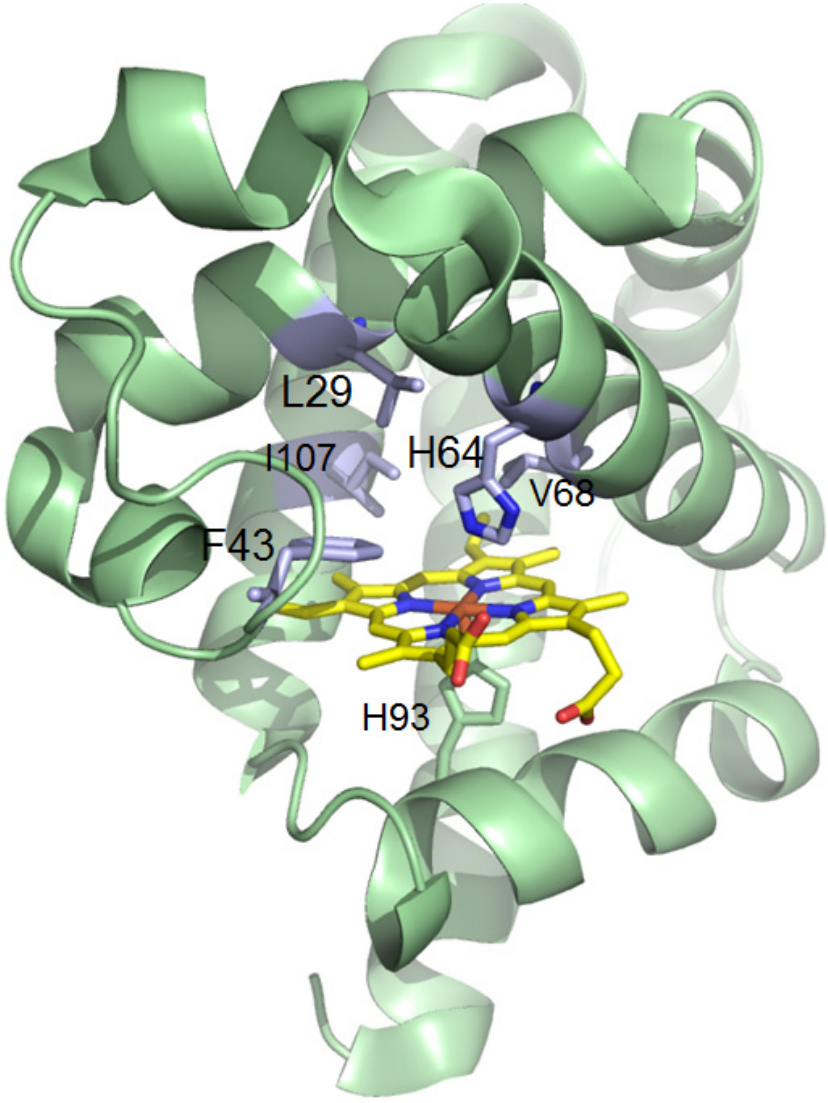
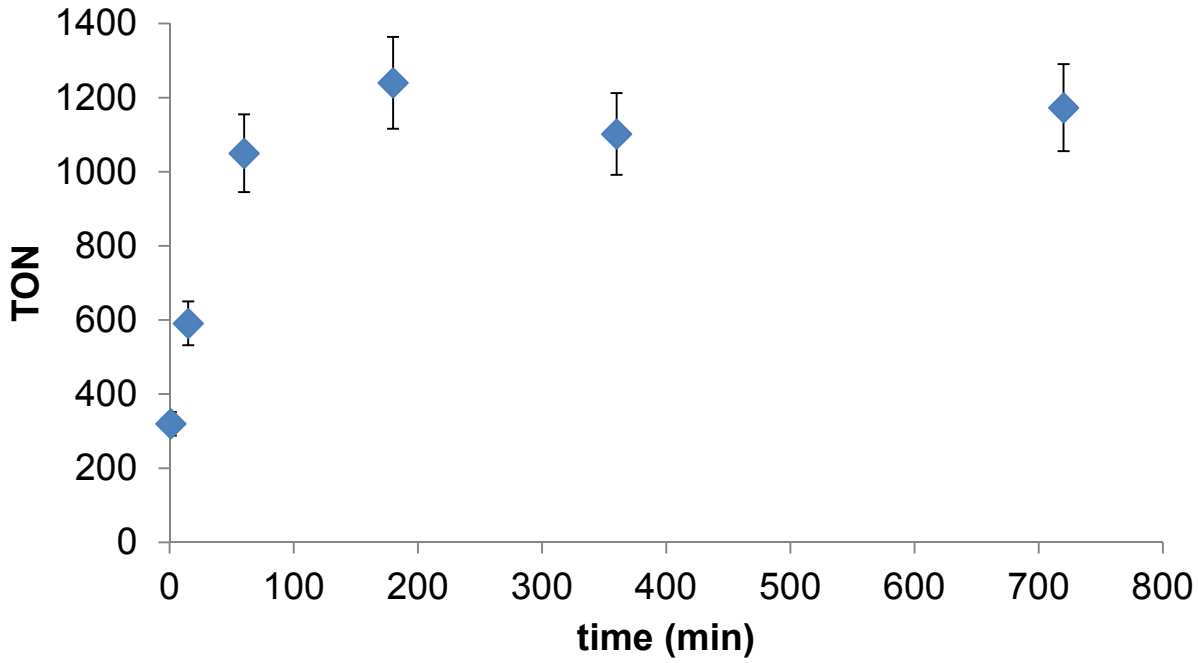
Table of contents:

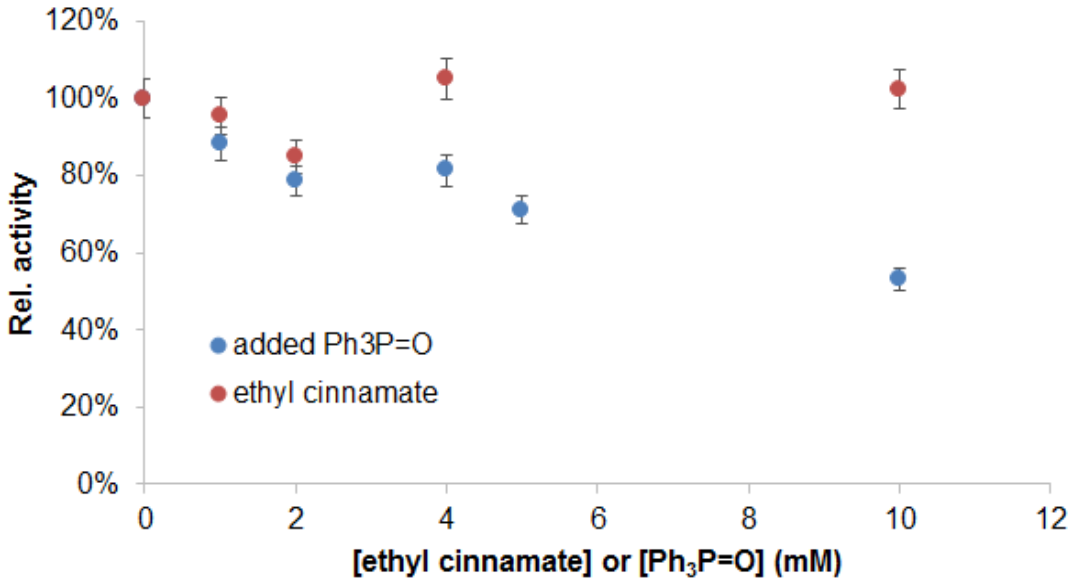
Supplementary Figure S1. Crystal structure of wild-type sperm whale myoglobin (pdb 1A6K). Residues targeted for mutagenesis (**Figure 1**) are highlighted in blue and displayed as stick models. The heme cofactor is colored in yellow.



Supplementary Figure S2: Time-course analysis of Mb(F43V,V68F)-catalyzed formation of ethyl cinnamate (**3a**) from benzaldehyde (**1**) in the presence of triphenylarsine and EDA (**2a**). Conversion was determined by gas chromatography using calibration curves with isolated **3a**. Reaction conditions: 1 μM Mb(F43V,V68F), 10mM benzaldehyde, 10 mM triphenylarsine, 10 mM EDA, 10 mM dithionite in oxygen-free phosphate buffer (pH 8.0).



Supplementary Figure S3: Product inhibition effects inMb(F43V,V68F)-catalyzed conversion of benzaldehyde (**1**) to ethyl cinnamate (**3a**) in the presence of $AsPh_3$ and EDA. The reaction mixtures (1 μM Mb(F43V,V68F), 10 mM benzaldehyde, 10 mM $AsPh_3$, 10 mM EDA, 10 mM dithionite in oxygen-free phosphate buffer at pH 8.0) were added with increasing amounts ofethyl cinnamate or phosphine oxide (0-10 mM). TON values were determined by GC and normalized to TON values in the absence of added ethyl cinnamate or phosphine oxide.



Experimental Procedures

Reagents and Analytical Methods. All the chemicals and reagents were purchased from commercial suppliers (Sigma-Aldrich, Alfa Aesar) and used without any further purification, unless otherwise stated. All dry reactions were carried out under argon atmosphere in oven-dried glassware with magnetic stirring using standard gas-tight syringes, cannulae and septa. ^{1}H and ^{13}C NMR spectra were measured on Bruker DPX-400 (operating at 400 MHz for ^{1}H and 100 MHz for ^{13}C) or Bruker DPX-500 (operating at 500 MHz for ^{1}H and 125 MHz for ^{13}C). Tetramethylsilane (TMS) served as the internal standard (0 ppm) for ^{1}H NMR and $CDCl_3$ was used as the internal standard (77.0 ppm) for ^{13}C NMR. Silica gel chromatography purifications were carried out using AMD Silica Gel 60 230-400 mesh. Gas chromatography (GC) analyses were carried out using a Shimadzu GC-2010 gas chromatograph equipped with a FID detector and aChiral Cyclosil-B column (30 m x 0.25 mm x 0.25 μm film). Separation methodfor calculation of TON and TTN values: 1 μL injection, injector temp.: 200 ºC, detector temp: 300 ºC. Gradient: column temperature set at 80 ºC for 3 min, then to 160 ºC at 2.80 ºC/min, then to 165 ºC at 1 ºC/min, then to 245 ºC at 25 ºC/min. Total run time was 45.77 min.

Protein expression and purification. Wild-type Mb and the engineered Mb variants were expressed in *E. coli* BL21(DE3) cells as described previously (M. Bordeaux, V. Tyagi, R. Fasan, *Angew. Chem. Int. Ed.***2015**, 54, 1744–1748).Briefly, cells were grown in TB medium (ampicillin, 100 mg L^{-1}) at 37 °C (150 rpm) until OD_{600} reached 0.6. Cells were then induced with 0.25 mM β-D-1-thiogalactopyranoside (IPTG) and 0.3 mM δ-aminolevulinic acid (ALA). After induction, cultures were shaken at 150 rpm and 27 °C

and harvested after 20 h by centrifugation at 4000 rpm at 4 °C. After cell lysis by sonication, the proteins were purified by Ni-affinity chromatography using the following buffers: loading buffer (50 mM Kpi, 800 mM NaCl, pH 7.0), wash buffer 1 (50 mM Kpi, 800 mM NaCl, pH 6.2), wash buffer 2 (50 mM Kpi, 800 mM NaCl, 250 mM glycine, pH 7.0) and elution buffer (50 mM Kpi, 800 mM NaCl, 300 mM L-histidine, pH 7.0). After buffer exchange (50 mM Kpi, pH 7.0), the proteins were stored at +4 °C. Myoglobin concentration was determined using an extinction coefficient ε_{410} = 157 mM^{-1} cm^{-1}.[2]

Aldehyde olefination reaction. Initial reactions (**Table 1**) were carried out at a 400 µL scale using 20 µM myoglobin, 10 mM benzaldehyde, 10 mM EDA, 10 mM triphenylphosphine (or trialkyl phosphines, $AsPh_3$, $SbPh_3$, $BiPh_3$) and 10 mM sodium dithionite. In a typical procedure, a solution containing sodium dithionate (100 mM stock solution) in potassium phosphate buffer (50 mM, pH 8.0) was degassed by bubbling argon into the mixture for 4 min in a sealed vial. A buffered solution containing myoglobin was carefully degassed in a similar manner in a separate vial. The two solutions were then mixed together via cannula. Reactions were initiated by addition of 10 µL of benzaldehyde (from a 0.4 M stock solution in DMSO), 10 µL triphenylphosphine (from a 0.4 M stock solution in DMSO) of followed by the addition of 10µL of EDA (from a 0.4 M stock solution in DMSO) with a syringe, and the reaction mixture was stirred for 12 h at room temperature, under positive argon pressure. For the optimization of the benzaldehyde: triphenylarsine:EDA ratio, reactions were performed according to the general procedure described above, using 20 µM of protein, 10 mM of benzaldehyde and variable amounts of triphenylarsine and EDA (5 mM EDA to 20mM EDA). Optimization of the substrate loading was done in a similar manner, using 20 µM

Mb, variable quantities of benzaldehyde (from 1 to 40mM final concentration), and variable quantities of triphenylarsine and EDA (from 1 to 40 mM final concentration), maintaining an benzaldehyde: triphenylarsine: EDA ratio of 1:1:1 at all times. Enzyme concentration optimization was carried according to the general procedure along with varying the enzyme concentration from 20 μM to 1 μM of Mb(F43V V68F)and 10 mM benzaldehyde (10 μL of 0.4 M stock solution in DMSO), 10 mM triphenylarsine (10 μL of 0.4 M stock solution in DMSO) and 10 mM EDA (10 μL of 0.4 M stock solution in DMSO). Reactions for TON determination were carried out according to the general procedure described above using 1 μM Mb(F43V V68F), benzaldehyde (10 μL of 0.4 M stock solution in DMSO), 10 mM triphenylarsine (10 μL of 0.4 M stock solution in DMSO) and 10 mM EDA (10 μL of 0.4 M stock solution in DMSO).

Product analysis. The reactions were analyzed by adding 20 μL of internal standard (benzodioxole, 50 mM in methanol) to the reaction mixture, followed by extraction with 400 μL of dichloromethane and separated organic layer was analyzed by GC-FID (see **Reagents and Analytical Methods** section for details on GC analyses). Calibration curves for quantification of the different aldehyde olefination products were constructed using authentic standards prepared synthetically as described in **Synthetic Procedures**. Benzyl cinnamate (**3c**) was purchased from Sigma-Aldrich. All measurements were performed at least in duplicate. For each experiment, negative control samples containing either no enzyme or no reductant were included.

Synthetic Procedures:

Synthesis of authentic ethyl cinnamate and *tert*-butyl cinnamate products (procedure 1):

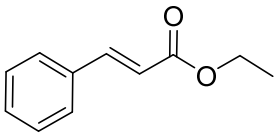
To a flame dried round bottom flask under argon, equipped with a stir bar was added aryl aldehydes (1 equiv.), triphenylphosphine (1.5 equiv.), and Fe(TPP)Cl (1.5 mol%) in toluene (4-5 mL). A solution of EDA or *t*-BDA (1.5 equiv) in 2-3 mL of toluene was added dropwise over approximately 5 min. The resulting mixture was stirred at 80^{o}C for overnight. The solvent was removed under vacuum and the crude mixture was purified by 9:1 hexanes to diethyl ether using flash chromatography to obtained aryl substituted ethyl cinnamate or *tert*-butyl cinnamate products. The identity of the ethyl cinnamate or *tert*-butyl cinnamate products was determined using GC-MS, ^{1}H and ^{13}C NMR.

Synthesis of authentic standard for aryl substituted cyclohexyl cinnamate products (procedure 2):

To a flame dried round bottom flask under argon, equipped with a stir bar was added cinnamic acid (1 equiv.) and the cyclohexanol (1.2 equiv.) in THF (10 mL). After addition of DCC (1.2 equiv.) and DMAP (catalytic amount), the resulting mixture was stirred at room temperature until complete disappearance of the starting material. After evaporation and column chromatography on silica gel in 9:1 hexanes to diethyl ether using flash chromatography the desired product was obtained.

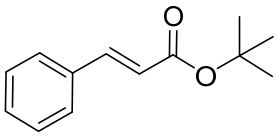
Compound Characterization Data:

Ethyl cinnamate (3a)



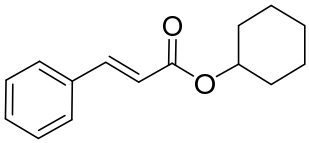
Following the standard procedure 1, 89% yield, GC-MS m/z (% relative intensity): 176(29.0), 148(15.9), 131(100), 103(48.3); ^{1}H NMR ($CDCl_3$, 500 MHz): δ 7.70 (d, J = 16 Hz, 1H), 7.51-7.50 (m, 2H), 7.37-7.36 (m, 3H), 6.45 (d, J = 16 Hz, 1H), 4.28 (q, J = 7.0 Hz, 2H), 1.34 (t, J = 7.0 Hz, 3H) ppm, ^{13}C NMR ($CDCl_3$, 125 MHz): δ 166.9, 144.5, 134.5, 130.2, 128.8, 128.0, 118.3, 60.4, 14.3 ppm.

Cyclohexyl cinnamate (3b)



Following the standard procedure 1, 72% yield, GC-MS m/z (% relative intensity): 204(7.9), 147(100), 131(65.2), 103(31.8); ^{1}H NMR ($CDCl_3$, 500 MHz): δ 7.61 (d, J =16 Hz, 1H), 7.50-7.49 (m, 2H), 7.36-7.35 (m, 3H), 6.39 (d, J = 16 Hz, 1H), 1.54 (s, 9H) ppm, ^{13}C NMR ($CDCl_3$, 125 MHz): δ 166.3, 143.5, 134.7, 129.9, 128.8, 127.9, 120.2, 80.4, 28.2 ppm.

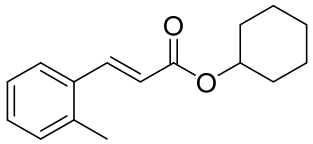
Cyclohexyl cinnamate (3d)



Following the standard procedure 2, 86% yield, GC-MS m/z (% relative intensity): 230(3.6), 149(37.7), 131(100), 103(38.7); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.69 (d, J = 16.0

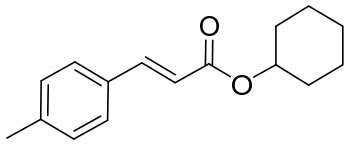
Hz, 1H), 7.51-7.50 (m, 2H) 7.37-7.35 (m, 3H), 6.45 (d, J = 16 Hz, 1H), 4.92-4.87 (m, 1H), 1.92-1.91 (m, 2H), 1.78-1.75 (m, 2H), 1.58-1.27 (m, 6H) ppm, ^{13}C NMR ($CDCl_3$, 100 MHz): δ 166.1, 144.0, 134.3, 129.8, 128.6, 127.7, 118.7, 72.4, 31.5, 25.2, 23.6 ppm.

(E)-Cyclohexyl 3-(o-tolyl)acrylate (5b)



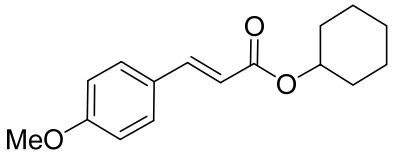
Following the standard procedure 2, 68% yield, GC-MS m/z (% relative intensity): 244(5.7), 162(28.1), 145(100), 116(68.4); ^1H NMR ($CDCl_3$, 400 MHz): δ 7.98 (d, J = 16 Hz 1H), 7.55 (d, J = 7.5 Hz, 1H), 7.26-7.17 (m, 3H), 6.37 (d, J = 16 Hz, 1H), 4.92-4.88 (m, 1H), 2.43 (s, 3H), 1.92-1.76 (m, 2H), 1.58-1.55 (m, 2H), 1.54-1.31 (m, 6H) ppm, ^{13}C NMR ($CDCl_3$, 100 MHz): δ 166.5, 141.9, 137.5, 133.5, 130.7, 129.8, 126.4, 126.3, 119.9, 72.6, 31.7, 25.5, 23.8, 19.7 ppm.

(E)-Cyclohexyl 3-(4-methyl-phenyl)acrylate (6b)



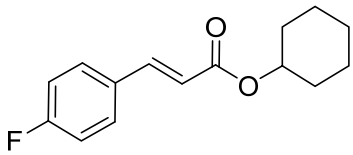
Following the standard procedure 2, 70% yield, GC-MS m/z (% relative intensity): 246(13.0), 164(100), 147(69.4), 120(18.4); ^1H NMR ($CDCl_3$, 400 MHz): δ 7.66 (d, J = 15.6 Hz, 1H), 7.42 (d, J = 6.0 Hz, 2H), 7.18 (d, J = 5.6 Hz, 2H), 6.40 (d, J = 15.6 Hz, 1H), 4.89-4.88 (m, 1H), 2.36 (s, 3H), 2.00 (m, 2H), 1.90 (m, 2H), 1.58-1.26 (m, 6H) ppm, ^{13}C NMR ($CDCl_3$, 100 MHz): δ 166.4, 144.0, 140.2, 131.6, 129.3, 127.7, 117.6, 72.4, 31.5, 25.2, 23.6, 21.2 ppm.

(E)-Cyclohexyl 3-(4-methoxy-phenyl)acrylate (7b)



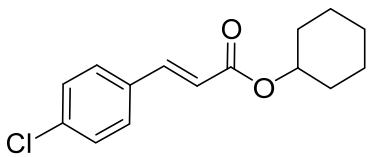
Following the standard procedure 2, 71% yield, GC-MS m/z (% relative intensity): 260(25.4), 178(100), 161(74.8), 134(42.8); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.64 (d, J = 16 Hz, 1H), 7.48 (d, J = 8.4 Hz, 2H), 6.90 (d, J = 8.4 Hz, 2H), 6.32 (d, J = 16 Hz, 1H), 4.90-4.84 (m, 1H), 3.82 (s, 3H), 1.91-1.90 (m, 2H), 1.78-1.75 (m, 2H), 1.58-1.27 (m, 6H) ppm, ^{13}C NMR ($CDCl_3$, 100 MHz): δ 166.5, 161.0, 143.6, 129.4, 127.1, 116.2, 114.0, 72.2, 55.1, 31.5, 25.2, 23.6 ppm.

(E)-Cyclohexyl 3-(4-fluoro-phenyl)acrylate (8b)



Following the standard procedure 2, 62% yield, GC-MS m/z (% relative intensity): 248(3.1), 166(61.9), 149(100), 28.8(121), 101(30.5); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.64 (d, J = 16 Hz, 1H), 7.51-7.48 (m, 2H), 7.08-7.04 (m, 2H), 6.37 (d, J = 16 Hz, 1H), 4.89-4.86 (m, 1H), 1.91-1.89 (m, 2H), 1.76-1.75 (m, 2H), 1.57-1.25 (m, 6H) ppm, ^{13}C NMR ($CDCl_3$, 100 MHz): δ 166.0, 142.7, 130.6, 129.6, 129.5, 118.4, 115.8, 115.6, 72.5, 31.5, 25.2, 23.6 ppm.

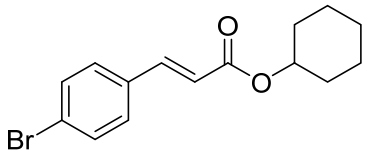
(E)-Cyclohexyl 3-(4-chloro-phenyl)acrylate (9b)



Following the standard procedure 2, 76% yield, GC-MS m/z (% relative intensity): 264(5.7), 182(86.8), 165(100), 137(33.1), 102(42.0); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.62 (d, J =16 Hz, 1H), 7.46 (d, J = 8.4 Hz, 2H), 7.36 (d, J = 7.6 Hz, 2H), 6.42 (d, J = 16 Hz,

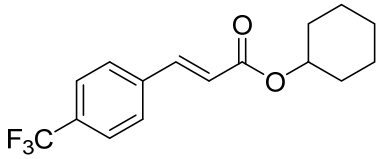
1H), 4.90-4.86 (m, 1H), 1.91-1.90 (m, 2H), 1.78-1.75 (m, 2H), 1.56-1.25 (m, 6H) ppm, ^{13}C NMR ($CDCl_3$, 100 MHz): δ 165.9, 142.5, 135.7, 132.8, 129.0, 128.9, 119.2, 72.7, 31.5, 25.2, 23.6 ppm.

(E)-Cyclohexyl 3-(4-bromo-phenyl)acrylate (10b)



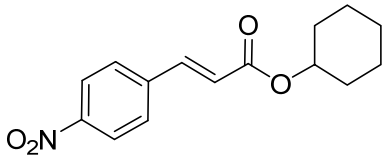
Following the standard procedure 2, 82% yield, GC-MS m/z (% relative intensity): 308(4.1), 226(73.1), 209(59.5), 102(100); ^1H NMR ($CDCl_3$, 400 MHz): δ 7.61(d, J = 16 Hz, 1H), 7.51 (d, J = 8.4 Hz, 2H), 7.39 (d, J = 8.4 Hz, 2H), 6.43 (d, J = 16 Hz, 1H), 4.90-4.85 (m, 1H), 1.91-1.90 (m, 2H), 1.78-1.75 (m, 2H), 1.60-1.25 (m, 6H) ppm, ^{13}C NMR ($CDCl_3$, 100 MHz): δ 165.9, 142.6, 133.2, 131.8, 129.1, 124.1, 119.4, 72.6, 31.5, 25.2, 23.5 ppm.

(E)-Cyclohexyl 3-(4-(trifluoromethyl)phenyl)acrylate (11b)



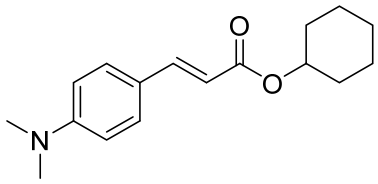
Following the standard procedure 2, 72% yield, GC-MS m/z (% relative intensity):217(73.8), 199(100), 171(30.4), 151(45.7);^1H NMR ($CDCl_3$, 400 MHz): δ 7.69-7.63 (m, 5H), 6.52 (d, J = 16 Hz, 1H), 4.90 (m, 1H), 1.91 (m, 2H), 1.76 (m, 2H), 1.58-1.25 (m, 6H) ppm, ^{13}C NMR ($CDCl_3$, 100 MHz): δ 165.6, 142.1, 137.7, 127.8, 125.5, 121.3, 72.9, 31.5, 25.1, 23.5 ppm.

(E)-Cyclohexyl 3-(4-nitro-phenyl)acrylate (12b)



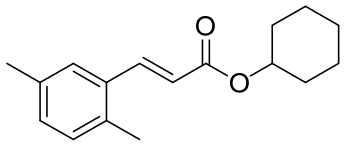
Following the standard procedure 2, 55% yield, GC-MS m/z (% relative intensity): 194(85.8), 176(100), 130(37.9), 102(44.1); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.24 (d, J = 7.2 Hz, 2H), 7.70-7.65 (m, 3H), 6.57 (d, J = 16 Hz, 1H), 4.91-4.90 (m, 1H), 1.90 (m, 2H), 1.75 (m, 2H), 1.58-1.25 (m, 6H) ppm, ^{13}C NMR ($CDCl_3$, 100 MHz): δ 165.2, 148.2 141.0, 140.5, 128.3, 123.9, 123.0, 73.1, 31.4, 25.1, 23.5 ppm.

(E)-Cyclohexyl 3-(4-(dimethylamino)-phenyl)acrylate (13b)



Following the standard procedure 2, 62% yield, GC-MS m/z (% relative intensity):273(54.9), 191(100), 174(34.2), 147(49.9); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.62 (d, J = 15.6 Hz, 1H), 7.42 (d, J = 8.8 Hz, 2H), 6.66 (d, J = 8.4 Hz, 2H), 6.23 (d, J = 15.6 Hz, 1H), 4.89-4.84 (m, 1H), 2.99 (s, 6H), 1.92-1.91 (m, 2H), 1.78-1.76 (m, 2H), 1.58-1.26 (m, 6H) ppm, ^{13}C NMR ($CDCl_3$, 100 MHz): δ 167.1, 151.4, 144.6, 129.4, 122.1, 112.9, 111.5, 71.9, 39.9, 31.6, 25.2, 23.7 ppm.

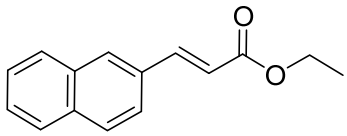
(E)-Cyclohexyl 3-(2,5-dimethylphenyl)acrylate (14b)



Following the standard procedure 2, 60% yield, GC-MS m/z (% relative intensity): 258(17.6), 176(52.8), 159(100), 130(94.9), 115(44.6);^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.96

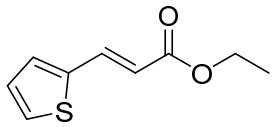
(d, J = 16 Hz, 1H), 7.35 (s, 1H), 7.05 (s, 2H), 6.37 (d, J = 15.6 Hz, 1H), 4.94-4.87 (m, 1H), 2.37 (s, 3H), 2.30 (s, 3H), 1.93-1.91 (m, 2H), 1.79-1.76 (m, 2H), 1.58-1.27 (m, 6H) ppm, ^{13}C NMR ($CDCl_3$, 100 MHz): δ 166.2, 141.9, 141.8, 135.3, 134.3, 132.9, 130.5, 130.4, 126.6, 119.2, 72.3, 31.5, 25.3, 23.6 ppm.

(E)-Ethyl 3-(naphthalen-2-yl)acrylate (15b)



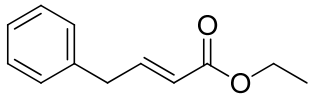
Following the standard procedure 2, 82% yield, GC-MS m/z (% relative intensity): 226(73.3), 198(14.7), 181(100), 152(92.5); ^{1}H NMR ($CDCl_3$, 500 MHz): δ 7.85-7.75 (m, 4H), 7.61 (d, J = 8.5 Hz, 1H), 7.49-7.45 (m, 2H), 6.55 (d, J = 16 Hz, 1H), 4.33 (q, J = 7.0 Hz, 2H), 1.38 (t, J = 7.0 Hz, 3H) ppm, ^{13}C NMR ($CDCl_3$, 125 MHz): δ 167.0, 144.6, 134.2, 133.3, 131.9, 129.9, 128.6, 128.5, 127.8, 127.2, 126.7, 123.5, 118.4, 60.5, 14.4 ppm.

(E)-Ethyl 3-(thiophen-2-yl)acrylate (16b)



Following the standard procedure 2, 75% yield, GC-MS m/z (% relative intensity): 182(35.4), 154(11.5), 137(100), 109(40.1);^{1}H NMR ($CDCl_3$, 500 MHz): δ 7.76 (d, J = 15.5 Hz, 1H), 7.32 (d, J = 4.5 Hz, 1H), 7.20 (d, J = 3.0 Hz, 1H), 7.01-6.99 (m, 1H), 6.22 (d, J = 15.5 Hz, 1H), 4.23 (q, J = 7.0 Hz, 2H), 1.30 (t, J = 7.5 Hz, 3H) ppm, ^{13}C NMR ($CDCl_3$, 125 MHz): δ 166.7, 139.5, 136.9, 130.8, 128.3, 128.0, 117.0, 60.4, 14.3 ppm.

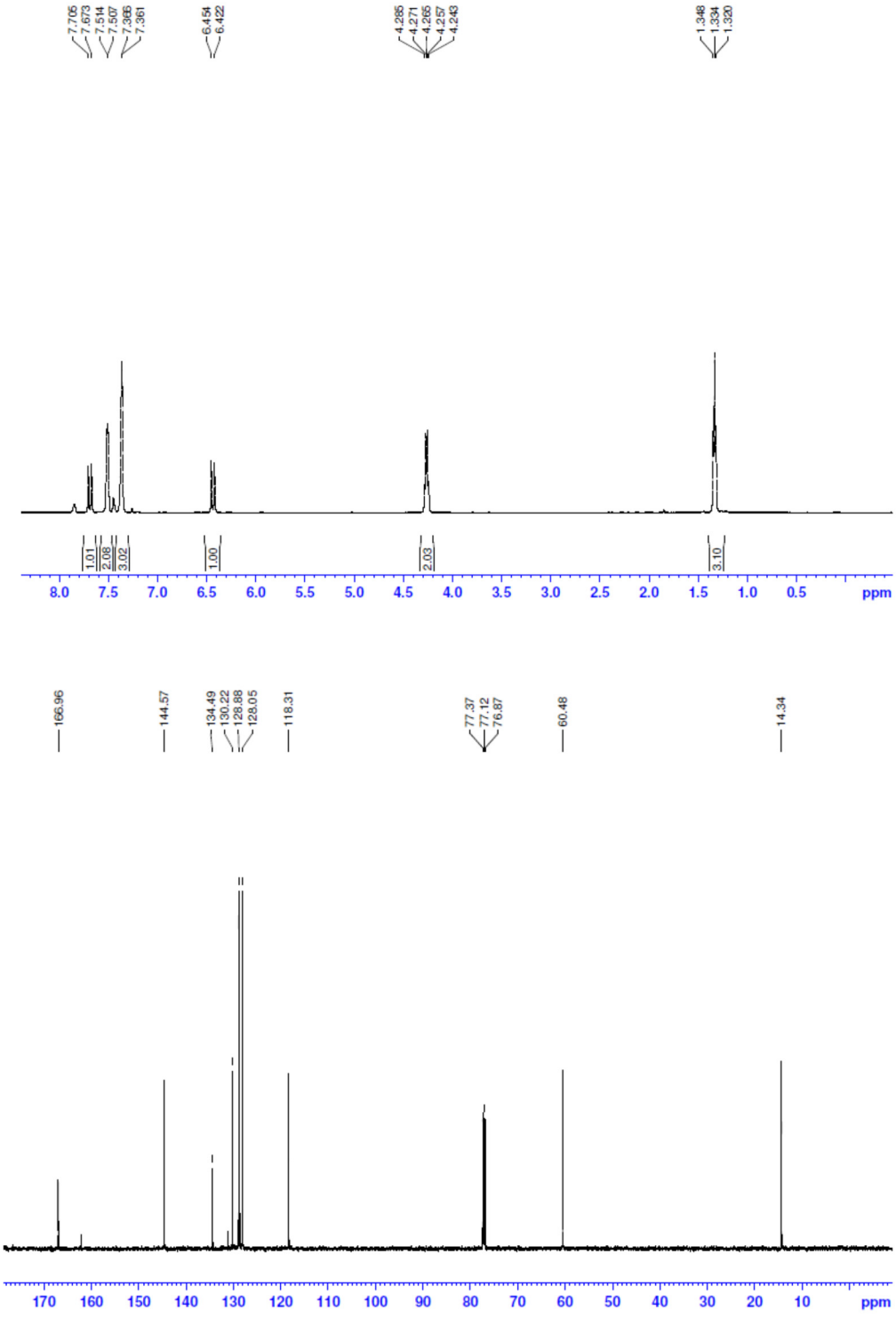
(E)-Ethyl 4-phenylbut-2-enoate (17b)



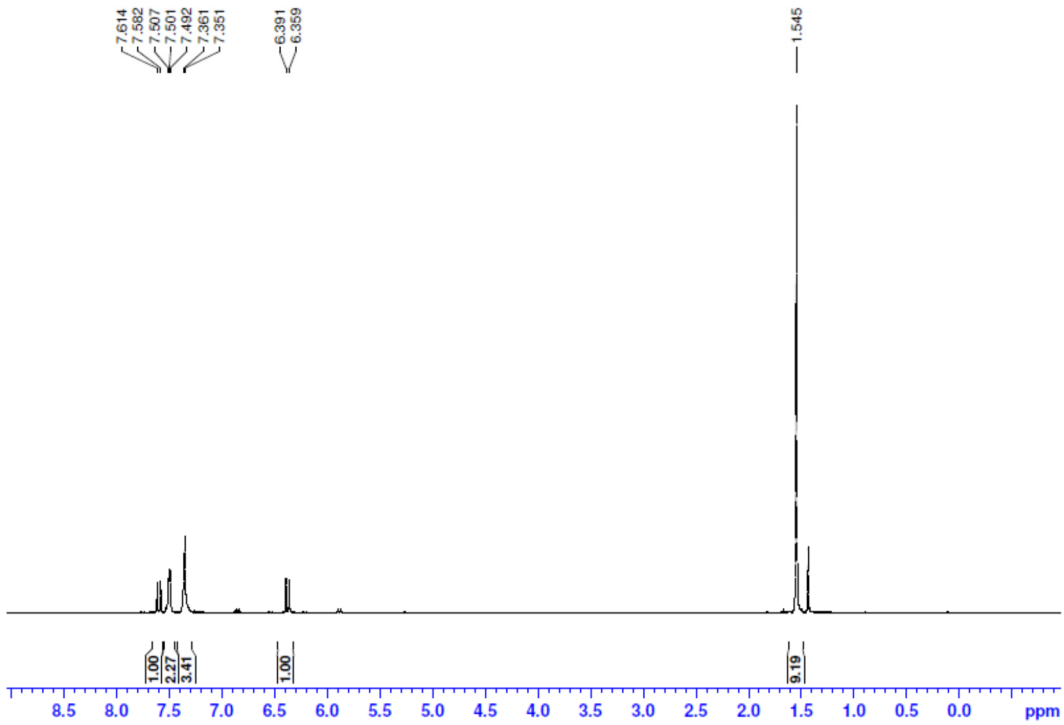
Following the standard procedure, % yield (67), GC-MS m/z (% relative intensity): 190(40.8), 145(39.0), 127(18.7), 117(100);^{1}H NMR ($CDCl_3$, 500 MHz): δ 7.33(t, J = 7.0 Hz, 2H), 7.26(t, J =7.5 Hz, 1H), 7.19 (d, J = 7.5 Hz, 2H), 7.14-7.08 (m, 1H), 5.84 (d, J = 15.5 Hz, 1H), 4.21(q, J = 7.0Hz, 2H), 3.53 (d, J = 6.5 Hz, 2H), 1.29 (t, J = 7.0 Hz, 3H) ppm, ^{13}C NMR ($CDCl_3$, 125 MHz): δ 166.4, 147.3, 137.7, 128.8, 128.7, 126.6, 122.4, 60.2, 38.4, 14.3 ppm.

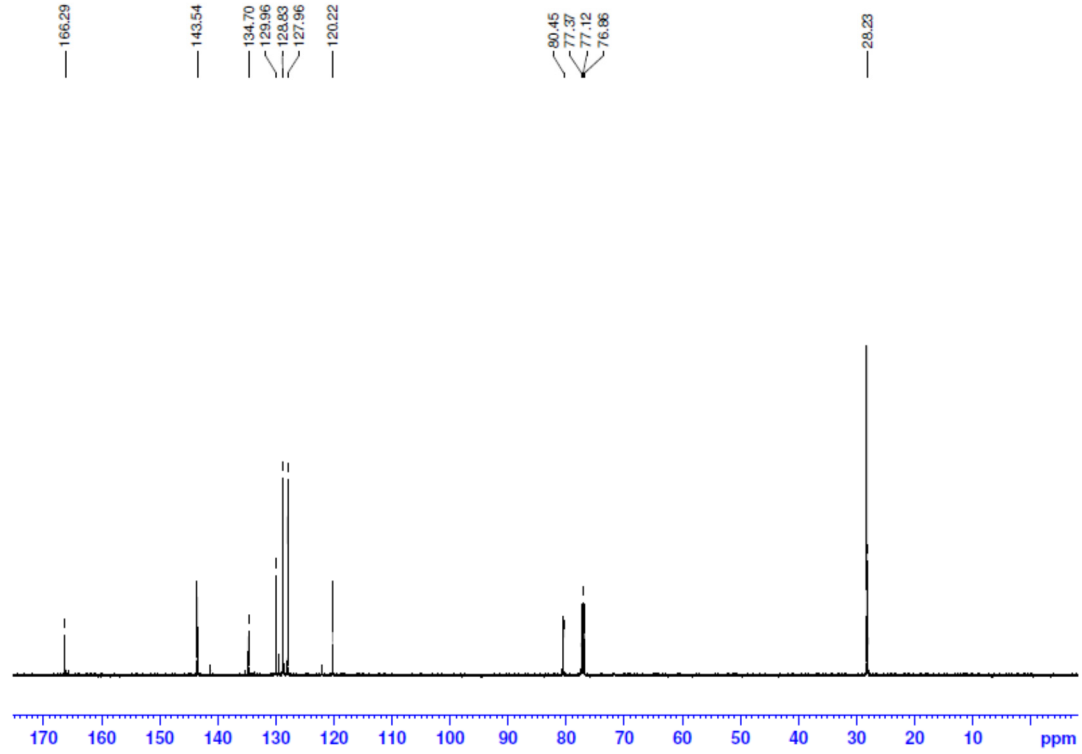
^{1}H and ^{13}C NMR spectra:

3a:

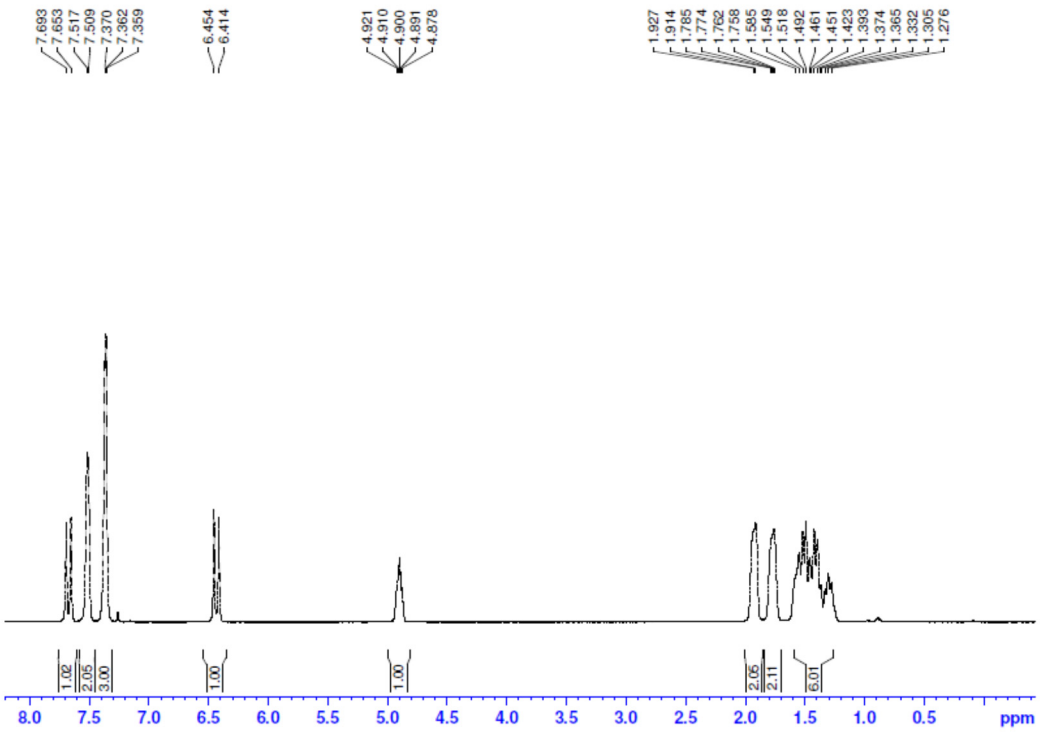


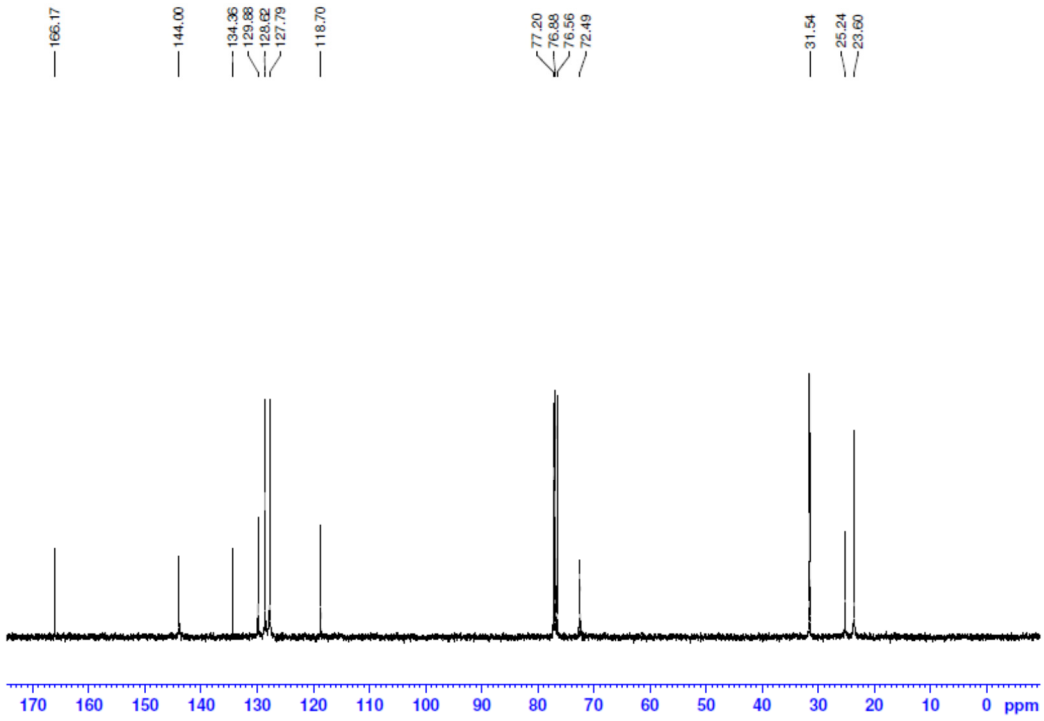
3b:


7.614
7.582
7.507
7.501
7.492
7.361
7.351
6.391
6.359
1.545
1.00
2.27
3.41
1.00
9.19
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm

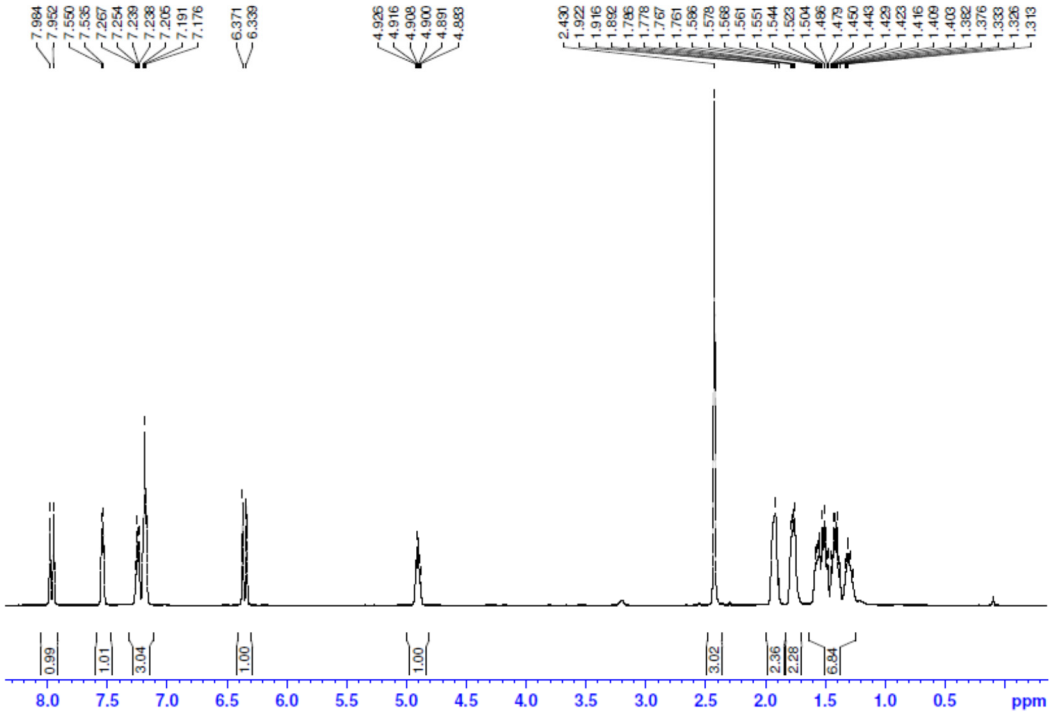

166.29
143.54
134.70
129.96
128.83
127.96
120.22
80.45
77.37
77.12
76.86
28.23
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

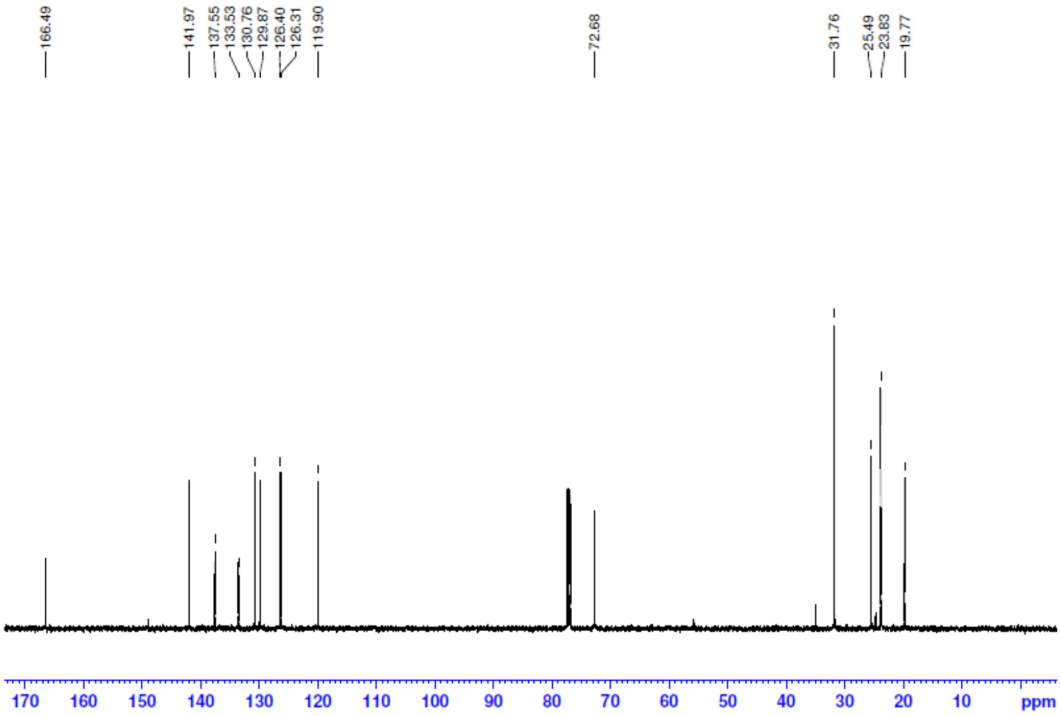
3d:


7.693
7.653
7.517
7.509
7.370
7.362
7.359
6.454
6.414
4.921
4.910
4.900
4.891
4.878
1.927
1.914
1.785
1.774
1.762
1.758
1.585
1.549
1.518
1.492
1.461
1.451
1.423
1.393
1.374
1.365
1.332
1.305
1.276
1.02
2.05
3.00
1.00
1.00
2.06
2.11
6.01
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm

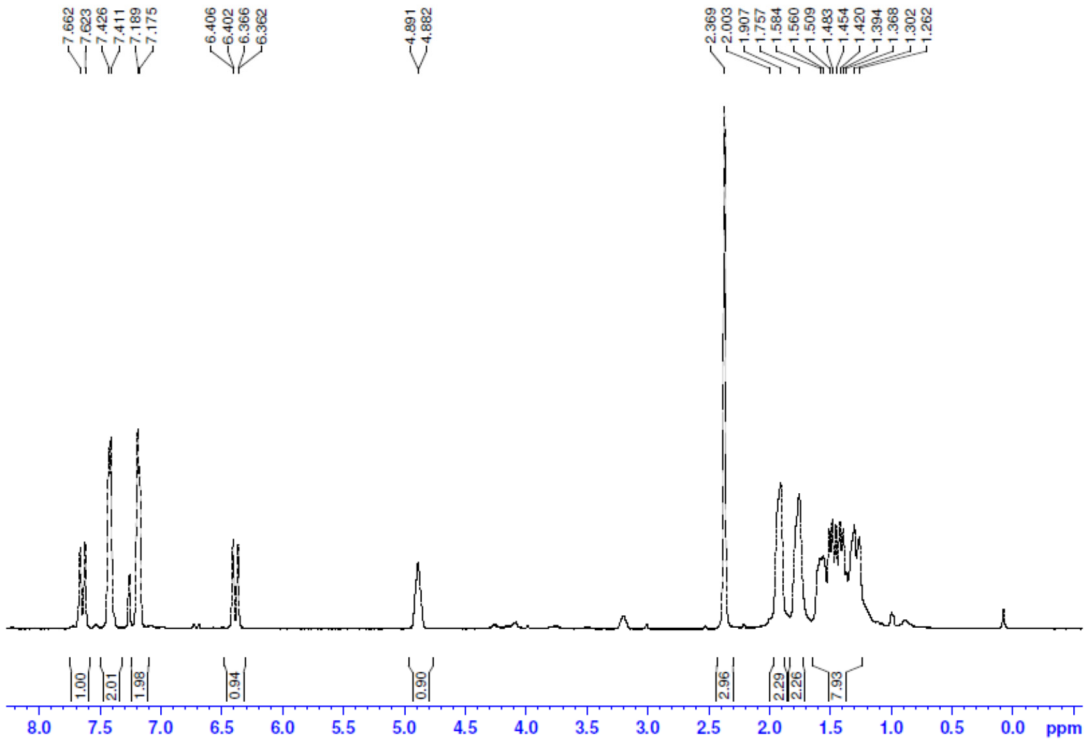

166.17
144.00
134.36
129.88
128.62
127.79
118.70
77.20
76.88
76.56
72.49
31.54
25.24
23.60
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

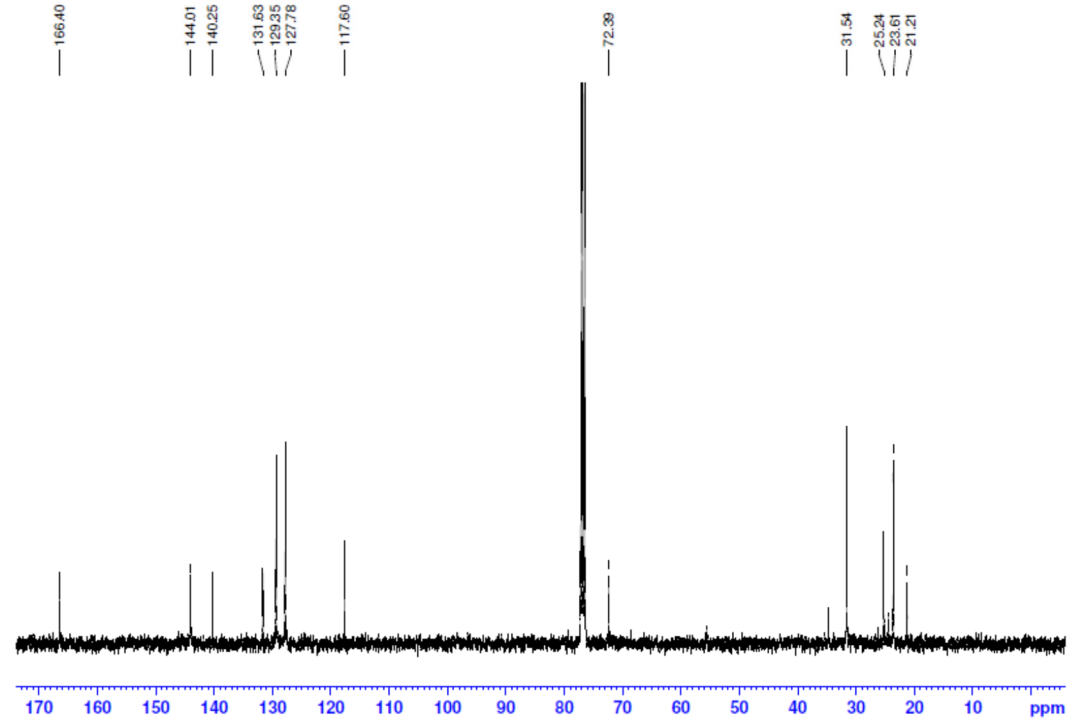
5b:


7.984
7.952
7.550
7.535
7.267
7.254
7.239
7.238
7.205
7.191
7.176
6.371
6.339
4.926
4.916
4.908
4.900
4.891
4.883
2.430
1.922
1.916
1.892
1.785
1.778
1.767
1.761
1.566
1.578
1.568
1.561
1.551
1.544
1.523
1.504
1.486
1.479
1.450
1.443
1.429
1.423
1.416
1.409
1.403
1.382
1.376
1.333
1.326
1.313
0.99
1.01
3.04
1.00
1.00
3.02
2.36
2.28
6.84
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm

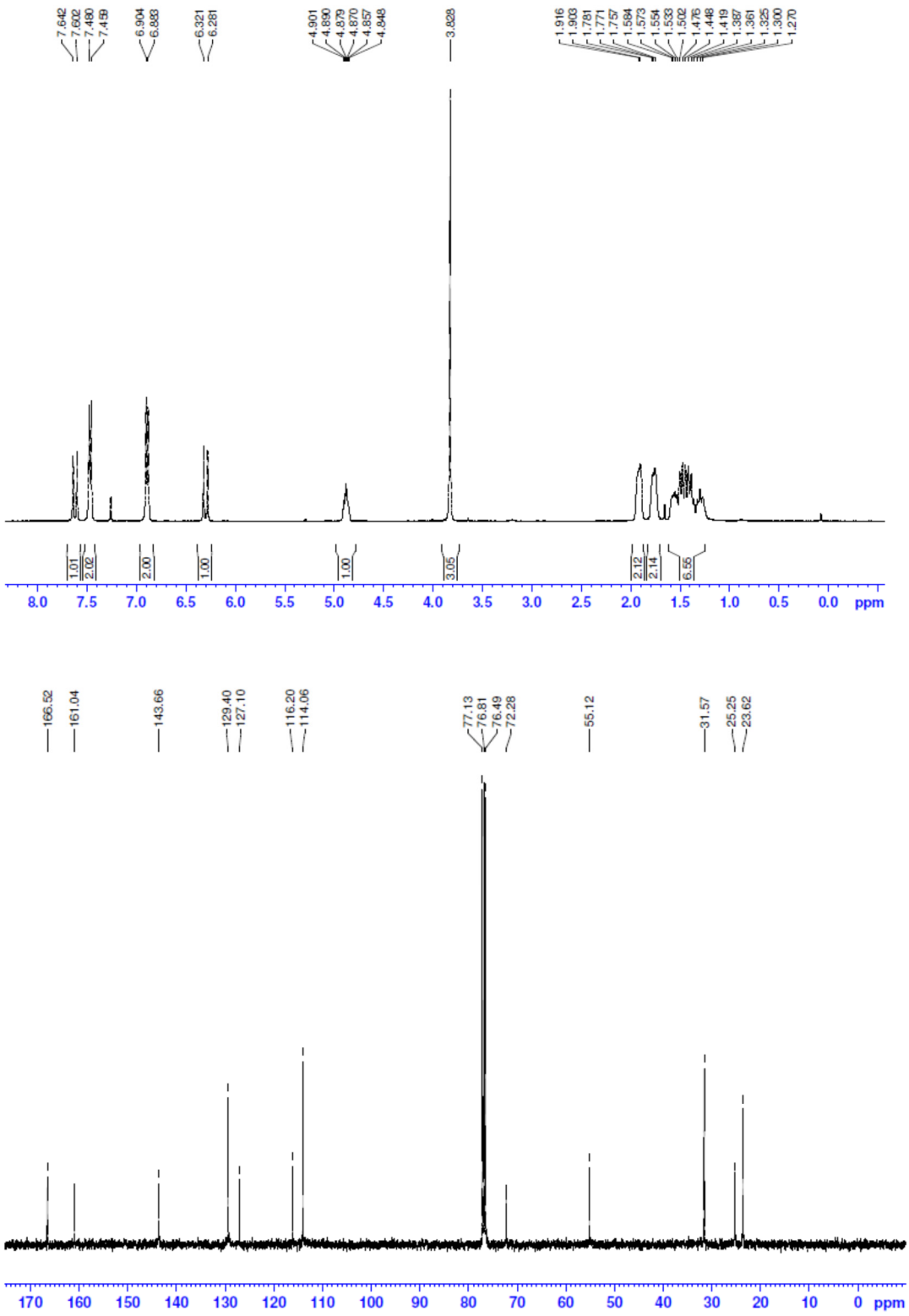

166.49
141.97
137.55
133.53
130.76
129.87
126.40
126.31
119.90
72.68
31.76
25.49
23.83
19.77
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

6b:

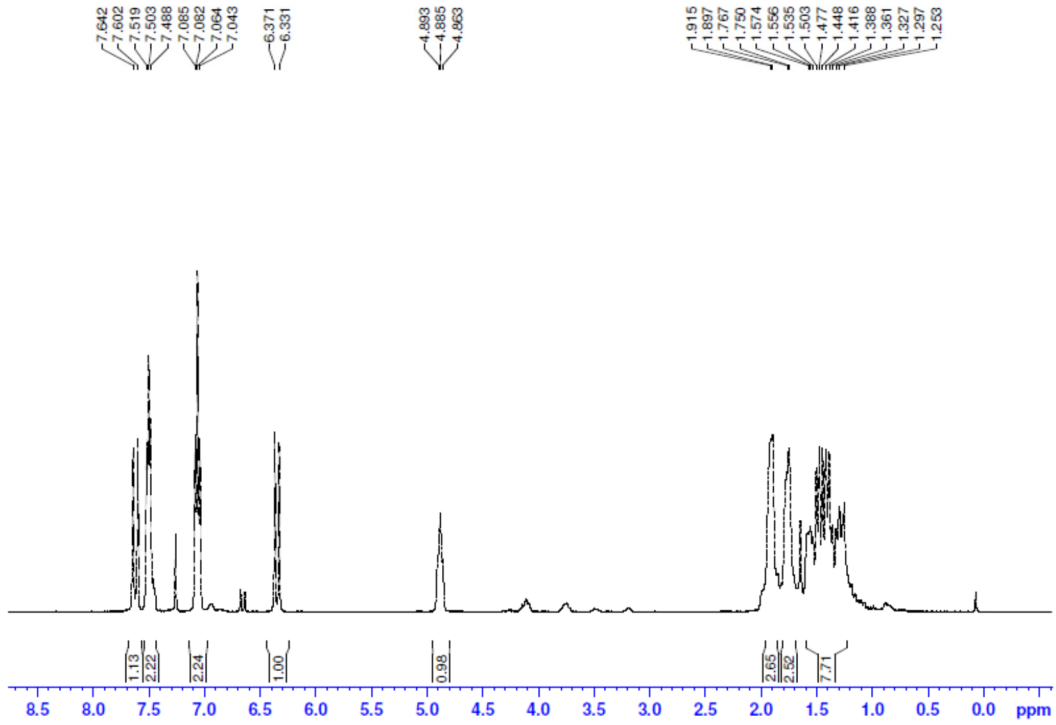

7.662
7.623
7.426
7.411
7.189
7.175
6.406
6.402
6.366
6.362
4.891
4.882
2.369
2.003
1.907
1.757
1.584
1.560
1.509
1.483
1.454
1.420
1.394
1.368
1.302
1.262
1.00
2.01
1.98
0.94
0.90
2.96
2.29
2.26
7.93
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm

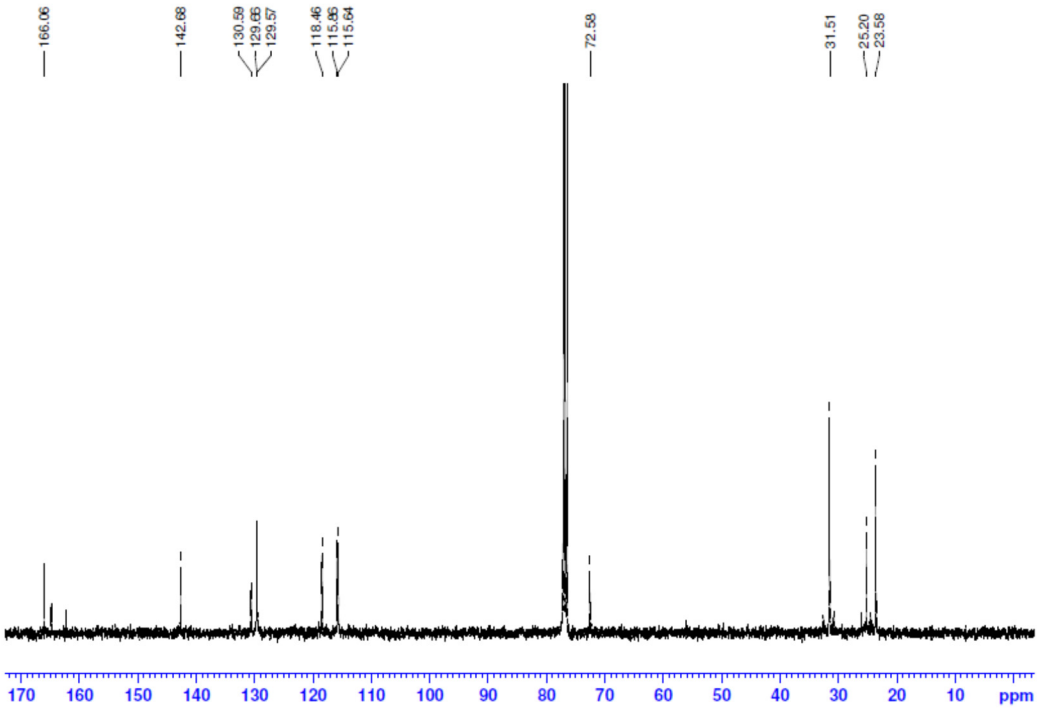

166.40
144.01
140.25
131.63
129.35
127.78
117.60
72.39
31.54
25.24
23.61
21.21
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

7b:

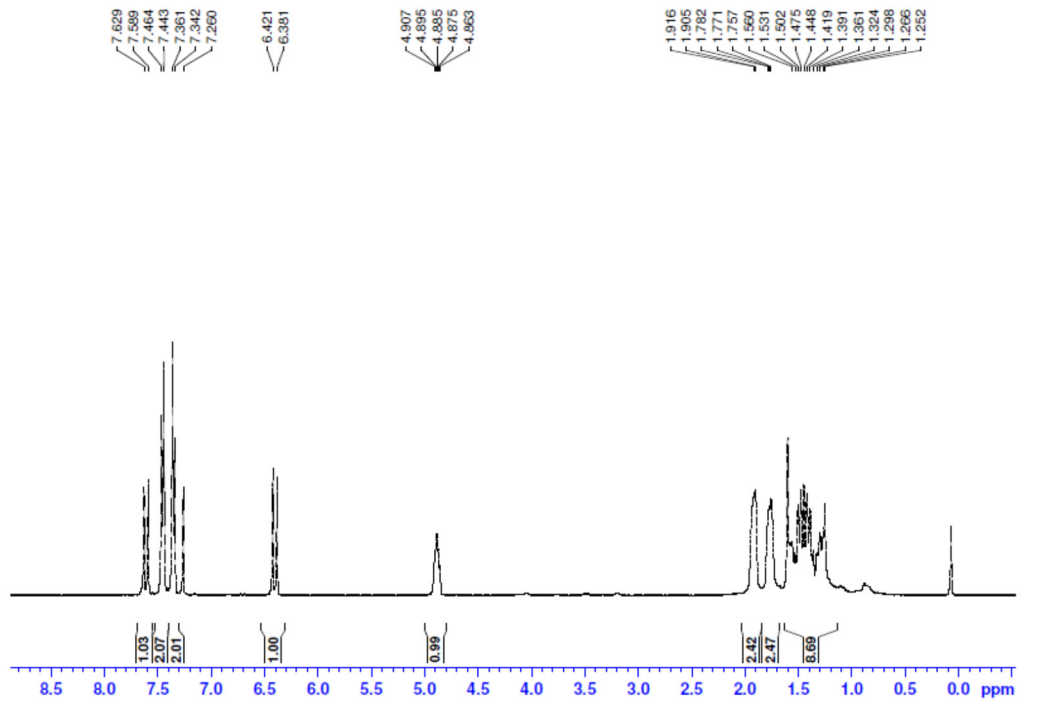

7.642
7.602
7.480
7.459
6.904
6.883
6.321
6.281
4.901
4.890
4.879
4.870
4.857
4.848
3.828
1.916
1.903
1.781
1.771
1.757
1.584
1.573
1.554
1.533
1.502
1.476
1.448
1.419
1.387
1.361
1.325
1.300
1.270
1.01
2.02
2.00
1.00
1.00
3.05
2.12
2.14
6.55
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
166.52
161.04
143.66
129.40
127.10
116.20
114.06
77.13
76.81
76.49
72.28
55.12
31.57
25.25
23.62
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

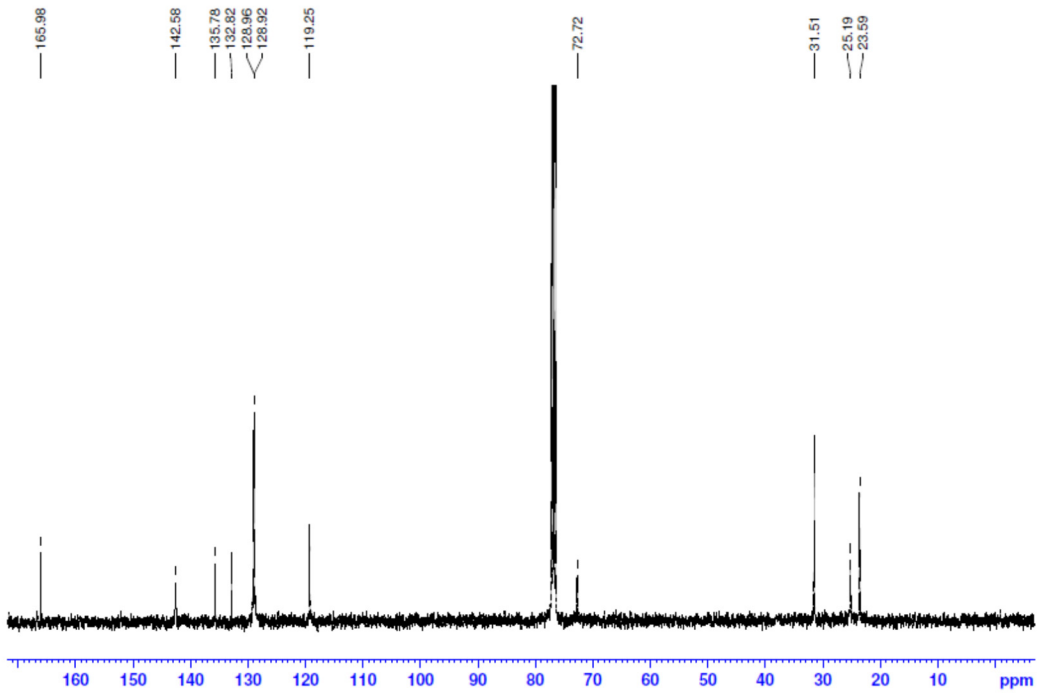
8b:


7.642
7.602
7.519
7.503
7.488
7.085
7.082
7.064
7.043
6.371
6.331
4.893
4.885
4.863
1.915
1.897
1.767
1.750
1.574
1.556
1.535
1.503
1.477
1.448
1.416
1.388
1.361
1.327
1.297
1.253
1.13
2.22
2.24
1.00
0.98
2.65
2.62
7.71
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm

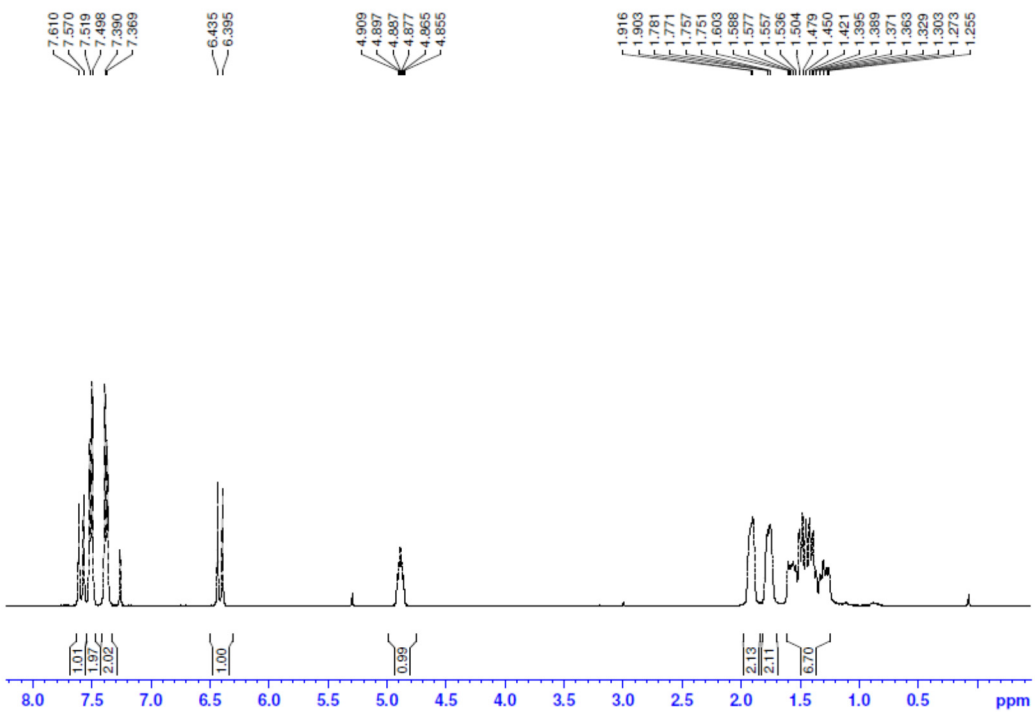

166.06
142.68
130.59
129.65
129.57
118.46
115.85
115.64
72.58
31.51
25.20
23.58
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

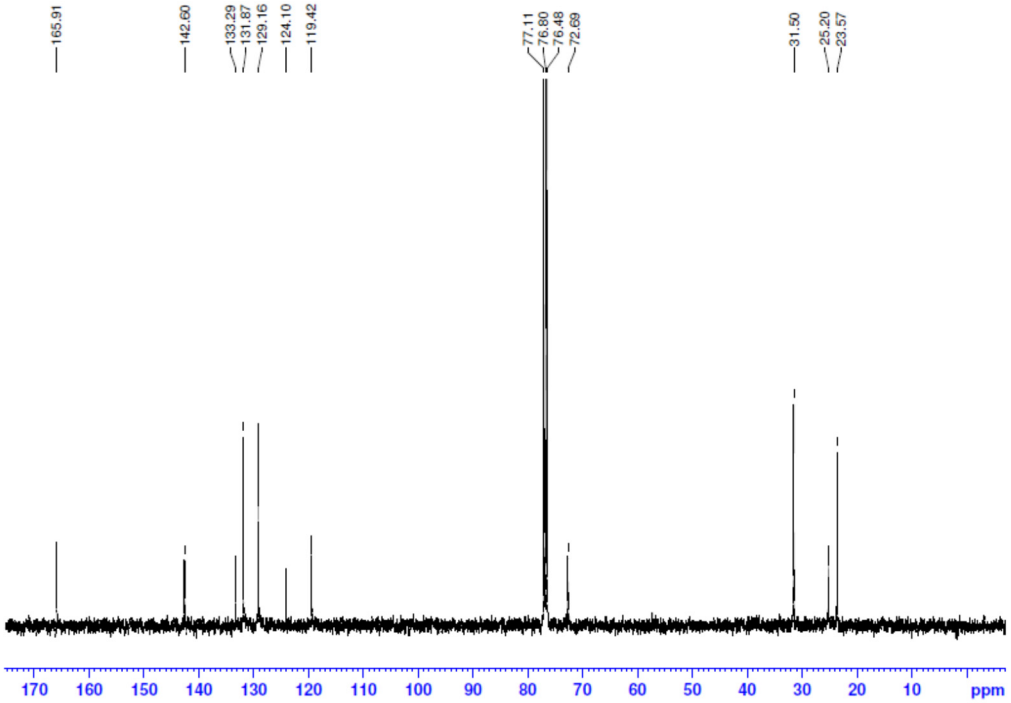
9b:


7.629
7.589
7.464
7.443
7.361
7.342
7.260
6.421
6.381
4.907
4.895
4.885
4.875
4.863
1.916
1.905
1.782
1.771
1.757
1.560
1.531
1.502
1.475
1.448
1.419
1.391
1.361
1.324
1.298
1.266
1.252
1.09
2.07
2.01
1.00
0.99
2.42
2.47
8.69
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm

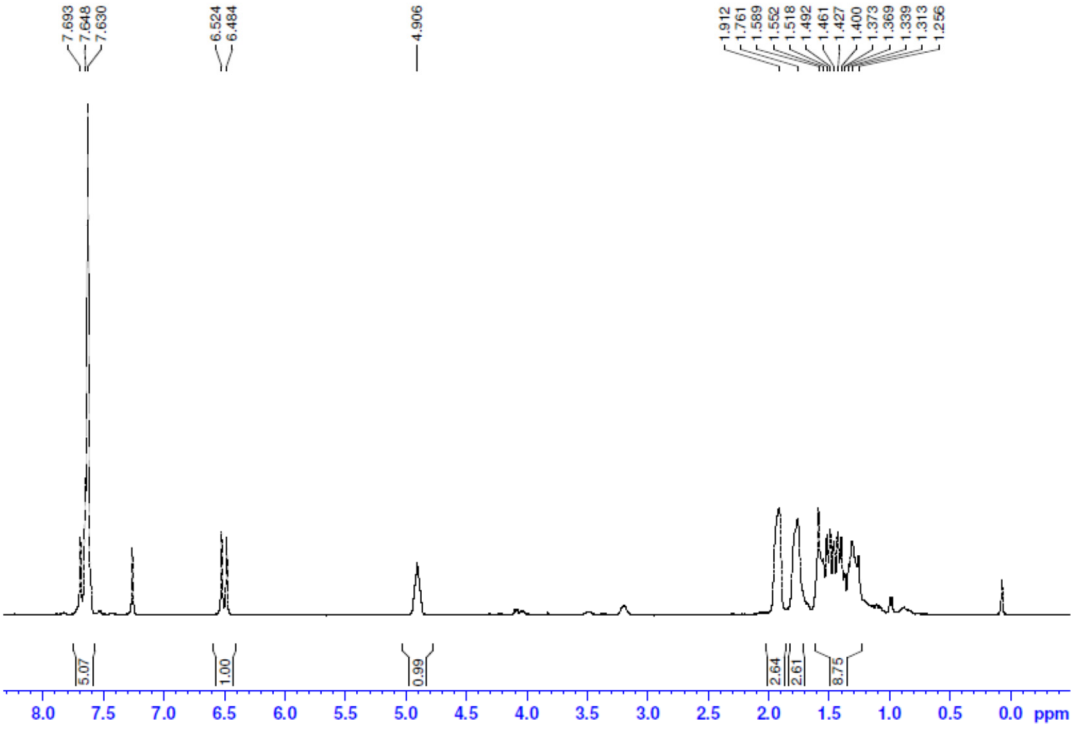

165.98
142.58
135.78
132.82
128.96
128.92
119.25
72.72
31.51
25.19
23.59
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

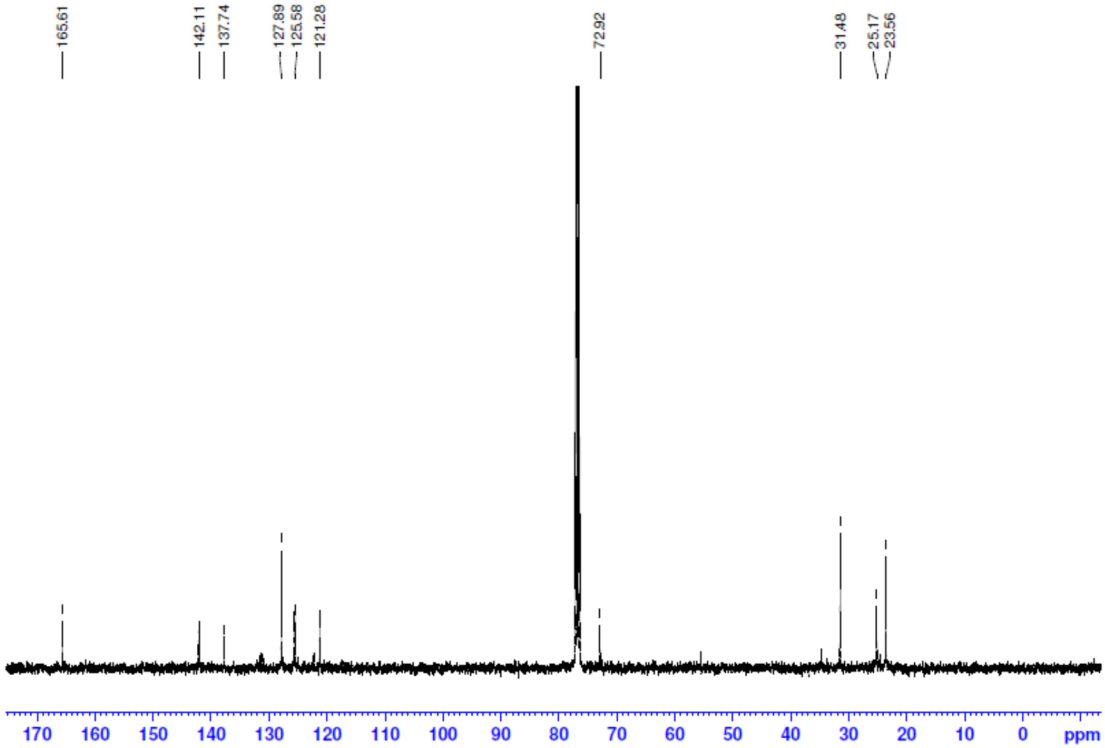
10b:


7.610
7.570
7.519
7.498
7.390
7.369
6.435
6.395
4.909
4.897
4.887
4.877
4.865
4.855
1.916
1.903
1.781
1.771
1.757
1.751
1.603
1.588
1.577
1.557
1.536
1.504
1.479
1.450
1.421
1.395
1.389
1.371
1.363
1.329
1.303
1.273
1.255
1.01
1.97
2.02
1.00
0.99
2.13
2.11
6.70
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm

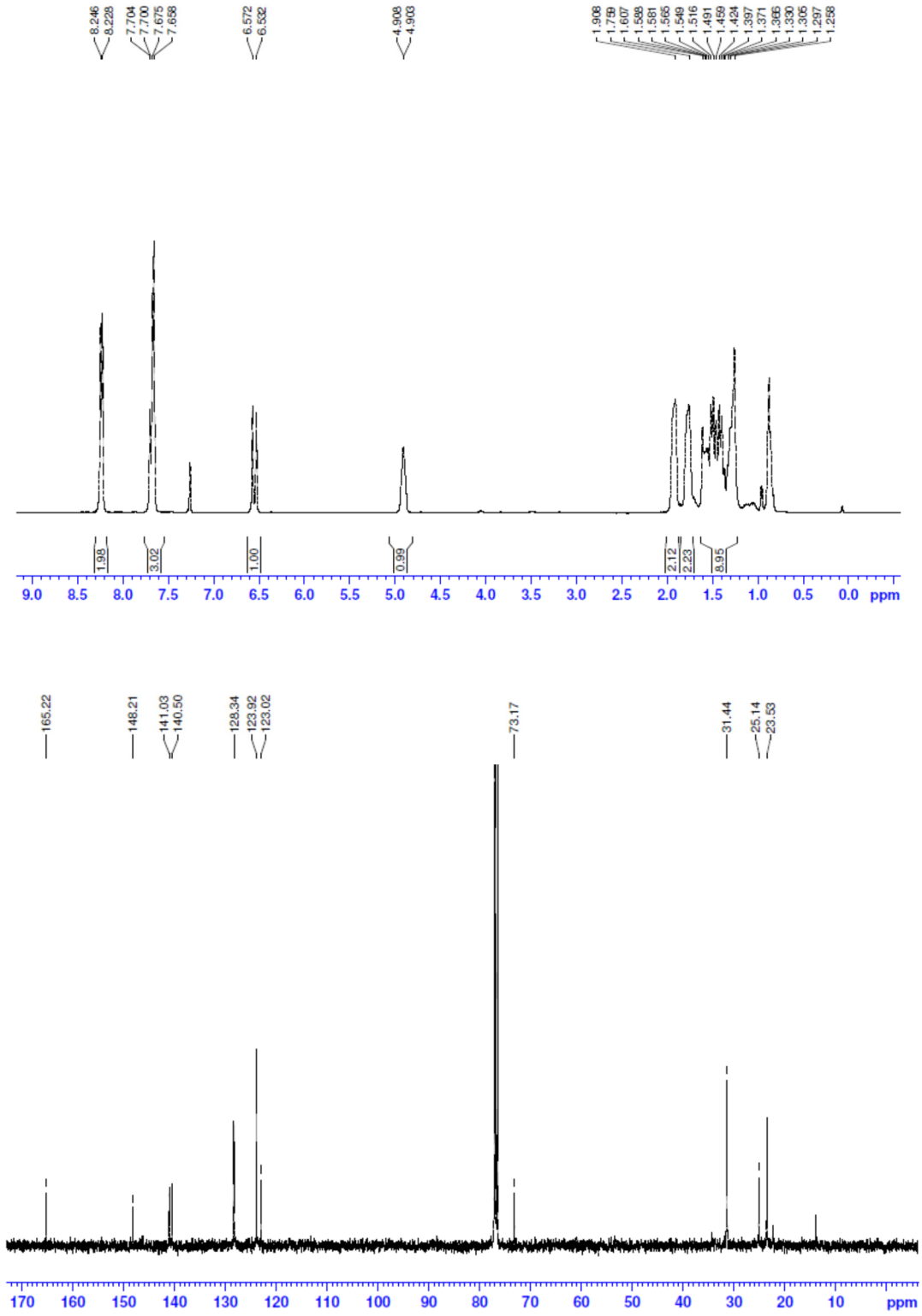

165.91
142.60
133.29
131.87
129.16
124.10
119.42
77.11
76.80
76.48
72.69
31.50
25.20
23.57
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

11b:

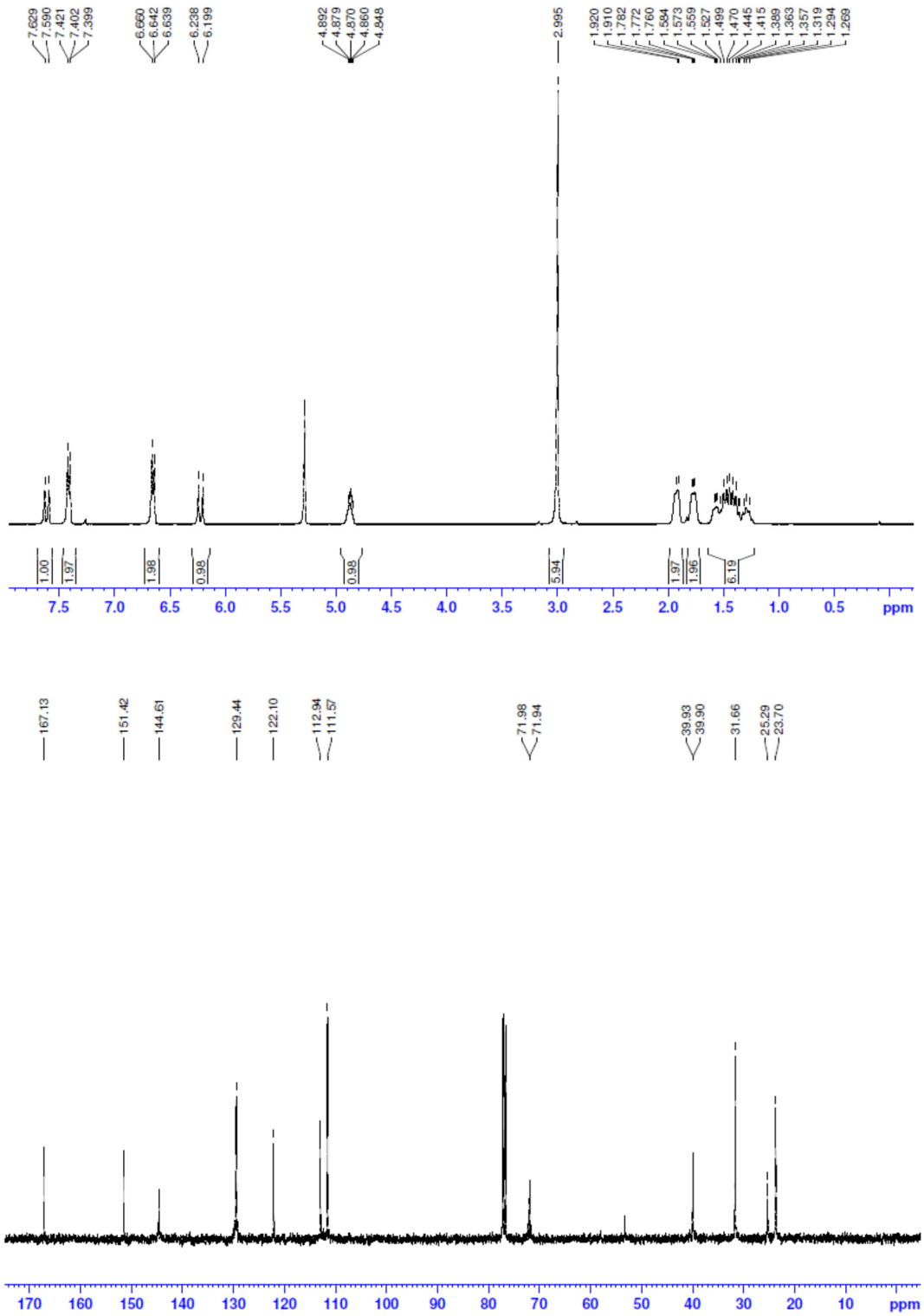

7.693
7.648
7.630
6.524
6.484
4.906
1.912
1.761
1.589
1.552
1.518
1.492
1.461
1.427
1.400
1.373
1.369
1.339
1.313
1.256
5.07
1.00
0.99
2.64
2.61
8.75
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm


165.61
142.11
137.74
127.89
125.58
121.28
72.92
31.48
25.17
23.56
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

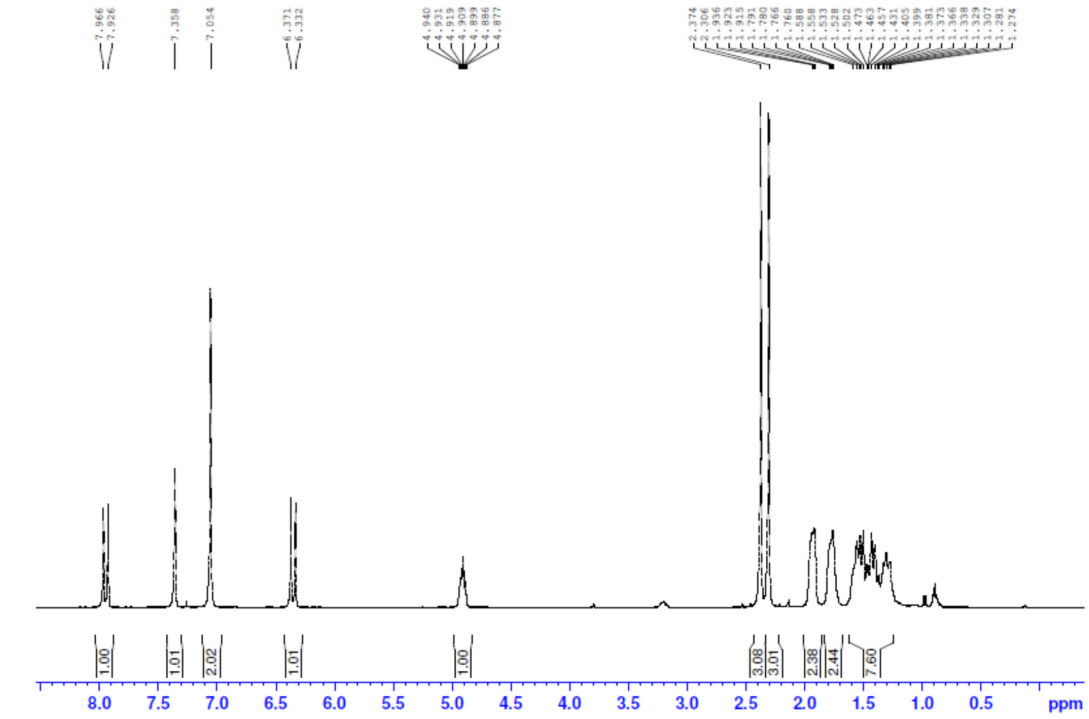
12b:

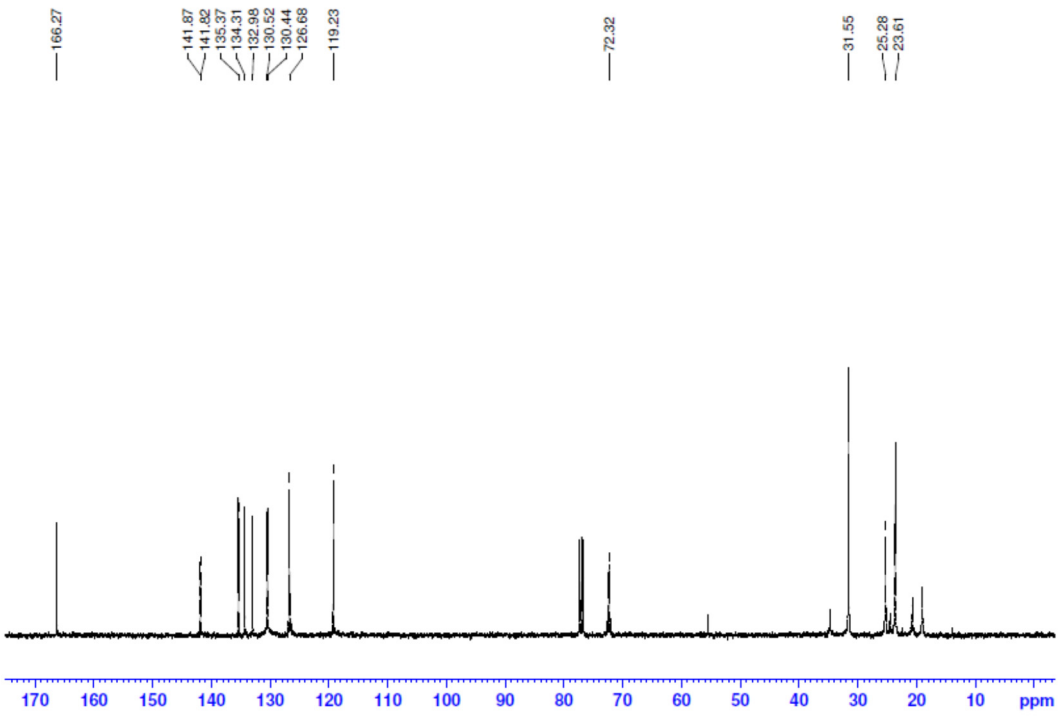

8.246
8.228
7.704
7.700
7.675
7.658
6.572
6.532
4.908
4.903
1.908
1.759
1.607
1.598
1.581
1.565
1.549
1.516
1.491
1.459
1.424
1.397
1.371
1.330
1.305
1.297
1.258
1.98
3.02
1.00
0.99
2.12
2.23
8.95
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
165.22
148.21
141.03
140.50
128.34
123.92
123.02
73.17
31.44
25.14
23.53
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

13b:

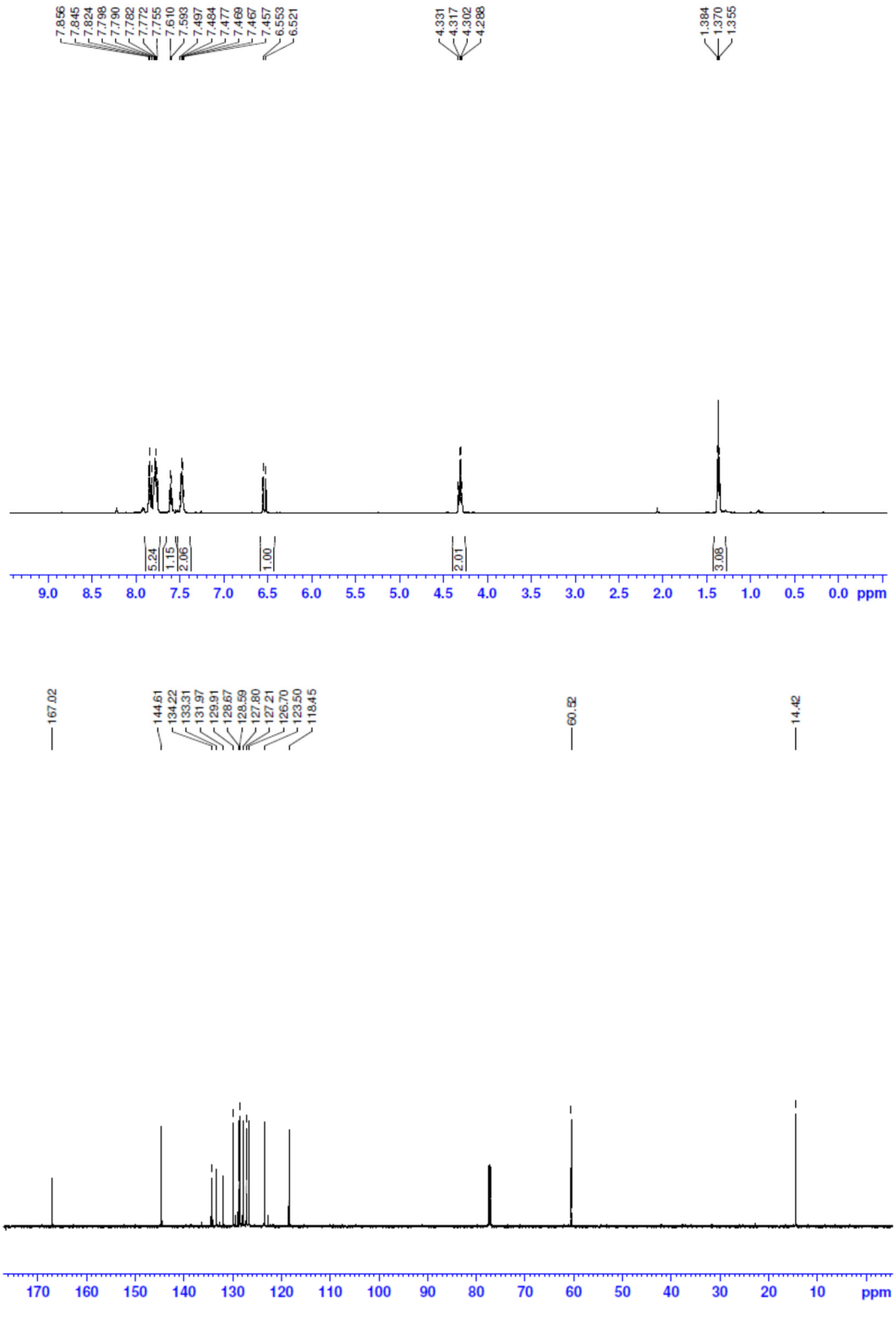

7.629
7.590
7.421
7.402
7.399
6.660
6.642
6.639
6.238
6.199
4.892
4.879
4.870
4.860
4.848
2.995
1.920
1.910
1.782
1.772
1.760
1.584
1.573
1.559
1.527
1.499
1.470
1.445
1.415
1.389
1.363
1.357
1.319
1.294
1.269
1.00
1.97
1.98
0.98
0.98
5.94
1.97
1.96
6.19
7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
167.13
151.42
144.61
129.44
122.10
112.94
111.57
71.98
71.94
39.93
39.90
31.66
25.29
23.70
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

14b:

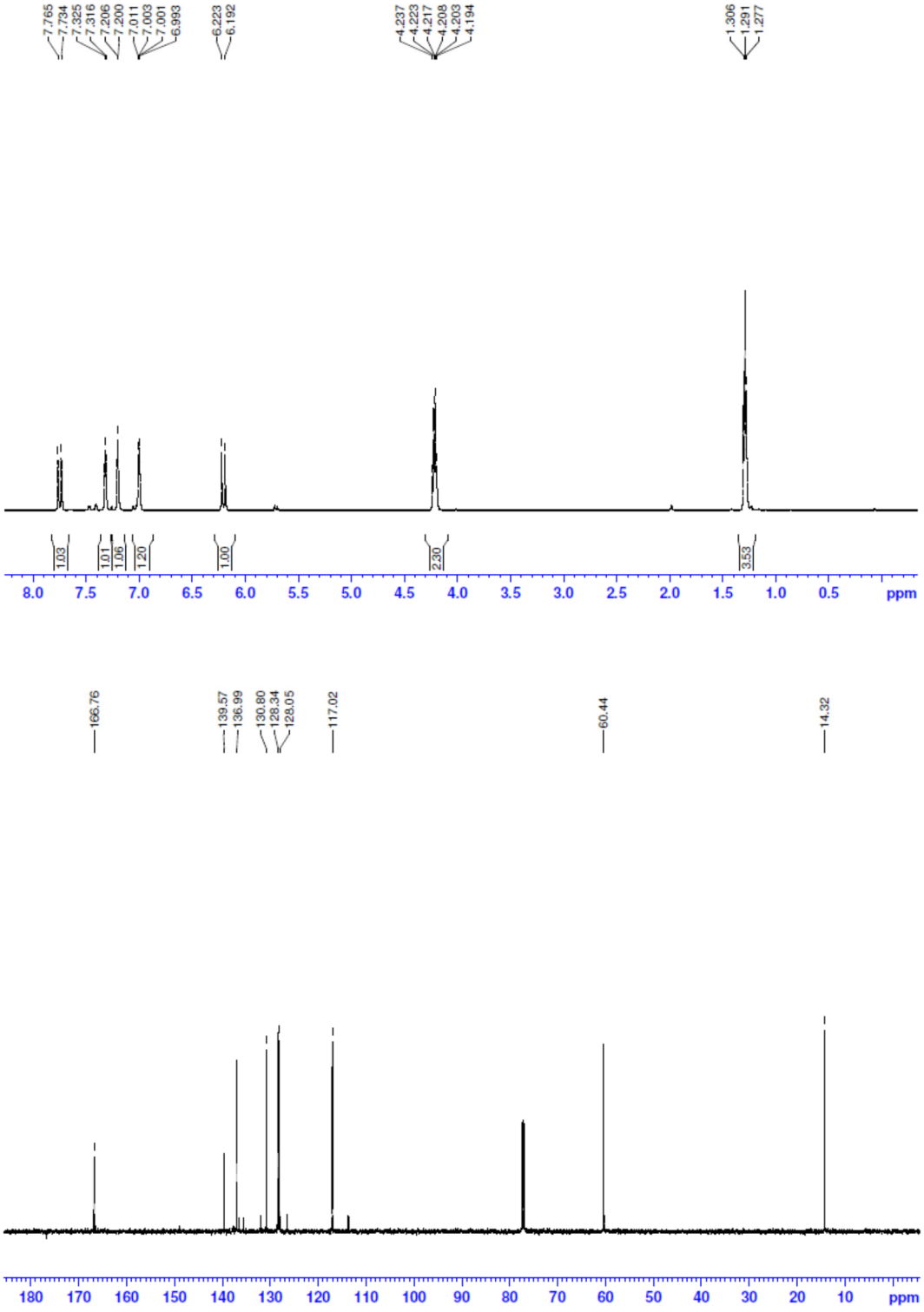

7.966
7.926
7.358
7.054
6.371
6.332
4.940
4.921
4.919
4.909
4.899
4.886
4.877
2.374
2.356
2.336
1.923
1.915
1.791
1.780
1.766
1.746
1.588
1.558
1.533
1.528
1.502
1.473
1.463
1.457
1.431
1.405
1.399
1.393
1.373
1.366
1.338
1.329
1.307
1.281
1.274
1.00
1.01
2.02
1.01
1.00
3.08
3.01
2.38
2.44
7.60
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm


166.27
141.87
141.82
135.37
134.31
132.98
130.52
130.44
126.68
119.23
72.32
31.55
25.28
23.61
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

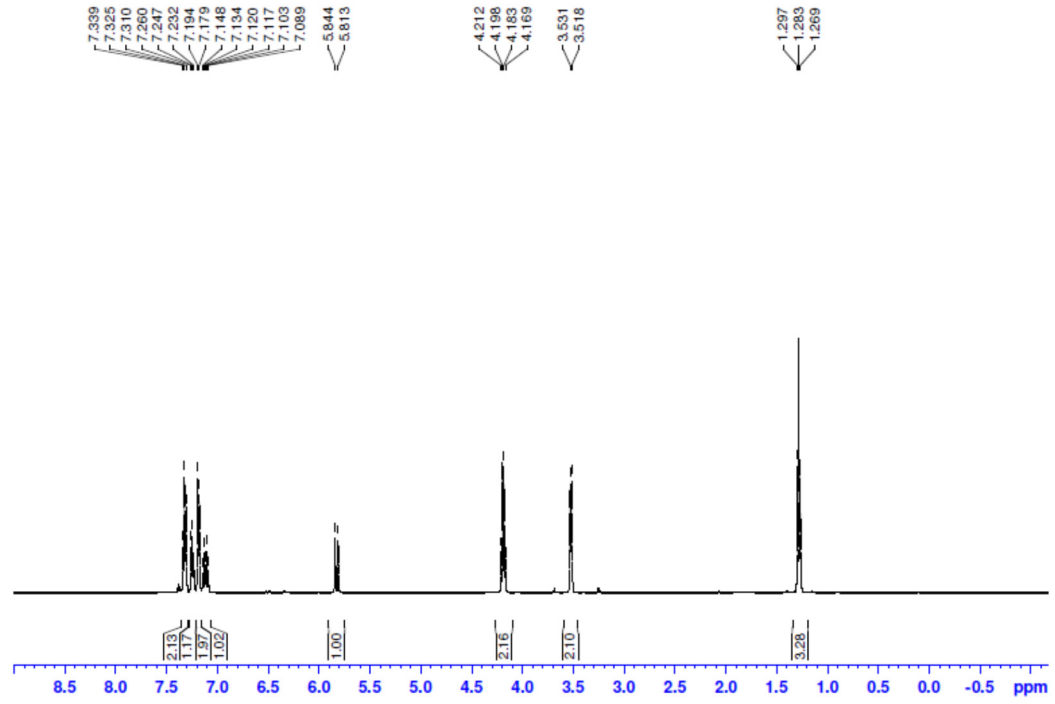
15b:

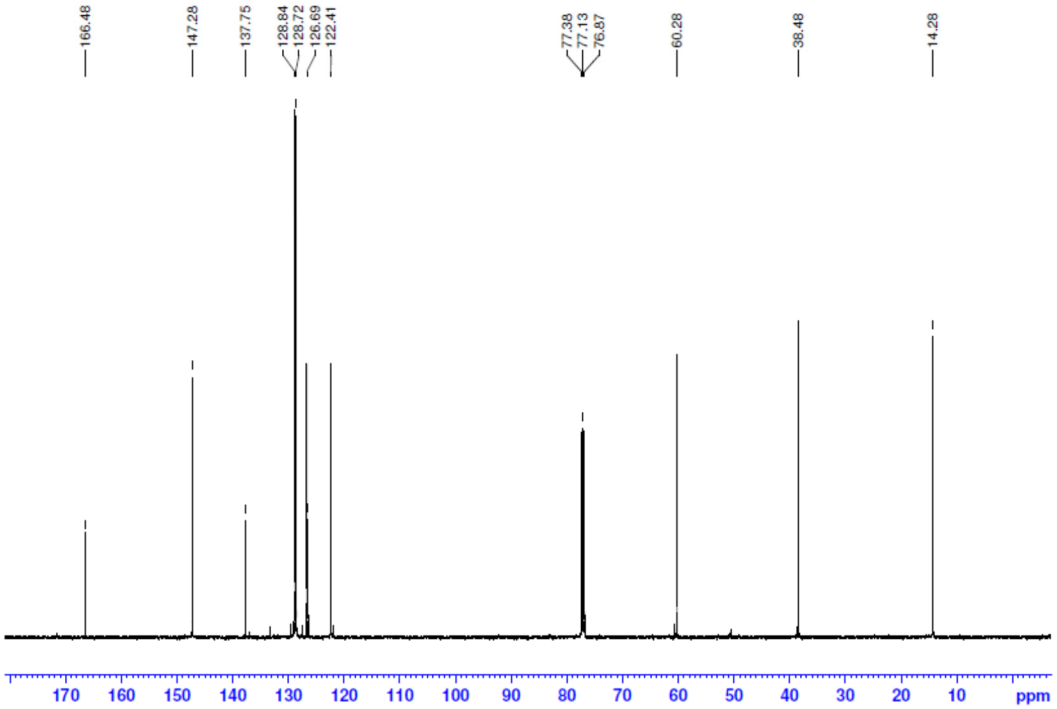

7.856
7.845
7.824
7.798
7.790
7.782
7.772
7.755
7.610
7.593
7.497
7.484
7.477
7.469
7.467
7.457
6.553
6.521
4.331
4.317
4.302
4.288
1.384
1.370
1.355
5.24
1.15
2.06
1.00
2.01
3.08
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
167.02
144.61
134.22
133.31
131.97
129.91
128.67
128.59
127.80
127.21
126.70
123.50
118.45
60.52
14.42
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

16b:


7.765
7.734
7.325
7.316
7.206
7.200
7.011
7.003
7.001
6.993
6.223
6.192
4.237
4.223
4.217
4.208
4.203
4.194
1.306
1.291
1.277
1.03
1.01
1.06
1.20
1.00
2.30
3.53
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
166.76
139.57
136.99
130.80
128.34
128.05
117.02
60.44
14.32
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

17b:


7.339
7.325
7.310
7.260
7.247
7.232
7.194
7.179
7.148
7.134
7.120
7.117
7.103
7.089
5.844
5.813
4.212
4.198
4.183
4.169
3.531
3.518
1.297
1.283
1.269
2.13
1.17
1.97
1.02
1.00
2.16
2.10
3.28
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 ppm


166.48
147.28
137.75
128.84
128.72
126.69
122.41
77.38
77.13
76.87
60.28
38.48
14.28
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm