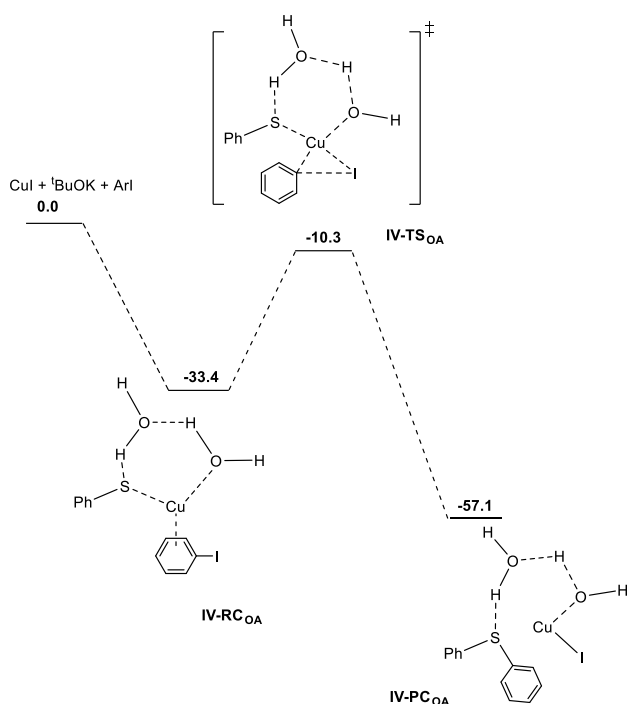
Scheme S2. Reaction Profile diagram for pathway **II** initiated by $[\text{Cu}(\text{SPh})_2]\text{K}$



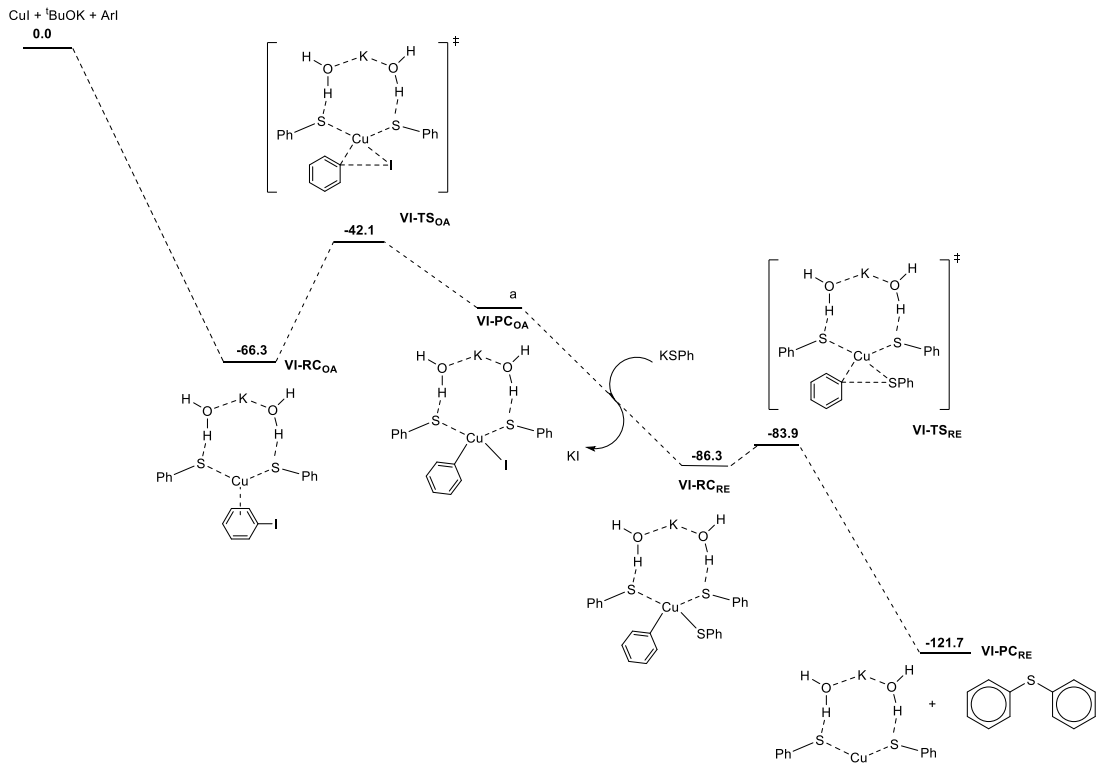
Scheme S3. Reaction Profile diagram for pathway–**III** initiated by $[\text{Cu}(\text{SPh})(\text{O}^t\text{Bu})]\text{K}$



Scheme S4. Reaction Profile diagram for pathway–**IV** initiated by $\text{Cu}_2[\mu-({}^t\text{BuO})_2]$



Scheme S5. Reaction Profile diagram for pathway-V (Solvent Assisted). ^aDespite of repeated attempts, we failed to locate **V-TS_{RE}** (transition state for reductive elimination).



Scheme S6. Reaction Profile diagram for pathway-VI (Solvent Assisted). ^aOptimization of **VI-PC_{OA}** failed to locate a desired intermediate.

Table S3. Optimized geometries (M062X, Cartesian coordinates in Å) and energies of reactants transition state and intermediates (in a.u.). Parenthesis value indicate single point energies obtained at M062X/6-311+G**, LANL2DZ. Notation: E = total electronic energy, Tc = thermal correction at 298K to obtain the Gibbs free energy, Nimag = number of imaginary frequencies

ArI E = -242.9333067 (-242.9369025) Nimag = 0 Tc = 0.058750	CuI E = -1651.7452036 (-1651.8238898) Nimag = 0 Tc = -0.025146
C -2.92328034 -0.87301586 0.00000000 C -1.52812034 - 0.87301586 0.00000000 C - 0.83058234 0.33473514 0.00000000 C -1.52823634 1.54324414 -0.00119900 C -2.92306134 1.54316614 -0.00167800 C -3.62066234 0.33496014 -0.00068200 H -3.47303934 -1.82533286 0.00045000 H 0.26909766 0.33481514 0.00063400 H -0.97803634 2.49538714 -0.00125800 H -3.47318334 2.49544714 -0.00263100 H -4.72026634 0.33514314 -0.00086200 I -0.47873078 -2.69201977 0.00251124	Cu 0.00000000 0.00000000 - 1.64355900 I 0.00000000 0.00000000 0.89930600
t-BuOH E = -233.6314384 (-233.636819) Nimag = 0 Tc = 0.107023	KO ^t Bu E = -833.0001613 (-833.0113823) Nimag = 0 Tc = 0.090052
8 -0.056170 -0.000213 1.446198 6 0.006649 -0.000005 0.014711 6 -0.676914 -1.254404 -0.525190 1 -1.735942 -1.259658 -0.250331 1 -0.608589 -1.299621 -1.614657 1 -0.206294 -2.146151 -0.105995 6 1.491690 -0.005185 -0.320202 1 1.642032 -0.004118 -1.401437 1 1.973137 0.879235 0.102505 1 1.966393 -0.894524 0.099828 6 -0.667920 1.259704 -0.524213 1 -0.191068 2.147618 -0.103913 1 -0.598947 1.305567 -1.613629 1 -1.726890 1.272027 -0.249456 1 -0.985506 0.000671 1.696871	19 2.626532 -0.000466 0.000370 8 0.272278 -0.000165 0.000135 6 -1.094164 0.000009 0.000001 6 -1.648168 -0.377540 1.392870 1 -1.278354 0.337824 2.133817 1 -2.743306 -0.386660 1.433086 1 -1.280885 -1.370721 1.669639 6 -1.646495 -1.017959 -1.024015 1 -2.741690 -1.048189 -1.053752 1 -1.277915 -0.761823 -2.022020 1 -1.276769 -2.017031 -0.773345 6 -1.644194 1.396415 -0.369813 1 -1.271058 1.679915 -1.358855 1 -2.739151 1.440218 -0.383578 1 -1.275093 2.131090 0.352631
PhSH E = -630.3845473 (-630.3879579) Nimag = 0 Tc = 0.069916	KI E = -611.3950276 (-611.3950799) Nimag = 0 Tc = -0.025664
6 0.200079 -1.206317 0.002854 6 -0.503679 -0.001149 0.001008 6 0.191722 1.207885 -0.001658	53 0.000000 0.000000 0.896875 19 0.000000 0.000000 -2.501809

6 1.582580 1.204998 -0.001192 6 2.287733 0.005890 -0.000479 6 1.589784 -1.198102 0.001108 1 -0.337382 -2.147833 0.006943 1 -0.346186 2.148621 -0.004578 1 2.114498 2.148996 -0.002498 1 3.370523 0.009460 -0.000835 1 2.126791 -2.139132 0.002611 16 -2.282156 -0.083551 -0.004694 1 -2.503053 1.237469 0.063613	
PhSK E = -1229.805225 (-1229.8083453) Nimag = 0 Tc = 0.053905	
6 0.743847 -0.443805 1.201357 6 0.096391 -0.797417 0.002605 6 0.748006 -0.457397 -1.197838 6 1.975039 0.198035 -1.198515 6 2.597520 0.539833 -0.000616 6 1.970864 0.211700 1.198919 1 0.269450 -0.694299 2.143940 1 0.276871 -0.718761 -2.139100 1 2.447233 0.441866 -2.143958 1 3.552163 1.051522 -0.001890 1 2.439679 0.466520 2.143140 16 -1.493619 -1.576274 0.004306 19 -1.783026 1.535150 -0.005605	
H ₂ O E = -76.4194597 (-76.4285158) Nimag = 0 Tc = 0.003938	Cu(SPh) E = -2270.1792007 (-2270.2445866) Nimag = 0 Tc = 0.055958
8 0.000000 0.000000 0.118797 1 0.000000 0.754674 -0.475188 1 0.000000 -0.754674 -0.475188	29 2.272764 0.469168 -0.063742 16 0.935868 -1.282702 0.105194 6 -0.641266 -0.466424 0.045622 6 -0.779953 0.926260 0.115194 6 -1.806519 -1.236628 -0.063953 6 -2.035181 1.522164 0.076039 1 0.100156 1.553618 0.212107 6 -3.060009 -0.638243 -0.104129 1 -1.719311 -2.315881 -0.118742 6 -3.184980 0.746835 -0.035809 1 -2.111628 2.602158 0.132957 1 -3.944122 -1.260028 -0.189932 1 -4.161699 1.213697 -0.068753
[Cu(SPh) ₂] E = -3500.0549097 (-3500.1125278) Nimag = 0 Tc = 0.134211	[Cu(SPh ₂)(^t BuO)] E = -3103.2623226 (-3103.3188491) Nimag = 0 Tc = 0.170090

29	0.770967	1.035450	-0.626539	6	3.356043	0.082585	-0.383438
16	2.491102	-0.368956	-0.970409	6	1.989104	-0.139934	-0.599493
6	1.314996	-1.534601	-0.291314	6	1.443433	-1.359426	-0.166287
6	0.844188	-1.417545	1.024465	6	2.238997	-2.310257	0.461474
6	0.812785	-2.572431	-1.083708	6	3.593997	-2.073673	0.678168
6	-0.102649	-2.304711	1.523905	6	4.147230	-0.871095	0.249481
1	1.224606	-0.626504	1.660764	1	3.799234	1.011985	-0.725299
6	-0.139345	-3.454952	-0.582964	1	0.390643	-1.562352	-0.335743
1	1.165707	-2.674060	-2.103340	1	1.792278	-3.244536	0.782237
6	-0.604376	-3.325842	0.722698	1	4.209368	-2.817784	1.168614
1	-0.456999	-2.189108	2.541844	1	5.201861	-0.672029	0.402391
1	-0.518737	-4.246339	-1.219512	16	1.011950	1.123783	-1.389736
1	-1.349637	-4.010383	1.109575	29	-0.980316	0.216851	-1.097474
16	-0.922252	2.424602	-0.279997	8	-2.576321	-0.704531	-0.793783
6	-2.273133	1.292210	-0.040690	6	-3.144704	-0.447714	0.448272
6	-2.180654	-0.079476	-0.314975	6	-2.171259	-0.831294	1.578400
6	-3.499766	1.786190	0.425037	1	-1.878901	-1.878906	1.464145
6	-3.273369	-0.919508	-0.126321	1	-1.262822	-0.222948	1.499701
1	-1.250769	-0.503632	-0.679855	1	-2.599352	-0.688786	2.575979
6	-4.589279	0.944341	0.612082	6	-3.496790	1.044344	0.584238
1	-3.591288	2.844727	0.641590	1	-4.130759	1.341561	-0.255266
6	-4.484876	-0.417365	0.338384	1	-4.013892	1.276781	1.520885
1	-3.166321	-1.976615	-0.343676	1	-2.579059	1.640689	0.536638
1	-5.524601	1.355819	0.975335	6	-4.424210	-1.283696	0.582096
1	-5.333014	-1.075066	0.484901	1	-4.919627	-1.140980	1.547294
19	4.231278	1.168679	1.150995	1	-5.121144	-1.009024	-0.214088
				1	-4.176384	-2.342153	0.466803
				19	1.418212	2.148236	1.546371
Cu ₂ [μ-(^t BuO) ₂] E = -3746.8553261 (-3746.950334) Nimag = 0 Tc = 0.207299				Cu ₂ [μ-(SPh) ₂] E = -4540.4621171 (-4540.5608186) Nimag = 0 Tc = 0.137624			
29	-0.141697	-1.242422	-0.276975	29	0.188304	1.124583	-1.108069
6	-2.493861	0.071518	0.140500	16	2.465359	-1.269005	1.336990
29	0.141686	1.242474	-0.276953	6	1.723196	0.338598	1.133127
6	2.493871	-0.071546	0.140498	6	2.252734	1.269979	0.221667
8	1.549968	-0.490871	-0.797424	6	0.562961	0.699715	1.840880
8	-1.549953	0.490875	-0.797406	6	1.571718	2.459366	-0.076475
6	2.392468	1.463255	0.287859	1	3.169217	1.030943	-0.302689
1	3.183404	1.894893	0.905798	6	-0.137859	1.856037	1.522164
1	2.444085	1.926795	-0.701602	1	0.161513	0.012824	2.576109
1	1.464584	1.769870	0.833435	6	0.342093	2.738240	0.544569
6	3.897130	-0.423622	-0.360280	1	2.003236	3.165110	-0.775868
1	4.680459	-0.098548	0.330067	1	-1.066213	2.076429	2.035179
1	3.969996	-1.506230	-0.488553	1	-0.196945	3.645321	0.306025
1	4.066542	0.046518	-1.332202	16	-0.495612	-0.921311	-1.913658
6	2.246759	-0.743177	1.495904	29	1.079345	-1.578656	-0.416958
1	2.995281	-0.479793	2.248554	6	-1.704367	-0.667423	-0.605511
1	1.262218	-0.452250	1.876460	6	-2.573344	0.425778	-0.671358

1	2.246830	-1.826778	1.355495	6	-1.804370	-1.549983	0.471903
6	-3.897108	0.423762	-0.360196	6	-3.498025	0.652052	0.341269
1	-4.680445	0.098659	0.330128	1	-2.529883	1.092921	-1.525708
1	-3.969897	1.506391	-0.488330	6	-2.730025	-1.318329	1.483236
1	-4.066568	-0.046245	-1.332173	1	-1.170192	-2.428752	0.511178
6	-2.392571	-1.463309	0.287676	6	-3.573016	-0.212351	1.429587
1	-2.444277	-1.926745	-0.701826	1	-4.159003	1.508597	0.279041
1	-1.464680	-1.770098	0.833151	1	-2.790311	-2.007685	2.317191
1	-3.183502	-1.894945	0.905624	1	-4.289372	-0.032603	2.221665
6	-2.246662	0.742951	1.495988				
1	-1.262138	0.451891	1.876485				
1	-2.246667	1.826574	1.355743				
1	-2.995188	0.479507	2.248614				
I-RC_{oA} E = -2513.1684757 (-2513.2158003) Nimag = 0 Tc = 0.136752				I-TS_{oA} E = -2513.1226565 (-2513.1681468) Nimag = 1 (-133.40 cm ⁻¹) Tc = 0.136007			
29	-1.266650	1.586808	0.554935	29	0.070694	-0.536362	-0.000118
53	2.648685	-0.360391	0.279381	53	-0.090019	1.953891	0.000054
6	1.075188	0.728872	-0.619172	6	-1.844444	-0.219385	0.000012
6	0.868021	2.057202	-0.234295	6	-2.489194	-0.363996	1.215730
6	-0.167949	2.790520	-0.836055	6	-3.845657	-0.686550	1.205346
6	-1.003929	2.170054	-1.778820	6	-4.520602	-0.849796	0.000050
6	-0.770065	0.846997	-2.150285	6	-3.845787	-0.686145	-1.205265
6	0.282156	0.125638	-1.588181	6	-2.489327	-0.363585	-1.215683
1	1.510467	2.526241	0.498665	1	-1.967262	-0.221705	2.153616
1	-0.301169	3.835129	-0.584489	1	-4.365991	-0.808071	2.147873
1	-1.813355	2.729358	-2.229230	1	-5.576154	-1.092275	0.000068
1	-1.408231	0.369385	-2.882825	1	-4.366227	-0.807339	-2.147777
1	0.447045	-0.905418	-1.873989	1	-1.967497	-0.220962	-2.153574
16	-2.494414	0.192249	1.774704	16	0.635863	-2.730828	-0.000101
6	-1.977314	-1.125390	0.674754	6	1.993180	-1.570508	-0.000034
6	-2.724577	-1.447757	-0.464142	6	2.514705	-1.065950	-1.210816
6	-0.833558	-1.880735	0.952652	6	2.514694	-1.066068	1.210801
6	-2.319838	-2.469952	-1.315958	6	3.505809	-0.095153	-1.205615
1	-3.618231	-0.876159	-0.688755	1	2.124137	-1.447850	-2.146845
6	-0.429137	-2.903223	0.100615	6	3.505807	-0.095285	1.205701
1	-0.246200	-1.645697	1.833086	1	2.124098	-1.448033	2.146792
6	-1.168099	-3.203430	-1.040432	6	4.000171	0.397651	0.000069
1	-2.910084	-2.696149	-2.197038	1	3.888372	0.283168	-2.145820
1	0.470636	-3.463157	0.329780	1	3.888355	0.282951	2.145945
1	-0.853096	-3.999018	-1.704871	1	4.769092	1.160274	0.000115
I-PC_{oA} E = -2513.2035824 (-2513.25276623) Nimag = 0 Tc = 0.138196							
29	0.185933	0.000006	-0.000017				
53	2.839636	-0.000002	0.000001				
6	-2.303854	1.311604	-0.142922				

6	-2.249823	2.347717	0.775971		
6	-1.196683	3.267607	0.716600		
6	-0.193336	3.130040	-0.228481		
6	-0.261704	2.099254	-1.175238		
6	-1.343981	1.220226	-1.166771		
1	-2.995922	2.417664	1.557978		
1	-1.151350	4.071118	1.441382		
1	0.642419	3.817830	-0.243214		
1	0.479036	2.027260	-1.961755		
1	-1.465434	0.484871	-1.955687		
16	-3.519910	-0.000019	0.000010		
6	-2.303802	-1.311594	0.142943		
6	-2.249840	-2.347729	-0.775924		
6	-1.343904	-1.220177	1.166739		
6	-1.196721	-3.267632	-0.716558		
1	-2.995989	-2.417700	-1.557880		
6	-0.261641	-2.099233	1.175204		
1	-1.465358	-0.484839	1.955672		
6	-0.193325	-3.130040	0.228475		
1	-1.151419	-4.071167	-1.441314		
1	0.479128	-2.027221	1.961689		
1	0.642411	-3.817855	0.243190		
I-TS_{RE}				I-PC_{RE}	
E = -3131.5691543 (-3131.605537)				E = -3131.6378498 ()	
Nimag = 1(-80.92)				Nimag = 0	
Tc = 0.224629				Tc = 0.223290	
29	-0.579829	0.379288	-0.107093	29	-0.655853 -0.336463 -0.504926
6	-2.441413	-0.115293	-0.068994	6	-2.562466 -0.014685 0.639632
6	-3.258047	0.448993	-1.033820	6	-2.320742 -1.113044 1.478165
6	-4.638248	0.274172	-0.920158	6	-2.502253 -2.408136 0.998265
6	-5.169689	-0.451253	0.139679	6	-2.906875 -2.621718 -0.316351
6	-4.323860	-1.007481	1.094701	6	-3.107819 -1.538735 -1.165866
6	-2.942916	-0.841690	0.997452	6	-2.957432 -0.231987 -0.692880
1	-2.848876	1.008998	-1.866278	1	-2.018120 -0.942624 2.503990
1	-5.290836	0.709314	-1.667940	1	-2.328807 -3.248431 1.658718
1	-6.241195	-0.587149	0.220481	1	-3.045925 -3.629919 -0.684807
1	-4.731902	-1.571515	1.925235	1	-3.417448 -1.697760 -2.191060
1	-2.290681	-1.276803	1.744743	1	-3.179195 0.614550 -1.331907
16	-0.530092	2.054117	1.362824	16	0.984621 -1.330355 -1.681540
6	1.055131	1.877881	0.573447	6	2.273039 -1.118847 -0.475371
6	2.190360	1.437134	1.283330	6	3.534769 -0.661868 -0.871035
6	1.184251	2.148114	-0.802230	6	2.068682 -1.400343 0.882119
6	3.406728	1.305034	0.641315	6	4.547808 -0.461041 0.061429
1	2.095327	1.213220	2.338990	1	3.710122 -0.442721 -1.918127
6	2.411702	1.986921	-1.444872	6	3.081504 -1.199957 1.813085
1	0.337871	2.550409	-1.349732	1	1.107122 -1.780482 1.212209
6	3.522231	1.574969	-0.726646	6	4.326473 -0.720947 1.411230
1	4.273638	0.974425	1.201084	1	5.513001 -0.095381 -0.270647
1	2.491775	2.200950	-2.503764	1	2.895136 -1.417863 2.858815

1	4.478350	1.455428	-1.221908	1	5.112786	-0.560115	2.138694
16	-0.416894	-1.320030	-1.480070	16	-2.424229	1.660870	1.272261
6	1.072800	-1.650603	-0.552745	6	-0.859108	2.067758	0.484860
6	2.327425	-1.496746	-1.150477	6	0.329438	1.532657	0.995752
6	0.991206	-2.126542	0.763708	6	-0.829767	2.922914	-0.616996
6	3.479358	-1.830934	-0.446637	6	1.545492	1.866101	0.404469
1	2.393015	-1.119619	-2.163729	1	0.305030	0.906011	1.880821
6	2.148420	-2.418400	1.472946	6	0.390240	3.239927	-1.206501
1	0.019330	-2.285041	1.217703	1	-1.754699	3.331348	-1.005506
6	3.395032	-2.280626	0.866519	6	1.574828	2.714107	-0.697503
1	4.446969	-1.718672	-0.922000	1	2.465074	1.456292	0.806894
1	2.075396	-2.775080	2.493374	1	0.412566	3.898419	-2.066285
1	4.295806	-2.525504	1.416269	1	2.521957	2.964904	-1.159516
II-RC_{oA}				II-TS_{oA}			
E = -3743.0060532 (-3743.0596345)				E = -3742.9759986 (-3743.0223605)			
Nimag = 0				Nimag = 1(-104.96 cm ⁻¹)			
Tc = 0.213778				Tc = 0.217936			
29	0.023976	0.601446	-0.189906	29	0.568472	-0.134914	-0.683658
53	-1.191241	-3.046755	-0.868161	53	1.837498	2.068312	-1.244786
6	-0.094994	-1.869065	0.509877	6	-0.464893	1.380670	-0.010253
6	-0.773347	-0.886994	1.243300	6	-0.303134	1.514745	1.360911
6	-0.025698	-0.090186	2.124487	6	-1.314041	2.135118	2.095849
6	1.331635	-0.340271	2.332805	6	-2.441843	2.634226	1.455851
6	1.967652	-1.358274	1.635566	6	-2.570773	2.505859	0.075424
6	1.260919	-2.112798	0.700630	6	-1.578278	1.877761	-0.669290
1	-1.845501	-0.757747	1.158792	1	0.594217	1.165611	1.860581
1	-0.536639	0.679988	2.690008	1	-1.199913	2.232222	3.169790
1	1.891168	0.270432	3.030041	1	-3.219798	3.124999	2.028498
1	3.026381	-1.540672	1.779821	1	-3.452711	2.882546	-0.429279
1	1.763342	-2.882100	0.128623	1	-1.681770	1.772268	-1.742622
16	1.943733	1.590430	-1.006207	16	-1.172984	-1.631639	-1.072214
6	3.366396	0.853228	-0.242916	6	-2.692691	-0.986405	-0.436432
6	3.893908	1.358132	0.950142	6	-2.878112	-0.827846	0.940633
6	3.977140	-0.265897	-0.819171	6	-3.727295	-0.621783	-1.304470
6	4.990363	0.752660	1.556153	6	-4.069873	-0.313317	1.435852
1	3.426252	2.222127	1.408879	1	-2.073770	-1.097026	1.616851
6	5.074187	-0.869647	-0.214100	6	-4.922927	-0.117147	-0.804681
1	3.573257	-0.668166	-1.741377	1	-3.582434	-0.731585	-2.373198
6	5.586239	-0.366273	0.979637	6	-5.097857	0.043125	0.567132
1	5.379392	1.157300	2.483996	1	-4.193286	-0.182696	2.505211
1	5.528567	-1.738868	-0.676271	1	-5.716382	0.159258	-1.489759
1	6.438847	-0.838295	1.452807	1	-6.026822	0.443668	0.955735
16	-1.880709	1.399004	-1.438330	16	2.293869	-1.793487	-0.660257
6	-2.888301	1.424802	0.022285	6	2.165586	-1.280192	1.047093
6	-2.512529	2.156182	1.158889	6	1.141687	-1.756615	1.879821
6	-4.070657	0.675615	0.085277	6	3.079705	-0.360731	1.583417
6	-3.285231	2.129219	2.315676	6	1.026011	-1.315808	3.194388
1	-1.605687	2.752520	1.129440	1	0.419246	-2.460931	1.484155
6	-4.839914	0.647199	1.244159	6	2.961490	0.078271	2.896669

1	-4.373603	0.101966	-0.783474	1	3.873707	0.017692	0.950537
6	-4.451798	1.370917	2.368785	6	1.931664	-0.392688	3.709351
1	-2.970592	2.702696	3.180839	1	0.221835	-1.694094	3.815281
1	-5.746783	0.053150	1.266905	1	3.676464	0.793733	3.286782
1	-5.049975	1.346974	3.271530	1	1.839153	-0.045392	4.731187
19	0.078833	3.899608	-1.939846	19	0.381498	-4.340513	-1.102844
II-PC_{oA} E = -3742.9790908 (-3743.028367) Nimag = 0 Tc = 0.215066				II-RC_{RE} E = -4361.4220666 (-4361.465579) Nimag = 0 Tc = 0.303084			
29	0.085985	-0.008560	0.336998	29	0.344852	-0.447061	-0.533123
53	1.436822	-2.277512	0.463230	6	-1.282243	0.563246	-0.576185
6	-1.405087	-1.033225	-0.329829	6	-1.772289	0.939855	-1.816928
6	-2.329898	-1.597953	0.532953	6	-2.986281	1.624161	-1.893098
6	-3.377446	-2.351456	0.007060	6	-3.696725	1.919653	-0.734927
6	-3.491961	-2.528853	-1.368781	6	-3.196532	1.527031	0.503661
6	-2.553728	-1.955813	-2.220618	6	-1.983269	0.847650	0.585325
6	-1.501140	-1.201578	-1.701548	1	-1.223876	0.716249	-2.725996
1	-2.252877	-1.455594	1.605392	1	-3.370189	1.924581	-2.861859
1	-4.102922	-2.796652	0.678650	1	-4.638692	2.452214	-0.796250
1	-4.310424	-3.110976	-1.775238	1	-3.747116	1.750714	1.410844
1	-2.634238	-2.090164	-3.293500	1	-1.597396	0.550918	1.555398
1	-0.773069	-0.761574	-2.374454	16	1.428284	1.500139	-0.285398
16	1.752311	1.487285	0.998399	6	0.412643	2.830900	0.307604
6	3.239711	0.947616	0.184313	6	-0.281102	3.661576	-0.576252
6	4.367173	0.614602	0.939931	6	0.343042	3.088111	1.679493
6	3.322808	0.879003	-1.210476	6	-1.046408	4.715849	-0.093053
6	5.547126	0.220956	0.316629	1	-0.229681	3.464019	-1.640090
1	4.310143	0.655893	2.021440	6	-0.416625	4.149586	2.160268
6	4.500982	0.479337	-1.831518	1	0.886709	2.448368	2.364971
1	2.452516	1.127028	-1.809376	6	-1.117840	4.963743	1.275907
6	5.620330	0.150653	-1.071248	1	-1.588487	5.347272	-0.787749
1	6.410252	-0.037154	0.919710	1	-0.461817	4.338312	3.226612
1	4.543841	0.426276	-2.913423	1	-1.714571	5.787623	1.649005
1	6.538219	-0.159344	-1.555988	16	-0.840734	-2.395926	-0.640751
16	-1.309074	1.747786	0.278736	6	-2.515463	-2.176793	-0.096693
6	-3.038832	1.367170	0.265183	6	-2.849854	-2.333879	1.251277
6	-3.726562	1.245915	1.475508	6	-3.519896	-1.858241	-1.013635
6	-3.729759	1.209030	-0.938388	6	-4.163629	-2.163846	1.674724
6	-5.086492	0.957508	1.480860	1	-2.072486	-2.577299	1.966899
1	-3.186650	1.368623	2.407065	6	-4.830774	-1.684174	-0.586937
6	-5.087801	0.914555	-0.928124	1	-3.261760	-1.732174	-2.058107
1	-3.194653	1.301204	-1.875658	6	-5.157579	-1.833329	0.758422
6	-5.768557	0.784489	0.279808	1	-4.408743	-2.285528	2.723604
1	-5.611416	0.861930	2.424109	1	-5.599164	-1.427207	-1.307158
1	-5.614554	0.782445	-1.866024	1	-6.179901	-1.696020	1.090097
1	-6.826917	0.552165	0.284467	16	2.270512	-1.758937	-0.775407
19	0.816349	4.101021	-0.575038	6	3.699334	-0.786766	-0.362119
				6	4.237697	-0.823250	0.928119

	6	4.324066	0.006584	-1.328563				
	6	5.370502	-0.080850	1.243639				
	1	3.758590	-1.432902	1.686080				
	6	5.457011	0.749160	-1.010900				
	1	3.910328	0.042417	-2.329714				
	6	5.985430	0.708945	0.275733				
	1	5.773152	-0.120130	2.249325				
	1	5.926083	1.361220	-1.772723				
	1	6.867574	1.287424	0.522946				
	19	1.219075	-4.004696	1.220529				
II-TS_{RE} E = -4361.4187697 (-4361.4628999) Nimag = 1 (-153.67 cm ⁻¹) Tc = 0.302704	II-PC_{RE} E = -4361.476006 (-4361.5287855) Nimag = 0 Tc = 0.303128							
29	0.335437	-0.628443	-0.562504		29	1.167654	0.842436	-0.984748
6	-1.116151	0.676199	-0.640269		6	-1.731724	1.504285	-1.824422
6	-1.622243	0.974251	-1.897824		6	-1.231240	2.675260	-2.397458
6	-2.918902	1.477459	-2.006317		6	-0.063643	2.631815	-3.147081
6	-3.685603	1.690782	-0.866632		6	0.591663	1.421522	-3.378378
6	-3.167111	1.377231	0.387571		6	0.048765	0.236716	-2.870187
6	-1.879364	0.868045	0.505314		6	-1.102202	0.283459	-2.074467
1	-1.012164	0.847144	-2.784935		1	-1.723565	3.623188	-2.213477
1	-3.317039	1.714416	-2.986497		1	0.338749	3.548931	-3.559895
1	-4.686633	2.096442	-0.954083		1	1.494570	1.391333	-3.975003
1	-3.767687	1.520020	1.278556		1	0.501058	-0.720753	-3.099418
1	-1.472571	0.642159	1.485379		1	-1.510090	-0.636697	-1.674959
16	1.133931	1.450883	-0.461726		16	-3.170374	1.667653	-0.788229
6	0.330396	2.868377	0.256504		6	-3.323571	0.032486	-0.087285
6	-0.338613	3.786011	-0.555187		6	-4.242420	-0.865290	-0.628136
6	0.412421	3.086108	1.631591		6	-2.543291	-0.330484	1.011946
6	-0.939097	4.903149	0.011431		6	-4.383257	-2.130984	-0.065619
1	-0.397541	3.608545	-1.622345		1	-4.839150	-0.573095	-1.483879
6	-0.189360	4.207979	2.193766		6	-2.683393	-1.600296	1.562207
1	0.940760	2.373530	2.253645		1	-1.834625	0.374893	1.432492
6	-0.869697	5.114395	1.387039		6	-3.605433	-2.497879	1.027938
1	-1.463296	5.609721	-0.621131		1	-5.099743	-2.828005	-0.483269
1	-0.126972	4.371467	3.263098		1	-2.073322	-1.881424	2.412771
1	-1.340734	5.985220	1.826892		1	-3.715876	-3.483916	1.463980
16	-0.885565	-2.612865	-0.349337		16	2.937926	-0.769486	-0.904581
6	-2.552727	-2.194993	0.082504		6	2.002433	-2.261181	-0.680775
6	-2.969274	-2.200148	1.418498		6	0.641270	-2.253570	-0.339201
6	-3.476024	-1.844370	-0.906668		6	2.622832	-3.507015	-0.856552
6	-4.276245	-1.864089	1.754861		6	-0.068998	-3.441381	-0.191507
1	-2.257216	-2.462183	2.193075		1	0.128446	-1.312220	-0.172168
6	-4.780008	-1.504233	-0.567521		6	1.912592	-4.691446	-0.704778
1	-3.158149	-1.828340	-1.942678		1	3.674029	-3.534490	-1.120829
6	-5.187691	-1.511879	0.763369		6	0.559025	-4.668647	-0.375194
1	-4.581115	-1.873206	2.795507		1	-1.121213	-3.398034	0.067715
1	-5.478195	-1.221801	-1.347667		1	2.419527	-5.639046	-0.849632

1	-6.204681	-1.244466	1.025440	1	0.005355	-5.592749	-0.262312
16	2.339356	-1.839366	-0.888551	16	0.898971	2.564018	0.563498
6	3.659785	-0.757325	-0.395756	6	0.396899	1.596421	1.966035
6	4.214134	-0.834882	0.886972	6	0.783687	0.256777	2.123881
6	4.182458	0.184156	-1.289536	6	-0.418329	2.161283	2.957475
6	5.259780	0.001278	1.263089	6	0.355040	-0.494271	3.213750
1	3.817918	-1.555158	1.594050	1	1.397918	-0.215100	1.364215
6	5.229326	1.019749	-0.912218	6	-0.851025	1.407337	4.041941
1	3.758795	0.257676	-2.284626	1	-0.728882	3.194879	2.855626
6	5.774763	0.932743	0.364966	6	-0.471375	0.072655	4.178337
1	5.674157	-0.077657	2.261898	1	0.661954	-1.531664	3.294152
1	5.618788	1.741565	-1.621383	1	-1.494227	1.865030	4.785142
1	6.590651	1.582338	0.658100	1	-0.814843	-0.513376	5.022072
19	1.429578	-4.135630	1.148361	19	3.717989	1.305857	1.476239
III-RC_{oA}				III-TS_{oA}			
E = -3346.2037578 (-3346.25202600)				E = -3346.1815283 (-3346.2267274)			
Nimag = 1(-15.9 cm ⁻¹)				Nimag = 1 (-145.37 cm ⁻¹)			
Tc = 0.250208				Tc = 0.249326			
29	-1.090355	0.114861	0.720488	29	-0.902460	0.343737	-0.239802
53	-0.170878	-1.514170	-1.993650	53	-2.706227	-1.590936	-0.495248
6	-0.215261	-1.758077	0.132484	6	-0.418017	-1.543046	0.179084
6	-1.456761	-2.013943	0.747297	6	-0.216878	-1.590222	1.559490
6	-1.462769	-2.450313	2.086524	6	0.882550	-2.280749	2.060404
6	-0.278424	-2.648402	2.767482	6	1.743947	-2.952973	1.199344
6	0.949828	-2.449220	2.118352	6	1.520374	-2.913123	-0.173994
6	0.990791	-2.036877	0.801710	6	0.435491	-2.217699	-0.691715
1	-2.374109	-2.027127	0.173486	1	-0.916565	-1.115809	2.238234
1	-2.414272	-2.644566	2.566290	1	1.049133	-2.304985	3.131014
1	-0.296588	-2.984996	3.796655	1	2.588550	-3.503439	1.594979
1	1.880298	-2.631390	2.642613	1	2.196472	-3.419960	-0.852264
1	1.939894	-1.902811	0.296684	1	0.253746	-2.198111	-1.759363
16	0.681551	1.720589	0.761770	16	1.273168	1.422127	-0.446661
6	2.224075	0.868298	0.572343	6	2.648536	0.327018	-0.223347
6	2.953715	0.431099	1.688090	6	3.207693	0.121656	1.046901
6	2.738294	0.581507	-0.700316	6	3.239857	-0.326377	-1.315675
6	4.130410	-0.291804	1.535391	6	4.300882	-0.719516	1.220500
1	2.570326	0.643107	2.679734	1	2.760314	0.615733	1.902679
6	3.918754	-0.141601	-0.852893	6	4.333109	-1.167347	-1.140690
1	2.183362	0.899169	-1.576611	1	2.821121	-0.175174	-2.304646
6	4.617446	-0.590469	0.263529	6	4.865643	-1.374765	0.129414
1	4.667567	-0.629842	2.414679	1	4.707645	-0.870693	2.214479
1	4.285816	-0.361370	-1.849224	1	4.767211	-1.667061	-1.999651
1	5.532143	-1.158882	0.146474	1	5.714398	-2.034306	0.265915
8	-2.721515	1.040427	1.229169	8	-1.792202	2.024640	-0.553307
6	-3.536251	1.485294	0.201684	6	-2.581247	2.571002	0.451000
6	-4.661702	2.344969	0.798166	6	-2.298428	4.078436	0.548873
1	-4.223213	3.193161	1.331221	1	-2.474619	4.542421	-0.425357
1	-5.350719	2.726456	0.037980	1	-2.928987	4.575542	1.293072
1	-5.229225	1.748610	1.517853	1	-1.249597	4.237368	0.816082

6	-4.163416	0.301309	-0.558817	6	-2.276448	1.926581	1.817697
1	-4.875569	0.621863	-1.326343	1	-2.829186	2.396118	2.637340
1	-3.374031	-0.277758	-1.050628	1	-2.548136	0.864903	1.797665
1	-4.677998	-0.355015	0.148803	1	-1.205435	2.007319	2.030271
6	-2.740805	2.334918	-0.807726	6	-4.069968	2.356774	0.128035
1	-3.375978	2.762727	-1.590477	1	-4.730399	2.773501	0.895682
1	-2.230354	3.144673	-0.278378	1	-4.304548	2.830743	-0.829110
1	-1.973060	1.717425	-1.286977	1	-4.268982	1.285609	0.035038
19	2.359595	3.935981	-0.568736	19	3.803347	3.199286	-0.456765
III-PC_{oA} E = -3346.1944779 (-3346.2338355) Nimag = 1(-18.5 cm ⁻¹) Tc = 0.252735				III-RC_{RE} E = -3964.6453166 (-3964.6804161) Nimag = 1(-8.37 cm ⁻¹) Tc = 0.340174			
29	-0.822845	0.131564	-0.319485	29	0.493194	-0.378486	-0.595758
53	-2.944465	-1.482676	-0.215175	6	-1.148382	0.371588	-1.223089
6	0.216941	-1.385838	0.198262	6	-1.705555	-0.147582	-2.384999
6	0.325647	-1.643868	1.557922	6	-2.965645	0.284837	-2.795910
6	1.088878	-2.725782	1.995890	6	-3.659635	1.233025	-2.050746
6	1.733527	-3.544833	1.074717	6	-3.092125	1.745069	-0.887320
6	1.612017	-3.281783	-0.286846	6	-1.834539	1.313931	-0.469631
6	0.855895	-2.197656	-0.727820	1	-1.167460	-0.876605	-2.982434
1	-0.181718	-1.019724	2.286983	1	-3.399077	-0.120714	-3.703507
1	1.173414	-2.925667	3.058244	1	-4.637815	1.569565	-2.373353
1	2.327209	-4.385271	1.414635	1	-3.628685	2.480001	-0.297419
1	2.110314	-3.916102	-1.011500	1	-1.401623	1.717826	0.440845
1	0.780443	-1.990565	-1.790221	16	1.319316	1.363245	-1.793782
16	1.092851	1.274734	-0.568316	6	1.487149	2.369545	-0.338848
6	2.596694	0.332956	-0.471691	6	0.789450	3.577565	-0.240643
6	3.136304	-0.063972	0.756213	6	2.331758	1.982623	0.711073
6	3.287845	0.028998	-1.649356	6	0.934714	4.385419	0.883217
6	4.335496	-0.766400	0.801366	1	0.132019	3.874534	-1.049366
1	2.599717	0.161310	1.670636	6	2.463186	2.788902	1.836277
6	4.493821	-0.661255	-1.599607	1	2.862959	1.040153	0.627360
1	2.867853	0.332797	-2.601207	6	1.768604	3.993697	1.926001
6	5.017479	-1.066551	-0.374962	1	0.391154	5.321175	0.943819
1	4.736019	-1.082183	1.757797	1	3.118393	2.480119	2.643154
1	5.020031	-0.890592	-2.518797	1	1.877553	4.622254	2.801724
1	5.951816	-1.613762	-0.337101	16	-0.626423	-1.861788	0.733456
8	-1.736124	1.689227	-0.809265	6	-2.311348	-1.391395	1.028790
6	-2.276477	2.536511	0.166598	6	-2.642111	-0.628033	2.153500
6	-1.628672	3.921342	0.027766	6	-3.329277	-1.778032	0.152676
1	-1.786411	4.296753	-0.986460	6	-3.960025	-0.255117	2.392886
1	-2.043502	4.642992	0.738396	1	-1.855875	-0.321615	2.834427
1	-0.551508	3.836128	0.196900	6	-4.645556	-1.400215	0.391051
6	-2.018474	2.014185	1.591261	1	-3.078172	-2.365376	-0.722653
1	-2.433533	2.688530	2.345561	6	-4.966452	-0.635921	1.509900
1	-2.478877	1.030926	1.725398	1	-4.200752	0.337128	3.268536
1	-0.941590	1.928263	1.772797	1	-5.423024	-1.700627	-0.302298
6	-3.790360	2.650835	-0.056314	1	-5.993115	-0.341772	1.693430

1	-4.254800	3.345582	0.650527	6	2.960787	-1.892841	-0.789969
1	-3.980388	3.006282	-1.072534	19	1.901018	-1.354272	2.591535
1	-4.254162	1.667542	0.055597	8	2.104734	-1.188670	0.072298
19	3.039096	3.519070	0.571604	6	4.173728	-1.024520	-1.147688
				1	3.835576	-0.107071	-1.632924
				1	4.710484	-0.752891	-0.233858
				1	4.865981	-1.549663	-1.813064
				6	2.226405	-2.309440	-2.074252
				1	2.857743	-2.929976	-2.716331
				1	1.328325	-2.881705	-1.819971
				1	1.930080	-1.428317	-2.652262
				6	3.436445	-3.158936	-0.065203
				1	2.574319	-3.770727	0.216501
				1	4.101910	-3.760782	-0.690886
				1	3.983499	-2.886623	0.842730
III-TS_{RE} E = -3964.644581 (-3964.6807175) Nimag = 1(-135.06 cm ⁻¹) Tc = 0.339463				III-PC_{RE} E = -3964.6815088 (-3864.7298454) Nimag = 0 Tc = 0.336730			
29	0.480867	-0.386890	-0.577161	29	-0.188833	-0.412106	-0.589266
6	-1.076462	0.550853	-1.243922	6	0.578058	1.657660	-1.061105
6	-1.648396	0.054820	-2.412752	6	-0.453424	1.314447	-1.956446
6	-2.970977	0.368883	-2.716323	6	-1.777430	1.671269	-1.667280
6	-3.715036	1.180619	-1.865852	6	-2.095448	2.317994	-0.485407
6	-3.134499	1.666821	-0.697799	6	-1.079065	2.608620	0.427313
6	-1.815070	1.356457	-0.383005	6	0.242255	2.291621	0.149116
1	-1.067569	-0.555293	-3.096852	1	-0.209142	0.886822	-2.923407
1	-3.413450	-0.020859	-3.626407	1	-2.556846	1.410836	-2.372822
1	-4.742038	1.427562	-2.107694	1	-3.126249	2.563993	-0.259104
1	-3.710852	2.287979	-0.021384	1	-1.316576	3.100362	1.363312
1	-1.367211	1.751948	0.523603	1	1.024449	2.562673	0.847405
16	1.078027	1.465295	-1.715295	16	2.261341	1.516970	-1.645558
6	1.391113	2.406408	-0.239933	6	3.192894	1.552390	-0.120549
6	0.811962	3.671155	-0.099840	6	4.095958	2.591107	0.092392
6	2.234752	1.916061	0.764779	6	3.036547	0.534360	0.821805
6	1.079361	4.440293	1.028590	6	4.859564	2.609383	1.257324
1	0.152814	4.042466	-0.875890	1	4.198080	3.378389	-0.645012
6	2.489362	2.688472	1.892117	6	3.791794	0.575297	1.988755
1	2.671246	0.928887	0.646732	1	2.341074	-0.282467	0.625928
6	1.916340	3.951432	2.026919	6	4.704971	1.605413	2.207061
1	0.629878	5.421402	1.127806	1	5.566780	3.413156	1.422798
1	3.145443	2.305981	2.665699	1	3.675828	-0.210318	2.727004
1	2.123224	4.551028	2.905332	1	5.295594	1.623929	3.115350
16	-0.652319	-1.975781	0.700048	16	-2.238588	-1.507075	0.110372
6	-2.325493	-1.461088	0.975422	6	-3.579374	-0.377300	0.360722
6	-2.675663	-0.761982	2.136994	6	-3.756063	0.278153	1.586621
6	-3.322928	-1.733703	0.034536	6	-4.478652	-0.084806	-0.672946
6	-3.986189	-0.350277	2.351592	6	-4.781128	1.200249	1.767465
1	-1.907927	-0.540184	2.870134	1	-3.066537	0.069639	2.397425

6	-4.631228	-1.315659	0.247175	6	-5.502873	0.839508	-0.493775
1	-3.060890	-2.265490	-0.872567	1	-4.357501	-0.582182	-1.628959
6	-4.970879	-0.623571	1.405925	6	-5.659502	1.492784	0.726526
1	-4.237525	0.189527	3.257797	1	-4.890667	1.696414	2.725649
1	-5.387580	-1.523643	-0.501712	1	-6.180401	1.051744	-1.313569
1	-5.991317	-0.297531	1.569392	1	-6.454703	2.215349	0.865247
6	3.042435	-1.773432	-0.879032	6	1.655452	-2.668695	-0.833372
19	1.903515	-1.669409	2.506368	19	-0.128984	-2.476841	2.213649
8	2.142595	-1.210174	0.033787	8	1.066032	-1.820089	0.104337
6	4.166318	-0.777402	-1.198695	6	3.168506	-2.411834	-0.911864
1	3.739823	0.137043	-1.617649	1	3.354455	-1.388421	-1.250099
1	4.697568	-0.517661	-0.278105	1	3.614046	-2.527578	0.080683
1	4.888029	-1.190697	-1.910378	1	3.664568	-3.102339	-1.601186
6	2.322532	-2.169072	-2.178427	6	1.047235	-2.445197	-2.228441
1	2.983760	-2.703522	-2.866521	1	1.486324	-3.101918	-2.985637
1	1.470743	-2.815221	-1.943987	1	-0.032007	-2.626338	-2.197168
1	1.952686	-1.278795	-2.696981	1	1.220407	-1.408017	-2.537237
6	3.648290	-3.035910	-0.249708	6	1.413224	-4.128580	-0.418036
1	2.851976	-3.745844	-0.005927	1	0.336859	-4.320742	-0.355123
1	4.360288	-3.527134	-0.919300	1	1.848178	-4.841507	-1.125062
1	4.177017	-2.775267	0.672625	1	1.857542	-4.311117	0.565963
IV-RC_{OA}				IV-TS_{OA}			
E = -3989.81121 (-3989.8962993)				E = -3989.7750618 (-3989.8962993)			
Nimag = 0				Nimag = 1 (-118.63 cm ⁻¹)			
Tc = 0.279084				Tc = 0.283639			
29	-2.362123	-1.616781	-0.500913	29	1.703639	0.104086	-0.449265
53	0.208542	2.522332	-0.076864	53	-0.019325	-2.228501	0.120874
6	0.117595	0.408900	-0.090379	6	-0.285631	0.393175	-0.039537
6	-0.078224	-0.285132	-1.290209	6	-0.109110	1.153094	-1.207747
6	-0.369313	-1.671016	-1.256726	6	0.100224	2.534448	-1.079049
6	-0.421716	-2.352547	-0.034965	6	0.191939	3.120125	0.173782
6	-0.156388	-1.649733	1.159288	6	0.099216	2.334503	1.324534
6	0.152624	-0.300351	1.135873	6	-0.114192	0.964426	1.231596
1	-0.116162	0.243814	-2.233846	1	-0.271038	0.719680	-2.187228
1	-0.437286	-2.210540	-2.193445	1	0.177137	3.133621	-1.977780
1	-0.549183	-3.427522	-0.013136	1	0.351598	4.187116	0.260488
1	-0.148944	-2.178947	2.103645	1	0.205936	2.782439	2.304885
1	0.345934	0.229503	2.059795	1	-0.202072	0.358882	2.124307
8	-4.165781	-1.176128	-0.480158	8	3.519112	-0.175399	-0.746616
6	-4.515557	-0.152237	0.400273	6	4.358190	0.527656	0.117925
6	-3.481442	0.986227	0.345729	6	4.270519	-0.060111	1.534993
1	-3.318251	1.279148	-0.695508	1	4.543002	-1.118543	1.507459
1	-3.781155	1.867191	0.921642	1	4.921730	0.454712	2.248191
1	-2.523673	0.635985	0.750189	1	3.238516	0.011335	1.896715
6	-4.586946	-0.690833	1.837032	6	3.955205	2.010901	0.160251
1	-4.849063	0.083365	2.564978	1	4.648537	2.625928	0.741987
1	-5.329005	-1.491672	1.891997	1	3.903888	2.397880	-0.860922
1	-3.614100	-1.112272	2.112487	1	2.959161	2.114071	0.607496
6	-5.888016	0.391409	-0.013665	6	5.796553	0.405996	-0.397599

1	-6.242288	1.178910	0.657832	1	6.513099	0.919161	0.250262
1	-5.830310	0.793826	-1.028470	1	6.071244	-0.650274	-0.457190
1	-6.614899	-0.424889	-0.011942	1	5.863038	0.832692	-1.401801
29	2.034698	-0.253341	-0.501773	29	-1.893795	-0.643482	-0.346021
8	3.798809	-0.756064	-0.813677	8	-3.504577	0.080059	-0.844942
6	4.580022	-0.815937	0.340318	6	-4.201863	0.832312	0.108421
6	6.041282	-1.012154	-0.079630	6	-5.681189	0.851239	-0.285815
1	6.355407	-0.172281	-0.704687	1	-6.072739	-0.169005	-0.293443
1	6.714245	-1.082378	0.779905	1	-6.279020	1.452572	0.404747
1	6.127807	-1.928306	-0.669443	1	-5.783906	1.265329	-1.291684
6	4.141239	-1.994011	1.224602	6	-3.646652	2.263422	0.123823
1	3.099655	-1.856450	1.536130	1	-2.577777	2.236875	0.357761
1	4.199112	-2.921380	0.648763	1	-3.765445	2.714578	-0.864625
1	4.755925	-2.096030	2.124306	1	-4.148747	2.893724	0.863550
6	4.451875	0.491267	1.140416	6	-4.047141	0.206845	1.502379
1	3.419406	0.615017	1.490818	1	-2.997894	0.248992	1.821673
1	5.108646	0.523889	2.015125	1	-4.642677	0.719046	2.262714
1	4.684351	1.336401	0.487468	1	-4.349509	-0.843261	1.464133
IV-PCoA E = -3989.7853548 (-3989.8673758) Nimag = 0 Tc = 0.285019				IV-RCRE + KI E = -5219.676311 (-5219.7438055) Nimag = 0 Tc = 0.366007			
29	1.269724	0.255232	-0.472925	29	0.981556	0.004257	-0.416395
53	0.246771	-2.449154	0.324144	53	-0.544728	2.960715	0.737616
6	-0.504010	0.799688	0.176785	6	-0.768541	-0.741173	-0.957331
6	-0.363390	1.837632	-0.750527	6	-0.710697	-2.111002	-1.238682
6	-0.086479	3.130929	-0.284416	6	-0.597431	-2.525864	-2.557706
6	0.017066	3.370729	1.075039	6	-0.556523	-1.589291	-3.594893
6	-0.128858	2.324600	1.991352	6	-0.622513	-0.234588	-3.315130
6	-0.398979	1.034668	1.555193	6	-0.736785	0.204585	-1.988820
1	-0.581360	1.671905	-1.798585	1	-0.738788	-2.842527	-0.438060
1	0.006324	3.940128	-0.998064	1	-0.541932	-3.585072	-2.777775
1	0.214940	4.373074	1.433758	1	-0.473780	-1.927072	-4.620521
1	-0.021818	2.509741	3.053188	1	-0.602637	0.496386	-4.114516
1	-0.491143	0.225873	2.268719	1	-0.856982	1.262196	-1.775259
8	3.011202	0.052158	-1.096032	8	2.805645	0.544006	-0.313674
6	3.973964	0.650500	-0.280610	6	3.471147	0.500798	-1.548923
6	4.154759	-0.170466	1.005280	6	3.024577	1.679908	-2.423219
1	4.439322	-1.193802	0.746810	1	3.259657	2.622666	-1.921498
1	4.911436	0.251039	1.674203	1	3.509562	1.672951	-3.403653
1	3.202694	-0.214168	1.545958	1	1.940506	1.637756	-2.572956
6	3.543740	2.079829	0.091541	6	3.145565	-0.817191	-2.269750
1	4.315364	2.624507	0.643783	1	3.679180	-0.915599	-3.219063
1	3.298144	2.632055	-0.819646	1	3.406871	-1.663931	-1.628715
1	2.642876	2.051533	0.717951	1	2.071361	-0.874913	-2.485584
6	5.297585	0.701742	-1.050550	6	4.978121	0.585753	-1.294212
1	6.103507	1.145715	-0.459111	1	5.550838	0.574619	-2.225665
1	5.589752	-0.311800	-1.336823	1	5.207799	1.509763	-0.756460
1	5.166243	1.289252	-1.963103	1	5.295915	-0.259426	-0.677803

29	-1.501970	-0.754185	-0.369813	29	-1.570518	-0.339211	0.775852
8	-2.837031	0.183835	-1.075839	8	-3.288306	-0.728151	0.458443
6	-3.888759	0.668279	-0.266286	6	-4.230974	-0.198687	-0.434533
6	-5.155077	0.547367	-1.121567	6	-5.605249	-0.385703	0.220627
1	-5.328180	-0.497522	-1.386387	1	-5.643065	0.163228	1.164153
1	-6.023770	0.925063	-0.576601	1	-6.402814	-0.021955	-0.432741
1	-5.034588	1.125375	-2.039786	1	-5.774377	-1.444891	0.426872
6	-3.642087	2.133661	0.098128	6	-4.185568	-0.973712	-1.756645
1	-2.766913	2.230899	0.745436	1	-3.208021	-0.861290	-2.231477
1	-3.465450	2.712921	-0.811042	1	-4.353120	-2.036333	-1.563382
1	-4.504464	2.553215	0.622015	1	-4.952029	-0.617740	-2.450652
6	-4.025763	-0.184946	0.997306	6	-3.972464	1.288870	-0.673828
1	-3.138655	-0.079198	1.631765	1	-2.998155	1.432414	-1.145332
1	-4.891049	0.114525	1.592756	1	-4.735996	1.732871	-1.318157
1	-4.142580	-1.238769	0.727544	1	-3.959556	1.820845	0.280745
				16	0.328100	-0.386320	1.898203
				6	0.780610	-2.109273	1.789643
				6	1.989369	-2.451592	1.176295
				6	-0.046158	-3.104364	2.311867
				6	2.353956	-3.788024	1.071918
				1	2.625725	-1.667405	0.775633
				6	0.326889	-4.440644	2.200125
				1	-0.975354	-2.833110	2.799800
				6	1.523318	-4.784809	1.578895
				1	3.287536	-4.051267	0.588793
				1	-0.320376	-5.210992	2.601467
				1	1.808700	-5.825988	1.491380
				19	2.741664	2.007362	1.726786
IV-TS_{RE}				IV-PC_{RE}			
E = -4608.2460638 ()				E = -4608.2820786 (-4608.3701882)			
Nimag = 1(-107.55 cm ⁻¹)				Nimag = 0			
Tc = 0.373373				Tc = 0.369926			
29	-1.909354	0.061313	-1.123101	29	-2.639329	0.527109	-0.917296
6	-0.467180	-0.861591	-0.187794	6	-0.087821	-0.668842	-0.504740
6	-0.176849	-0.484605	1.129127	6	-0.151025	-0.613083	0.900511
6	0.104753	-1.476181	2.071075	6	-0.013899	-1.776429	1.637621
6	0.152318	-2.814292	1.693951	6	0.200377	-3.003732	1.000123
6	-0.042424	-3.167926	0.362362	6	0.294319	-3.059224	-0.379795
6	-0.328316	-2.195402	-0.597505	6	0.159909	-1.891448	-1.151363
1	-0.237204	0.553915	1.437897	1	-0.325069	0.334808	1.396382
1	0.289917	-1.186479	3.098274	1	-0.078607	-1.728440	2.717503
1	0.365676	-3.577756	2.431151	1	0.297335	-3.908473	1.586181
1	0.025775	-4.203792	0.053354	1	0.464443	-4.002399	-0.882854
1	-0.530956	-2.482569	-1.621397	1	0.122949	-1.953153	-2.233463
16	-0.106930	1.028089	-1.791461	16	-0.500838	0.750646	-1.534861
6	0.168703	2.229442	-0.514132	6	0.069954	2.102405	-0.507986
6	-0.890219	2.981009	-0.000318	6	-0.860868	2.928105	0.116988
6	1.470662	2.414416	-0.038274	6	1.440315	2.307420	-0.360693
6	-0.646609	3.910784	1.003948	6	-0.408153	3.993167	0.887946

1	-1.891462	2.854718	-0.395927	1	-1.922245	2.737107	0.006927
6	1.700977	3.355307	0.957761	6	1.875644	3.369047	0.423012
1	2.288086	1.816182	-0.434044	1	2.164065	1.649553	-0.833819
6	0.646662	4.097887	1.483509	6	0.956308	4.213013	1.040904
1	-1.467574	4.491500	1.406027	1	-1.125425	4.642390	1.374109
1	2.707730	3.499707	1.331398	1	2.938073	3.537773	0.548359
1	0.832238	4.825034	2.264573	1	1.304620	5.041447	1.645419
8	-3.559176	-0.655771	-0.848130	8	-4.370162	0.309822	-0.279674
6	-4.170818	-0.615619	0.411214	6	-4.489886	-0.727342	0.645590
6	-5.686928	-0.661967	0.200029	6	-5.980690	-1.029014	0.840908
1	-6.003205	0.206126	-0.383817	1	-6.493233	-0.120157	1.166336
1	-5.948926	-1.564497	-0.357118	1	-6.416915	-1.343434	-0.110997
1	-6.228719	-0.664804	1.149921	1	-6.152120	-1.814388	1.582898
6	-3.799278	0.677949	1.150547	6	-3.870959	-0.313633	1.990149
1	-4.311215	0.770643	2.112182	1	-3.948167	-1.096989	2.750953
1	-2.720992	0.708260	1.347432	1	-2.811209	-0.081267	1.840429
1	-4.061888	1.540327	0.530905	1	-4.365863	0.588745	2.358440
6	-3.725304	-1.831201	1.235432	6	-3.779890	-1.997273	0.139616
1	-2.638168	-1.822761	1.355030	1	-2.695070	-1.834900	0.101483
1	-4.183739	-1.842093	2.228586	1	-3.963254	-2.867720	0.777429
1	-4.002026	-2.748807	0.709966	1	-4.123151	-2.219089	-0.874243
29	1.505648	-0.582518	-0.653918	29	2.023842	-0.871860	-0.776953
8	3.338257	-0.282661	-0.933215	8	3.804710	-0.328570	-0.775667
6	4.178764	-0.718410	0.093459	6	4.483183	-0.548545	0.427296
6	5.620690	-0.714898	-0.425107	6	5.988398	-0.436607	0.161580
1	5.883717	0.292915	-0.756672	1	6.206720	0.544420	-0.267801
1	6.337045	-1.031645	0.338577	1	6.577800	-0.559088	1.074859
1	5.701199	-1.388048	-1.282658	1	6.294211	-1.200330	-0.558284
6	4.070035	0.220776	1.305559	6	4.069614	0.500711	1.469145
1	4.347999	1.237029	1.010231	1	4.309496	1.500984	1.098127
1	3.034103	0.243586	1.663036	1	2.986902	0.450854	1.631223
1	4.713006	-0.091361	2.134180	1	4.570133	0.353411	2.431001
6	3.793749	-2.141014	0.529438	6	4.164660	-1.949749	0.973823
1	2.783592	-2.137201	0.955442	1	3.104632	-2.010390	1.251677
1	3.786103	-2.798560	-0.344085	1	4.351094	-2.692807	0.194017
1	4.475243	-2.553397	1.279563	1	4.757027	-2.204728	1.857596
V-RCoA E = -2666.0505721 (-2666.1008909) Nimag = 0 Tc = 0.182763				V-TSoA E = -2666.0146131 (-2666.0639188) Nimag = 1 (-111.00 cm ⁻¹) Tc = 0.182549			
29	-0.705797	-1.092439	-0.979649	29	0.420375	-0.707556	-0.657337
53	2.999040	0.025795	0.527932	53	2.404168	-0.529797	0.937066
6	1.432385	0.663257	-0.748792	6	0.805449	1.189037	-0.415929
6	0.811015	1.874479	-0.511694	6	0.009337	1.906836	0.458993
6	-0.242036	2.277449	-1.341994	6	-0.165184	3.269617	0.223000
6	-0.664126	1.470674	-2.381896	6	0.460374	3.884414	-0.856178
6	-0.031174	0.240260	-2.619643	6	1.278020	3.141084	-1.702962
6	1.053529	-0.162599	-1.820553	6	1.465609	1.778902	-1.482425
1	1.116736	2.499540	0.317027	1	-0.475666	1.429808	1.303057

1	-0.732246	3.223405	-1.150141	1	-0.796508	3.843214	0.891747
1	-1.487392	1.777377	-3.014667	1	0.323471	4.944684	-1.029640
1	-0.285025	-0.338573	-3.499966	1	1.774117	3.614490	-2.541955
1	1.637572	-1.036262	-2.083030	1	2.109422	1.201258	-2.133758
16	-2.986143	-1.152631	-0.440612	16	-1.618178	-0.395877	-1.767332
6	-2.524338	0.296621	0.497734	6	-2.395136	-0.037819	-0.207590
6	-1.523205	0.237482	1.479257	6	-2.227553	-0.888816	0.893903
6	-3.151386	1.526520	0.267192	6	-3.146138	1.129529	-0.043521
6	-1.152809	1.375252	2.187033	6	-2.780417	-0.565216	2.128329
1	-1.044961	-0.709172	1.703633	1	-1.672932	-1.814879	0.780056
6	-2.781312	2.661508	0.980833	6	-3.703730	1.445724	1.190648
1	-3.928950	1.587417	-0.485849	1	-3.271137	1.799404	-0.886145
6	-1.774516	2.596090	1.940123	6	-3.517777	0.605277	2.284683
1	-0.371495	1.303809	2.935931	1	-2.633521	-1.232894	2.969331
1	-3.280864	3.603158	0.781375	1	-4.276724	2.359581	1.298448
1	-1.484014	3.481872	2.492236	1	-3.944375	0.857772	3.247723
8	0.207767	-2.493756	0.291373	8	0.393561	-2.711433	-0.759961
1	-0.425458	-2.878079	0.934831	1	-0.456395	-3.172601	-0.969270
1	1.027483	-2.321848	0.763990	1	0.896076	-3.254719	-0.144803
8	-1.886232	-3.143424	1.843179	8	-2.052264	-3.536421	-1.280140
1	-2.248865	-4.032364	1.896723	1	-2.257898	-4.158117	-1.984830
1	-2.479669	-2.649083	1.245108	1	-2.266356	-2.653205	-1.629283
V-PCoA				VI-RCoA			
E = -2666.0825569 (-2666.1387625)				E = -3895.8842714 (-3895.9367735)			
Nimag = 0				Nimag = 0			
Tc = 0.182784				Tc = 0.256852			
29	1.383608	1.001528	-0.375376	29	0.102003	0.244201	0.152479
53	2.516104	-1.397985	0.136299	53	-3.333600	-1.207987	-0.857842
6	-1.379606	1.766625	0.762047	6	-1.401843	-1.864264	-0.281064
6	-0.773402	1.267246	1.926864	6	-0.951420	-1.604540	1.016170
6	0.549474	1.560426	2.191639	6	0.323772	-2.055821	1.381936
6	1.284307	2.392187	1.324516	6	1.088928	-2.812253	0.500865
6	0.651831	2.956414	0.207266	6	0.601216	-3.095456	-0.769867
6	-0.684968	2.619283	-0.081531	6	-0.640100	-2.612854	-1.173739
1	-1.337255	0.622085	2.589749	1	-1.584956	-1.110224	1.741380
1	1.027831	1.152103	3.072607	1	0.689327	-1.834203	2.377866
1	2.302330	2.666464	1.569756	1	2.072757	-3.156350	0.798141
1	1.171899	3.671155	-0.418045	1	1.197078	-3.676066	-1.463885
1	-1.152839	3.008748	-0.977477	1	-1.009113	-2.816235	-2.170698
16	-3.045475	1.278742	0.346222	16	1.918762	0.294862	-1.293767
6	-2.835871	-0.500612	0.243844	6	3.147139	-0.659636	-0.442545
6	-1.654070	-1.075823	-0.223003	6	3.400737	-0.473667	0.921964
6	-3.914813	-1.306886	0.600167	6	3.866241	-1.648525	-1.121975
6	-1.548676	-2.458126	-0.311154	6	4.327752	-1.265809	1.589111
1	-0.803510	-0.461399	-0.492958	1	2.853569	0.290720	1.464139
6	-3.807904	-2.689763	0.484281	6	4.793528	-2.441375	-0.453264
1	-4.827199	-0.858619	0.975778	1	3.675293	-1.805945	-2.177463
6	-2.626229	-3.269386	0.034084	6	5.026565	-2.259947	0.907428
1	-0.614781	-2.890348	-0.651920	1	4.502370	-1.107436	2.647478

1	-4.648387	-3.313217	0.764767	1	5.331294	-3.209265	-0.998203
1	-2.542078	-4.346726	-0.039556	1	5.744762	-2.880971	1.428778
8	0.732234	0.592657	-2.293078	16	-1.220645	2.551113	-0.183634
1	-0.184815	0.831505	-2.546500	6	-1.148937	1.812242	1.431540
1	0.875836	-0.312416	-2.587240	6	0.078487	1.635708	2.106822
8	-1.836385	1.296692	-2.778200	6	-2.323607	1.393101	2.083722
1	-2.432947	1.256127	-2.017363	6	0.118689	1.024001	3.361866
1	-2.311884	0.879278	-3.502971	1	0.980918	2.072479	1.689803
				6	-2.272345	0.795361	3.333329
				1	-3.274756	1.537133	1.584977
				6	-1.047591	0.586182	3.974206
				1	1.074504	0.899910	3.859306
				1	-3.193236	0.481189	3.811798
				1	-1.011303	0.111326	4.946756
				19	1.621382	3.309137	-2.031331
				8	1.457066	4.236888	0.415811
				1	1.613265	4.731138	1.224149
				8	-0.194931	1.639782	-3.219584
				1	-0.745060	1.543319	-2.428934
				1	0.533079	3.933368	0.455669
				1	0.276412	0.800356	-3.282466
VI-TSoA E = -3895.8494208 (-3895.9014235) Nimag = 1 (-87.69) Tc = 0.259988				VI-PCoA E = -3895.9156633 (-3895.9784947) Nimag = 0 Tc = 0.256953			
29	-0.337450	-0.278859	-0.614829	29	-1.461420	-0.369326	0.311069
53	-0.398690	-2.718130	-1.507481	53	-2.052888	-2.922270	-0.597366
6	1.305630	-1.157568	-0.035761	6	0.963384	-0.089245	1.399165
6	1.224902	-1.529497	1.297465	6	-0.219834	0.412578	1.973924
6	2.410818	-1.713179	2.009952	6	-1.085673	-0.466990	2.635498
6	3.639669	-1.555159	1.380499	6	-0.710189	-1.797349	2.849289
6	3.691910	-1.200346	0.035198	6	0.490574	-2.261336	2.336458
6	2.518799	-0.998015	-0.685014	6	1.316984	-1.421431	1.588132
1	0.268452	-1.698655	1.781387	1	-0.440494	1.474023	1.931237
1	2.359015	-1.993892	3.055934	1	-1.991311	-0.073910	3.083035
1	4.557386	-1.711556	1.934709	1	-1.365487	-2.459980	3.399734
1	4.647024	-1.064424	-0.458661	1	0.786237	-3.291350	2.492246
1	2.558088	-0.714365	-1.729937	1	2.235929	-1.806651	1.164774
16	0.428878	1.908456	-0.610814	16	1.942580	1.089457	0.484929
6	2.116966	1.985475	-0.089709	6	3.534336	0.280176	0.383746
6	2.448290	1.781168	1.253106	6	4.514676	0.580697	1.327590
6	3.137170	2.246587	-1.009501	6	3.797660	-0.616393	-0.651908
6	3.774351	1.830506	1.664102	6	5.765726	-0.020271	1.232825
1	1.659023	1.566989	1.965510	1	4.295701	1.278130	2.126998
6	4.462417	2.305110	-0.592541	6	5.050973	-1.215009	-0.736780
1	2.882855	2.396805	-2.052445	1	3.011626	-0.864134	-1.357075
6	4.786651	2.093412	0.744753	6	6.034328	-0.915175	0.200908
1	4.018640	1.655120	2.705792	1	6.529791	0.211081	1.965014
1	5.243849	2.508050	-1.316062	1	5.256661	-1.916570	-1.536230

1	5.820292	2.130494	1.068018	1	7.010065	-1.380522	0.128894
16	-2.655536	0.312811	-0.546468	16	-1.774626	1.227888	-1.391853
6	-2.327671	-0.299863	1.103918	6	-1.873089	2.426315	-0.077752
6	-1.682762	0.506689	2.054511	6	-0.942580	3.464498	0.042142
6	-2.692698	-1.602204	1.474973	6	-2.856703	2.298346	0.914179
6	-1.393607	0.019474	3.324990	6	-0.977110	4.328330	1.134306
1	-1.382271	1.510322	1.777852	1	-0.180569	3.584240	-0.720106
6	-2.399939	-2.086106	2.744388	6	-2.890344	3.163185	2.001303
1	-3.192559	-2.234845	0.750878	1	-3.603935	1.517706	0.819050
6	-1.746080	-1.280429	3.675335	6	-1.943620	4.178491	2.124714
1	-0.886974	0.658403	4.039216	1	-0.238683	5.118376	1.212423
1	-2.683836	-3.098478	3.007923	1	-3.656908	3.039887	2.758137
1	-1.516891	-1.662694	4.662619	1	-1.963952	4.846415	2.977010
19	-2.318603	3.647298	-0.590280	19	1.161408	1.292467	-2.797749
8	-3.913430	2.737137	1.369101	8	-0.411566	3.350131	-3.394830
1	-3.719919	2.634034	2.305144	1	-0.563581	4.297542	-3.350690
8	-1.497436	2.768919	-3.007624	8	0.858855	-1.234727	-2.090143
1	-1.882675	1.961203	-3.360065	1	0.911550	-2.047187	-2.602717
1	-3.893466	1.837575	1.015186	1	-1.149591	2.941016	-2.916152
1	-0.621386	2.503960	-2.690424	1	0.151869	-1.411447	-1.454863
VI-RC_{RE} E = -4514.3020647 (-4514.3516302) Nimag = 0 Tc = 0.351231				VI-TS_{RE} E = -4514.2984466 (-4514.3484266) Nimag = 1(-157.33) Tc = 0.351759			
29	0.169773	-0.494447	-0.689273	29	-0.139026	0.736023	-0.715674
6	-1.511975	0.417827	-0.709640	6	1.329405	-0.548114	-0.685854
6	-1.985376	0.853833	-1.935795	6	1.829252	-0.950211	-1.915859
6	-3.212206	1.518379	-1.988761	6	3.125511	-1.459543	-1.981711
6	-3.941883	1.735886	-0.825689	6	3.889992	-1.580724	-0.826705
6	-3.449825	1.287623	0.397555	6	3.373393	-1.164153	0.397907
6	-2.227992	0.622790	0.458007	6	2.087311	-0.642709	0.474660
1	-1.421312	0.690737	-2.847906	1	1.215532	-0.901184	-2.808137
1	-3.589810	1.864504	-2.944626	1	3.524005	-1.777264	-2.938504
1	-4.892598	2.254191	-0.870886	1	4.889941	-1.994676	-0.880038
1	-4.012807	1.454502	1.309094	1	3.974255	-1.234043	1.297199
1	-1.846238	0.274593	1.413156	1	1.676874	-0.329349	1.429762
16	1.169472	1.483994	-0.243344	16	-0.891643	-1.354975	-0.422961
6	0.044224	2.708620	0.378493	6	-0.034776	-2.767070	0.247548
6	-0.612362	3.569394	-0.504480	6	0.526307	-3.706868	-0.618241
6	-0.174861	2.846977	1.751380	6	0.032064	-2.965579	1.626368
6	-1.488264	4.534536	-0.023227	6	1.164974	-4.828733	-0.103828
1	-0.443694	3.463876	-1.569345	1	0.470255	-3.545217	-1.687951
6	-1.046088	3.819086	2.231272	6	0.668170	-4.092627	2.135709
1	0.327196	2.183212	2.445255	1	-0.393330	-2.234008	2.302119
6	-1.710568	4.661464	1.345636	6	1.239042	-5.023325	1.273159
1	-2.000416	5.188128	-0.719981	1	1.603384	-5.552657	-0.780475
1	-1.209780	3.912688	3.298614	1	0.720246	-4.239627	3.207859
1	-2.395342	5.413505	1.719275	1	1.736838	-5.898820	1.672080
16	-0.957408	-2.473368	-0.822225	16	1.077886	2.750526	-0.642940

6	-2.660695	-2.333363	-0.336197	6	2.749250	2.344077	-0.206059
6	-3.033850	-2.545242	0.994120	6	3.175946	2.440750	1.123753
6	-3.643922	-2.028054	-1.280313	6	3.667649	1.933501	-1.176798
6	-4.366695	-2.433782	1.375264	6	4.487189	2.135363	1.472114
1	-2.275606	-2.778688	1.733138	1	2.469583	2.750633	1.886160
6	-4.973527	-1.912840	-0.894641	6	4.976303	1.624740	-0.825176
1	-3.355649	-1.862974	-2.311439	1	3.343883	1.848436	-2.207558
6	-5.339504	-2.111356	0.434470	6	5.393628	1.724677	0.499129
1	-4.642140	-2.595776	2.410944	1	4.799274	2.216763	2.507225
1	-5.726361	-1.664603	-1.634026	1	5.671416	1.295545	-1.589649
1	-6.376817	-2.019125	0.733504	1	6.414583	1.482282	0.770032
16	2.141702	-1.760685	-0.878693	16	-2.157756	1.943856	-0.924196
6	3.585903	-0.720983	-0.934736	6	-3.564677	0.856684	-0.909078
6	4.642195	-0.948686	-0.043469	6	-4.626841	1.096434	-0.025239
6	3.719394	0.301889	-1.880842	6	-3.661338	-0.236078	-1.779873
6	5.790196	-0.161841	-0.083961	6	-5.738734	0.259233	-0.000834
1	4.569531	-1.756338	0.677979	1	-4.579109	1.948182	0.645614
6	4.866479	1.085628	-1.917709	6	-4.773834	-1.069885	-1.753012
1	2.916205	0.480335	-2.585849	1	-2.860165	-0.424261	-2.484577
6	5.905426	0.862449	-1.017557	6	-5.816445	-0.830990	-0.862076
1	6.595077	-0.356441	0.615262	1	-6.546851	0.466460	0.691164
1	4.949357	1.874510	-2.656430	1	-4.825399	-1.909770	-2.436299
1	6.797743	1.475815	-1.048739	1	-6.682101	-1.481773	-0.844555
19	2.479489	-0.221667	2.207662	19	-2.483359	0.166582	2.053780
8	0.182148	-1.752737	2.271543	8	-0.098534	1.546236	2.221586
1	0.845551	-2.438944	2.443554	1	-0.725791	2.244996	2.464789
8	2.679663	-2.941322	2.070105	8	-2.528656	2.886959	2.128669
1	3.187283	-3.715255	2.330536	1	-3.009450	3.652597	2.455213
1	2.588079	-2.976198	1.102076	1	-2.465662	2.983989	1.161264
1	-0.221278	-2.043607	1.440095	1	0.362654	1.933843	1.459470
VI-PCRE							
E = -4514.346925 (-4514.4052455)							
Nimag = 0							
Tc = 0.348441							
29	-0.594201	-1.052826	-0.626482				
6	0.117192	1.026295	-1.078563				
6	0.316828	1.098791	-2.469598				
6	-0.771278	1.197631	-3.319637				
6	-2.069835	1.278689	-2.801462				
6	-2.278214	1.232270	-1.434137				
6	-1.191807	1.069940	-0.560337				
1	1.328264	1.100375	-2.856590				
1	-0.610372	1.246576	-4.389494				
1	-2.911810	1.393834	-3.472841				
1	-3.277284	1.316704	-1.022686				
1	-1.346413	1.154602	0.511007				
16	1.523608	1.218680	0.014531				
6	1.261497	2.884166	0.615387				
6	0.516206	3.837899	-0.076266				

6	1.903625	3.226886	1.805707
6	0.406565	5.126433	0.437228
1	0.020205	3.583098	-1.005432
6	1.796941	4.520703	2.302972
1	2.481926	2.484209	2.344428
6	1.044701	5.473894	1.623591
1	-0.178239	5.862754	-0.101079
1	2.297788	4.778405	3.228423
1	0.955476	6.479235	2.016190
16	-2.445821	-2.387333	-0.063758
6	-3.709832	-1.166140	0.177993
6	-3.683210	-0.296445	1.275962
6	-4.755682	-1.035176	-0.743131
6	-4.645047	0.697003	1.424259
1	-2.886276	-0.394026	2.006163
6	-5.721187	-0.044804	-0.591560
1	-4.792062	-1.705056	-1.594569
6	-5.667770	0.833600	0.487743
1	-4.595400	1.366309	2.275793
1	-6.514934	0.044565	-1.324808
1	-6.415347	1.609222	0.601932
16	1.225713	-2.546847	-0.519219
6	2.767621	-1.759671	-0.915196
6	3.805627	-1.704911	0.023577
6	2.975922	-1.173254	-2.169228
6	4.994621	-1.043459	-0.266902
1	3.683103	-2.197583	0.983408
6	4.165206	-0.513567	-2.458095
1	2.193215	-1.240289	-2.916613
6	5.177375	-0.433454	-1.505087
1	5.781582	-1.007465	0.478018
1	4.301289	-0.061201	-3.434309
1	6.101870	0.084443	-1.729254
19	1.399433	-0.987373	2.498671
8	-0.805074	-2.485038	2.819516
1	-0.188280	-3.226703	2.737524
8	1.719176	-3.674572	2.388186
1	2.220841	-4.460072	2.622344
1	1.677269	-3.645568	1.413419
1	-1.389026	-2.549339	2.044475