Supporting Information

Boric acid catalyzed Ugi three-component reaction in aqueous media

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General: All the reagents and solvents were purchased from Sigma-Aldrich or Merck chemical Co. Column chromatography was performed using Spectrochem siliga gel (100-200). Organic solvents were concentrated under reduced pressure on Ika rotary evaporator. The progress of reaction was checked by thin-layer chromatography. The plates were visualized first with UV illumination followed by iodine. ^{1}H and ^{13}C NMR spectra were obtained using either a Bruker DRX-200 or AV-300 spectrometer. Chemical shifts are reported in ppm from tetramethylsilane with the solvent resonance as the internal standard and ^{1}H NMR Spectra are reported in the order: multiplicity, coupling constant (J value) in hertz (Hz) and no of protons; signals were characterized as s (singlet), d (doublet), t (triplet), m (multiplet). ^{13}C NMR spectra were recorded at 50 or 75 MHz. Mass spectra were obtained using JEOL SX-102 (ESI) instrument. Elemental analysis was performed using a Perkin-Elmer Autosystem XL Analyzer.

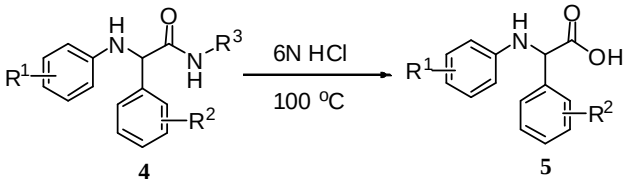
General experiment procedure for the synthesis of 2-arylamino-2-phenylacetamide (4)

Aniline (1 mmol), Aldehyde (1 mmol), Isocyanide (1 mmol) and Boric acid (10 mol %) were placed into a 50 mL flask and (5 mL) water was added to the mixture and stirred for 1h at room temperature for an appropriate time given in Table 3 and the progress of the reaction was monitored by TLC. After completion of the reaction, the reaction mixture was extracted with ethyl acetate. The solvent was evaporated to yield a crude residue, which upon purification *via* silica gel column chromatography using EtOAc/Hexane gave pure products.

General procedure for the synthesis of α-Amino Acid (5)

In a 25 mL round-bottom flask, 2-arylamino-2-phenylacetamide 4 (1 mmol) in 6N HCl (20 mL) was heated at 100 ºC for 24 h, cooled at room temperature than extracted with ethyl acetate/water and apply column chromatography to yield compound.

Table 4. Synthesis of α-Amino acid by acidic hydrolysis of 2-arylamino-2-phenylacetamide.



4 5

Entry	R^1	R^2	R^3	Prod.	Time (h)	Yield (%)[b]
4a	H	H	*t*BuNC	**5a**	22	70
4b	4-OMe	4-Cl	*c*Hex	**5b**	20	65
4c	4-OMe	4-Cl	*t*BuNC	**5b**	21	72
4d	2,4-diMe	H	*c*Hex	**5c**	22	69

[a]Reaction Conditions: 2-arylamino-2-phenylacetamide 4 in 6N HCl at 100 °C for a given time. [b]Isolated Yield.

Characterization data for synthesized compounds:

N-*tert*-butyl-2-phenyl-2-(phenylamino)acetamide (4a)

White solid, ESI MS (*m/z*) = 283 (M+H).^{1}H NMR (300 MHz; $CDCl_3$) δ_H : 1.49 (s, 9H), 4.49 (s, 1H, NH) 4.95 (s, 1H, CH), 6.06 (s, 1H, NH), 6.57 (d, *J* = 5.7 Hz, 2H), 6.66 (t, *J* = 5.5 Hz, 1H), 6.98 (d, *J* = 3.7 Hz, 2H), 7.14 (t, *J* = 5.8 Hz, 2H), 7.28 (m, 3H).^{13}C NMR (75 MHz; $CDCl_3$) δ_C : 29.0, 49.6, 63.3, 112.7, 118.4, 127.4, 127.8, 127.8, 128.0, 128.8, 128.9, 139.2, 145.8, 169.7. Analysis calculated for: $C_{18}H_{22}N_2O$: C 76.56, H 7.85, N 9.92, Found : C 76.42, H 7.97, N 9.81.

2-(4-Chlorophenyl)-N-cyclohexyl-2-(4-methoxyphenylamino)acetamide (4b)

White solid, ESI MS (*m/z*) = 373 (M+H), ^{1}H NMR (300 MHz; $CDCl_3$) δ_H : 1.13-1.28 (m, 5H), 1.45 (t, *J* = 4.31 Hz, 3H), 1.65 (t, *J* = 10.6 Hz, 2H), 3.39-3.61 (m, 1H), 3.67 (s, 3H, OCH_3), 4.13 (s, 1H, NH), 4.43 (s, 1H, CH), 6.03 (s, 1H, NH), 6.76 (q, *J* = 6.6 Hz, 4H), 7.06 (d, *J* = 6.2 Hz, 2H), 7.16 (d, *J* = 6.3 Hz, 2H). ^{13}C NMR (75 MHz; $CDCl_3$) δ_C : 25.2, 26.3, 32.8, 49.6, 55.3, 61.6, 114.1, 115.1, 128.6, 129.0, 133.1, 135.8, 140.9, 153.8, 169.5. Analysis calculated for: $C_{21}H_{25}ClN_2O_2$, C 67.64, H 6.76, N 7.51, Found : C 67.77, H 6.52, N 7.40.

N-*tert*-butyl-2-(4-chlorophenyl)-2-(4-methoxyphenylamino)acetamide (4c)

White solid, mp- 126-128 ^{o}C ESI MS (*m/z*) = 347 (M+H), ^{1}H NMR (300 MH; $CDCl_3$) δ_H :1.49 (s, 9H), 3.67 (s, 3H, OCH_3), 4.45 (s. 1H, NH), 4.91 (s, 1H, CH), 6.06 (s, 1H, NH), 6.74 (dd, *J* = 6.6, 6.6 Hz, 4H), 7.06 (dd, *J* = 6.4, 6.3 Hz, 4H). ^{13}C NMR (75MHz; $CDCl_3$) δ_C : 28.9, 49.6, 55.3, 63.1, 114.1, 114.5, 128.3, 128.5, 133.1, 137.0, 140.6, 153.8, 168.8. Analysis calculated for: $C_{19}H_{23}ClN_2O_2$, C 65.79, H 6.68, N 8.08, Found : C 65.86, H 6.78, N 7.98.

N-cyclohexyl-2-(2,4-dimethylphenylamino)-2-phenylacetamide (4d)

Yellow solid, ESI MS (*m/z*) = 337 (M+H), ^{1}H NMR (300 MHz; $CDCl_3$) δ_H :1.18-1.47 (m, 6H), 1.68 (d, *J* = 16.8 Hz, 4H), 2.28 (s, 6H, CH_3), 3.59-3.79 (m, 1H), 4.07 (s, 1H, NH), 4.53 (s, 1H, CH), 6.03 (s, 1H, NH), 6.35 (d, *J* =3.4 Hz, 1H), 6.76 (s, 1H), 6.84 (d, *J* = 6.09 Hz, 1H), 7.01 (d, *J* = 4.71 Hz, 2H), 7.32 (t, *J* = 5.52 Hz, 3H). ^{13}C NMR (75 MHz; $CDCl_3$) δ_C : 18.3, 20.5, 25.2, 26.3, 32.8, 49.8, 62.4, 113.2, 122.4, 127.7, 127.8, 128.0, 128.9, 130.8, 132.0, 139.1, 142.6, 170.2. Analysis calculated for: $C_{22}H_{28}N_2O$, C 78.53, H 8.39, N 8.33, Found : C 78.68, H 8.47, N 8.21.

N-*tert*-butyl-2-(4-chlorophenyl)-2-(4-chlorophenylamino)acetamide (4e)

White solid, ESI MS (*m/z*) = 351 (M+H), ^{1}H NMR (300 MHz; $CDCl_3$) δ_H : 1.48 (s, 9H), 4.45 (s, 1H, NH), 4.98 (s, 1H, CH), 6.06 (s, 1H, NH), 6.55 (d, *J* = 5.6 Hz, 2H), 7.06-7.16 (m, 6H), ^{13}C NMR (75 MHz; $CDCl_3$) δ_C : 29.0, 49.6, 63.4, 113.8, 123.9, 128.3, 128.5, 128.9, 129.3, 133.1, 137.0, 144.3, 168.8. Analysis calculated for: $C_{18}H_{20}Cl_2N_2O$, C 61.55, H 5.74, N 7.97, Found: C 61.46, H 5.82, N 7.88.

N-*tert*-butyl-2-(4-chlorophenylamino)-2-phenylacetamide (4f)

White solid, ESI MS (*m/z*) = 317 (M+H), ^{1}H NMR (300 MHz; $CDCl_3$) δ_H : 1.49 (s, 9H), 4.19 (s, 1H, NH), 4.73 (s, 1H, CH), 6.08 (s, 1H, NH), 6.56 (d, *J* = 5.6 Hz, 2H), 7.01 (d, *J* = 3.6 Hz, 2H), 7.14 (d, *J* = 5.9 Hz, 2H), 7.28-7.34 (m, 3H), ^{13}C NMR (75 MHz; $CDCl_3$) δ_C : 28.8, 49.6, 63.8, 113.5, 123.9, 127.4, 127.7, 127.8, 128.0, 128.9, 129.3, 139.0, 144.5, 169.3. Analysis calculated for : $C_{18}H_{21}ClN_2O$, C 68.24, H 6.68, N 8.84, Found : C 68.14, H 6.76, N 8.96.

2-(4-Bromophenyl)-N-*tert*-butyl-2-(4-methoxyphenylamino)acetamide (4g)

White solid, ESI MS (*m/z*) = 391(M+H),.^{1}H NMR (300 MHz; $CDCl_3$) δ_H: 1.48 (s, 9H), 3.67 (s, 3H, OCH_3), 4.59 (s, 1H, NH), 4.85 (s, 1H, CH), 6.09 (s, 1H, NH), 6.74-6.83 (m, 4H), 6.90 (d, *J* = 6.3 Hz, 2H), 7.47 (d, *J* = 6.1 Hz, 2H), ^{13}C NMR (50 MHz; $CDCl_3$) δ_C : 29.1, 49.6, 55.3, 63.6, 114.2, 114.5, 121.8, 128.7, 131.6, 137.7, 140.6, 153.8, 169.8. Analysis calculated for: $C_{19}H_{23}BrN_2O_2$, C 58.32, H 5.92, N 7.16, Found : C 58.21, H 6.02, N 7.28.

2-(4-Chlorophenyl)-N-cyclohexyl-2-(3-methoxyphenylamino)acetamide (4h)

White solid, ESI MS (*m/z*) = 373 (M+H), ^{1}H NMR (300 MHz; $CDCl_3$) δ_H : 1.10-1.39 (m, 5H), 1.35 (t, *J* = 4.3 Hz, 3H), 1.65 (t, *J* = 7.2 Hz, 2H), 3.39-3.60 (m, 1H), 3.67 (s, 3H, OCH_3), 4.50 (s, 1H, NH), 5.01 (s, 1H, CH), 6.03 (s, 1H, NH), 6.78 (d, *J* =8.7 Hz, 4H), 7.01 (d, *J* = 5.4 Hz, 1H), 7.33 (d, *J* =5.6 Hz, 3H), ^{13}C NMR (50 MHz; $CDCl_3$) δ_C : 25.2, 26.3, 32.8, 49.7, 55.4, 61.3, 101.1, 104.3, 106.1, 128.6, 129.4, 133.1, 135.8, 147.3, 159.6, 169.8. Analysis calculated for : $C_{21}H_{25}ClN_2O_2$, C 67.64, H 6.76, N 7.51, Found : C 67.77, H 6.84, N 7.41.

N-cyclohexyl-2-(4-methoxyphenylamino)-2-phenylacetamide (4i)

White solid, MS (*m/z*) = 339 (M+H), ^{1}H NMR (300 MHz; $CDCl_3$) δ_H : 1.27-1.61 (m, 7H), 1.65 (t, *J* = 11.7 Hz, 3H), 3.41-3.61 (m, 1H), 3.69 (s, 3H, OCH_3), 4.39 (s, 1H, NH), 4.73 (s, 1H, CH), 6.03 (s, 1H, NH), 6.76-6.83 (m, 4H), 6.98 (d, *J* = 4.5 Hz, 2H), 7.32 (d, *J* = 5.3 Hz, 3H), ^{13}C NMR (50 MHz; $CDCl_3$) δ_C : 25.3, 26.4, 32.7, 49.8, 55.2, 62.5, 114.2, 115.2, 128.0, 128.1, 128.3, 128.6, 128.8, 138.3, 141.3, 153.8, 169.9. Analysis calculated for: $C_{21}H_{26}N_2O_2$, C 74.52, H 7.74, N 8.28, Found : C 74.60, H 7.67, N 8.36.

N-*tert*-butyl-2-(4-chlorophenyl)-2-(2,4-dimethylphenylamino)acetamide (4j)

Yellow solid, MS (*m/z*) = 345 (M+H), ^{1}H NMR (300 MHz; $CDCl_3$) δ_H : 1.51 (s, 9H), 2.28 (s, 6H, CH_3), 4.23 (s, 1H, NH), 4.98 (s, 1H, CH), 6.06 (s, 1H, NH), 6.33 (d, *J* = 7.8 Hz, 1H), 6.76 (s, 1H), 6.84 (d, *J* = 9.27 Hz, 1H), 7.07-7.14 (m, 4H). ^{13}C NMR (75 MHz; $CDCl_3$) δ_C : 18.5, 20.5, 29.0, 49.5, 63.7, 112.9, 122.8, 127.8, 128.2, 128.7, 130.8, 132.0, 133.1, 137.5, 141.7, 169.1. Analysis calculated for : $C_{20}H_{25}ClN_2O$, C 69.65, H 7.31, N 8.12, Found : C 69.77, H 7.21, N 8.11.

N-*tert*-butyl-2-(3,5-dimethoxyphenyl)-2-(phenylamino)acetamide (4k)

White solid, MS (*m/z*) = 343 (M+H), ^{1}H NMR (300 MHz; $CDCl_3$) δH : 1.48 (s, 9H), 3.75, (s, 3H, OCH_3), 3.80 (s, 3H, OCH_3) 4.40 (s, 1H, NH), 4.95 (s, 1H, CH), 6.06 (s, 1H, NH), 6.29 (s, 2H), 6.47 (d, *J* = 1.4 Hz, 1H), 6.57 (d, *J* = 5.6 Hz, 2H), 6.66 (t, *J* = 4.5 Hz, 1H), 7.14 (t, *J* = 5.2 Hz, 2H), ^{13}C NMR (50 MHz; $CDCl_3$) δC : 29.0, 49.3, 55.2, 63.4, 99.5, 104.8, 112.2, 118.4, 128.8, 143.1, 146.1, 161.5, 168.8 . Analysis calculated for : $C_{20}H_{26}N_2O_3$, C 70.15, H 7.65, N 8.18, Found : C 70.28, H 7.52, N 8.28.

N-cyclohexyl-2-(3,5-dimethoxyphenyl)-2-(phenylamino)acetamide (4l)

White solid, MS (*m/z*) = 369 (M+H), ^{1}H NMR (300 MHz; $CDCl_3$) δ_H : 1.29-1.49 (m, 5H), 1.50-171(m, 5H), 3.40-3.59 (m ,1H), 3.74, (s, 3H, OCH_3), 3.79 (s, 3H, OCH_3), 4.76 (s, 1H, NH), 5.05 (s, 1H, CH), 5.83 (s, 1H, NH), 6.29 (s, 2H), 6.47 (d, *J* = 1.4 Hz, 1H), 6.59-6.70 (m, 3H), 7.14 (t, *J* = 4.6 Hz, 2H), ^{13}C NMR (75 MHz:$CDCl_3$) δ_C : 25.2, 26.3, 32.8, 50.0, 55,2, 99.5, 104.7, 112.7, 118.4, 128.8, 142.5, 146.7, 161.2, 169.1. Analysis calculated for : $C_{22}H_{28}N_2O_3$, C 71.71, H 7.66, N 7.60, Found : C 71.62, H 7.76, N 7.51.

2-(4-Bromophenyl)-N-*tert*-butyl-2-(3-methoxyphenylamino)acetamide (4m)

White solid, MS (*m/z*) = 391 (M+H), ^{1}H NMR (300 MHz; $CDCl_3$) δ_H : 1.49 (s, 9H), 3.67 (s, 3H, OCH_3), 4.39 (s, 1H, NH), 4.93 (s, 1H, CH), 5.78 (s, 1H, NH), 6.74 (dd, *J* = 6.3, 6.3 Hz, 4H), 6.97 (d, *J* = 5.1 Hz, 1H), 7.19 (t, *J* = 4.6 Hz, 2H), 7.43 (d, *J* = 5.8 Hz, 1H).^{13}C NMR (50 MHz; $CDCl_3$) δ_C : 28.9, 49.4, 55.3, 62.1, 114.1, 114.3, 121.4, 126.6, 130.0, 130.1, 141.7, 141.8, 159.8, 168.5. Analysis calculated for : $C_{19}H_{23}BrN_2O_2$, C 58.32, H 5.92, N 7.16, Found : C 58.42, H 5.81, N 7.27.

N-*tert*-butyl-2-(4-fluorophenylamino)-2-(4-methoxyphenyl)acetamide (4n)

White solid, MS (*m/z*) = 331 (M+H), ^{1}H NMR (300 MHz; $CDCl_3$) δ_H : 1.49 (s, 9H), 3.76 (s, 3H, OCH_3), 4.50 (s, 1H, NH), 4.92 (s, 1H, CH), 5.96 (s, 1H, NH), 6.47 (s, 2H), 6.82 (m, 4H), 7.07 (t, *J* = 6.3 Hz, 2H), , ^{13}C NMR (50 MHz; $CDCl_3$) δ_C : 29.0, 49.6, 55.1, 64.6, 113.8, 114.3, 114.4, 115.4, 115.6, 128.3, 129.7, 134.3, 141.2, 141.3, 153.2, 160.8, 169.4 . Analysis calculated for : $C_{19}H_{23}FN_2O_2$, C 69.07, H 7.02, N 8.48, Found : C 68.98, H 6.98, N 8.55.

2-(4-Bromophenyl)-N-*tert*-butyl-2-(phenylamino)acetamide (4o)

Pale Yellow solid, MS (*m/z*) = 361 (M+H), ^{1}H NMR (300 MHz; $CDCl_3$) δ_H : 1.50 (s, 9H), 4.50 (s, 1H, NH), 4.69 (s, 1H, CH), 6.06 (s, 1H, NH), 6.57 (d, *J* = 5.6 Hz, 2H), 6.66 (t, *J* = 5.4 Hz, 1H), 6.90 (d, *J* = 6.4 Hz, 2H), 7.14 (t, *J* = 5.5 Hz, 2H), 7.46 (d, *J* = 6.4 Hz, 2H). ^{13}C NMR (50 MHz; $CDCl_3$) δc : 29.1, 49.6, 63.3, 112.7, 118.4, 121.8, 128.7, 128.8, 131.6, 137.7, 145.5, 169.5. Analysis calculated for : $C_{18}H_{21}BrN_2O$, C 59.84, H 5.86, N 7.75, Found : C 59.96, H 5.75, N 7.67.

2-Phenyl-2-(phenylamino)acetic acid (5a)

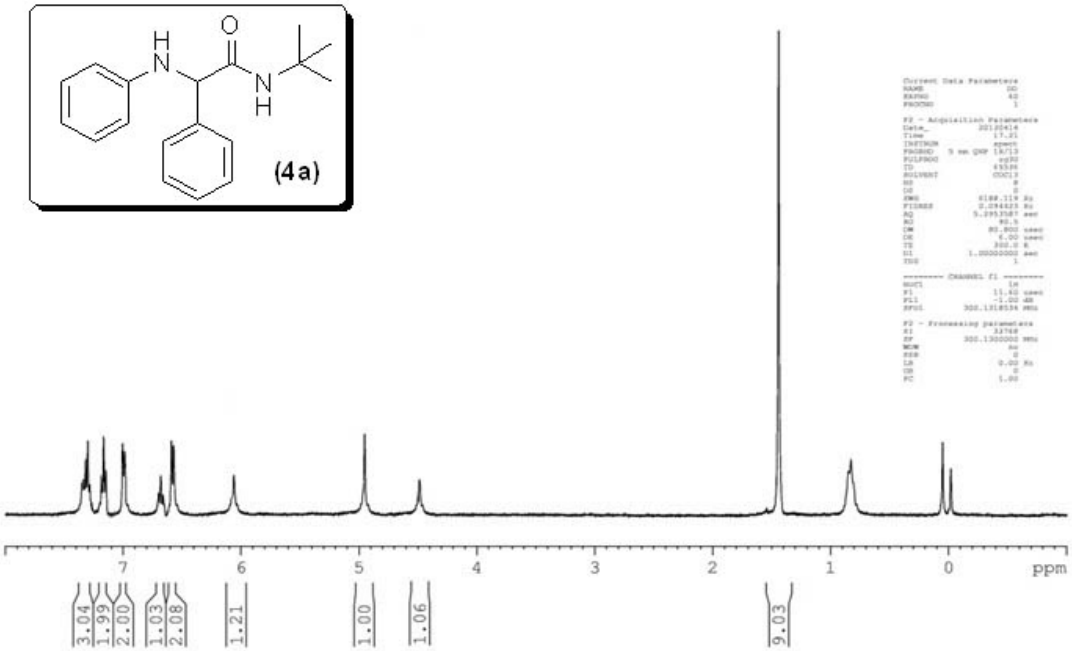
White solid, ESI MS (*m/z*) = 228 (M+H). ^{1}H NMR (300 MHz DMSO) δ_H **:** 4.33 (s, 1H, NH), 4.92 (s, 1H, CH), 6.29 (d, *J* = 5.7 Hz, 2H), 6.69 (t, *J* = 1.0 Hz, 1H), 7.14 (t, *J* = 5.7 Hz, 2H), 7.30-7.35 (m, 5H), 8.35 (s, 1H), ^{13}C NMR (75 MHz, DMSO) δ_C **:** 60.3, 114.2, 118.4, 127.19, 127.7, 128.1, 128.3, 128.9, 129.3, 136.5, 145.8, 169.4. Analysis calculated for : $C_{14}H_{13}NO_2$, C 73.99, H 5.77, N 6.16, Found : C 74.09, H 5.62, N 6.25.

2-(4-Chlorophenyl)-2-(4-methoxyphenylamino)acetic acid (5b)

White Solid, ESI MS (*m/z*) = 292 (M+H), ^{1}H NMR (300 MHz, DMSO) δ_H **:** 3.67 (s, 3H, OCH_3), 4.48 (s, 1H, NH), 4.80 (s, 1H, CH), 6.51 (d, *J* = 6.5 Hz, 2H), 6.80 (d, *J* = 6.5 Hz, 2H), 7.26 (d, *J* = 6.4 Hz, 2H), 7.42 (d, *J* = 6.4 Hz, 2H), 8.30 (s, 1H), ^{13}C NMR (50 MHz, DMSO) δ_C **:** 55.3, 59.6, 115.3, 116.1, 128.5, 128.8, 129.2, 130.3, 133.6, 135.7, 141.4, 153.8, 170.3. Analysis calculated for : $C_{15}H_{14}ClNO_3$, C 61.76, H 4.84, N 4.80, Found : C 61.85, H 4.73, N 4.93.

2-(2,4-Dimethylphenylamino)-2-phenylacetic acid (5c)

White solid, ESI MS (*m/z*) = 256 (M+H), ^{1}H NMR (300 MHz, DMSO) δ_H **:** 2.25 (s, 6H, CH_3), 4.30 (s, 1H, NH), 4.90 (s, 1H, CH), 6.04 (d, *J* = 6.0 Hz, 1H), 6.76 (s, 1H), 6.84 (d, *J* = 6.0 Hz, 1H), 7.30-7.35 (m, 5H), 8.35 (s, 1H). ^{13}C NMR (50 MHz, DMSO) δ_C **:** 18.2, 20.5, 60.7, 113.8, 121.7, 127.9, 128.1, 128.8, 129.0, 130.8, 132.7, 137.94, 142.8, 168.7. Analysis calculated for : $C_{16}H_{17}NO_2$, C 75.27, H 6.71, N 5.49, Found : C 75.37, H 6.62, N 5.58.



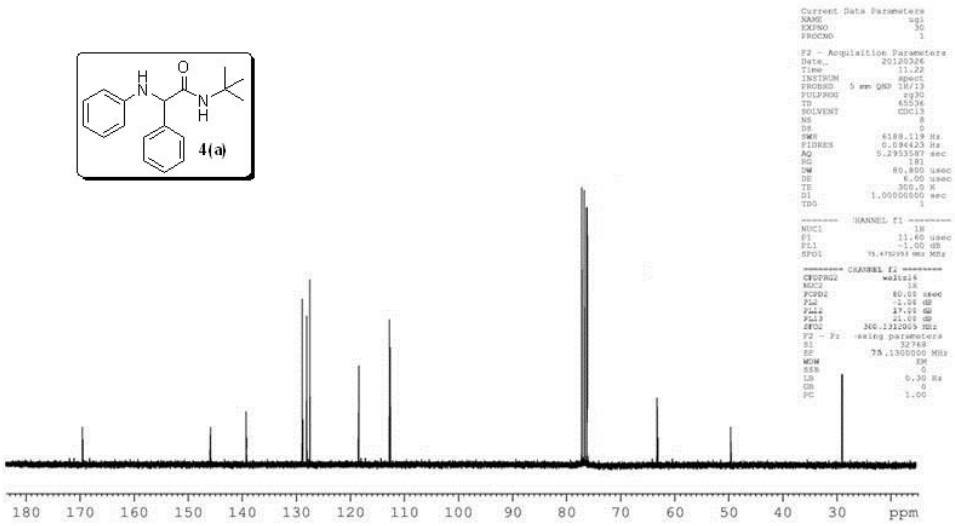
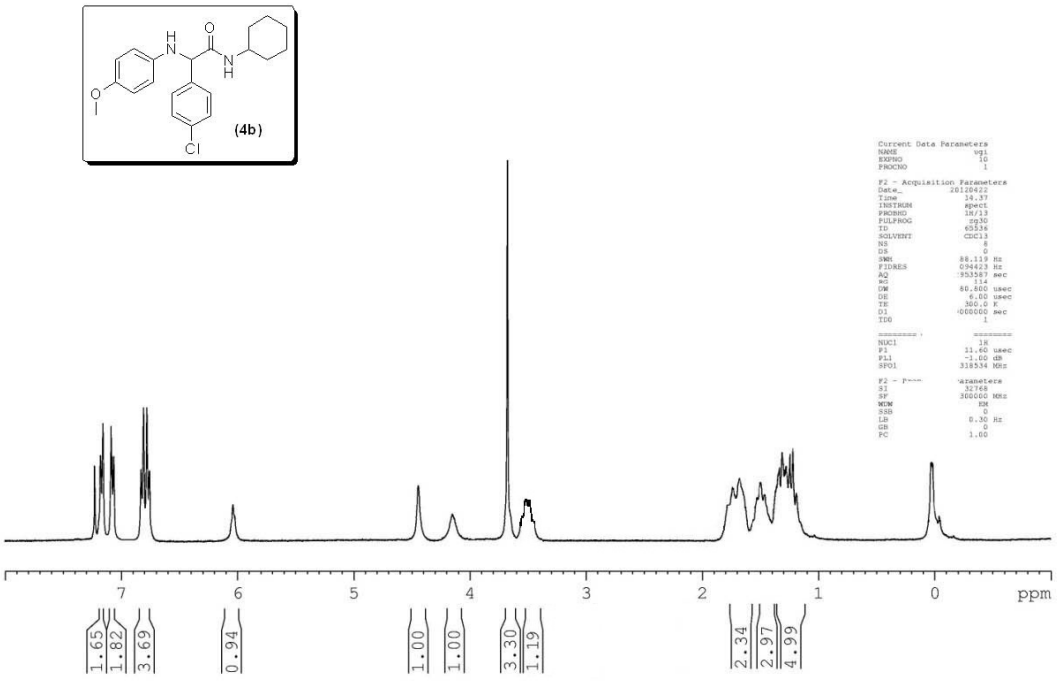


Fig. (4a)



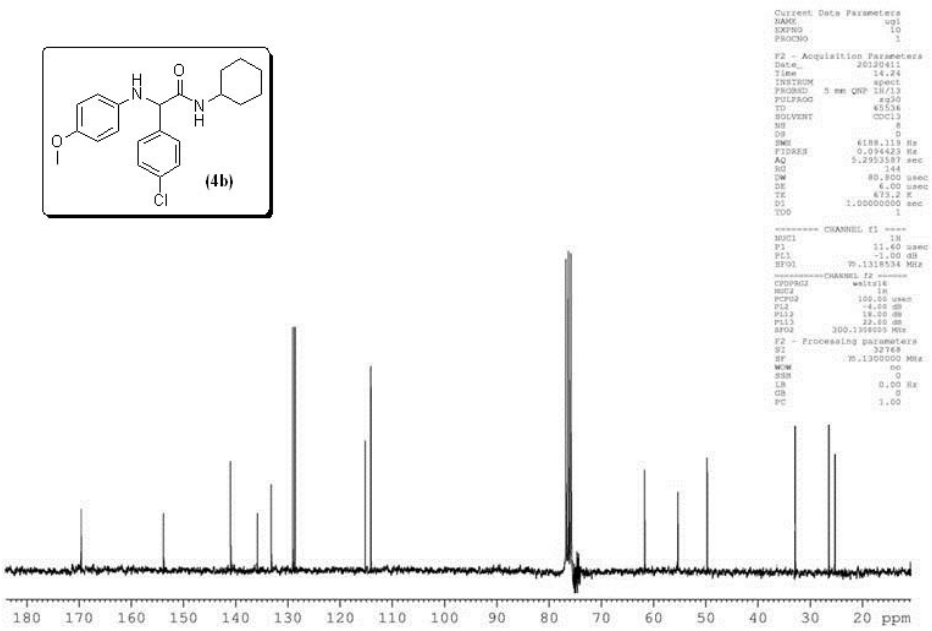
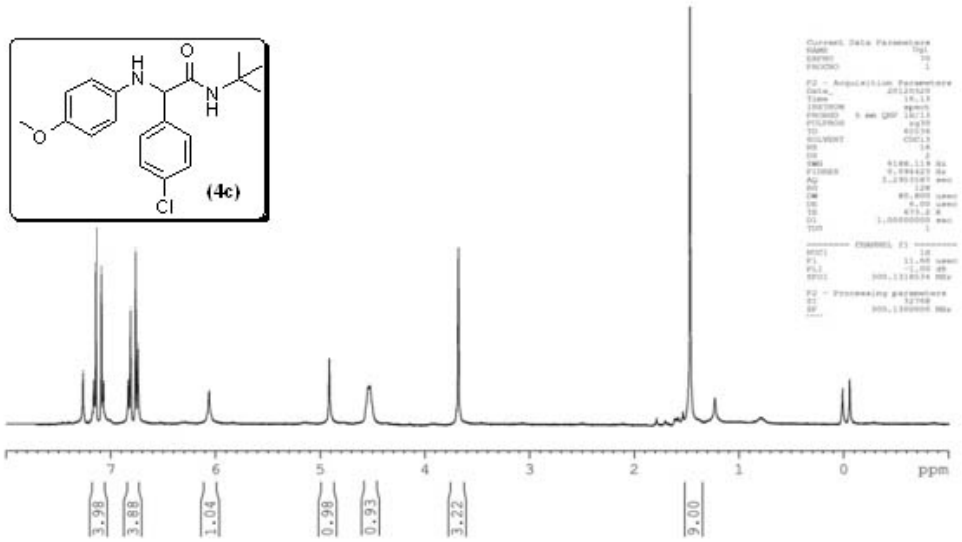


Fig. (4b)



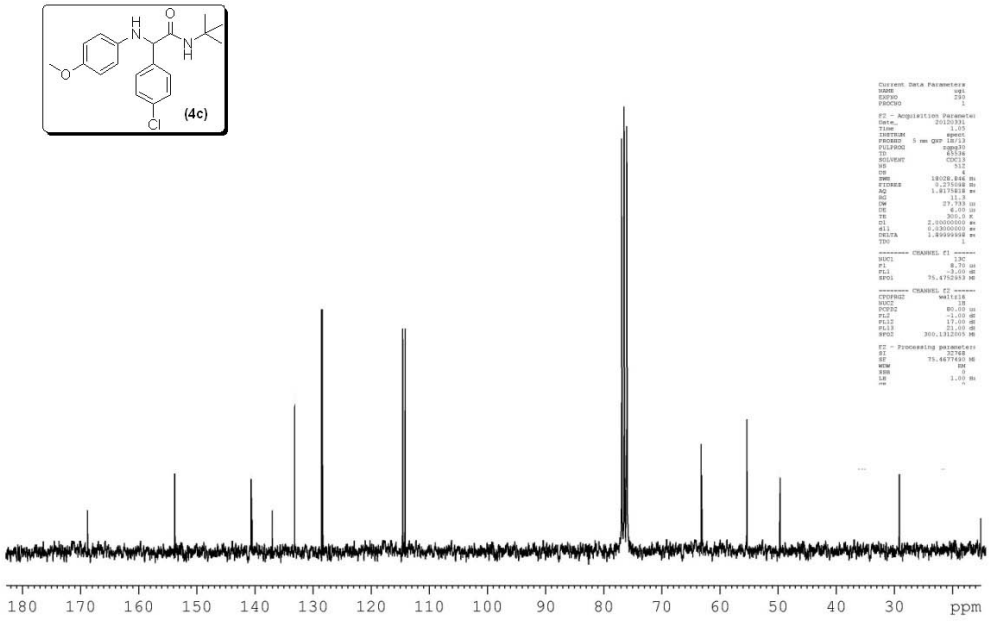


Fig. (4c)

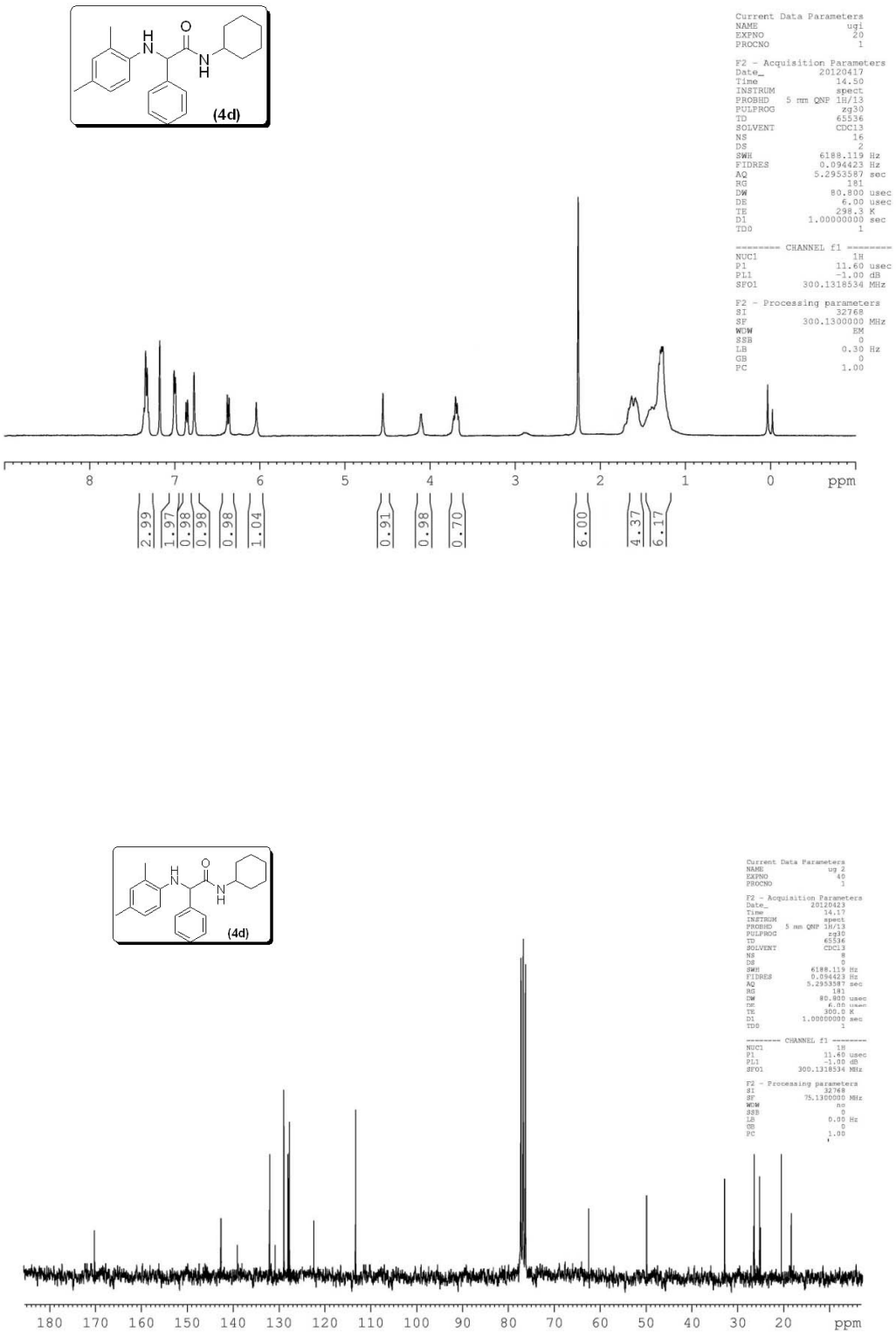

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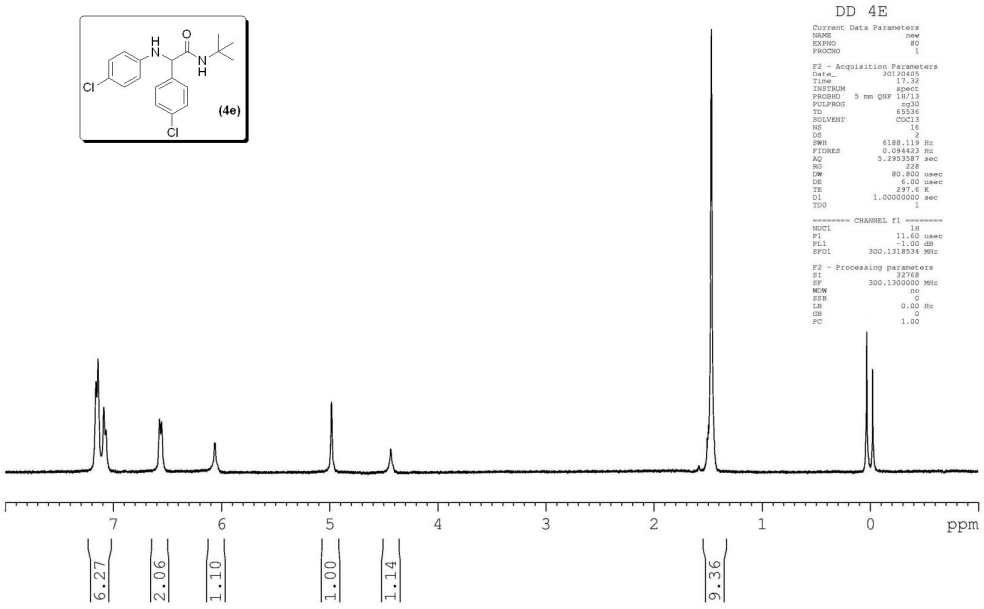
Fig. (4d)



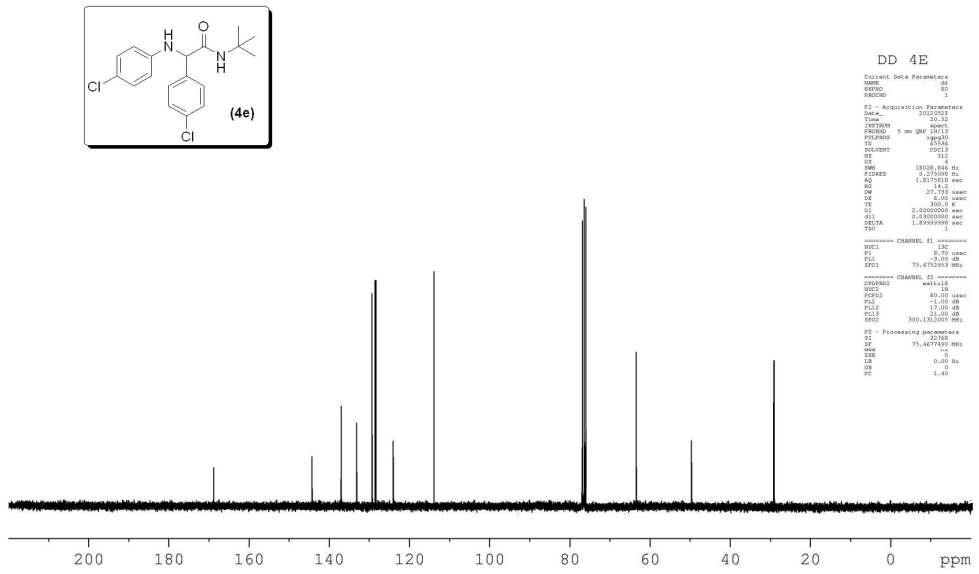


Fig. (4e)

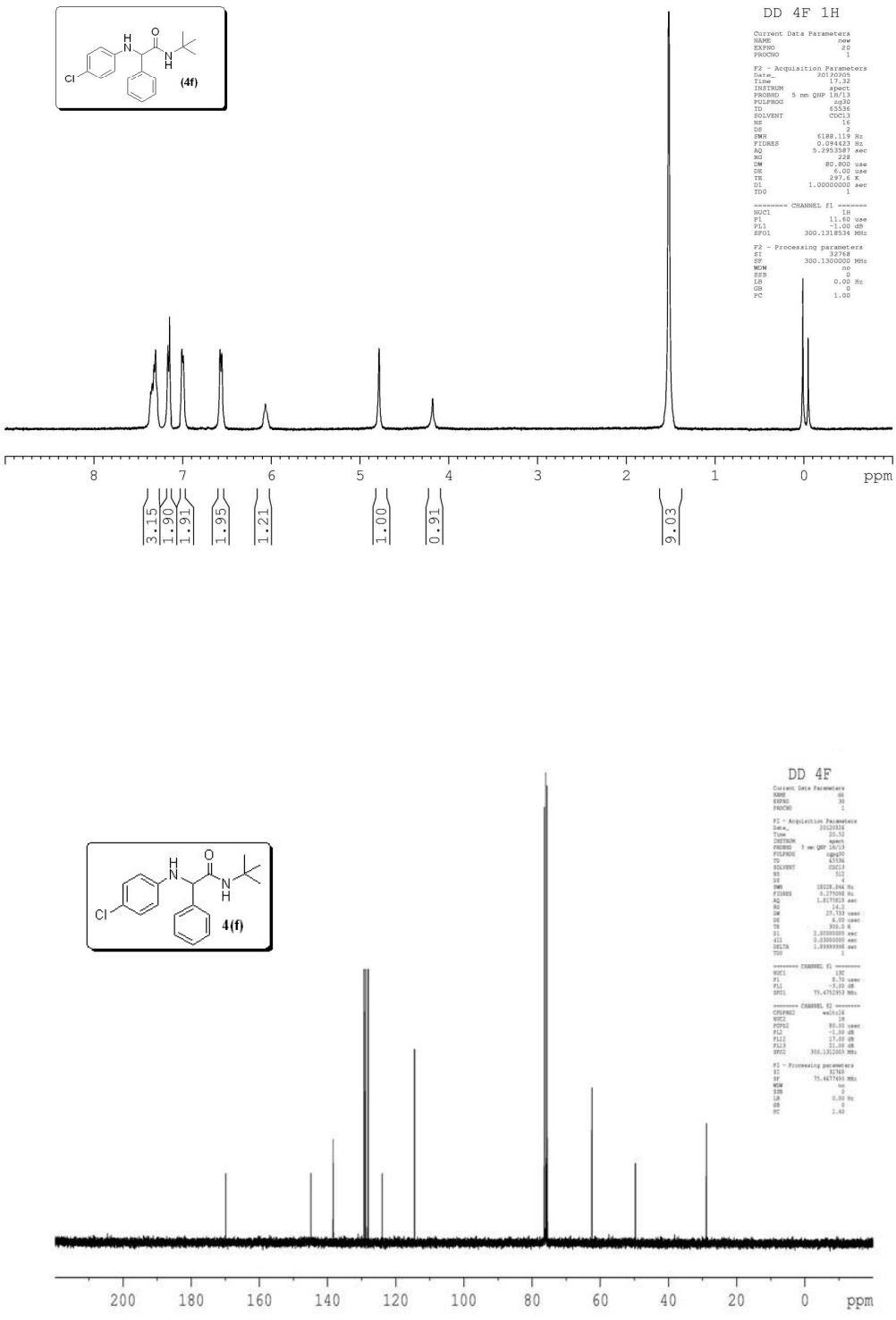
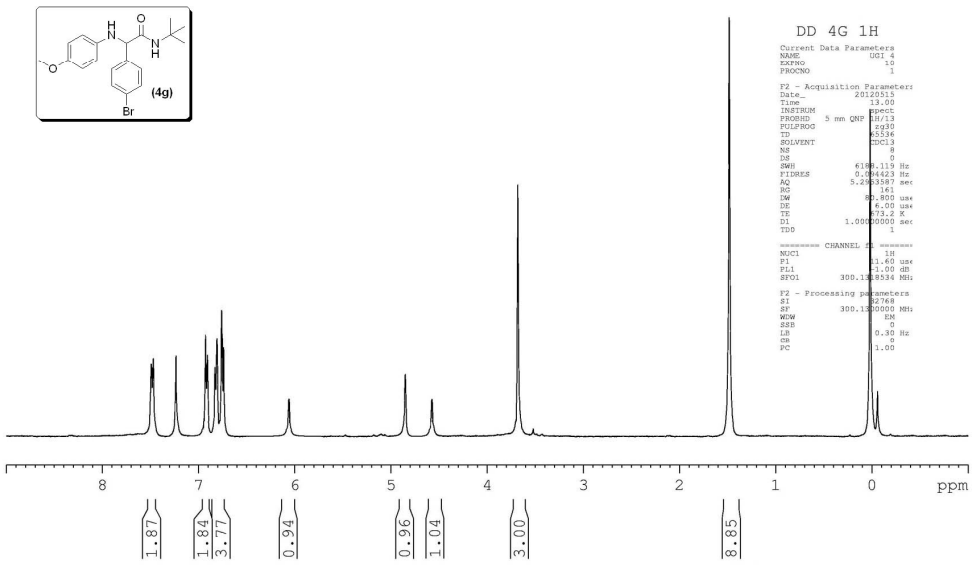


Fig. (4f)


(4g)
Br
DD 4G 1H
8
7
6
5
4
3
2
1
0
ppm
1.87
1.84
3.77
0.94
0.96
1.04
3.00
8.85

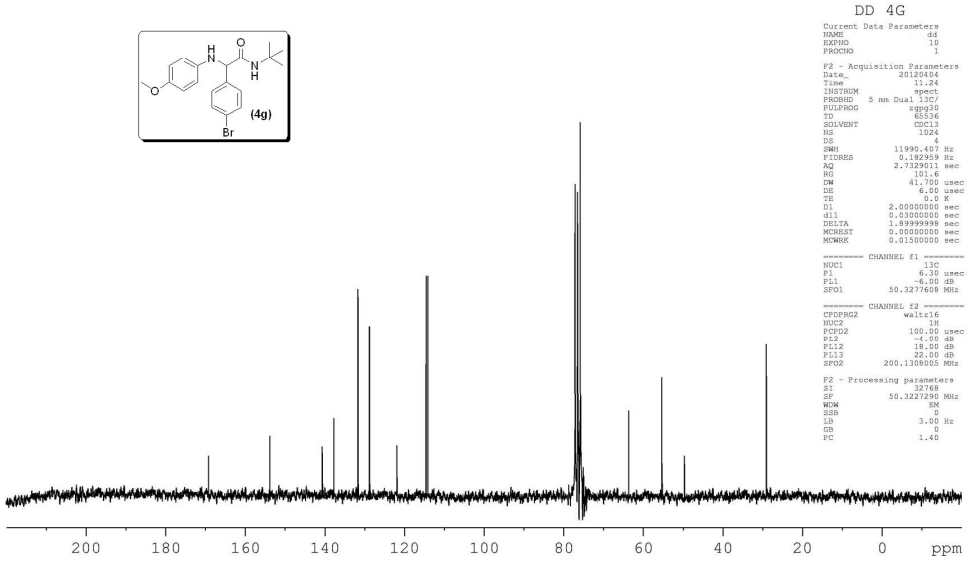
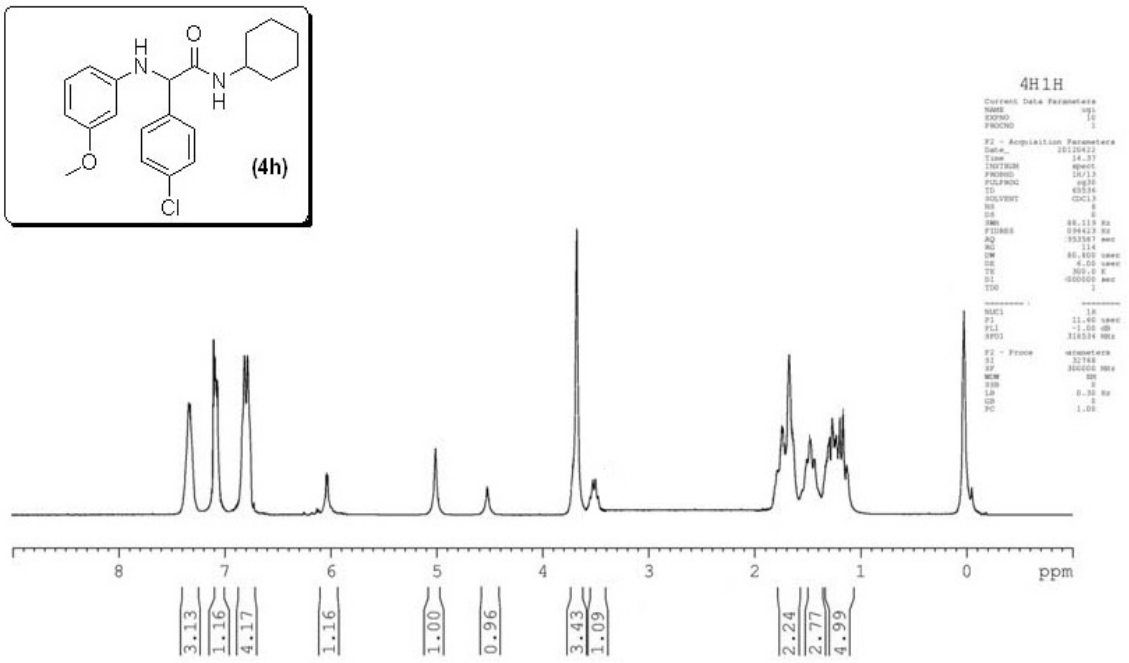

(4g)
Br
DD 4G
200
180
160
140
120
100
80
60
40
20
0
ppm

Fig. (4g)



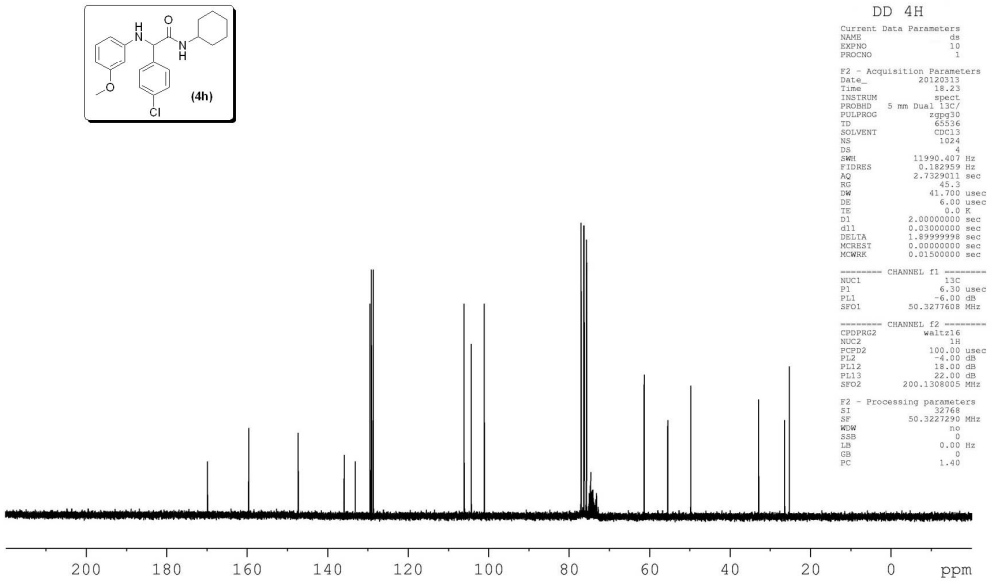
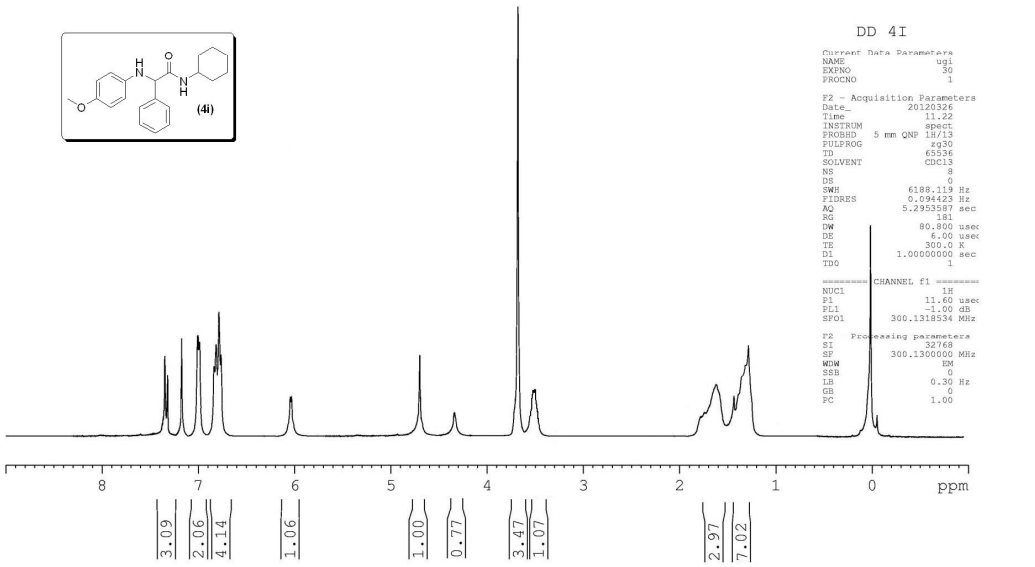


Fig. (4h)



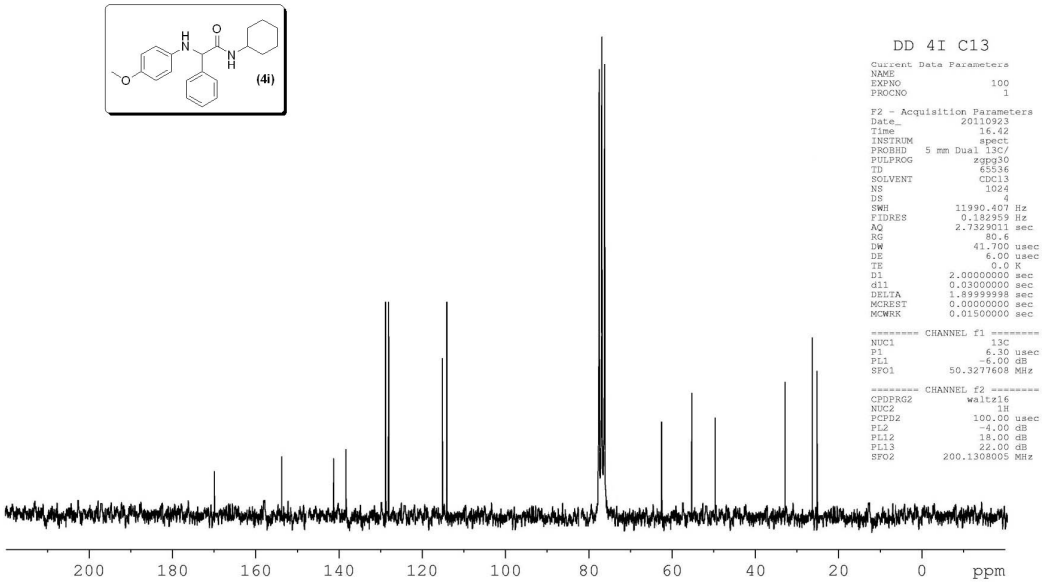
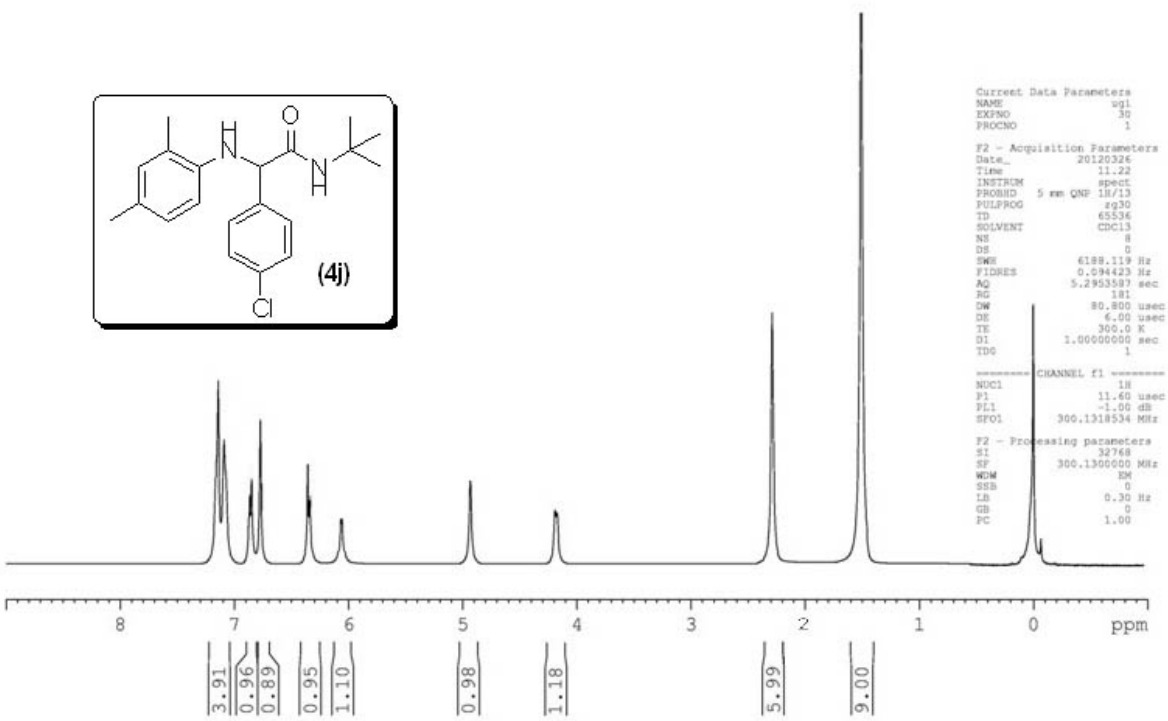


Fig. (4i)



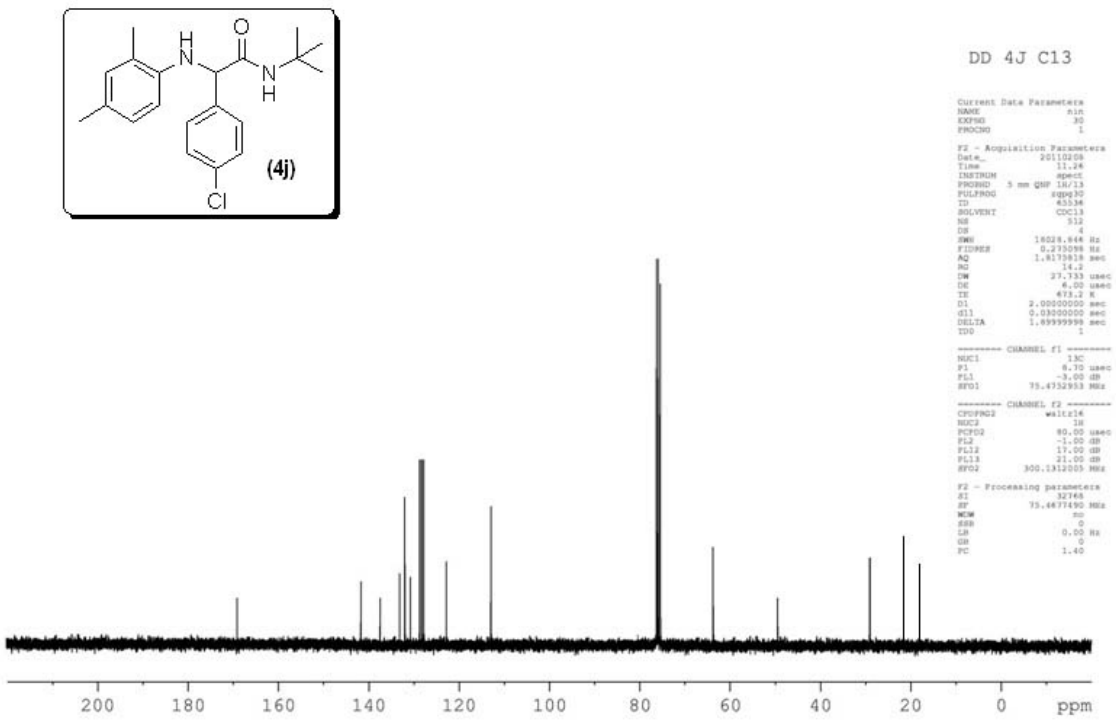


Fig. (4j)

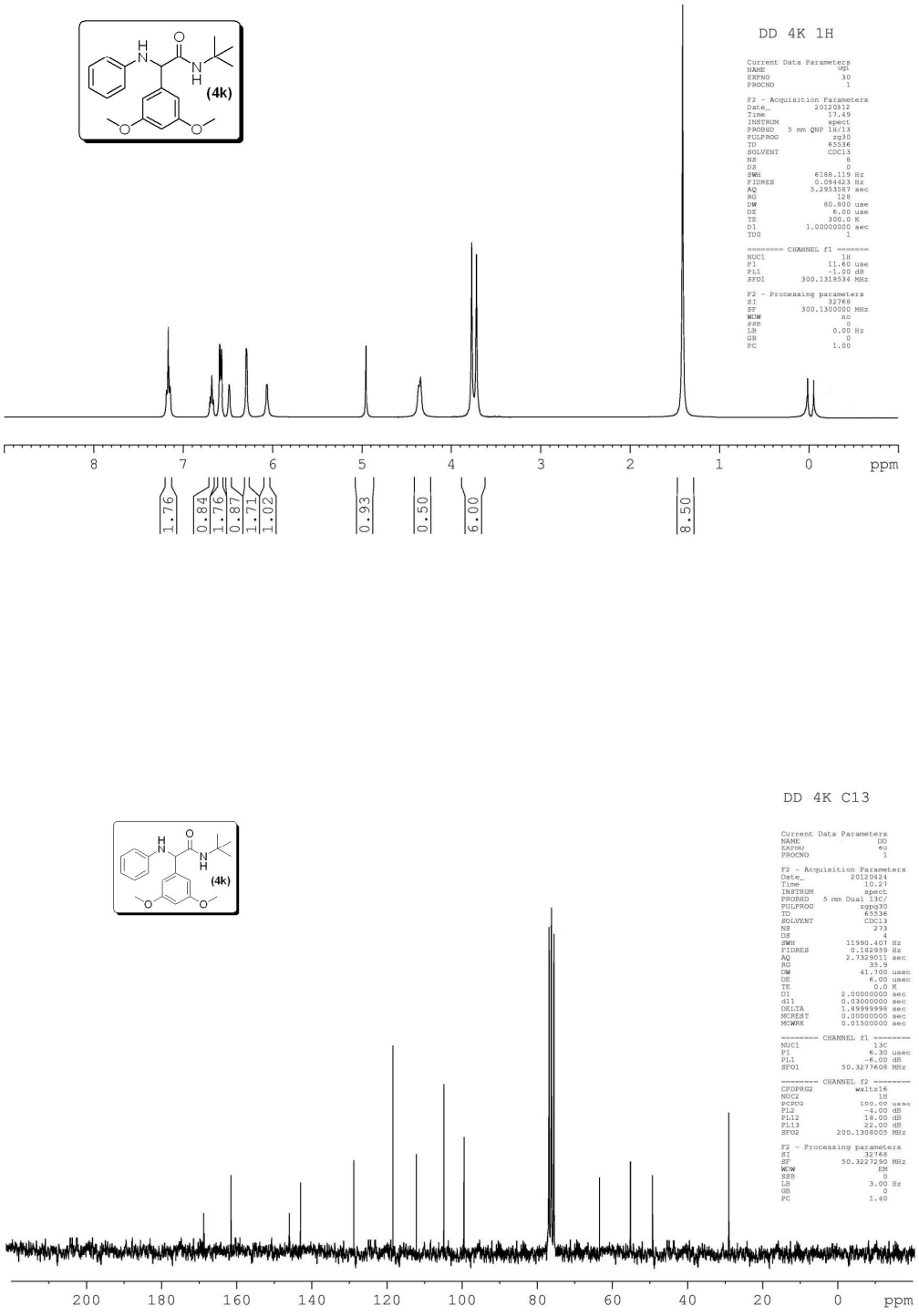
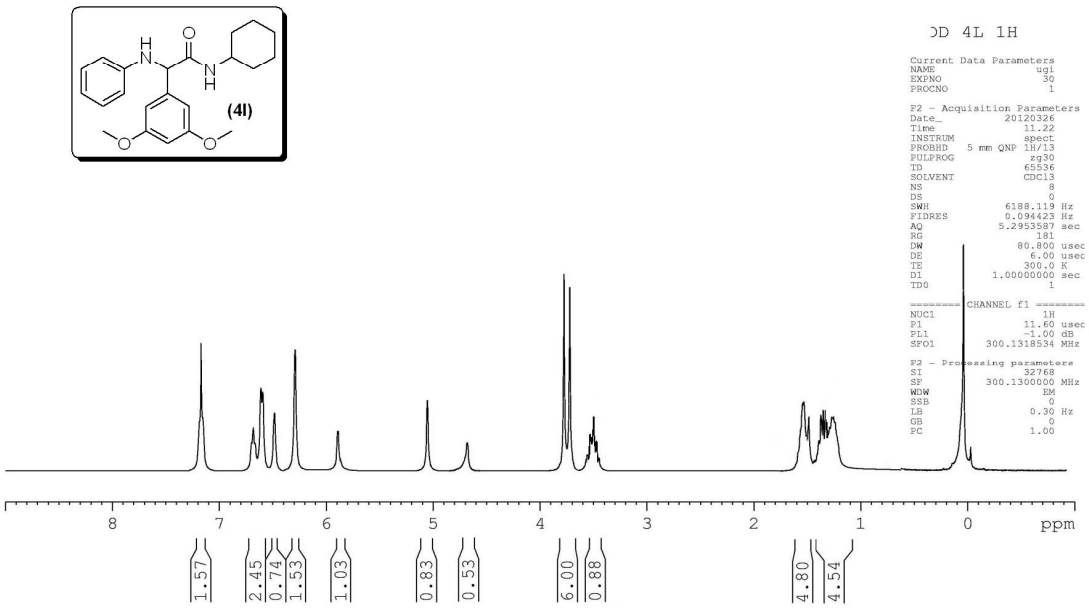


Fig. (4k)


(4l)
DD 4L 1H
ppm
1.57
2.45
0.74
1.53
1.03
0.83
0.53
6.00
0.88
4.80
4.54

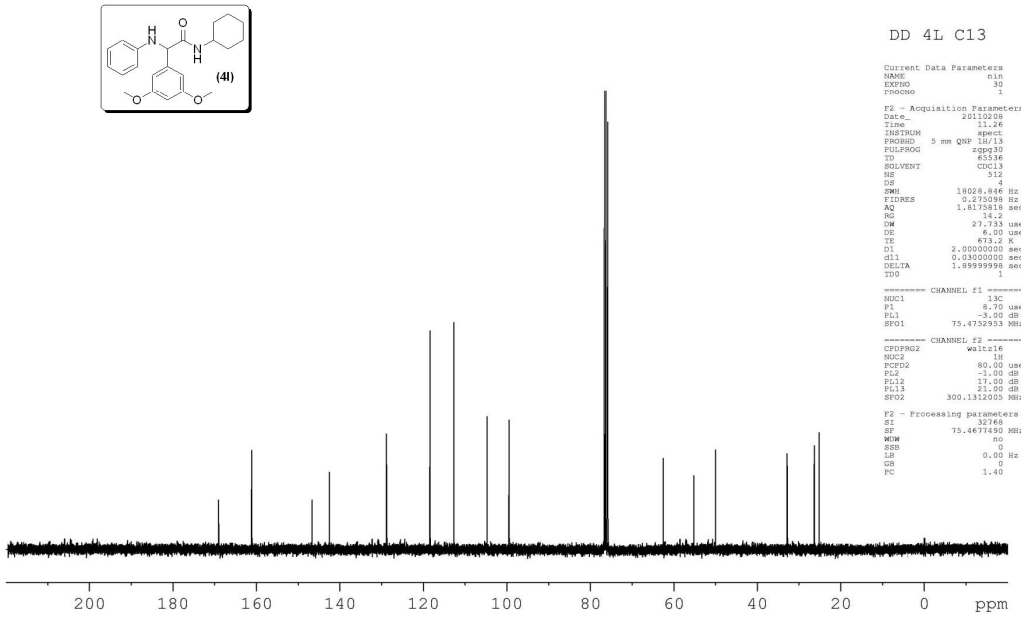
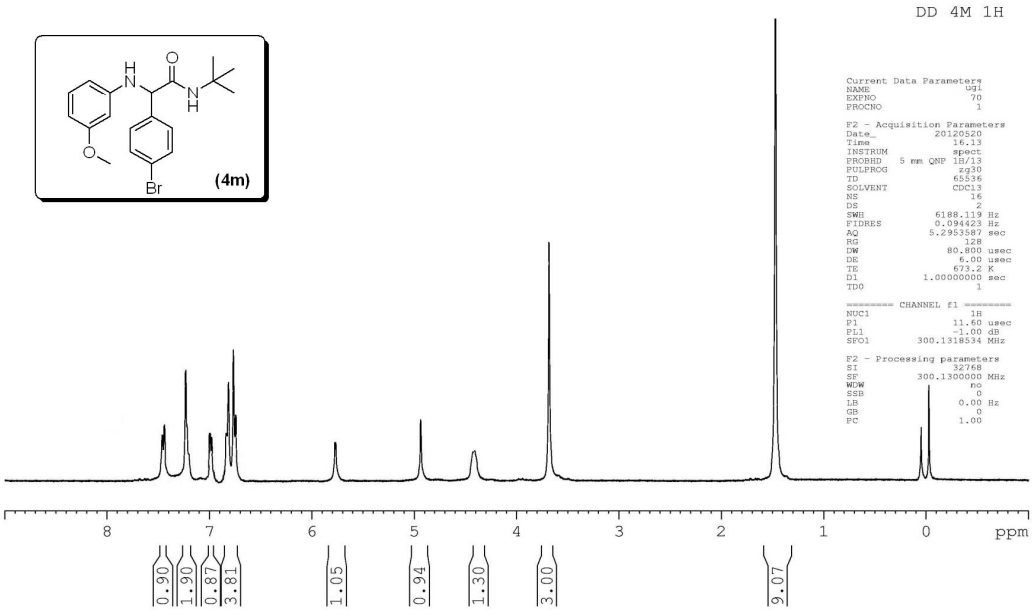

(4l)
DD 4L C13
ppm

Fig. (4l)


DD 4M 1H
(4m)
Br
8
7
6
5
4
3
2
1
0
ppm
0.90
1.90
0.87
3.81
1.05
0.94
1.30
3.00
9.07

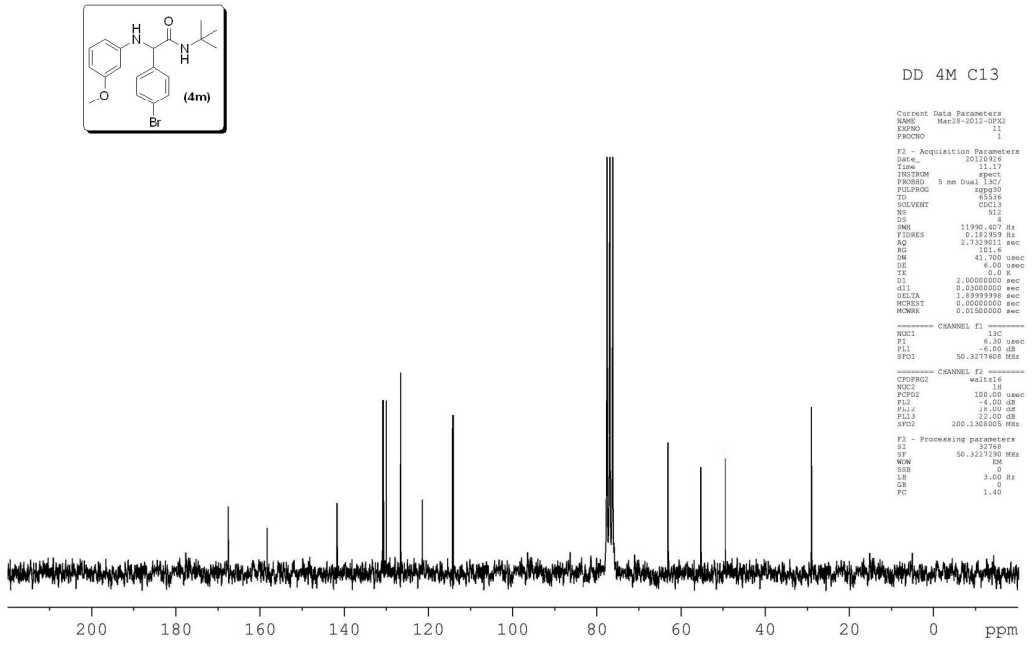
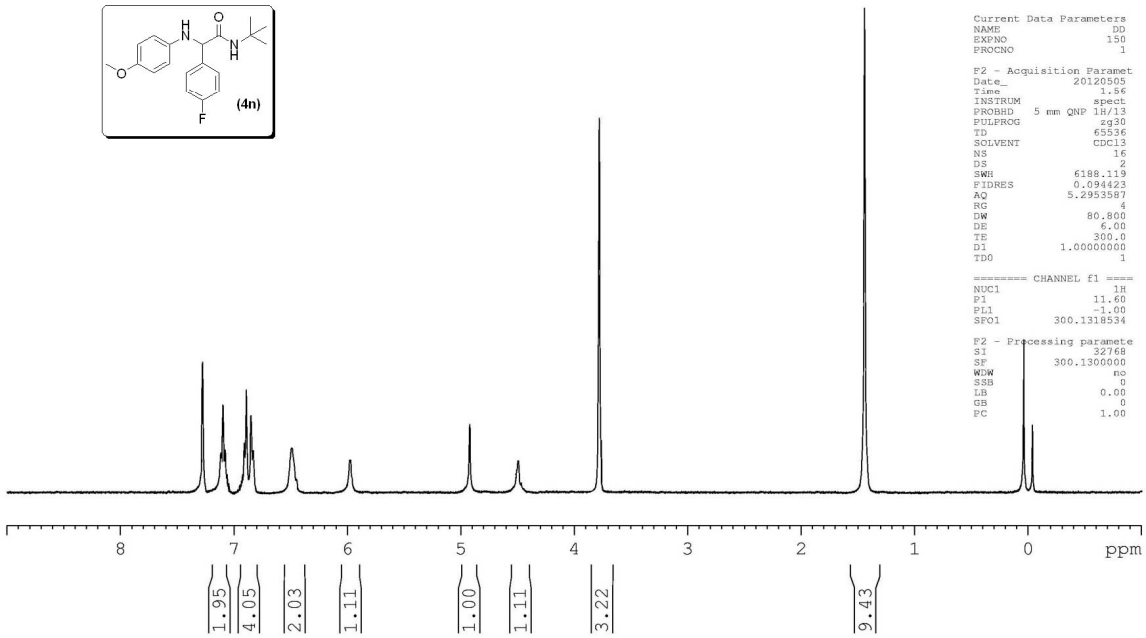

DD 4M C13
(4m)
Br
200
180
160
140
120
100
80
60
40
20
0
ppm

Fig. (4m)



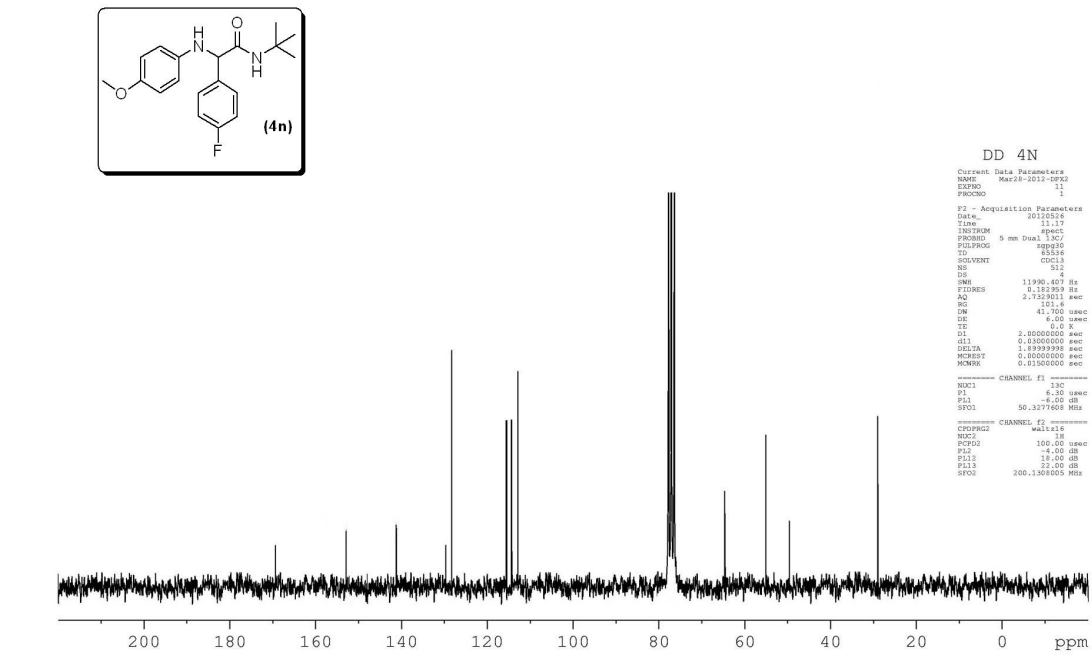


Fig. (4n)

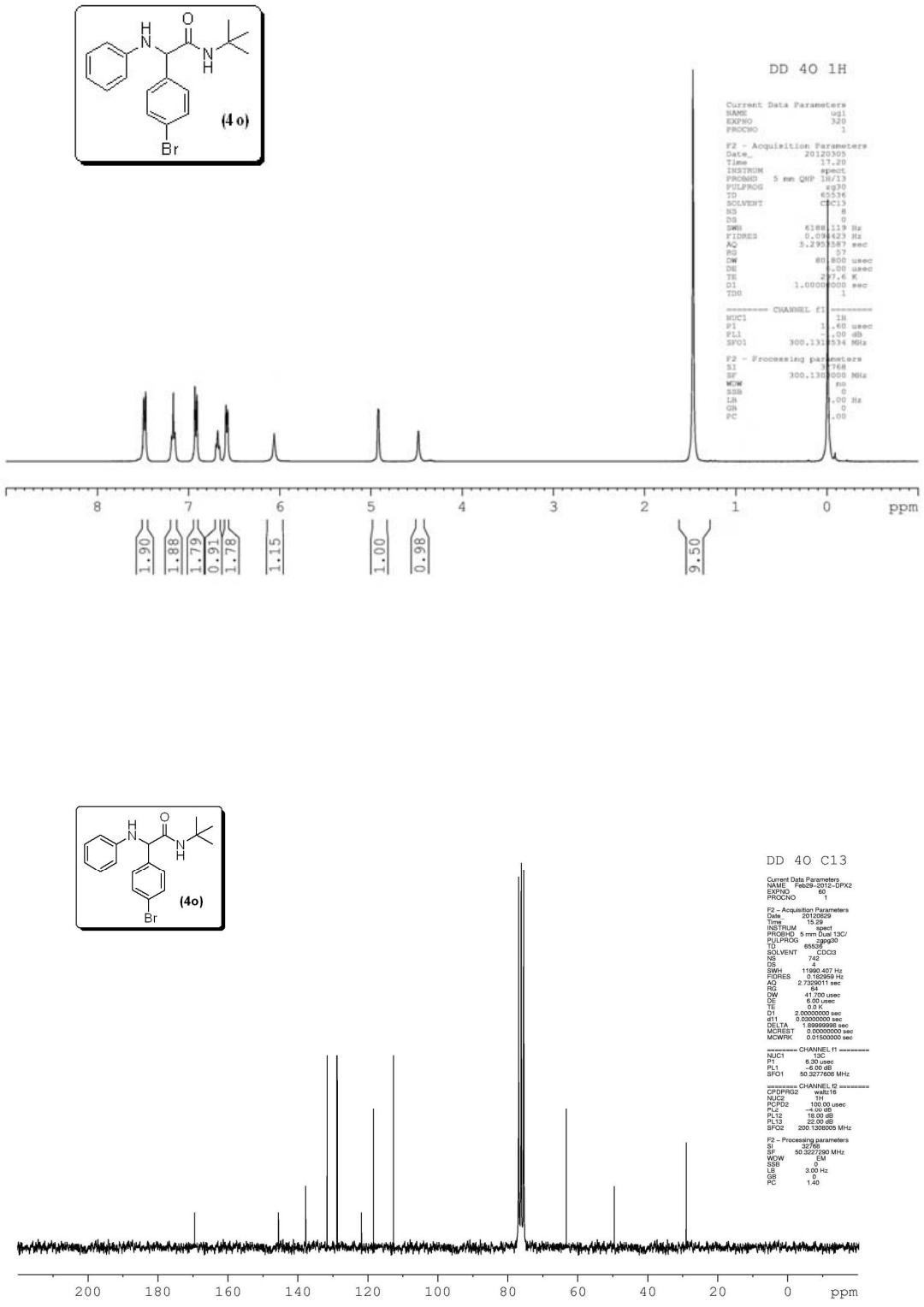
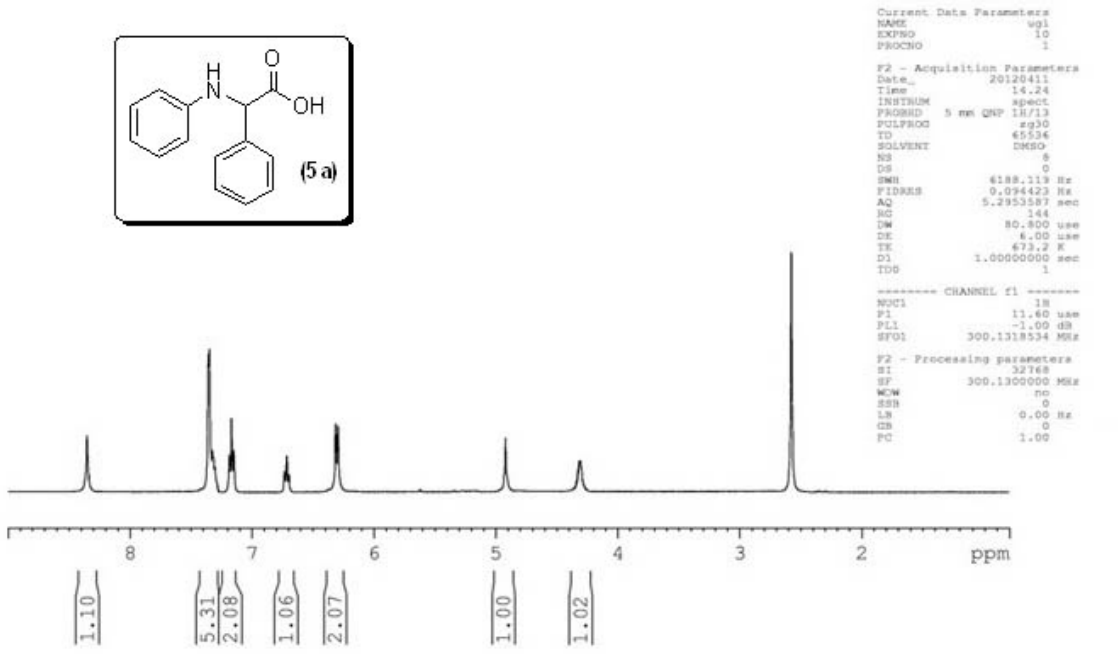

(4o)
Br
DD 4O 1H
ppm
1.90
1.88
1.79
0.91
1.78
1.15
1.00
0.98
9.50
(4o)
Br
DD 4O C13
200
180
160
140
120
100
80
60
40
20
0
ppm

Fig. (4o)



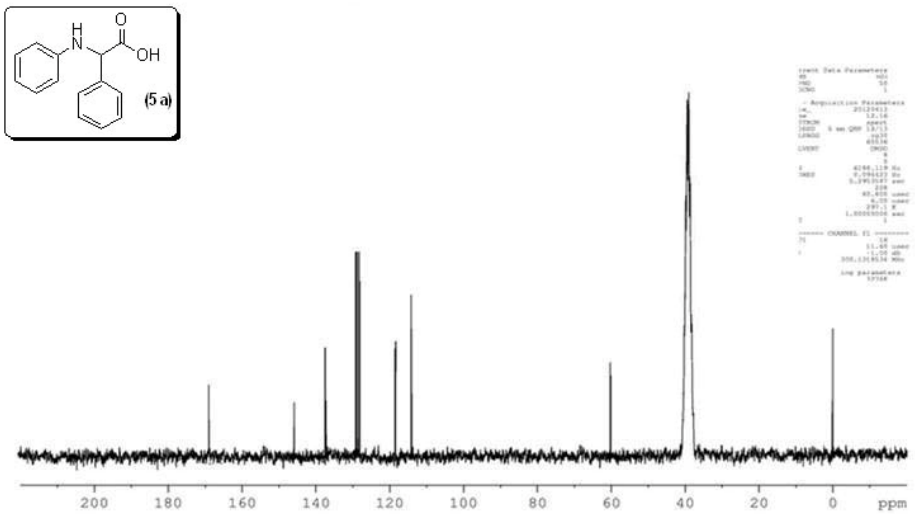
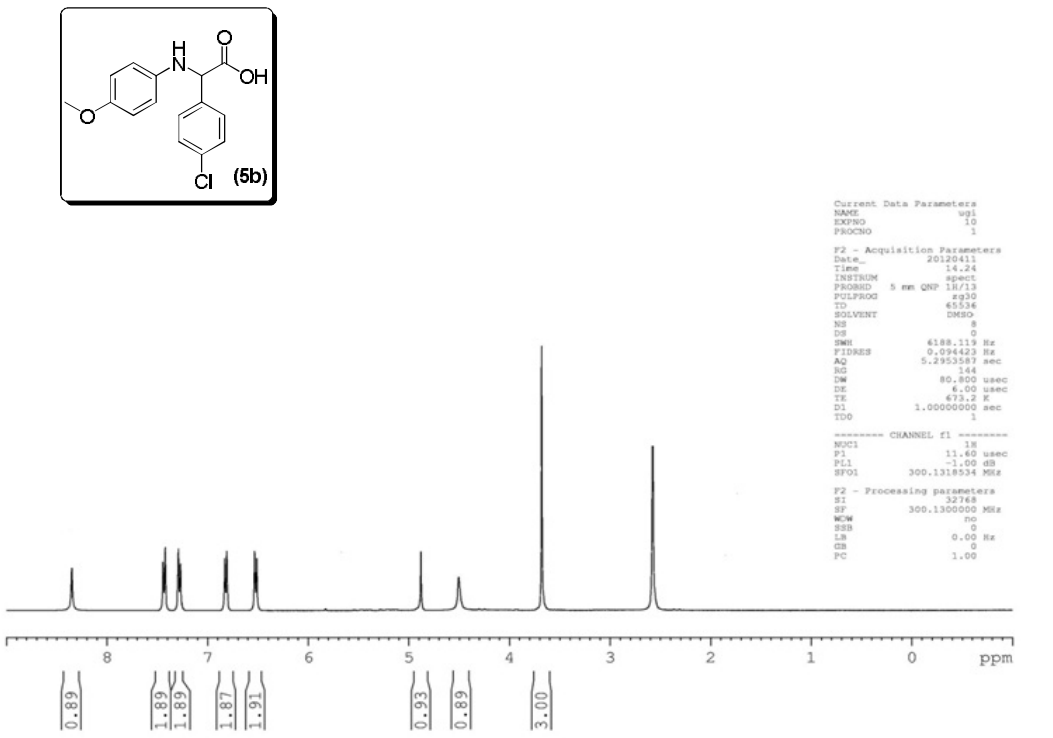


Fig. (5a)



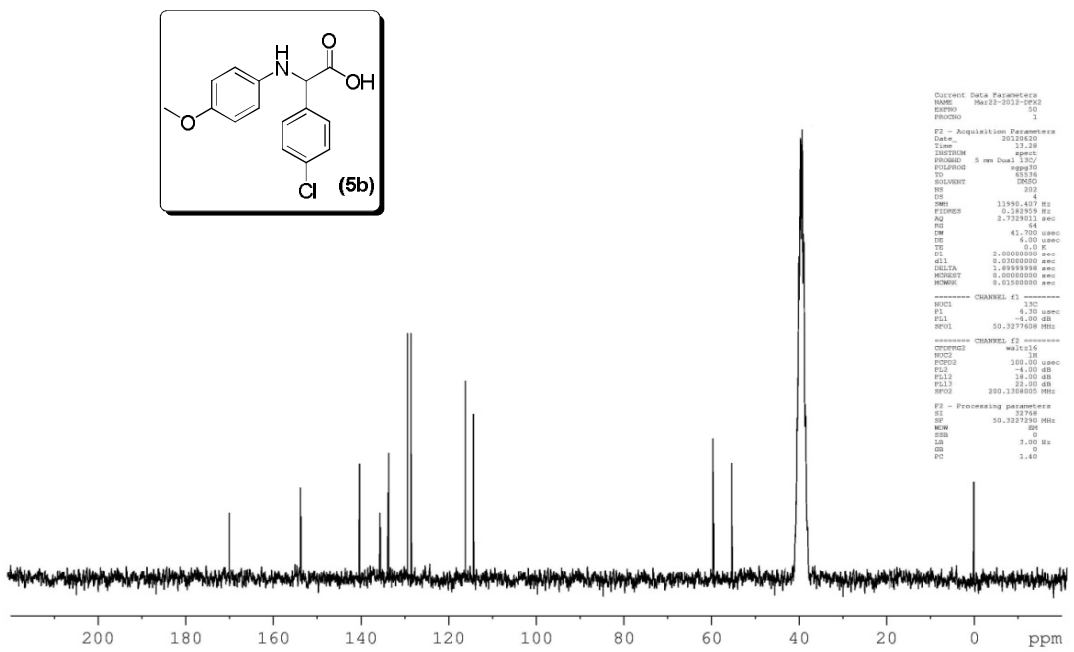
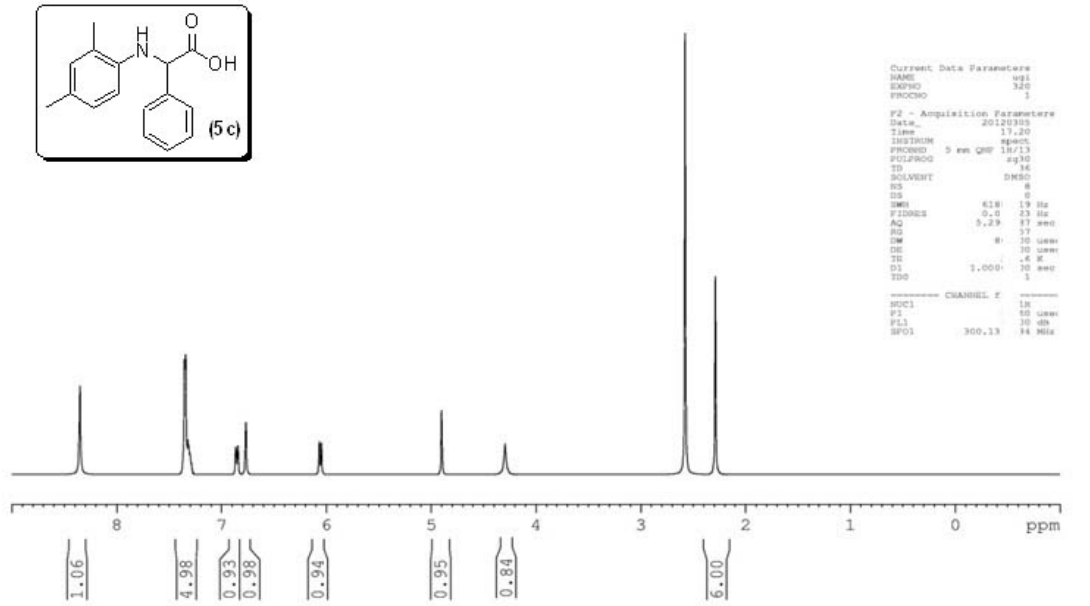


Fig. (5b)



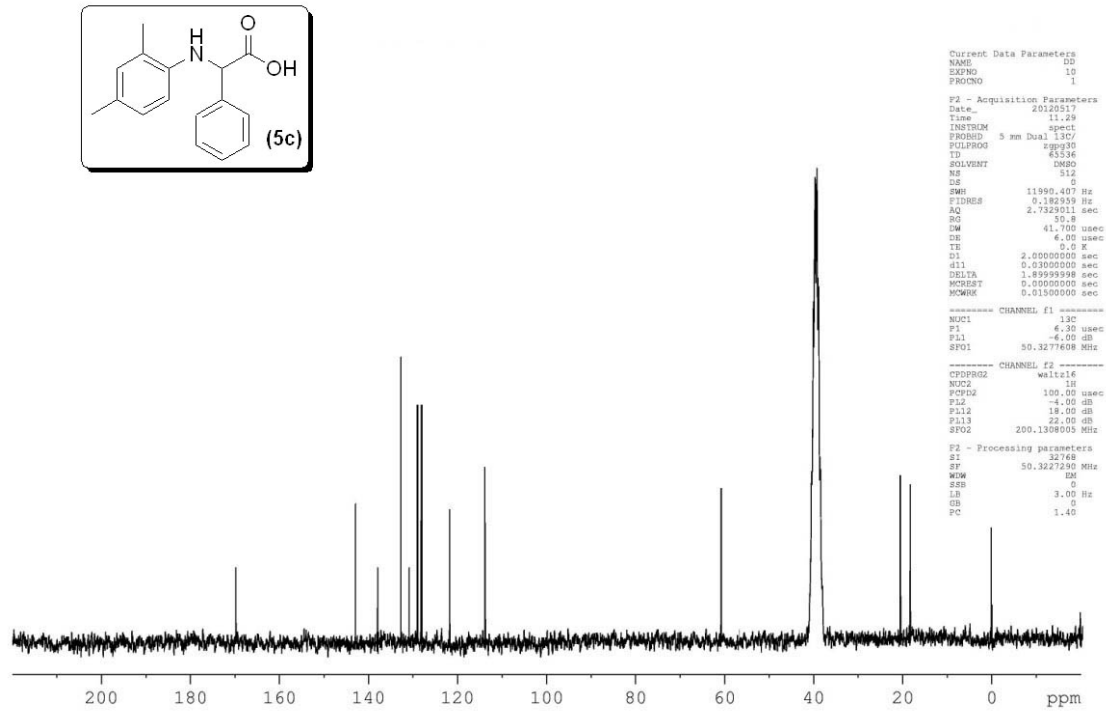


Fig. (5c)