Supporting Information

Synthesis of Tetrahydro-β-Carbolines via Isomerization of *N*-Allyltryptamines: A Metal-Catalyzed Variation on the Pictet-Spengler Theme

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General Methods

Unless otherwise stated, all reactions were run under an argon atmosphere. The glassware was dried over a Bunsen flame under vacuum, before contact with any of the reactants or solvents. All flasks were equipped with a rubber-septum, through which transport of chemicals, from or to the flask, was performed by use of a syringe equipped with a needle. Solvents were typically freshly distilled or dried over molecular sieves. All reactions were monitored by thin layer chromatography (TLC), reversed-phase high-performance liquid chromatography (RP-HPLC), and/or reversed-phase ultra-performance liquid chromatography mass spectrometry (RP-UPLC/MS).

All solvents were of HPLC quality, and all commercially available reagents were used without further purification. Typically all new compounds were characterized with ^{1}H NMR and ^{13}C NMR, IR, TLC, RP-HPLC, MS (ESI), HRMS (ESI) and melting point. Some compounds were characterized by HSQC, HMBC and/or melting point. Known compounds were characterized with ^{1}H- and ^{13}C NMR, TLC, RP-HPLC and MS alone. Intermediates, *N*-benzyl-(6-methoxy)tryptamine (**3j**), *N*-benzyl-(7-methyl)tryptamine, *N*-benzyl-(5-methyl)tryptamine, *N*-benzyl-(5-fluoro)tryptamine, and *N*-benzyl-(5-bromo)tryptamine were only characterized by ^{1}H NMR.

I*n vacuo* evaporation of solvents was performed using a rotary evaporator under house vacuum at various temperatures.

Analytical TLC was conducted using Merck aluminium sheets covered with silicagel C-60 F_{254}. The plates were either visualized under UV-light or stained by dipping in a developing agent followed by heating. $KMnO_4$ (3 g in H_2O (300 mL) along with K_2CO_3 (20 g) and 5% aqueous NaOH (5 mL)) and/or phosphomolybdic acid (PMA) (10 g in 200 mL EtOH) were used as developing agent.

Flash chromatography was performed using a glass column which was packed with Matrex 60 Å silicagel (35 – 70 µm particles) as stationary phase. The liquid phase is specified in the experimental procedures.

Analytical HPLC was conducted on a Water Alliance 2695 RP-HPLC system using a Symmetry® C-18 column (*d* 2.5 µm, 4.6 x 75 mm, column temp: 25 °C flow 1 mL/min) with detection at 215 nm and 254 nm. Eluents A (0.1% TFA in H_2O) and B (0.1% TFA in MeCN) were used in a linear gradient (100% A to 100% B) in a run time of 13 min. HPLC analysis of screening experiments was performed using a linear gradient (100% A to 100% B) in a run time of 23 min.

For the recording of ^{1}H NMR and ^{13}C NMR either a Varian Mercury-300 spectrometer (operating at 300 MHz for proton and 75 MHz for carbon), or a Varian Unity Inova-500 spectrometer (operating at 500 MHz for ^{1}H NMR) were used. HSQC and HMBC were also recorded on a Varian Unity Inova-500 spectrometer. The chemical shifts (δ) are reported in parts per million (ppm) and the coupling constants (*J*) in Hz. Usually DMSO-d_6 and $CDCl_3$ were used as the solvent and signal positions were measured relative to the signal for DMSO (δ 2.50 ppm for ^{1}H NMR and δ 39.43 ppm for ^{13}C NMR) and $CHCl_3$ (δ 7.26 ppm, for ^{1}H NMR and δ 77.36 ppm for ^{13}C NMR). Multiplicities of peaks in ^{1}H NMR are given as: s (singlet), d (doublet), t (triplet),), dd (double doublet), ddd (double double doublet), dddd (double double double doublet), dt (double triplet), ddt (double double triplet), t (triplet) td (triplet of doublet), tt (triplet of triplet), ddq (double double quartet), dqd (double quartet of doublets), dp (double pentet), and m (multiplet).

IR analysis was performed on a Bruker Alpha FT-IR spectrometer and reported in frequency of absorption (cm^{-1}).

Analytical LC/MS (ESI) analysis was performed on a Waters AQUITY RP-UPLC system equipped with a diode array detector using an AQUITY UPLC BEH C-18 column (*d* 1.7 µm, 2.1 x 50 mm; column temp: 65 °C; flow: 0.6 mL/min). Eluents A (0.1% HCO_2H in H_2O) and B (0.1% HCO_2H in acetonitrile) were used in a linear gradient (5% B to 100% B) in a total run time of 2.6 min. The LC system was coupled to a SQD mass spectrometer. Analytical LC-HRMS (ESI) analysis was performed on an Agilent 1100 RP-LC system equipped with a diode array detector using a Phenomenex Luna C-18 column (*d* 3 µm, 2.1 x 50 mm; column temp: 40 °C; flow: 0.4 mL/min). Eluents A (0.1% HCO_2H in H_2O) and B (0.1% HCO_2H in acetonitrile) were used in a linear gradient (20% B to 100% B) in a total run time of 15 min. The LC system was coupled to a Micromass LCT orthogonal time-of-flight mass spectrometer equipped with a Lock Mass probe operating in positive electrospray mode.

Melting points were measured using a Thomas Hoover capillary melting point apparatus.

Optimization of Metal-Catalyzed THBC Synthesis (1a to 2a)

General method for catalyst screening

Screening experiments were carried out in carousel equipment for parallel synthesis. All reactions were run in 20 – 30 mg scale (0.1 M concentration of starting material). Analysis aliquots of the reaction mixtures were taken out with the tip of a Pasteur pipette, followed by argon flush of the reaction tube. The samples were evaporated to dryness under reduced pressure prior to RP-HPLC analysis.

Structures of selected catalysts

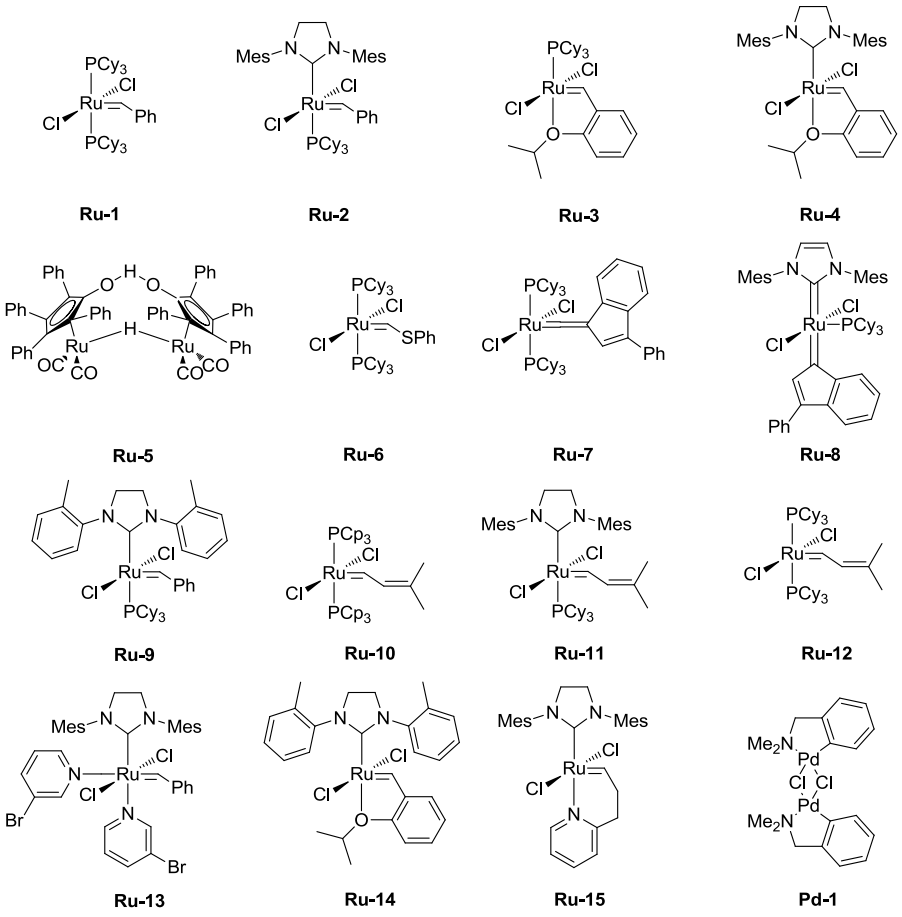
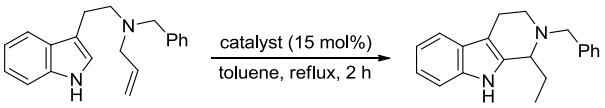


Table SI-1. Catalyst abbreviations and names

Entry	Catalyst abbreviation	Catalyst name (commercial)
1	Ru-1	Grubbs catalyst 1st generation
2	Ru-2	Grubbs catalyst 2nd generation
3	Ru-3	Hoveyda-Grubbs catalyst 1st generation
4	Ru-4	Hoveyda-Grubbs catalyst 2nd generation
5	Ru-5	1-Hydroxytetraphenylcyclopentadienyl-(tetraphenyl-2,4-cyclopentadien-1-one)-μ-hydrotetracarbonyldiruthenium(II)
6	Ru-6	Bis(tricyclohexylphosphine)[(phenylthio)methylene]ruthenium (IV) dichloride
7	Ru-7	Bis(tricyclohexylphosphine)-3-phenyl-1H-inden-1-ylideneruthenium(IV) dichloride
8	Ru-8	Tricyclohexylphosphine[1,3-bis(2,4,6-trimethylphenyl)imidazol-2-ylidene][3-phenyl-1H-inden-1-ylidene]ruthenium(II) dichloride
9	Ru-9	[1,3-Bis(2-methylphenyl)-2-imidazolidinylidene]dichloro(phenylmethylene)(tricyclohexylphosphine)ruthenium(II)
10	Ru-10	Dichloro(3-methyl-2-butenylidene)bis(tricyclopentylphosphine)ruthenium(II))
11	Ru-11	Dichloro[1,3-bis(2,4,6-trimethylphenyl)-2-imidazolidinylidene](3-methyl-2-butenylidene)(tricyclohexylphosphine)ruthenium(II)
12	Ru-12	Dichloro(3-methyl-2-butenylidene)bis(tricyclohexylphosphine)ruthenium(II)
13	Ru-13	Dichloro[1,3-bis(2,4,6-trimethylphenyl)-2-imidazolidinylidene](benzylidene)bis(3-bromopyridine)ruthenium(II)
14	Ru-14	Dichloro[1,3-bis(2-methylphenyl)-2-imidazolidinylidene](2-isopropoxyphenylmethylene)ruthenium(II)
15	Ru-15	Dichloro[1,3-bis(2,4,6-trimethylphenyl)-2-imidazolidinylidene][3-(2-pyridinyl)propylidene]ruthenium(II)
16	Pd-1	Di-μ-chlorobis[2-[(dimethylamino)methyl]phenyl-C,N]dipalladium(II)
17	*(R)*-TRIP	(*R*)-(–)-3,3′-Bis(triphenylsilyl)-1,1′-binaphthyl-2,2′-diyl hydrogenphosphate

Table SI-2. Transition metal catalysts for the synthesis of THBC 2a

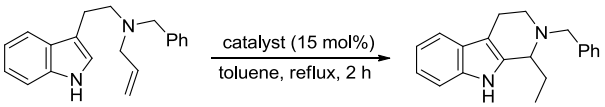


1a **2a**

Entry	Catalyst	Conversion (%)[a, b]
1	None	0
2	TFA	0[c]
3	(*R*)-TRIP	0[c]
4	[Rh((*S*,*S*)MeBPE)(cod)]BF_4	100[d]
5	Rh(cod)Cl dimer	13
6	$Rh(PPh_3)_3Cl$	100
7	$Rh(acac)(CO)_2$	42
8	$Pd(P(o\text{-tolyl})_3)_2Cl_2$	0
9	$Pd(PPh_3)_4$	100
10	$Pd_2(dba)_3$	63
11	$Pd(PPh_3)_2Cl_2$	0
12	Pd-1	0
13	$Pd(cod)Cl_2$	0
14	$Pd(Pt\text{-}Bu_3)_2$	100
15	$Pd(PhCN)_2Cl_2$	0

[a] Determined by RP-HPLC (215 nm); [b] Reaction mixtures were generally clean (>85% of **1a** and **2a** as determined by RP-HPLC); [c] Reaction carried out with 5 mol% of catalyst. [d] The reaction product was analyzed by chiral RP-HPLC and the enantiomeric excess was found to be <1%.

Table SI-3. Ruthenium catalysts for the synthesis of THBC 2a

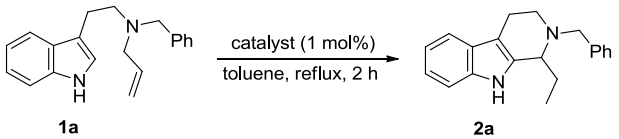


1a **2a**

Entry	Catalyst	Conversion (%)[a, b]
1	Ru-1	78
2	Ru-2	100
3	Ru-2 + *(R)*-TRIP	100[c]
4	Ru-3	100
5	Ru-4	100
6	Ru-5	NA[d]
7	Ru-6	100
8	Ru-7	100
9	Ru-8	100
10	Ru-9	100
11	Ru-10	100
12	Ru-11	95
13	Ru-12	100
14	Ru-13	100
15	Ru-14	100
16	Ru-15	36

[a] Determined by RP-HPLC (215 nm); [b] Reaction mixtures were generally clean (>85% of **1a** and **2a** as determined by RP-HPLC); [c] The reaction product was analyzed by chiral RP-HPLC and the enantiomeric excess was found to be 17%; [d] Complex reaction mixture.

Table SI-4. Transition metal catalysts (1 mol%) for the synthesis of THBC 2a

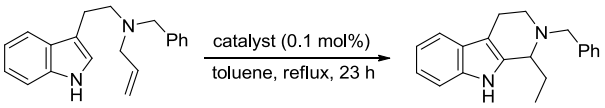


1a **2a**

Entry	Catalyst	Conversion (%)[a, b]	
		6 h	23 h
1	[Rh((*S*,*S*)MeBPE)(cod)]BF_4	16	25
2	$Rh(PPh_3)_3Cl$	76	100
3	$Pd(PPh_3)_4$	58	66
4	$Pd(P(t\text{-}Bu)_3)_2$	5	14
5	Ru-2	95	95
6	Ru-2 + *(R)*-TRIP	23	25
7	Ru-3	6	10
8	Ru-4	30	47
9	Ru-6	21	40
10	Ru-7	17	26
11	Ru-8	29	47
12	Ru-9	95	100
13	Ru-10	12	19
14	Ru-11	19	42
15	Ru-13	31	55
16	Ru-14	100	100

[a] Determined by RP-HPLC (215 nm); [b] Reaction mixtures were generally clean (>85% of **1a** and **2a** as determined by RP-HPLC).

Table SI-5. Transition metal catalysts (0.1 mol%) for the synthesis of THBC 2a



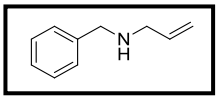
1a **2a**

entry	Catalyst	Conversion (%)[a, b]
1	$Rh(PPh_3)_3Cl$	33
2	$RuHCl(CO)(PPh_3)_3$	14
3	Ru-2	97
4	Ru-9	42
5	Ru-14	95

[a] Determined by RP-HPLC (215 nm); [b] Reaction mixtures were generally clean (>85% of **1a** and **2a** as determined by RP-HPLC).

Synthetic Procedures and Analytical Data for Tryptamine Derivatives (3a-e, 3j and 1a-s)

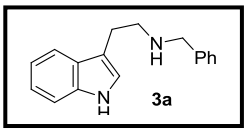
N-benzyl-allylamine[1]



In a round-bottomed flask fitted with a magnetic stirring bar, benzyl bromide (4.99 g, 3.46 mL, 29.2 mmol) was added dropwise to a stirred suspension of K_2CO_3 (4.83 g, 35.1 mmol) in allyl amine (13.32 g, 17.5 mL, 233 mmol) over 45 min. The reaction was stirred at rt overnight, whereupon the reaction mixture was filtered through a pad of celite, which was washed with CH_2Cl_2 (2 x 25 mL). The filtrate was then evaporated *in vacuo*, and the crude product was distilled at 3.1 mbar, 75°C (kugehlror) to give the title compound as a clear oil (2.43 g, 57%). R_f = 0.26 (EtOAc; UV; $KMnO_4$); HPLC purity: 93% (R_t = 4.01 min); ^{1}H NMR (300 MHz, DMSO-d_6) δ 7.34 – 7.26 (m, 4H), 7.21 (ddd, *J* = 10.7, 5.2, 2.9 Hz, 1H), 5.93 – 5.78 (m, 1H), 5.15 (ddd, *J* = 17.3, 3.8, 1.7 Hz, 1H), 5.09 – 5.00 (m, 1H), 3.66 (s, 2H), 3.12 (dd, *J* = 5.7, 1.4 Hz, 2H), 2.18 (br. s, 1H); ^{13}C NMR (75 MHz, DMSO-d_6) δ 140.7, 137.5, 127.9, 127.8, 126.3, 115.0, 52.2, 50.1; MS (ESI) *m/z*: calcd for $C_{10}H_{14}N$ $[M + H]^+$ 148.1, found 148.1.

N-Benzyltryptamine (3a)[2]

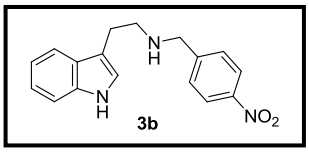
General procedure (I): *Reductive alkylation of tryptamine*



In a round-bottomed flask fitted with a magnetic stirring bar, tryptamine (2.50 g, 15.6 mmol) and benzaldehyde (1.66 g, 1.59 mL, 15.6 mmol) were dissolved in MeOH (63 mL). The reaction mixture was added molecular sieves (3Å) and stirred at rt. The reaction was monitored by TLC, and upon full conversion of benzaldehyde (24 h), solid $NaBH_4$ (590 mg, 15.6 mmol) was added. After further 16 h of stirring, the reaction mixture was filtered through a pad of celite, which was washed with MeOH (2 x 50 mL). The filtrate was evaporated *in vacuo*. The residue was taken up in sat. $NaHCO_3$ (50 mL), H_2O (50 mL) and EtOAc (100 mL) and transferred to a separatory funnel. The organic layer was separated and washed with H_2O (50 mL) and brine (50 mL). The organic layer was dried over Na_2SO_4 and evaporated *in vacuo* to give the title compound as a brown oil (3.89g, >95%). The compound was used in the next step without further purification. R_f = 0.25 (EtOAc; UV; $KMnO_4$); HPLC purity: > 95% (R_t = 5.77min); ^{1}H NMR (300 MHz, DMSO-d_6) δ 10.79 (s, 1H), 7.49 (d, *J* = 7.8 Hz, 1H), 7.37 – 7.25 (m, 5H), 7.24 – 7.16 (m, 1H), 7.12 (d, *J* = 2.3 Hz, 1H), 7.09 – 7.01 (m, 1H), 6.99 – 6.90 (m, 1H), 3.87 (s, 2H), 2.91 – 2.74 (m, 4H); ^{13}C NMR (75 MHz, DMSO-d_6) δ 140.8, 136.2, 128.0, 127.9, 127.2, 126.4, 122.5, 120.8, 118.2, 118.0, 112.5, 111.3, 52.8, 49.5, 25.4; MS (ESI) *m/z*: calcd for $C_{17}H_{19}N_2$ $[M + H]^+$ 251.2, found 251.3.

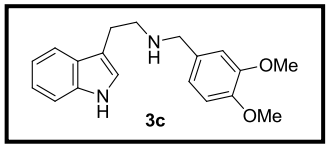
[1] Mukharjee. S.; List. B. *J. Am. Chem. Soc.* **2007,** *129*, 11336-11337
[2] David. B.; Martin. C.; Vanderwal. C. D. *J. Am. Chem. Soc.* **2009,** *131*, 3472-3473

N-(4-Nitro)benzyltryptamine (3b)



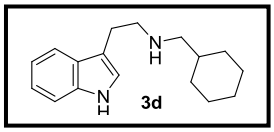
Following **general procedure (I)**, the reaction of tryptamine (300 mg, 1.87 mmol), 4-nitrobenzaldehyde (283 mg, 1.87 mmol) and $NaBH_4$ (71 mg, 1.87 mmol) gave, after aqueous work-up, the title compound as brown amorphous solid (525 mg, 95%). The compound was used in the next step without further purification; HPLC purity: > 95% (R_t = 5.86 min); IR (neat) cm^{-1}: 3404, 3052, 2920, 2850, 1559, 1507, 1452, 1100; ^1H NMR (300 MHz, DMSO-d_6) δ 10.80 (s, 1H), 8.20 – 8.09 (m, 2H), 7.58 (d, *J* = 5.6 Hz, 2H), 7.49 (d, *J* = 7.6 Hz, 1H), 7.33 (d, *J* = 8.0 Hz, 1H), 7.13 (d *J* = 2.3 Hz, 1H), 3.86 (s, 2H), 2.91 – 2.83 (m, 2H), 2.83 – 2.75 (m, 2H); ^{13}C NMR (75 MHz, DMSO-d_6) δ 149.6, 146.1, 136.2, 128.7, 127.2, 123.1, 122.5, 120.8, 118.2, 118.0, 112.4, 111.3, 52.0, 49.5, 25.5; MS (ESI) *m/z*: calcd for $C_{17}H_{18}N_3O_2$ $[M + H]^+$ 296.1, found 296.3.

N-(3,4-Dimethoxy)benzyltryptamine (3c)



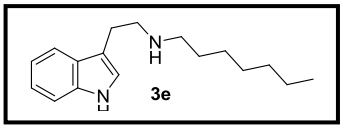
Following **general procedure (I)**, the reaction of tryptamine (300 mg, 1.87 mmol), 3,4-dimethoxybenzaldehyde (311 mg, 1.87 mmol) and $NaBH_4$ (71 mg, 1.87 mmol) gave, after aqueous work-up, the title compound as a brown oil (550 mg, 95%). The compound was used in the next step without further purification. R_f = 0.32 (MeOH:CH_2Cl (1:3); UV; $KMnO_4$); HPLC purity: > 95% (R_t = 5.61 min); IR (neat) cm^{-1}: 3368, 2913, 2833, 1607, 1513, 1259, 1231, 1137, 1024; ^1H NMR (300 MHz, DMSO-d_6) δ 10.79 (s, 1H), 7.49 (d, *J* = 7.7 Hz, 1H), 7.32 (d, *J* = 8.1 Hz, 1H), 7.13 (d, *J* = 2.2 Hz, 1H), 7.05 (t, *J* = 7.0 Hz, 1H), 6.95 (t, *J* = 7.1 Hz, 2H), 6.88 – 6.79 (m, 2H), 3.71 (s, 6H), 3.70 (s, 2H), 3.35 (br. s, 1H), 2.93 – 2.64 (m, 4H); ^{13}C NMR (75 MHz, DMSO-d_6) δ 148.5, 147.5, 136.2, 132.9, 127.2, 122.5, 120.8, 119.9, 118.3, 118.1, 112.4, 111.7, 111.4, 111.3, 55.4, 55.2, 52.4, 49.3, 25.2; HRMS (ESI) m/z: calcd for $C_{19}H_{23}N_2O_2$ $[M + H]^+$ 311.1760, found 311.1755.

N-Cyclohexylmethyltryptamine (3d)



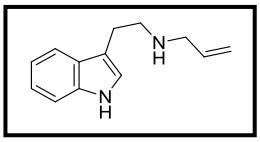
Following **general procedure (I)**, the reaction of tryptamine (300 mg, 1.87 mmol), cyclohexanecarbaldehyde (210 mg, 227 µL, 1.87 mmol) and $NaBH_4$ (71 mg, 1.87 mmol) gave, after aqueous work-up, the title compound as a yellow oil (471 mg, >95%). The compound was used in the next step without further purification. R_f = 0.22 (MeOH:CH_2Cl_2 (1:1); UV; $KMnO_4$); HPLC purity: > 95% (R_t = 6.30 min); IR (neat) cm^{-1}: 3410, 3326, 3050, 2915, 2839, 1619, 1447, 1355, 1341, 1192; ^1H NMR (300 MHz, DMSO-d_6) δ 10.78 (s, 1H), 7.50 (d, *J* = 7.7 Hz, 1H), 7.32 (d, *J* = 8.0 Hz, 1H), 7.12 (d, *J* = 2.2 Hz, 1H), 7.05 (t, *J* = 7.5 Hz, 1H), 6.96 (t, *J* = 7.4 Hz, 1H), 2.85 – 2.71 (m, 4H), 2.37 (d, *J* = 6.6 Hz, 2H), 1.75 – 1.56 (m, 5H), 1.41 – 1.27 (m, 1H), 1.26 – 1.01 (m, 3H), 0.89 - 0.78 (m, 2H); ^{13}C NMR (75 MHz, DMSO-d_6) δ 136.2, 127.2, 122.4, 120.7, 118.2, 118.0, 112.6, 111.2, 56.2, 50.5, 37.6, 31.1, 26.3, 25.6, 25.5; HRMS (ESI) m/z: calcd for $C_{17}H_{25}N_2$ $[M + H]^+$ 257.2018, found 257.2013.

N-Heptyltryptamine (3e)



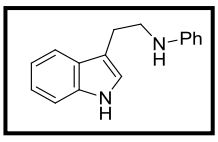
Following **general procedure (I)**, the reaction of tryptamine (300 mg, 1.87 mmol), heptanal (214 mg, 261 µL, 1.87 mmol) and $NaBH_4$ (71 mg, 1.87 mmol) gave, after aqueous, work-up the title compound as a brown oil (449 mg, 93%). The compound was used in the next step without further purification. R_f = 0.18 (MeOH:CH_2Cl_2 (1:1); UV; $KMnO_4$); HPLC purity: 93% (R_t = 6.71 min); IR (neat) cm^{-1}: 3413, 2923, 2853, 1454, 1353, 1107; ^{1}H NMR (300 MHz, DMSO-d_6) δ 10.73 (s, 1H), 7.46 (d, *J* = 7.8 Hz, 1H), 7.28 (d, *J* = 8.0 Hz, 1H), 7.08 (d, *J* = 2.2 Hz, 1H), 7.07 (dt, *J* = 7.5, 1.2 Hz, 1H), 6.96 – 6.88 (m, 1H), 2.85 – 2.62 (m, 4H), 2.48 – 2.4 (m, 2H), 1.45 – 1.03 (m, 10H), 0.81 (t, *J* = 6.6 Hz, 3H); ^{13}C NMR (75 MHz, DMSO-d_6) δ 136.2, 127.2, 122.4, 120.7, 118.2, 118.0, 112.6, 111.3, 50.2, 49.3, 31.3, 29.6, 28.7, 26.8, 25.5, 22.1, 13.9; HRMS (ESI) *m/z*: calcd for $C_{17}H_{27}N_2$ $[M + H]^+$ 259.2174, found 259.2169.

N-Allyltryptamine[3]



In a round-bottomed flask fitted with a magnetic stirring bar, 3-(2-bromoethyl)indole (1.00 g, 4.46 mmol) was added in portions to a stirred suspension of K_2CO_3 (740 mg, 5.35 mmol) in allylamine (7.96 g, 10.4 mL, 89.2 mmol) over 30 min. The reaction was stirred at rt overnight, whereupon the reaction mixture was filtered through a pad of celite, which was washed with CH_2Cl_2 (2 x 25 mL). The filtrate was then evaporated *in vacuo*, and the residue was then purified by flash column chromatography on silica gel (Et_3N:MeOH:CH_2Cl_2; 1:10:89), to give the title compound as a brown oil (876 mg, >95%). R_f = 0.26 (MeOH:CH_2Cl_2 (1:9); UV; $KMnO_4$); HPLC purity: >95% (R_t = 4.90 min); ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.11 (s, 1H), 7.63 (dd, *J* = 7.8, 0.7 Hz, 1H), 7.37 (dt, *J* = 8.1, 0.9 Hz 1H), 7.20 (ddd, *J* = 8.2, 7.1, 1.3 Hz, 1H), 7.15 – 7.09 (m, 1H), 7.05 (d, *J* = 2.3 Hz, 1H), 5.89 (ddt, *J* = 17.2, 10.2, 6.0 Hz, 1H), 5.14 (ddd, *J* = 17.1, 3.3, 1.6 Hz, 1H), 5.06 (ddd, *J* = 10.2, 3.0, 1.3 Hz, 1H), 3.27 (dt, *J* = 6.0, 1.4 Hz, 2H), 3.01 – 2.92 (m, 4H), 1.64 (br. s, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 137.1, 136.7, 127.7, 122.4, 122.3, 119.5, 119.2, 116.2, 114.2, 111.5, 52.7, 49.7, 26.1; MS (ESI) *m/z*: calcd for $C_{13}H_{17}N_2$ $[M + H]^+$ 201.1, found 201.3.

N-Phenyltryptamine

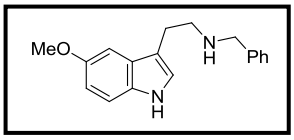


In a round-bottomed flask fitted with a magnetic stirring bar, 3-(2-bromoethyl)indole (500 mg, 2.23 mmol) was added in portions over 30 min to a stirred suspension of K_2CO_3 (370 mg, 2.68 mmol) in aniline (4.16 g, 4.01 mL, 44.6 mmol). The reaction was stirred at rt, whereupon the reaction mixture was filtered through a pad of celite, which was washed with CH_2Cl_2 (2 x 10 mL). The CH_2Cl_2 was removed *in vacuo*. Excess of aniline was removed by distillation (73 °C, 16 mbar), and the residue was then purified by flash column chromatography on silica gel (Et_3N:EtOAc:heptane; 1:35:64), to give the title compound as a brown solid (515 mg, >95%). m.p.: 83 – 86 °C; R_f = 0.39 (EtOAc:heptane (35:65); UV; $KMnO_4$); HPLC purity: >95% (R_t = 5.75 min); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.99 (s, 1H), 7.64 (ddt, *J* = 7.7, 1.4, 0.8 Hz, 1H), 7.39 (dt, *J* = 8.1, 1.0 Hz, 1H), 7.28 – 7.11 (m, 3H), 7.05 (d, *J* = 2.4 Hz, 1H), 6.83 – 6.68 (m, 2H), 6.67 – 6.58 (m, 2H), 3.72 (br. s, 1H), 3.49 (t, *J* = 6.8 Hz, 2H), 3.11 (t, *J* = 6.7 Hz, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 148.5, 136.6, 129.6, 127.7, 122.4, 122.4,

[3] Ascic. E.; Jensen. J. F.; Nielsen. T. E. *Angew. Chem. Int. Ed.* **2011**, *50*, 5188-5191.

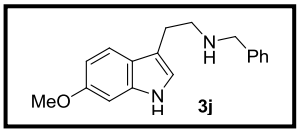
119.7, 119.04 117.6, 115.4, 113.3, 111.5, 44.2, 25.3; MS (ESI) *m/z*: calcd for $C_{16}H_{17}N_2$ $[M + H]^+$ 237.1, found 237.4.

_N_-Benzyl-(5-methoxy)tryptamine



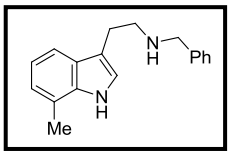
Following **general procedure (I)**, the reaction of (5-methoxy)tryptamine (120 mg, 0.63 mmol), benzaldehyde (67 mg, 64 µL, 0.63 mmol) and $NaBH_4$ (24 mg, 0.63 mmol) gave, after aqueous work-up, the title compound as a yellow oil (128 mg, 73%). The compound was used in the next step without further purification. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.85 (s, 1H), 7.16 – 7.14 (m, *J* = 5.9, 4.4 Hz, 6H), 6.95 (dd, *J* = 9.2, 2.3 Hz, 2H), 6.78 (dd, *J* = 8.8, 2.4 Hz, 1H), 3.77 (s, 3H), 3.76 (s, 2H), 2.92 (s, 4H), 2.05 (br. s, 1H).

_N_-Benzyl-(6-methoxy)tryptamine (3j)



Following general **procedure (I)**, the reaction of (6-methoxy)tryptamine (100 mg, 0.53 mmol), benzaldehyde (56 mg, 54 µL, 0.53 mmol) and $NaBH_4$ (20 mg, 0.53 mmol) gave, after aqueous work-up, the title compound as a brown oil (143 mg, >95%). The compound was used in the next step without further purification. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.86 (s, 1H), 7.39 (d, *J* = 8.4 Hz, 1H), 7.24 – 7.16 (m, 5H), 6.82 (d, *J* = 2.2 Hz, 1H), 6.76 (d, *J* = 2.0 Hz, 1H), 6.71 (dd, *J* = 8.6, 2.3 Hz, 1H), 3.76 (s, 3H), 3.74 (s, 2H), 2.90 (s, 4H), 1.74 (br. s, 1H).

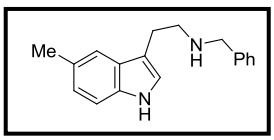
_N_-Benzyl-(7-methyl)tryptamine



Following **general procedure (I)**, the reaction of (7-methyl)tryptamine (100 mg, 0.57 mmol), benzaldehyde (61 mg, 58 µL, 0.57 mmol) and $NaBH_4$ (22 mg, 0.57 mmol) gave, after aqueous work-up, the title compound as a brown oil (112 mg, 74%). The compound was used in the next step without further purification. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.87 (s, 1H), 7.39 (d, *J* = 7.4 Hz, 1H), 7.27 – 7.11 (m, 5H), 6.99 – 6.91 (m, 3H), 3.74 (s, 2H), 2.95 – 2.88 (m, 4H), 2.39 (s, 3H), 1.76 (br. s, 1H).

_N_-Benzyl-(5-methyl)tryptamine

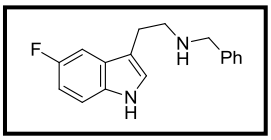
General procedure (II): *Reductive alkylation of tryptamine HCl salts*



In a round-bottomed flask fitted with a magnetic stirring bar, Et_3N (96 mg, 132 µL, 0.95 mmol) was added to a stirred suspension of (5-methyl)tryptamine (hydrochloride salt) (200 mg, 0.95 mmol) in MeOH (4 mL). After 5 min, the reaction mixture was added benzaldehyde (101 mg, 97 µL, 0.95 mmol) and molecular sieves (3Å), and stirred at rt. The reaction was monitored by TLC, and upon full conversion of benzaldehyde (24 h), solid $NaBH_4$ (36 mg, 0.95 mmol) was added. After further 16 h of stirring, the reaction mixture was filtered through a pad of celite, which was washed with MeOH (2 x 15 mL). The filtrate was

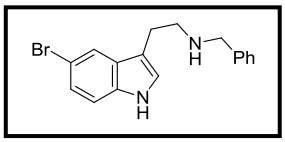
evaporated *in vacuo*. The residue was taken up in sat. $NaHCO_3$ (25 mL), H_2O (25 mL) and EtOAc (50 mL) and transferred to a separatory funnel. The organic layer was separated and washed with H_2O (25 mL) and brine (25 mL). The organic layer was dried over Na_2SO_4 and evaporated *in vacuo* to give the title compound as a brown oil (236 mg, 94%). The compound was used in the next step without further purification. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.98 (s, 1H), 7.36 – 7.06 (m, 6H), 6.96 – 6.91 (dd, *J* = 8.4, 1.5 1H), 6.87 (d, *J* = 2.1 Hz, 1H), 3.74 (s, 2H), 2.91 (s, 4H), 2.37 (s, 3H), 2.03 (br. s, 1H).

_N_-Benzyl-(5-fluoro)tryptamine



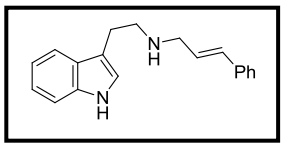
Following **general procedure (II)**, the reaction of (5-fluoro)tryptamine hydrochloride (200 mg, 0.93 mmol), Et_3N (94 mg, 130 µL, 0.93 mmol), benzaldehyde (99 mg, 95 µL, 0.93 mmol) and $NaBH_4$ (35 mg, 0.93 mmol) gave after aqueous work-up the title compound as a brown oil (231 mg, 92%). The compound was used in the next step without further purification. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.00 (s, 1H), 7.28 – 7.08 (m, 7H), 6.98 (d, *J* = 2.1 Hz, 1H), 6.86 (td, *J* = 9.1, 2.4 Hz, 1H), 3.75 (s, 2H), 2.92 – 2.83 (m, 4H), 1.78 (s, 1H).

_N_-Benzyl-(5-bromo)tryptamine



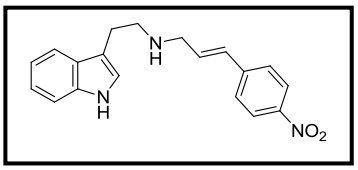
Following **general procedure (II)**, the reaction of (5-bromo)tryptamine hydrochloride (250 mg, 0.91 mmol), Et_3N (92 mg, 126 µL, 0.91 mmol), benzaldehyde (96 mg, 92 µL, 0.91 mmol) and $NaBH_4$ (34 mg, 0.91 mmol) gave after aqueous work-up the title compound as a brown oil (282 mg, 95%). The compound was used in the next step without further purification. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.36 (s, 1H), 7.60 (d, *J* = 1.6 Hz, 1H), 7.24 – 7.08 (m, 7H), 6.91 (s, 1H), 4.19 (br. s, 1H), 3.77 (s, 2H), 2.93 – 2.82 (m, 4H).

_N_-3-Phenylprop-2-en-1-tryptamine



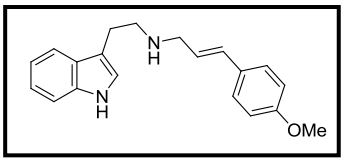
Following **general procedure (I)**, the reaction of tryptamine (300 mg, 1.87 mmol), cinnamaldehyde (247 mg, 236 µL, 1.87 mmol) and $NaBH_4$ (142 mg, 3.75 mmol) gave, after aqueous work-up, the title compound as a brown oil (439 mg, 85%). The compound was used in the next step without further purification. R_f = 0.41 (MeOH:CH_2Cl_2 (1:3); UV; $KMnO_4$); HPLC purity: > 95% (R_t = 6.41 min); IR (neat) cm^{-1}: 3412, 2915, 2838, 1448, 1353, 1229, 966, 736;^{1}H NMR (300 MHz, DMSO-d_6) δ 10.79 (s, 1H), 7.52 (d, *J* = 7.8 Hz, 1H), 7.44 – 7.24 (m, 5H), 7.20 (t, *J* = 6.8 Hz, 1H), 7.14 (d, *J* = 2.0 Hz, 1H), 7.05 (t, *J* = 7.5 Hz, 1H), 6.95 (t, *J* = 7.4 Hz, 1H), 6.50 (d, *J* = 16.0 Hz, 1H), 6.31 (dt, *J* = 15.9, 5.9 Hz, 1H), 3.35 (d, *J* = 5.9 Hz, 2H), 2.84 (s, 4H); ^{13}C NMR (75 MHz, DMSO-d_6) δ 136.9, 136.2, 129.7, 129.5, 128.5, 127.2, 127.1, 126.0, 122.5, 120.8, 118.3, 118.1, 112.6, 111.3, 51.0, 49.6, 25.5; HRMS (ESI) *m/z*: calcd for $C_{19}H_{21}N_2$ $[M + H]^+$ 277.1705, found 277.1702.

_N_-3-(4-Nitrophenyl)prop-2-en-1-tryptamine



Following **general procedure (I)**, the reaction of tryptamine (600 mg, 3.75 mmol), *trans*-4-nitrocinnamaldehyde (664 mg, 3.75 mmol) and $NaBH_4$ (284 mg, 7.50 mmol) gave after aqueous work-up the title compound as a yellow powder (1.17 g, >95%). The compound was used in the next step without further purification. m.p.: 83 – 86 °C; R_f = 0.37 (EtOAc; UV; $KMnO_4$); HPLC purity: > 95% (R_t = 6.40 min); IR (neat) cm^{-1}: 3412, 2914, 2839, 1594, 1507, 1454, 1336, 1105; ^1H NMR (300 MHz, DMSO-d_6) δ 10.79 (s, 1H), 8.19 – 8.13 (m, 2H), 7.70 – 7.60 (m, 2H), 7.52 (d, *J* = 7.7 Hz, 1H), 7.33 (d, *J* = 8.0 Hz, 1H), 7.15 (d, *J* = 2.3 Hz, 1H), 7.09 – 7.02 (dt, *J* = 8.1, 0.9, 1H), 6.99 – 6.91 (m, 1H), 3.41 (d, *J* = 4.0 H012z, 2H), 2.85 (s, 4H); ^{13}C NMR (75 MHz, DMSO-d_6) δ 145.9, 143.8, 136.2, 135.3, 127.7, 127.2, 126.8, 123.8, 122.5, 120.8, 118.3, 118.1, 112.5, 111.3, 50.8, 49.6, 25.5; HRMS (ESI) m/z: calcd for $C_{19}H_{20}N_3O_2$ $[M + H]^+$ 322.1556, found 322.1550.

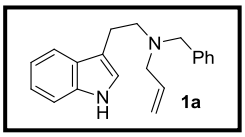
_N_-3-(4-Methoxyphenyl)prop-2-en-1-tryptamine



Following **general procedure (I)**, the reaction of tryptamine (600 mg, 3.75 mmol), *trans*-4-methoxycinnamaldehyde (608 mg, 3.75 mmol) and $NaBH_4$ (284 mg, 7.50 mmol) gave, after aqueous work-up, the title compound as a brown oil (1.10 g, >95%). The compound was used in the next step without further purification. R_f = 0.45 (MeOH:CH_2Cl_2 (1:3); UV; $KMnO_4$); HPLC purity: > 95% (R_t = 6.45 min); IR (neat) cm^{-1}: 3411, 2923, 2832, 1607, 1151, 1449, 1245. 1149, 1035; ^1H NMR (300 MHz, DMSO-d_6) δ 10.80 (s, 1H), 7.52 (d, *J* = 7.5 Hz, 1H), 7.35 – 7.29 (m, 3H), 7.14 (d, *J* = 2.3 Hz, 1H), 7.05 (dt, *J* = 25, 1.2 Hz, 1H), 6.99 – 6.92 (m, 1H), 6.90 – 6.84 (m, 2H), 6.43 (d, *J* = 16.0 Hz, 1H), 6.15 (dt, *J* = 16.0, 6.1 Hz, 1H), 3.73 (S, 3H), 3.29 (dd, *J* = 23.7, 5.6 Hz, 2H), 2.84 (s, 4H); ^{13}C NMR (75 MHz, DMSO-d_6) δ 158.4, 136.2, 129.5, 129.4, 127.2, 127.1, 126.9, 122.5, 120.7, 118.3, 118.0, 113.9, 112.5, 111.3, 55.0, 51.0, 49.5, 25.4; HRMS (ESI) m/z: calcd for $C_{20}H_{23}N_2O$ $[M + H]^+$ 307.1810, found 307.1804.

_N_-Allyl-_N_- benzyltryptamine (1a)

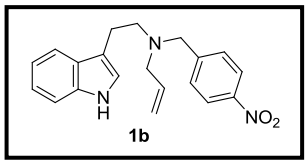
General procedure (III): *Alkylation of secondary amines*



In a round-bottomed flask fitted with a magnetic stirring bar, allyl bromide (1.55 g, 1.11 mL, 12.8 mmol) was added to a stirred suspension of *N*-benzyltryptamine (1.6 g, 6.4 mmol) and K_2CO_3 (2.85 g, 19.8 mmol) in DMF (20 mL). The reaction was stirred at rt, and was monitored by TLC. Upon full conversion of the starting material (30 min), the reaction mixture was evaporated *in vacuo*. The residue was taken up in CH_2Cl_2 (100 mL) and water (80 mL) and transferred to a separatory funnel. The organic layer was separated and the aqueous phase was further extracted with CH_2Cl_2 (1 x 100 mL). The combined organic layers were dried over Na_2SO_4 and evaporated *in vacuo*. The residue was purified by flash column chromatography on silica gel (Et_3N:MeOH:CH_2Cl_2; 1:2:97), to give the title compound as a brown/yellow oil (1.76 g, 94%). R_f = 0.38 (EtOAc:heptane (1:1); UV; $KMnO_4$); HPLC purity: > 95% (R_t = 6.28 min); IR (neat) cm^{-1}: 3417, 3058, 2972, 2801, 1454, 735; ^1H NMR (300 MHz, DMSO-d_6) δ 10.75 (s, 1H), 7.41 – 7.18 (m, 7H), 7.10 – 6.98 (m, 2H), 6.95 – 6.85 (m, 1H), 5.91 (ddt, *J* = 16.4, 10.2, 6.3 Hz, 1H), 5.24 (dd, *J* = 17.2, 2.0 Hz, 1H), 5.15 (dd, *J* =

10.2, 2.1 Hz, 1H)., 3.66 (s, 2H), 3.16 (d, *J* = 6.3 Hz, 2H), 2.85 (dd, J = 9.8, 5.8 Hz, 2H), 2.68 (dd, J = 9.7, 5.7 Hz, 2H); ^{13}C NMR (75 MHz, DMSO-d_6) δ 139.5, 136.1, 136.0, 128.5, 128.0, 127.1, 126.7, 122.3, 120.7, 118.1, 118.0, 117.1, 112.4, 111.2, 57.3, 56.1, 53.6, 22.3; HRMS (ESI) m/z: calcd for $C_{20}H_{23}N_2$ $[M + H]^+$ 291.1861, found 291.1855.

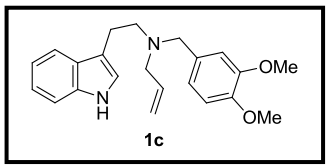
_N_-Allyl-_N_-(4-nitro)benzyltryptamine (1b)



1b

Following **general procedure (III)**, the reaction of *N*-(4-nitro)benzyltryptamine (370 mg, 1.25 mmol), allyl bromide (303 mg, 217 µL, 2.50 mmol) and K_2CO_3 (519 mg, 3.75 mmol) gave after purification by flash column chromatography on silica gel (Et_3N:MeOH:CH_2Cl_2; 1:2:97), the title compound as a yellow oil (409 mg, >95%). R_f = 0.19 (EtOAc:heptane (1:3); UV; $KMnO_4$); HPLC purity: >95% (R_t = 6.31 min); IR (neat) cm^{-1}: 3415, 2920, 2808, 1559, 1513, 1340; ^{1}H NMR (300 MHz, DMSO-d_6) δ 10.77 (s, 1H), 8.17 – 8.09 (m, 2H), 7.57 (d, *J* = 8.7 Hz, 2H), 7.36 (d, *J* = 7.9 Hz, 1H), 7.31 (d, *J* = 8.1 Hz, 1H), 7.08 (d, *J* = 2.3 Hz, 1H), 7.03 (dt, *J* = 1.2, 6.9 Hz, 1H), 6.94 – 6.85 (m, 1H), 5.91 (ddt, *J* = 16.5, 10.2, 6.3 Hz, 1H), 5.25 (dd, *J* = 17.2, 1.9 Hz, 1H), 5.16 (dd, *J* = 10.2, 2.0 Hz, 1H), 3.77 (s, 2H), 3.19 (d, *J* = 6.3 Hz, 2H), 2.91 – 2.78 (m, 2H), 2.80 – 2.56 (m, 2H); ^{13}C NMR (75 MHz, DMSO-d_6) δ 148.4, 146.3, 136.1, 135.7, 129.3, 127.1, 123.2, 122.5, 120.7, 118.1, 118.0, 117.5, 112.3, 111.3, 56.6, 56.3, 53.9, 22.5; HRMS (ESI) *m/z*: calcd for $C_{20}H_{22}N_3O_2$ $[M + H]^+$ 336.1712, found 336.1707.

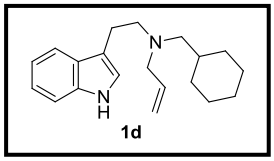
_N_-Allyl-_N_-(3,4-dimethoxy)benzyltryptamine (1c)



1c

Following **general procedure (III)**, the reaction of *N*-(3,4-dimethoxy)benzyltryptamine (400 mg, 1.29 mmol), allyl bromide (312 mg, 223 µL, 2.58 mmol) and K_2CO_3 (534 mg, 3.87 mmol) gave after purification by flash column chromatography on silica gel (Et_3N:MeOH:CH_2Cl_2; 1:2:97), the title compound as a brown oil (434 mg, >95%). R_f = 0.20 (EtOAc:heptane (1:3); UV; $KMnO_4$); HPLC purity: 86% (R_t = 6.04 min); IR (neat) cm^{-1}: 3372, 2932, 2833, 1591, 1511, 1455, 1259. 1228, 1146, 1025; ^{1}H NMR (300 MHz, DMSO-d_6) δ 10.76 (s, 1H), 7.38 (d, *J* = 7.7 Hz, 1H), 7.30 (d, *J* = 8.1 Hz, 1H), 7.12 – 7.00 (m, 2H), 6.96 – 6.79 (dt, *J* = 11.8, 8.1 Hz, 4H), 5.99 – 5.84 (m, 1H), 5.24 (d, *J* = 17.2 Hz, 1H), 5.15 (d, *J* = 10.1 Hz, 1H), 3.79 – 3.71 (s, 3H), 3.67 (s, 3H), 3.58 (s, 2H), 3.16 (d, *J* = 5.9 Hz, 2H), 2.92 – 2.78 (m, 2H), 2.74 – 2.64 (m, 2H); ^{13}C NMR (75 MHz, DMSO-d_6) δ 148.5, 147.6, 136.2, 136.1, 131.8, 127.2, 122.4, 120.7, 120.5, 118.2, 118.0, 117.1, 112.5, 112.0, 111.3, 111.2, 57.0, 56.0, 55.4, 55.21, 53.4, 22.3; HRMS (ESI) *m/z*: calcd for $C_{22}H_{27}N_2O_2$ $[M + H]^+$ 351.2073, found 351.2067.

_N_-Allyl-_N_-cyclohexylmethyltryptamine (1d)

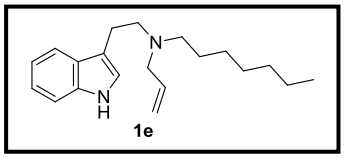


1d

Following **general procedure (III)**, the reaction of *N*-cyclohexylmethyltryptamine (330 mg, 1.17 mmol), allyl bromide (283 mg, 202 µL, 2.34 mmol) and K_2CO_3 (485 mg, 3.57 mmol) gave after purification by flash column chromatography on silica gel (Et_3N:MeOH:CH_2Cl_2; 1:2:97), the title compound as a brown oil (282 mg, 81%). R_f = 0.26 (EtOAc:heptane (1:3); UV; $KMnO_4$); HPLC purity: 86% (R_t = 6.80 min); IR (neat) cm^{-1}: 3418, 2920, 2848, 2798, 1454; ^{1}H NMR (500 MHz, DMSO-d_6) δ 10.71 (d, *J* = 31.3 Hz,

1H), 7.46 (d, *J* = 7.8 Hz, 1H), 7.30 (t, *J* = 12.7 Hz, 1H), 7.11 (d, *J* = 1.6 Hz, 1H), 7.04 (t, *J* = 7.4 Hz, 1H), 6.96 (t, *J* = 7.3 Hz, 1H), 5.91 – 5.74 (m, 1H), 5.21 (dd, *J* = 16.3, 8.4 Hz, 1H), 5.11 (d, *J* = 10.4 Hz, 1H), 3.12 (d, *J* = 5.7 Hz, 2H), 2.83 – 2.75 (m, 2H), 2.70 – 2.63 (m, 2H), 2.26 (d, *J* = 6.9 Hz, 2H), 1.74 (d, *J* = 12.7 Hz, 2H), 1.64 (d, *J* = 11.8 Hz, 3H), 1.44 (ddd, *J* = 10.6, 7.1, 3.5 Hz, 1H), 1.25 – 1.05 (m, 3H), 0.88 – 0.70 (m, 2H); ^{13}C NMR (75 MHz, DMSO-d_6) δ 137.2, 136.9, 127.9, 123.1, 121.4, 118.8, 118.7, 117.4, 113.3, 112.0, 61.1, 57.9, 55.4, 36.3, 32.0, 27.1, 26.3, 23.2; HRMS (ESI) *m/z*: calcd for $C_{20}H_{31}N_2$ $[M + H]^+$ 297.2331, found 297.2325.

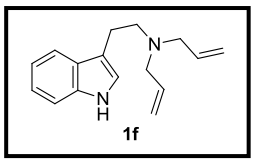
N-Allyl-*N*-heptyltryptamine (1e)



1e

Following **general procedure (III)**, the reaction of *N*-heptyltryptamine (310 mg, 1.20 mmol), allyl bromide (290 mg, 207 µL, 2.40 mmol) and K_2CO_3 (497 mg, 3.60 mmol) gave after purification by flash column chromatography on silica gel (Et_3N:MeOH:CH_2Cl_2; 1:2:97), the title compound as a brown oil (223 mg, 63%). R_f = 0.23 (EtOAc:heptane (1:1); UV; $KMnO_4$); HPLC purity: 81% (R_t = 7.16 min); IR (neat) cm^{-1}: 3416, 2924, 2854, 1455, 1352, 1091; ^{1}H NMR (500 MHz, DMSO-d_6) δ 10.78 (s, 1H), 7.50 (d, *J* = 7.8 Hz, 1H), 7.35 (d, *J* = 8.1 Hz, 1H), 7.13 (d, *J* = 1.5 Hz, 1H), 7.07 (t, *J* = 7.7 Hz, 1H), 6.98 (t, *J* = 7.1 Hz, 1H), 5.95 – 5.81 (m, 1H), 5.27 – 5.20 (m, 1H), 5.16 (dd, *J* = 14.4, 5.3 Hz, 1H), 3.20 – 3.14 (m, 2H), 2.88 – 2.77 (m, 2H), 2.74 – 2.62 (m, 2H), 1.49 – 1.41 (m, 1H), 1.38 – 1.13 (m, 11H), 0.94 – 0.80 (m, 3H); ^{13}C NMR (75 MHz, DMSO-d_6) δ 136.5, 136.1, 127.2, 122.4, 120.7, 118.1, 118.0, 116.6, 112.6, 111.3, 56.6, 56.1, 54.1, 52.9, 31.3, 28.6, 26.8, 26.6, 22.4, 22.1, 13.9; HRMS (ESI) *m/z*: calcd for $C_{20}H_{31}N_2$ $[M + H]^+$ 299.2487, found 299.2484.

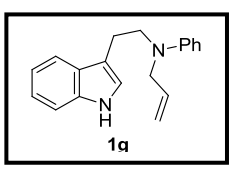
N,N-Diallyltryptamine (1f)



1f

In a round-bottomed flask fitted with a magnetic stirring bar, and a reflux condenser, diallylamine (257 mg, 326 µL, 2.67 mmol) was added to a stirred suspension of 3-(2-bromoethyl)indole (500 mg, 2.23 mmol) and K_2CO_3 (431 mg, 3.12 mmol) in MeCN (2 mL). The reaction was stirred at reflux, and was monitored by TLC. Upon full conversion of the starting material (16 h), the reaction mixture was filtered through a pad of celite, which was washed with CH_2Cl_2 (2 x 10 mL). The filtrate was evaporated *in vacuo*, to give the title compound as a light green oil (319 mg, 59%). R_f = 0.26 (EtOAc:heptane (1:1); UV; $KMnO_4$); HPLC purity: >95% (R_t = 5.41 min); IR (neat) cm^{-1}: 3441, 2921, 2897, 1455, 1418, 1352, 1105, 994, 917, 736; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.11 (s, 1H), 7.51 (d, *J* = 7.5 Hz, 1H), 7.23 (d, *J* = 7.9 Hz, 1H), 7.16 – 7.00 (m, 2H), 6.88 (s, 1H), 5.91 – 5.76 (m, 2H), 5.21 – 5.11 (m, 2H), 5.10 – 5.04 (m, 4H), 3.16 (d, *J* = 6.5 Hz, 4H), 2.92 – 2.81 (m, 2H), 2.80 – 2.70 (m, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 136.5, 135.9, 127.8, 122.1, 121.8, 119.4, 119.2, 118.0, 114.7, 111.4, 57.2, 54.2, 23.0; HRMS (ESI) *m/z*: calcd for $C_{16}H_{21}N_2$ $[M + H]^+$ 241.1705, found 241.1697.

N-Allyl-*N*-phenyltryptamine (1g)

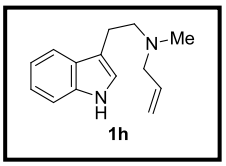


1g

In a round-bottomed flask fitted with a magnetic stirring bar, allyl bromide (888 mg, 549 µL, 6.35 mmol) was added to a stirred suspension of *N*-phenyltryptamine (300 mg,

1.27 mmol) and K_2CO_3 (526 mg, 3.81 mmol) in DMF (3.5 mL). The reaction was stirred at rt, and was monitored by TLC. Upon full conversion of the starting material (4 h) the reaction mixture was evaporated *in vacuo*. The residue was taken up in CH_2Cl_2 (50 mL) and water (30 mL) and transferred to a separatory funnel. The organic layer was separated and the aqueous phase was further extracted with CH_2Cl_2 (1 x 50 mL). The combined organic layers were dried over Na_2SO_4 and evaporated *in vacuo*, to give the title compound as a light brown powder (342 mg, >95%). m.p.: 66 – 68 °C; R_f = 0.36 (EtOAc:heptane (1:3); UV; $KMnO_4$); HPLC purity: >95% (R_t = 6.86 min); IR (neat) cm^{-1}: 3388, 1667, 1594, 1503, 1358, 1231, 1165; ^1H NMR (300 MHz, $CDCl_3$) δ 7.89 (s, 1H), 7.55 (dd, *J* = 7.8, 0.7 Hz, 1H), 7.30 (dt, *J* = 8.2, 0.9 Hz, 1H), 7.22 – 7.12 (m, 3H), 7.12 – 7.03 (m, 1H), 6.94 (d, *J* = 2.3 Hz, 1H), 6.70 (dd, *J* = 8.8, 0.9 Hz, 2H), 6.66 – 6.58 (m, 1H), 5.84 – 5.67 (m, 1H), 5.14 – 5.07 (m, 1H), 5.06 – 5.02 (m, 1H), 3.84 (dt, *J* = 4.8, 1.7 Hz, 2H), 3.60 – 3.51 (m, 2H), 2.99 (dd, *J* = 9.0, 6.6 Hz, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 148.4, 136.5, 134.5, 129.7, 129.4, 127.7, 122.3, 122.0, 119.6, 119.0, 116.2, 113.9, 112.4, 111.5, 53.6, 51.7, 23.3; HRMS (ESI) *m/z*: calcd for $C_{19}H_{21}N_2$ $[M + H]^+$ 277.1705, found 277.1700.

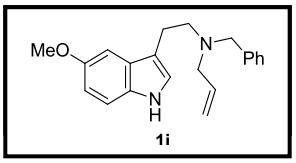
N-Allyl-*N*-methyltryptamine (1h)



1h

In a round-bottomed flask fitted with a magnetic stirring bar, and a reflux condenser *N*-methyl-allylamine (190 mg, 257 µL, 2.68 mmol) was added to a stirred suspension of 3-(2-bromoethyl)indole (500 mg, 2.23 mmol) and K_2CO_3 (432 mg, 3.12 mmol) in MeCN (2 mL). The reaction was stirred at reflux, and was monitored by TLC. Upon full conversion of the starting material (16 h), the reaction mixture was filtered through a pad of celite, which was washed with CH_2Cl_2 (2 x 10 mL). The filtrate was evaporated *in vacuo*, to give the title compound as a light green oil (247 mg, 52%). R_f = 0.19 (EtOAc; UV; $KMnO_4$); HPLC purity: >95% (R_t = 4.92 min); IR (neat) cm^{-1}: 3414, 2920, 2850, 2793, 1454, 1352, 1338, 1010, 994, 921, 735; ^1H NMR (300 MHz, $CDCl_3$) δ 8.06 (s, 1H), 7.62 (ddt, *J* = 7.7, 1.4, 0.7 Hz, 1H), 7.37 – 7.33 (m, 1H), 7.22 – 7.09 (m, 2H), 7.02 (d, *J* = 2.3 Hz, 1H), 5.93 (ddt, *J* = 16.7, 10.1, 6.6 Hz, 1H), 5.25 – 5.18 (m, 1H), 5.18 – 5.13 (m, 1H), 3.13 (dt, *J* = 6.6, 1.2 Hz, 2H), 3.01 – 2.93 (m, 2H), 2.77 – 2.70 (m, 2H), 2.37 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 136.5, 135.5, 127.7, 123.0, 122.0, 119.2, 119.0, 118.2, 114.1, 111.5, 61.1, 58.0, 42.2, 23.4; MS (ESI) *m/z*: calcd for $C_{14}H_{18}N_2$ $[M + H]^+$ 215,2, found 215.3.

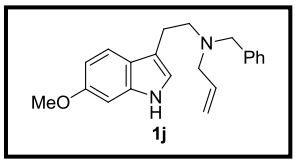
N-Allyl-*N*-benzyl-(5-methoxy)tryptamine (1i)



1i

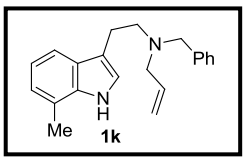
Following **general procedure (III)**, the reaction of *N*-benzyl-(5-methoxy)tryptamine (120 mg, 0.43 mmol), allyl bromide (104 mg, 74 µL, 0.86 mmol) and K_2CO_3 (177 mg, 1.28 mmol) gave after purification by flash column chromatography on silica gel (Et_3N:MeOH:CH_2Cl_2; 1:2:97), the title compound as a brown oil (116 mg, 85%). R_f = 0.25 (EtOAc:heptane (1:3); UV; $KMnO_4$); HPLC purity: 81% (R_t = 6.13 min); IR (neat) cm^{-1}: 3416, 2930, 2828, 1584, 1484, 1452, 1214, 1027, 920;^1H NMR (300 MHz, $CDCl_3$) δ 7.76 (s, 1H), 7.36 – 7.10 (m, 5H), 6.86 (dd, *J* = 7.5, 2.4 Hz, 2H), 6.75 (dd, *J* = 8.8, 2.4 Hz, 1H), 5.89 (ddt, *J* = 16.7, 10.2, 6.4 Hz, 1H), 5.18 (dd, *J* = 17.2, 1.7 Hz, 1H), 5.11 (d, *J* = 10.1 Hz, 1H), 3.73 (s, 3H), 3.65 (s, 2H), 3.17 (d, *J* = 6.3 Hz, 2H), 2.89 – 2.83 (m, 2H), 2.78 – 2.71 (m, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 154.2, 131.8, 131.7, 129.7, 128.6, 128.7, 122.9, 122.8, 112.5, 112.2, 100.8, 58.2, 56.3, 54.8, 53.8, 22.8; HRMS (ESI) *m/z*: calcd for $C_{21}H_{25}N_2O$ $[M + H]^+$ 321.1967, found 321.1960.

_N_-Allyl-_N_-benzyl-(6-methoxy)tryptamine (1j)



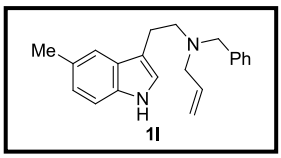
Following **general procedure (III)**, the reaction of *N*-benzyl-(6-methoxy)tryptamine (130 mg, 0.46 mmol), allyl bromide (112 mg, 80 µL, 0.93 mmol) and K_2CO_3 (192 mg, 1.39 mmol) gave after purification by flash column chromatography on silica gel (Et_3N:MeOH:CH_2Cl_2; 1:2:97), the title compound as a brown oil (131 mg, 86%). R_f = 0.21 (EtOAc:heptane (1:3); UV; $KMnO_4$); HPLC purity: >95% (R_t = 6.07 min); IR (neat) cm^{-1}: 3412, 2923, 2831, 1627, 1498, 1453, 1305, 1258, 1198, 1131; ^1H NMR (300 MHz, $CDCl_3$) δ 7.74 (s, 1H), 7.33 – 7.09 (m, 6H), 6.77 (d, *J* = 2.2 Hz, 1H), 6.74 (d, *J* = 2.1 Hz, 1H), 6.67 (dd, *J* = 8.6, 2.3 Hz, 1H), 5.86 (ddt, *J* = 16.5, 10.2, 6.4 Hz, 1H), 5.19 – 5.11 (m, 1H), 5.11 – 5.05 (m, 1H), 3.75 (s, 3H), 3.62 (s, 2H), 3.13 (d, *J* = 6.4 Hz, 2H), 2.88 – 2.79 (m, 2H), 2.73 (ddd, *J* = 11.6, 6.7, 2.6 Hz, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 156.6, 139.8, 137.2, 136.2, 129.3, 128.5, 127.11, 122.3, 120.6, 119.7, 117.7, 114.6, 109.3, 94.9, 58.4, 57.2, 55.9, 54.3, 23.2; MS (ESI) *m/z*: calcd for $C_{21}H_{25}N_2O$ $[M + H]^+$ 321.2, found 321.4.

_N_-Allyl-_N_- benzyl-(7-methyl)tryptamine (1k)



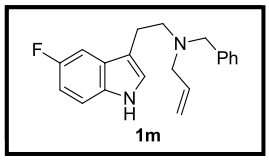
Following **general procedure (III)**, the reaction of *N*-benzyl-(7-methyl)tryptamine (100 mg, 0.49 mmol), allyl bromide (118 mg, 85 µL, 0.98 mmol) and K_2CO_3 (203 mg, 1.47 mmol) gave after purification by flash column chromatography on silica gel (Et_3N:MeOH:CH_2Cl_2; 1:2:97), the title compound as a brown oil (108 mg, 72%). R_f = 0.45 (EtOAc:heptane (1:1); UV; $KMnO_4$); HPLC purity: 90% (R_t = 6.58 min); IR (neat) cm^{-1}: 3421, 2919, 2799, 1494, 1452, 1340, 1066, 917; ^1H NMR (300 MHz, $CDCl_3$): δ 7.74 (s, 1H), 7.36 – 7.07 (m, 6H), 6.98 – 6.85 (m, 3H), 5.87 (ddt, *J* = 16.6, 10.1, 6.4 Hz, 1H), 5.15 (ddd, *J* = 17.2, 3.4, 1.5 Hz, 1H), 5.11 – 5.06 (m, 1H), 3.63 (s, 2H), 3.14 (d, *J* = 6.4 Hz, 2H), 2.94 – 2.82 (m, 2H), 2.79 – 2.67 (m, 2H), 2.38 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 139.6, 136.0, 129.3, 128.5, 127.3, 127.2, 122.7, 121.6, 120.5, 119.7, 117.9, 116.9, 115.2, 58.4, 57.1, 54.3, 23.3, 16.9; HRMS (ESI) *m/z*: calcd for $C_{21}H_{25}N_2$ $[M + H]^+$ 305.2018, found 305.2012.

_N_-Allyl-_N_-benzyl-(5-methyl)tryptamine (1l)



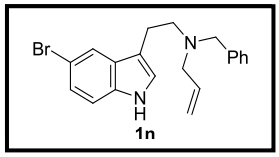
Following **general procedure (III)**, the reaction of *N*-benzyl-(5-methyl)tryptamine (220 mg, 0.83 mmol), allyl bromide (201 mg, 144 µL, 1.66 mmol) and K_2CO_3 (345 mg, 2.50 mmol) gave after purification by flash column chromatography on silica gel (Et_3N:MeOH:CH_2Cl_2; 1:2:97), the title compound as a brown oil (193 mg, 76%). R_f = 0.18 (EtOAc:heptane (1:3); UV; $KMnO_4$); HPLC purity: 92% (R_t = 6.61 min); IR (neat) cm^{-1}: 3416, 3027, 2918, 2803, 1452, 1227, 1091, 994, 918; ^1H NMR (300 MHz, $CDCl_3$) δ 7.74 (s, 1H), 7.35 – 7.10 (m, 7H), 6.91 (dd, *J* = 8.3, 1.6 Hz, 1H), 6.85 (d, *J* = 2.3 Hz, 1H), 5.89 (ddt, *J* = 16.6, 10.2, 6.4 Hz, 1H), 5.17 (dd, *J* = 17.2, 1.8 Hz, 1H), 5.10 (d, *J* = 10.4 Hz, 1H), 3.64 (s, 2H), 3.16 (d, *J* = 6.4 Hz, 2H), 2.91 – 2.79 (m, 2H), 2.80 – 2.68 (m, 2H), 2.35 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 139.5, 136.0, 134.6, 129.1, 128.4, 128.3, 127.8, 127.0, 123.5, 121.8, 118.7, 117.6, 114.0, 110.8, 58.2, 57.0, 54.0, 23.0, 21.6; HRMS (ESI) *m/z*: calcd for $C_{21}H_{25}N_2$ $[M + H]^+$ 305.2018, found 305.2013.

_N_-Allyl-_N_-benzyl-(5-fluoro)tryptamine (1m)



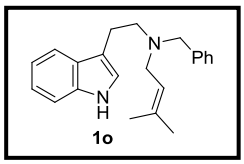
Following **general procedure (III)**, the reaction of *N*-benzyl-(5-fluoro)tryptamine (210 mg, 0.78 mmol), allyl bromide (189 mg, 136 µL, 1.56 mmol) and K_2CO_3 (324 mg, 2.35 mmol) gave after purification by flash column chromatography on silica gel (Et_3N:MeOH:CH_2Cl_2; 1:2:97), the title compound as a brown oil (131 mg, 54%). R_f = 0.45 (EtOAc:heptane (1:1); UV; $KMnO_4$); HPLC purity: >95% (R_t = 6.38 min); IR (neat) cm^{-1}: 3428, 2918, 2803, 1582 1484, 1420, 1173, 934, 792, 738, 698; ^1H NMR (300 MHz, $CDCl_3$) δ 7.87 (s, 1H), 7.31 – 7.09 (m, 6H), 7.03 (dd, *J* = 9.7, 2.5 Hz, 1H), 6.90 (d, *J* = 2.3 Hz, 1H), 6.82 (td, *J* = 9.0, 2.5 Hz, 1H), 5.86 (ddt, *J* = 16.6, 10.2, 6.4 Hz, 1H), 5.19 – 5.12 (m, 1H), 5.12 – 5.06 (m, 1H), 3.62 (s, 2H), 3.14 (dt, *J* = 6.4, 1.2 Hz, 2H), 2.87 – 2.75 (m, 2H), 2.75 – 2.63 (m, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 157.8 (d, J_{C-F} 232.5 Hz, 1C), 139.4, 135.9, 133.3, 129.3, 128.5, 127.2, 123.8, 117.9, 114.6, 114.5, 112.0 (d, J_{C-F} = 9.8 Hz, 1C), 110.2 (d, J_{C-F} = 26.2 Hz, 1C), 103.9 (d, J_{C-F} = 22.5 Hz, 1C), 58.4, 57.1, 54.0, 23.0; HRMS (ESI) *m/z*: calcd for $C_{20}H_{22}FN_2$ $[M + H]^+$ 309.1767, found 309.1767.

_N_-Allyl-_N_-benzyl-(6-bromo)tryptamine (1n)



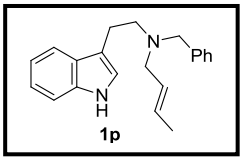
Following **general procedure (III)**, the reaction of *N*-benzyl-(5-bromo)tryptamine (240 mg, 0.73 mmol), allyl bromide (176 mg, 126 µL, 1.46 mmol) and K_2CO_3 (302 mg, 2.19 mmol) gave after purification by flash column chromatography on silica gel (Et_3N:MeOH:CH_2Cl_2; 1:2:97), the title compound as a brown oil (209 mg, 78%). R_f = 0.31 (EtOAc:heptane (1:3); UV; $KMnO_4$); HPLC purity: >95% (R_t = 6.90 min); IR (neat) cm^{-1}: 3425, 2923, 2803, 1665, 1452, 1093, 791, 737, 698; ^1H NMR (300 MHz, $CDCl_3$) δ 8.02 (s, 1H), 7.52 (d, *J* = 1.8 Hz, 1H), 7.29 – 7.11 (m, 6H), 7.07 (d, *J* = 8.6 Hz, 1H), 6.85 (d, *J* = 2.2 Hz, 1H), 5.92 – 5.77 (m, 1H), 5.19 – 5.11 (m, 1H), 5.11 – 5.06 (m, 1H), 3.60 (s, 2H), 3.12 (d, *J* = 6.4 Hz, 2H), 2.83 – 2.75 (m, 2H), 2.73 – 2.60 (m, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 139.7, 136.2, 135.1, 129.7, 129.2, 128.5, 127.3, 124.9, 123.1, 121.8, 117.8, 114.6, 112.8, 112.7, 58.5, 57.2, 54.0, 23.1; HRMS (ESI) *m/z*: calcd for $C_{20}H_{22}BrN_2$ $[M + H]^+$ 369.0966, found 369.0964.

_N_-Benzyl-_N_-(3,3-dimethyl)allyltryptamine (1o)



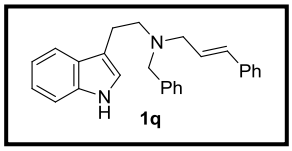
Following **general procedure (III)**, the reaction of *N*-benzyltryptamine (400 mg, 1.60 mmol), (3,3-dimethyl)allyl bromide (262 mg, 203 µL, 1.76 mmol) and K_2CO_3 (662 mg, 4.79 mmol) gave after purification by flash column chromatography (Et_3N:MeOH:CH_2Cl_2; 1:2:97), the title compound as a light yellow oil (468 mg, 92%). R_f = 0.21 (EtOAc:heptane (1:3); UV; $KMnO_4$); HPLC purity: > 95% (R_t = 6.84 min); IR (neat) cm^{-1}: 3417, 3027, 2915, 2807, 1493, 1354, 1092; ^1H NMR (300 MHz, DMSO-d_6) δ 10.74 (s, 1H), 7.41 – 7.15 (m, 7H), 7.10 – 6.97 (m, 2H), 6.91 (dd, *J* = 7.9, 7.0 Hz, 1H), 5.28 (t, *J* = 6.3 Hz, 1H), 3.62 (s, 2H), 3.10 (d, *J* = 6.7 Hz, 2H), 2.91 – 2.78 (m, 2H), 2.67 (dd, *J* = 9.5, 6.0 Hz, 2H), 1.70 (s, 3H), 1.59 (s, 3H); ^{13}C NMR (75 MHz, DMSO-d_6) δ 139.8, 136.1, 133.9, 128.5, 128.0, 127.1, 126.6, 122.3, 121.9, 120.7, 118.1, 118.0, 112.5, 111.2, 57.5, 53.7, 50.7, 25.7, 22.5, 17.8; HRMS (ESI) *m/z*: calcd for $C_{21}H_{25}N_2$ $[M + H]^+$ 319.2174, found 319.2169.

_N_-Benzyl-_N_-crotyltryptamine (1p)



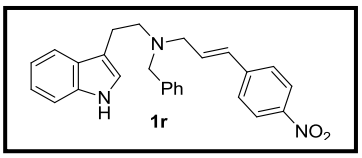
Following **general procedure (III)**, the reaction of *N*-benzyltryptamine (720 mg, 2.88 mmol), crotyl bromide (777 mg, 592 µL, 5.75 mmol) and K_2CO_3 (1.19 g, 8.62 mmol) gave after purification by flash column chromatography on silica gel (Et_3N:MeOH:CH_2Cl_2; 1:2:97), the title compound as a yellow oil (682 mg, 78%). R_f = 0.23 (EtOAc:heptane (1:3); UV; $KMnO_4$); HPLC purity: 88% (R_t = 6.67 min); IR (neat) cm^{-1}: 3418, 3025, 2916, 2801, 1454, 1353, 1228, 996; ^1H NMR (300 MHz, DMSO-d_6) δ 10.75 (s, 1H), 7.41 – 7.26 (m, 6H), 7.26 – 7.17 (m, 1H), 7.08 – 7.05 (m, 1H), 7.01 (d, *J* = 8.0 Hz, 1H), 6.91 (td, *J* = 7.8, 0.9 Hz, 1H), 5.71 – 5.40 (m, 2H), 3.63 (s, 1H), 3.09 (d, *J* = 5.7 Hz, 2H), 2.90 – 2.78 (m, 2H), 2.71 – 2.60 (m, 2H), 1.67 (d, *J* = 5.8 Hz, 2H); ^{13}C NMR (75 MHz, DMSO-d_6) δ 139.7, 136.1, 128.5, 128.4, 128.0, 127.6, 127.1, 126.6, 122.3, 120.7, 118.1, 117.9, 112.5, 111.2, 57.2, 55.2, 53.4, 22.3, 17.6; HRMS (ESI) m/z: calcd for $C_{21}H_{25}N_2$ $[M + H]^+$ 305.2018, found 305.2012.

_N_-Benzyl-_N_-3-phenylprop-2-en-1-tryptamine (1q)



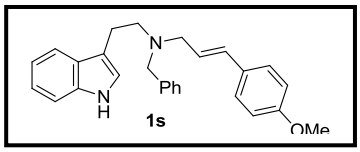
Following **general procedure (III)**, the reaction of *N*-3-phenylprop-2-en-1-tryptamine (380 mg, 1.38 mmol), benzyl bromide (263 mg, 183 µL, 1.53 mmol) and K_2CO_3 (577 mg, 4.18 mmol) gave after purification by flash column chromatography on silica gel (EtOAc:heptane; 1:3), the title compound as a yellow oil (330 mg, 66%). R_f = 0.25 (EtOAc:heptane (1:3); UV; $KMnO_4$); HPLC purity: 91% (R_t = 7.41 min); IR (neat) cm^{-1}: 3420, 3025, 2919, 2799, 1493, 1454;^1H NMR (300 MHz, DMSO-d_6) δ 10.74 (s, 1H), 7.46 – 7.17 (m, 12H), 7.08 (d, *J* = 1.9 Hz, 1H), 7.01 (dd, *J* = 8.0, 7.1 Hz, 1H), 6.84 (dd, *J* = 7.9, 7.0 Hz, 1H), 6.59 (d, *J* = 15.9 Hz, 1H), 6.45 – 6.30 (m, 1H), 3.69 (d, J = 19.7 Hz, 2H), 3.34 (s, 2H), 2.96 – 2.80 (m, 2H), 2.77 - 2.72 (m, 2H); ^{13}C NMR (75 MHz, DMSO-d_6) δ 139.6, 136.7, 136.1, 131.7, 128.6, 128.5, 128.1, 127.7, 127.2, 127.1, 126.7, 126.1, 122.4, 120.7, 118.2, 118.0, 112.5, 111.2, 57.5, 55.5, 53.7, 22.4; HRMS (ESI) *m/z*: calcd for $C_{26}H_{27}N_2$ $[M + H]^+$ 367.2174, found 367.2170.

_N_-Benzyl-_N_- 3-(4-nitrophenyl)prop-2-en-1-tryptamine (1r)



Following **general procedure (III)**, the reaction of *N*-3-(4-nitrophenyl)prop-2-en-1-tryptamine (200 mg, 0.62 mmol), benzyl bromide (117 mg, 81 µL, 0.69 mmol) and K_2CO_3 (258 mg, 1.87 mmol) gave after purification by flash column chromatography on silica gel (Et_3N:MeOH:CH_2Cl_2; 1:2:97), the title compound as a yellow oil (242 mg, 95%). R_f = 0.30 (EtOAc:heptane (3:7); UV; $KMnO_4$); HPLC purity: >95% (R_t = 7.28 min); IR (neat) cm^{-1}: 3415, 2924, 2803, 1666, 1619, 1493, 1454, 1107; ^1H NMR (300 MHz, DMSO-d_6) δ 10.74 (s, 1H), 8.16 (d, *J* = 8.8 Hz, 2H), 7.65 (d, *J* = 8.8 Hz, 2H), 7.41 – 7.20 (m, 8H), 7.09 (d, *J* = 2.1 Hz, 1H), 7.02 (t, *J* = 7.2 Hz, 1H), 6.85 (t, *J* = 7.3 Hz, 1H), 6.72 – 6.60 (m, 1H), 3.74 (s, 2H), 3.39 – 3.33 (m, 2H), 2.97 – 2.85 (m, 2H), 2.80 – 2.69 (m, 2H); ^{13}C NMR (75 MHz, DMSO-d_6) δ 162.2, 146.1, 143.5, 136.14, 128.7, 128.7, 128.1, 127.1, 127.01 126.9, 123.8, 122.5, 120.7, 118.2, 118.0, 111.3, 57.5, 55.2, 35.7, 30.7;HRMS (ESI) *m/z*: calcd for $C_{26}H_{26}N_3O_2$ $[M + H]^+$ 412.2025, found 412.2021.

_N_-Benzyl-_N_-3-(4-methoxyphenyl)prop-2-en-1-tryptamine (1s)

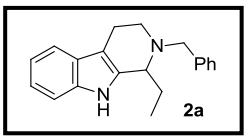


Following **general procedure (III)**, the reaction of _N_-3-(4-methoxyphenyl)prop-2-en-1-tryptamine (400 mg, 1.31 mmol), benzyl bromide (246 mg, 171 µL, 1.44 mmol) and K_2CO_3 (541 mg, 3.92 mmol) gave after purification by flash column chromatography on silica gel (Et_3N:MeOH:CH_2Cl_2; 1:2:97), the title compound as a yellow oil (495 mg, >95%). R_f = 0.43 (EtOAc:heptane (1:1); UV; $KMnO_4$); HPLC purity: >95% (R_t = 7.31 min); IR (neat) cm^{-1}: 3419, 2926, 2833, 1666, 1606, 1509, 1454, 1245, 1174, 1030; ^1H NMR (300 MHz, DMSO-d_6) δ 10.73 (s, 1H), 7.41 – 7.21 (m, 9H), 7.07 (d, J = 2.2 Hz, 1H), 7.01 (t, J = 7.5 Hz, 1H), 6.91 – 6.81 (m, 3H), 6.52 (d, J = 16.0 Hz, 1H), 6.21 (dt, J = 15.8, 6.4 Hz, 1H), 3.74 (s, 3H), 3.71 (s, 2H), 3.30 (d, J = 6.3 Hz, 2H), 2.94 – 2.82 (m, 2H), 2.78 – 2.65 (m, 2H); ^{13}C NMR (75 MHz, DMSO-d_6) δ 158.6, 139.7, 136.1, 131.3, 129.4, 128.6, 128.1, 127.3, 127.1, 126.6, 125.1, 122.4, 120.7, 118.2, 118.0, 113.9, 112.5, 111.2, 57.5, 55.6, 55.0, 53.6, 22.3; HRMS (ESI) _m/z_: calcd for $C_{26}H_{29}N_2O$ $[M + H]^+$ 397.2280, found 397.2276.

Synthesis of THBCs 2a-s

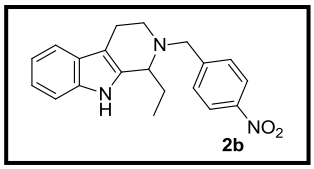
THBC 2a

***General procedure IV**: Formation of THBCs via tandem isomerization/N-alkylimimium ion cyclization*



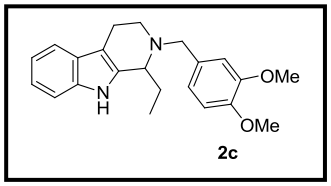
In a Schlenk tube fitted with a magnetic stirring bar and a reflux condenser, **1a** (200 mg, 0.69 mmol) and $Rh(PPh_3)_3Cl$ (31.9 mg, 0.034 mmol) were dissolved in toluene (6.9 mL). The reaction was stirred at reflux, and was monitored by TLC. Upon full conversion of the starting material (5 h), the reaction mixture was filtered through a pad of celite, which was washed with CH_2Cl_2 (2 x 20 mL). The filtrate was evaporated *in vacuo*, and the residue was then purified by flash column chromatography on silica gel (Et_3N:MeOH:CH_2Cl_2; 1:1:98), to give the title compound as a yellow oil (179 mg, 90%). R_f = 0.31 (EtOAc:heptane (1:3); UV; $KMnO_4$); HPLC purity: 89% (R_t = 6.34 min); IR (neat) cm^{-1}: 3408, 3082, 3027, 2929, 2841, 1449, 1227; ^1H NMR (300 MHz, DMSO-d_6) δ 10.66 (s, 1H), 7.38 - 7.26. (m, 7H), δ 7.02 (t, *J* = 7.3 Hz, 1H), 6.94 (t, *J* = 7.2 Hz, 1H), 3.79 (d, *J* = 13.5 Hz, 1H), 3.64 (d, *J* = 13.6 Hz, 1H), 3.54 (s, 1H), 3.19 – 2.98 (m, 1H), 2.85 – 2.67 (m, 2H), 2.52 (s, 1H), 1.91 – 1.71 (m, 2H), 0.88 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (75 MHz, DMSO-d_6) δ 139.8, 135.8, 135.6, 128.6, 128.1, 126.8, 126.7, 120.3, 118.1, 117.4, 110.8, 106.2, 57.7, 56.7, 44.9, 26.0, 18.0, 10.3; HRMS (ESI) m/z: calcd for $C_{20}H_{23}N_2$ $[M + H]^+$ 291.1861, found 291.1854.

THBC 2b



Following **general procedure (IV)**, the reaction of **1b** (250 mg, 0.75 mmol) and $Rh(PPh_3)_3Cl$ (34.5 mg, 0.037 mmol) gave after purification by flash column chromatography on silica gel (Et_3N:MeOH:CH_2Cl_2; 1:1:98), the title compound as a yellow powder (214 mg, 86%). m.p.: 56 – 58 °C; R_f = 0.22 (EtOAc:heptane (1:3); UV; $KMnO_4$); HPLC purity: >95% (R_t = 6.44 min); IR (neat) cm^{-1}: 3402, 2931, 1559, 1513, 1340; ^1H NMR (300 MHz, DMSO-d_6) δ 10.67 (s, 1H), 8.22 (d, *J* = 8.6 Hz, 2H), 7.68 (d, *J* = 8.0 Hz, 2H), 7.38 (d, *J* = 7.5 Hz, 1H), 7.28 (d, *J* = 7.8 Hz, 1H), 7.02 (t, *J* = 6.9 Hz, 1H), 6.94 (t, *J* = 7.1 Hz, 1H), 3.92 (d, *J* = 14.8 Hz, 1H), 3.80 (d, *J* = 14.7 Hz, 1H), 3.58 – 3.47 (m, 1H), 3.14 – 2.98 (m, 1H), 2.83 – 2.78 (m, 2H), 2.76 – 7.25 (m, 2H), 2.57 – 2.52 (m, 1H), 1.93 – 1-73 (m, 2H), 0.89 (t, *J* = 7.3 Hz, 3H); ^{13}C NMR (75 MHz, DMSO-d_6) δ 148.5, 146.4, 135.8, 135.3, 129.4, 126.7, 123.3, 120.3, 118.1, 117.4, 110.8, 106.1, 58.3, 56.0, 45.0, 26.0, 18.0, 10.3; HRMS (ESI) *m/z*: calcd for $C_{20}H_{22}N_3O_2$ $[M + H]^+$ 336.1712, found 336.1710.

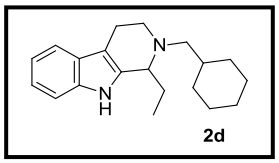
THBC 2c



Following **general procedure (IV)**, the reaction of **1c** (300 mg, 0.86 mmol) and $Rh(PPh_3)_3Cl$ (39.6 mg, 0.043 mmol) gave after purification by flash column chromatography on silica gel (Et_3N:EtOAc:heptane; 1:20:79), the title compound as a yellow crystal (232 mg, 77%). m.p.: 69 – 72 °C; R_f = 0.32 (EtOAc:heptane (1:1); UV; $KMnO_4$); HPLC purity: 88% (R_t = 6.28 min); IR (neat) cm^{-1}: 3366, 2932, 2835, 1511, 1462, 1451, 1257, 1257, 1229, 1135, 1024; ^1H NMR (300 MHz, DMSO-d_6) δ 10.63 (s, 1H), 7.37 (d, *J* = 7.5 Hz, 1H), 7.27 (d, *J* = 7.8 Hz, 1H), 7.05 – 6.79 (m, 5H), 3.73 (s,

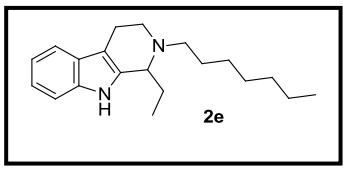
6H), 3.70 – 3.46 (m, 3H), 3.16 – 3.07 (m, 1H), 2.89 – 2.67 (m, 2H), 2.58 – 2.42 (m, 1H), 1.79 (ddq, *J* = 28.4, 14.2, 7.2 Hz, 2H), 0.90 (t, *J* = 7.3 Hz, 3H); ^{13}C NMR (75 MHz, DMSO-d_6) δ 148.5, 147.6, 135.8, 135.7, 132.1, 126.8, 120.5, 120.2, 118.0, 117.4, 112.1, 111.3, 110.7, 106.0, 57.1, 56.3, 55.4, 55.2, 44.9, 26.2, 18.0, 10.5; HRMS (ESI) *m/z*: calcd for $C_{22}H_{27}N_2O_2$ $[M + H]^+$ 351.2073, found 351.2067.

THBC 2d



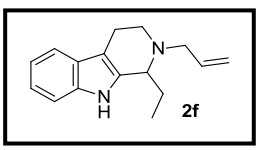
Following **general procedure (IV)**, the reaction of **1d** (200 mg, 0.67 mmol) and $Rh(PPh_3)_3Cl$ (31.2 mg, 0.034 mmol) gave after purification by flash column chromatography on silica gel (Et_3N:EtOAc:heptane; 1:10:89), the title compound as a brown oil (171 mg, 86%). R_f = 0.20 (EtOAc:heptane (1:3); UV; $KMnO_4$); HPLC purity: >95% (R_t = 6.74 min); IR (neat) cm^{-1}: 3407, 2918, 2846, 1464, 1446; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.53 (s, 1H), 7.41 (d, *J* = 8.3 Hz, 1H), 7.23 – 7.18 (m, 1H), 7.09 – 6.96 (m, 2H), 3.43 – 3.34 (m, 1H), 3.18 – 3.03 (m, 1H), 2.82 – 2.62 (m, 2H), 2.45 (dt, *J* = 10.5, 4.7 Hz, 1H), 2.28 (qd, *J* = 12.6, 7.0 Hz, 2H), 1.86 – 1.53 (m, 7H), 1.51 – 1.34 (m, 1H), 1.25 – 1.05 (m, 4H), 0.92 (t, *J* = 7.3 Hz, 3H), 0.88 – 0.72 (m, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 136.2, 136.0, 127.7, 121.4, 119.4, 118.3, 110.9, 108.6, 60.7, 59.8, 45.9, 36.8, 32.3, 32.0, 27.5, 27.3, 26.7, 18.5, 11.0; HRMS (ESI) *m/z*: calcd for $C_{20}H_{29}N_2$ $[M + H]^+$ 297.2331, found 297.2326.

THBC 2e



Following **general procedure (IV)**, the reaction of **1e** (150 mg, 0.50 mmol) and $Rh(PPh_3)_3Cl$ (23.2 mg, 0.025 mmol) gave after purification by flash column chromatography on silica gel (Et_3N:EtOAc:heptane; 1:5:94), the title compound as a brown oil (103 mg, 69%); R_f = 0.21 (EtOAc:heptane (1:3); UV; $KMnO_4$); HPLC purity: >95% (R_t = 7.39 min); IR (neat) cm^{-1}: 3408, 2925, 2854, 1464, 1452; ^{1}H NMR (300 MHz, DMSO-d_6) δ 10.62 (s, *J* = 24.5 Hz, 1H), 7.34 (d, *J* = 7.6 Hz, 1H), 7.26 (d, *J* = 7.9 Hz, 1H), 6.99 (dt, *J* = 8.1, 1.2 Hz, 1H), 6.92 (dt, *J* = 7.2, 0.9 Hz, 1H), 3.51 (dd, *J* = 7.0, 4.1 Hz, 1H), 3.08 (ddd, *J* = 14.0, 8.8, 4.9 Hz, 1H), 2.72 (ddd, *J* = 22.5, 8.5, 4.6 Hz, 2H), 2.60 – 2.40 (m, 2H), 1.94 – 1.59 (m, 2H), 1.53 – 1.45 (m, 2H), 1.39 – 1.22 (m, 8H), 0.96 – 0.73 (m, 6H); ^{13}C NMR (75 MHz, DMSO-d_6) δ 136.7, 136.5, 127.4, 120.9, 118.7, 118.0, 111.5, 107.1, 58.9, 53.2, 45.9, 32.1, 29.4, 28.3, 27.5, 26.6, 22.8, 18.9, 14.7, 11.1; HRMS (ESI) *m/z*: calcd for $C_{20}H_{31}N_2$ $[M + H]^+$ 299.2487, found 299.2482.

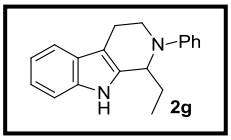
THBC 2f



Following **general procedure (IV)**, the reaction of **1f** (100 mg, 0.42 mmol) and $Rh(PPh_3)_3Cl$ (19.2 mg, 0.021 mmol) gave after purification by flash column chromatography on silica gel (Et_3N:EtOAc:heptane; 1:25:74), the title compound as a brown oil (71 mg, 71%). R_f = 0.17 (EtOAc:heptane (1:3); UV; $KMnO_4$); HPLC purity: >95% (R_t = 5.47 min); IR (neat) cm^{-1}: 3406, 2931, 1464, 1449, 1299, 918, 737; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.68 (s, 1H), 7.50 (ddd, *J* = 7.3, 1.5, 0.7 Hz, 1H), 7.34 – 7.29 (m, 1H), 7.19 – 7.07 (m, 2H), 5.96 (ddt, *J* = 16.9, 10.2, 6.4 Hz, 1H), 5.20 – 5.15 (m, 1H), 5.15 – 5.11 (m, 1H), 3.62 (t, *J* = 6.3 Hz, 1H), 3.29 – 3.23 (m, 2H), 3.23 – 3.19 (m, 1H), 2.95 (ddd, *J* = 13.1, 5.1, 3.7 Hz, 1H), 2.83 (dddd, *J* = 14.3, 9.2, 5.1, 1.3

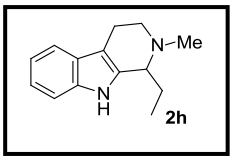
Hz, 1H), 2.60 (dddd, *J* = 5.9, 4.7, 3.7, 0.7 Hz, 1H), 1.89 – 1.72 (m, 2H), 1.03 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 137.0, 136.1, 135.5, 127.6, 121.6, 119.6, 118.4, 117.5, 110.9, 108.4, 57.9, 56.6, 45.6, 27.4, 18.5, 11.2; HRMS (ESI) *m/z*: calcd for $C_{16}H_{21}N_2$ $[M + H]^+$ 241.1705, found 241.1704.

THBC 2g



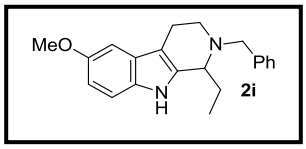
Following **general procedure (IV)**, the reaction of **1g** (130 mg, 0.47 mmol) and $Rh(PPh_3)_3Cl$ (65.3 mg, 0.071 mmol) gave after purification by flash column chromatography on silica gel (Et_3N:EtOAc:heptane; 1:10:89), the title compound as a brown oil (64 mg, 49%). R_f = 0.34 (EtOAc:heptane (1:4); UV; $KMnO_4$); HPLC purity: 86% (R_t = 7.13 min); IR (neat) cm^{-1}: 3399, 3340, 2957, 2923, 2853, 1695, 1595, 1452; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.64 (s, 1H), 7.39 (d, *J* = 7.6 Hz, 1H), 7.26 – 6.96 (m, 5H), 6.90 (dd, *J* = 8.8, 0.9 Hz, 2H), 6.69 (tt, *J* = 7.3, 1.0 Hz, 1H), 4.60 (t, *J* = 6.8 Hz, 1H), 3.86 (ddd, *J* = 13.9, 5.1, 1.2 Hz, 1H), 3.48 (ddd, *J* = 14.0, 11.4, 4.2 Hz, 1H), 2.89 (dddd, *J* = 16.6, 11.4, 5.2, 1.3 Hz, 1H), 2.58 (ddd, *J* = 15.3, 4.2, 1.7 Hz, 1H), 1.94 – 1.80 (m, 2H), 1.05 (t, *J* = 7.4 Hz, 3H).; ^{13}C NMR (75 MHz, $CDCl_3$) δ 151.1, 136.1, 135.9, 129.5, 127.5, 121.9, 119.7, 118.7, 118.4, 116.5, 111.0, 109.4, 57.6, 42.3, 27.9, 20.0, 11.7; HRMS (ESI) *m/z*: calcd for $C_{19}H_{21}N_2$ $[M + H]^+$ 277.1705, found 277.1705

THBC 2h



Following **general procedure (IV)**, the reaction of **1h** (100 mg, 0.47 mmol) and $Rh(PPh_3)_3Cl$ (21.6 mg, 0.023 mmol) gave after purification by flash column chromatography on silica gel (Et_3N: heptane:EtOAc; 1:20:79), the title compound as a yellow oil (75 mg, 75%). R_f = 0.17 (EtOAc; UV; $KMnO_4$); HPLC purity: 93% (R_t = 5.47 min); IR (neat) cm^{-1}: 3410, 2932, 2791, 1450, 1374, 1128; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.79 (s, 1H), 7.57 – 7.43 (m, 1H), 7.34 – 7.29 (m, 1H), 7.12 (dtd, *J* = 14.4, 7.1, 1.4 Hz, 2H), 3.47 (t, *J* = 5.2 Hz, 1H), 3.24 – 3.09 (m, 1H), 2.84 – 2.71 (m, 2H), 2.48 (s, 3H), 1.96 (dqd, *J* = 14.7, 7.4, 5.1 Hz, 1H), 1.78 (dqd, *J* = 14.6, 7.4, 5.3 Hz, 1H), 0.94 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 136.3, 135.1, 127.6, 121.6, 119.6, 118.3, 111.0, 109.0, 61.5, 50.6, 42.4, 25.7, 19.76, 9.9; MS (ESI) *m/z*: calcd for $C_{14}H_{18}N_2$ $[M + H]^+$ 215,2, found 215.3.

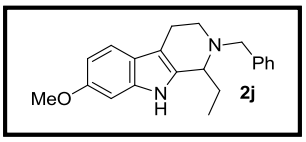
THBC 2i



Following **general procedure (IV)**, the reaction of **1i** (80 mg, 0.25 mmol) and $Rh(PPh_3)_3Cl$ (11.5 mg, 0.0012 mmol) gave after purification by flash column chromatography on silica gel (Et_3N:EtOAc:heptane; 1:10:89), the title compound as a brown oil (51 mg, 64%); R_f = 0.25 (EtOAc:heptane (1:3); UV; $KMnO_4$); HPLC purity: >95% (R_t = 6.20 min); IR (neat) cm^{-1}: 3406, 2930, 2830, 1589, 1481, 1452, 1434, 1295, 1211, 1150, 1027; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.46 (s, 1H), 7.35 – 7.16 (m, 5H), 7.12 (d, *J* = 8.7 Hz, 1H), 6.89 (d, *J* = 2.5 Hz, 1H), 6.73 (dd, *J* = 8.7, 2.5 Hz, 1H), 3.79 (s, 1H), 3.77 – 3.71 (d, 13.5, 1H), 3.63 (d, *J* = 13.5 Hz, 1H), 3.47 (t, *J* = 6.3 Hz, 1H), 3.14 (ddd, *J* = 14.9, 9.5, 5.1 Hz, 1H), 2.77 (dddd, *J* = 8.8, 7.0, 6.3, 3.1 Hz, 2H), 2.48 (dt, *J* = 8.8, 4.8 Hz, 1H), 1.81 – 1.64 (m, 2H), 0.89 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$)

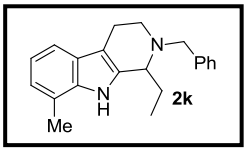
δ 154.1, 139.7, 136.3, 131.0, 129.0, 128.30, 127.8, 127.1, 111.4, 111.2, 107.9, 100.5, 58.3, 57.3, 56.1, 45.1, 27.3, 18.3, 10. 8; HRMS (ESI) *m/z*: calcd for $C_{21}H_{25}N_2$ $[M + H]^+$ 321.1967, found 321.1962.

THBC 2j



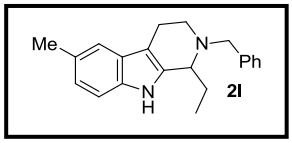
Following general **procedure (IV)**, the reaction of **1j** (100 mg, 0.31 mmol) and $Rh(PPh_3)_3Cl$ (14.4 mg, 0.017 mmol) gave after purification by flash column chromatography on silica gel (Et_3N:EtOAc:heptane; 1:10:89), the title compound as a brown oil (76 mg, 76%). R_f = 0.23 (EtOAc:heptane (1:3); UV; $KMnO_4$); HPLC purity: 69% (R_t = 6.18 min); IR (neat) cm^{-1}: 3368, 1687, 1458, 1200, 1158, 1048, 1003; ^1H NMR (300 MHz, $CDCl_3$) δ 7.44 (s, 1H), 7.37 – 7.10 (m, 6H), 6.75 (d, *J* = 2.2 Hz, 1H), 6.70 (dd, *J* = 8.5, 2.3 Hz, 1H), 3.75 (s, 3H), 3.70 (d, *J* = 2.7 Hz, 1H), 3.61 (d, *J* = 13.5 Hz, 1H), 3.44 (t, *J* = 6.3 Hz, 1H), 3.12 (ddd, *J* = 14.9, 9.5, 5.0 Hz, 1H), 2.76 (ddt, *J* = 7.5, 5.2, 4.4 Hz, 2H), 2.46 (dt, *J* = 8.5, 4.7 Hz, 1H), 1.78 – 1.65 (m, 2H), 0.88 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 156.3, 140.3, 136.8, 134.5, 129.2, 128.5, 127.2, 122.2, 118.8, 108.9, 108.2, 95.4, 58.4, 57.6, 56.2, 45.4, 27.5, 18.6, 11.0; MS (ESI) *m/z*: calcd for $C_{21}H_{24}N_2$ $[M + H]^+$ 321,2, found 321,5.

THBC 2k



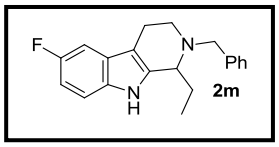
Following **general procedure (IV)**, the reaction of **1k** (80 mg, 0.26 mmol) and $Rh(PPh_3)_3Cl$ (12.2 mg, 0.013 mmol) gave after purification by flash column chromatography on silica gel (Et_3N:EtOAc:heptane; 1:10:89), the title compound as a yellow oil (64 mg, 80%). R_f = 0.34 (EtOAc:heptane (1:3); UV; $KMnO_4$); HPLC purity: 83% (R_t = 6.78 min); IR (neat) cm^{-1}: 3416, 2929, 1541, 1452, 1335, 903; ^1H NMR (300 MHz, $CDCl_3$) δ 7.46 (s, 1H), 7.34 – 7.14 (m, 6H), 6.99 – 6.93 (t, *J* = 7.3 Hz, 1H), 6.88 (d, *J* = 7.1 Hz, 1H), 3.74 (d, *J* = 13.5 Hz, 1H), 3.65 (d, *J* = 13.5 Hz, 1H), 3.51 (t, *J* = 6.4 Hz, 1H), 3.16 (ddd, *J* = 14.4, 9.7, 5.0 Hz, 1H), 2.90 – 2.70 (m, 2H), 2.50 (dt, *J* = 8.1, 4.9 Hz, 1H), 2.39 (s, 3H), 1.81 – 1.69 (m, 2H), 0.91 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 140.0, 135.4, 135.2, 129.0, 128.3, 127.0, 122.2, 119.9, 119.6, 115.9, 108.7, 58.1, 57.4, 45.0, 27.5, 18.3, 16.9, 10.9; HRMS (ESI) *m/z*: calcd for $C_{21}H_{25}N_2$ $[M + H]^+$ 305.2018, found 305.2013.

THBC 2l



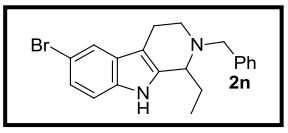
Following **general procedure (IV)**, the reaction of **1l** (150 mg, 0.49 mmol) and $Rh(PPh_3)_3Cl$ (22.8 mg, 0.025 mmol) gave after purification by flash column chromatography on silica gel (Et_3N:EtOAc:heptane; 1:10:89), the title compound as a brown oil (121 mg, 81%). R_f = 0.30 (EtOAc:heptane (1:3); UV; $KMnO_4$); HPLC purity: 94% (R_t = 6.76 min); IR (neat) cm^{-1}: 3405, 2929, 1451, 1388, 1315, 1300; ^1H NMR (300 MHz, $CDCl_3$) δ 7.51 (s, 1H), 7.34 – 7.08 (m, 7H), 6.90 (dd, *J* = 8.2, 1.4 Hz, 1H), 3.74 (d, *J* = 13.5 Hz, 1H), 3.69 (d, *J* = 20.6 Hz, 1H), 3.55 – 3.44 (m, 1H), 3.15 (ddd, *J* = 14.7, 9.5, 5.3 Hz, 1H), 2.91 – 2.67 (m, 2H), 2.61 – 2.42 (m, 1H), 2.38 (s, 3H), 1.84 – 1.65 (m, 2H), 0.89 (t, *J* = 7.5 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 140.0, 135.7, 134.2, 129.0, 128.4, 128.3, 127.6, 127.0, 123.0, 117.9, 110.5, 107.5, 77.1, 58.1, 57.3, 45.1, 27.2, 21.6, 18.3, 10.7; HRMS (ESI) *m/z*: calcd for $C_{21}H_{25}N_2$ $[M + H]^+$ 305.2018, found 305.2013.

THBC 2m



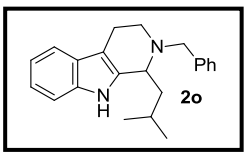
Following **general procedure (IV)**, the reaction of **1m** (100 mg, 0.32 mmol) and $Rh(PPh_3)_3Cl$ (15.0 mg, 0.016 mmol) gave after purification by flash column chromatography on silica gel (Et_3N:EtOAc:heptane; 1:10:89), the title compound as a brown oil (42 mg, 42%). R_f = 0.34 (EtOAc:heptane (1:3); UV; $KMnO_4$); HPLC purity: >95% (R_t = 6.41 min); IR (neat) cm^{-1}: 3419, 2930, 2803, 1584, 1482, 1318, 1130, 848, 765; ^1H NMR (300 MHz, $CDCl_3$) δ 7.55 (s, 1H), 7.34 – 7.10 (m, 6H), 7.06 (dd, *J* = 9.5, 2.5 Hz, 1H), 6.81 (dt, *J* = 9.0, 2.4 Hz, 1H), 3.74 (d, *J* = 13.5 Hz, 1H), 3.63 (d, *J* = 13.5 Hz, 1H), 3.49 (t, *J* = 6.3 Hz, 1H), 3.13 (ddd, *J* = 10.9, 7.9, 3.8 Hz, 1H), 2.87 – 2.66 (m, 2H), 2.46 (dt, *J* = 8.7, 5.1 Hz, 1H), 1.81 – 1.64 (m, 2H), 0.90 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 158.1 (d, J_{C-F} = 232.5 Hz, 1C), 140.1, 137.8, 132.6, 129.2, 128.5, 128.0 (d, J_{C-F} = 9.8 Hz, 1C), 127.3, 111.4 (d, J_{C-F} = 9.8 Hz, 1C), 109.5 (d, J_{C-F} = 26.3 Hz, 1C), 108.7 (d, J_{C-F} = 4.5 Hz, 1C), 103.5 (d, J_{C-F} = 23.3 Hz, 1C), 58.4, 57.6, 45.3, 27.4, 18.5, 11.0; HRMS (ESI) *m/z*: calcd for $C_{20}H_{22}FN_2$ $[M + H]^+$ 309.1767, found 309.1764.

THBC 2n



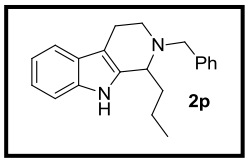
Following **general procedure (IV)**, the reaction of **1n** (80 mg, 0.22 mmol) and $Rh(PPh_3)_3Cl$ (10.0 mg, 0.011 mmol) gave after purification by flash column chromatography on silica gel (Et_3N:EtOAc:heptane; 1:10:89), the title compound as a brown oil (54 mg, 68%). R_f = 0.27 (EtOAc:heptane (1:3); UV; $KMnO_4$); HPLC purity: 78% (R_t = 7.00 min); IR (neat) cm^{-1}: 3418, 2961, 2928, 1579, 1436, 1312, 1298, 1261, 1207, 792; ^1H NMR (300 MHz, $CDCl_3$) δ 7.61 (s, 1H), 7.55 (d, *J* = 1.8 Hz, 1H), 7.34 – 7.07 (m, 7H), 3.73 (d, *J* = 13.6 Hz, 1H), 3.62 (d, *J* = 13.5 Hz, 1H), 3.49 (t, *J* = 6.2 Hz, 1H), 3.13 (ddd, *J* = 10.8, 7.9, 3.8 Hz, 1H), 2.87 – 2.67 (m, 2H), 2.46 (dt, *J* = 8.3, 4.9 Hz, 1H), 1.84 – 1.63 (m, 2H), 0.89 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 138.6, 135.9, 133.7, 128.3, 128.1, 127.5, 126.3, 119.9, 111.6, 111.3, 106.9, 57.3, 56.5, 53.63, 44.1, 26.2, 17.3; HRMS (ESI) *m/z*: calcd for $C_{20}H_{22}BrN_2$ $[M + H]^+$ 369.0966, found 369.0969

THBC 2o



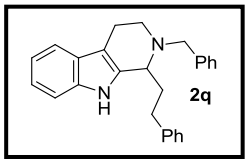
Following **general procedure (IV)**, the reaction of **1o** (200 mg, 0.63 mmol) and $Rh(PPh_3)Cl$ (87.2 mg, 0.094 mmol) gave after purification by flash column chromatography on silica gel (Et_3N:MeOH:CH_2Cl_2; 1:1:98), the title compound as a brown oil (52 mg, 26%). R_f = 0.21 (EtOAc:heptane (1:9); UV; $KMnO_4$); HPLC purity: 71% (R_t = 7.01 min); IR (neat) cm^{-1}: 3245, 2950, 2928, 2865, 2841, 1452, 1343, 1300, 1050, 1025, 1006; ^1H NMR (300 MHz, DMSO-d_6) δ 10.67 (s, 1H), 7.40 – 7.20 (m, 7H), 7.05 – 6.98 (m, 1H), 6.94 (td, *J* = 7.1, 0.8 Hz, 1H), 3.75 (d, *J* = 13.2 Hz, 1H), 3.69 – 3.56 (m, 2H), 3.19 – 3.02 (m, 1H), 2.94 – 2.78 (m, 2H), 2.47 – 2.39 (m, 1H), 1.96 – 1.84 (m, 1H), 1.68 (ddd, *J* = 14.0, 10.1, 4.1 Hz, 1H), 1.46 – 1.34 (m, 1H), 0.85 (d, *J* = 6.7 Hz, 3H), 0.66 (d, *J* = 6.5 Hz, 3H); ^{13}C NMR (75 MHz, DMSO-d_6) δ 139.8, 136.1, 135.7, 128.9, 128.0, 126.8, 126.8, 120.2, 118.0, 117.3, 110.7, 105.2, 56.6, 53.8, 43.5, 43.2, 24.1, 23.6, 21.5, 16.7; HRMS (ESI) *m/z*: calcd for $C_{21}H_{25}N_2$ $[M + H]^+$ 319.2174, found 319.2163

THBC 2p



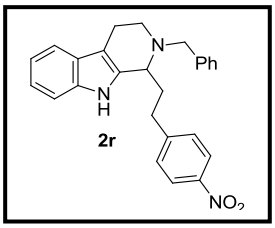
Following **general procedure (IV)**, the reaction of **1p** (150 mg, 0.49 mmol) and **Ru-9** (58.6 mg, 0.074 mmol) gave after purification by flash column chromatography on silica gel (Et_3N:MeOH:CH_2Cl_2; 1:1:98), the title compound as a brown oil (101 mg, 67%). R_f = 0.39 (EtOAc:heptane (1:3); UV; $KMnO_4$); HPLC purity: 73% (R_t = 6.67 min); IR (neat) cm^{-1}: 3406; 2954, 2929, 1600, 1493, 1452, 1052, 1008; ^1H NMR (300 MHz, $CDCl_3$) δ 7.55 (s, 1H), 7.43 (dd, *J* = 7.9, 1.0 Hz, 1H), 7.33 – 7.14 (m, 6H), 7.11 – 6.99 (m, 2H), 3.69 (d, *J* = 4.5 Hz, 2H), 3.60 – 3.50 (m, 1H), 3.22 – 3.12 (m, 1H), 2.91 – 2.76 (m, 2H), 2.56 – 2.44 (m, 1H), 1.77 – 1.52 (m, 2H), 1.51 – 1.29 (m, 2H), 0.78 (t, *J* = 7.3 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 140.0, 135.9, 135.8, 129.0, 128.3, 127.5, 127.0, 121.4, 119.3, 118.1, 110.8, 107.8, 57.4, 56.5, 44.8, 37.0, 19.6, 18.0, 14.3; HRMS (ESI) *m/z*: calcd for $C_{21}H_{25}N_2$ $[M + H]^+$ 305.2018, found 305.2011.

THBC 2q



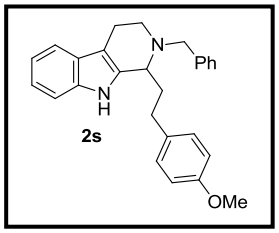
Following **general procedure (IV)**, the reaction of **1q** (150 mg, 0.41 mmol) and $Rh(PPh_3)_3Cl$ (18.9 mg, 0.0204 mmol) gave after purification by flash column chromatography on silica gel (Et_3N:MeOH:CH_2Cl_2; 1:1:98), the title compound as a brown oil (98 mg, 65%). R_f = 0.20 (EtOAc:heptane (1:9); UV; $KMnO_4$); HPLC purity: 93% (R_t = 7.35 min); IR (neat) cm^{-1}: 3402, 3227, 2934, 2842, 1494, 1452, 1050, 1034, 1006; ^1H NMR (500 MHz, DMSO-d_6) δ 10.71 (s, 1H), 7.46 – 7.31 (m, 5H), 7.31 – 7.18 (m, 3H), 7.14 (d, *J* = 7.7 Hz, 3H), 7.02 (t, *J* = 7.4 Hz, 1H), 6.95 (t, *J* = 7.3 Hz, 1H), 3.80 (d, *J* = 13.5 Hz, 1H), 3.70 (dd, *J* = 8.2, 4.9 Hz, 2H), 3.15 (ddd, *J* = 14.1, 9.0, 4.8 Hz, 1H), 2.87 – 2.74 (m, 2H), 2.65 (t, *J* = 7.2 Hz, 2H), 2.52 – 2.48 (m, 1H), 2.23 – 1.94 (m, 2H); ^{13}C NMR (75 MHz, DMSO-d_6) δ 142.4, 139.7, 135.9, 135.4, 128.7, 128.3, 128.2, 128.2, 126.8, 126.8, 125.5, 120.4, 118.1, 117.5, 110.9, 106.3, 56.7, 56.4, 44.6, 35.2, 31.6, 17.8; HRMS (ESI) *m/z*: calcd for $C_{26}H_{27}N_2$ $[M + H]^+$ 367.2174, found 367.2170.

THBC 2r



Following **general procedure (IV)**, the reaction of **1r** (150 mg, 0.36 mmol) and $Rh(PPh_3)_3Cl$ (50.6 mg, 0.055 mmol) gave after purification by flash column chromatography on silica gel (Et_3N:EtOAc:heptane; 1:10:89), the title compound as a brown oil (65 mg, 43%). R_f = 0.27 (EtOAc:heptane (1:3); UV; $KMnO_4$); HPLC purity: 82% (R_t = 7.37 min); IR (neat) cm^{-1}: 3406, 2938, 2840, 1598, 1512, 1450, 1299, 1007; ^1H NMR (300 MHz, $CDCl_3$) δ 8.00 – 7.97 (m, 1H), 7.97 – 7.93 (m, 1H), 7.56 (s, 1H), 7.44 (d, *J* = 8.5 Hz, 1H), 7.35 – 7.19 (m, 7H), 7.11 – 6.99 (m, 4H), 3.70 (s, 2H), 3.59 (dd, *J* = 8.7, 3.8 Hz, 1H), 3.28 – 3.15 (m, 1H), 3.00 – 2.62 (m, 5H), 2.60 – 2.47 (m, 1H), 2.12 – 1.86 (m, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 150.8, 146.4, 136.2, 129.5, 129.4, 128.7, 127.5, 127.4, 123.8, 121.9, 119.7, 118.4, 111.1, 108.4, 57.6, 55.9, 45.3, 36.0, 32.3, 18.1; HRMS (ESI) *m/z*: calcd for $C_{26}H_{26}N_3O_2$ $[M + H]^+$ 412.2025, found 412.2019.

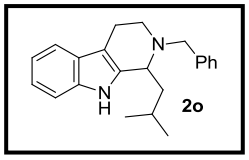
THBC 2s



2s

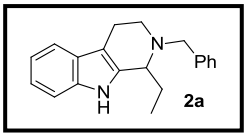
Following **general procedure (IV)**, the reaction of **1s** (250 mg, 0.63 mmol) and $Rh(PPh_3)_3Cl$ (87.5 mg, 0.095 mmol) gave after purification by flash column chromatography on silica gel (Et_3N:MeOH:CH_2Cl_2; 1:1:98), the title compound as a brown oil (97 mg, 39%). R_f = 0.26 (EtOAc:heptane (1:3); UV; $KMnO_4$); HPLC purity: 90% (R_t = 7.35 min); IR (neat) cm^{-1}: 3409, 2932, 2836, 1609, 1510, 1254, 1298, 1232, 1175, 1009; ^1H NMR (500 MHz, DMSO-d_6) δ 10.69 (s, 1H), 7.42 – 7.33 (m, 5H), 7.27 (dd, *J* = 7.5, 4.0 Hz, 2H), 7.04 (d, *J* = 8.6 Hz, 2H), 7.00 (d, *J* = 7.4 Hz, 1H), 6.94 (t, *J* = 7.4 Hz, 1H), 6.79 (d, *J* = 8.5 Hz, 2H), 3.78 (d, *J* = 13.6 Hz, 1H), 3.73 – 3.64 (m, 5H), 3.13 (ddd, *J* = 14.2, 9.2, 4.8 Hz, 1H), 2.84 – 2.73 (m, 2H), 2.58 (t, *J* = 7.7 Hz, 2H), 2.52 – 2.47 (m, 1H), 2.09 – 1.99 (m, 2H); ^{13}C NMR (75 MHz, DMSO-d_6) δ 157.2, 139.7, 135.9, 135.5, 134.2, 129.1, 128.7, 128.1, 126.8, 126.6, 120.3, 118.1, 117.4, 113.6, 110.8, 106.2, 56.7, 56.3, 54.8, 44.5, 35.5, 30.7, 17.8; HRMS (ESI) *m/z*: calcd for $C_{27}H_{29}N_2O$ $[M + H]^+$ 397.2280, found 397.2276.

Synthesis of THBC 2o



In a Schlenk tube fitted with a magnetic stirring bar and a reflux condenser, freshly titrated *n*-BuLi (0.57 mmol, 36.2 mg, 1.1 M in hexanes, 514 µL) was added to a suspension of $Rh(PPh_3)_3Cl$ (261 mg, 0.28 mmol) in toluene (4.2 mL). The mixture was stirred for 20 min at rt, after which a solution of **1o** (300 mg, 0.94 mmol) in toluene (4.2 mL) was added. The reaction was stirred at reflux and was monitored by TLC. After 23 hours, the reaction mixture was filtered through a pad of celite, which was washed with CH_2Cl_2 (2 x 20 mL). The filtrate was evaporated *in vacuo*, and the residue was purified by flash column chromatography on silica gel (Et_3N:EtOAc:heptane; 1:10:89), to give the title compound as a yellow oil (152 mg, 51%).

Synthesis of THBC 2a: One-Pot Reaction

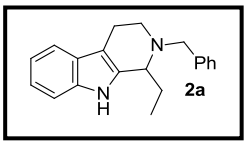


In a Schlenk tube fitted with a magnetic stirring bar and a reflux condenser, allyl bromide (16 mg, 11.4 µL, 0.13 mmol) was added to a stirred suspension of *N*-benzyltryptamine (30 mg, 0.12 mmol) and K_2CO_3 (23 mg, 0.17 mmol) in toluene (1.1 mL). The reaction was stirred at reflux and was monitored by TLC. Upon full conversion of the starting material (16 h), $Rh(PPh_3)_3Cl$ (16.6 mg, 0.018 mmol) was added. After further 2 h of stirring, the reaction mixture was filtered through a pad of celite, which was washed with CH_2Cl_2 (2 x 5 mL). The filtrate was evaporated *in vacuo*, and the residue was purified by flash column chromatography on silica gel (Et_3N:EtOAc:heptane; 1:10:89), to give the title compound as a yellow oil (25 mg, 71%).

Synthesis of THBCs 2a-e and 2j: Pd-Catalyzed Tandem Tsuji-Trost Allylation/Isomerization/Cyclization

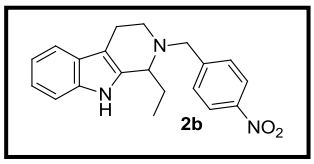
***General procedure V**: Synthesis of THBCs via Pd-catalyzed Tsuji-Trost /isomerization/ cyclization sequence*

THBC 2a



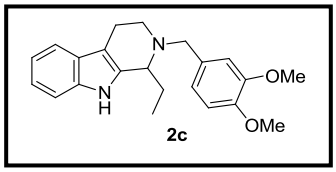
In a Schlenk tube fitted with a magnetic stirring bar and a reflux condenser, *N*-benzyltryptamine (48 mg, 0.19 mmol) was dissolved in toluene (1.6 ml). Allylmethylcarbonate (18.6 mg, 18.2 µl, 0.16 mmol) was added, followed by $Pd(PPh_3)_4$ (28.0 mg, 0.024 mmol). The reaction was stirred at reflux and was monitored by TLC. After 4 h, the reaction was cooled to room temperature and transferred to column chromatography for purification on silica gel (EtOAc:hexanes; 1:3), to give the title compound (40 mg, 85%).

THBC 2b



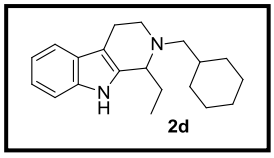
Following **general procedure (V)**, the reaction of *N*-(4-nitro)benzyltryptamine (61.0 mg, 0.20 mmol), allylcarbonate (20 mg, 19.6 µl, 0.17 mmol), and $Pd(PPh_3)_4$ (59 mg, 0.051 mmol), gave after purification by flash column chromatography on silica gel (EtOAc:hexanes; 1:6), the title compound (49 mg, 86%).

THBC 2c



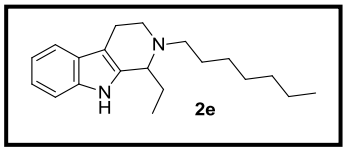
Following **general procedure (V)**, the reaction of *N*-(3,4-dimethoxy)benzyltryptamine (64.0 mg, 0.20 mmol), allylcarbonate (20 mg, 19.6 µl, 0.17 mmol), and $Pd(PPh_3)_4$ (59 mg, 0.051 mmol), gave after purification by flash column chromatography on silica gel (EtOAc:hexanes; 1:1), the title compound (49 mg, 81%).

THBC 2d



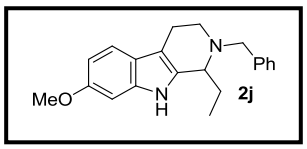
Following **general procedure (V)**, the reaction of *N*-cyclohexylmethyltryptamine (53.0 mg, 0.20 mmol), allylcarbonate (20 mg, 19.6 µl, 0.17 mmol), and $Pd(PPh_3)_4$ (59 mg, 0.051 mmol), gave after purification by flash column chromatography on silica gel (EtOAc:hexanes; 1:8), the title compound (34 mg, 67%).

THBC 2e



Following **general procedure (V)**, the reaction of *N*-heptyltryptamine (53.3 mg, 0.20 mmol), allylcarbonate (20 mg, 19.6 µl, 0.17 mmol), and $Pd(PPh_3)_4$ (59 mg, 0.051 mmol), gave after purification by flash column chromatography on silica gel (EtOAc:hexanes; 1:2), the title compound (25 mg, 48%).

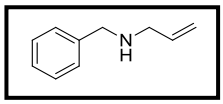
THBC 2j.



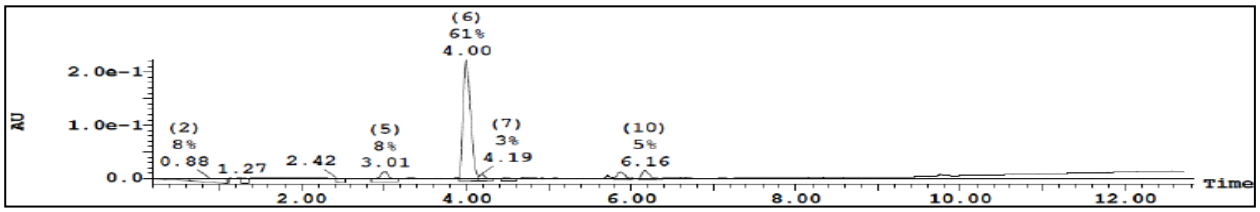
Following **general procedure (V)**, the reaction of *N*-benzyl-(6-methoxy)tryptamine (56.0 mg, 0.20 mmol), allylcarbonate (20 mg, 19.6 µl, 0.17 mmol), and $Pd(PPh_3)_4$ (29.0 mg, 0.025 mmol), gave after purification by flash column chromatography on silica gel (EtOAc:hexanes; 1:6), the title compound (37 mg, 67%).

RP-HPLC Chromatograms, IR, ^{1}H-, and ^{13}C NMR Spectra for all Compounds

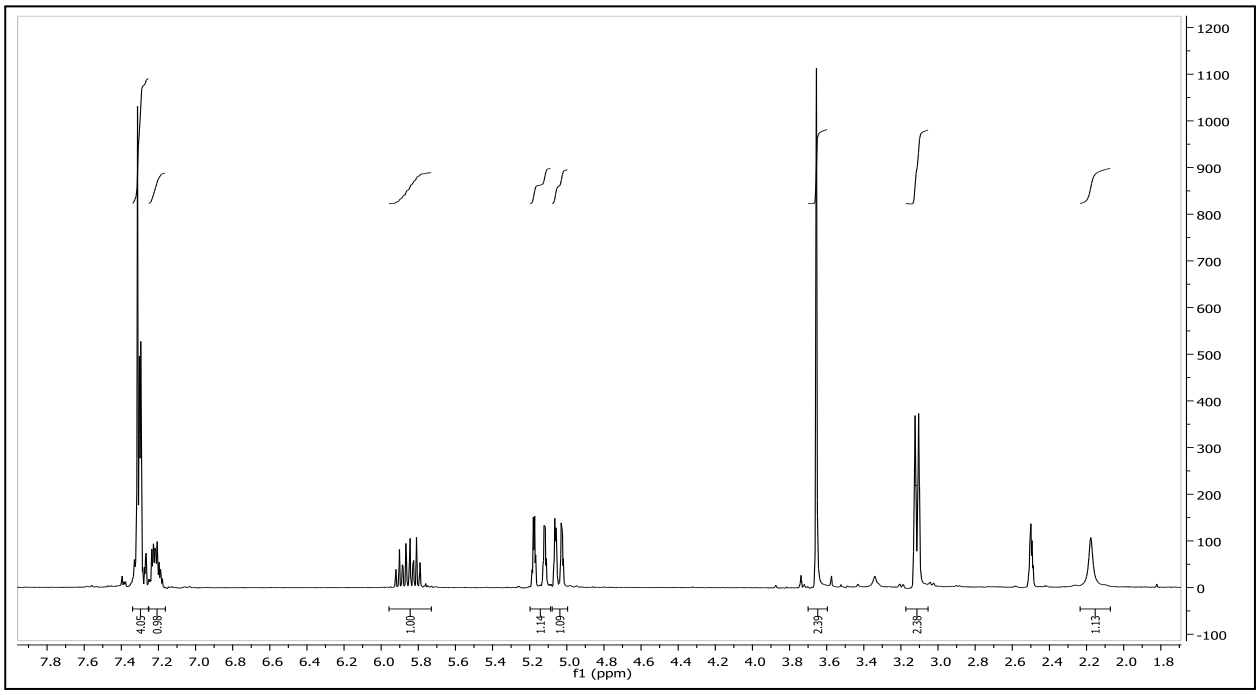
_N_-Benzyl-allylamine



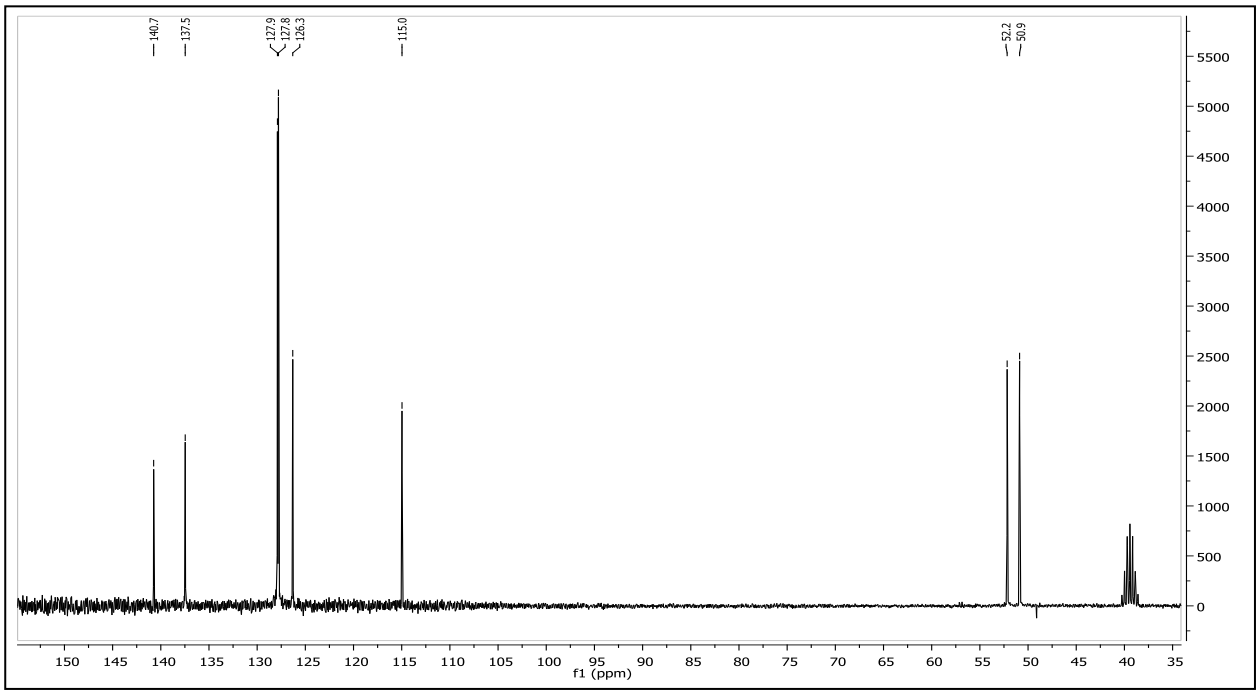
RP-HPLC of _N_-benzyl-allylamine



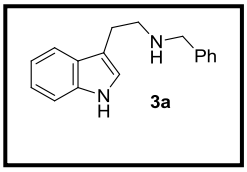
^{1}H NMR of *N*-benzyl-allylamine



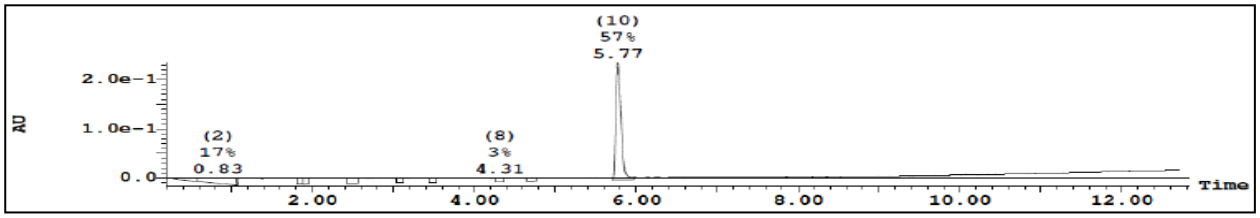
^{13}C NMR of *N*-benzyl-allylamine



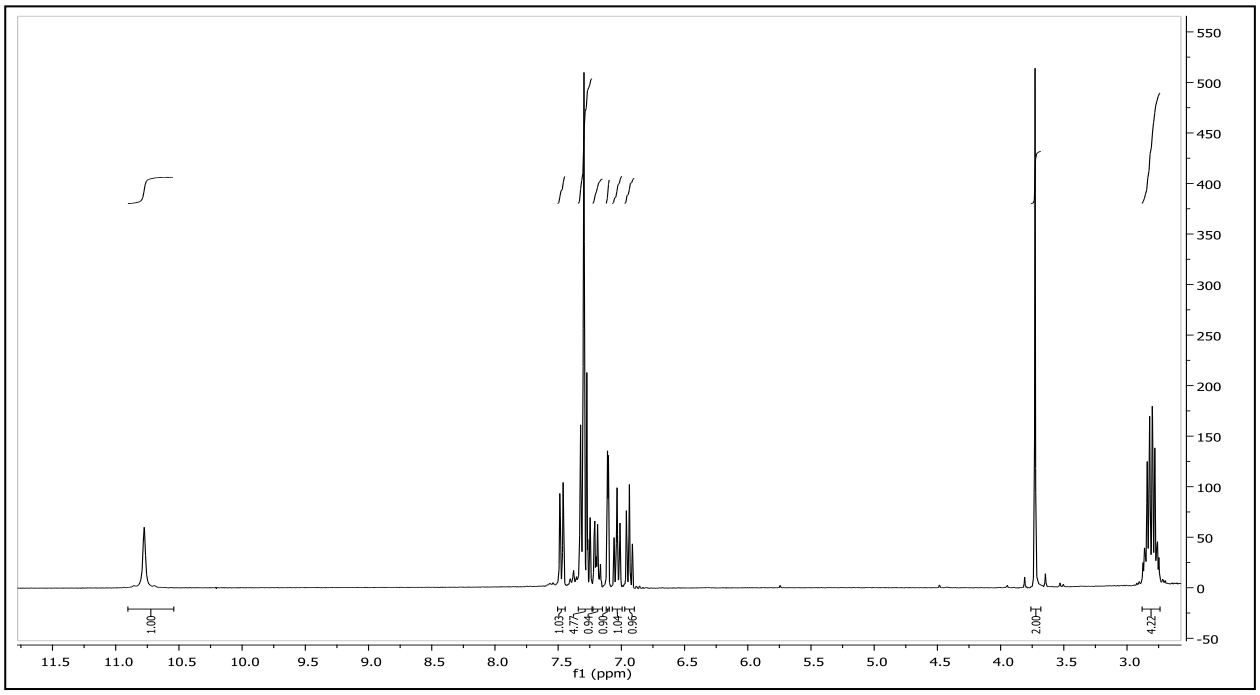
_N_-Benzyltryptamine (3a)



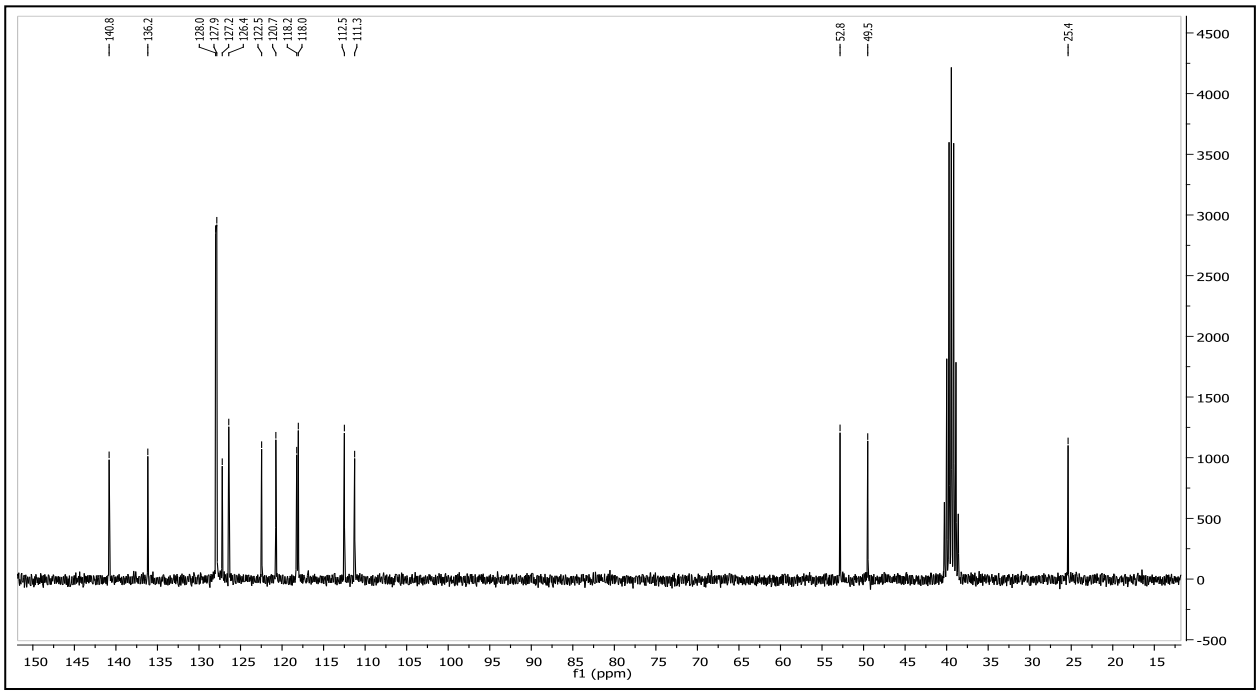
RP-HPLC of _N_-benzyltryptamine (3a)



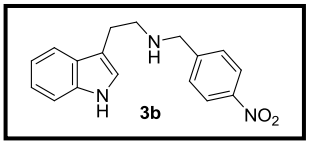
^{1}H NMR of *N*-benzyltryptamine (3a)



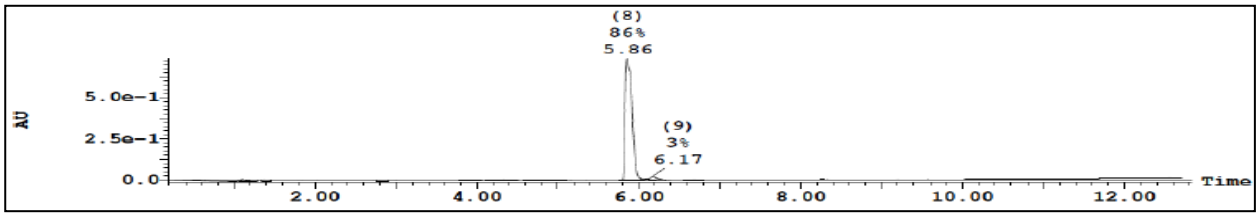
^{13}C NMR of *N*-benzyltryptamine (3a)



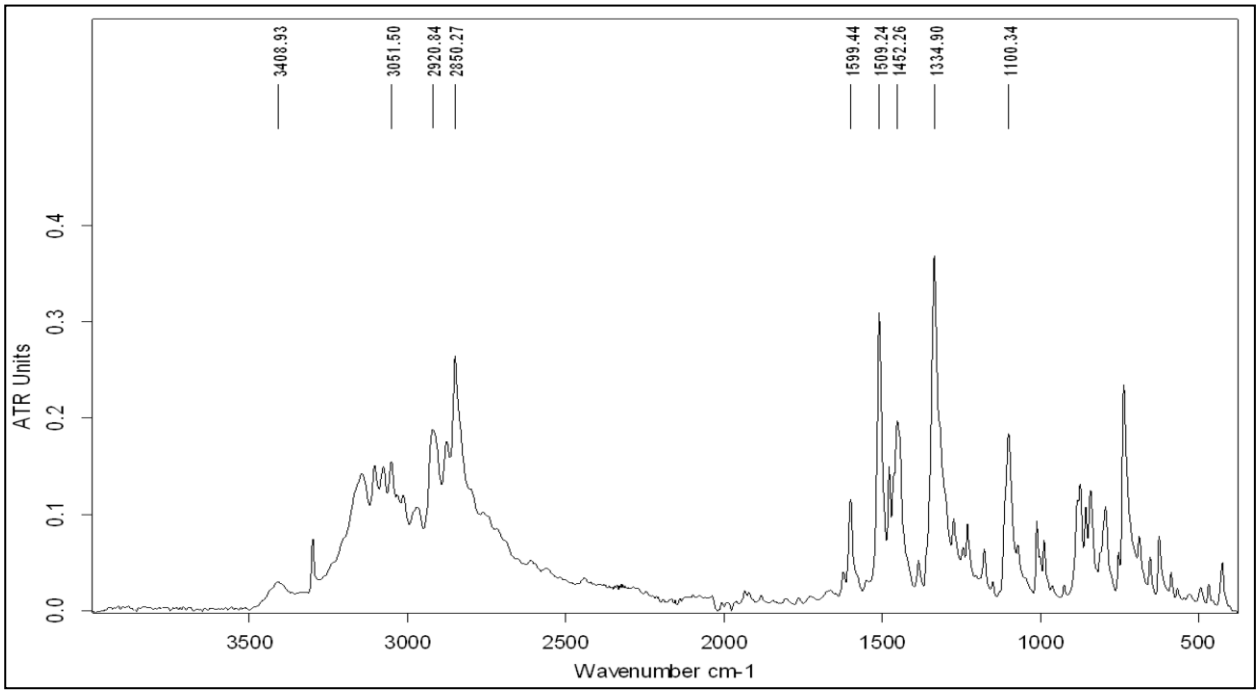
_N_-(4-Nitro)benzyltryptamine (3b)



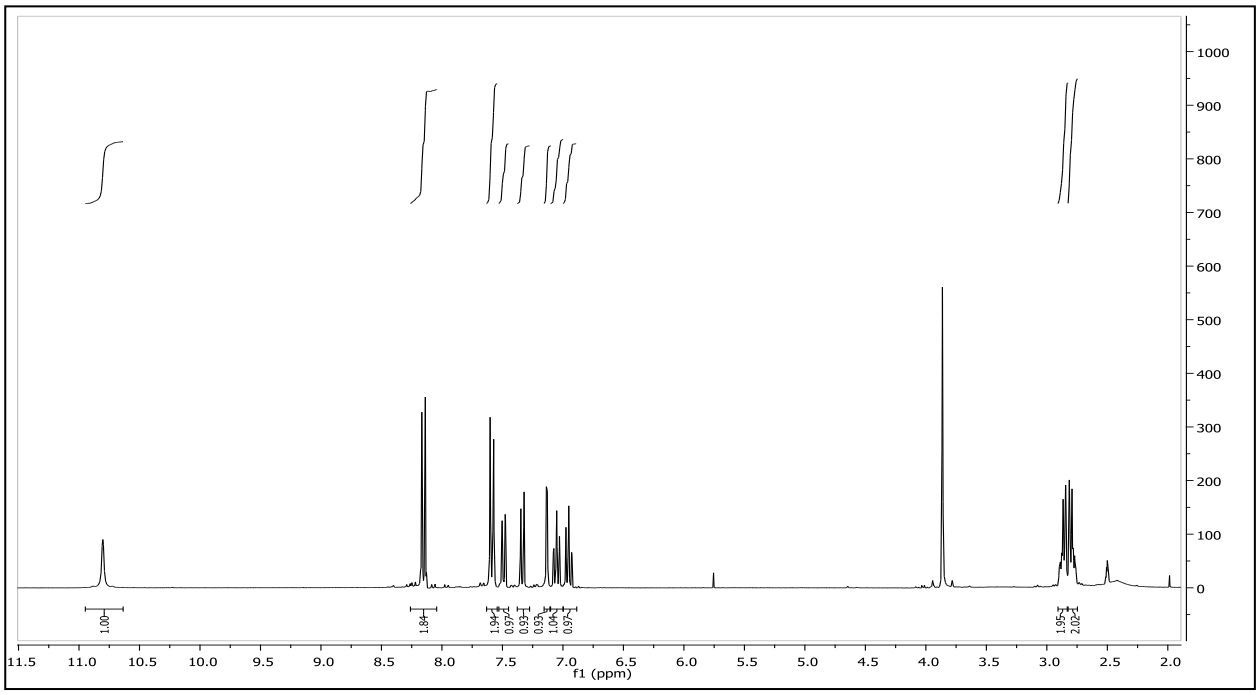
RP-HPLC of _N_-(4-nitro)benzyltryptamine (3b)



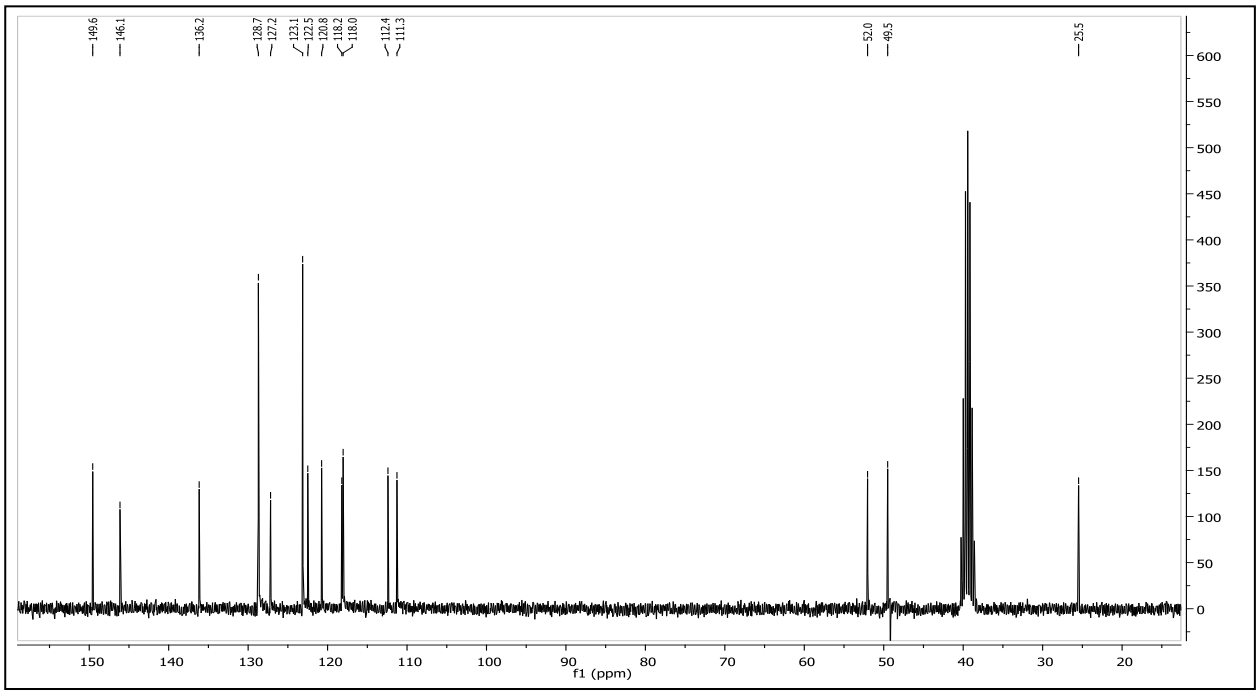
IR of _N_-(4-nitro)benzyltryptamine (3b)



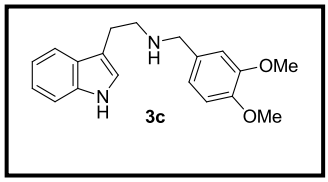
^{1}H NMR of *N*-(4-nitro)benzyltryptamine (3b)



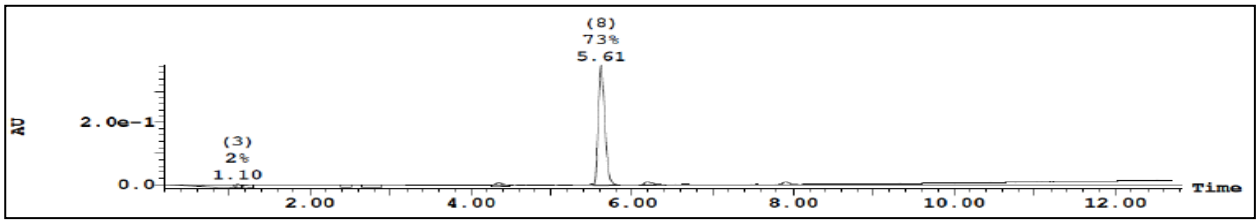
^{13}C NMR of *N*-(4-nitro)benzyltryptamine (3b)



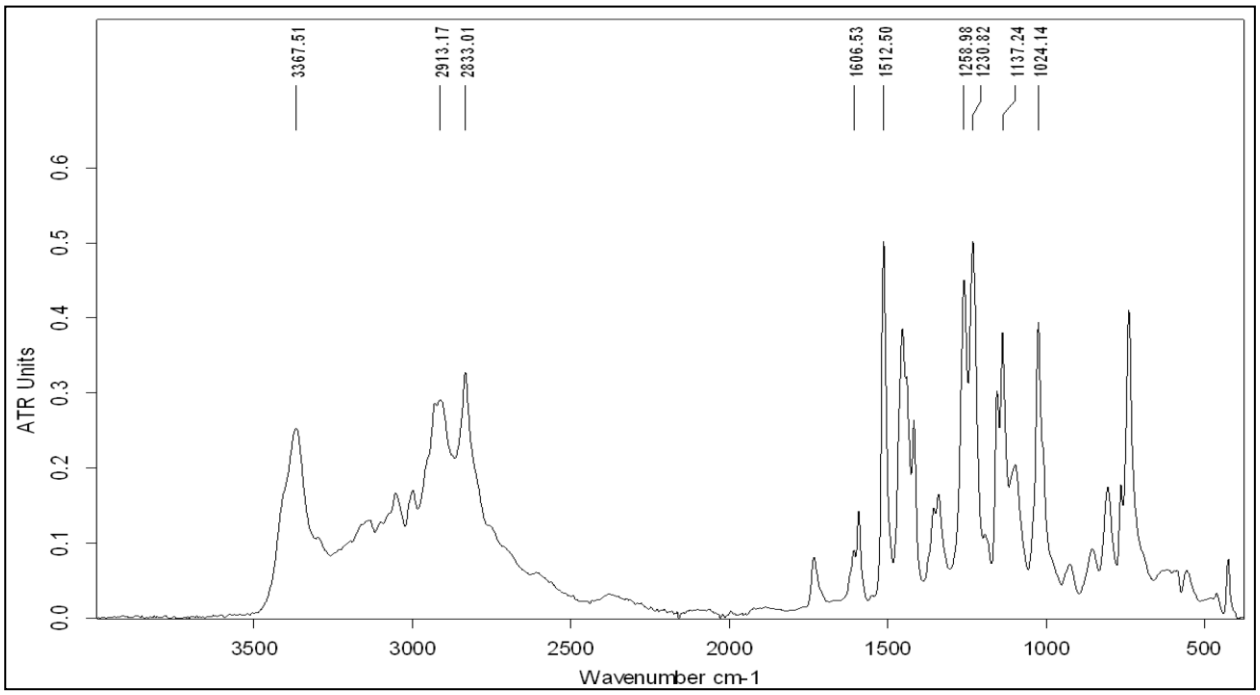
_N_-(3,4-Dimethoxy)benzyltryptamine (3c)



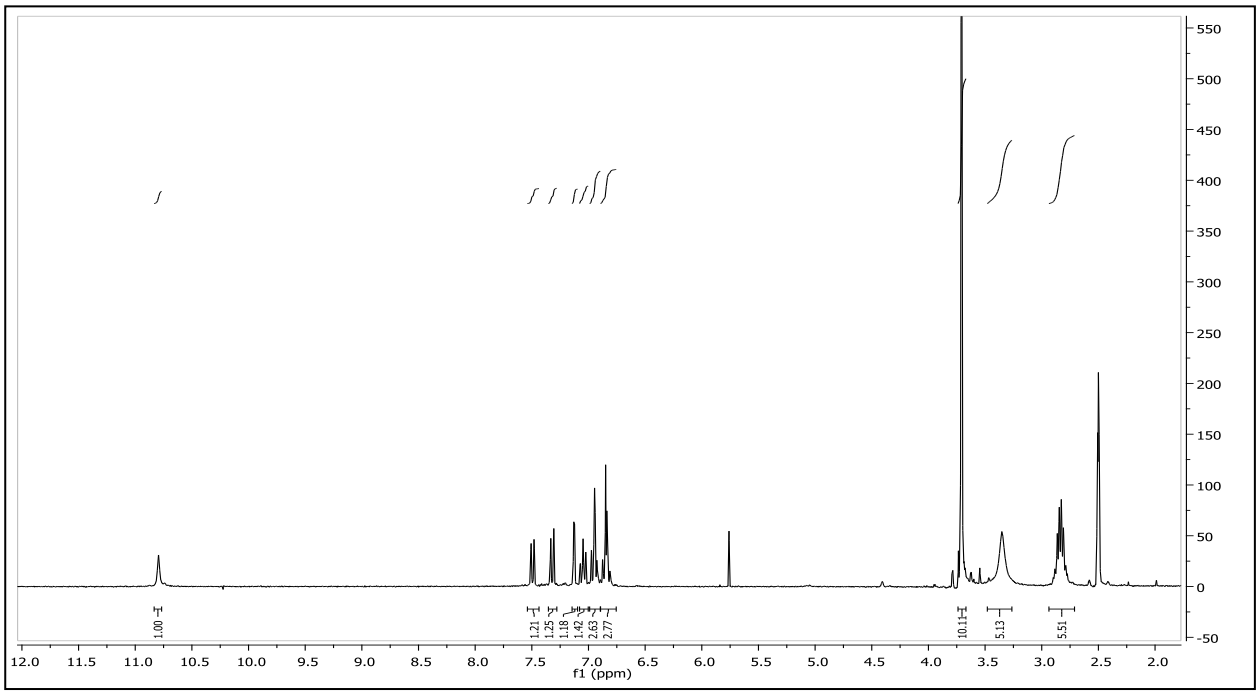
RP-HPLC of _N_-(3,4-dimethoxy)benzyltryptamine (3c)



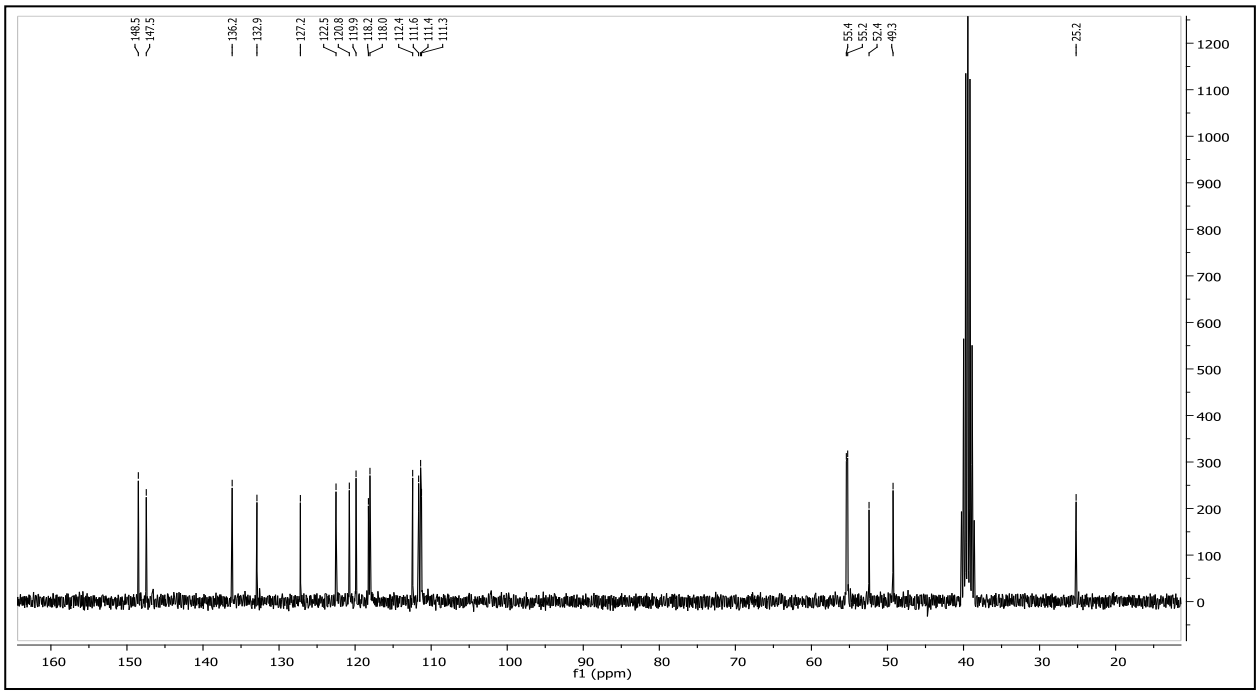
IR of _N_-(3,4-dimethoxy)benzyltryptamine (3c)



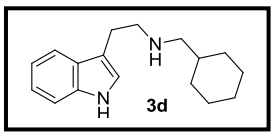
^{1}H NMR of *N*-(3,4-dimethoxy)benzyltryptamine (3c)



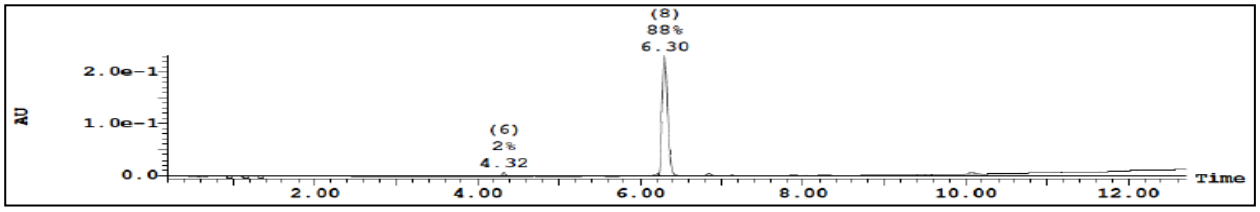
^{13}C NMR of *N*-(3,4-dimethoxy)benzyltryptamine (3c)



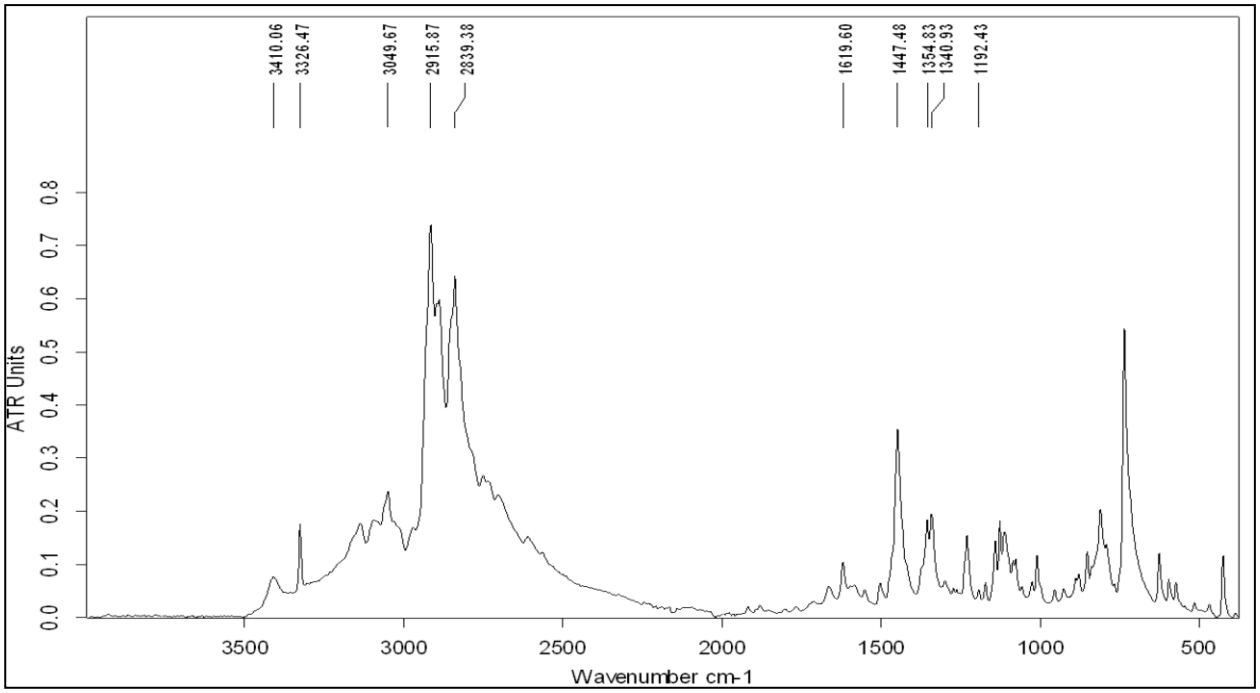
_N_-Cyclohexylmethyltryptamine (3d)



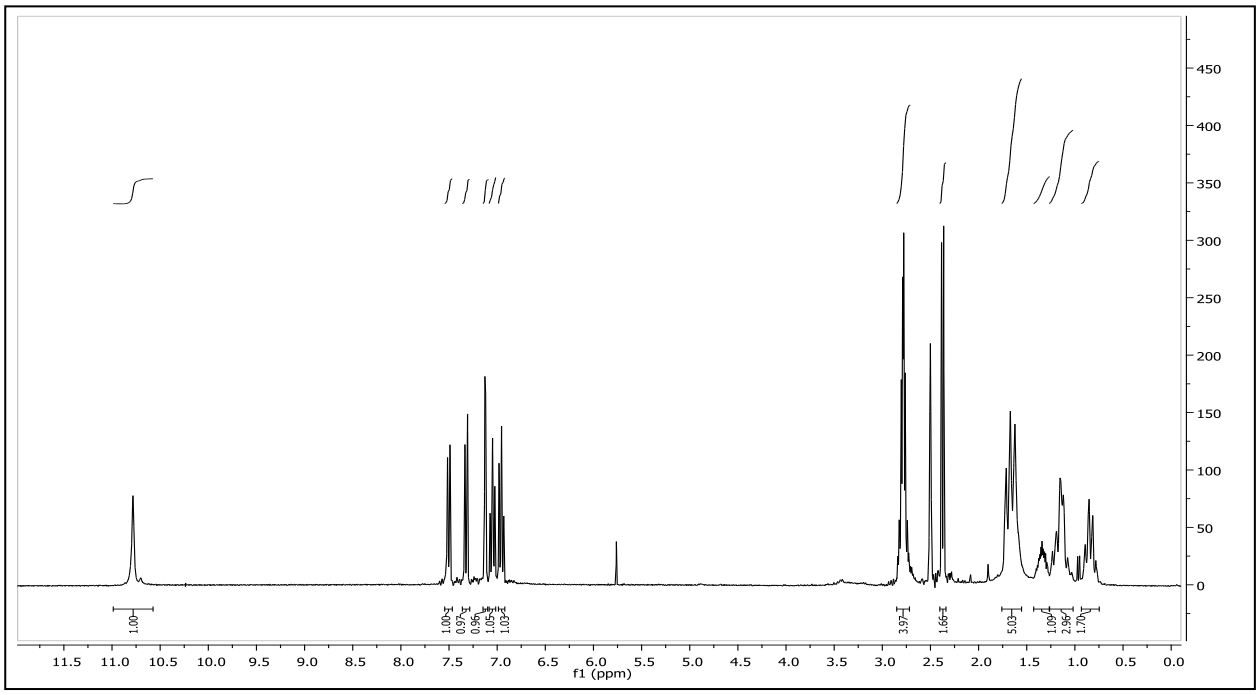
RP-HPLC of _N_-cyclohexylmethyltryptamine (3d)



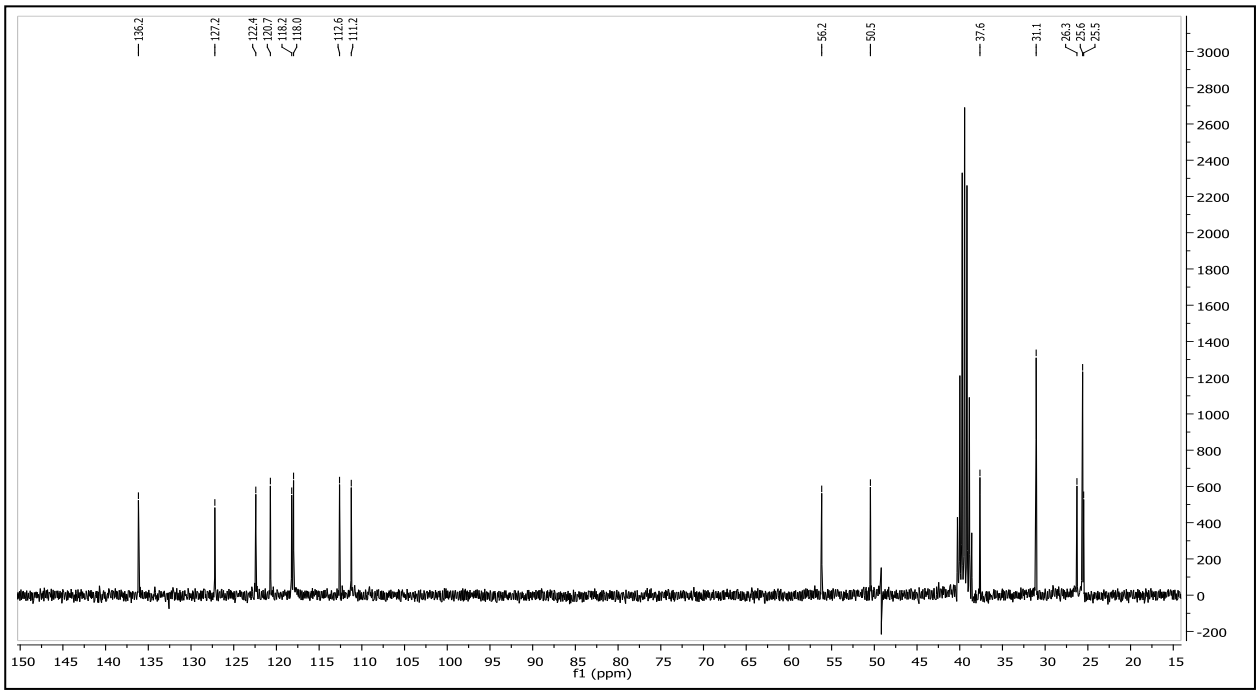
IR of _N_-cyclohexylmethyltryptamine (3d)



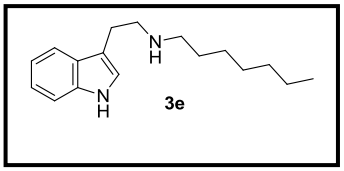
^{1}H NMR of *N*-cyclohexylmethyltryptamine (3d)



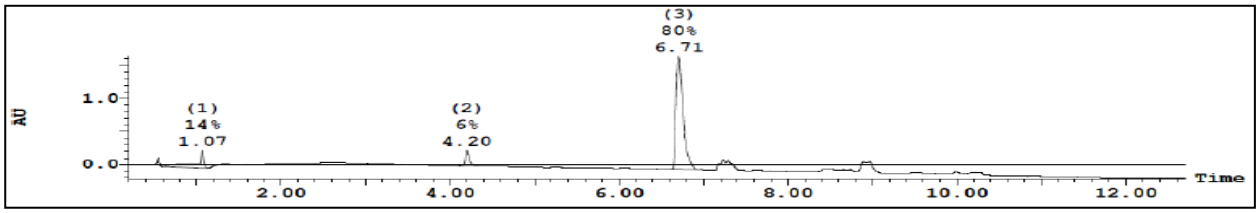
^{13}C NMR of *N*-cyclohexylmethyltryptamine (3d)



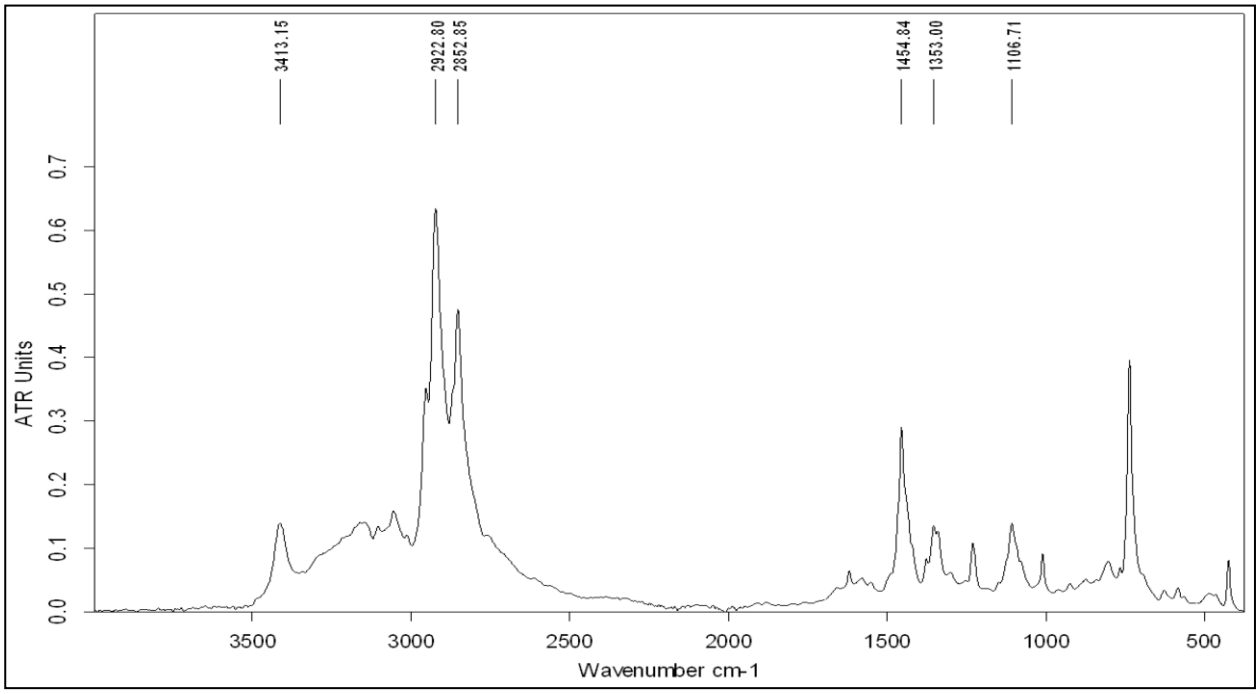
_N_-Heptyltryptamine (3e)



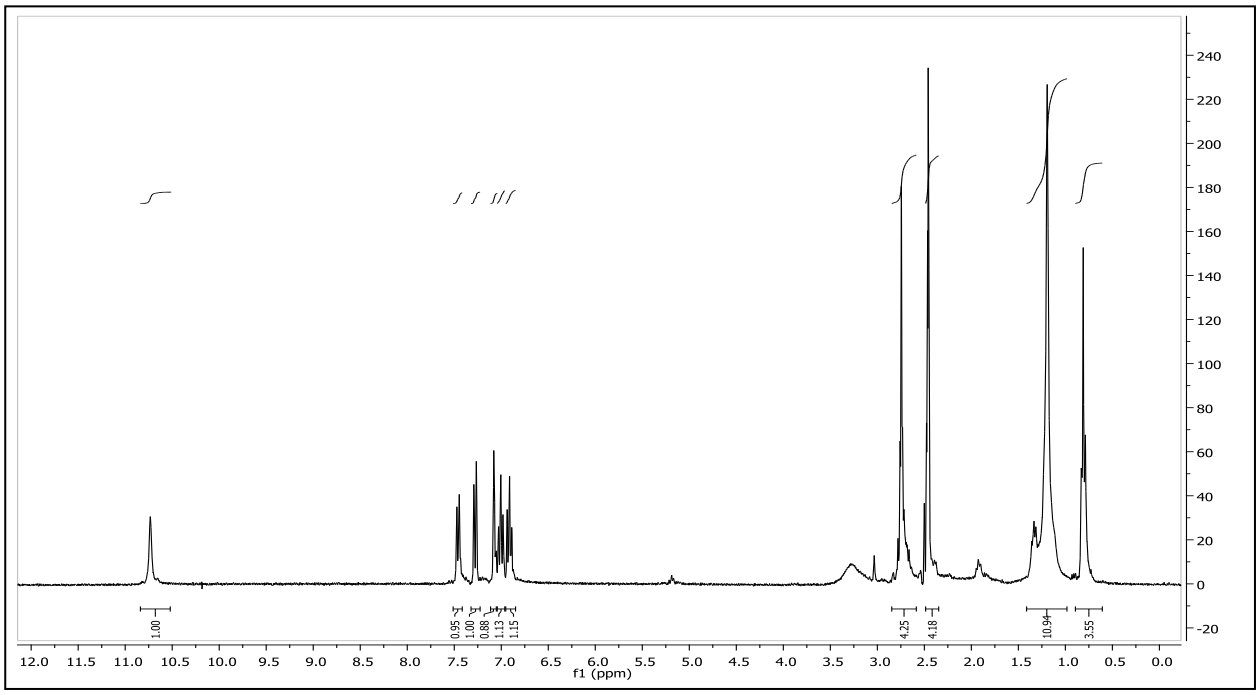
RP-HPLC of _N_-heptyltryptamine (3e)



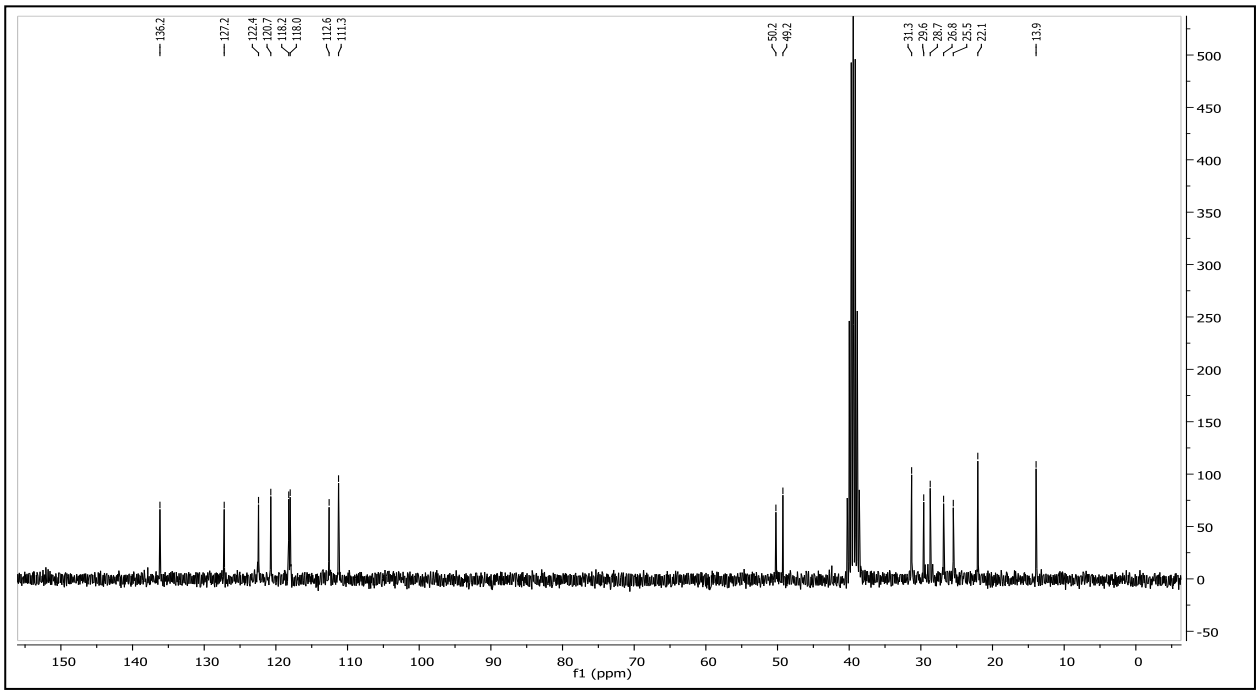
IR of _N_-heptyltryptamine (3e)



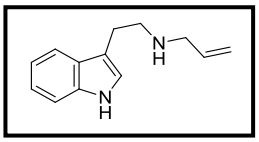
^{1}H NMR of *N*-heptyltryptamine (3e)



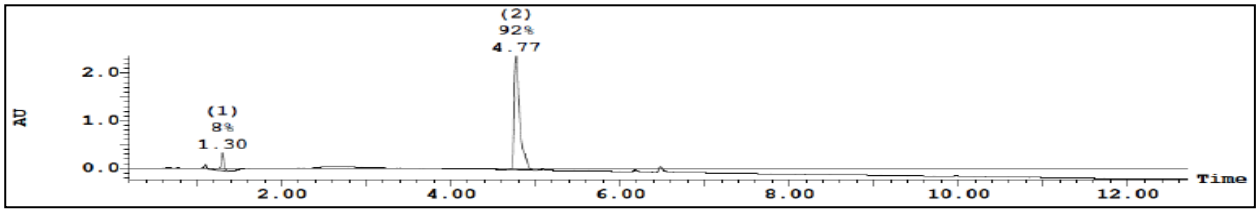
^{13}C NMR of *N*-heptyltryptamine (3e)



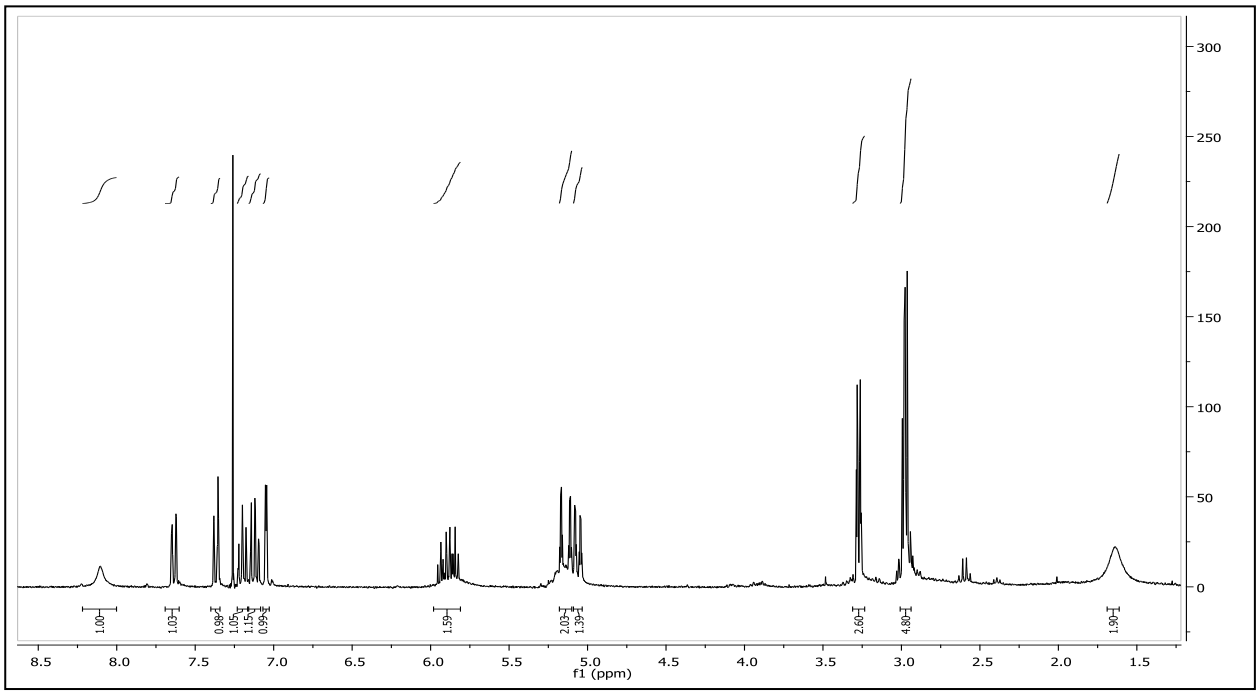
_N_-Allyltryptamine



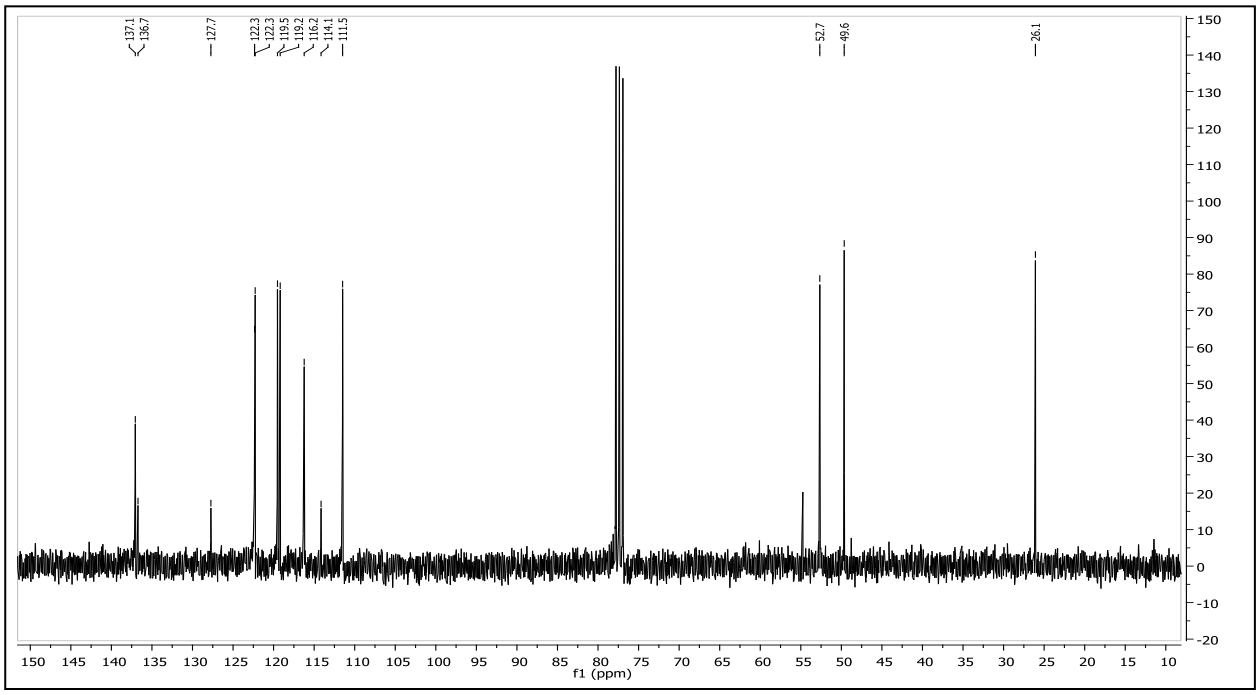
RP-HPLC of _N_-allyltryptamine



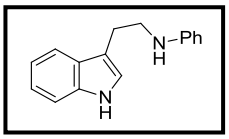
^{1}H NMR of *N*-allyltryptamine



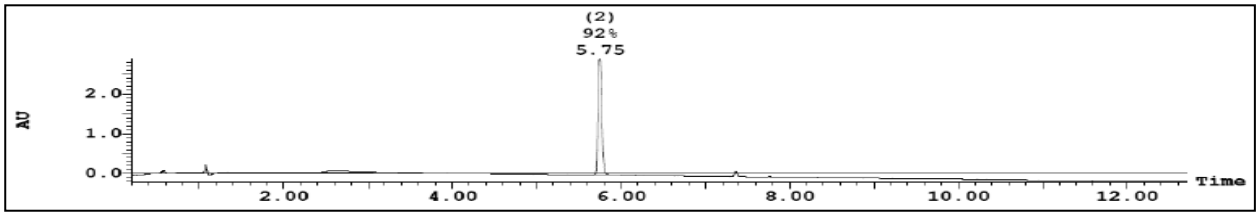
^{13}C NMR of *N*-Allyltryptamine



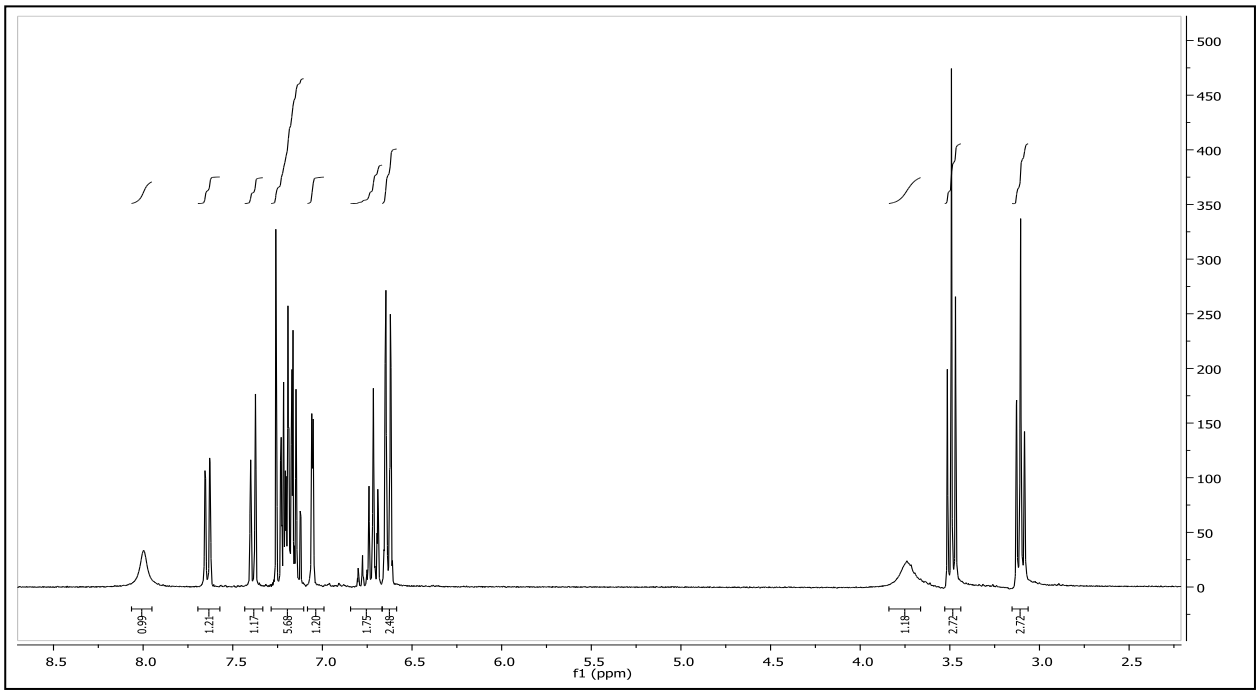
_N_-Phenyltryptamine



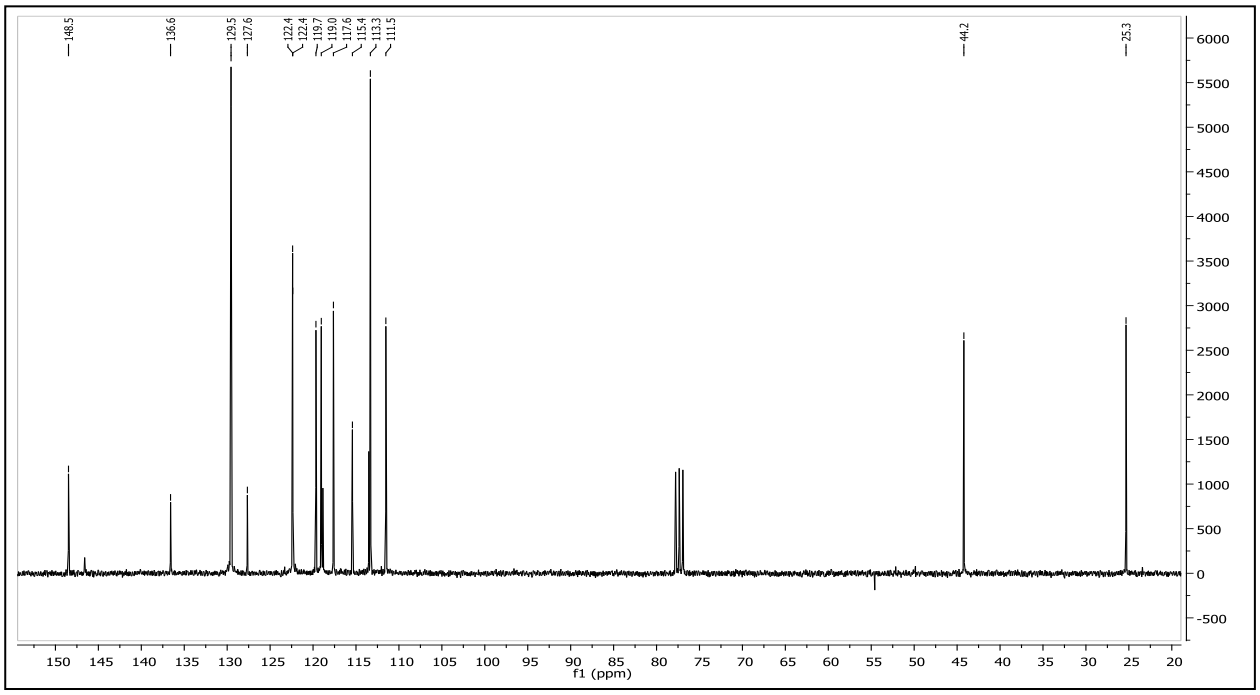
RP-HPLC of _N_-phenyltryptamine



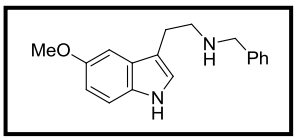
^{1}H NMR of *N*-phenyltryptamine



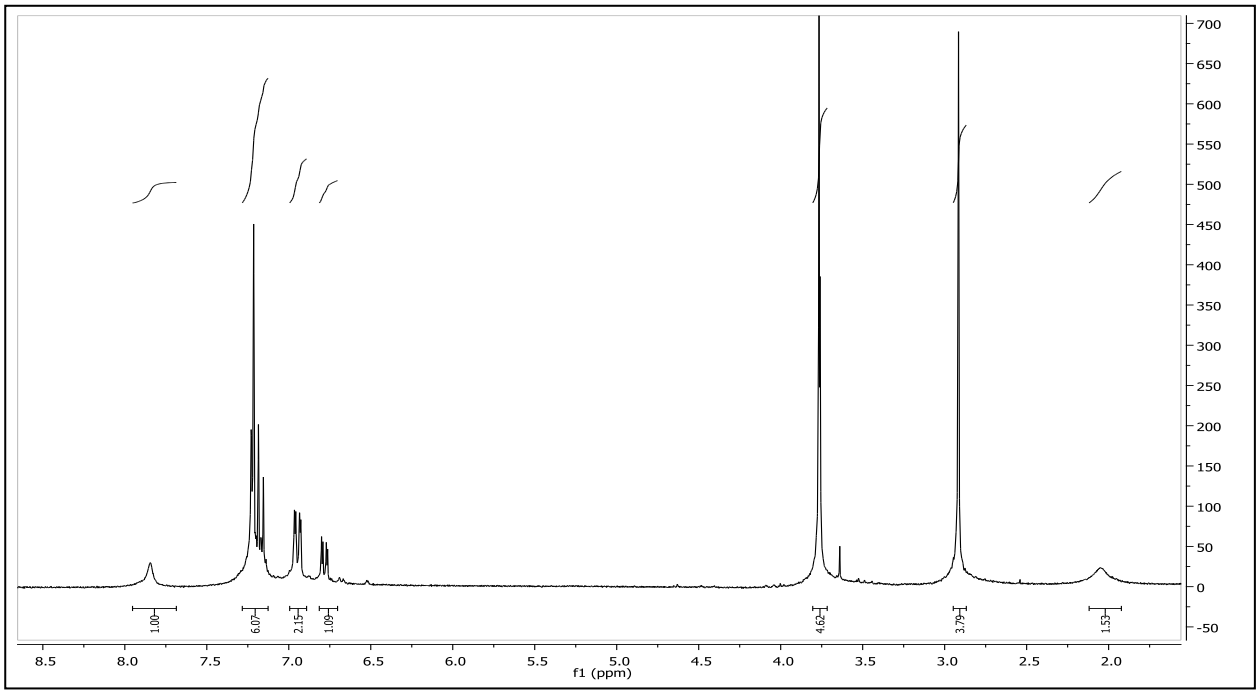
^{13}C NMR of *N*-phenyltryptamine



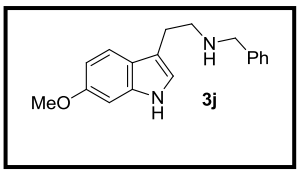
N-Benzyl-(5-methoxy)tryptamine



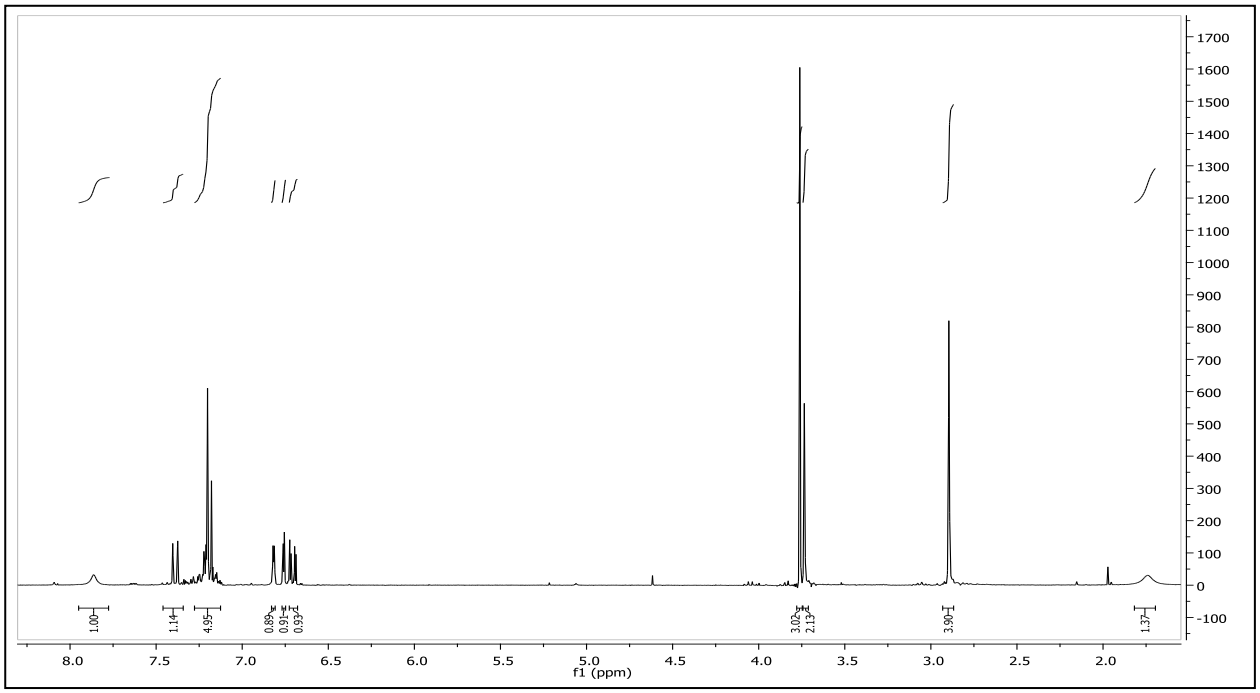
^{1}H NMR of *N*-benzyl-(5-methoxy)tryptamine



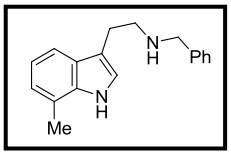
N-Benzyl-(6-methoxy)tryptamine (3j)



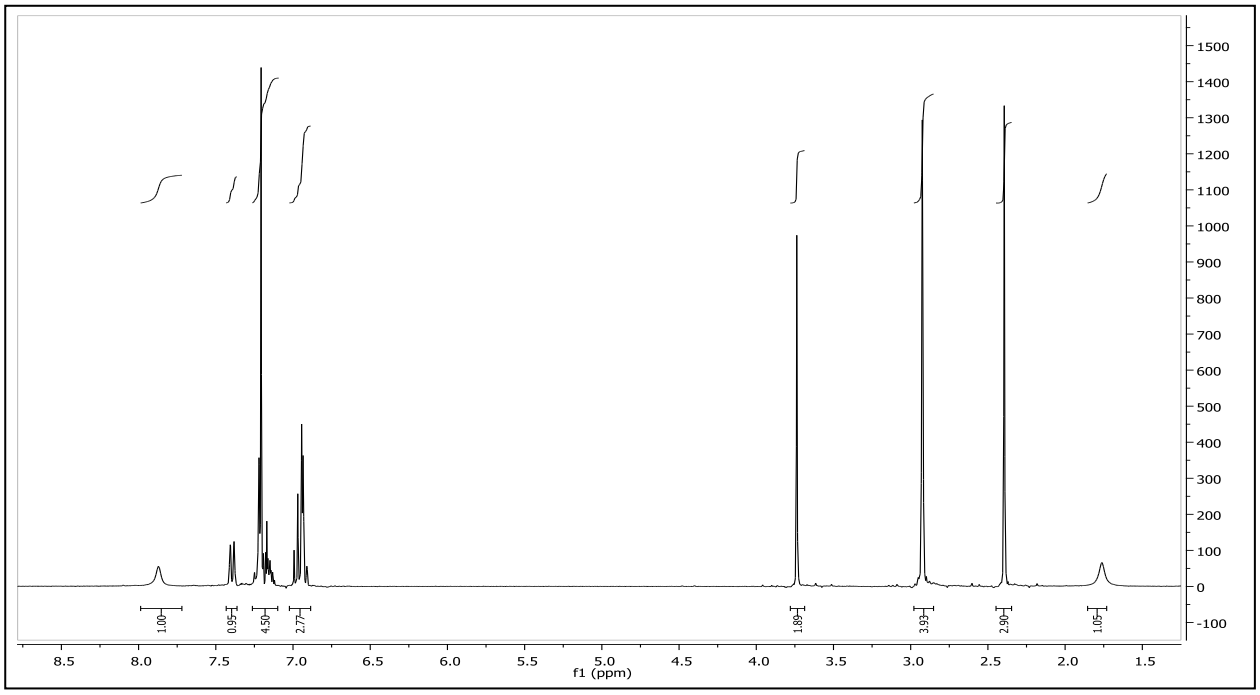
^{1}H NMR of *N*-benzyl-(6-methoxy)tryptamine (3j)



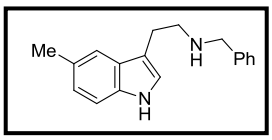
N-Benzyl-(7-methyl)tryptamine



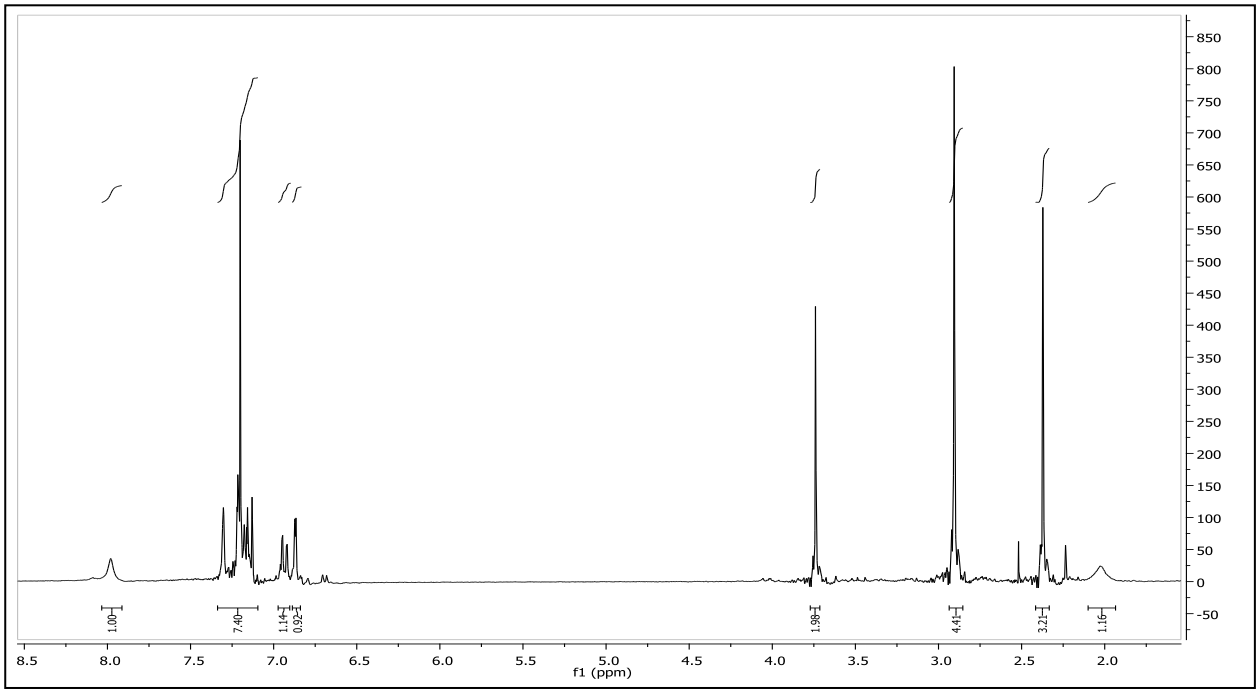
^{1}H NMR of *N*-benzyl-(7-methyl)tryptamine



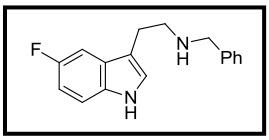
N-Benzyl-(5-methyl)tryptamine



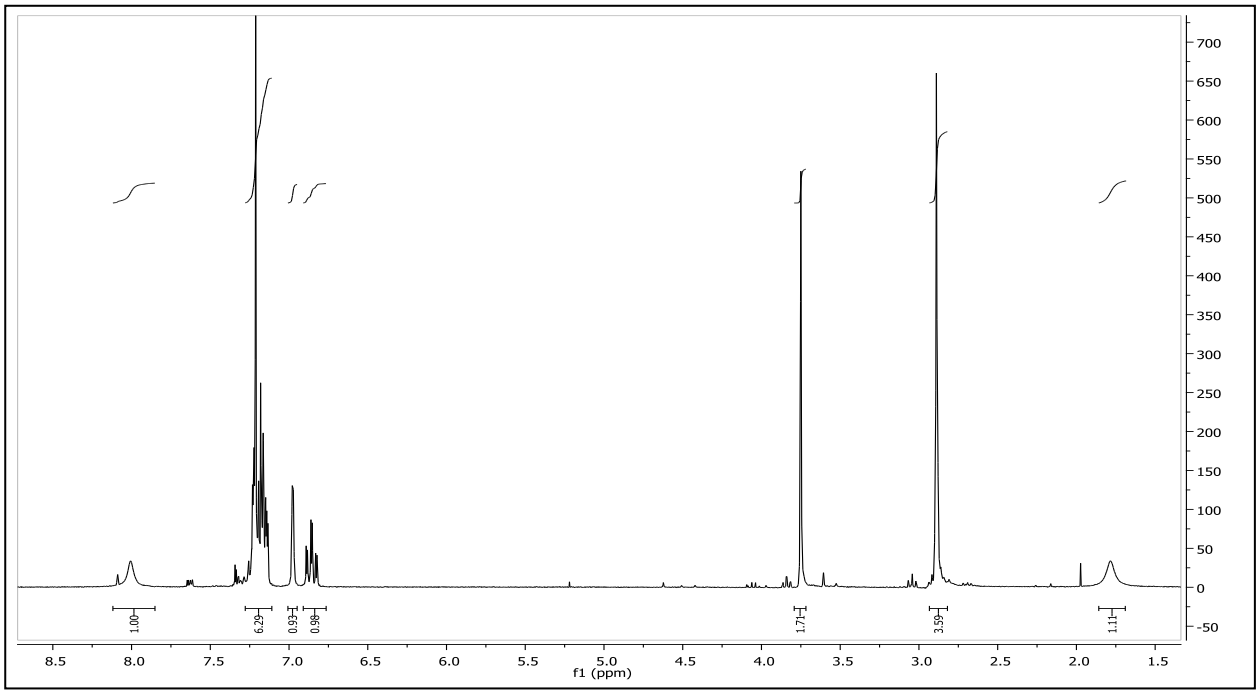
^{1}H NMR of *N*-benzyl-(5-methyl)tryptamine



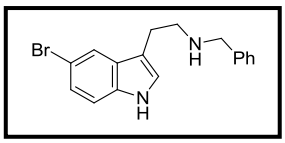
N-Benzyl-(5-fluoro)tryptamine



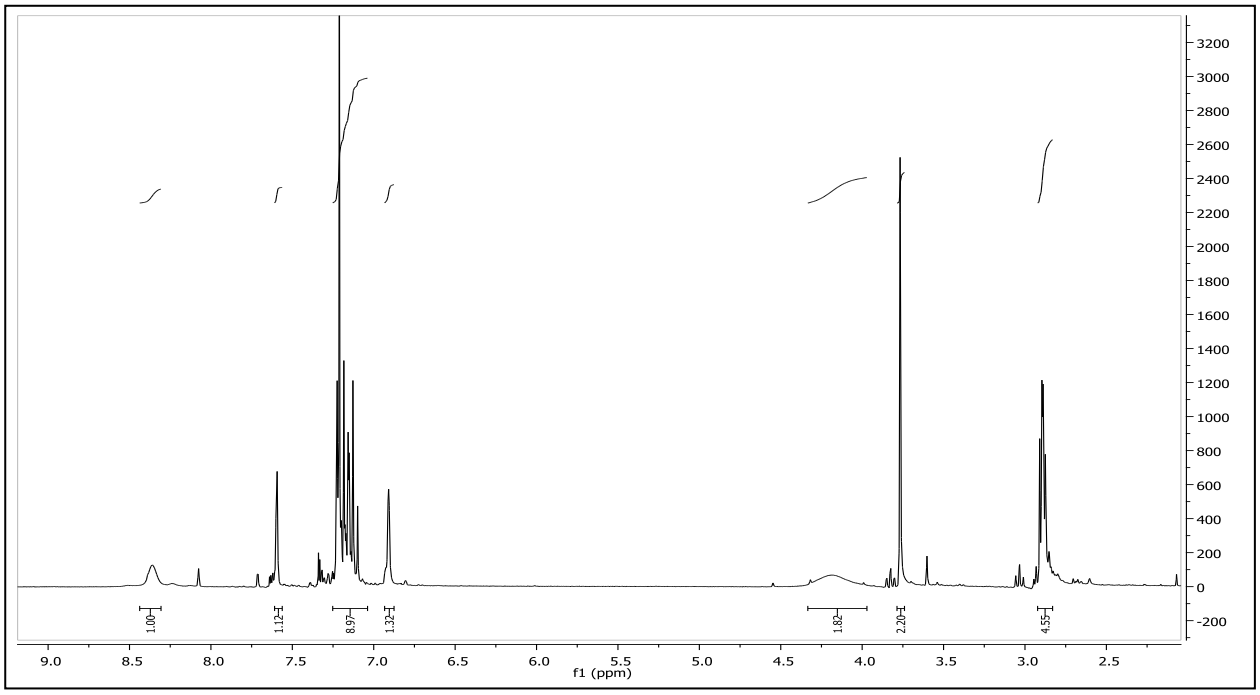
^{1}H NMR of *N*-benzyl-(5-fluoro)tryptamine



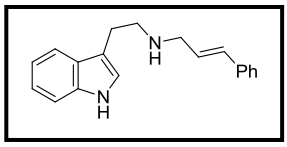
N-Benzyl-(5-bromo)tryptamine



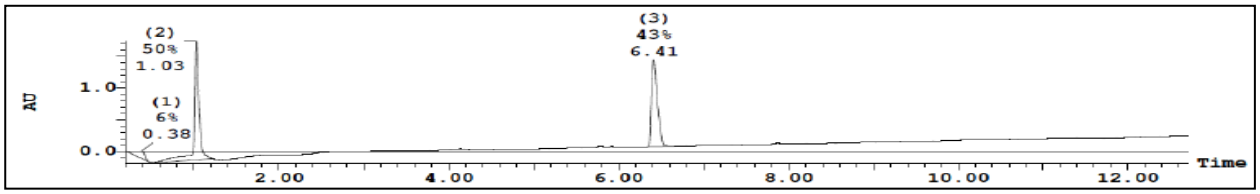
^{1}H NMR of *N*-benzyl-(5-bromo)tryptamine



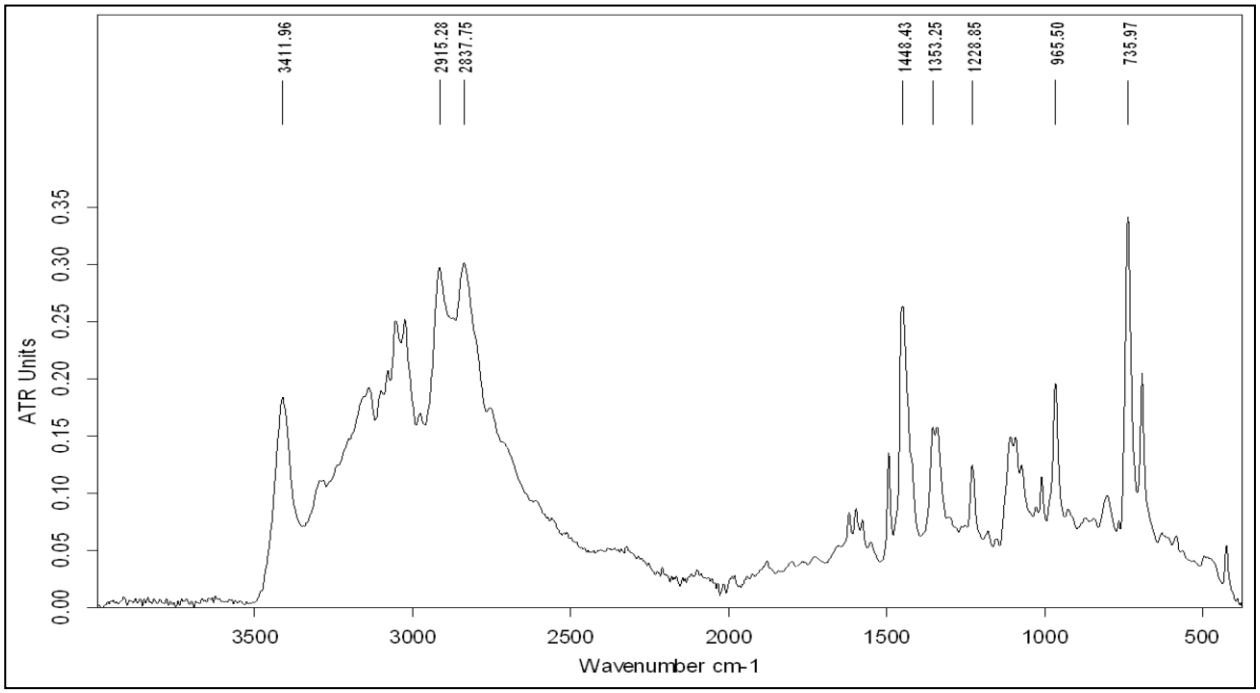
_N_-3-Phenylprop-2-en-1-tryptamine



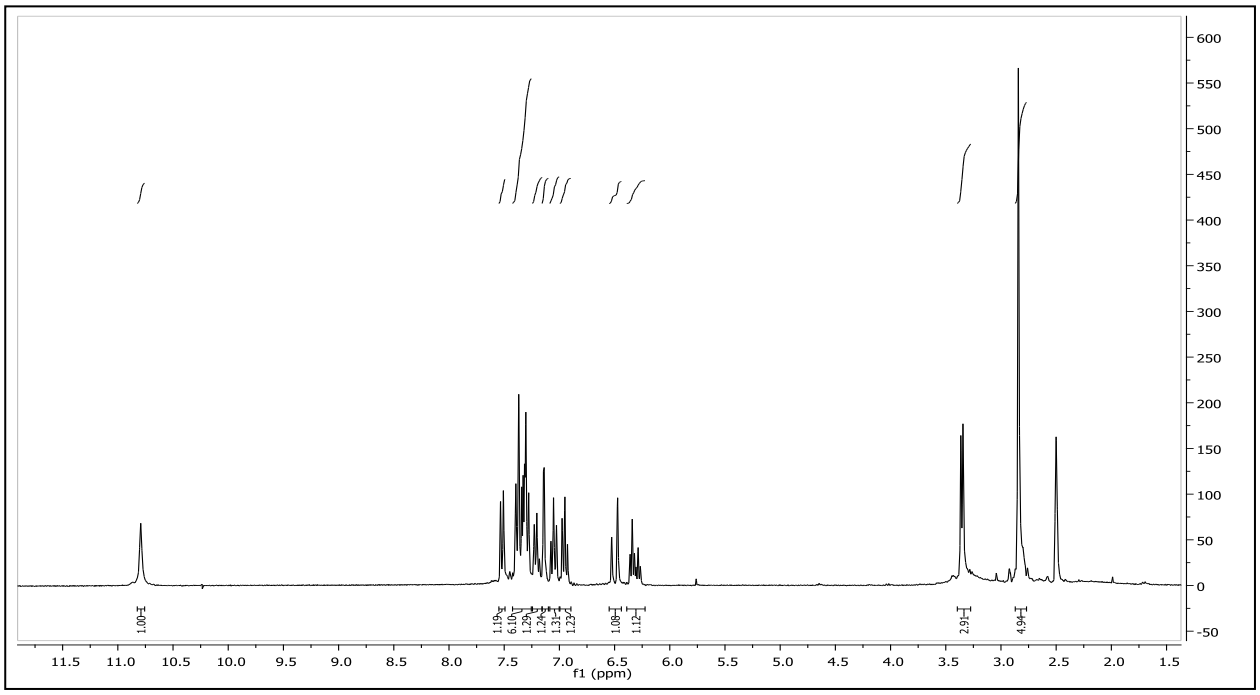
RP-HPLC of _N_-3-phenylprop-2-en-1-tryptamine



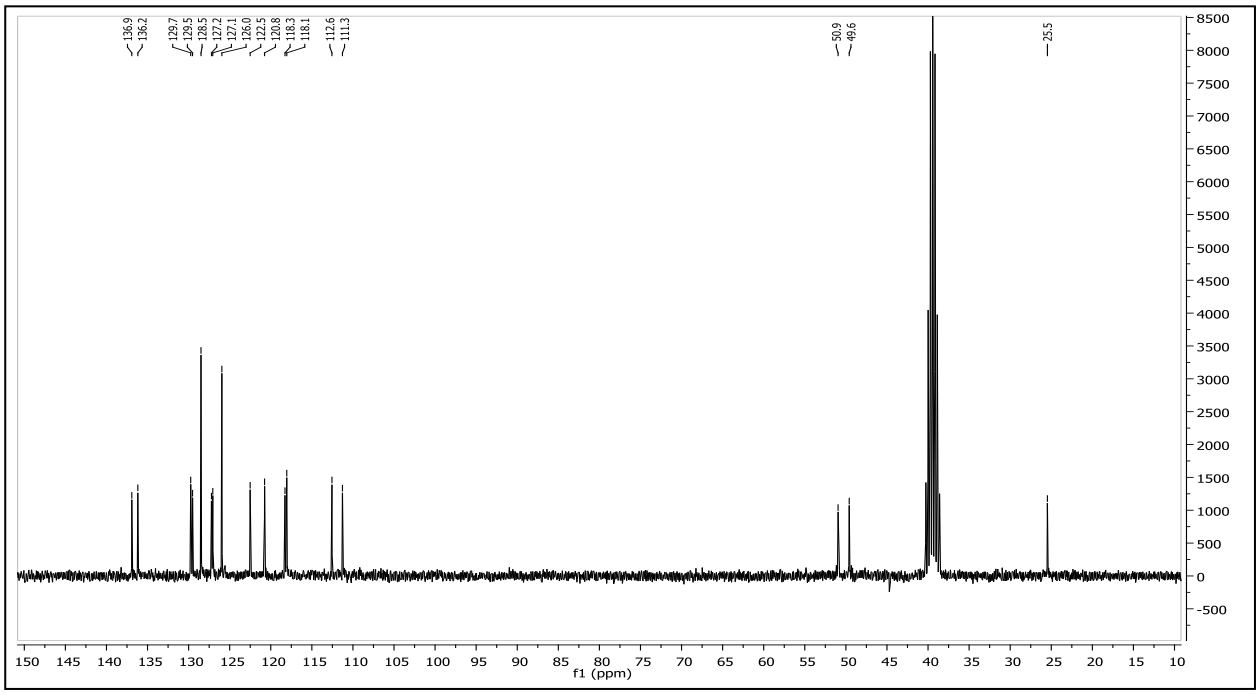
IR of _N_-3-phenylprop-2-en-1-tryptamine



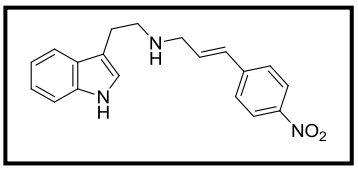
^{1}H NMR of *N*-3-phenylprop-2-en-1-tryptamine



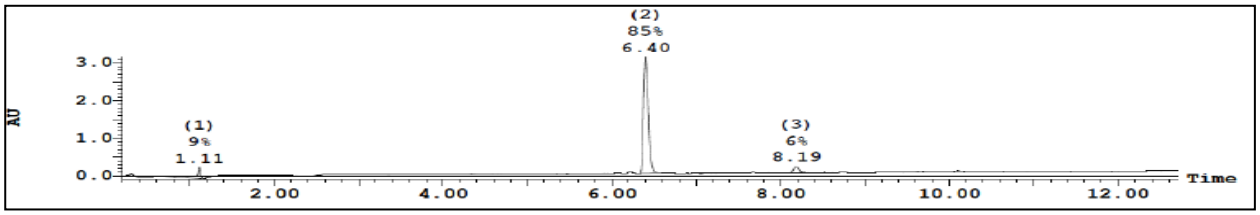
^{13}C NMR of *N*-3-phenylprop-2-en-1-tryptamine



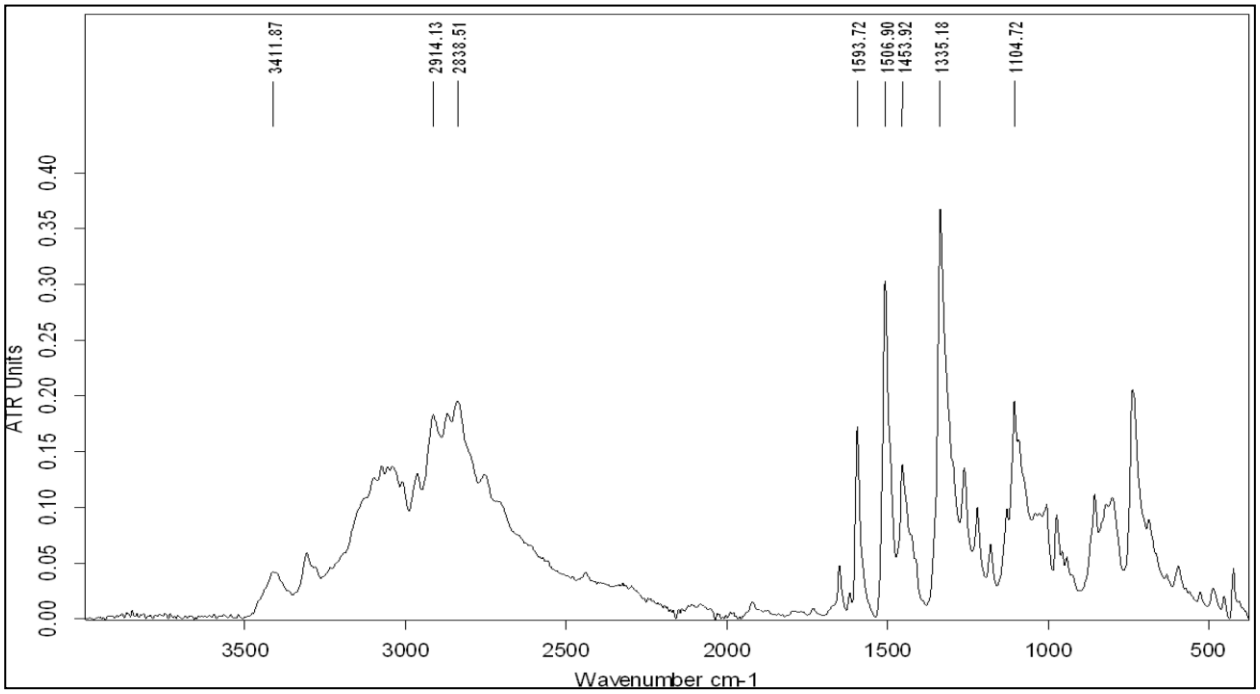
_N_-3-(4-Nitrophenyl)prop-2-en-1-tryptamine



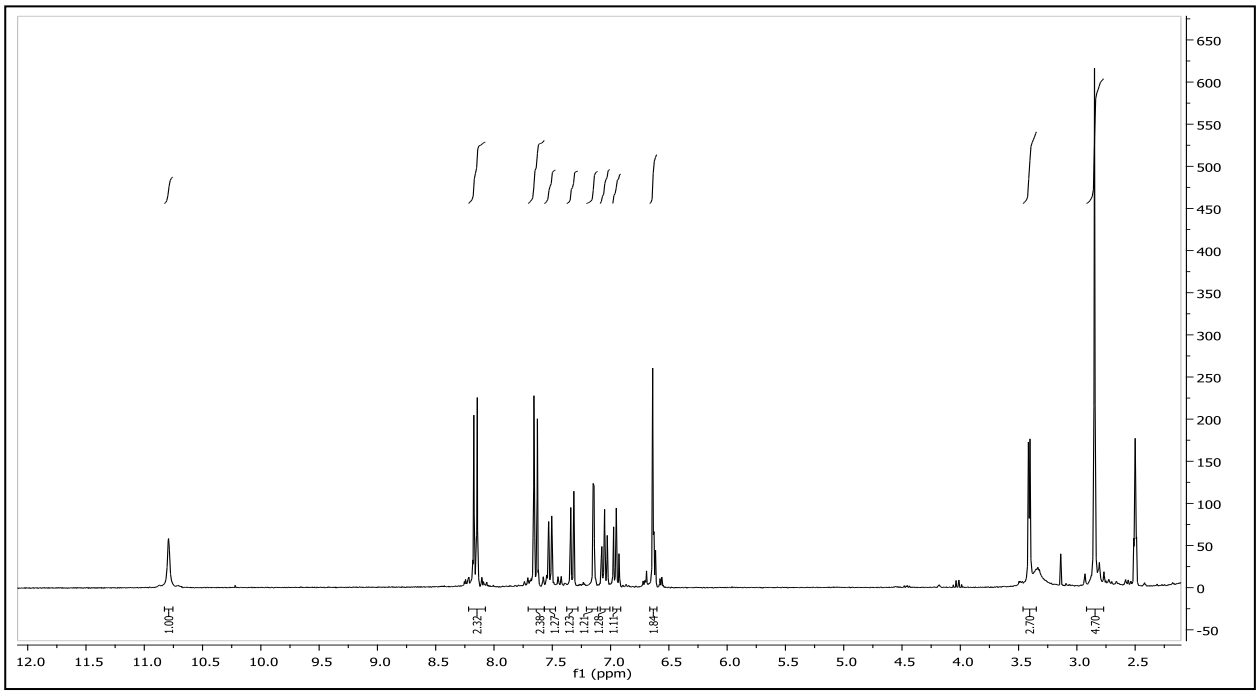
RP-HPLC of _N_-3-(4-nitrophenyl)prop-2-en-1-tryptamine



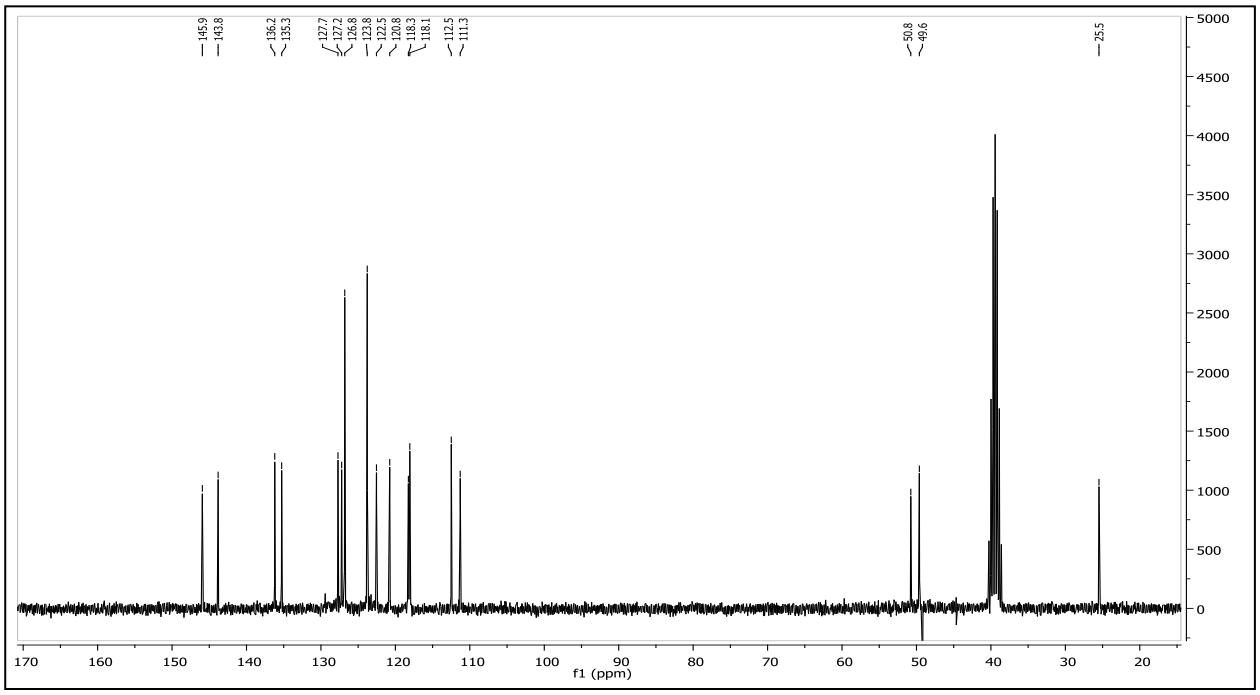
IR of _N_-3-(4-nitrophenyl)prop-2-en-1-tryptamine



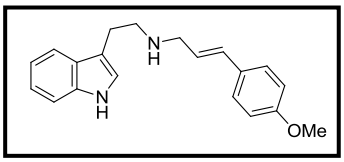
^{1}H NMR of *N*-3-(4-nitrophenyl)prop-2-en-1-tryptamine



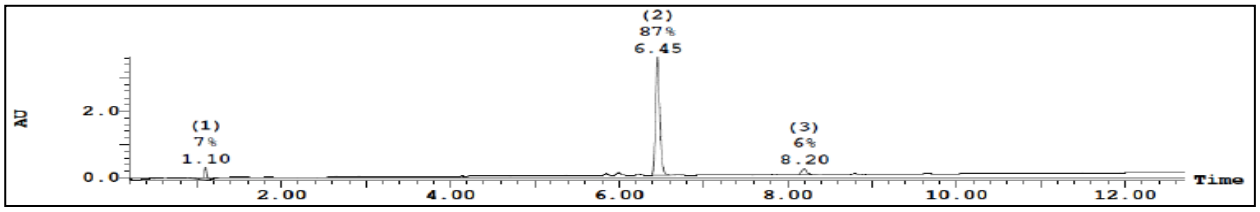
^{13}C NMR of *N*-3-(4-nitrophenyl)prop-2-en-1-tryptamine



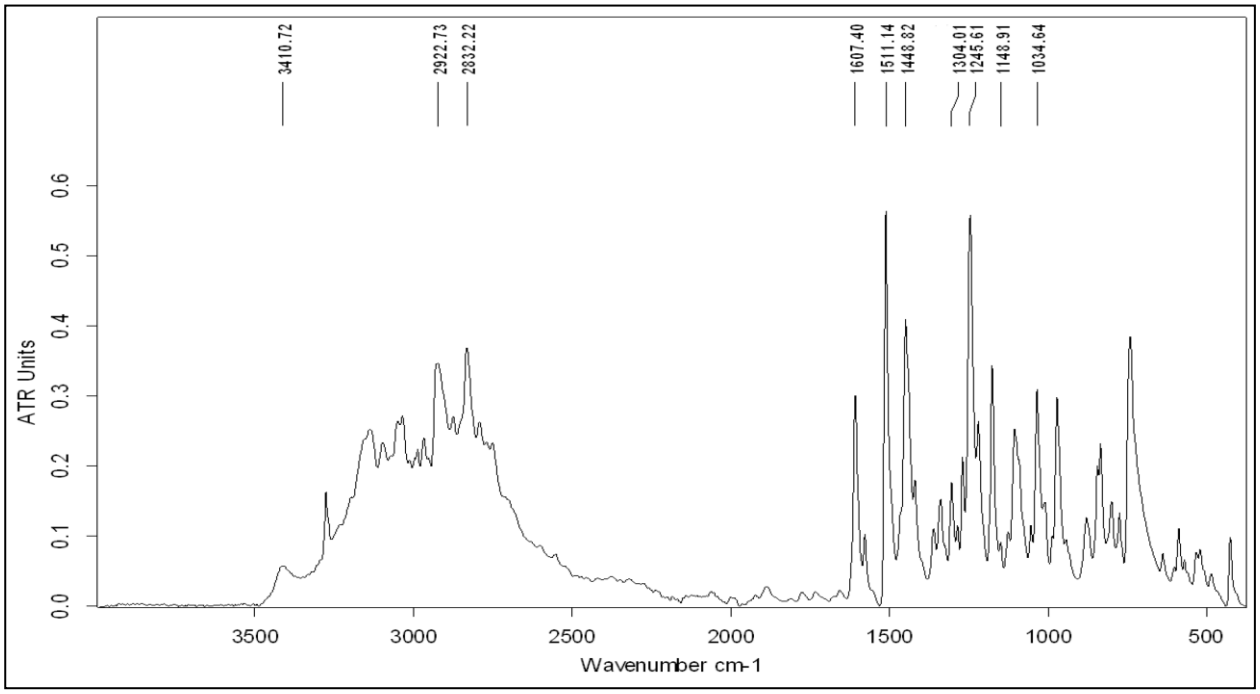
_N_-3-(4-Methoxyphenyl)prop-2-en-1-tryptamine



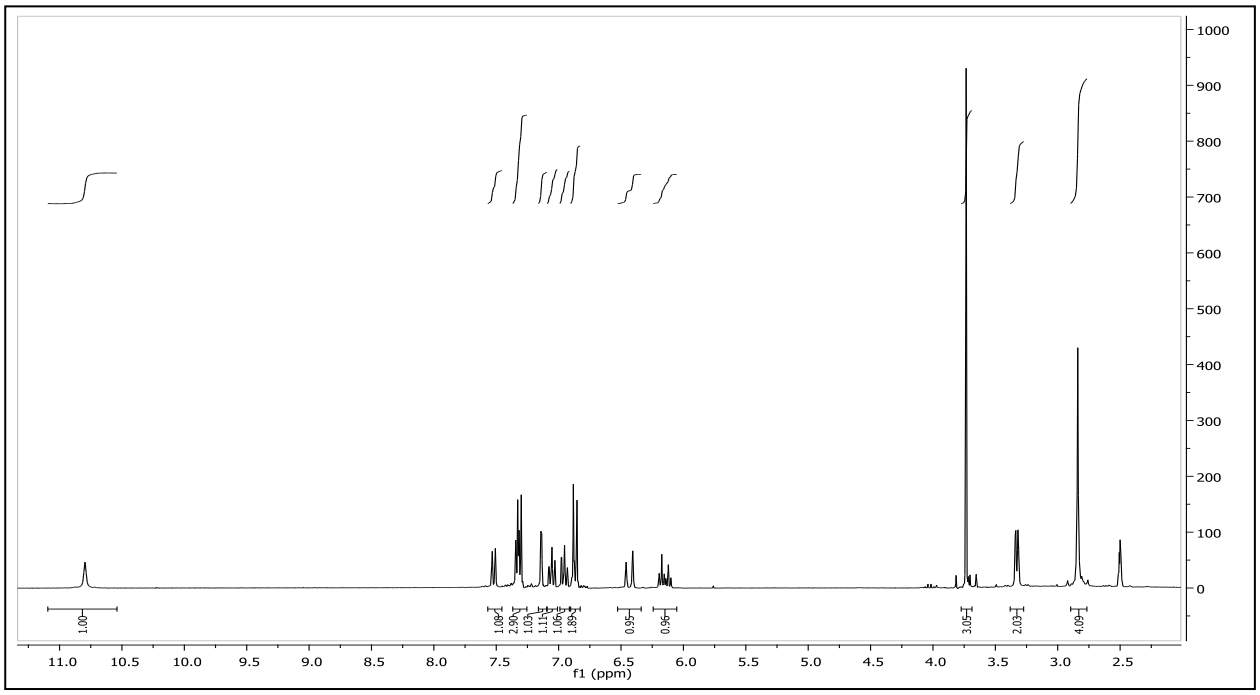
RP-HPLC of _N_-3-(4-methoxyphenyl)prop-2-en-1-tryptamine



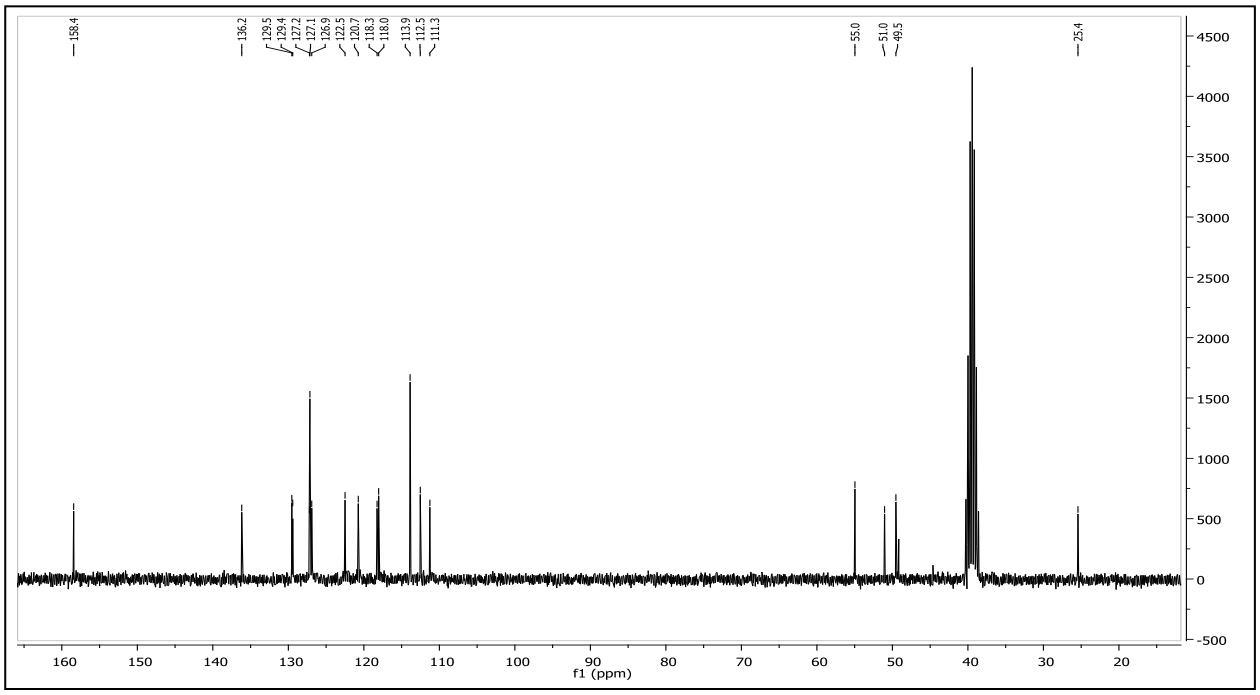
IR of _N_-3-(4-methoxyphenyl)prop-2-en-1-tryptamine



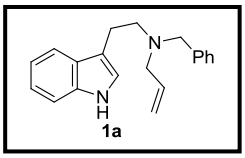
^{1}H NMR of *N*-3-(4-methoxyphenyl)prop-2-en-1-tryptamine



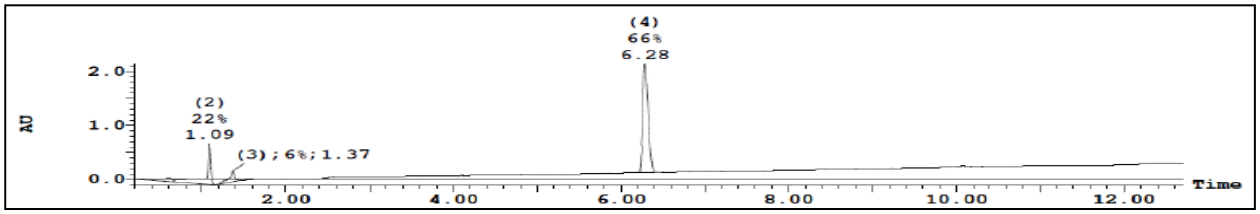
^{13}C NMR of *N*-3-(4-methoxyphenyl)prop-2-en-1-tryptamine



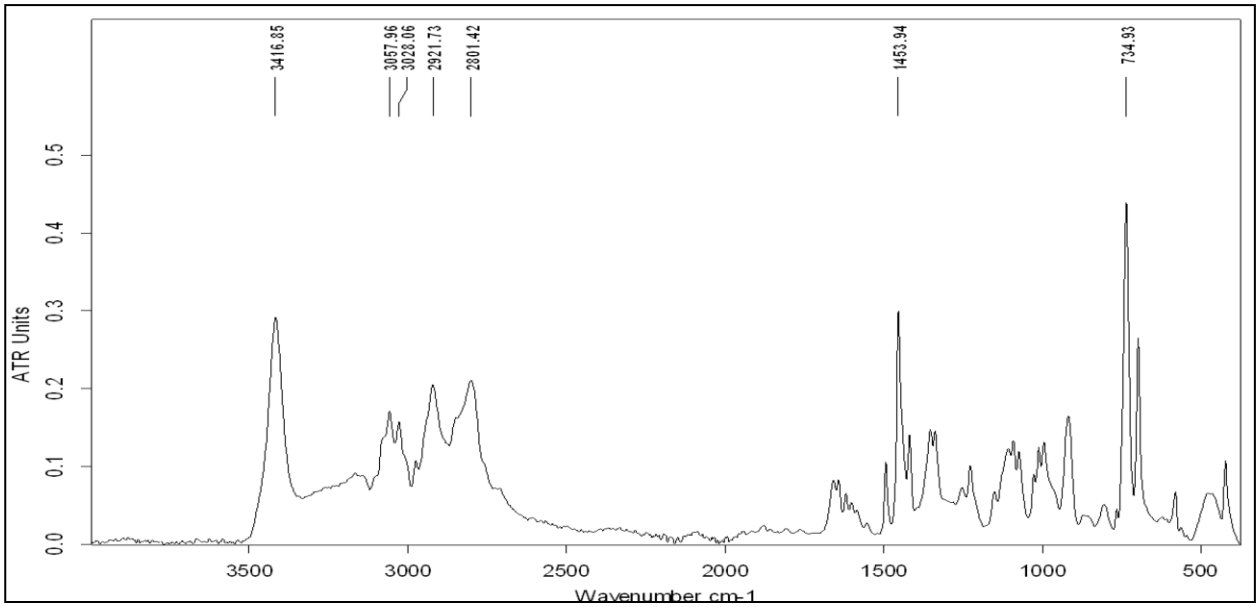
_N_-Allyl-_N_-benzyltryptamine (1a)



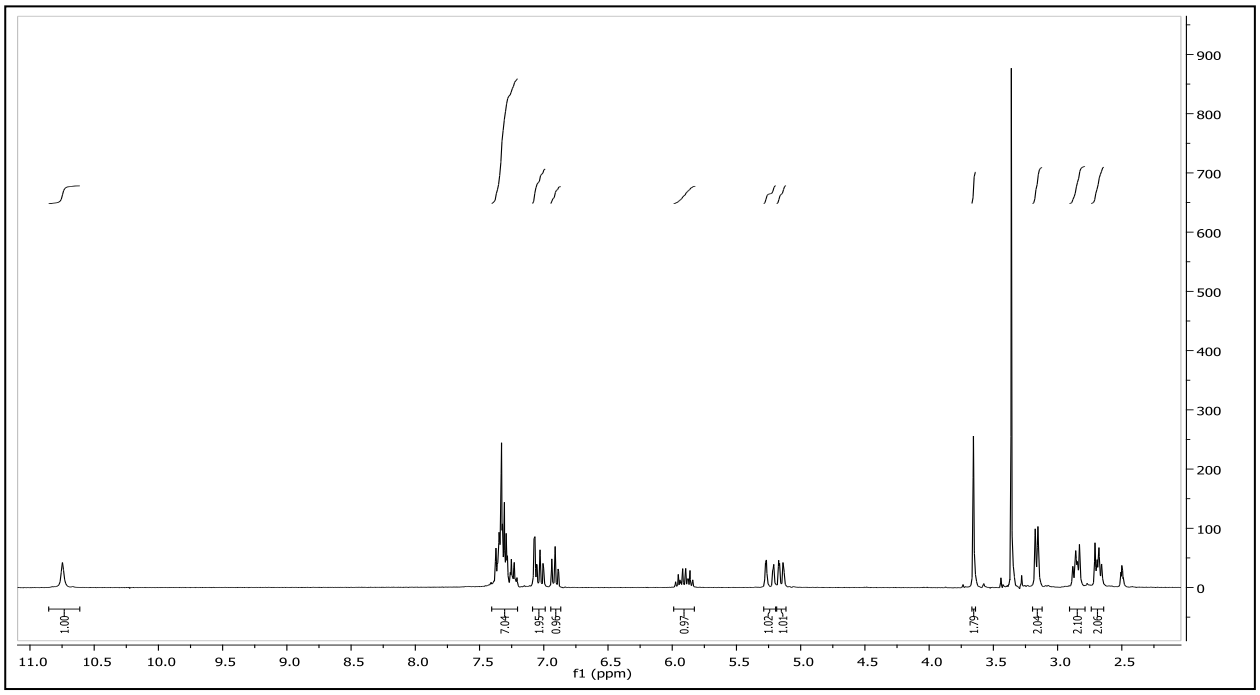
RP-HPLC of _N_-allyl-_N_-benzyltryptamine (1a)



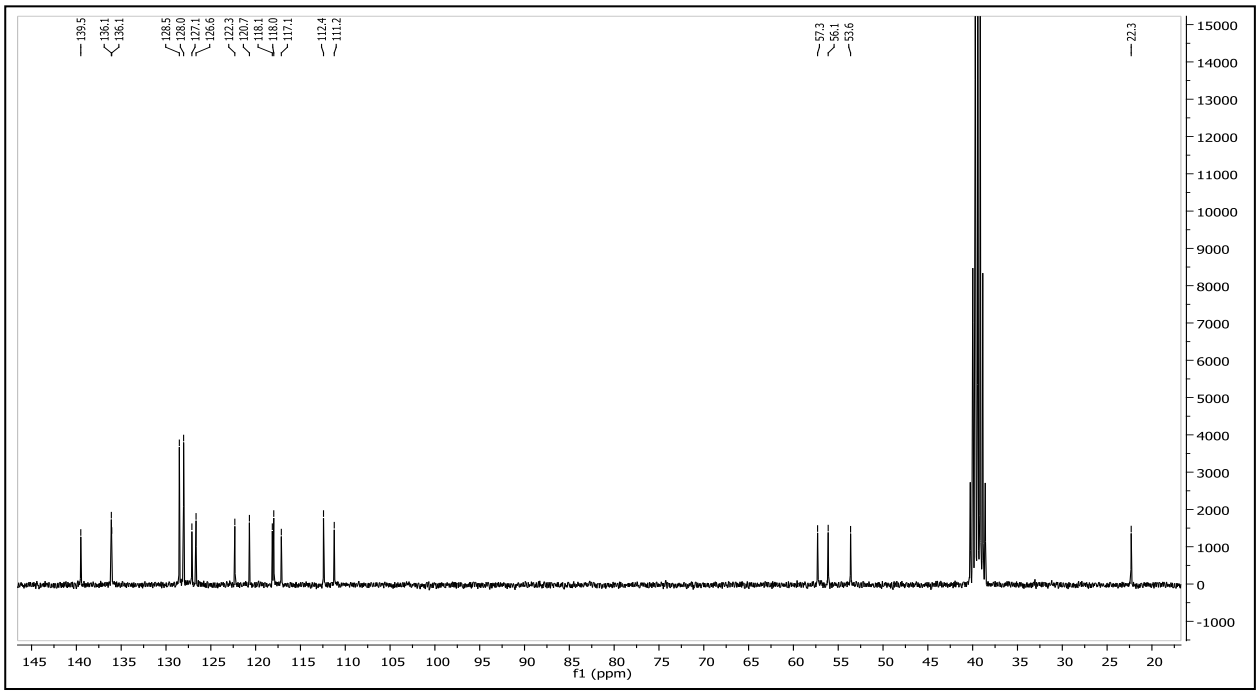
IR of _N_-allyl-_N_-benzyltryptamine (1a)



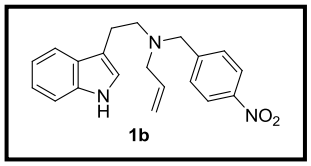
^{1}H NMR of *N*-allyl-*N*-benzyltryptamine (1a)



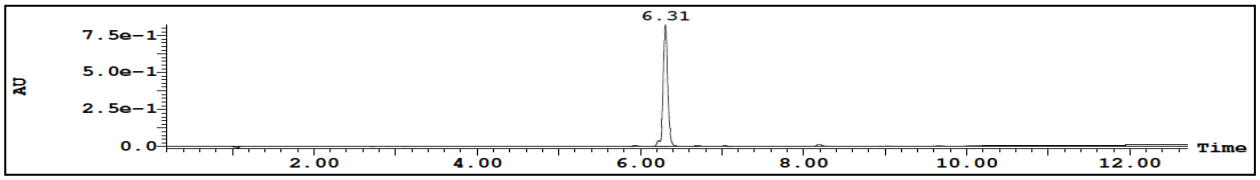
^{13}C NMR of *N*-allyl-*N*-benzyltryptamine (1a)



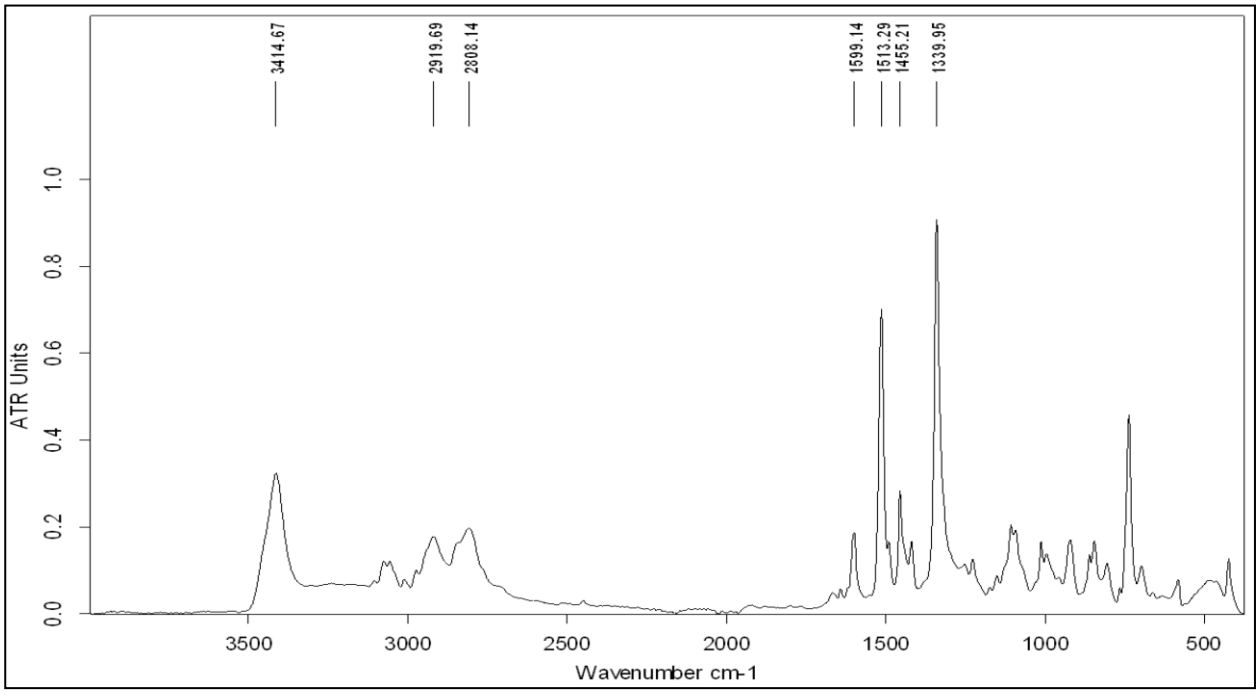
_N_-Allyl-_N_-(4-nitro)benzyltryptamine (1b)



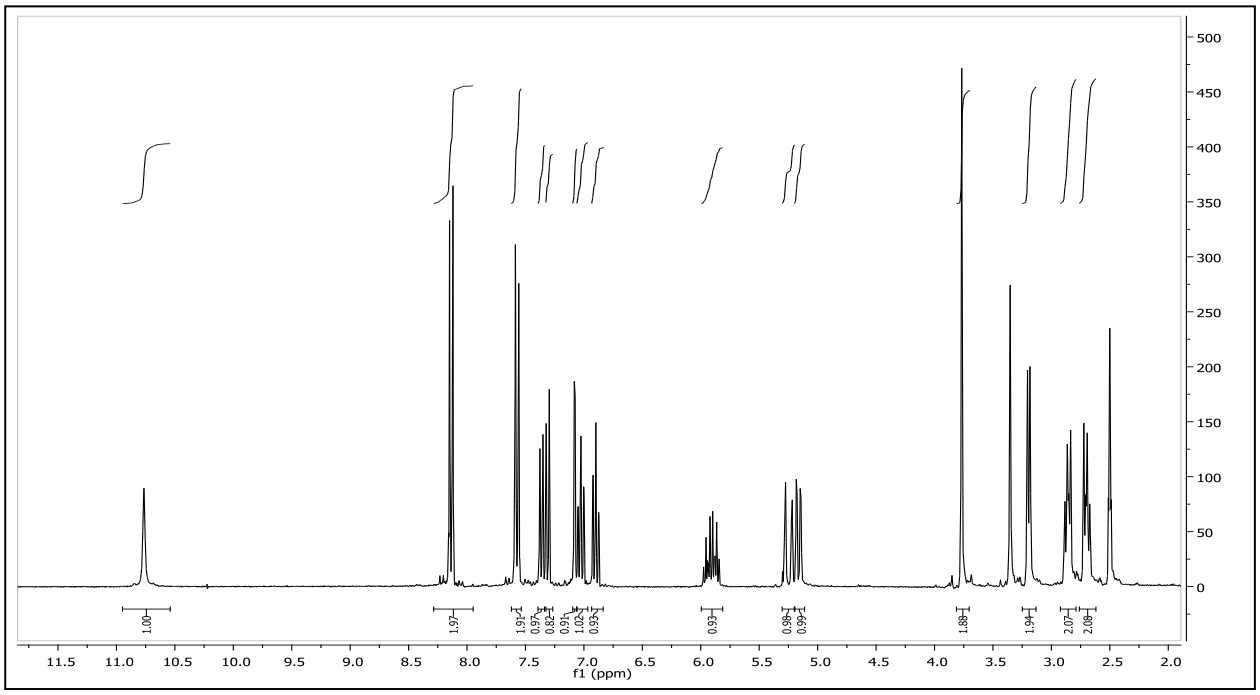
RP-HPLC of _N_-allyl-_N_-(4-nitro)benzyltryptamine (1b)



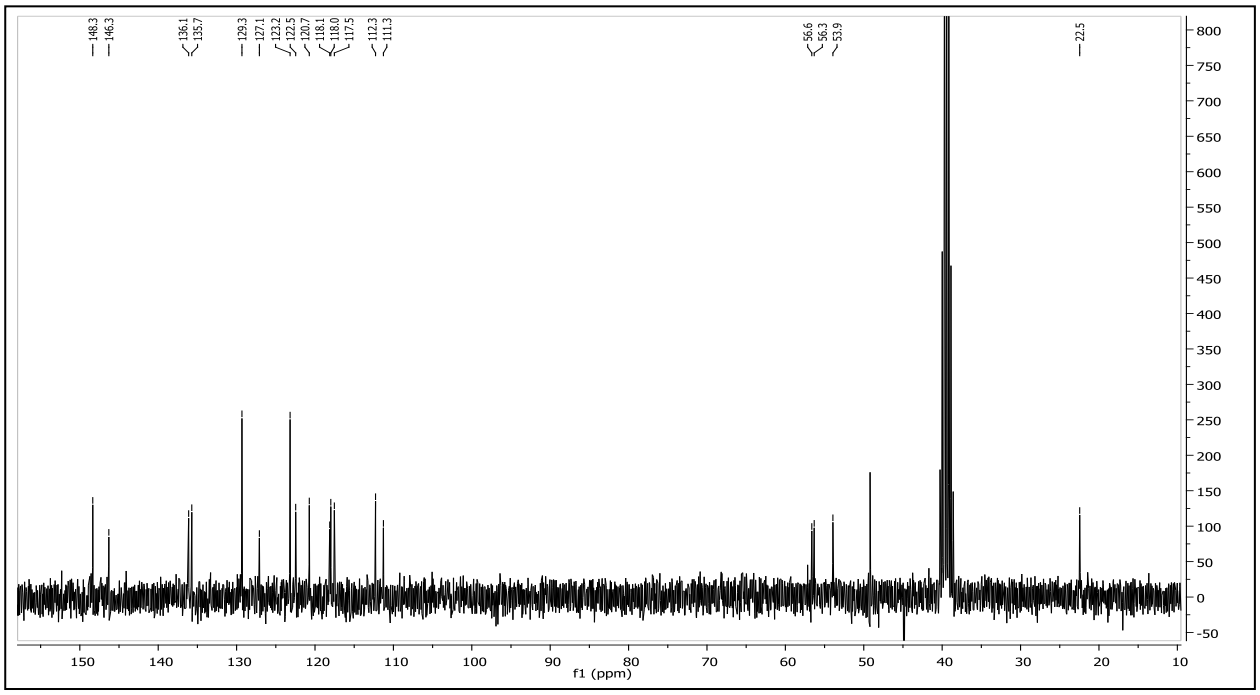
IR of _N_-allyl-_N_-(4-nitro)benzyltryptamine (1b)



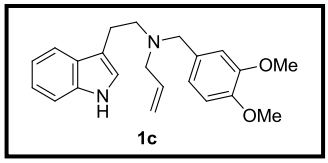
^{1}H NMR of *N*-allyl-*N*-(4-nitro)benzyltryptamine (1b)



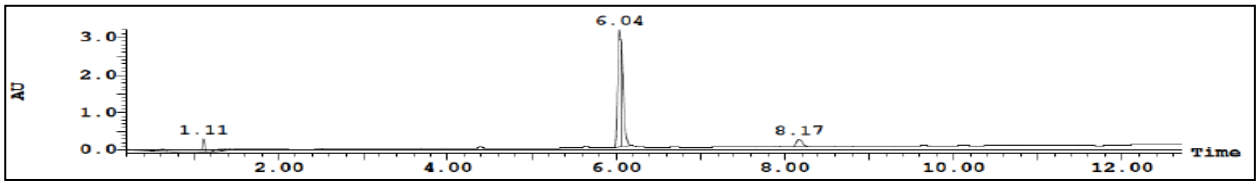
^{13}C NMR of *N*-allyl-*N*-(4-nitro)benzyltryptamine (1b)



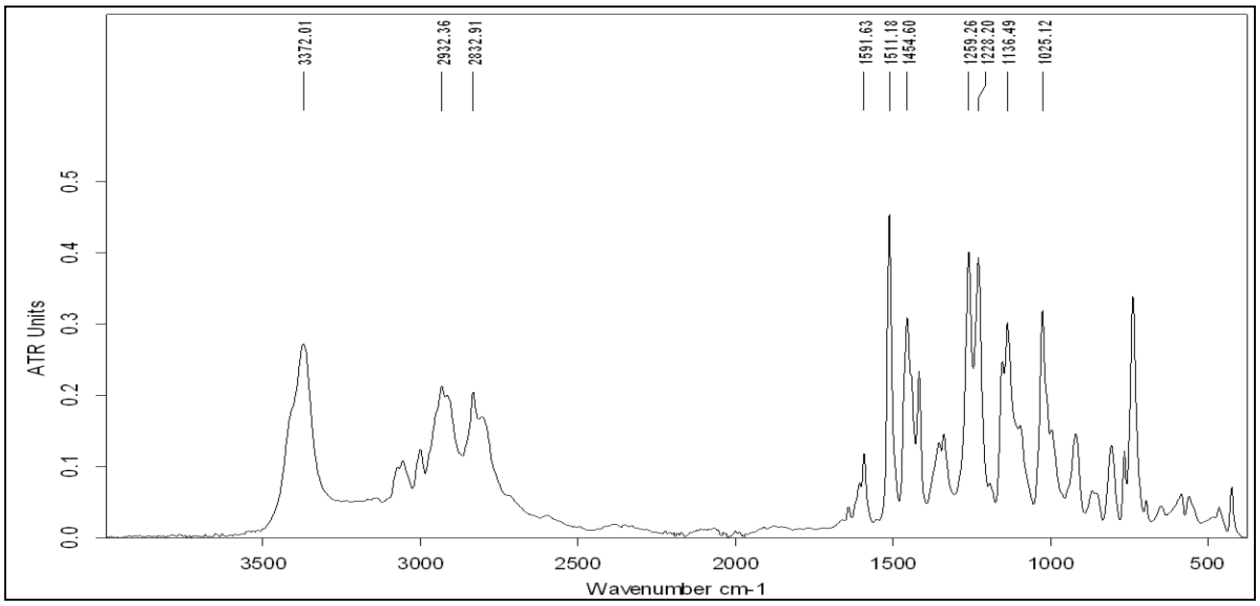
_N_-Allyl-_N_-(3,4-dimethoxy)benzyltryptamine (1c)



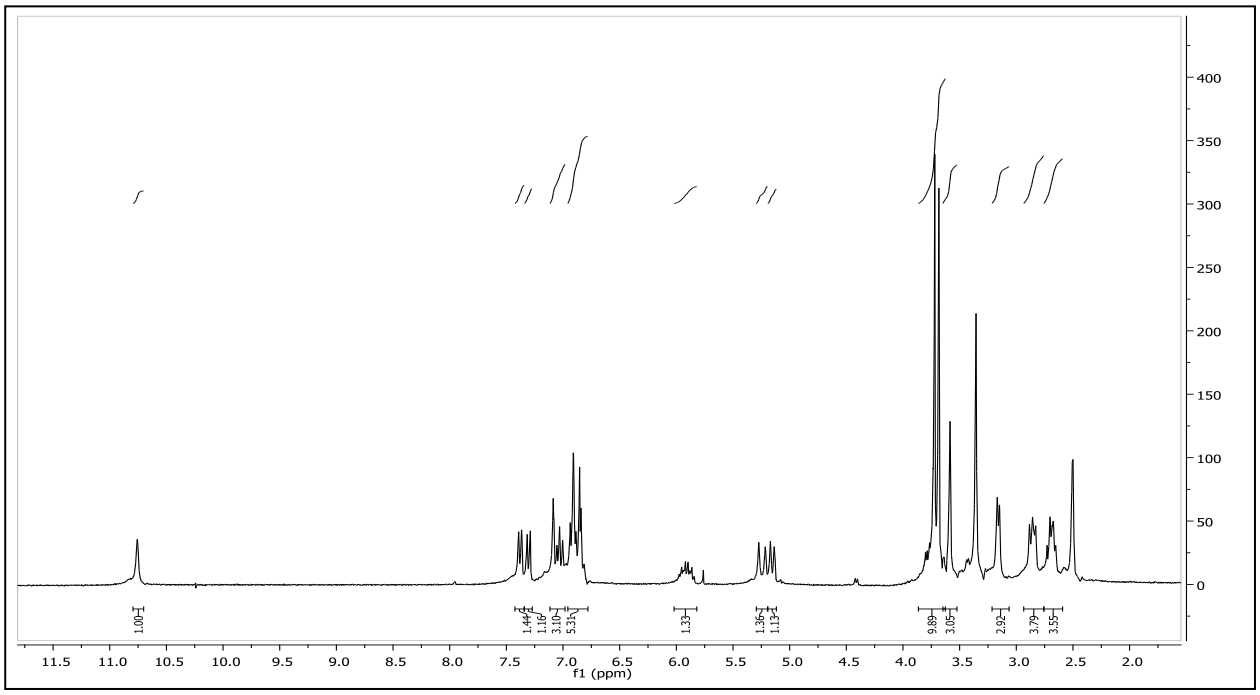
RP-HPLC of _N_-allyl-_N_-(3,4-dimethoxy)benzyltryptamine (1c)



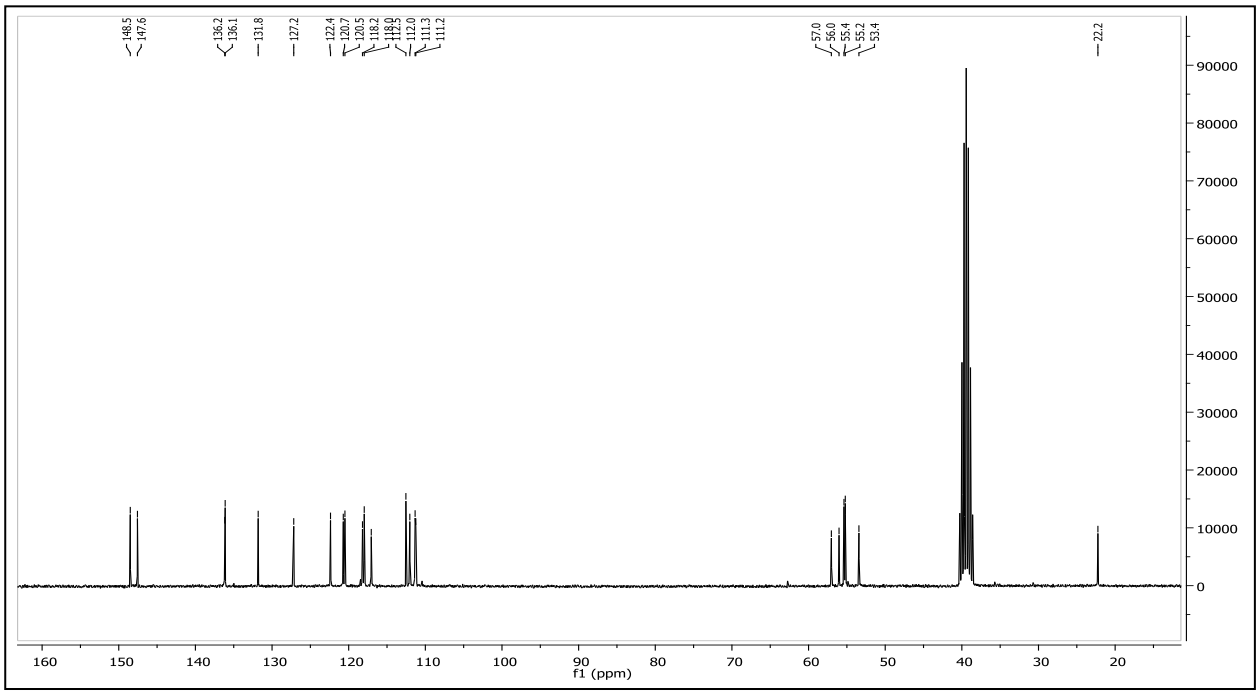
IR of _N_-allyl-_N_-(3,4-dimethoxy)benzyltryptamine (1c)



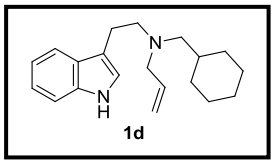
^{1}H NMR of *N*-allyl-*N*-(3,4-dimethoxy)benzyltryptamine (1c)



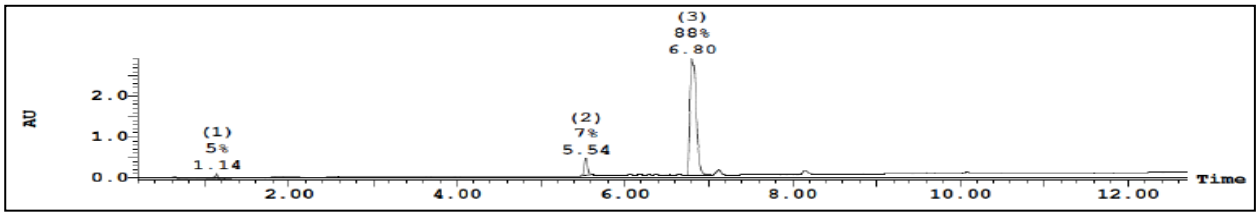
^{13}C NMR of *N*-allyl-*N*-(3,4-dimethoxy)benzyltryptamine (1c)



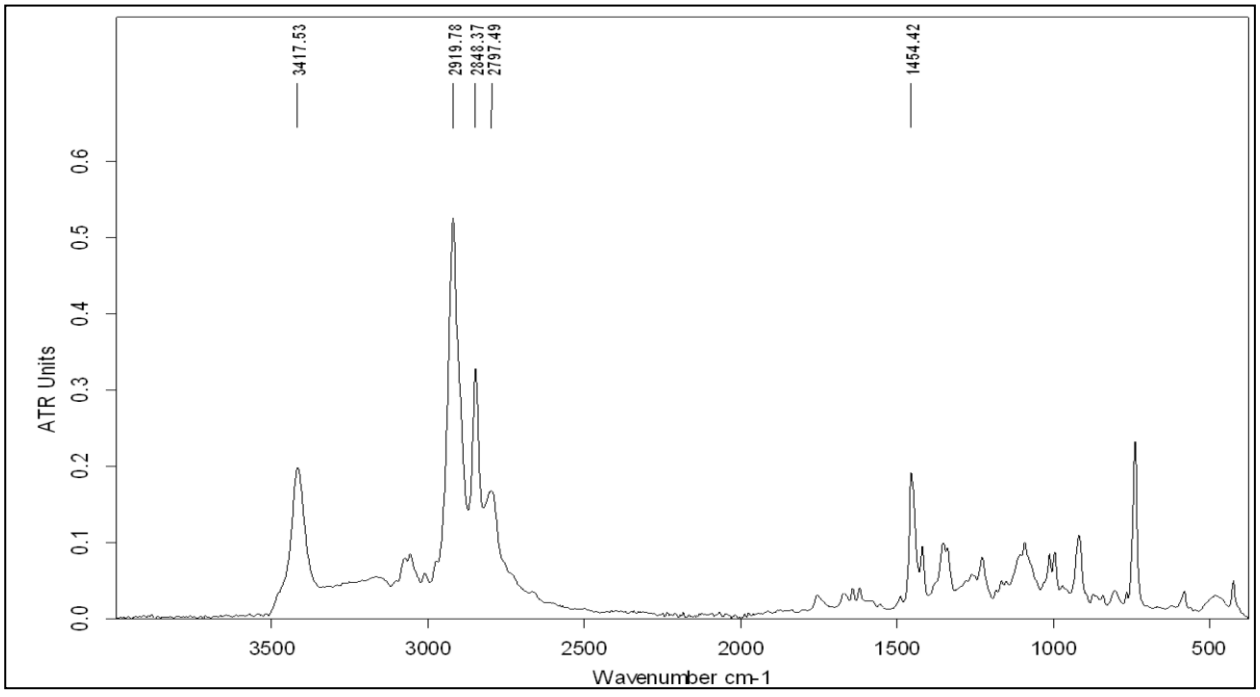
_N_-Allyl-_N_-cyclohexylmethyltryptamine (1d)



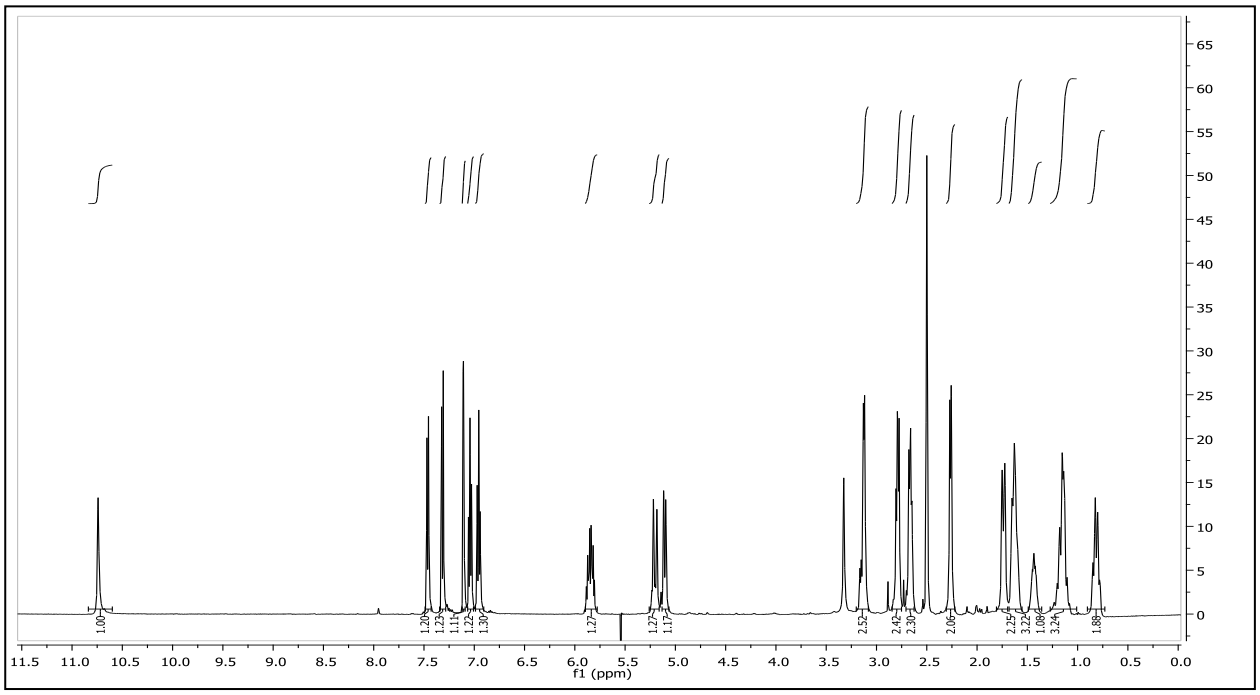
RP-HPLC of _N_-allyl-_N_-cyclohexylmethyltryptamine (1d)



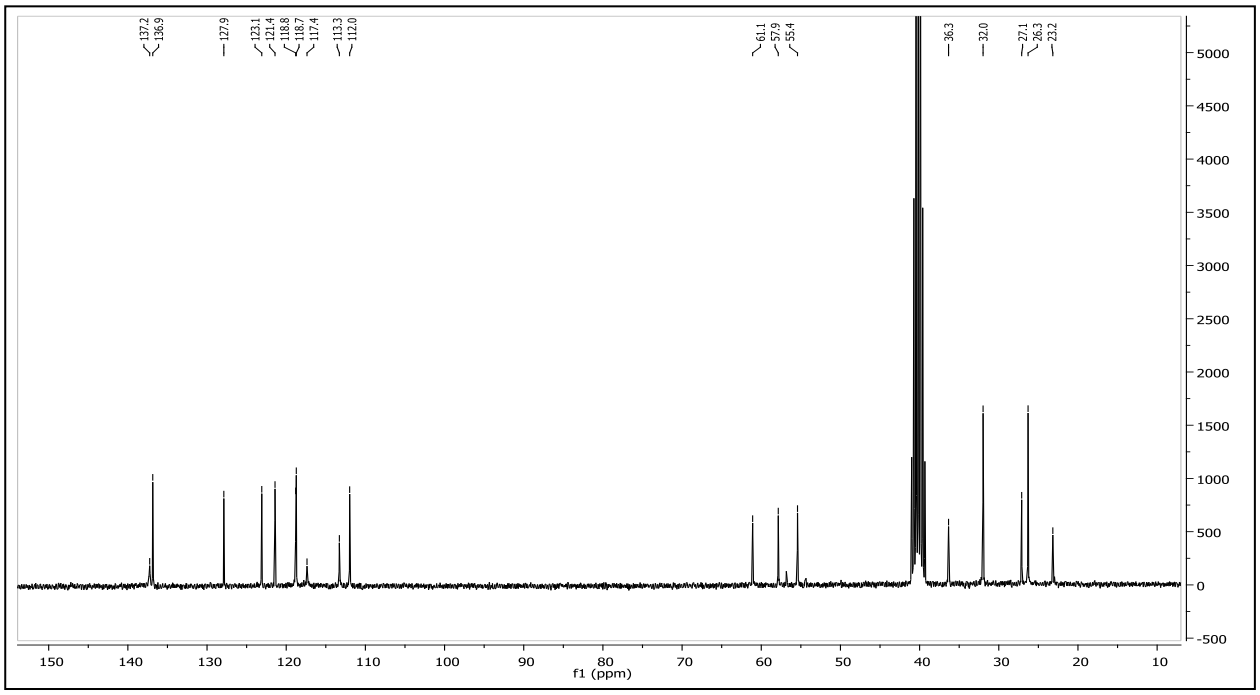
IR of _N_-allyl-_N_-cyclohexylmethyltryptamine (1d)



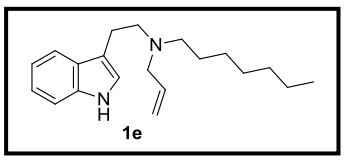
^{1}H NMR of *N*-allyl-*N*-cyclohexylmethyltryptamine (1d)



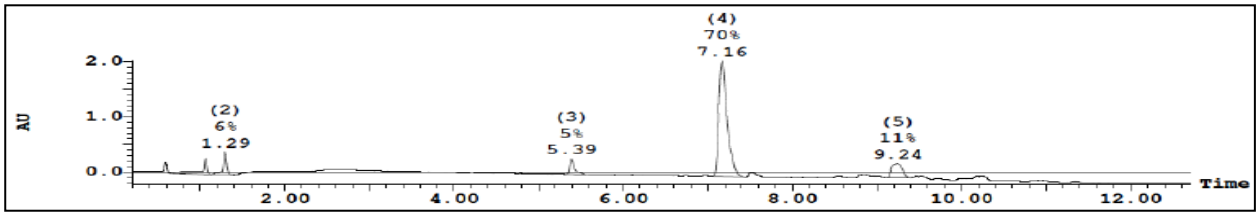
^{13}C NMR of *N*-allyl-*N*-cyclohexylmethyltryptamine (1d)



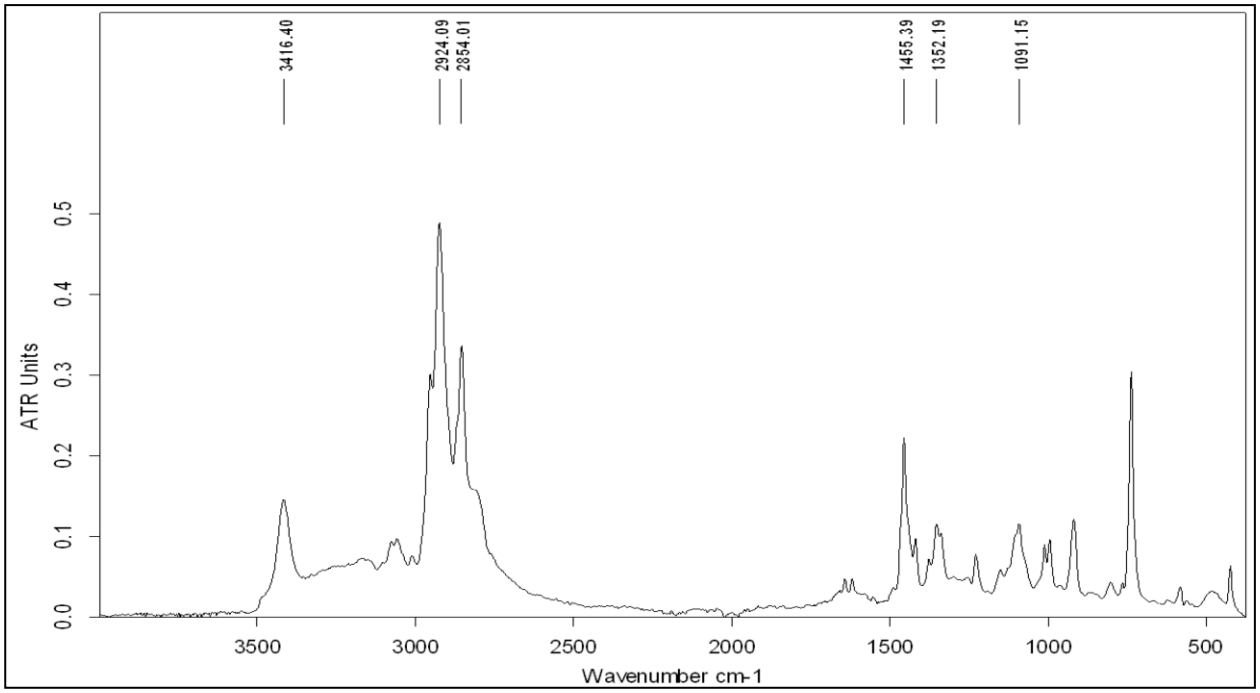
_N_-Allyl-_N_-heptyltryptamine (1e)



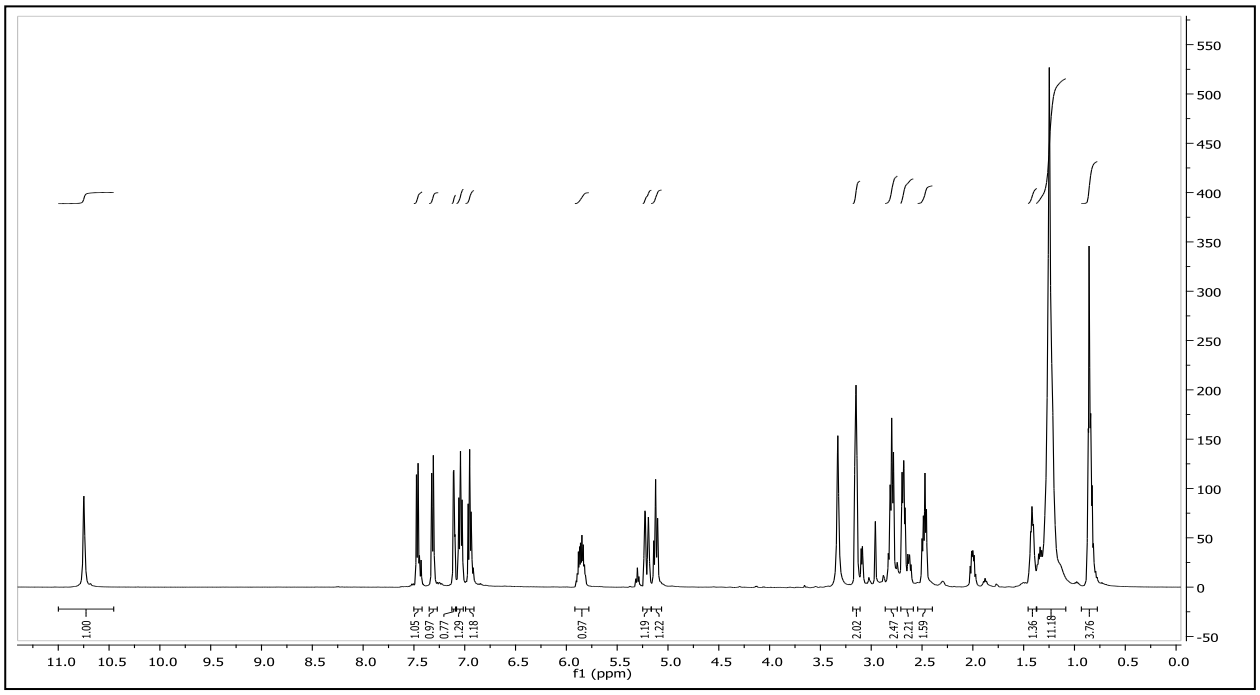
RP-HPLC of _N_-allyl-_N_-heptyltryptamine (1e)



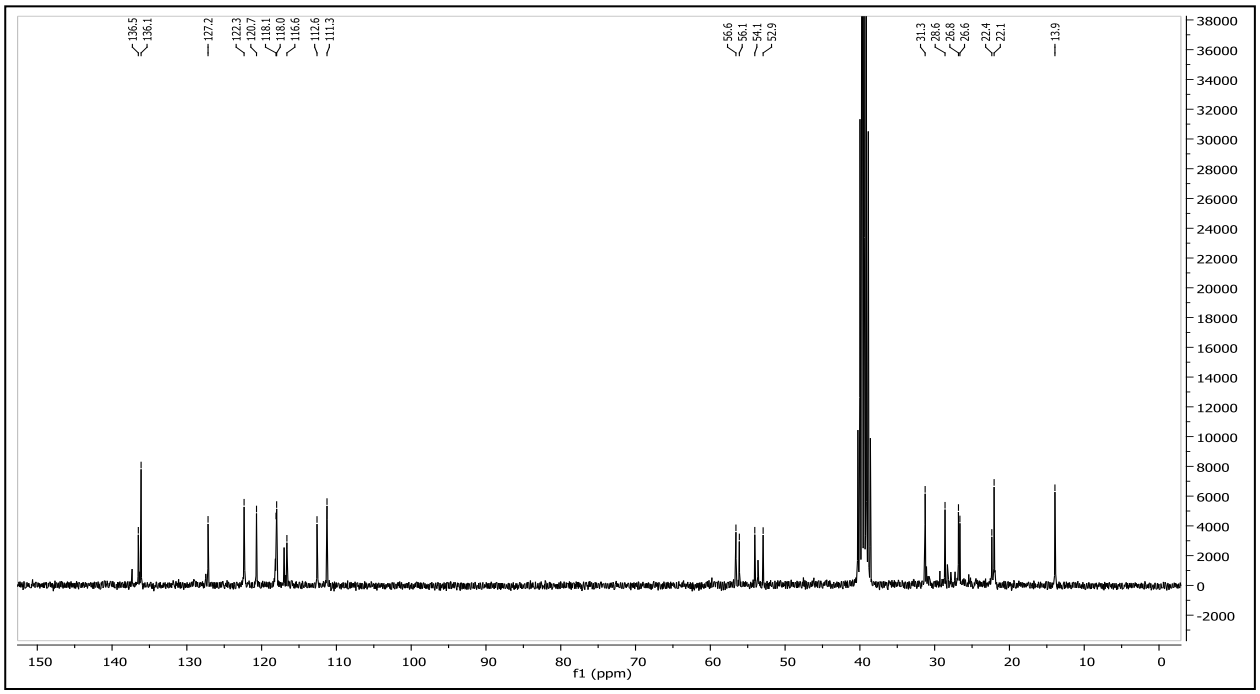
IR of _N_-allyl-_N_-heptyltryptamine (1e)



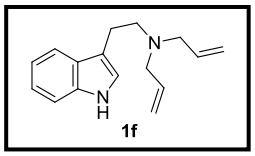
^{1}H NMR of *N*-allyl-*N*-heptyltryptamine (1e)



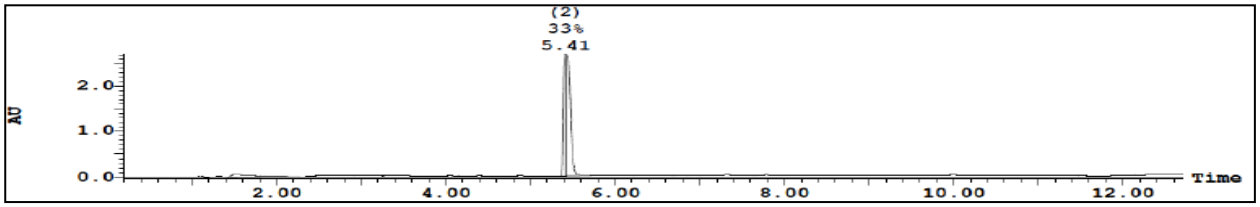
^{13}C NMR of *N*-allyl-*N*-heptyltryptamine (1e)



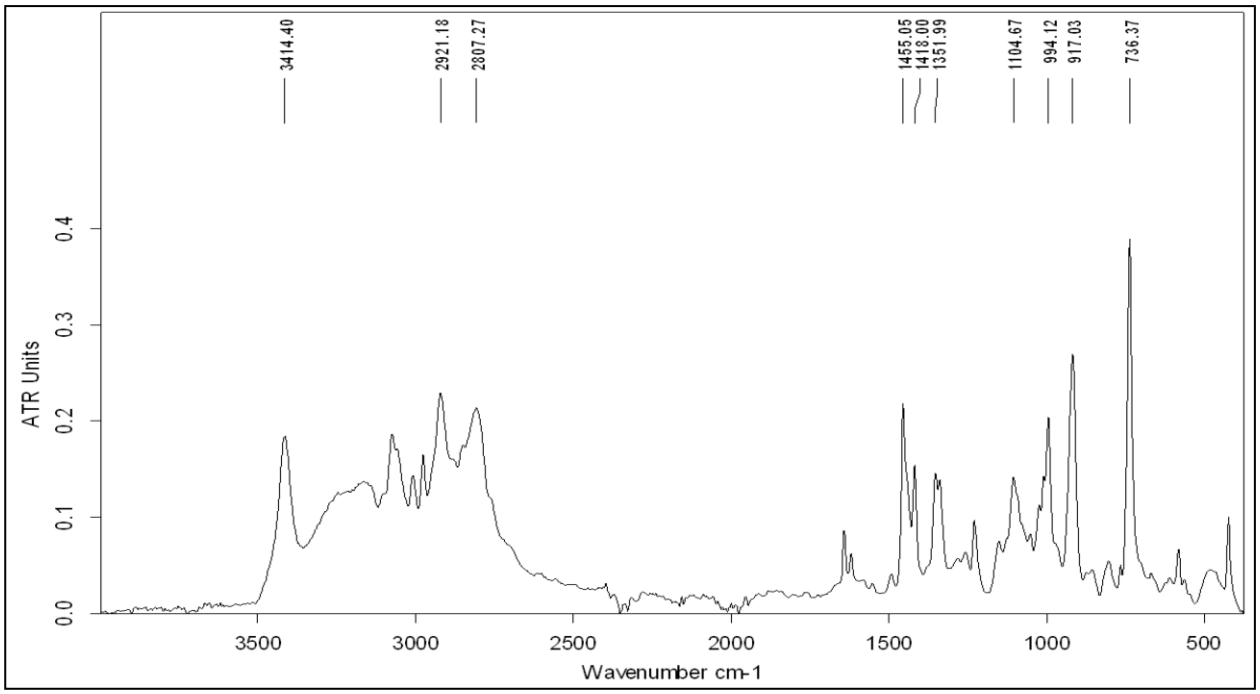
_N,N_-Diallyltryptamine (1f)



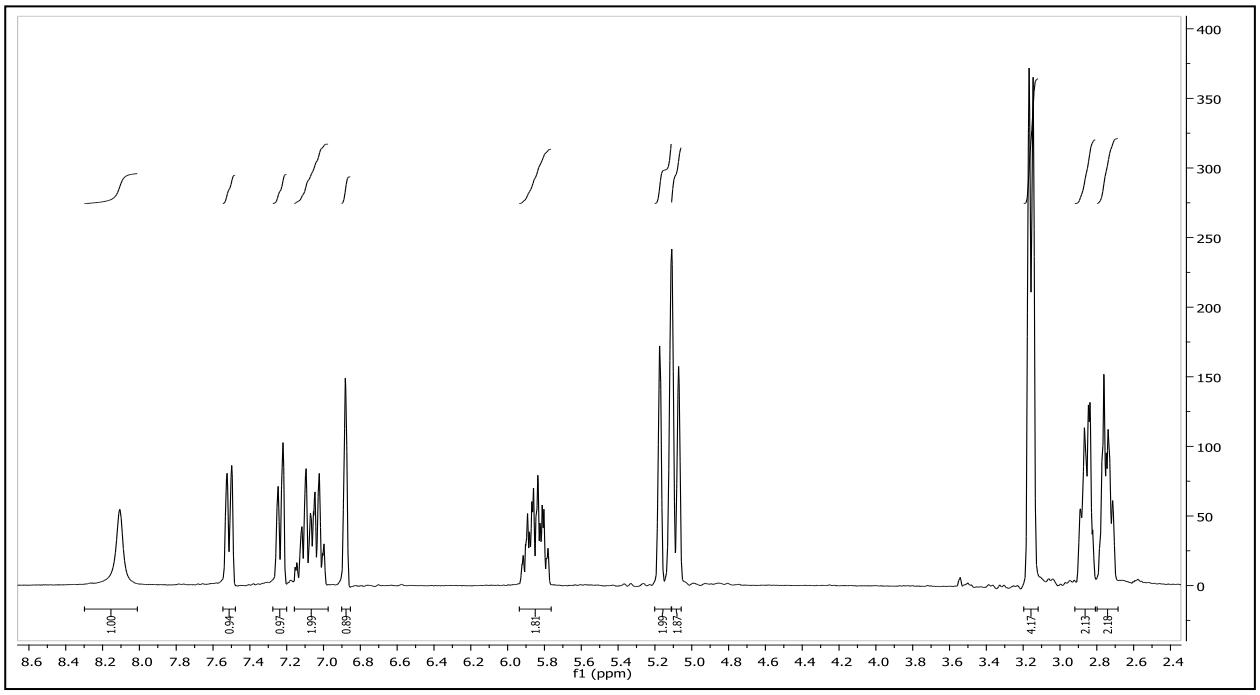
RP-HPLC of _N,N_-diallyltryptamine (1f)



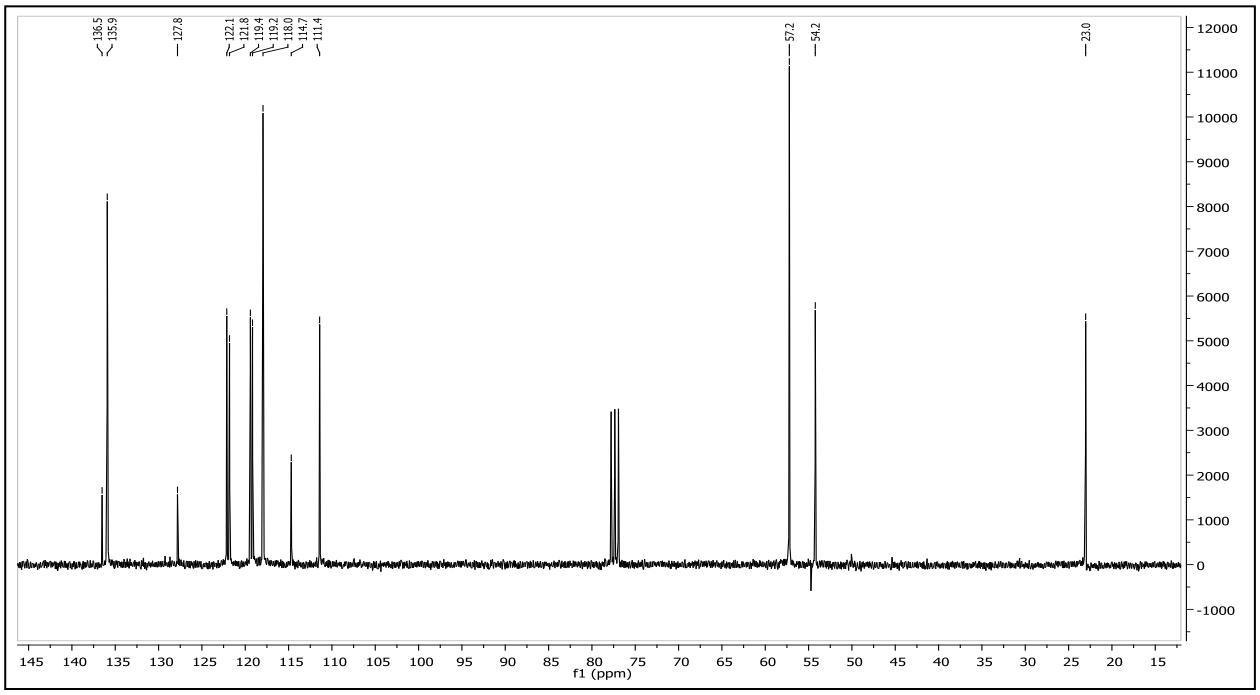
IR of _N,N_-diallyltryptamine (1f)



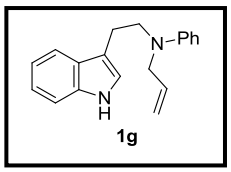
^{1}H NMR of *N,N*-diallyltryptamine (1f)



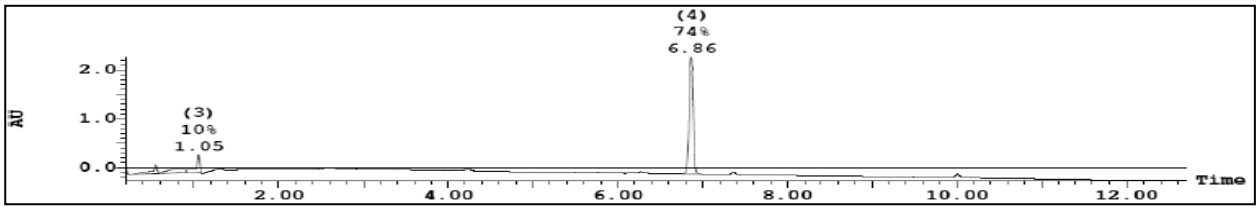
^{13}C NMR of *N,N*-diallyltryptamine (1f)



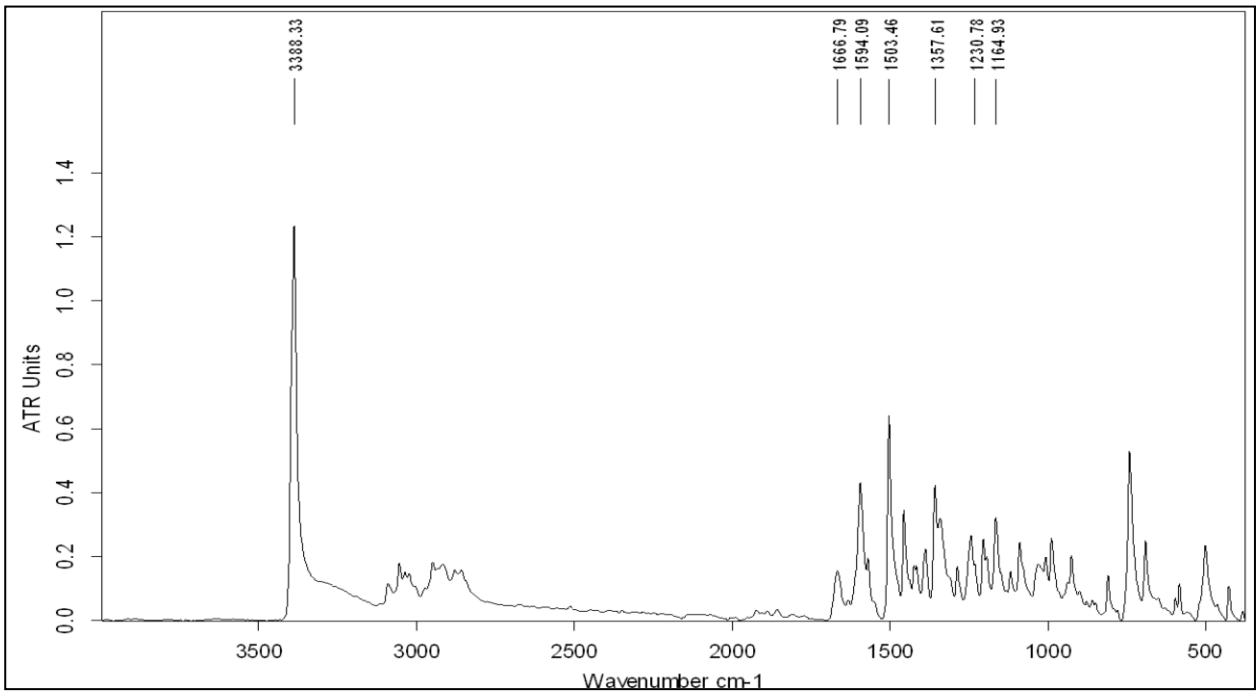
_N_-Allyl-_N_-phenyltryptamine (1g)



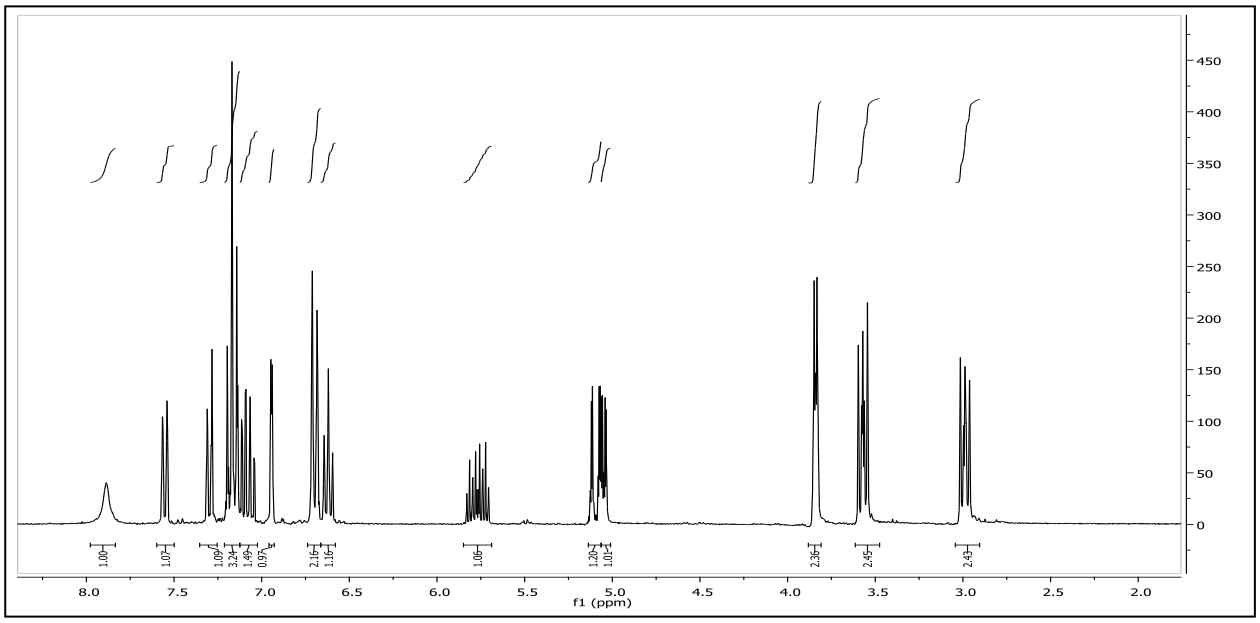
RP-HPLC of _N_-allyl-_N_-phenyltryptamine (1g)



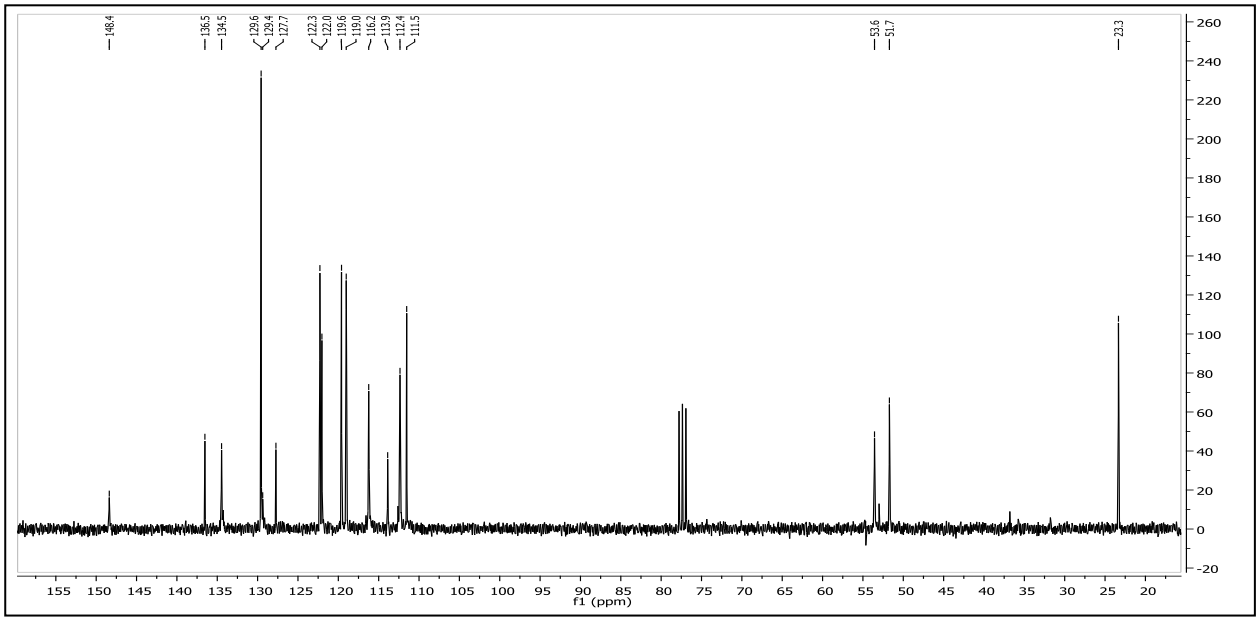
IR of _N_-allyl-_N_-phenyltryptamine (1g)



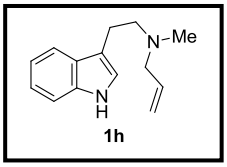
^{1}H NMR of *N*-allyl-*N*-phenyltryptamine (1g)



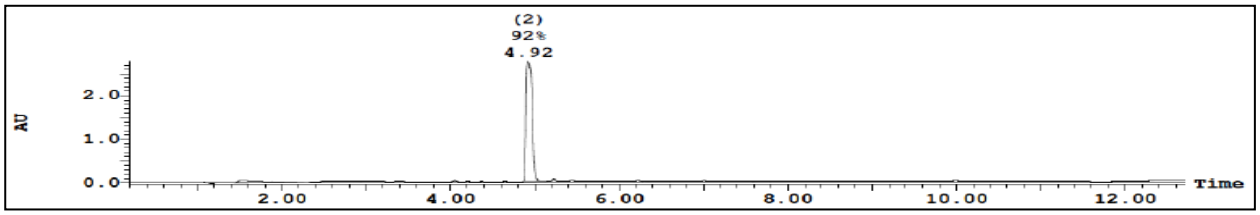
^{13}C NMR of *N*-allyl-*N*-phenyltryptamine (1g)



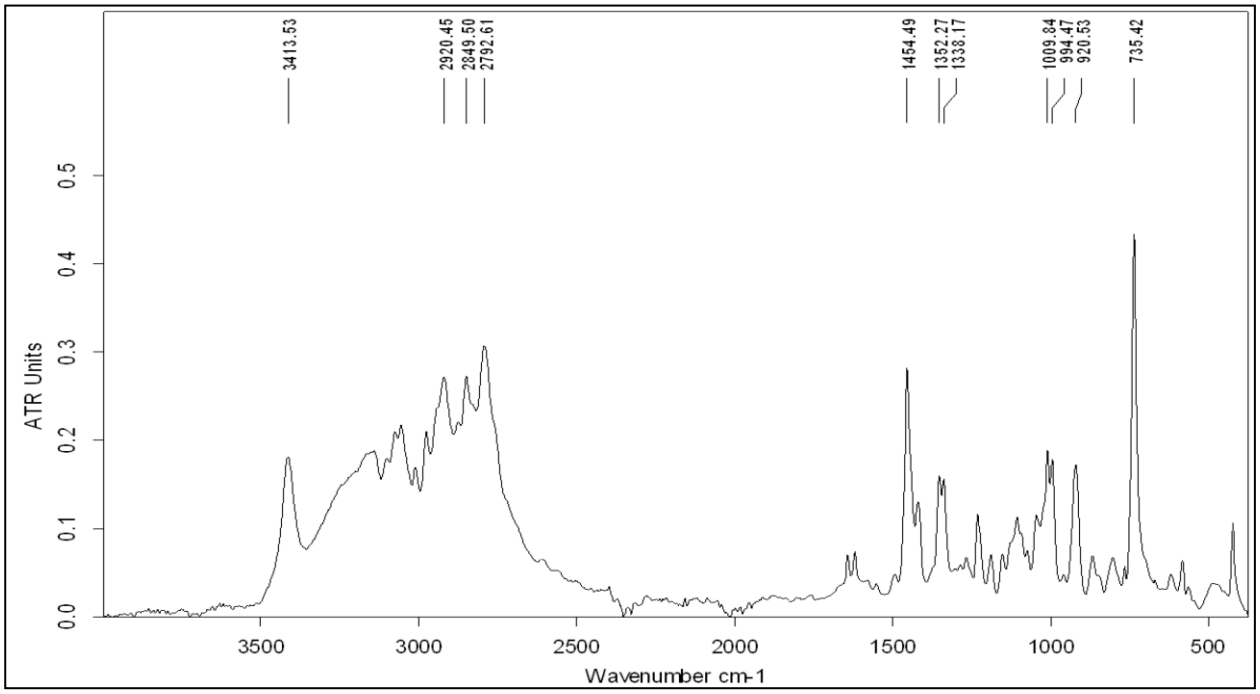
_N_-Allyl-_N_-methyltryptamine (1h)



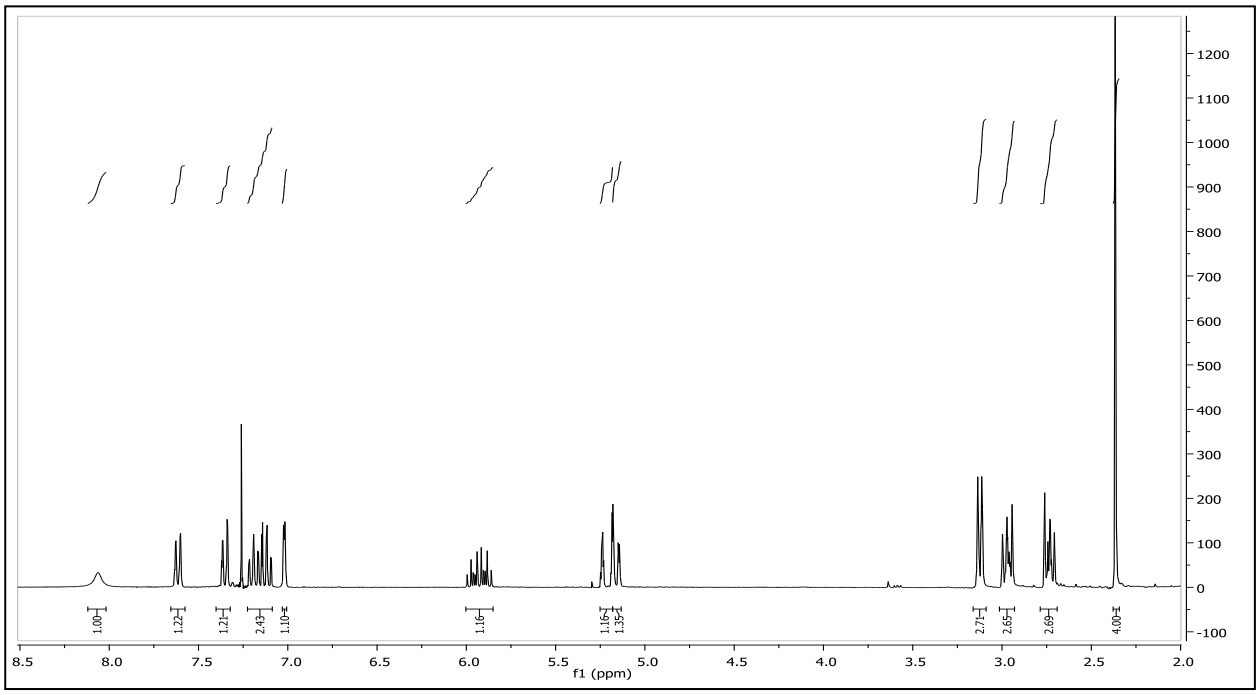
RP-HPLC of _N_-allyl-_N_-methyltryptamine (1h)



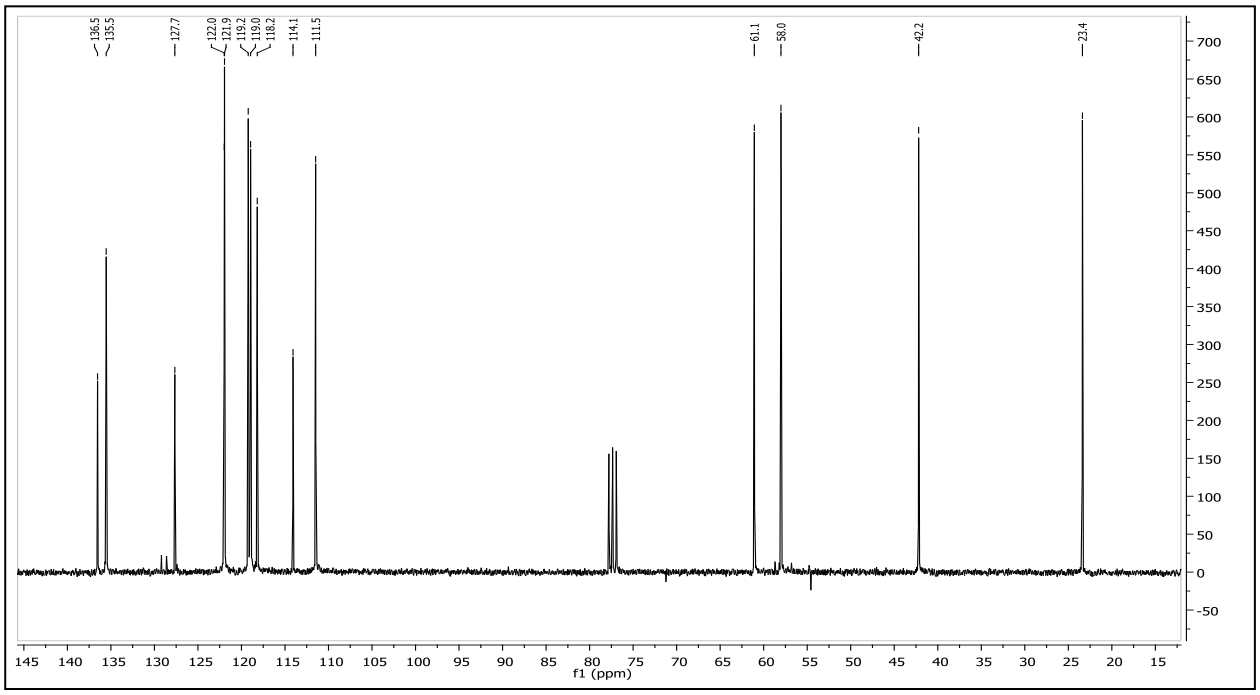
IR of _N_-allyl-_N_-methyltryptamine (1h)



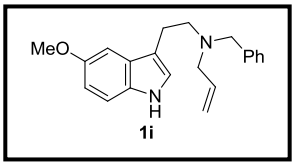
^{1}H NMR of *N*-allyl-*N*-methyltryptamine (1h)



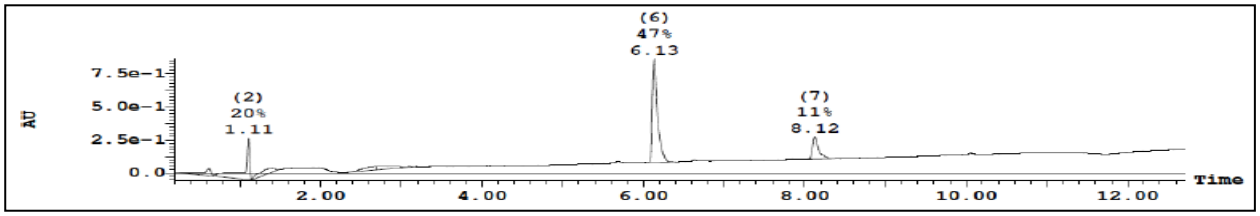
^{13}C NMR of *N*-allyl-*N*-methyltryptamine (1h)



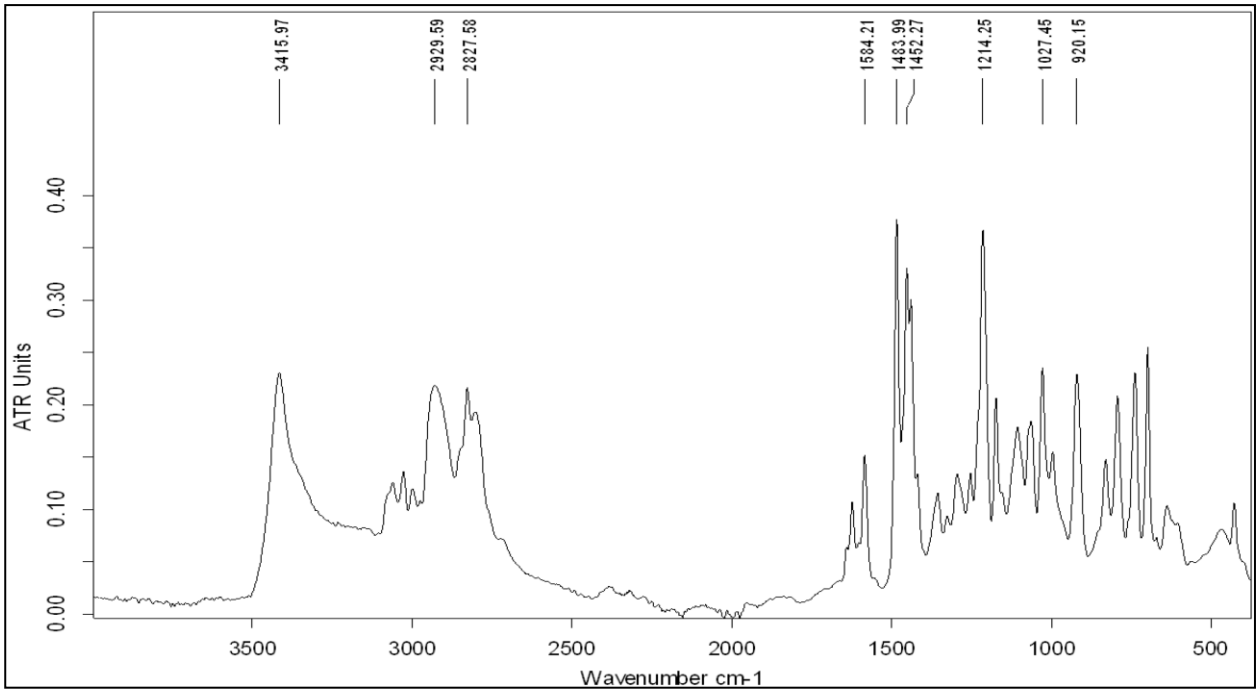
_N_-Allyl-_N_-benzyl-(5-methoxy)tryptamine (1i)



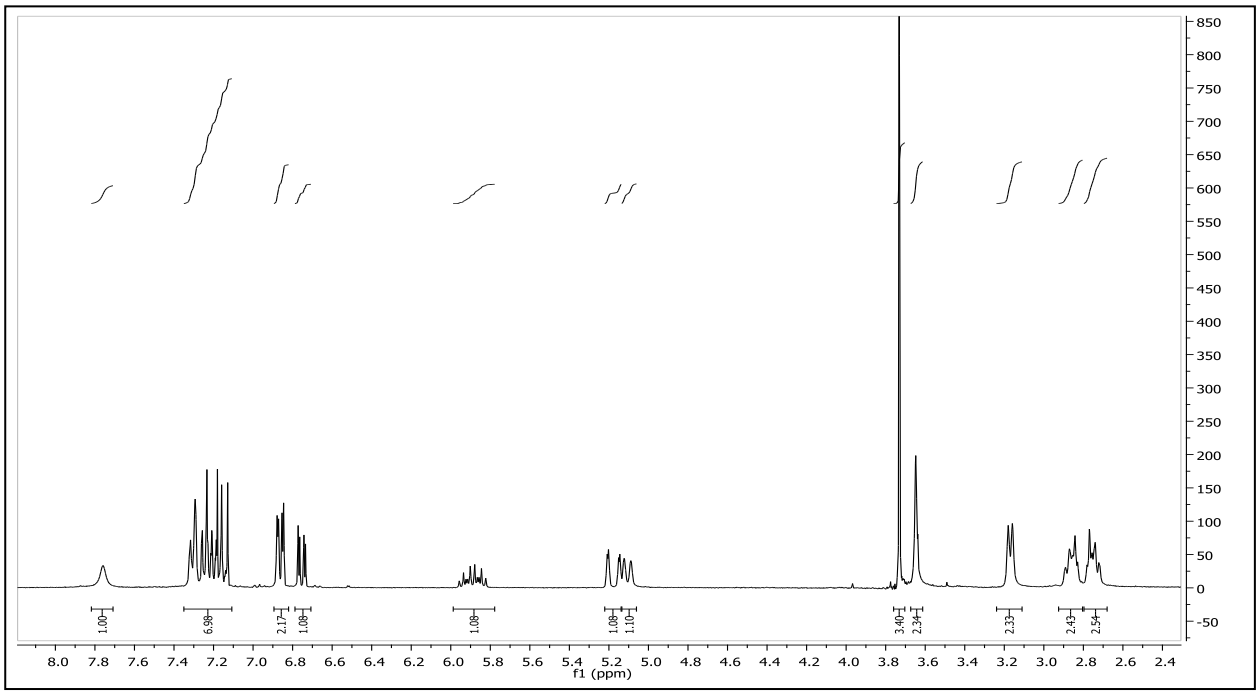
RP-HPLC of _N_-allyl-_N_-benzyl-(5-methoxy)tryptamine (1i)



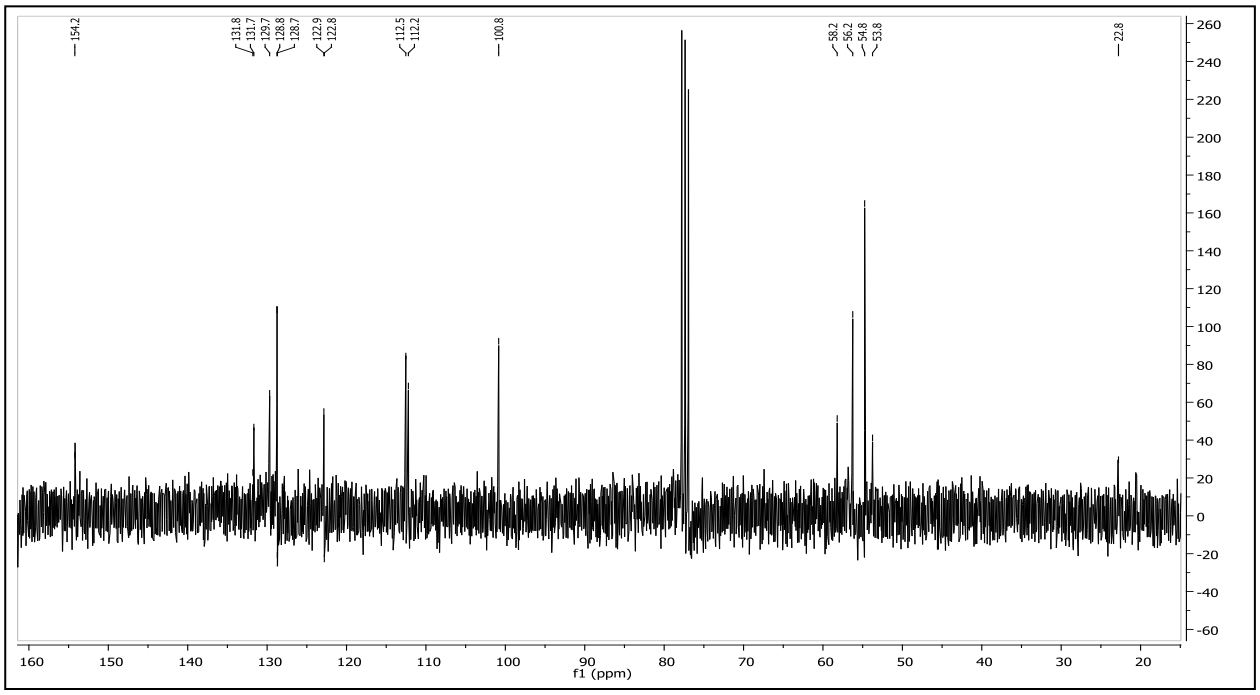
IR of _N_-allyl-_N_-benzyl-5-(methoxy)tryptamine (1i)



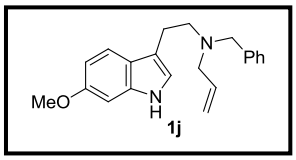
^{1}H NMR of *N*-allyl-*N*-benzyl-(5-methoxy)tryptamine (1i)



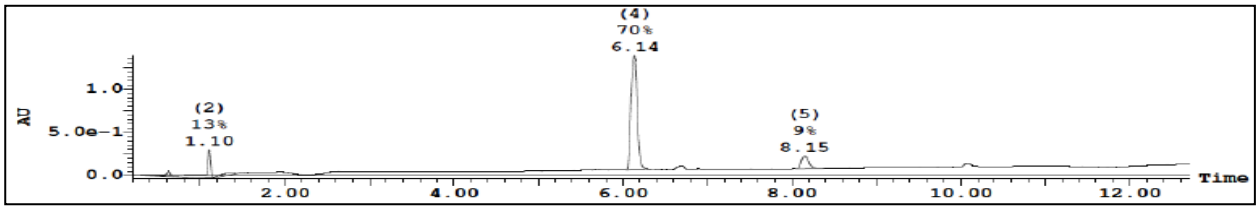
^{13}C NMR of *N*-allyl-*N*-benzyl-(5-methoxy)tryptamine (1i)



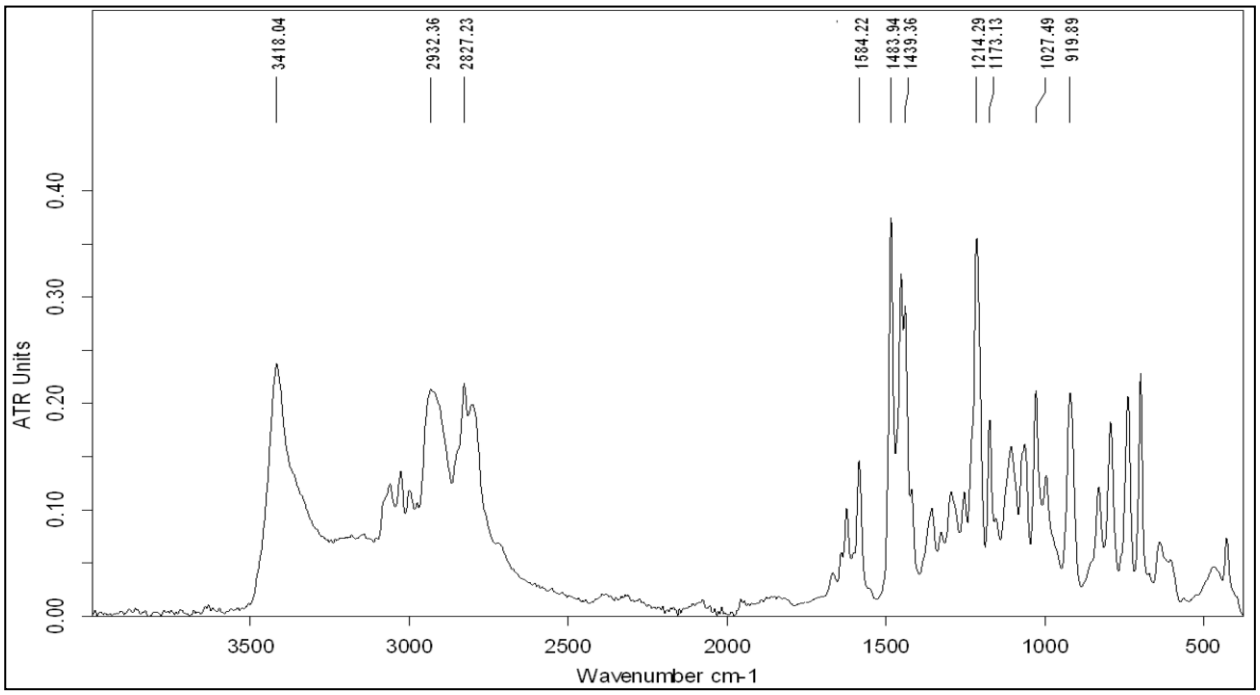
_N_-Allyl-_N_-benzyl-(6-methoxy)tryptamine (1j)



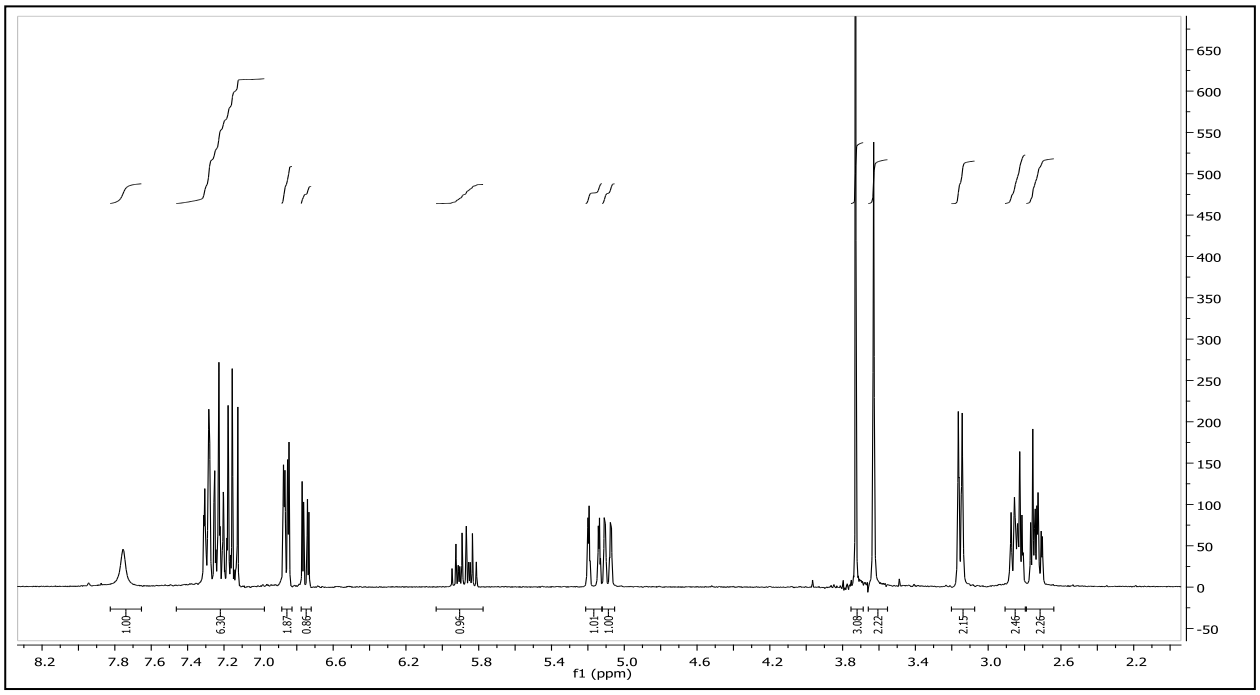
RP-HPLC of _N_-allyl-_N_-benzyl-(6-methoxy)tryptamine (1j)



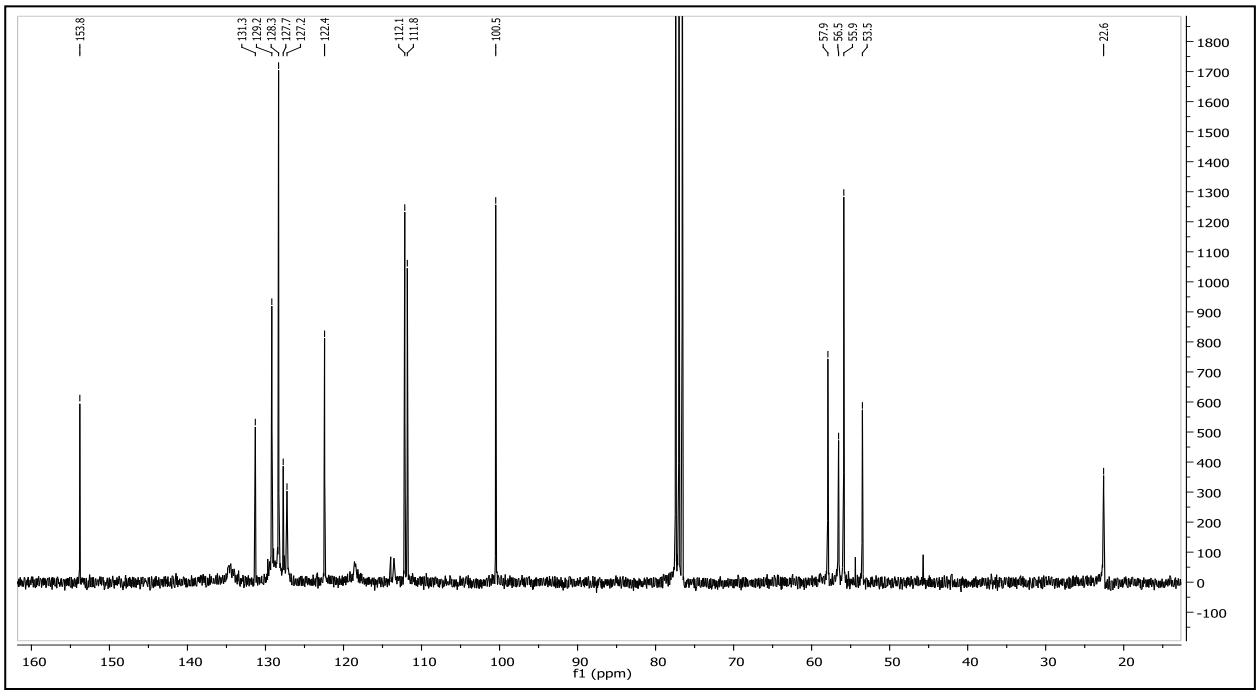
IR of _N_-allyl-_N_-benzyl-(6-methoxy)tryptamine (1j)



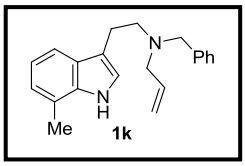
^{1}H NMR of *N*-allyl-*N*-benzyl-(6-methoxy)tryptamine (1j)



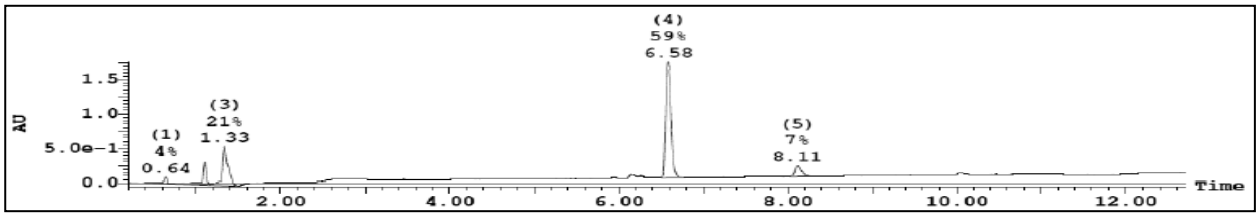
^{13}C NMR of *N*-allyl-*N*-benzyl-(6-methoxy)tryptamine (1j)



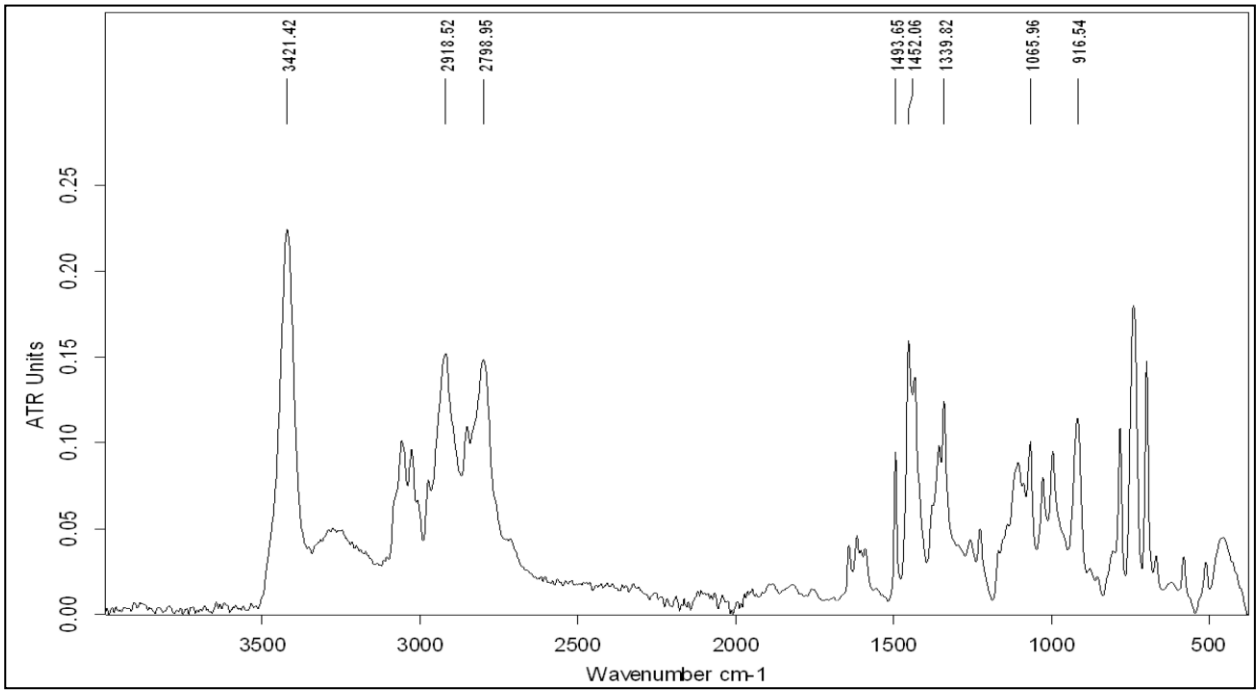
_N_-Allyl-_N_-benzyl-(7-methyl)tryptamine (1k)



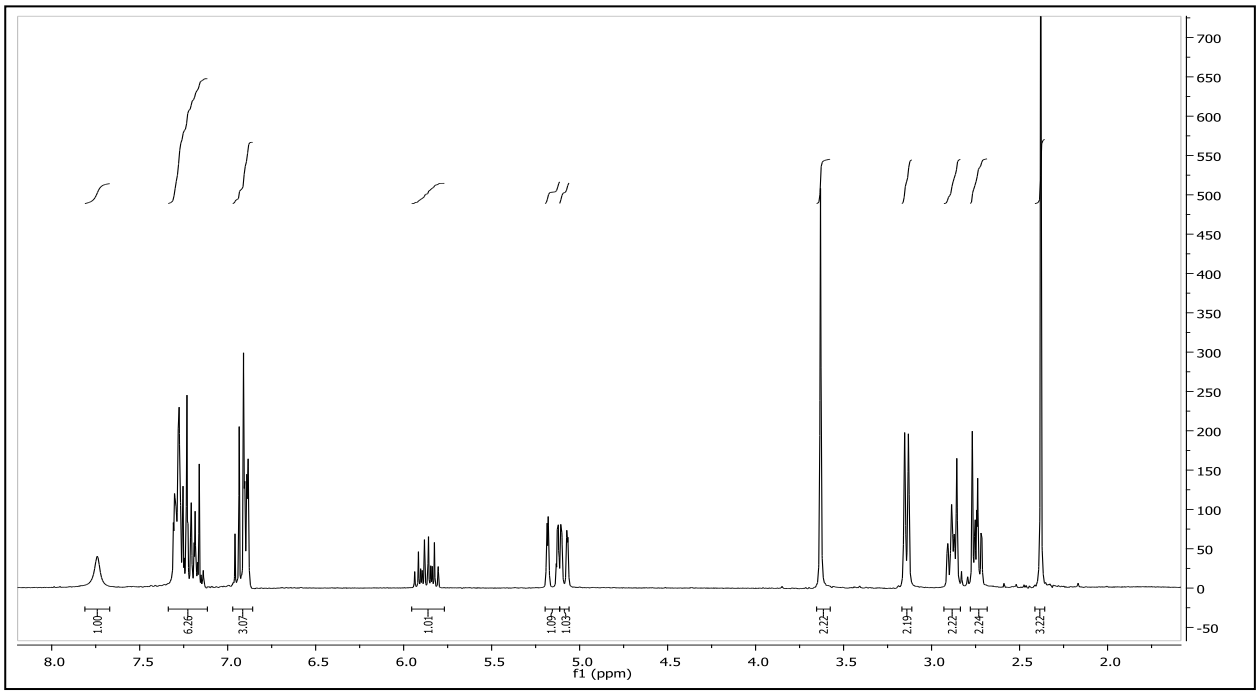
RP-HPLC of _N_-allyl-_N_-benzyl-(7-methyl)tryptamine (1k)



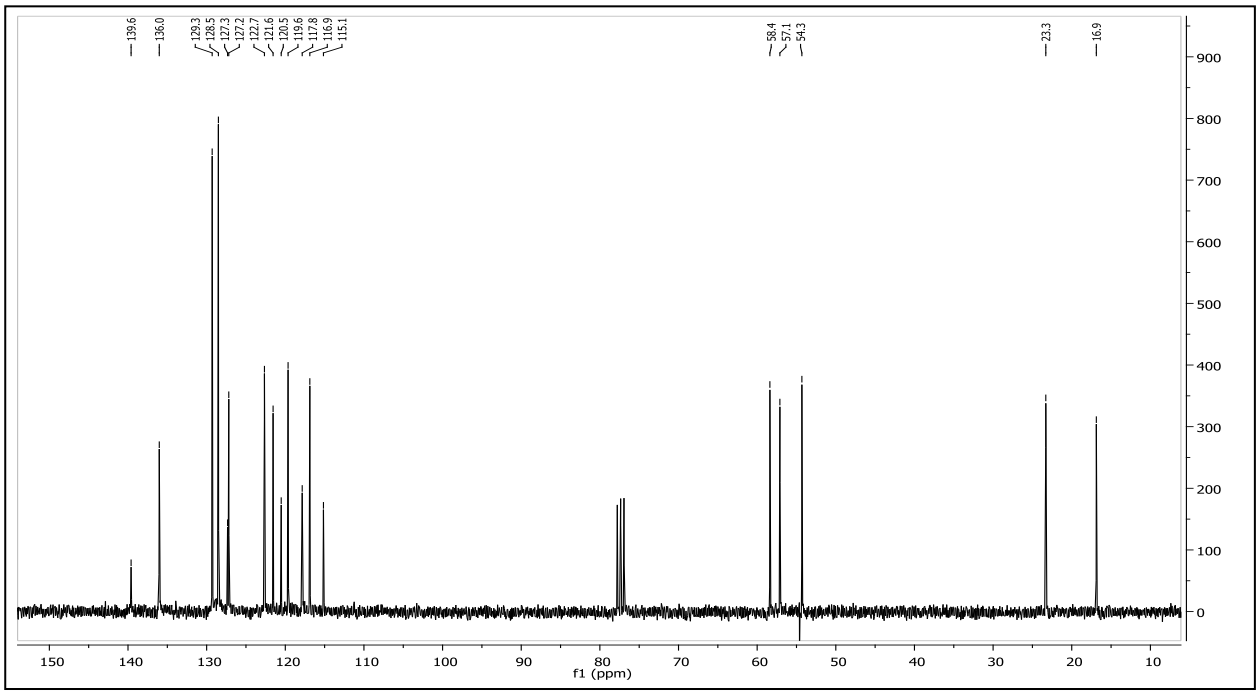
IR of _N_-allyl-_N_-benzyl-(7-methyl)tryptamine (1k)



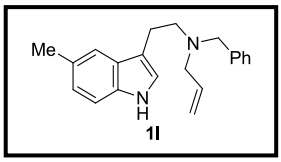
^{1}H NMR of *N*-allyl-*N*-benzyl-(7-methyl)tryptamine (1k)



^{13}C NMR of *N*-allyl-*N*-benzyl-(7-methyl)tryptamine (1k)

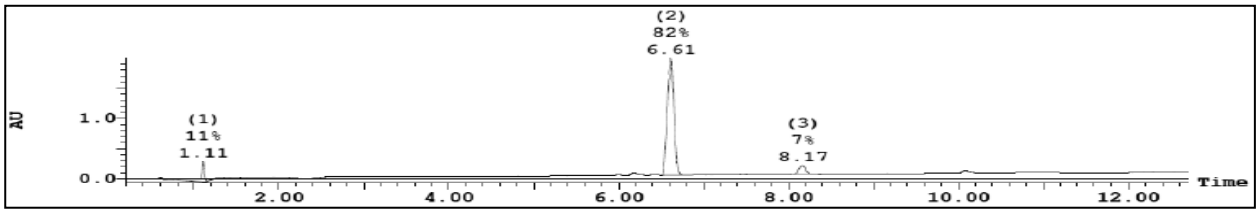


_N_-Allyl-_N_-benzyl-(5-methyl)tryptamine (1l)

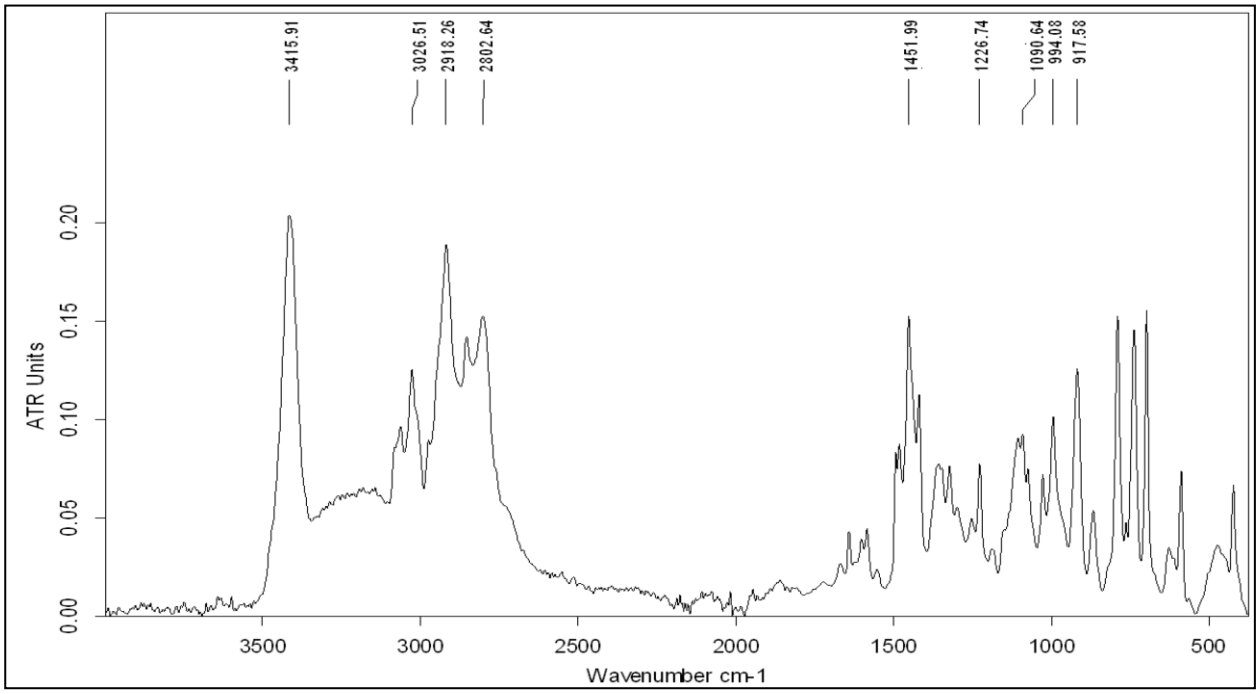


1l

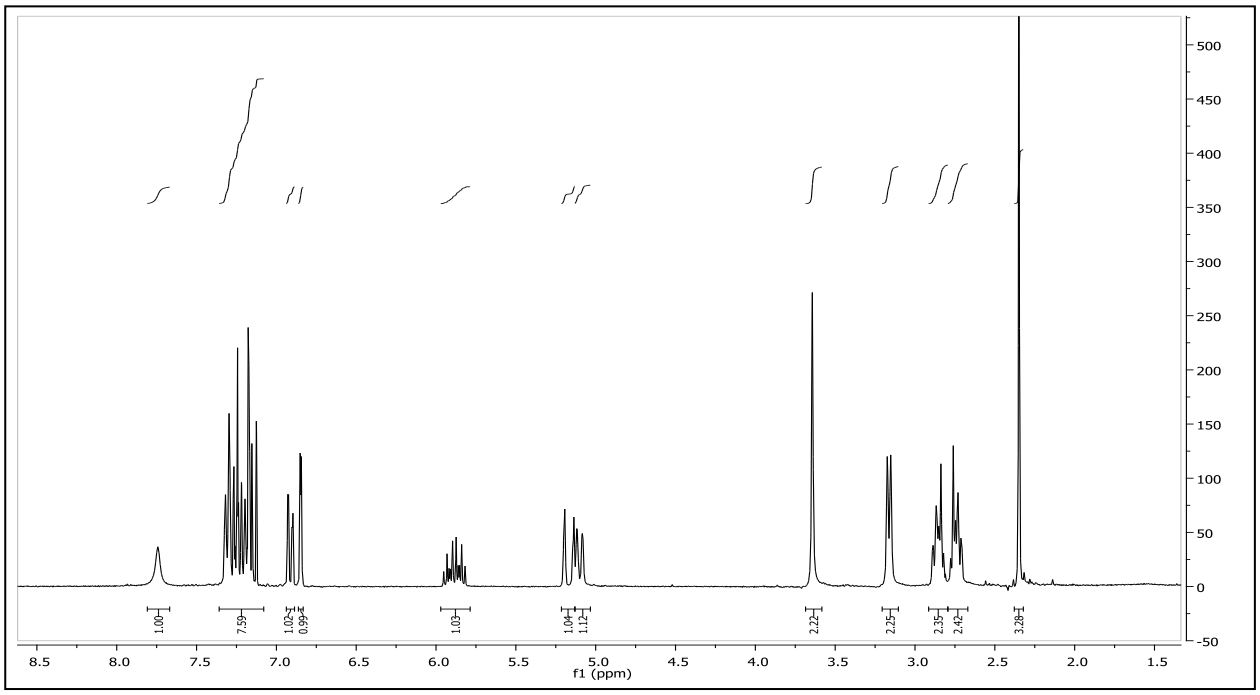
RP-HPLC of _N_-allyl-_N_-benzyl-(5-methyl)tryptamine (1l)



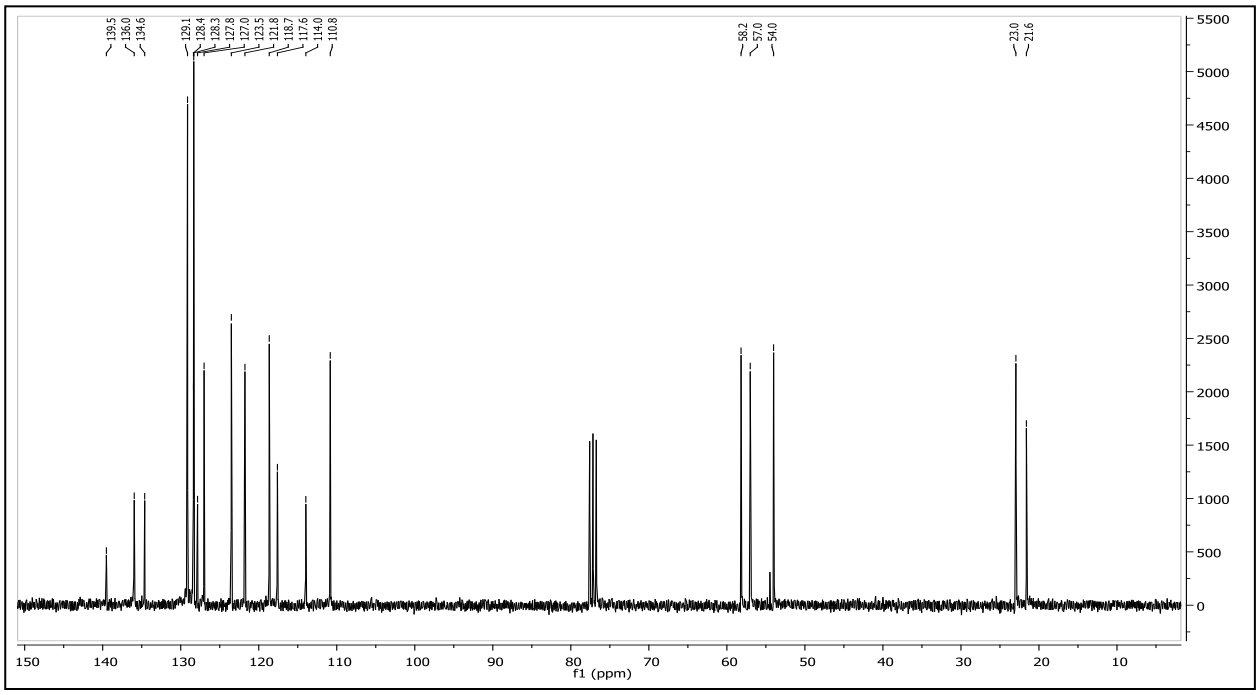
IR of _N_-allyl-_N_-benzyl-(5-methyl)tryptamine (1l)



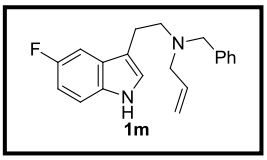
^{1}H NMR of *N*-allyl-*N*-benzyl-(5-methyl)tryptamine (1l)



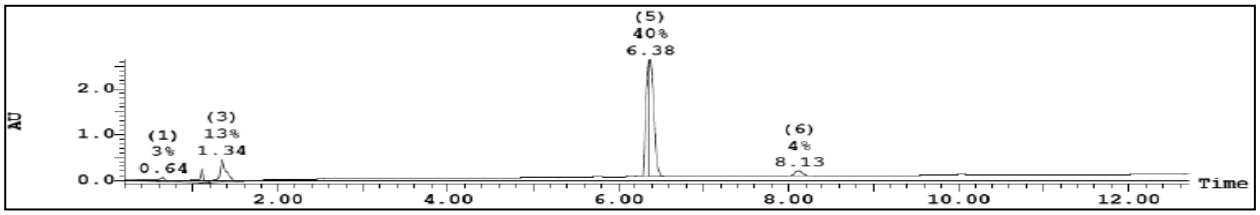
^{13}C NMR of *N*-allyl-*N*-benzyl-(5-methyl)tryptamine (1l)



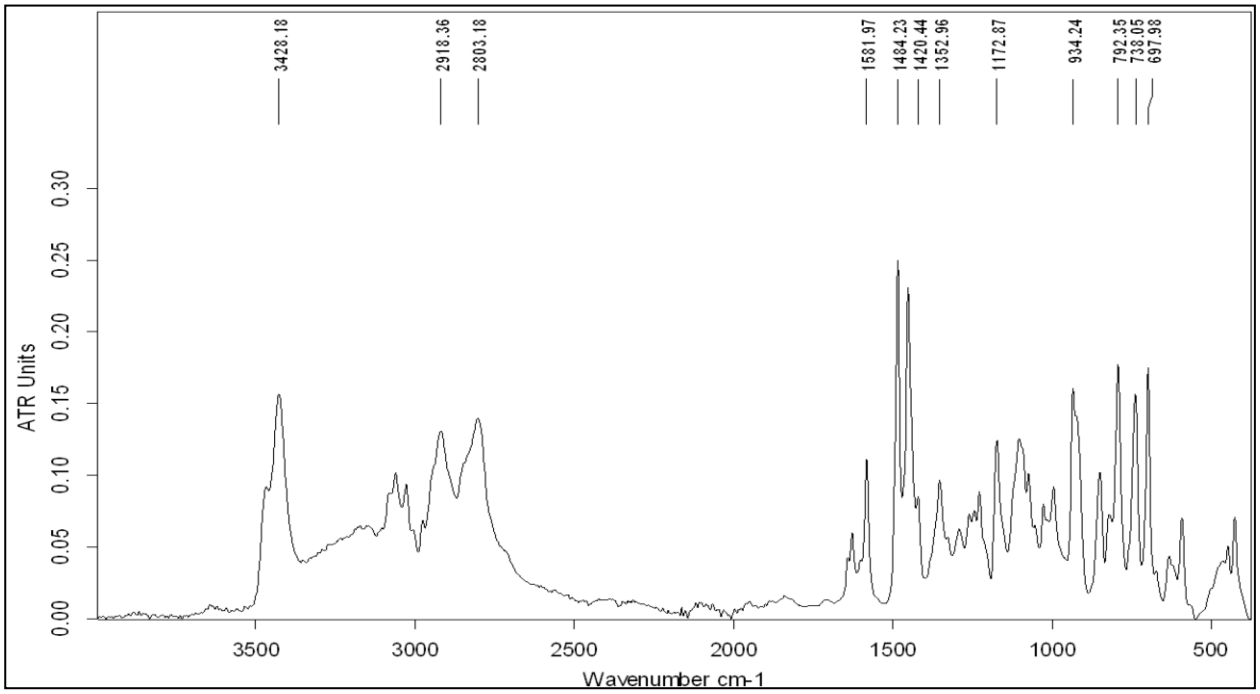
_N_-Allyl-_N_-benzyl-(5-fluoro)tryptamine (1m)



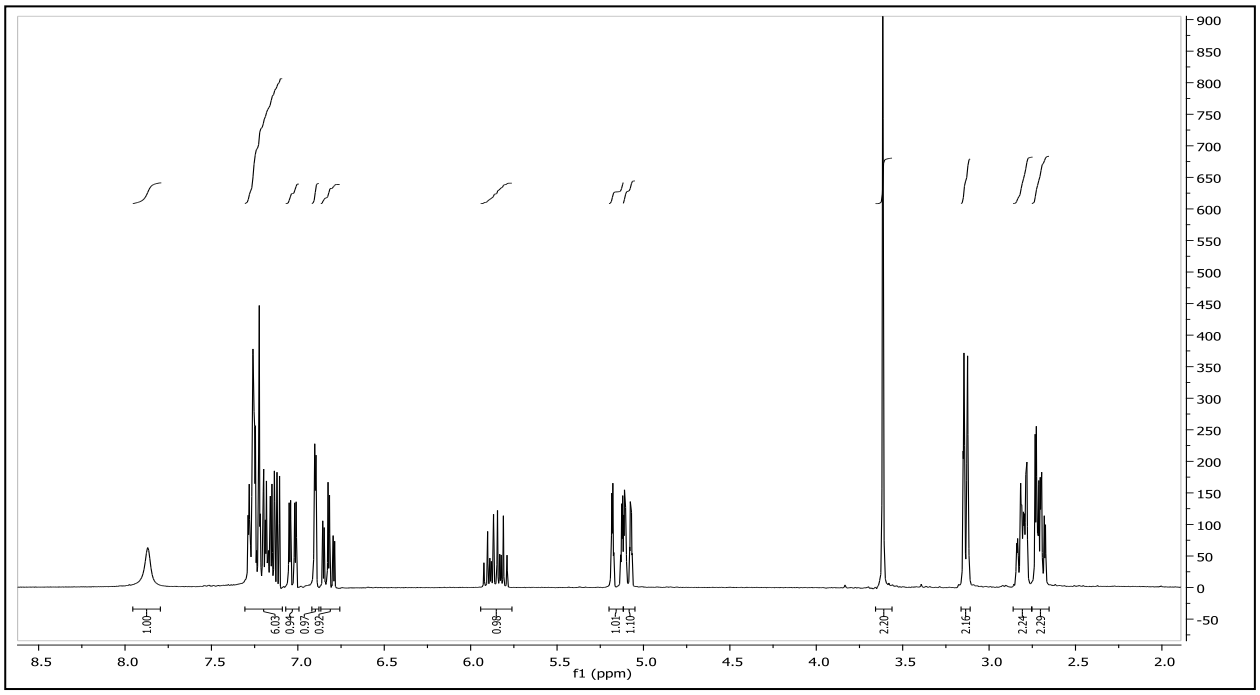
RP-HPLC of _N_-allyl-_N_-benzyl-(5-fluoro)tryptamine (1m)



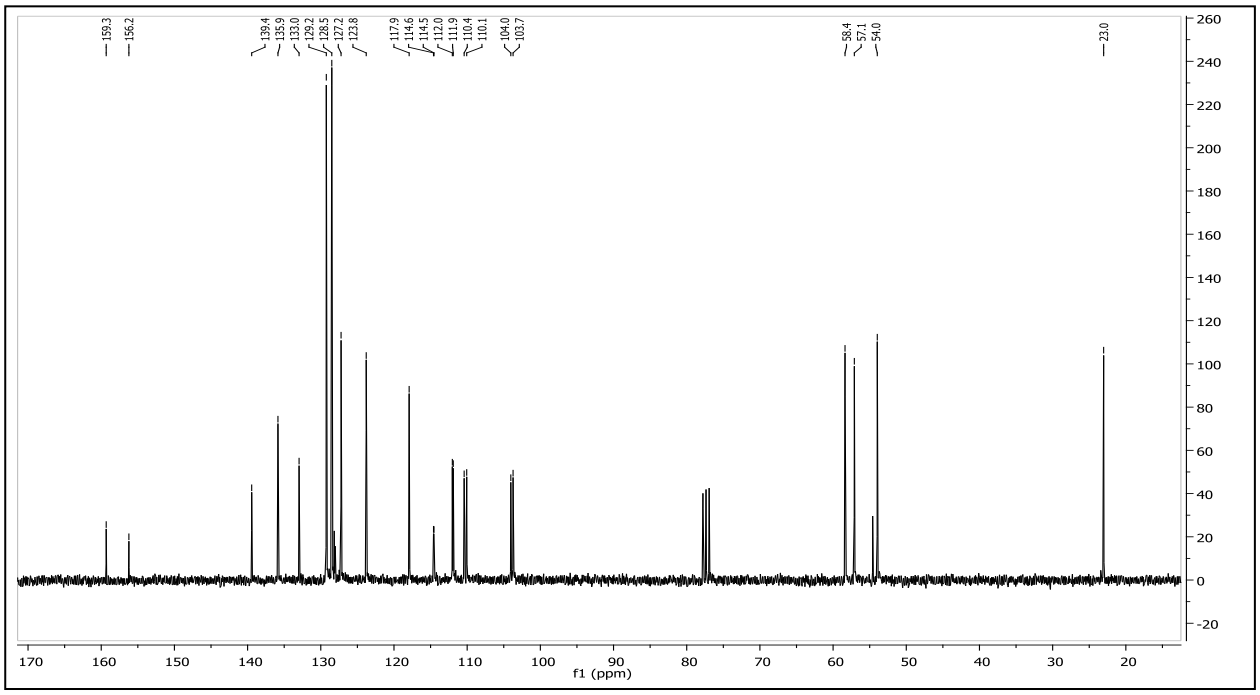
IR of _N_-allyl-_N_-benzyl-(5-fluoro)tryptamine (1m)



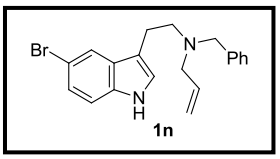
^{1}H NMR of *N*-allyl-*N*-benzyl-(5-fluoro)tryptamine (1m)



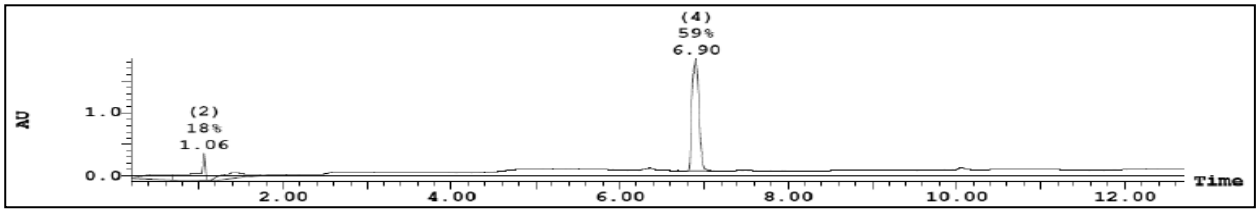
^{13}C NMR of *N*-allyl-*N*-benzyl-(5-fluoro)tryptamine (1m)



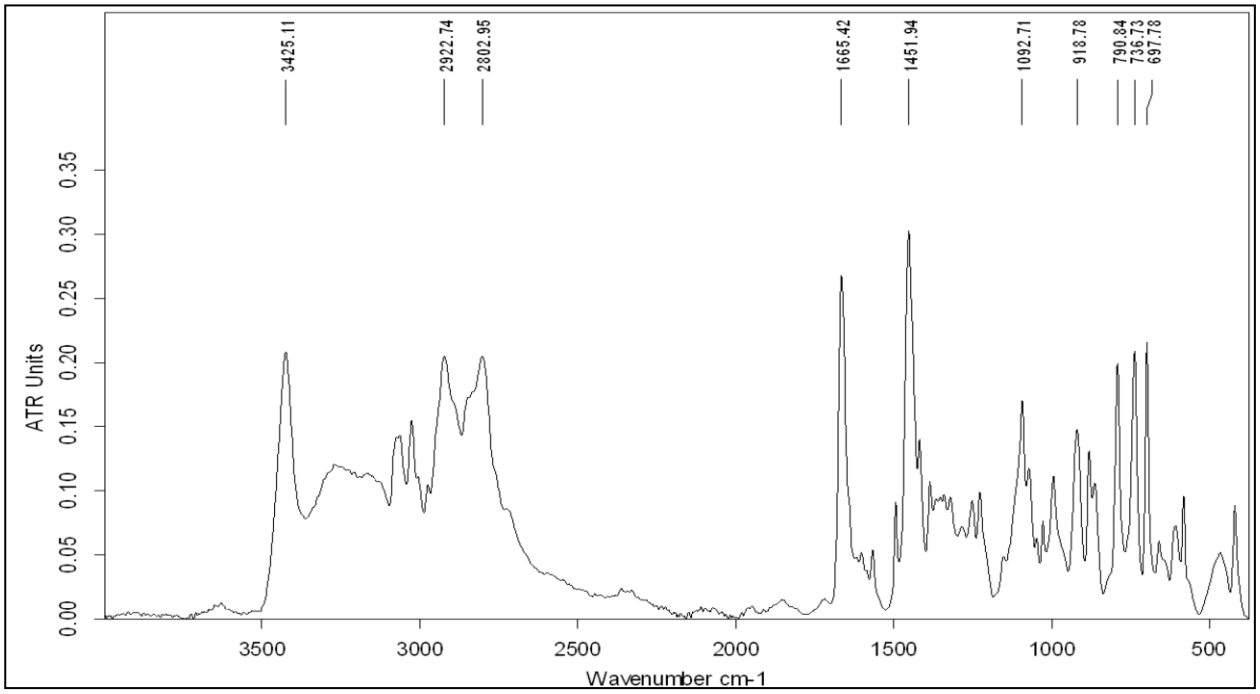
_N_-Allyl-_N_-benzyl-(5-bromo)tryptamine (1n)



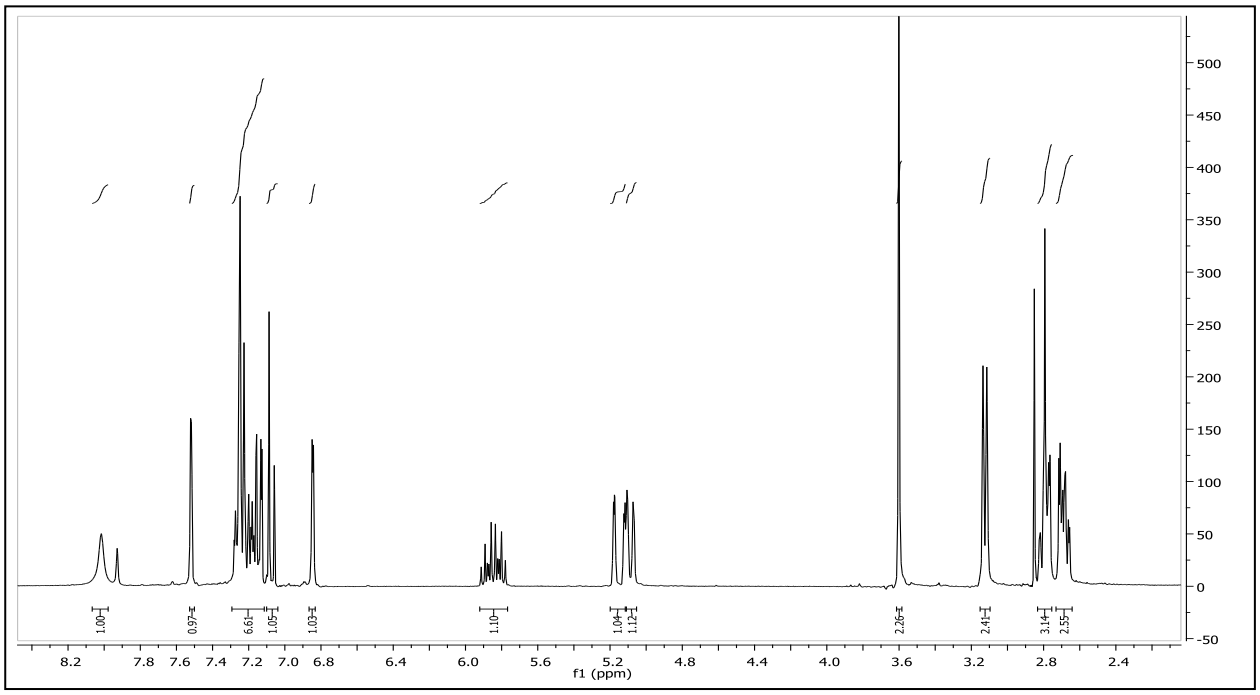
RP-HPLC of _N_-allyl-_N_-benzyl-(5-bromo)tryptamine (1n)



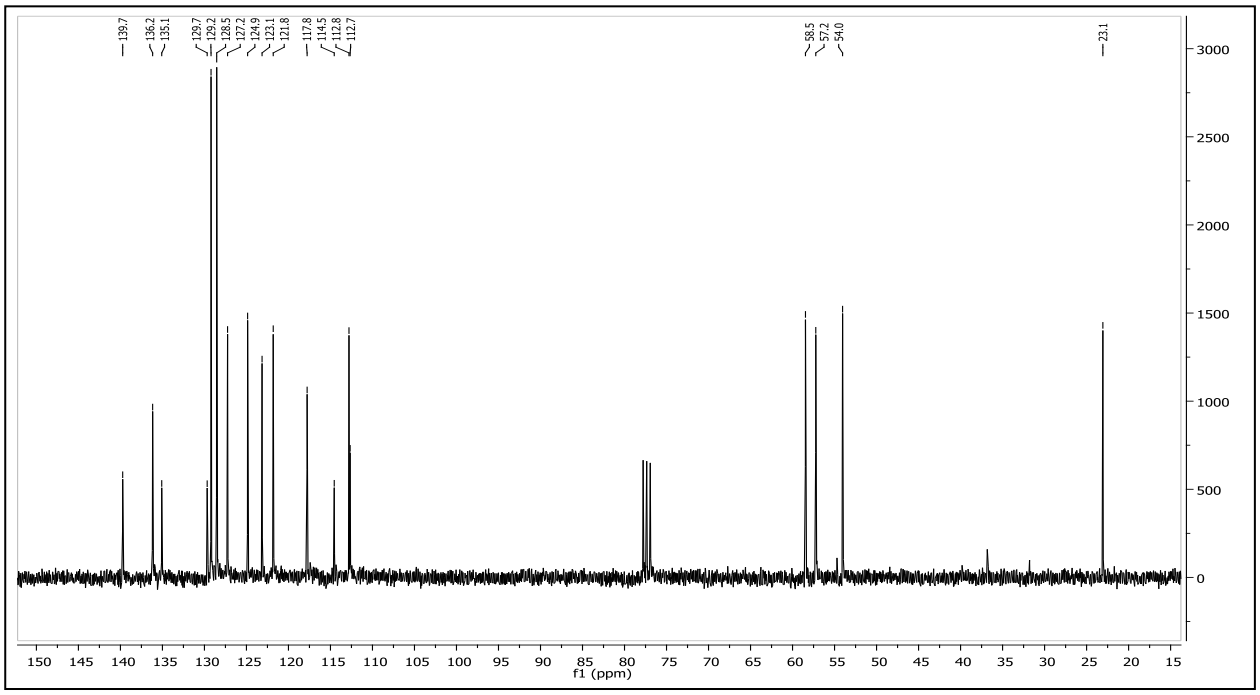
IR of _N_-allyl-_N_-benzyl-(5-bromo)tryptamine (1n)



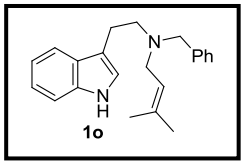
^{1}H NMR of *N*-allyl-*N*-benzyl-(5-bromo)tryptamine (1n)



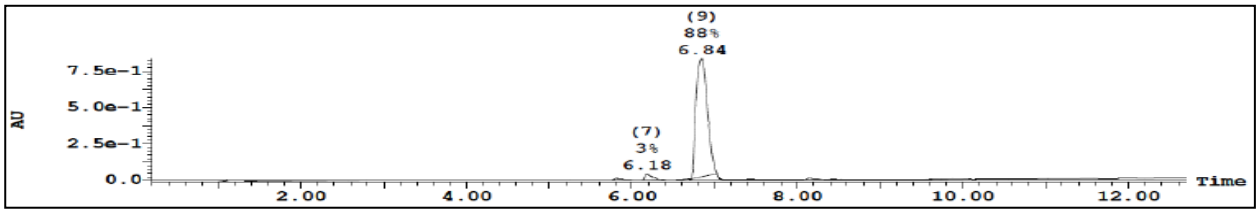
^{13}C NMR of *N*-allyl-*N*-benzyl-(5-bromo)tryptamine (1n)



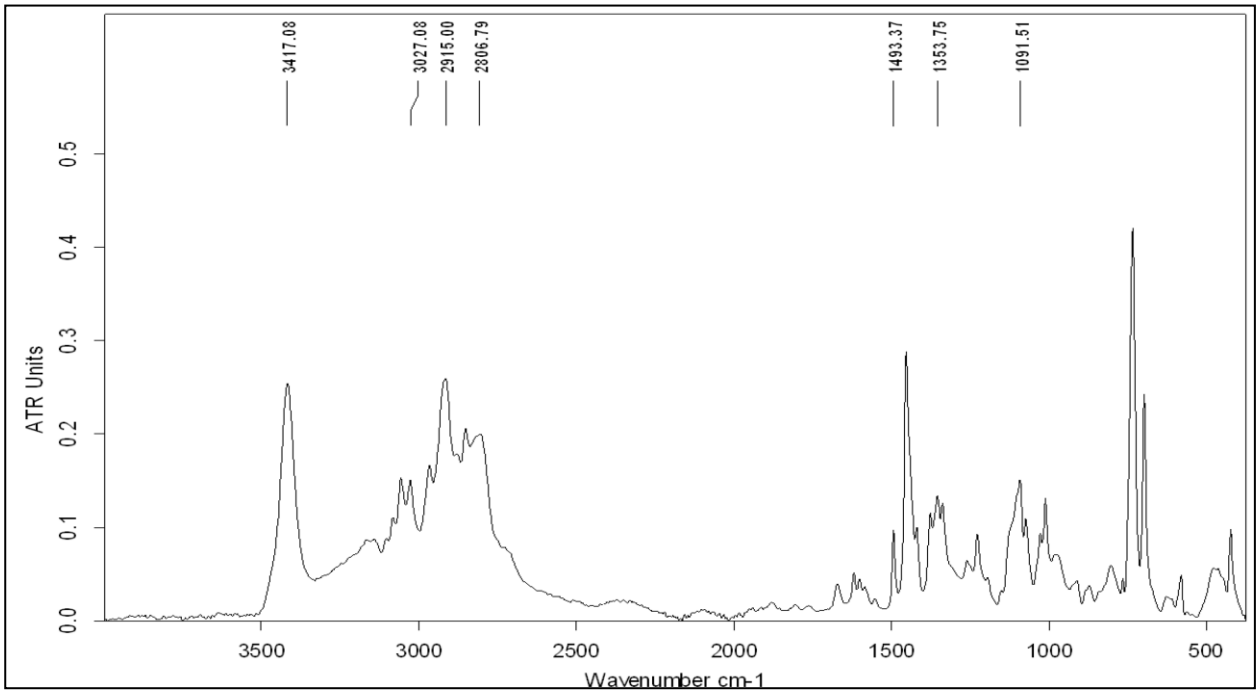
_N_-Benzyl-_N_-(3,3-dimethyl)allyltryptamine (1o)



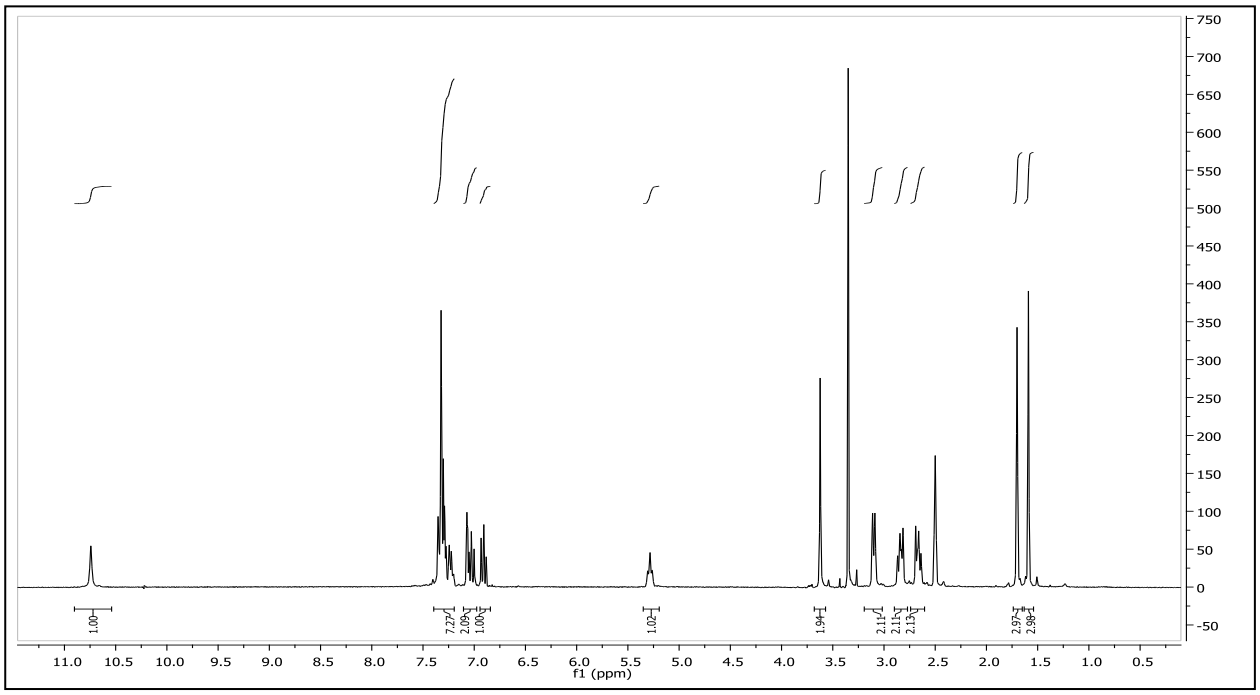
RP-HPLC of _N_-benzyl-_N_-(3,3-dimethyl)allyltryptamine (1o)



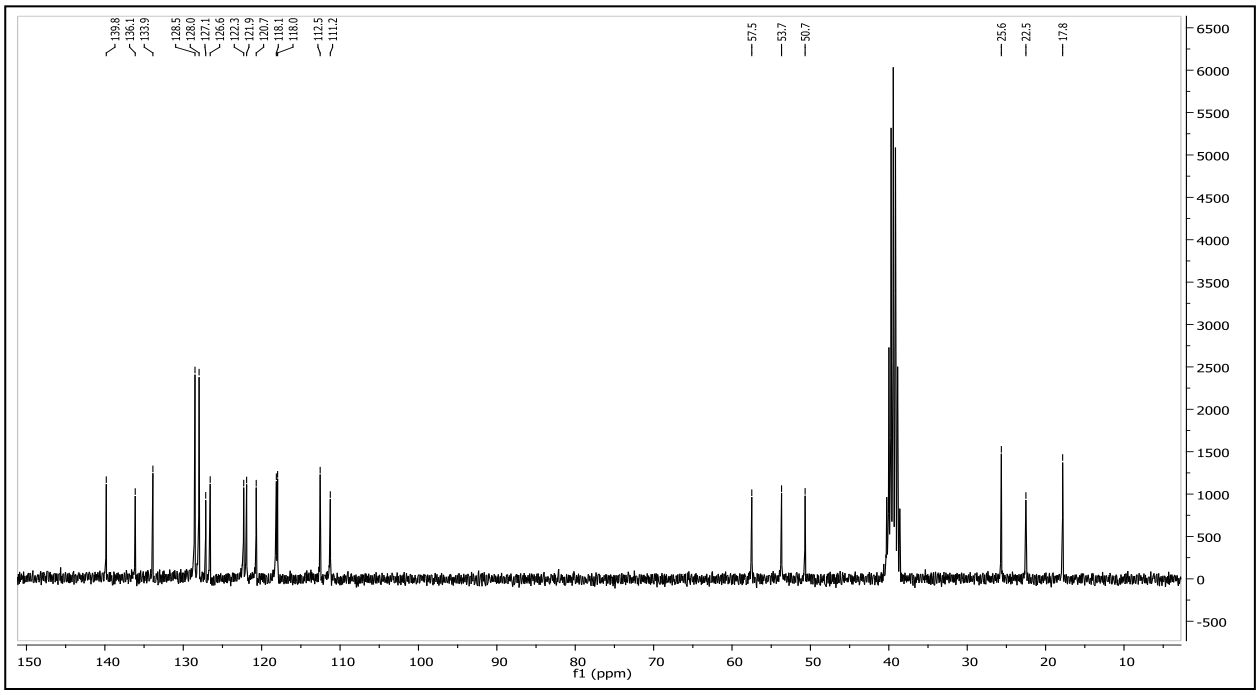
IR of _N_-benzyl-_N_-(3,3-dimethyl)allyltryptamine (1o)



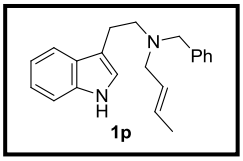
^{1}H NMR of *N*-benzyl-*N*-*(*3,3-dimethyl)allyltryptamine (1o)



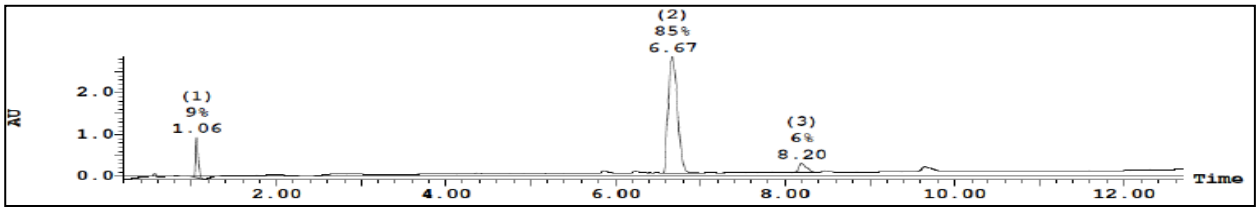
^{13}C NMR of *N*-benzyl-*N*-*(*3,3-dimethyl)allyltryptamine (1o)



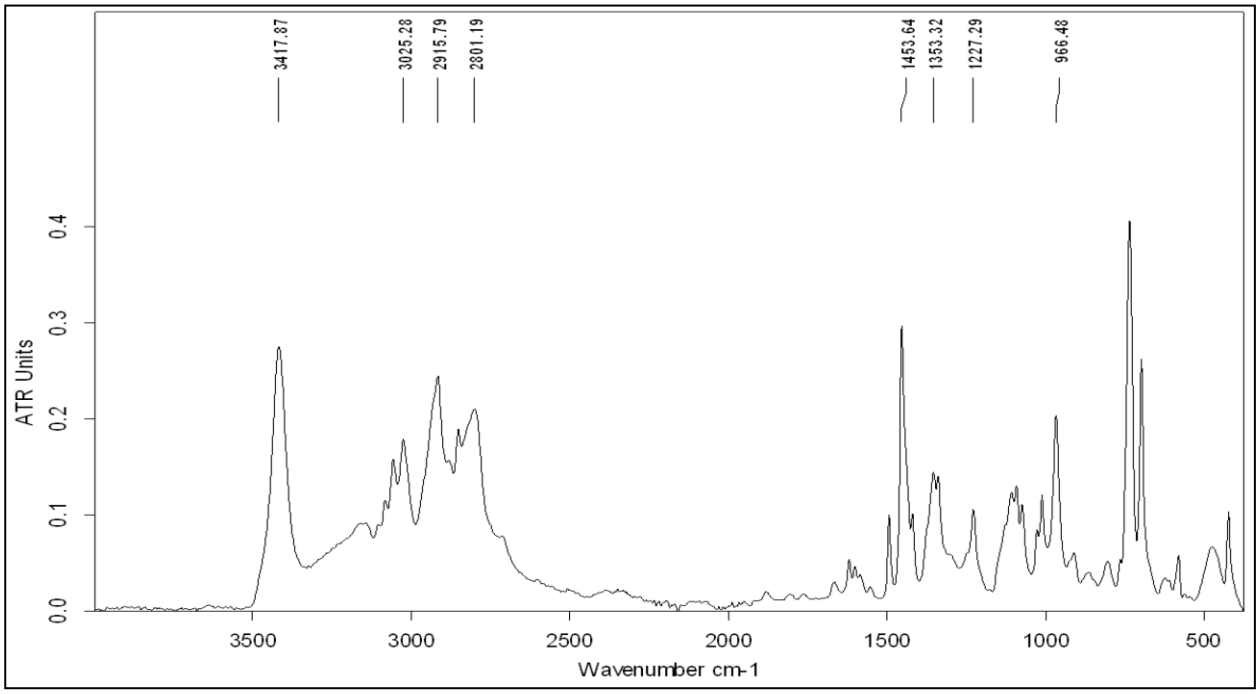
_N_-Benzyl-_N_-crotyltryptamine (1p)



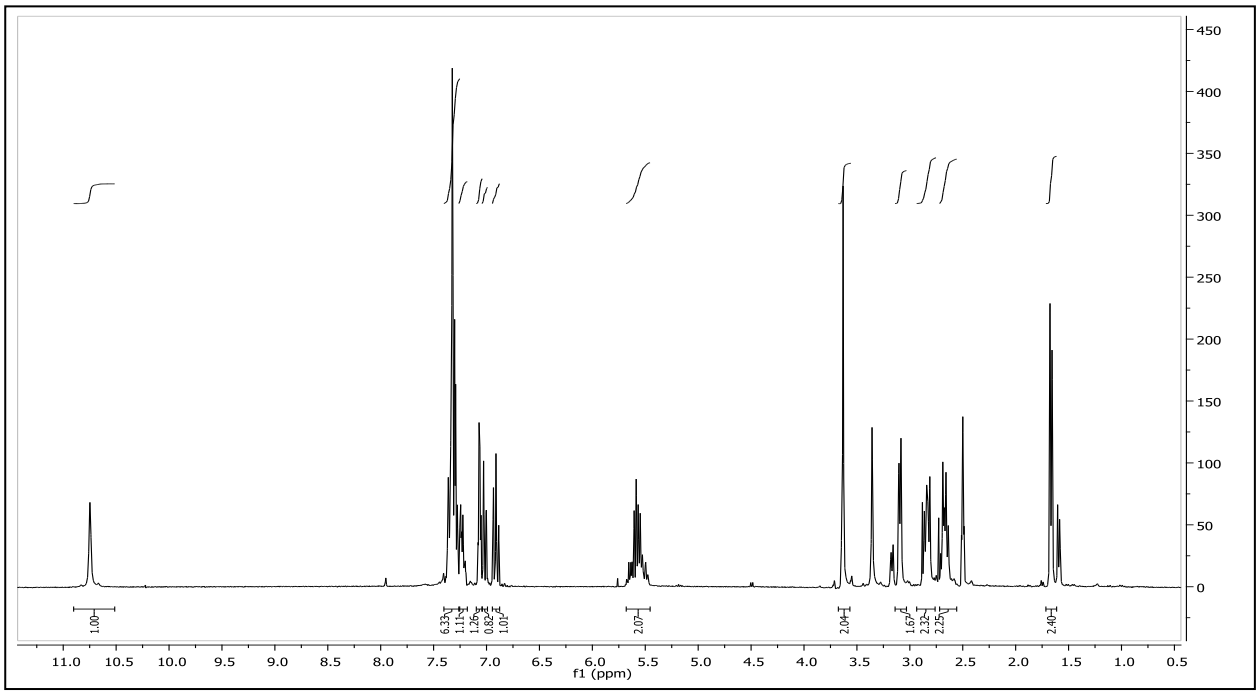
RP-HPLC of _N_-benzyl-_N_-crotyltryptamine (1p)



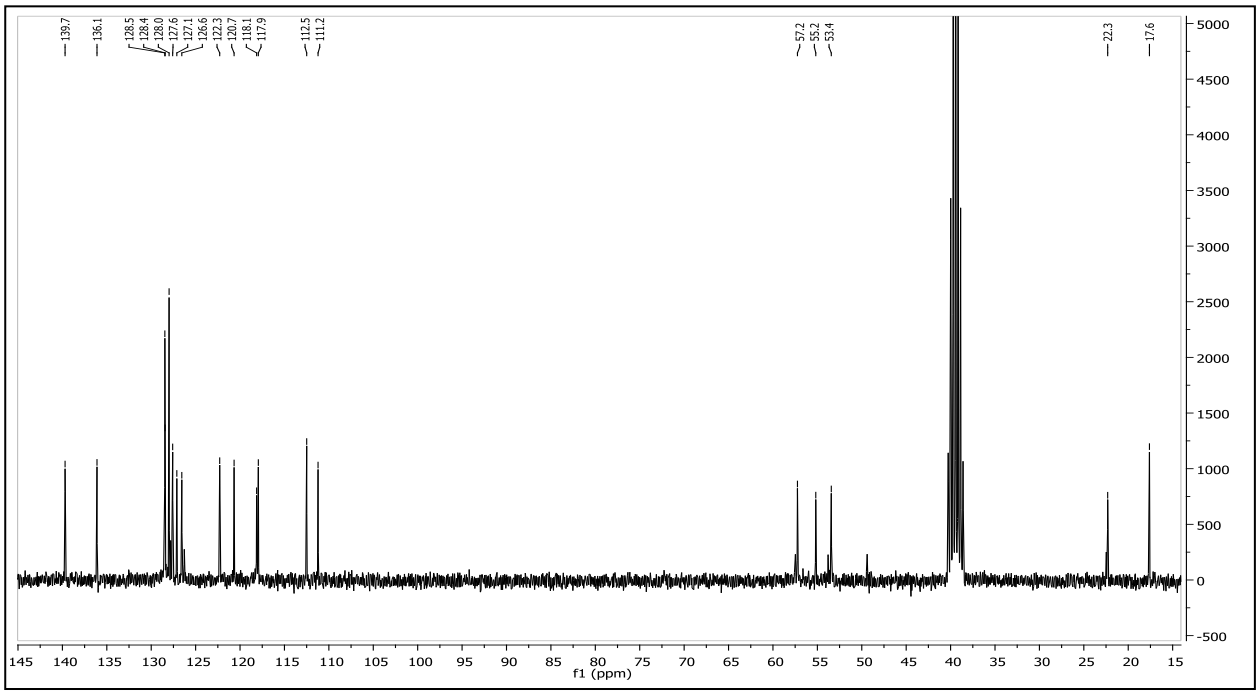
IR of _N_-benzyl-_N_-crotyltryptamine (1p)



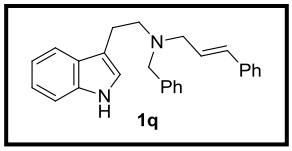
^{1}H NMR of *N*-benzyl-*N*-crotyltryptamine (1p)



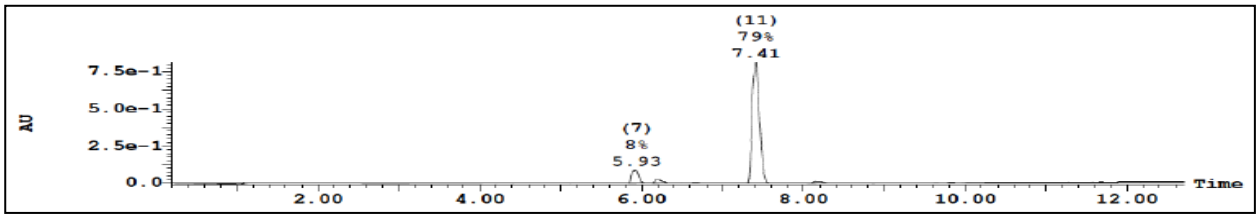
^{13}C NMR of *N*-benzyl-*N*-crotyltryptamine (1p)



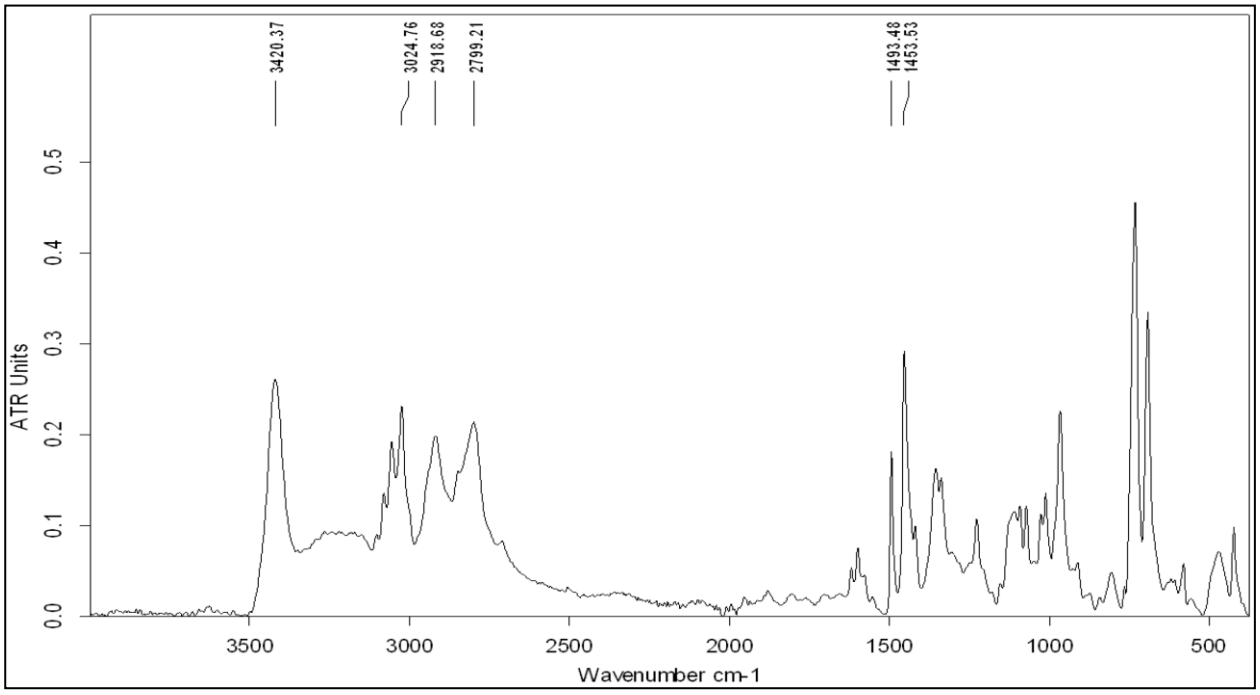
_N_-Benzyl-_N_-3-phenylprop-2-en-1-tryptamine (1q)



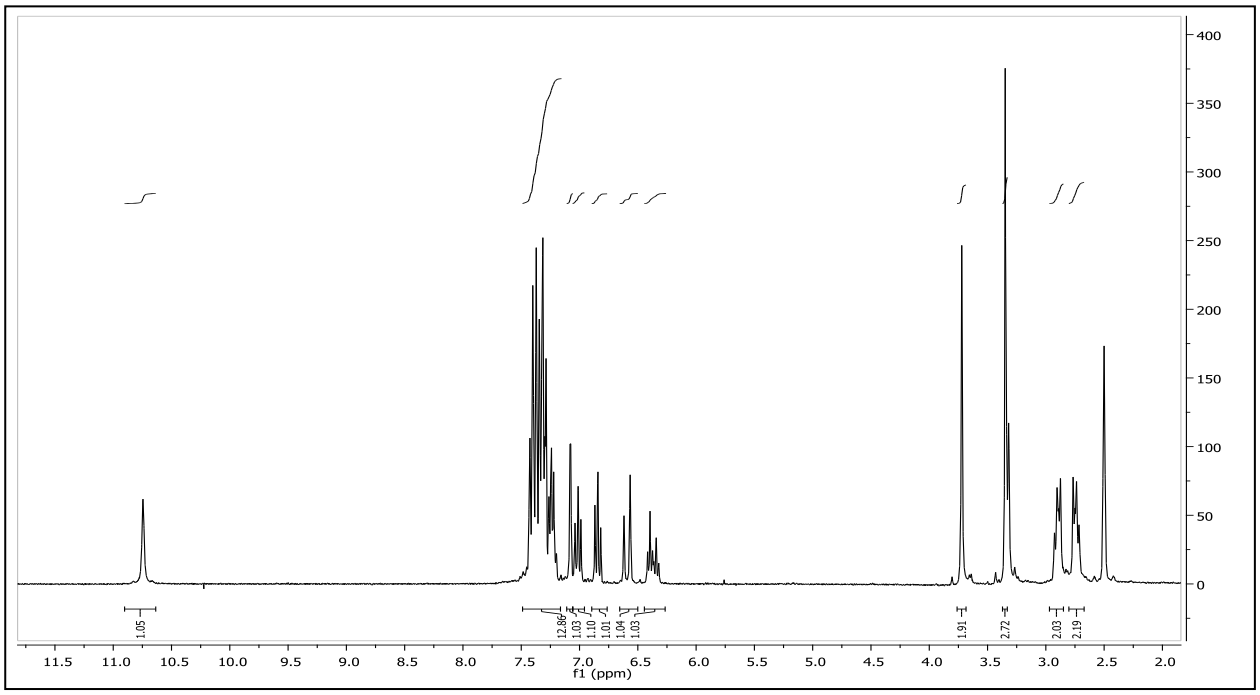
RP-HPLC of _N_-benzyl-_N_-3-phenylprop-2-en-1-tryptamine (1q)



IR of _N_-benzyl-_N_-3-phenylprop-2-en-1-tryptamine (1q)



^{1}H NMR of *N*-benzyl-*N*-3-phenylprop-2-en-1-tryptamine (1q)



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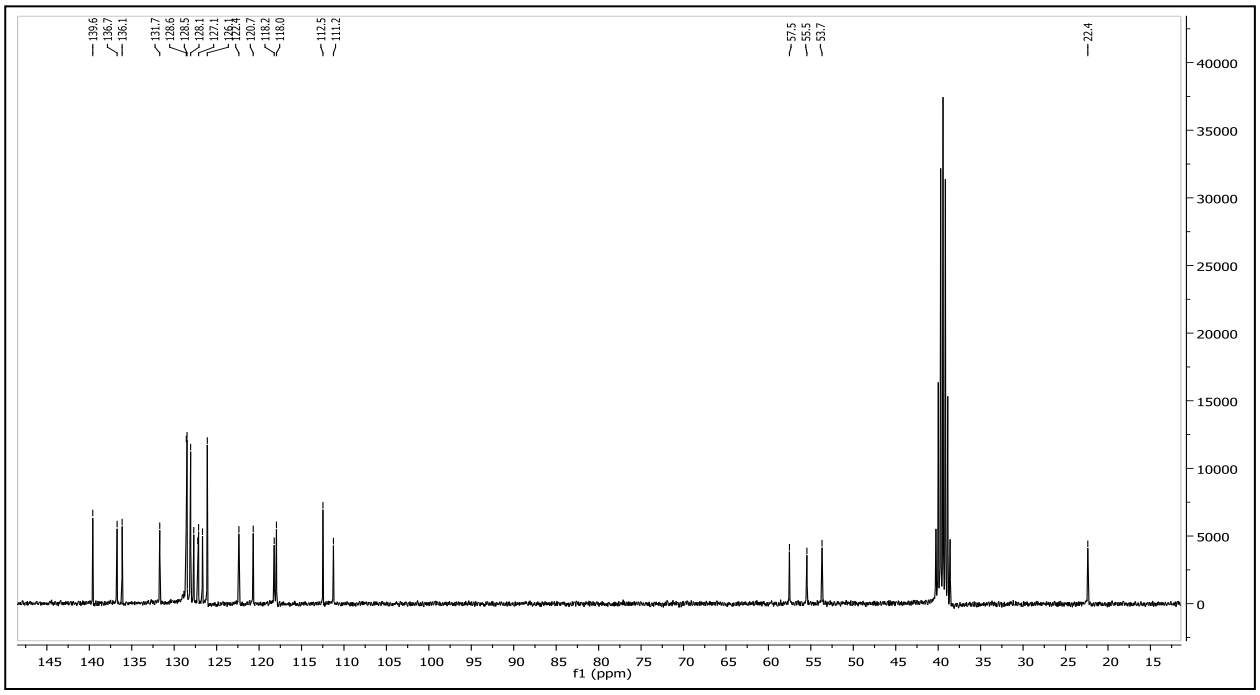

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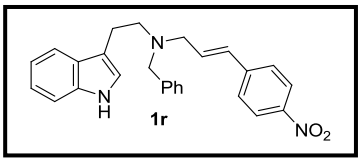
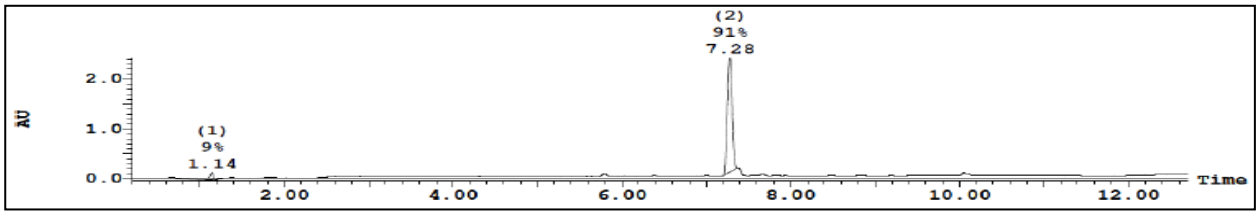
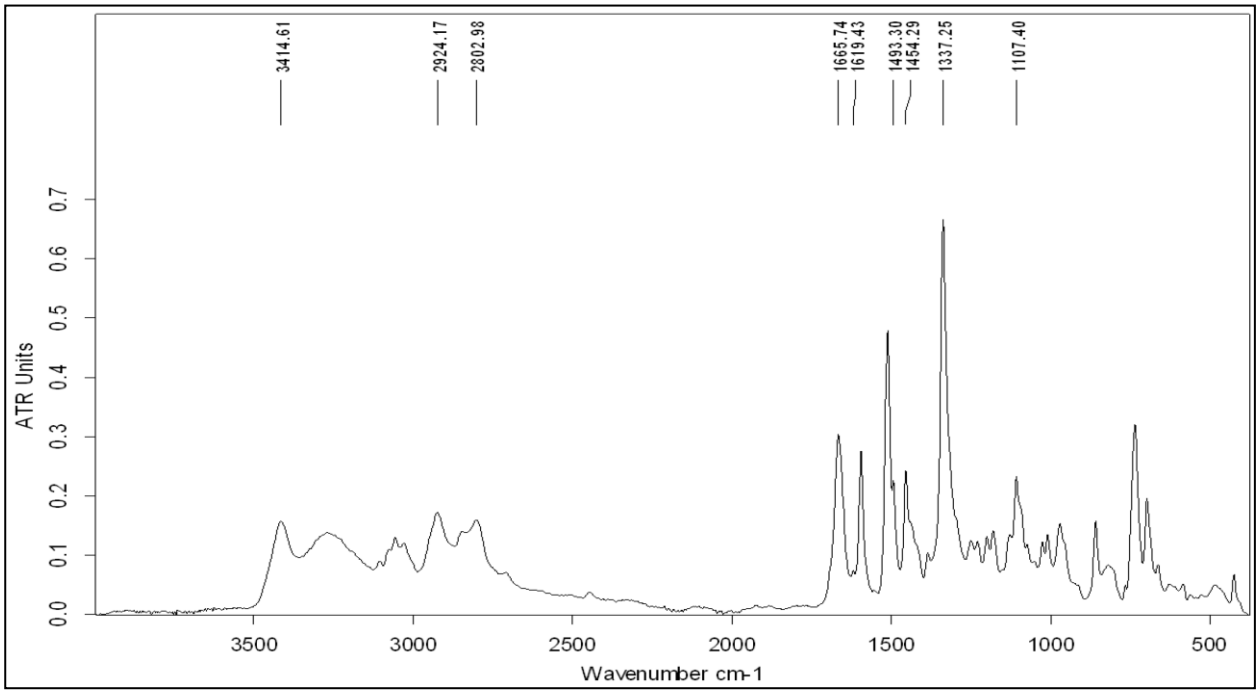


RP-HPLC of _N_-benzyl-_N_-3-(4-nitrophenyl)prop-2-en-1-tryptamine (1r)



IR of _N_-benzyl-_N_-3-(4-nitrophenyl)prop-2-en-1-tryptamine (1r)



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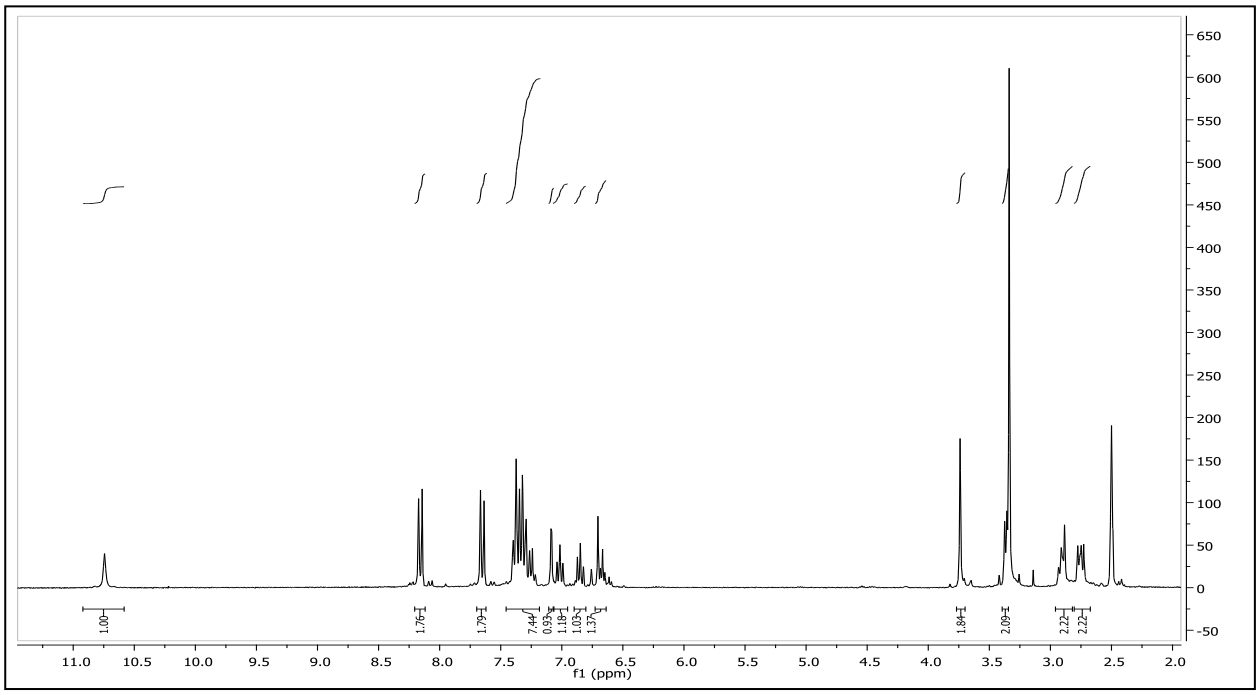

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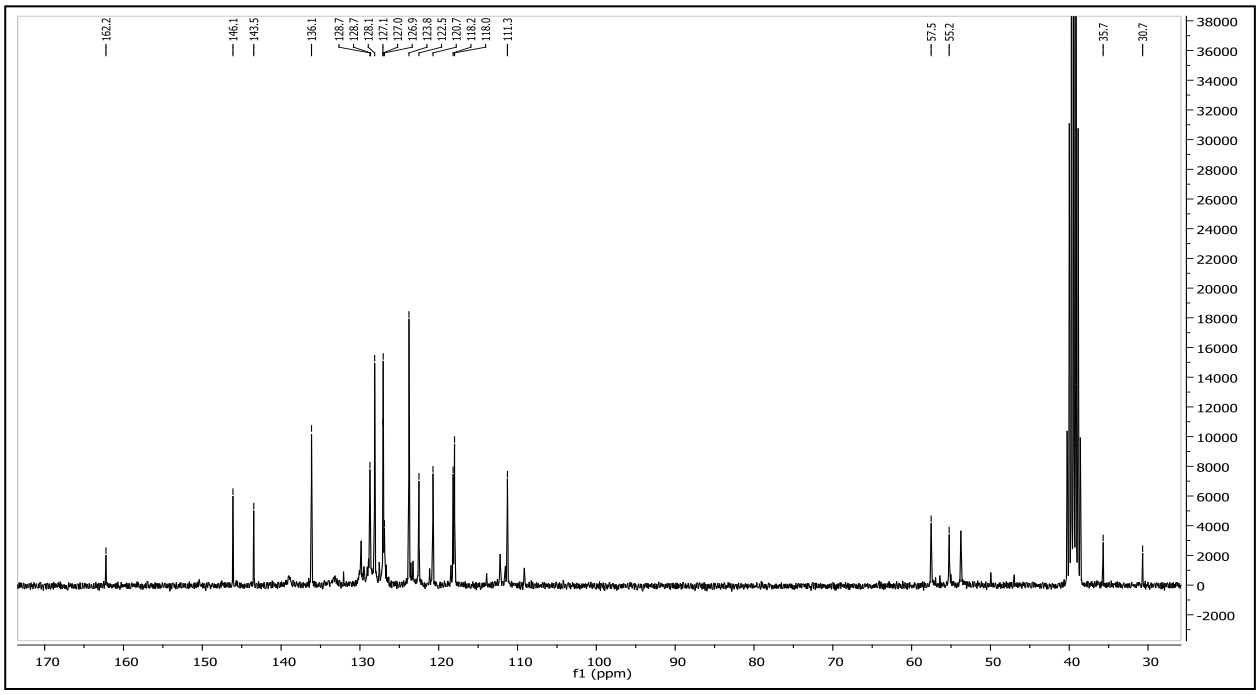

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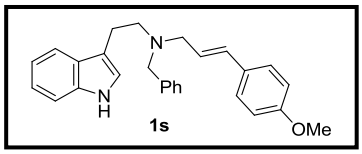
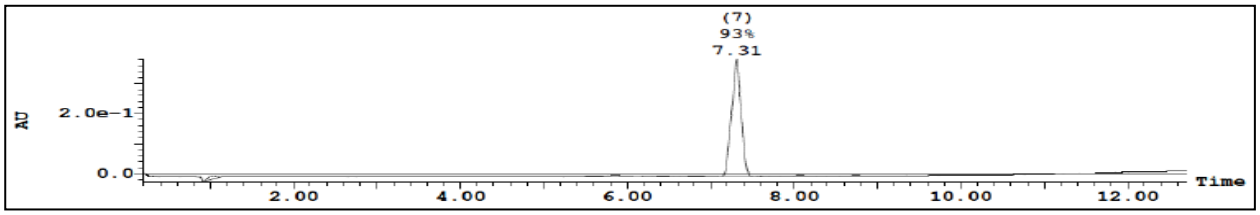
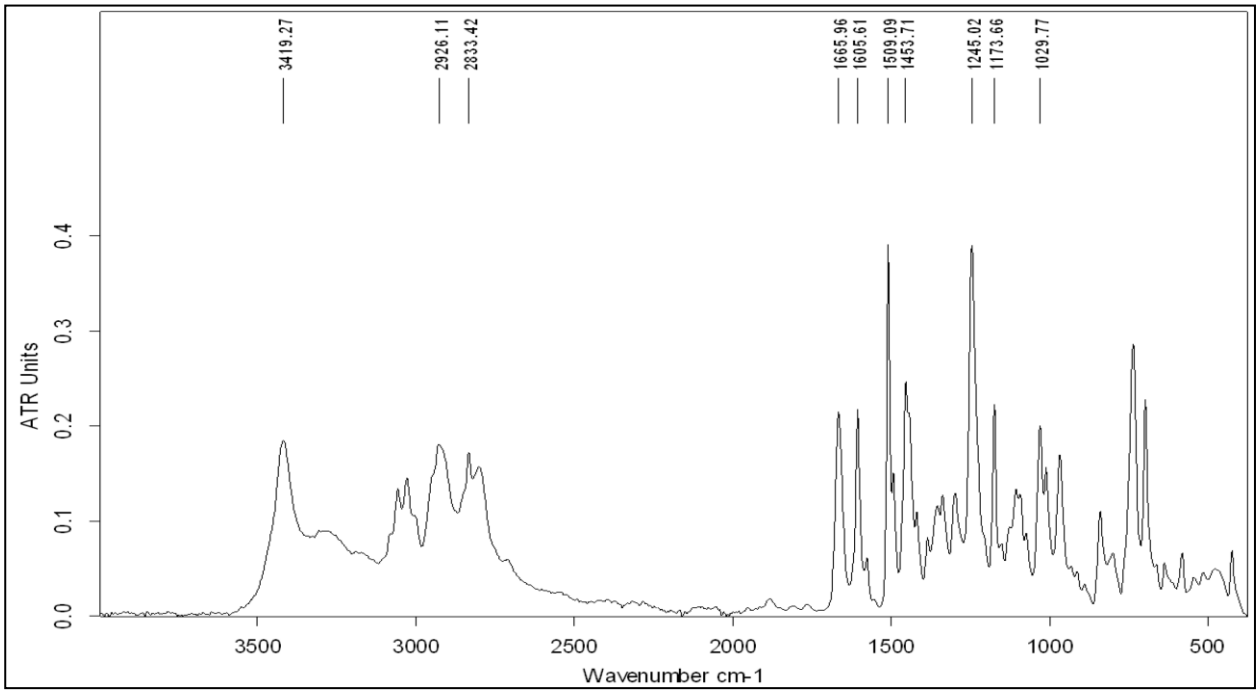


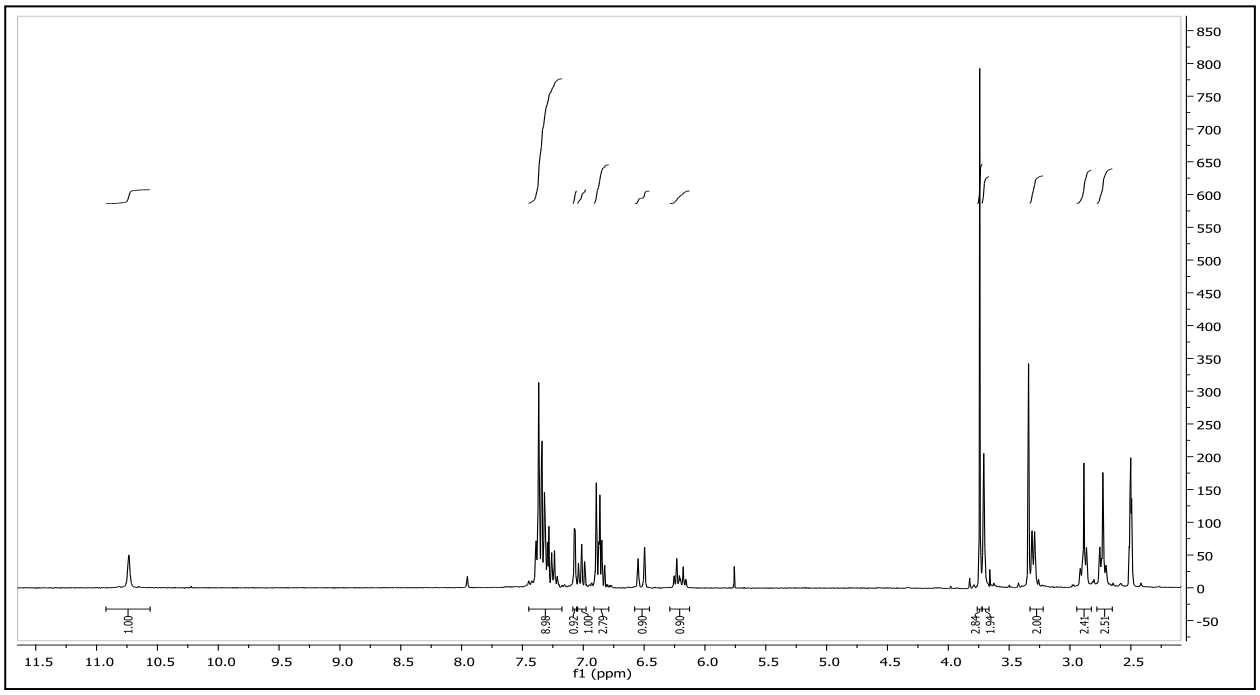
RP-HPLC of _N_-benzyl-_N_-3-(4-methoxyphenyl)prop-2-en-1-tryptamine (1s)



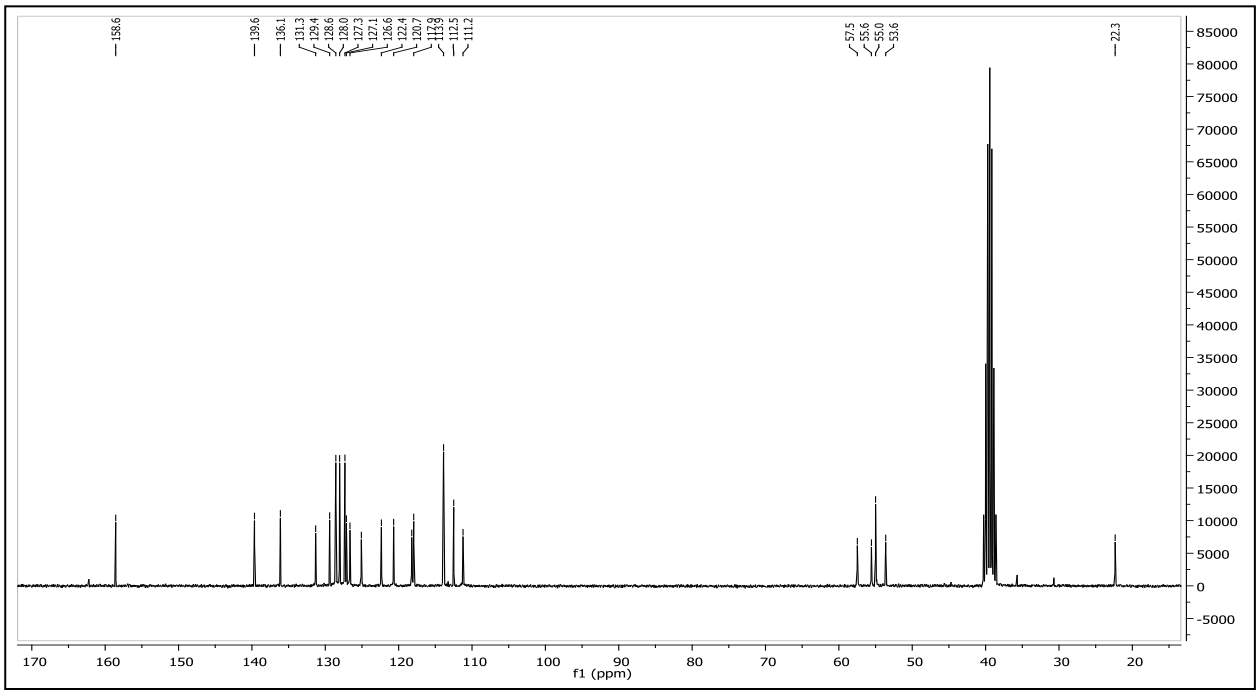
IR of _N_-benzyl-_N_-3-(4-methoxyphenyl)prop-2-en-1-tryptamine (1s)



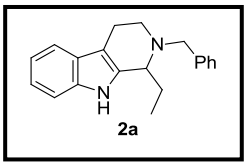
^{1}H NMR of *N*-benzyl-*N*-3-(4-methoxyphenyl)prop-2-en-1-tryptamine (1s)



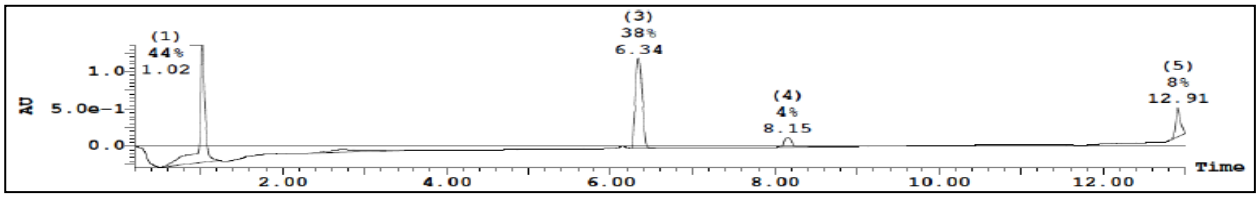
^{13}C NMR of *N*-benzyl-*N*-3-(4-methoxyphenyl)prop-2-en-1-tryptamine (1s)



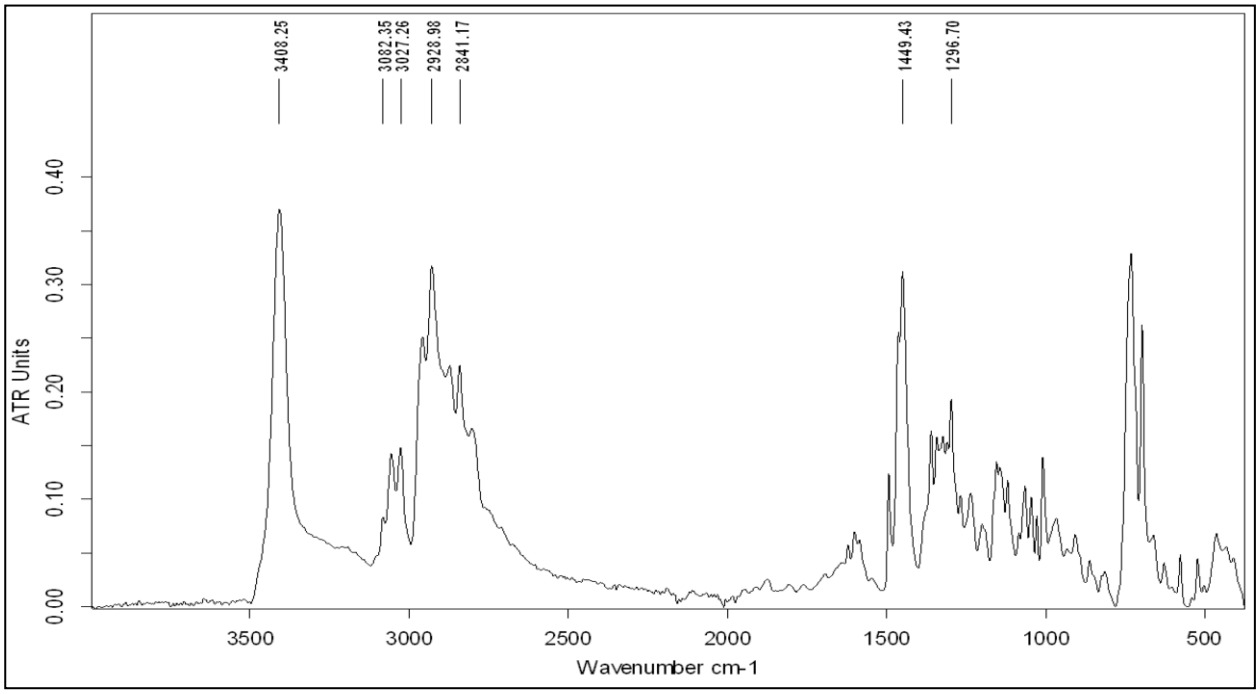
THBC 2a



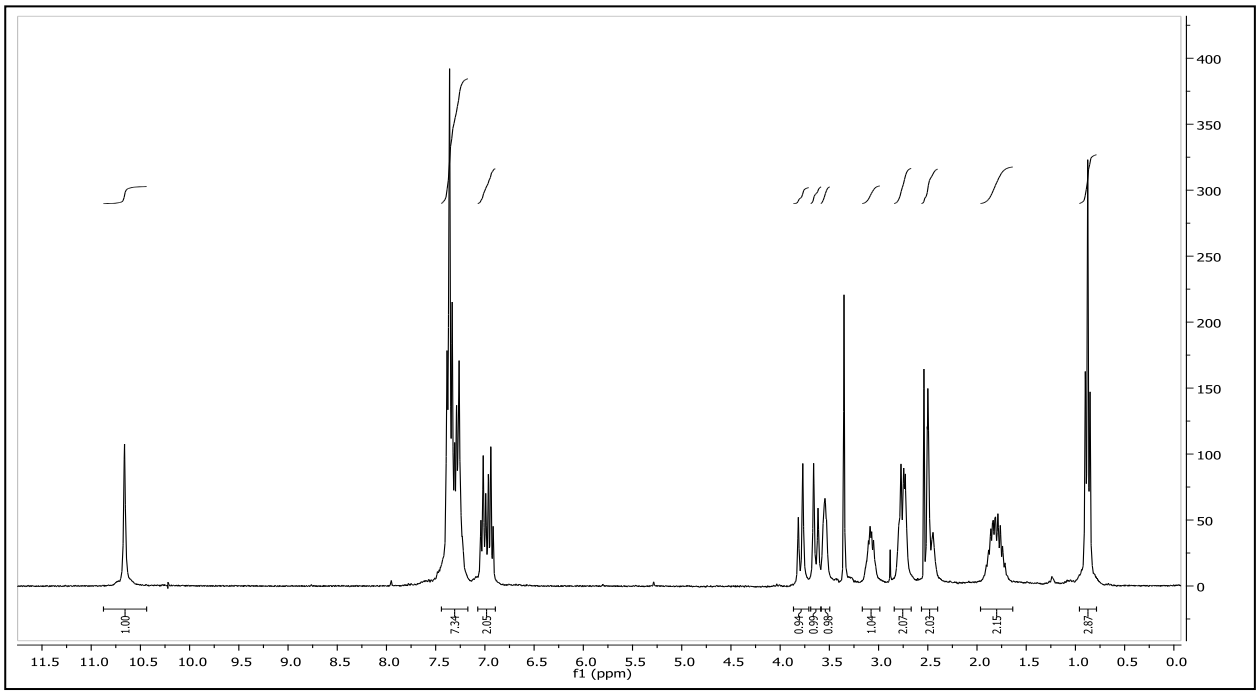
RP-HPLC of THBC 2a



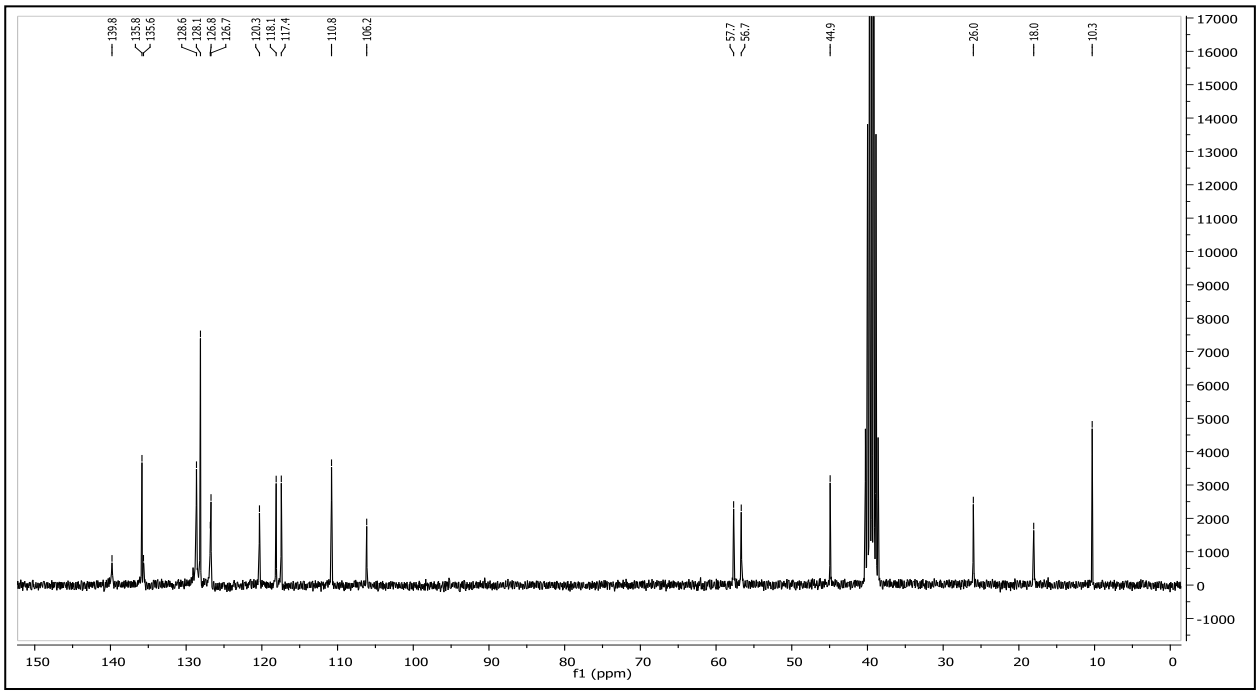
IR of THBC 2a



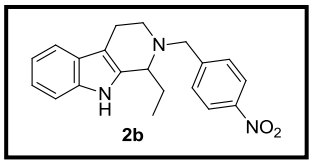
^{1}H NMR of THBC 2a



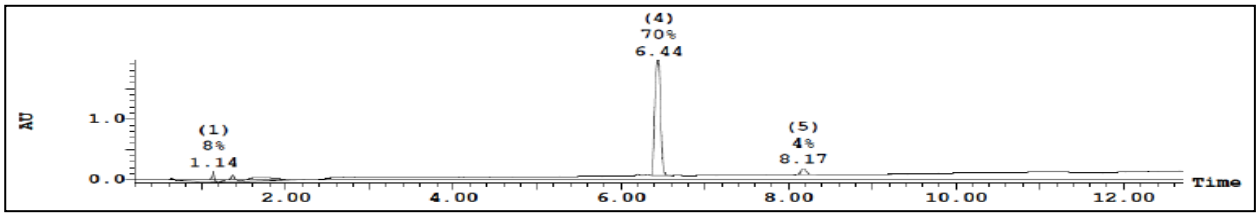
^{13}C NMR of THBC 2a



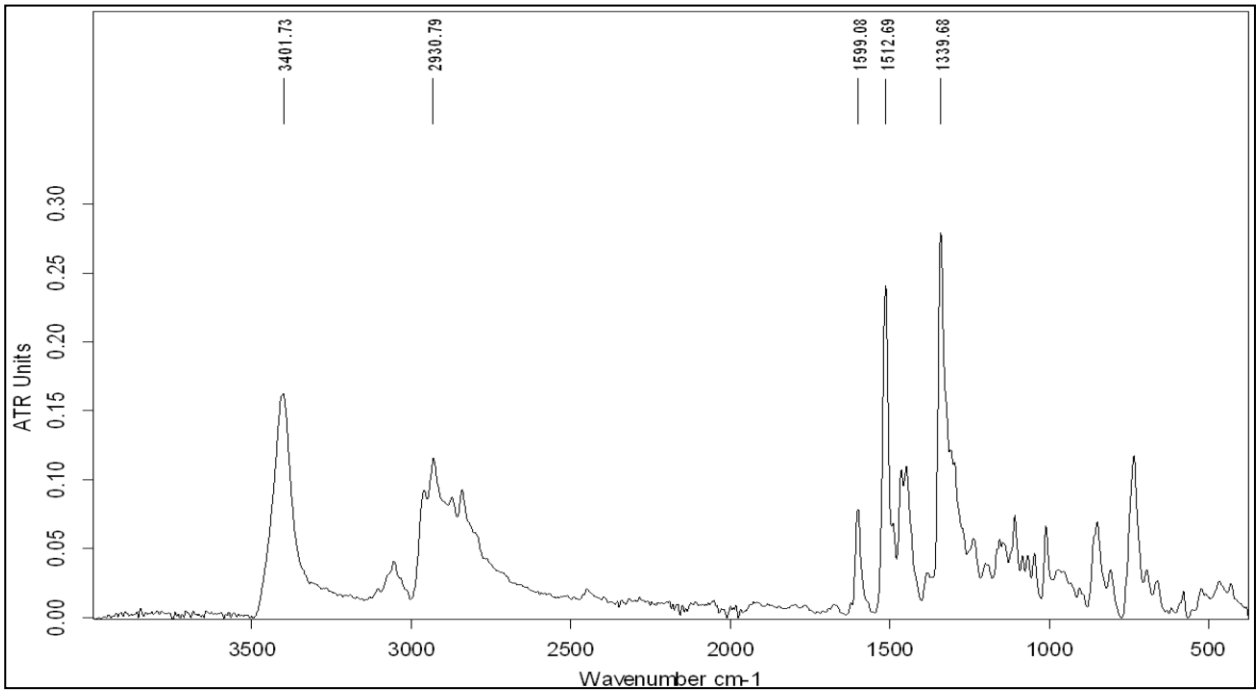
THBC 2b



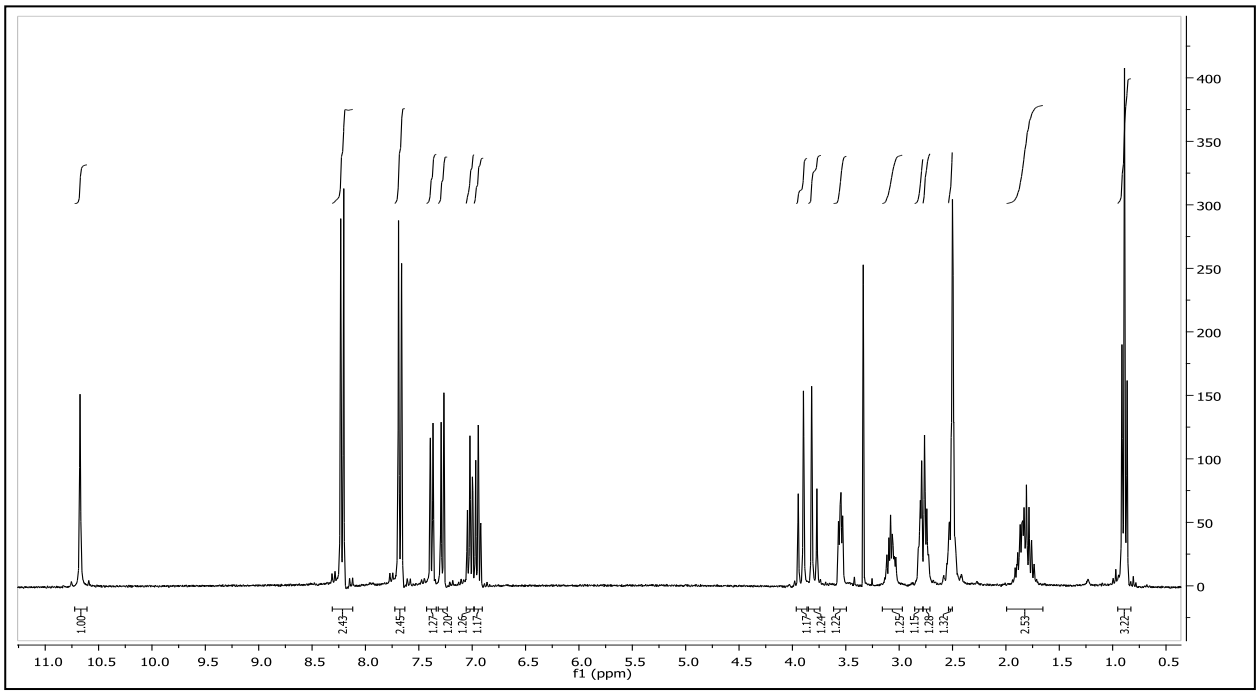
RP-HPLC of 2b



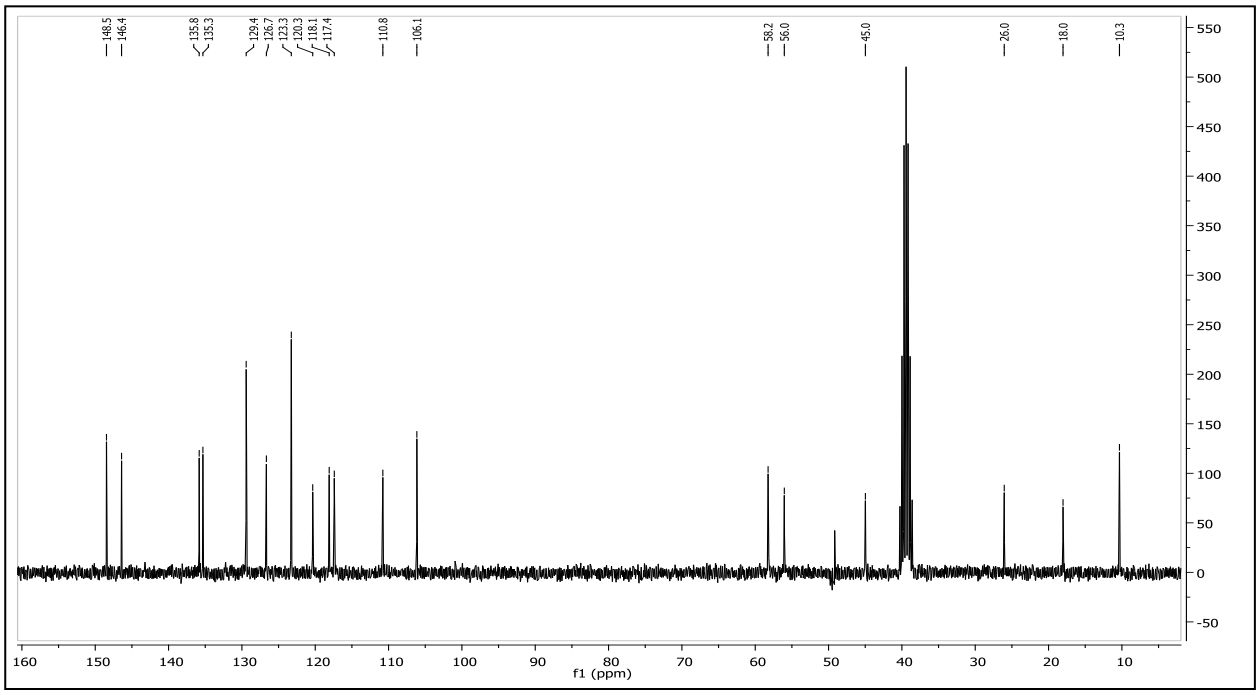
IR of 2b



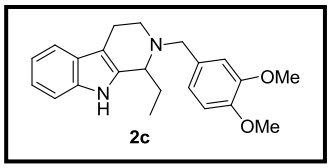
^{1}H NMR of 2b



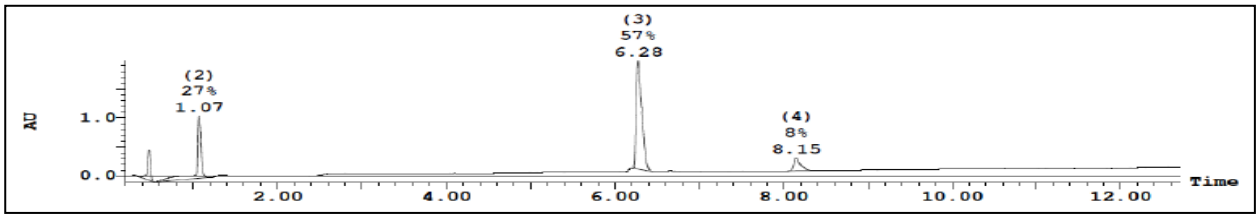
^{13}C NMR of 2b



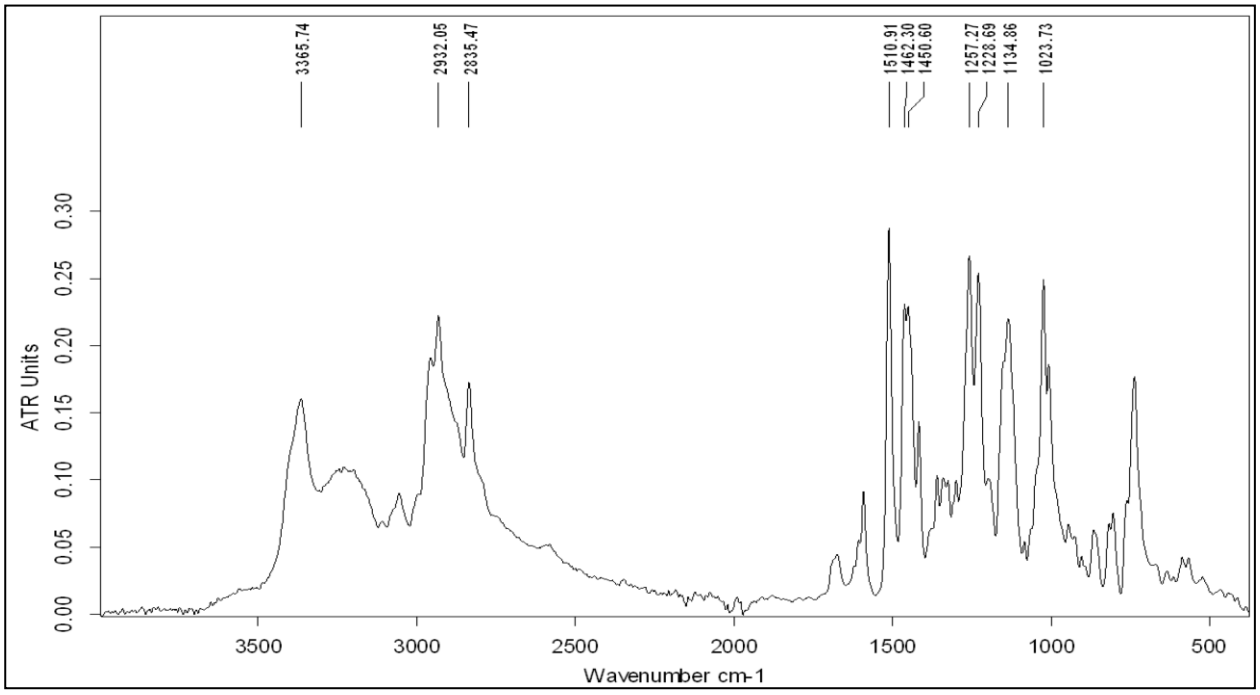
THBC 2c



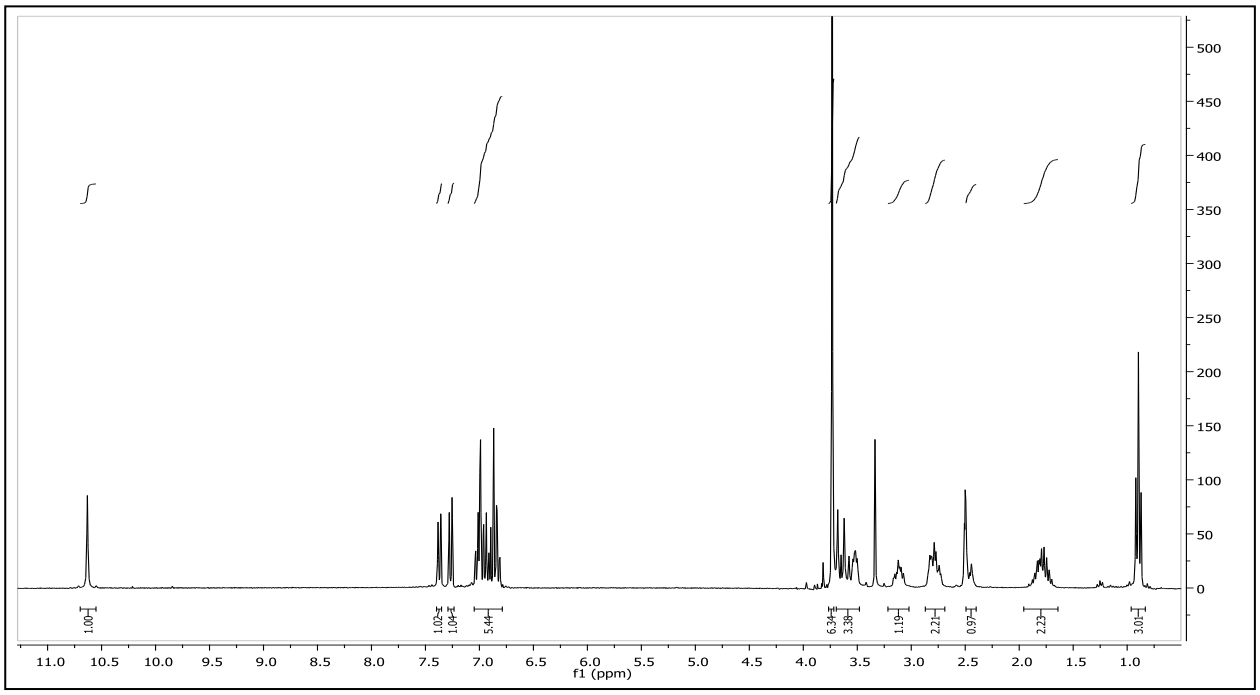
RP-HPLC of 2c



IR of 2c



^{1}H NMR of 2c



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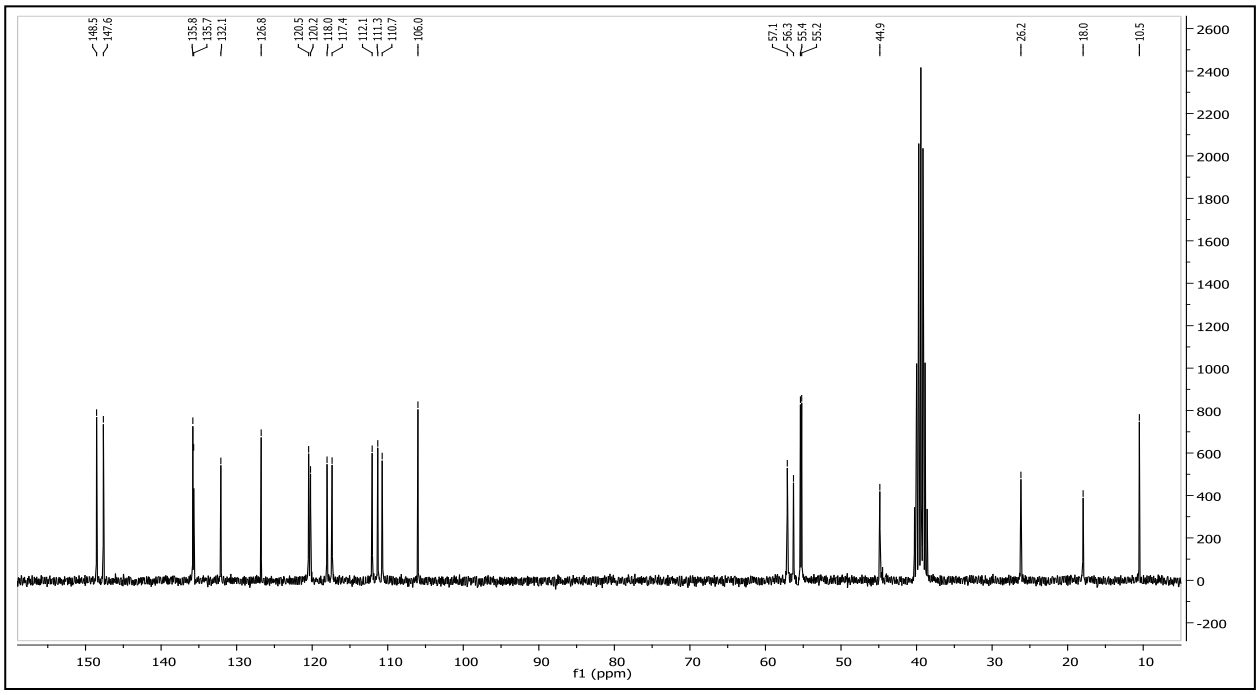
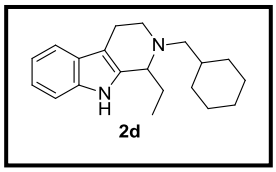
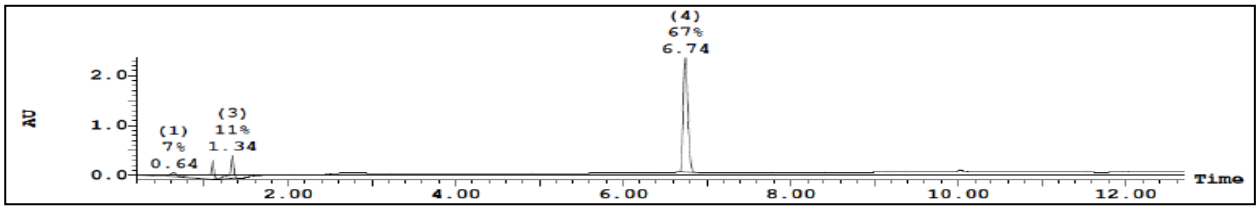


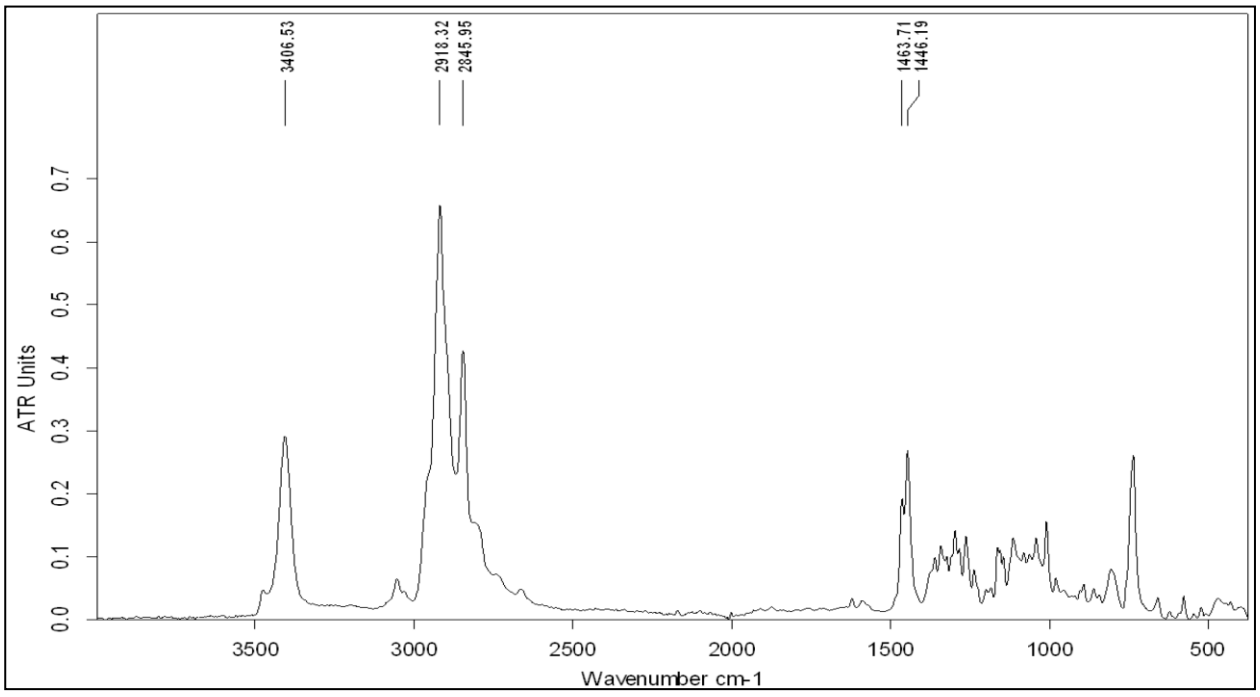
THBC 2d



RP-HPLC of 2d



IR of 2d



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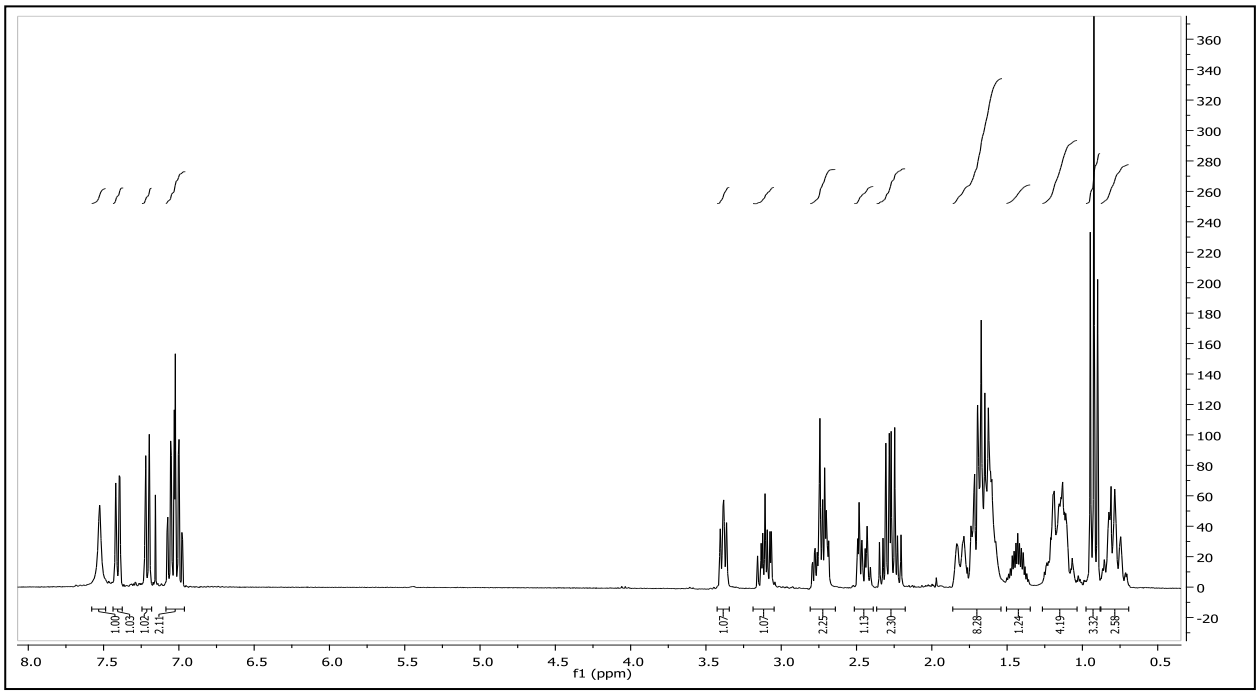

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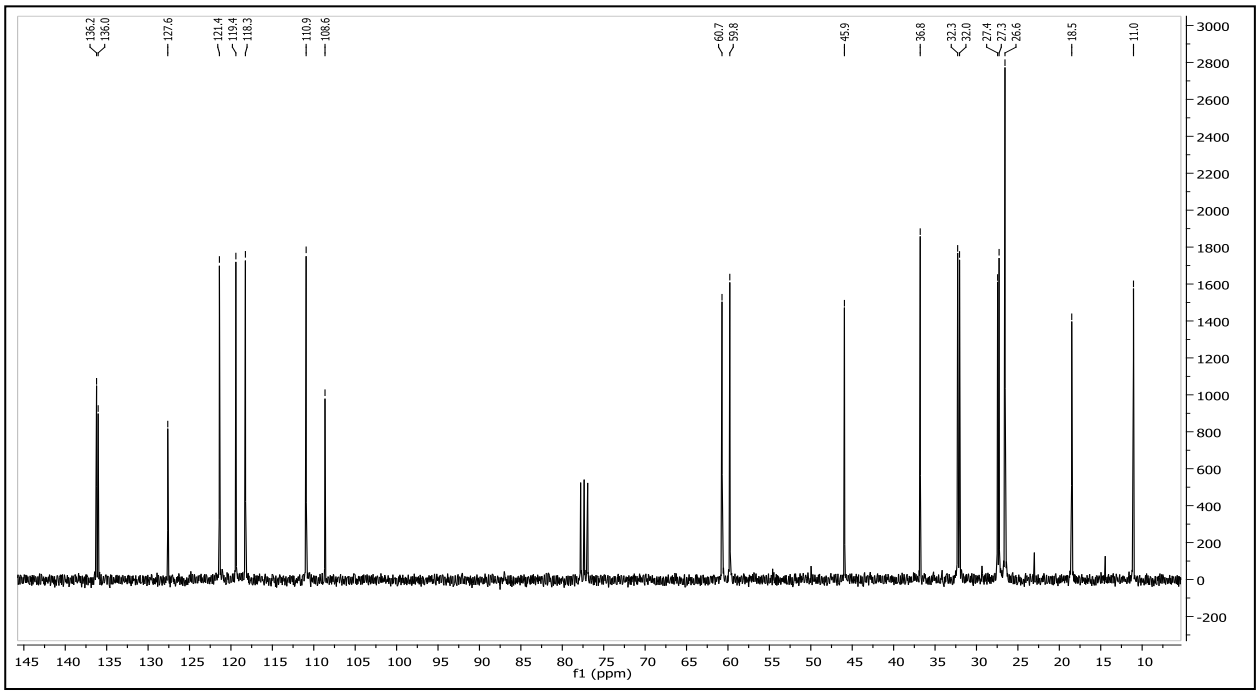
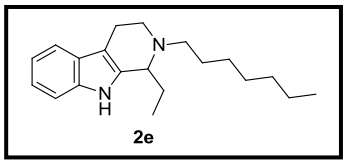
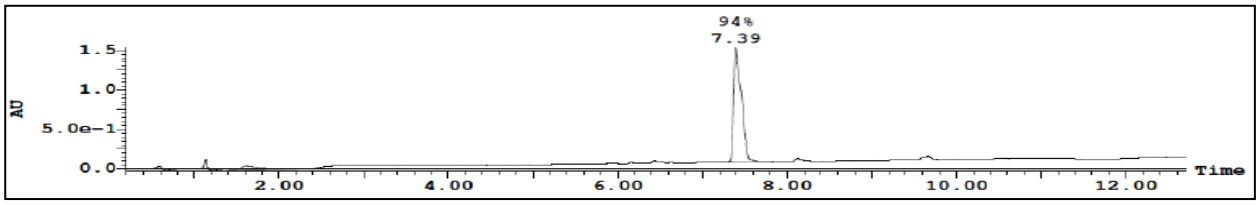


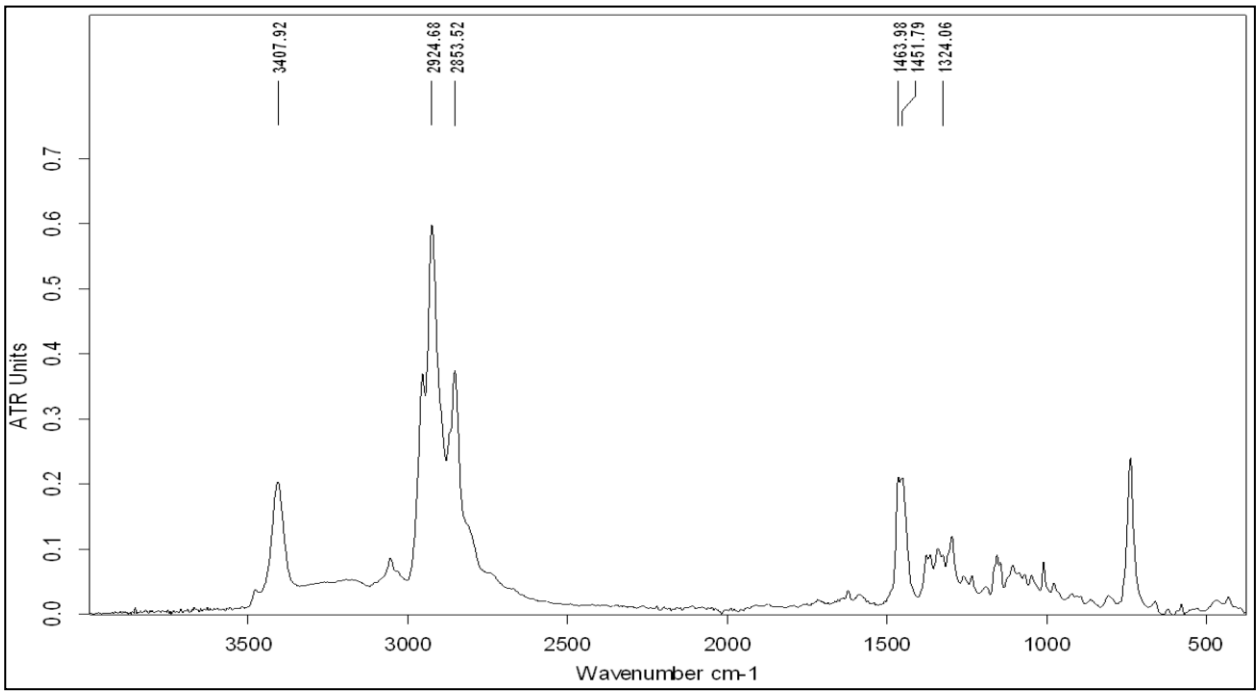
THBC 2e



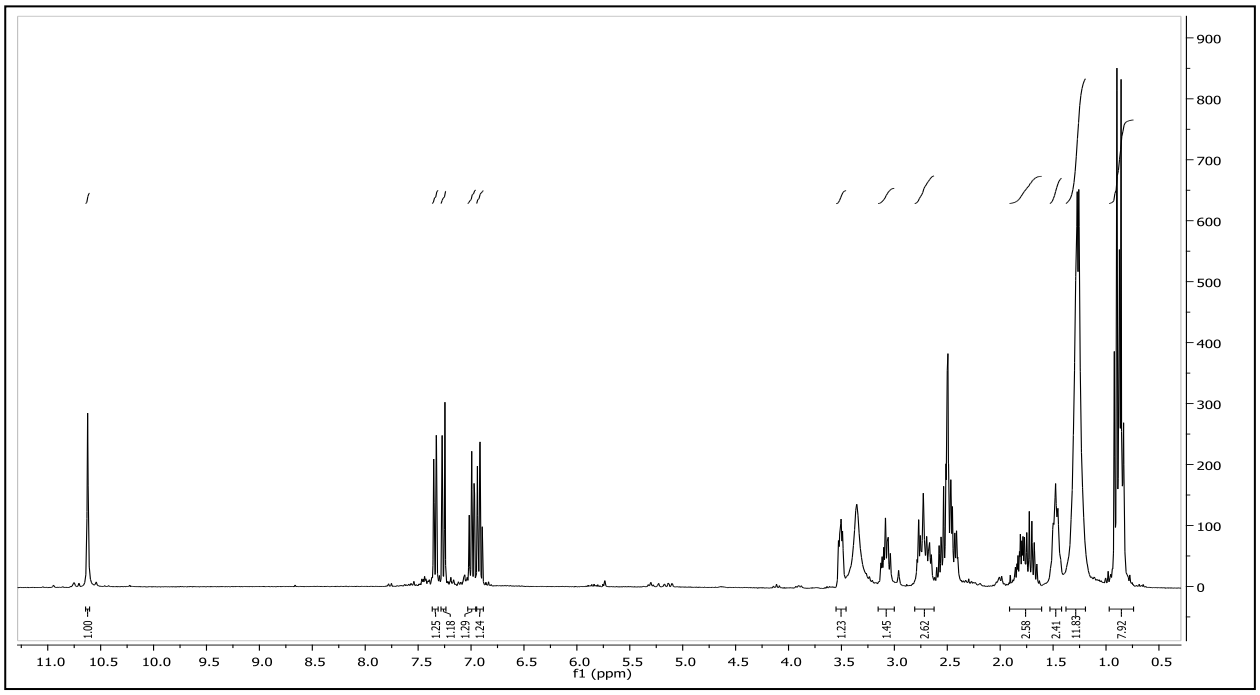
RP-HPLC of 2e



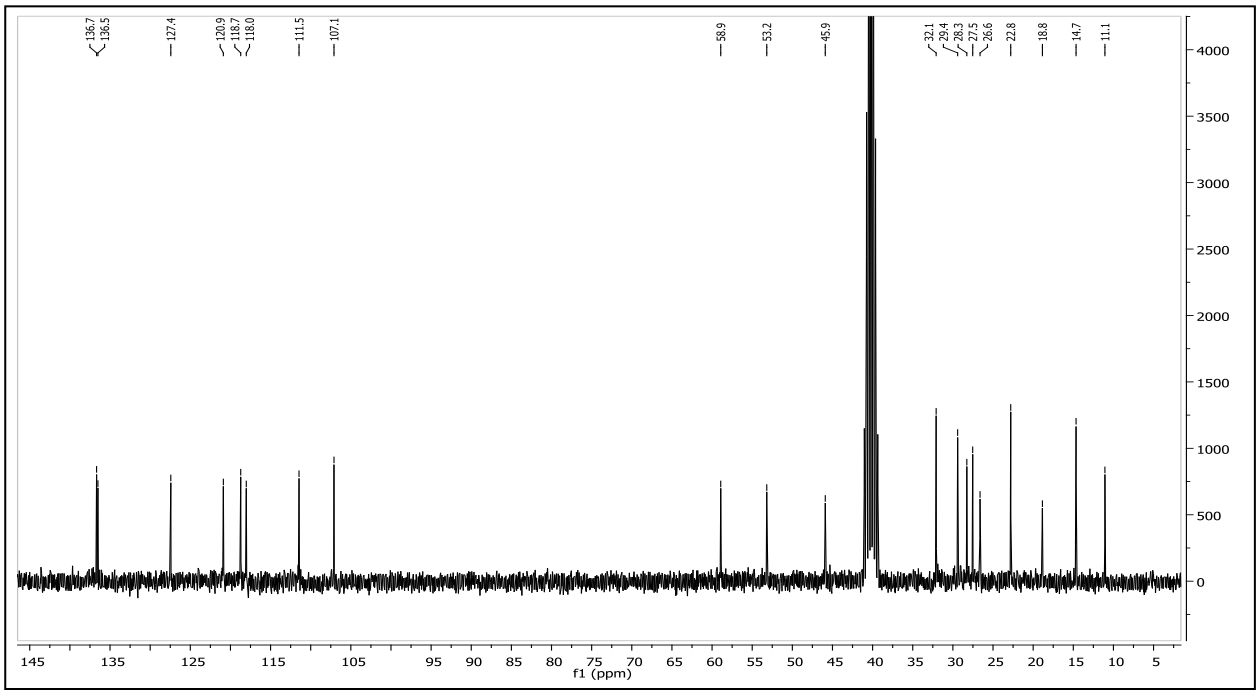
IR of 2e



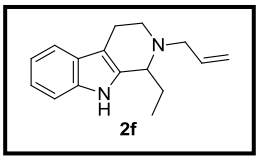
^{1}H NMR of 2e



^{13}C NMR of 2e



THBC 2f



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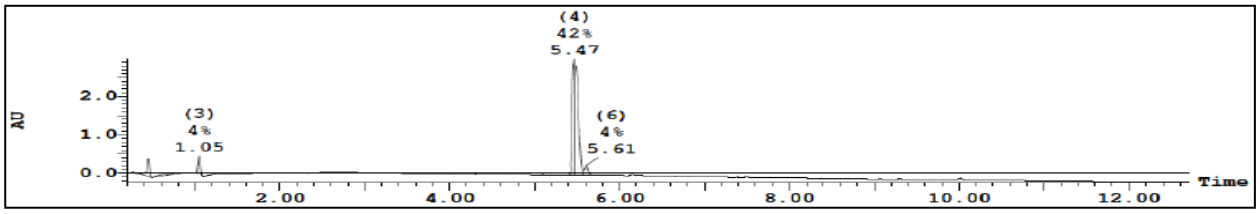

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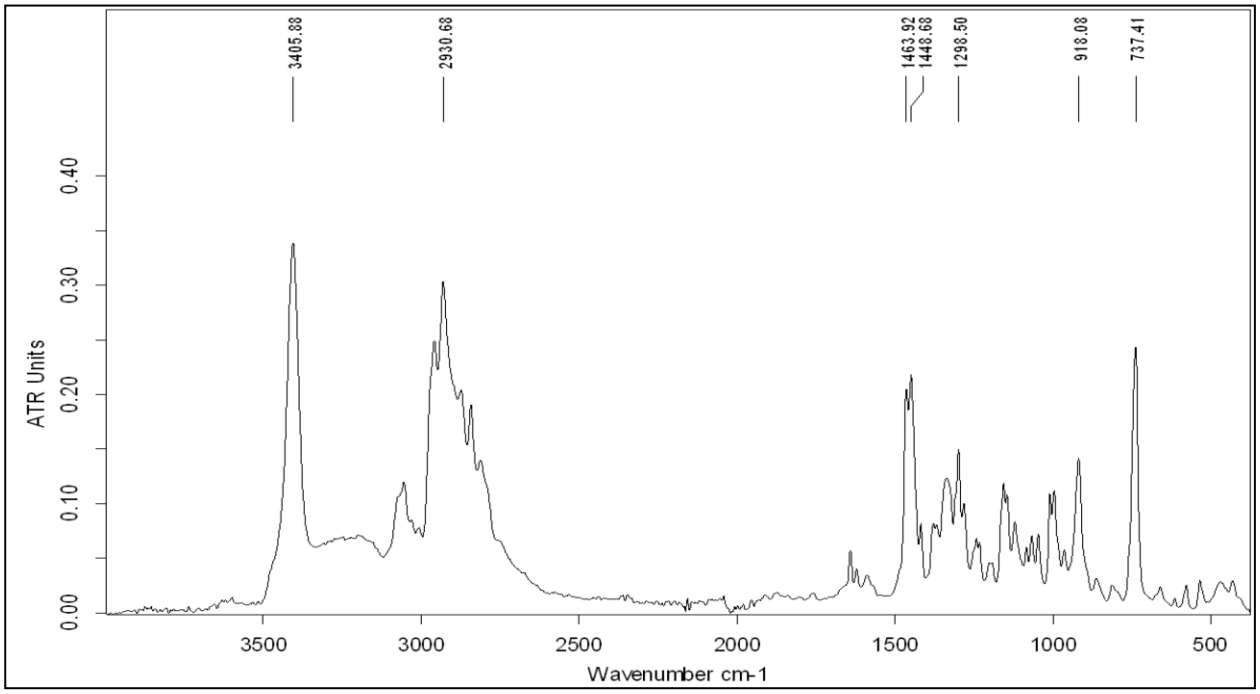

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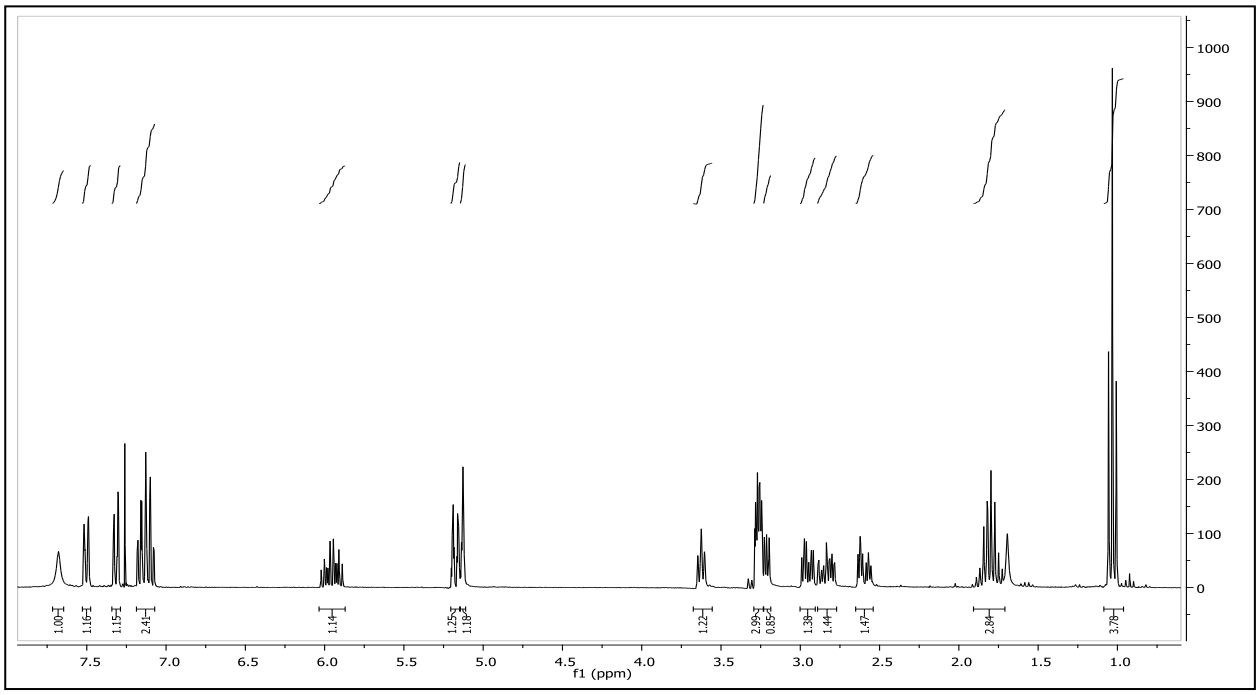

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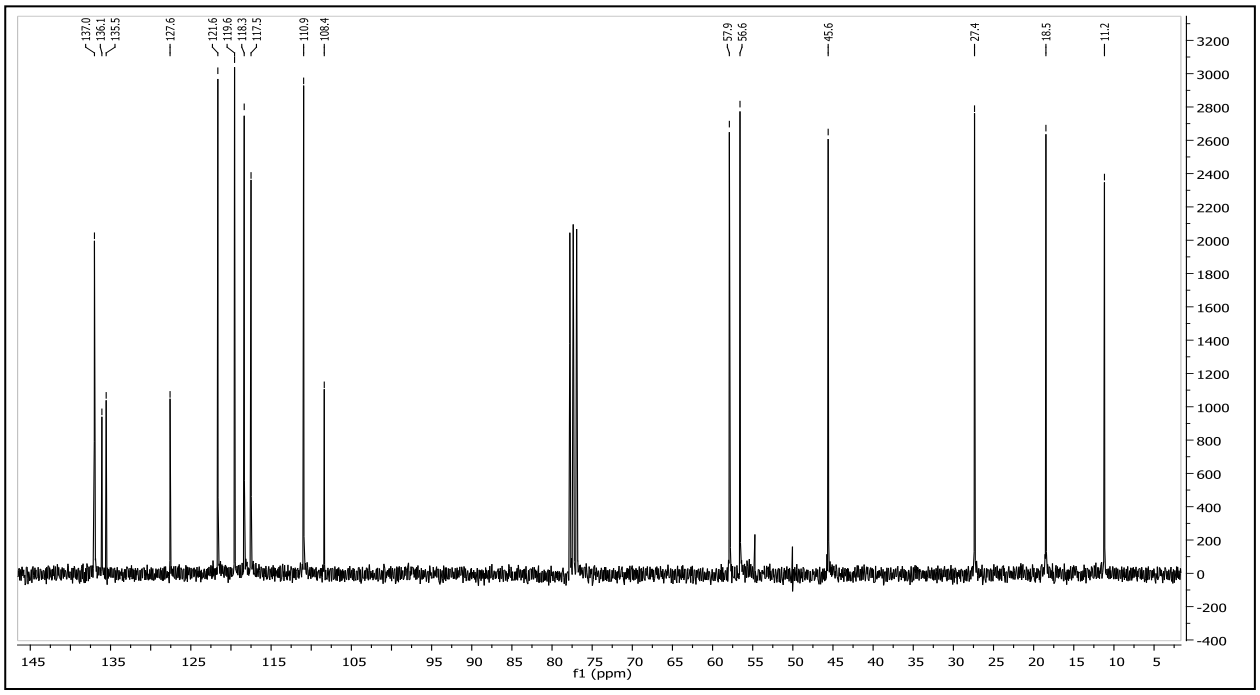
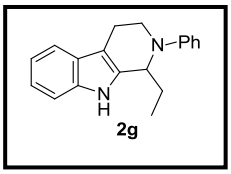


THBC 2g



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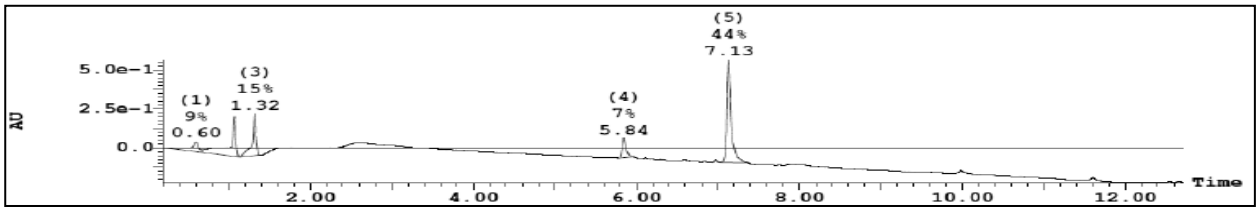
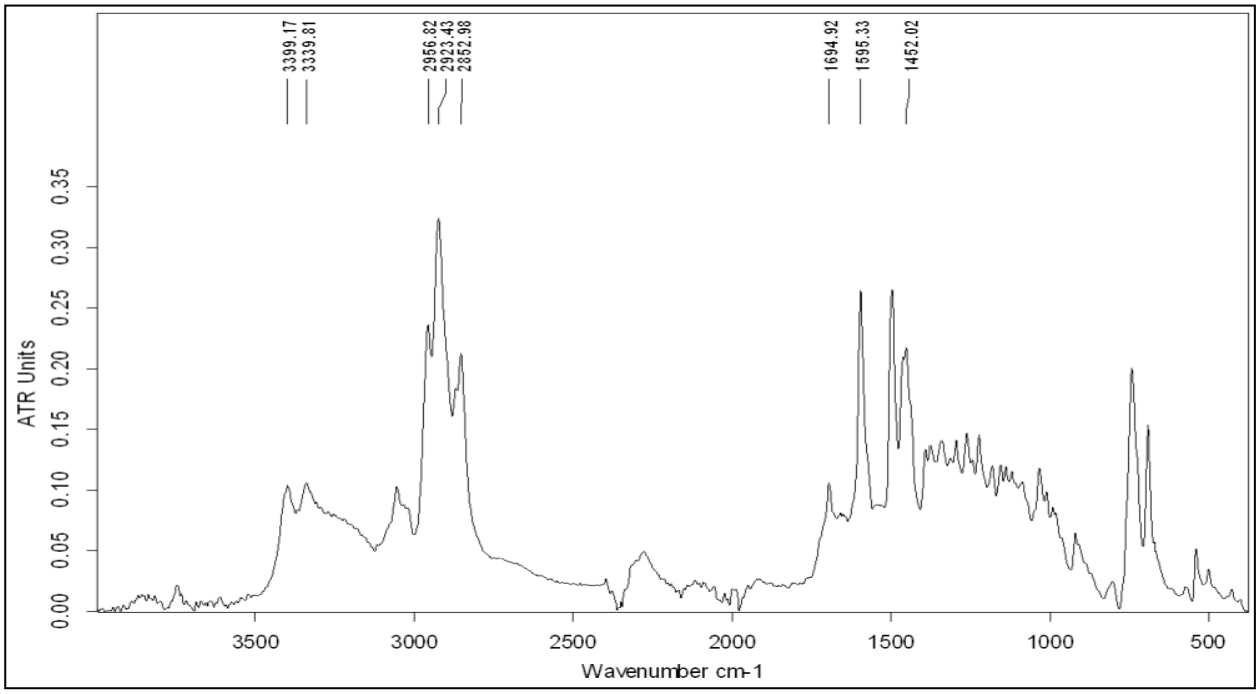


IR of 2g



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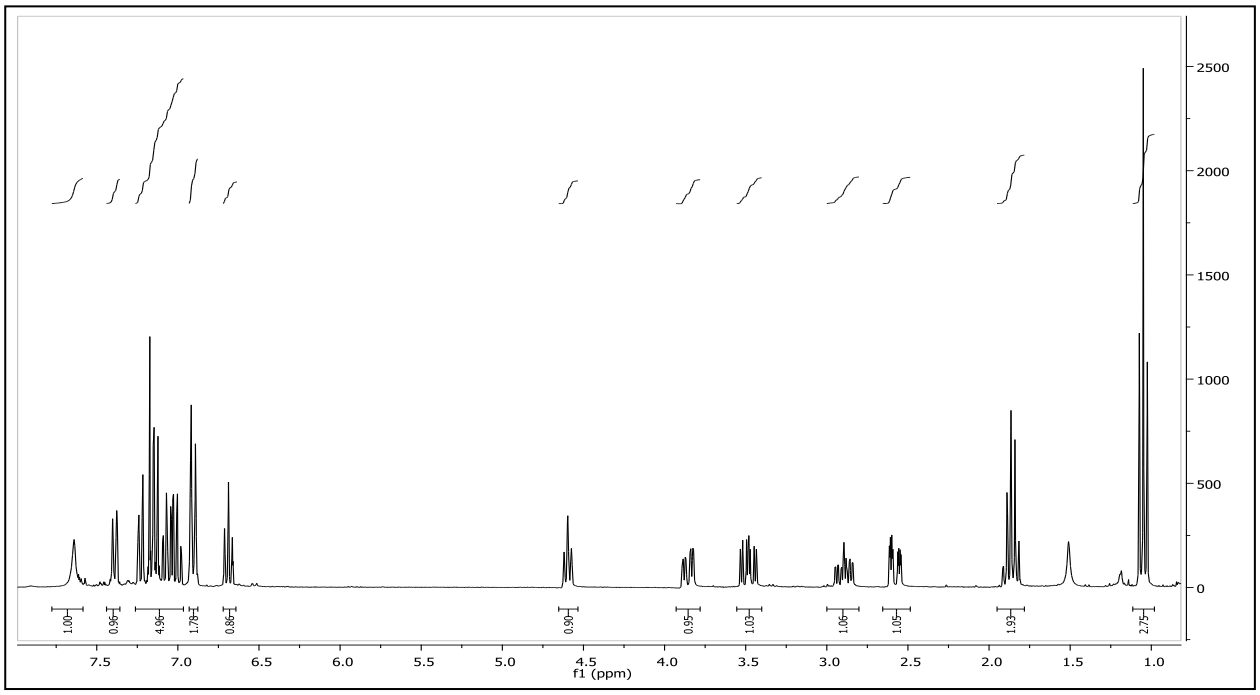

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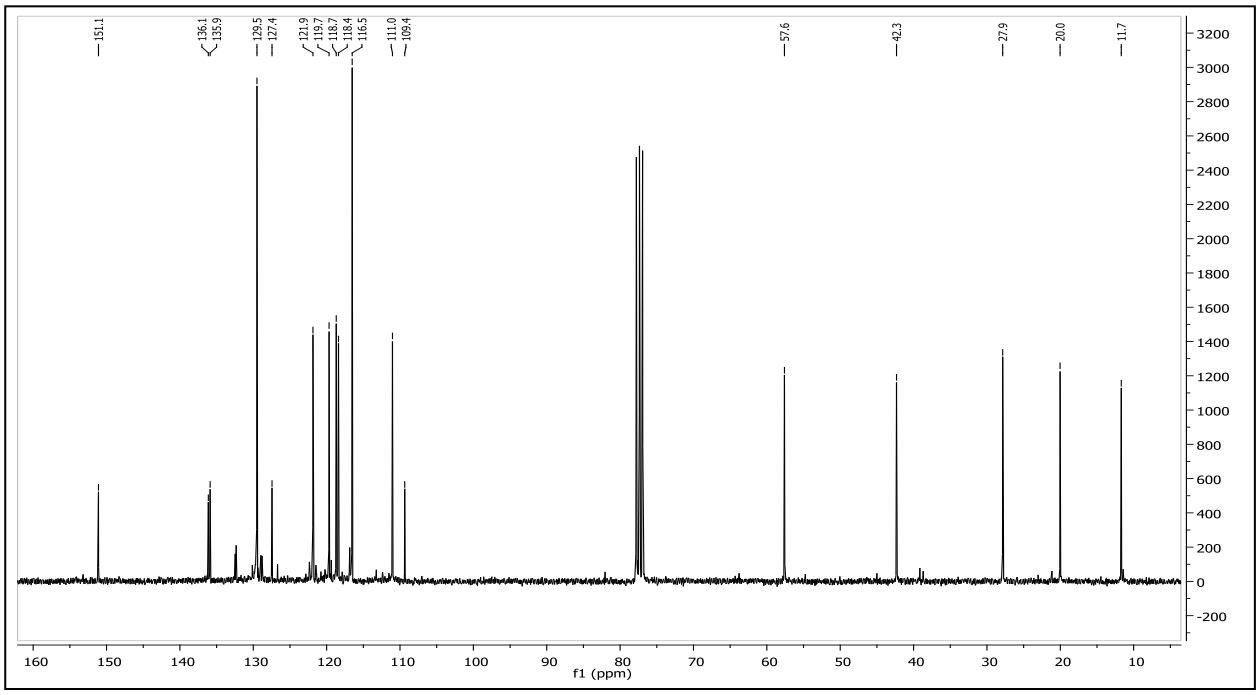
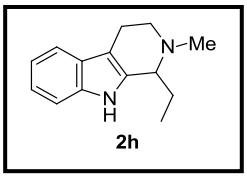
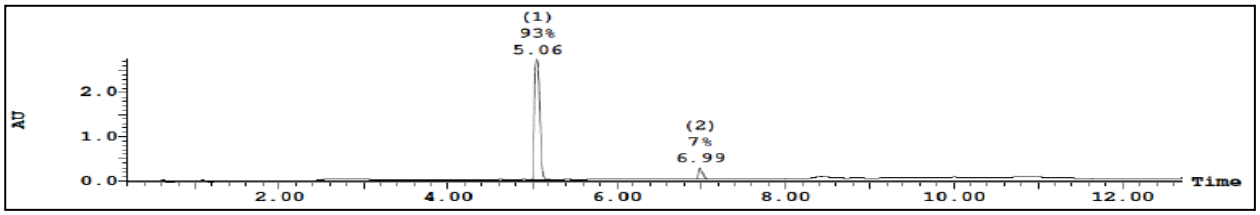


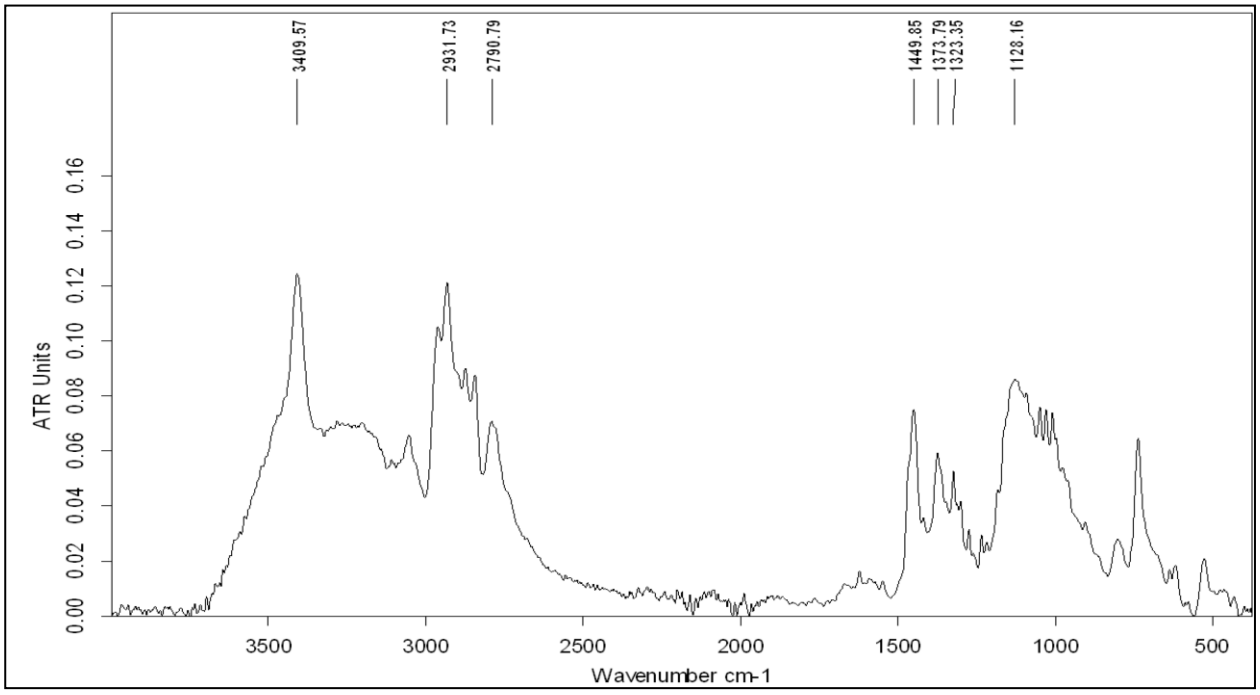
THBC 2h



RP-HPLC of 2h



IR of 2h



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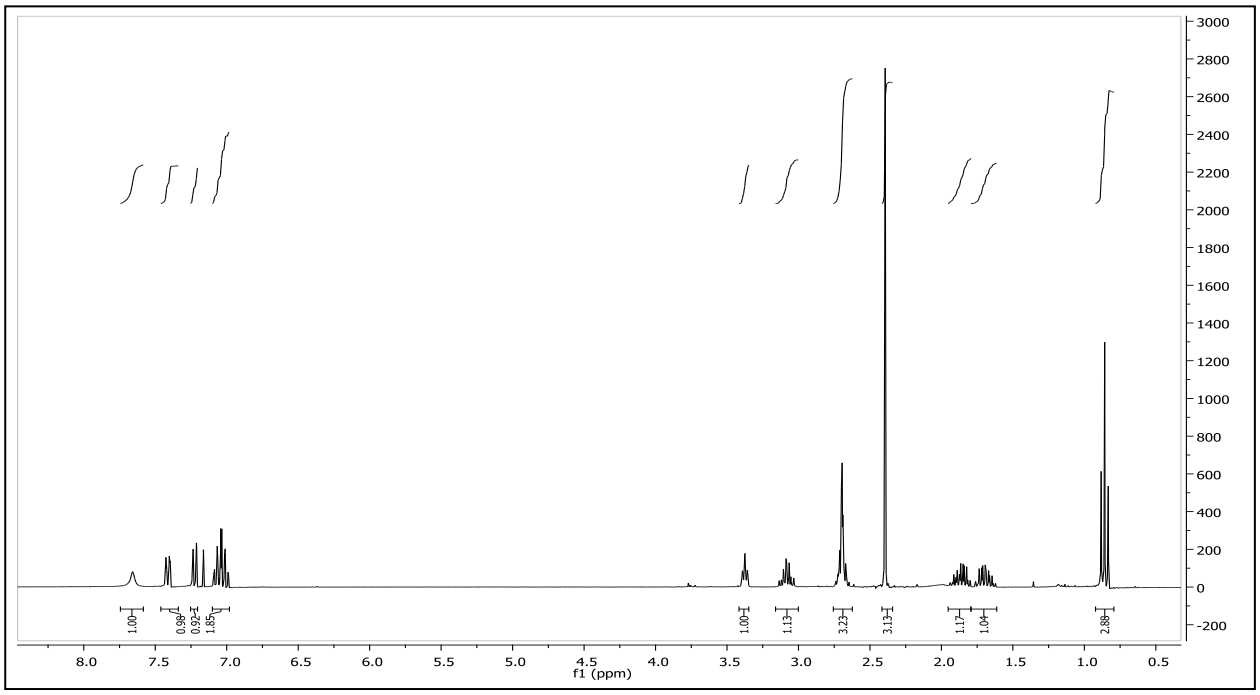

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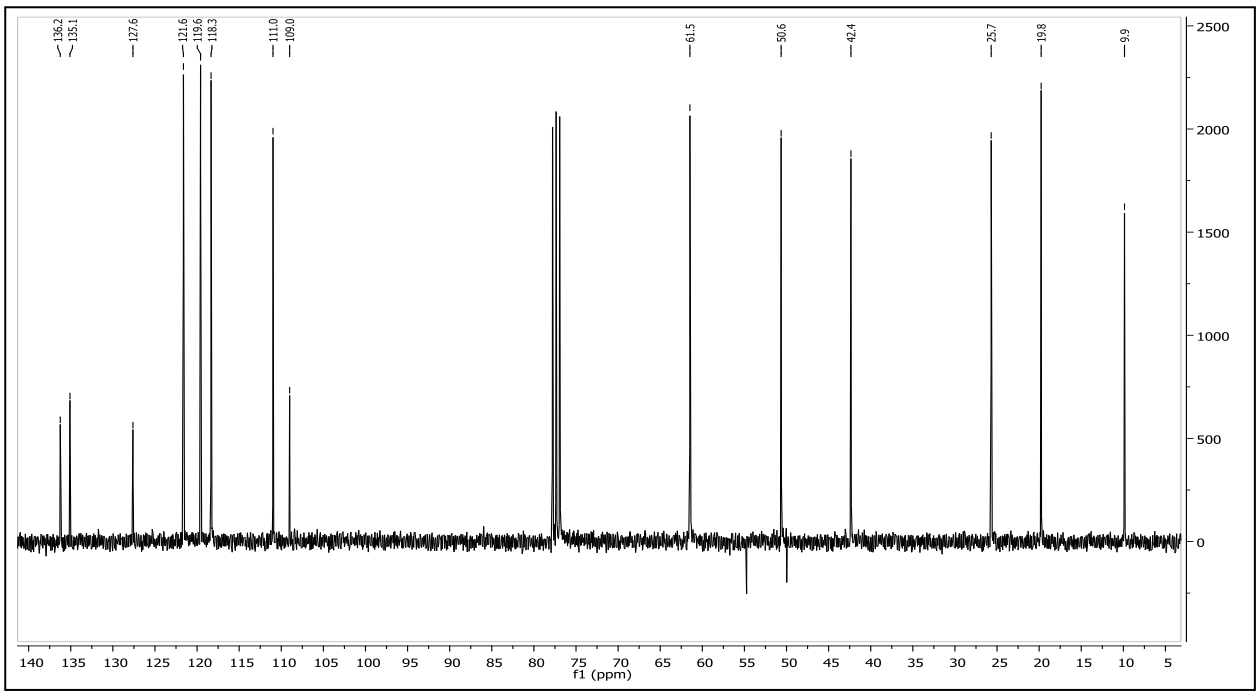
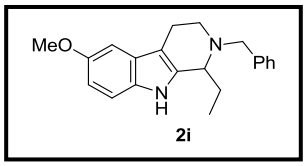
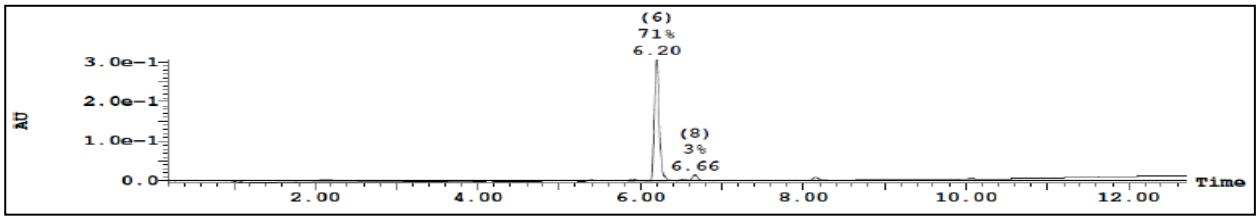


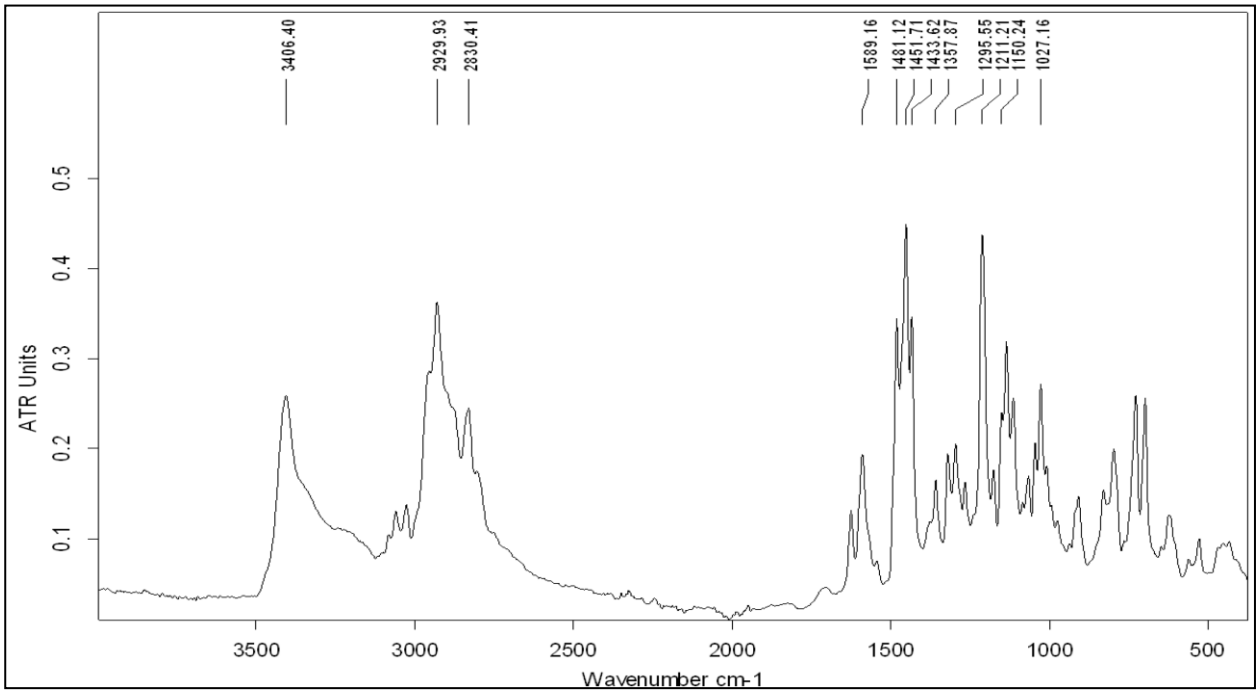
THBC 2i



RP-HPLC of 2i



IR of 2i



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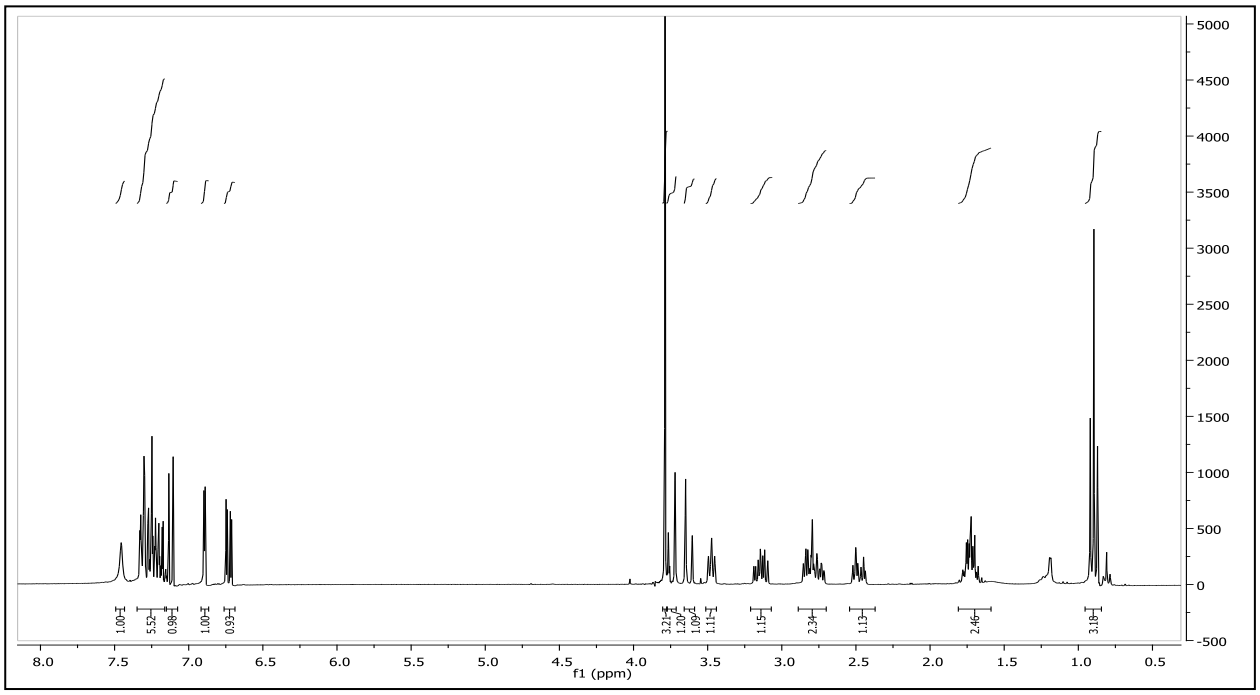

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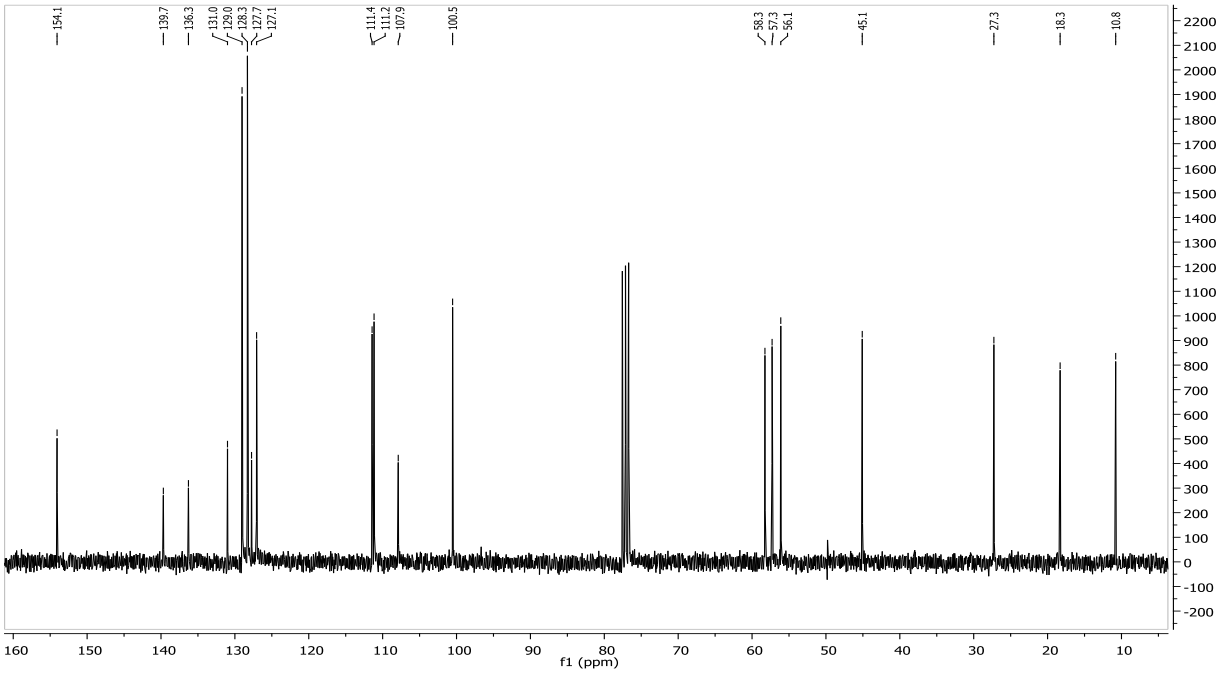

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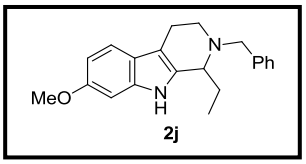
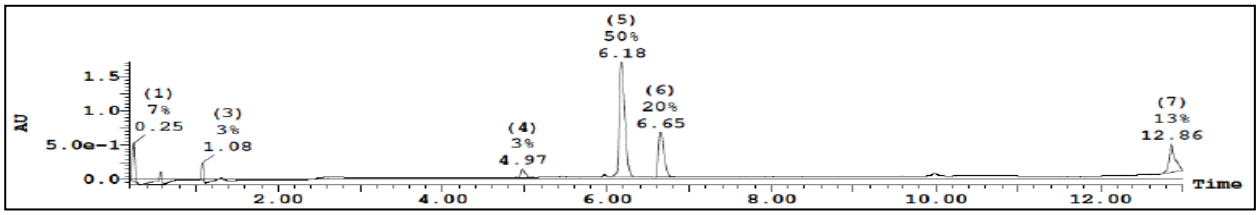
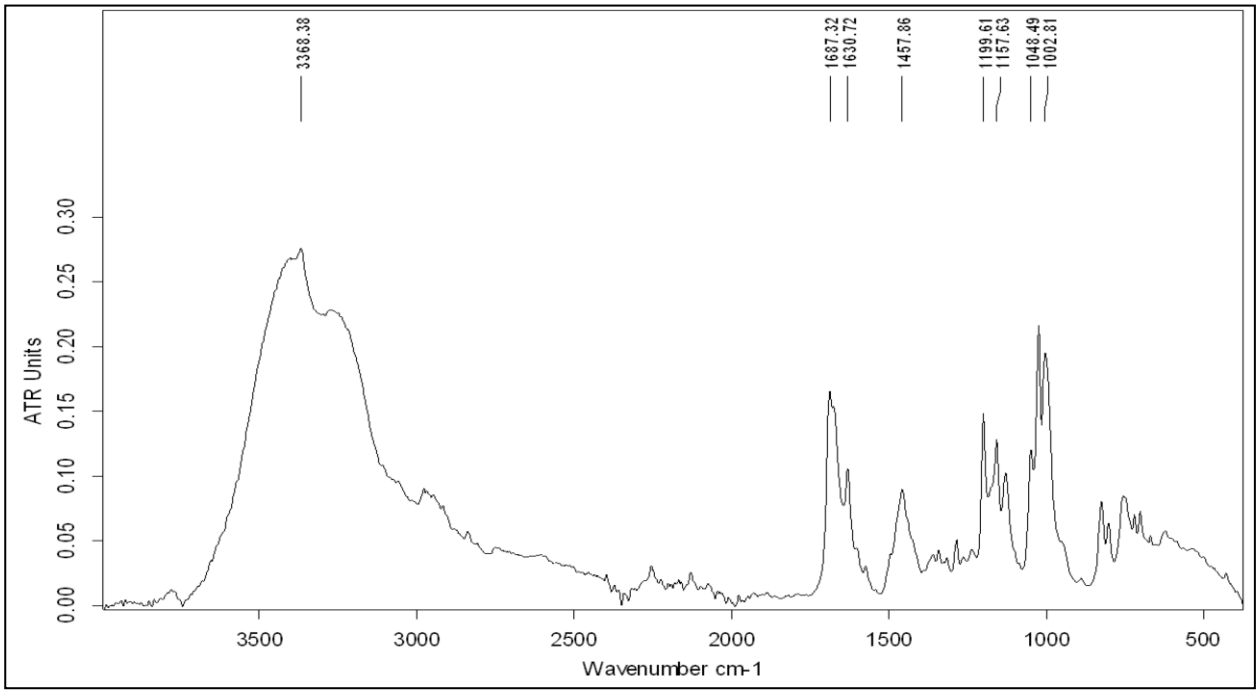


2j

RP-HPLC of 2j



IR of 2j



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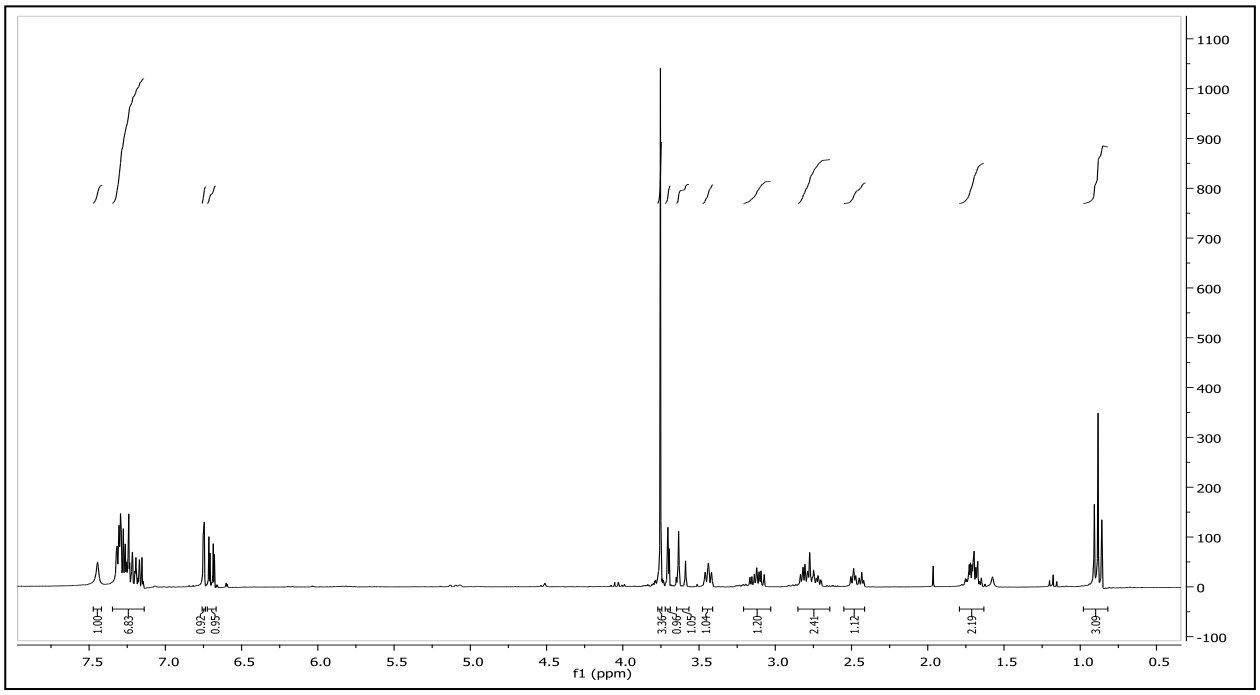

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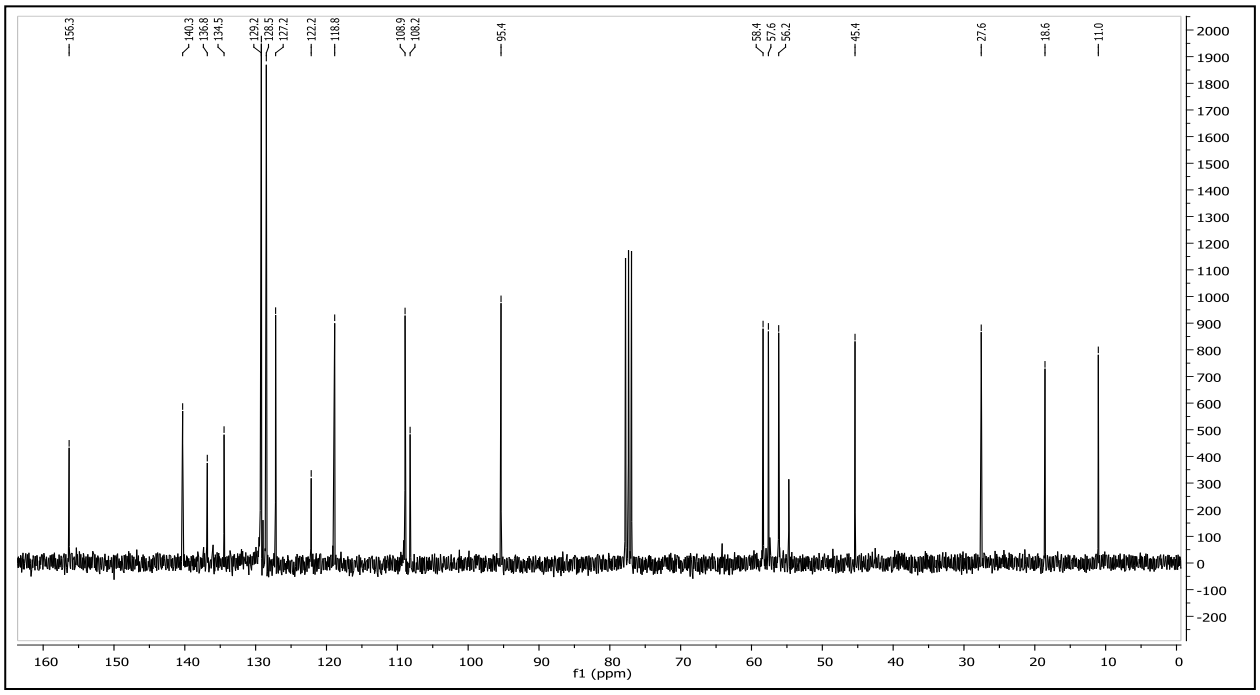
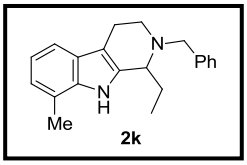


THBC of 2k



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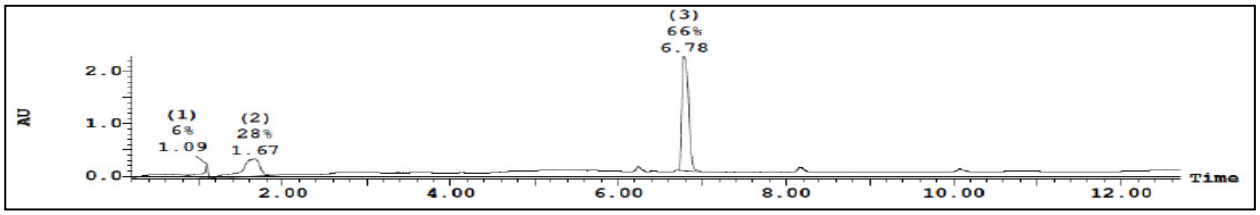

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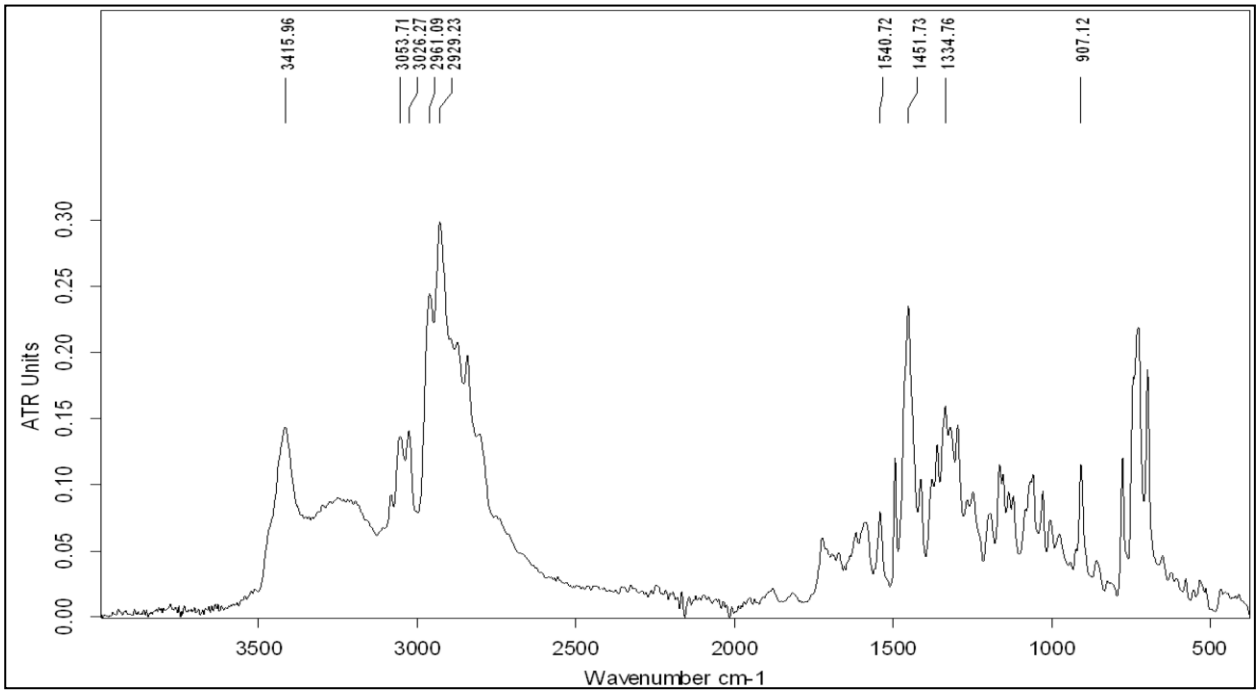

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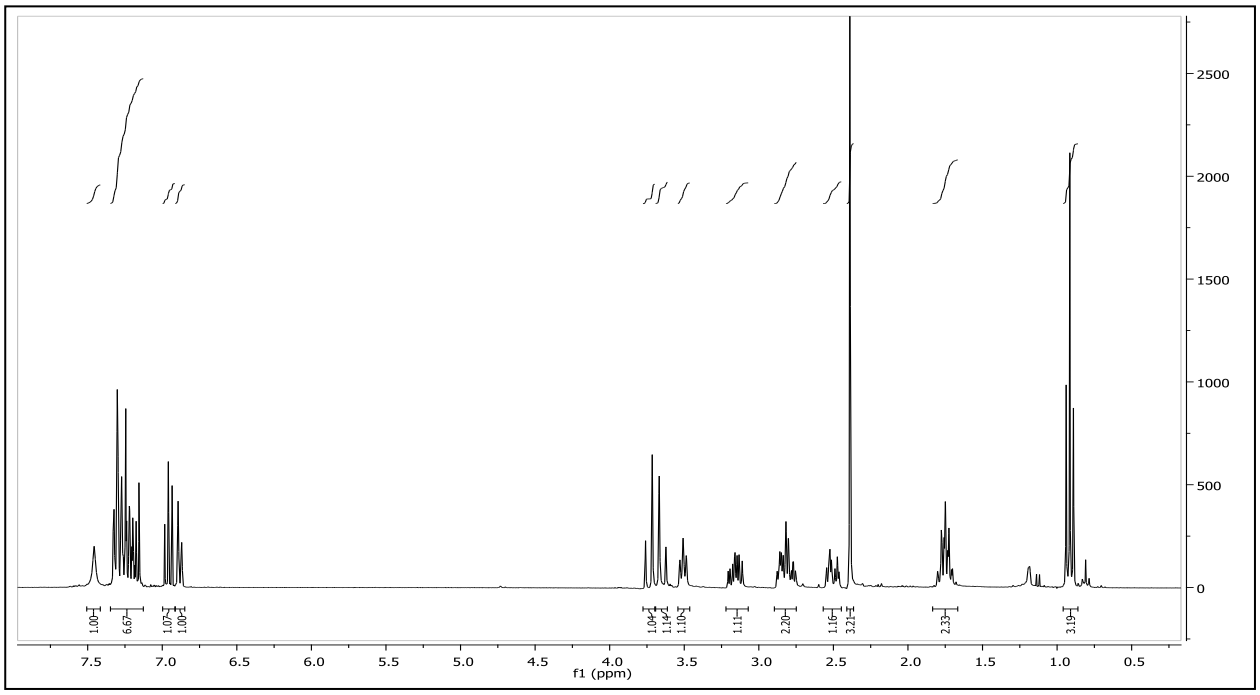

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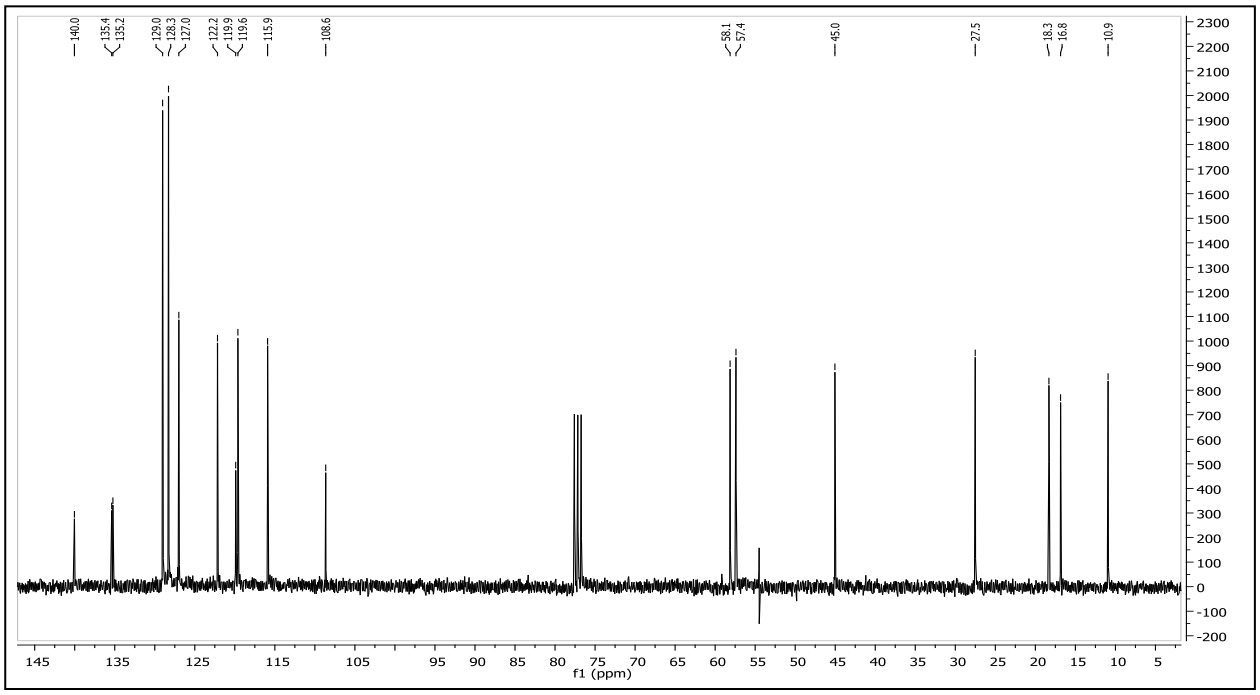
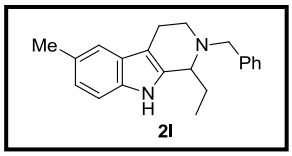


THBC 2l



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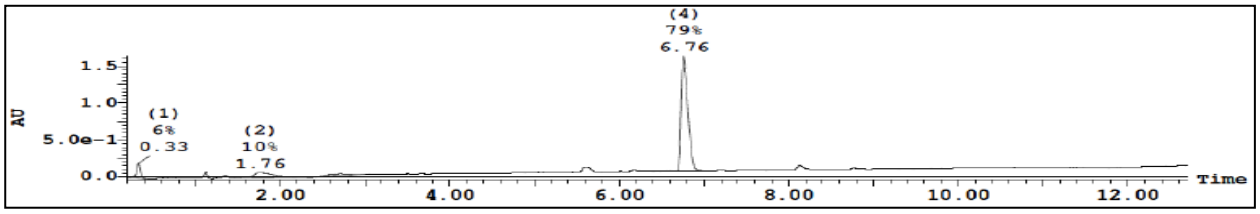
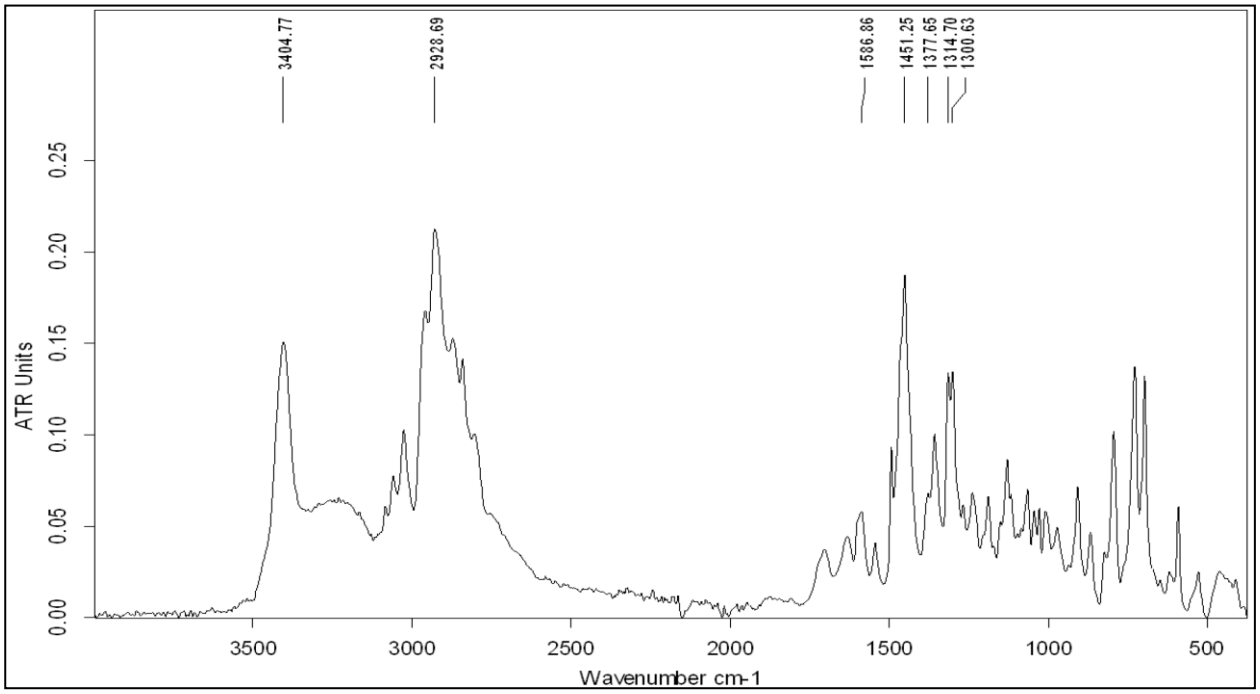


IR of 2l



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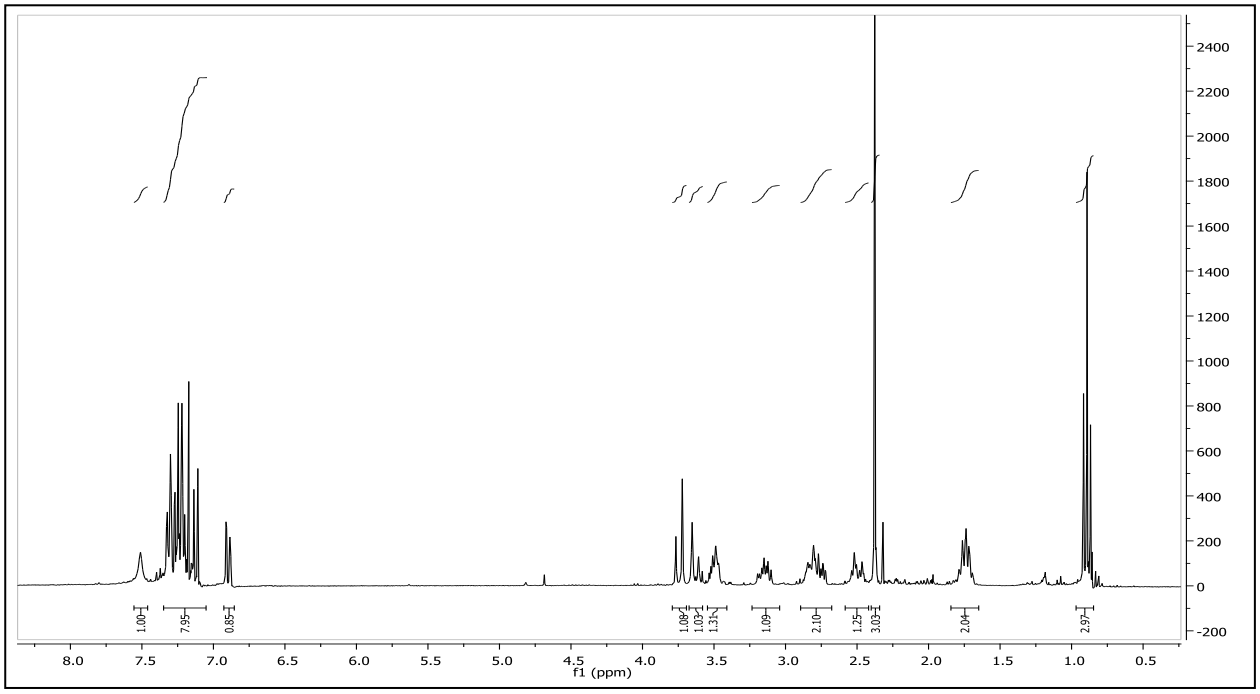

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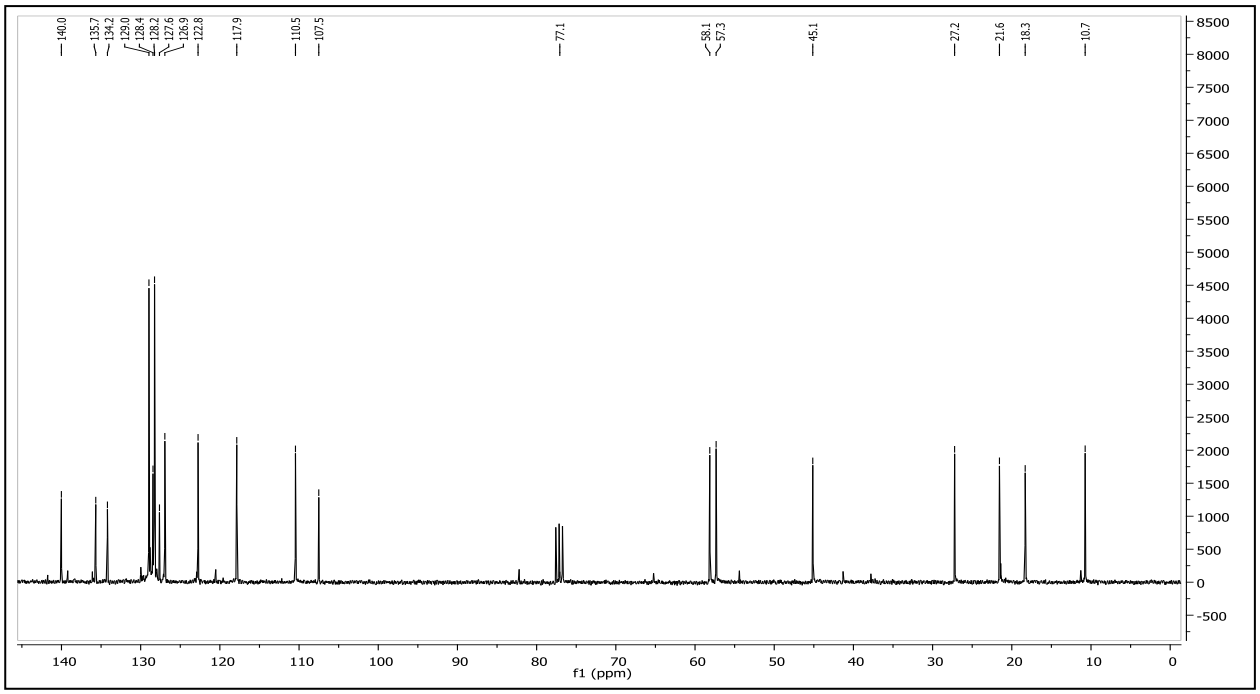
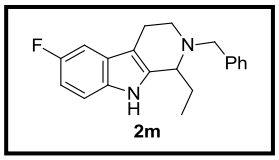
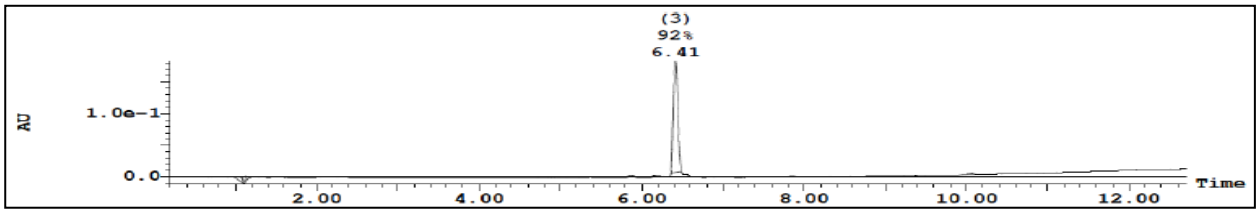


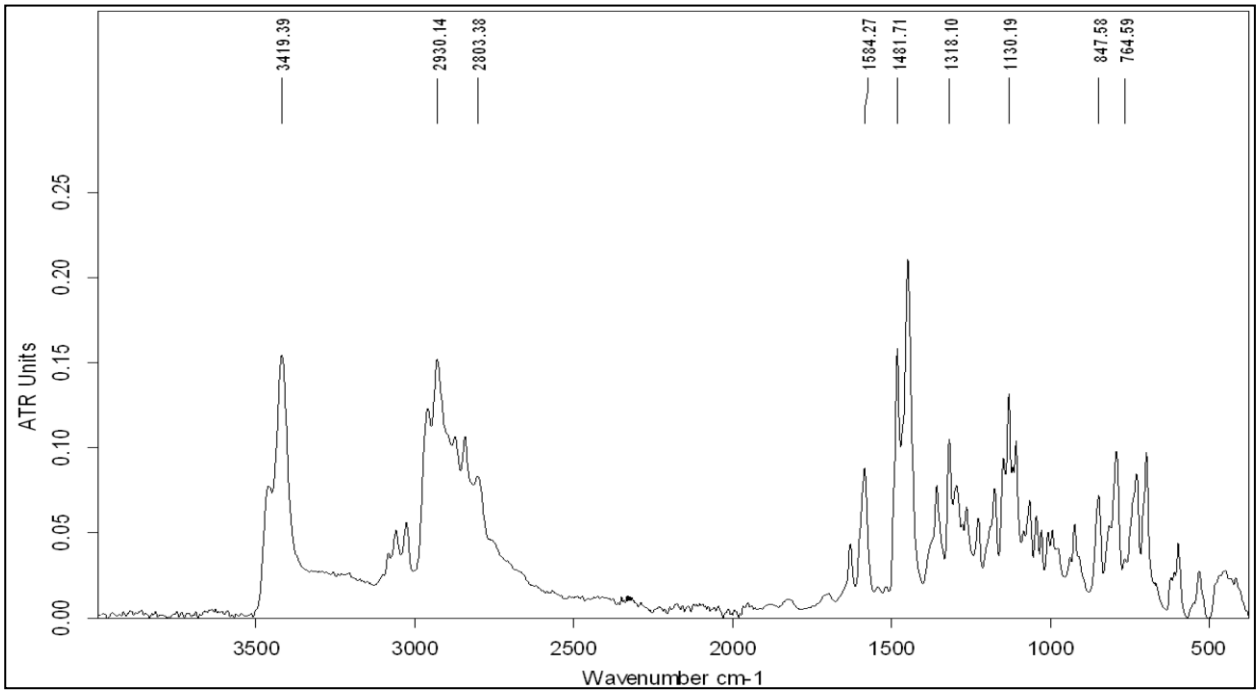
THBC 2m



RP-HPLC of 2m



IR of 2m



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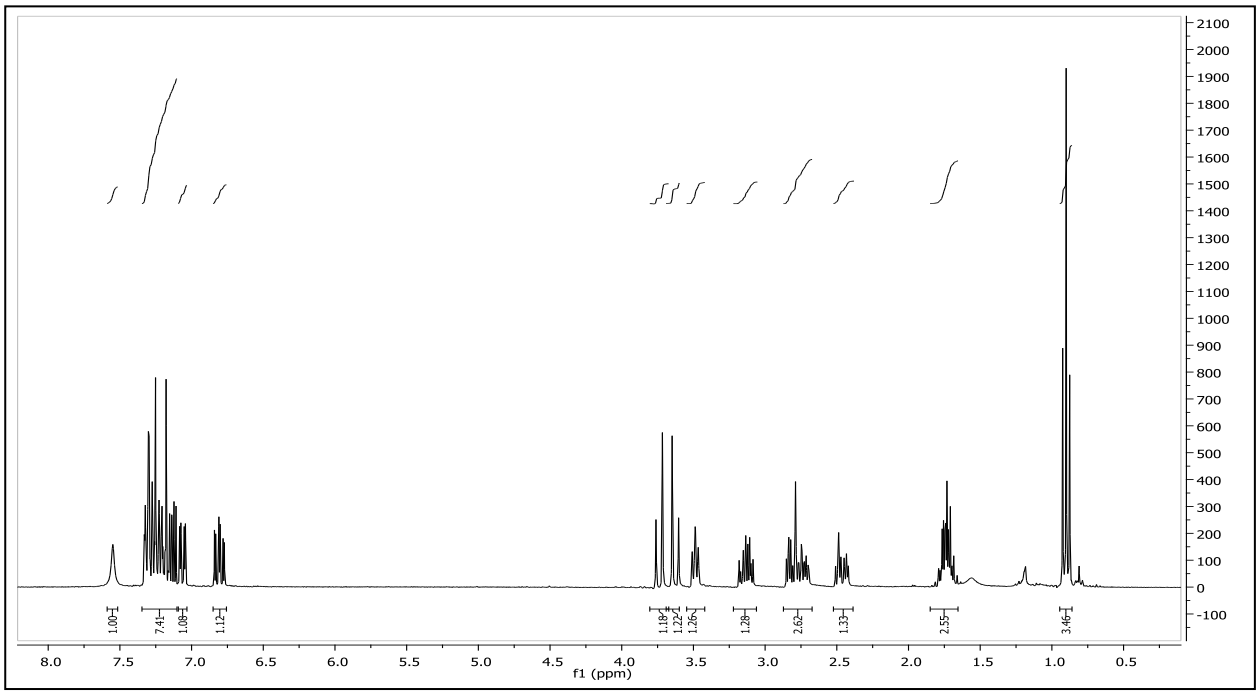

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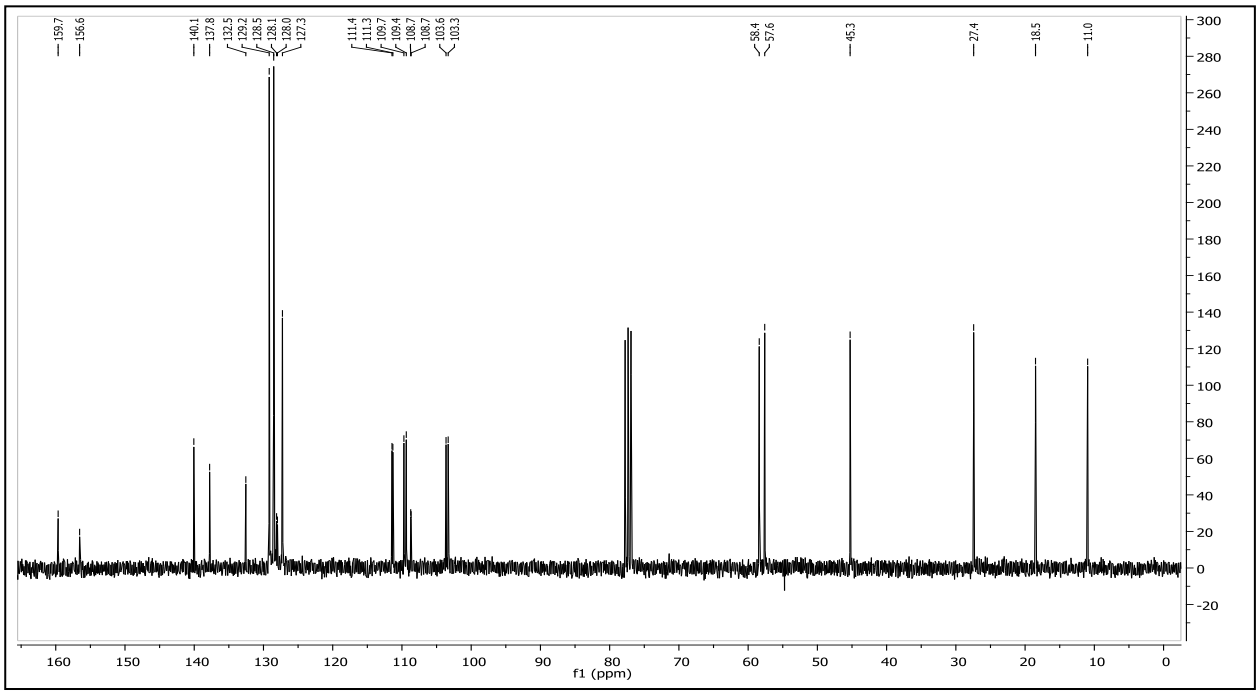
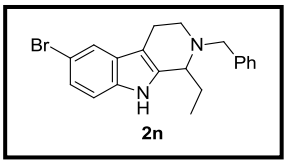
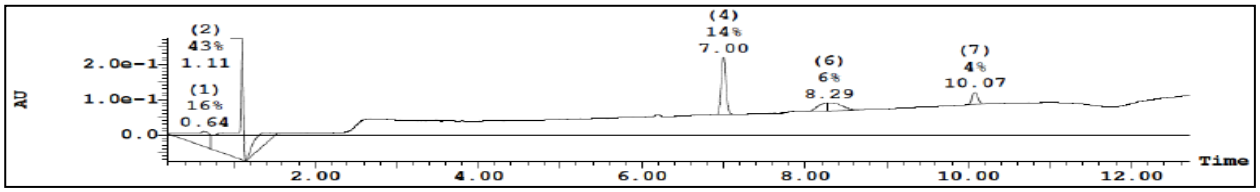


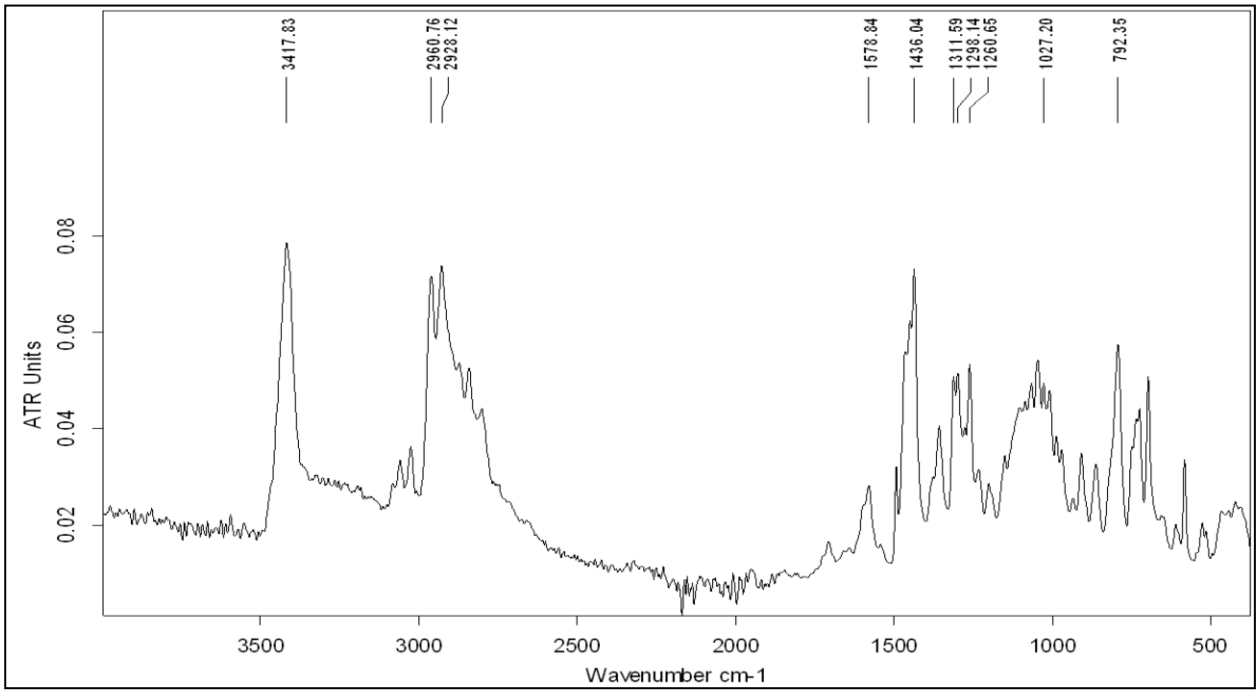
THBC 2n



RP-HPLC of 2n



IR of 2n



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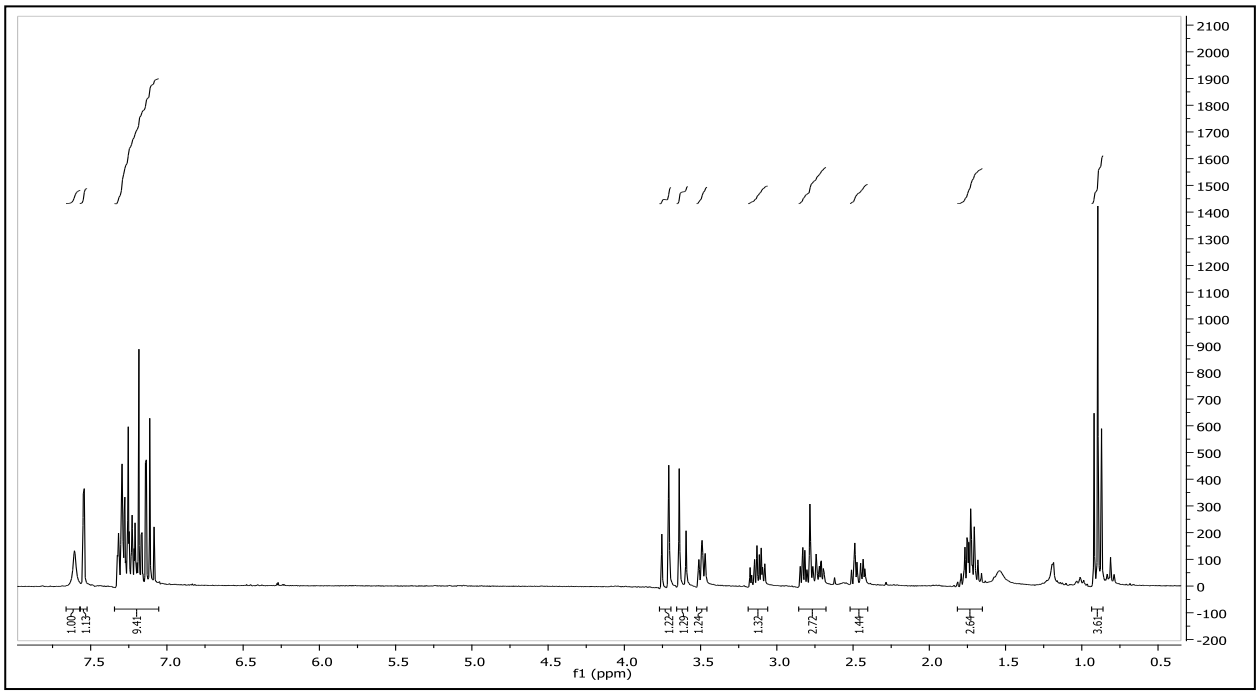

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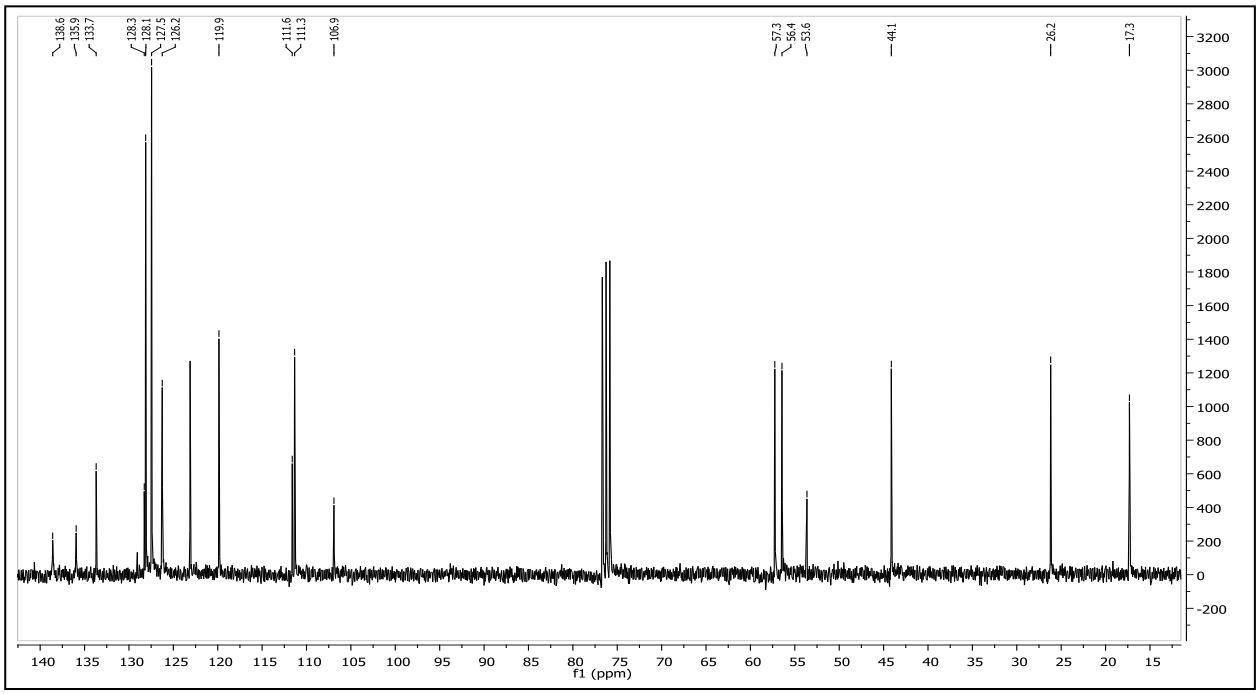
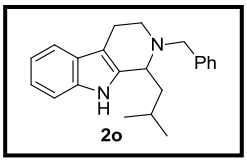
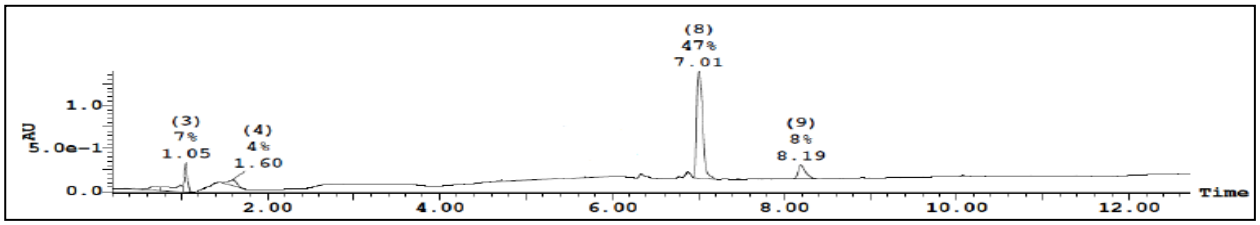


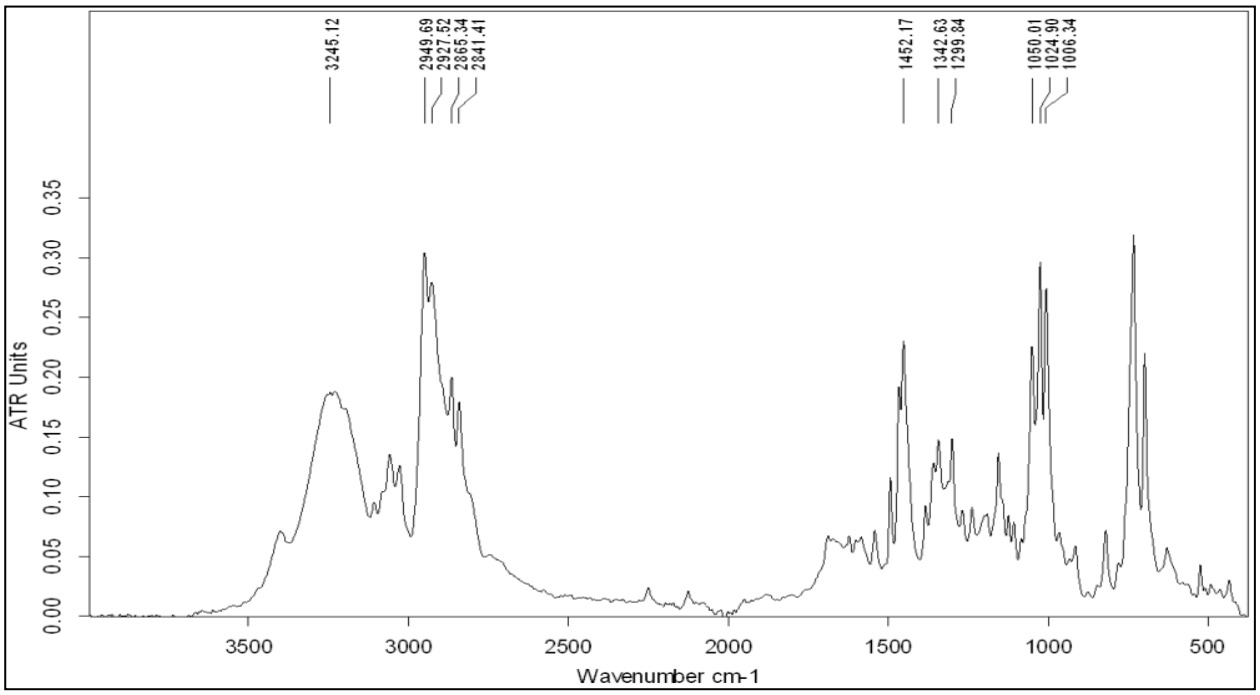
THBC 2o



RP-HPLC of 2o



IR of 2o



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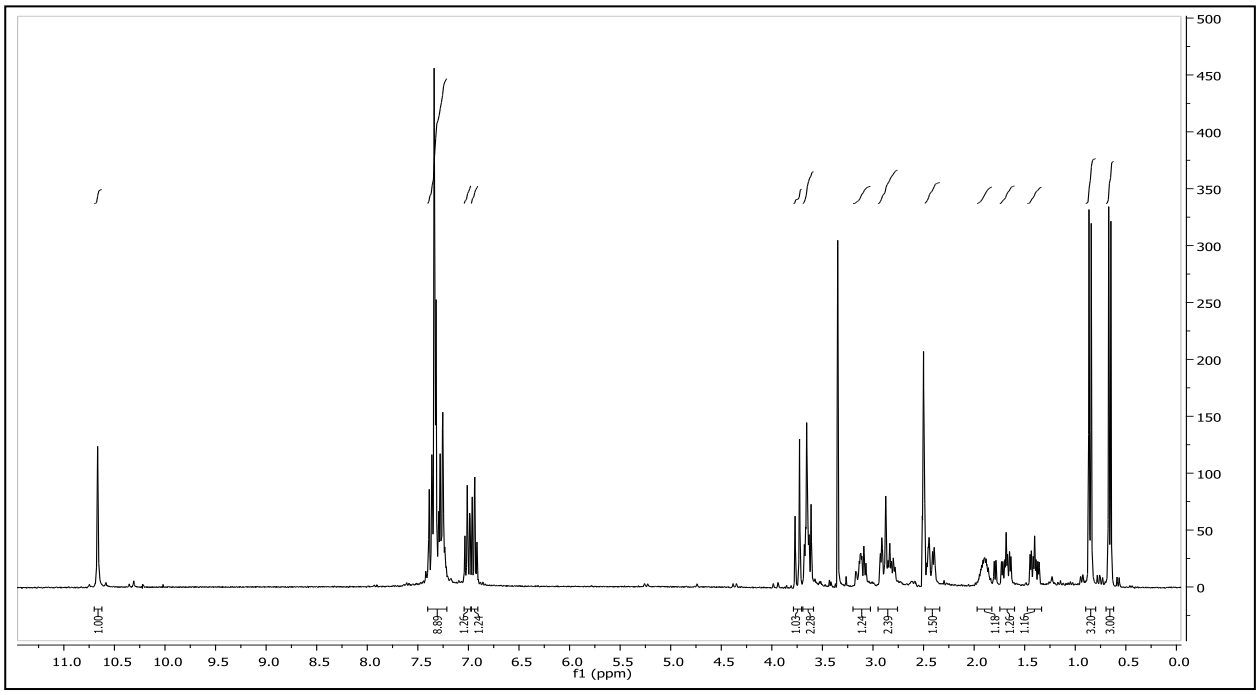

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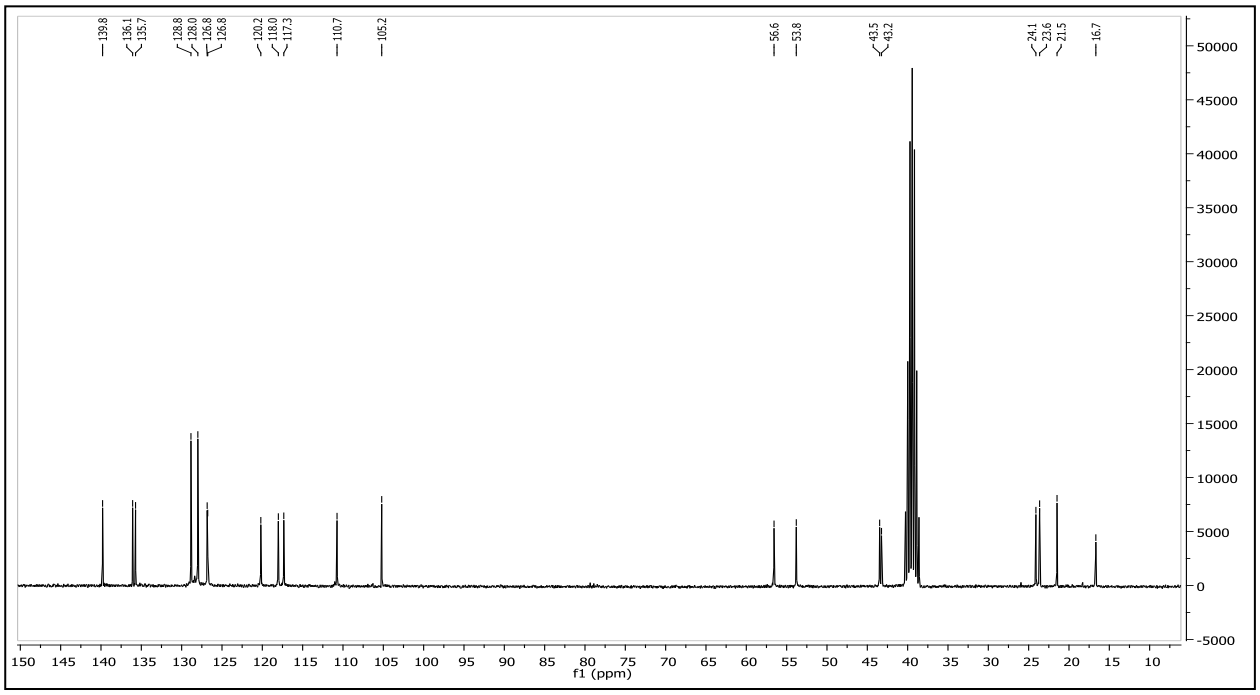
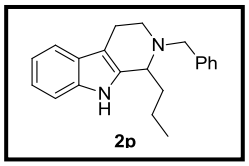
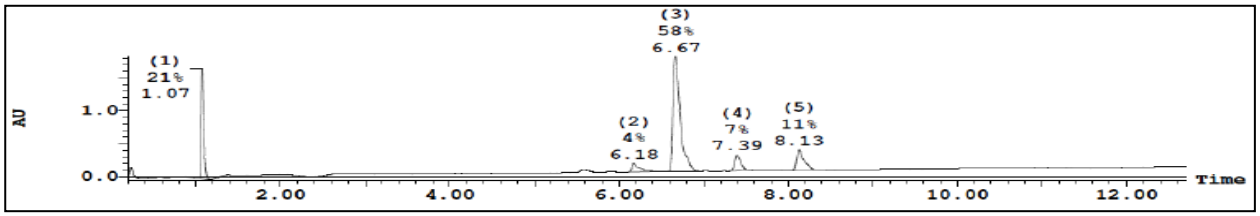


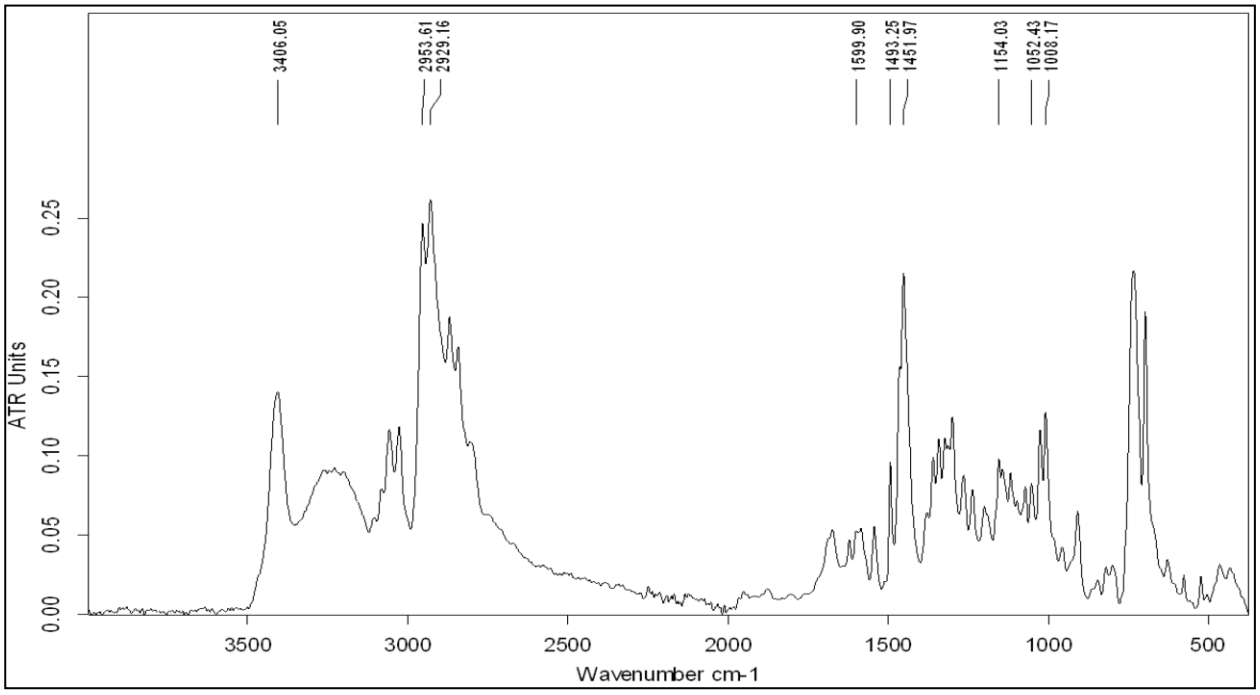
THBC 2p



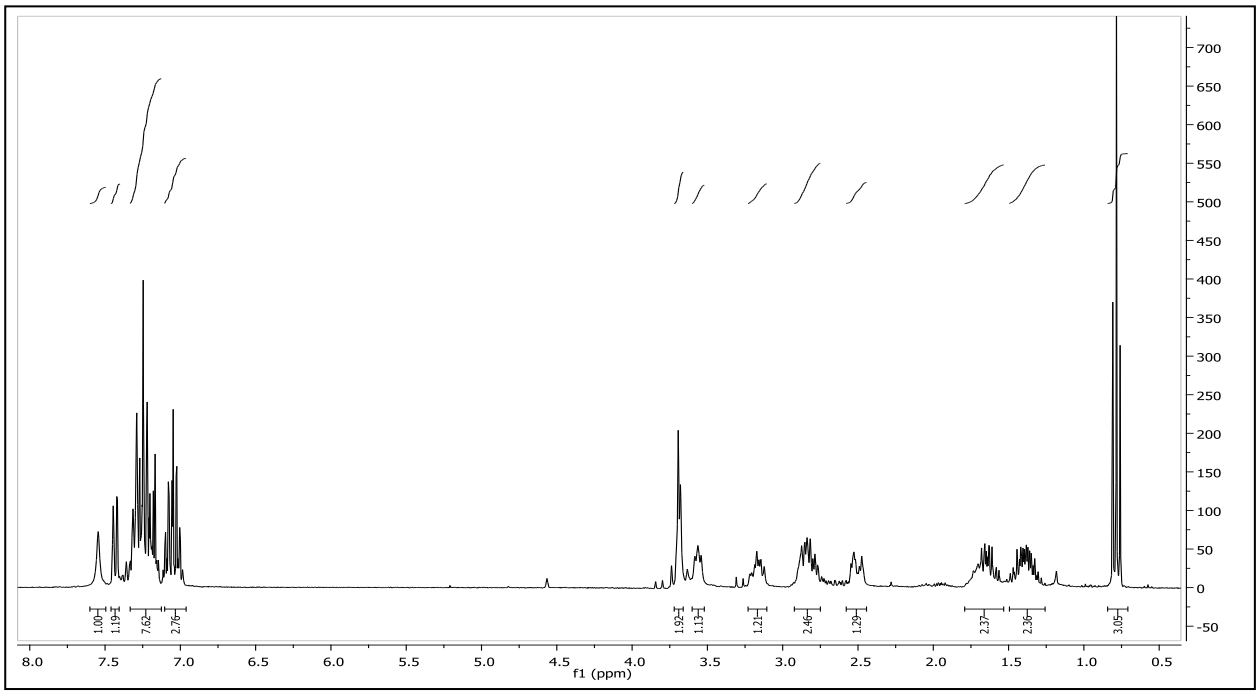
RP-HPLC of 2p



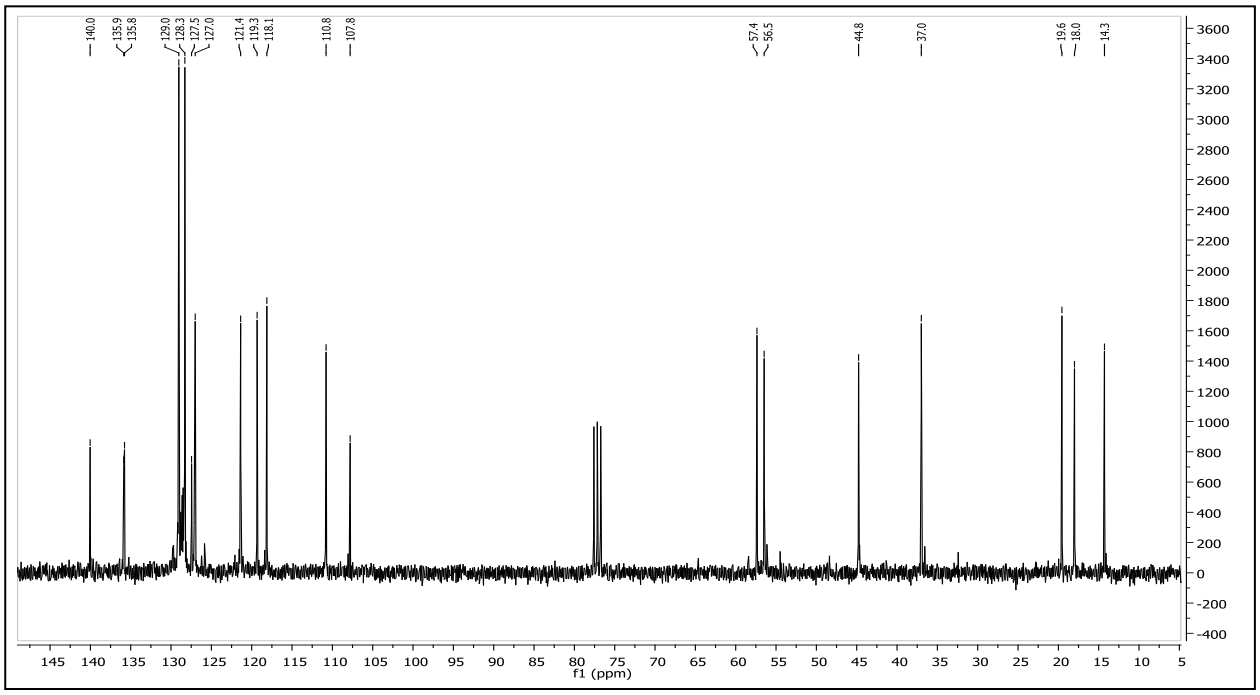
IR of 2p



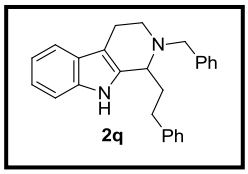
^{1}H NMR of 2p



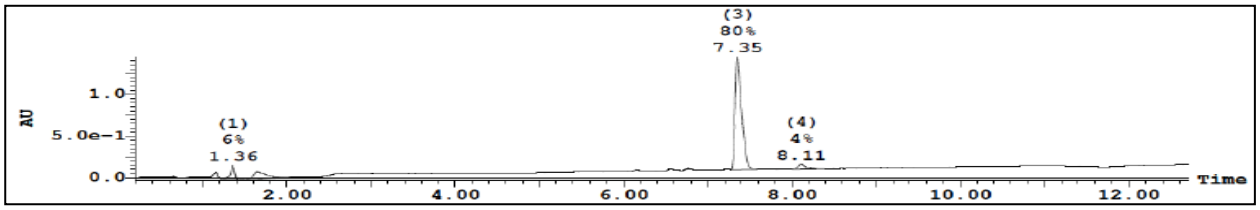
^{13}C NMR of 2p



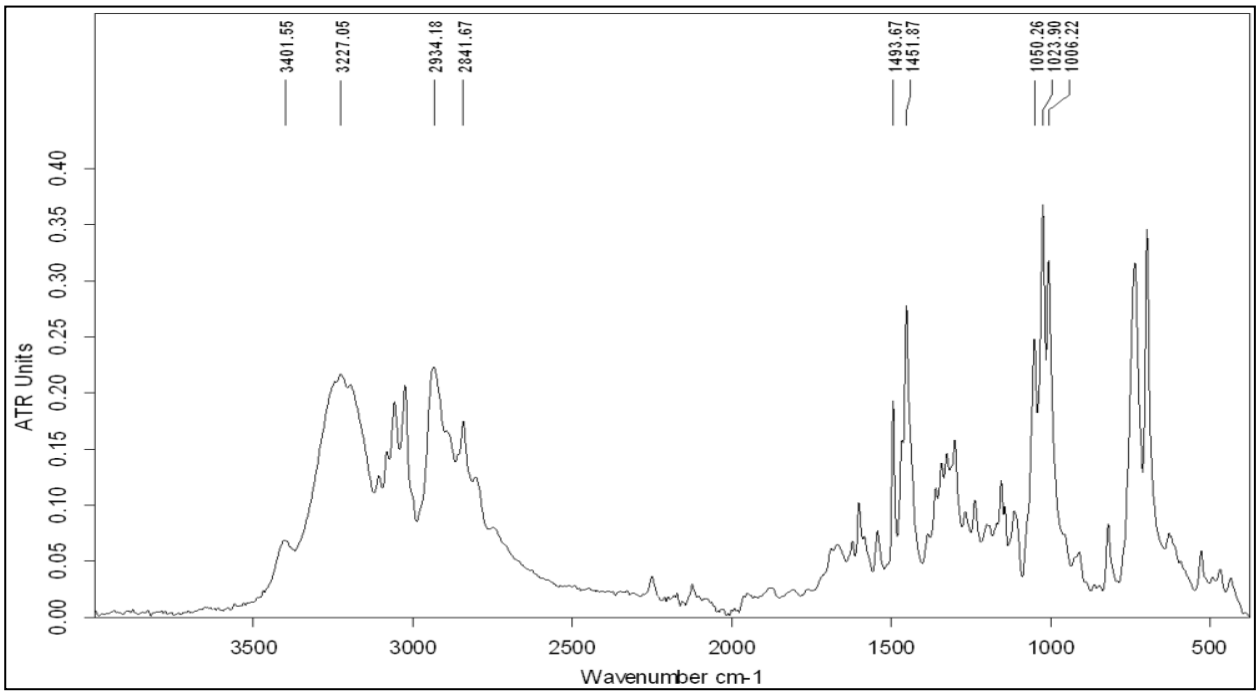
THBC 2q



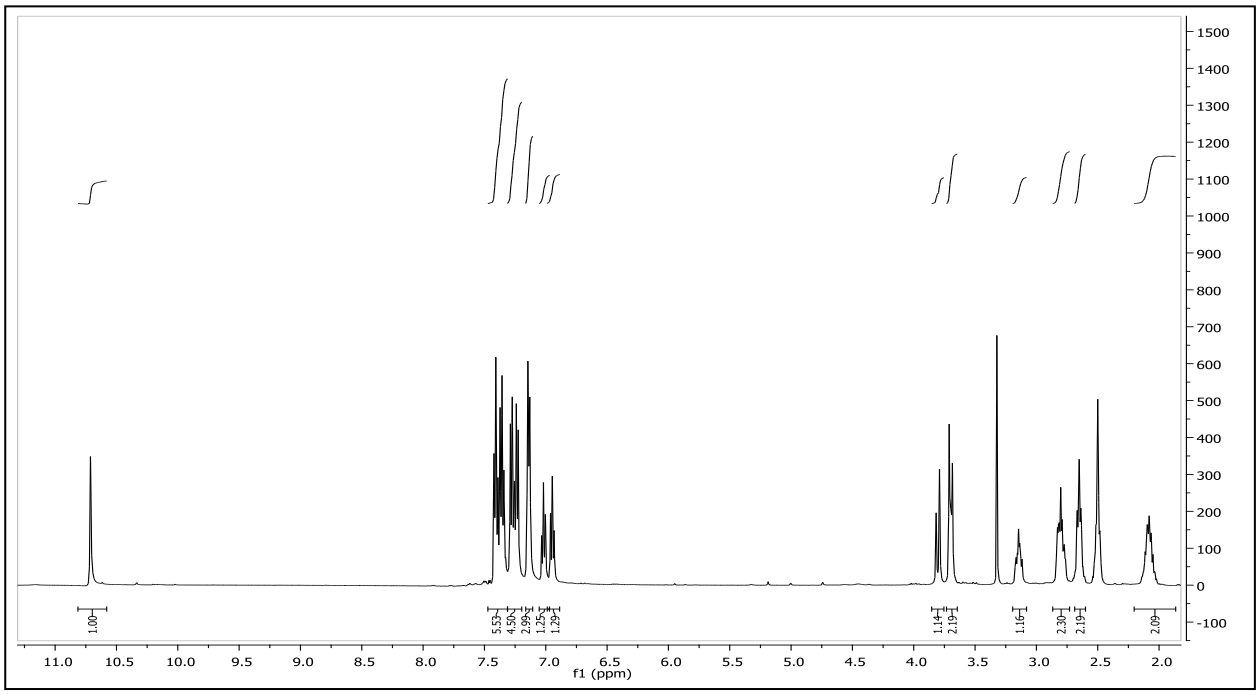
RP-HPLC of 2q



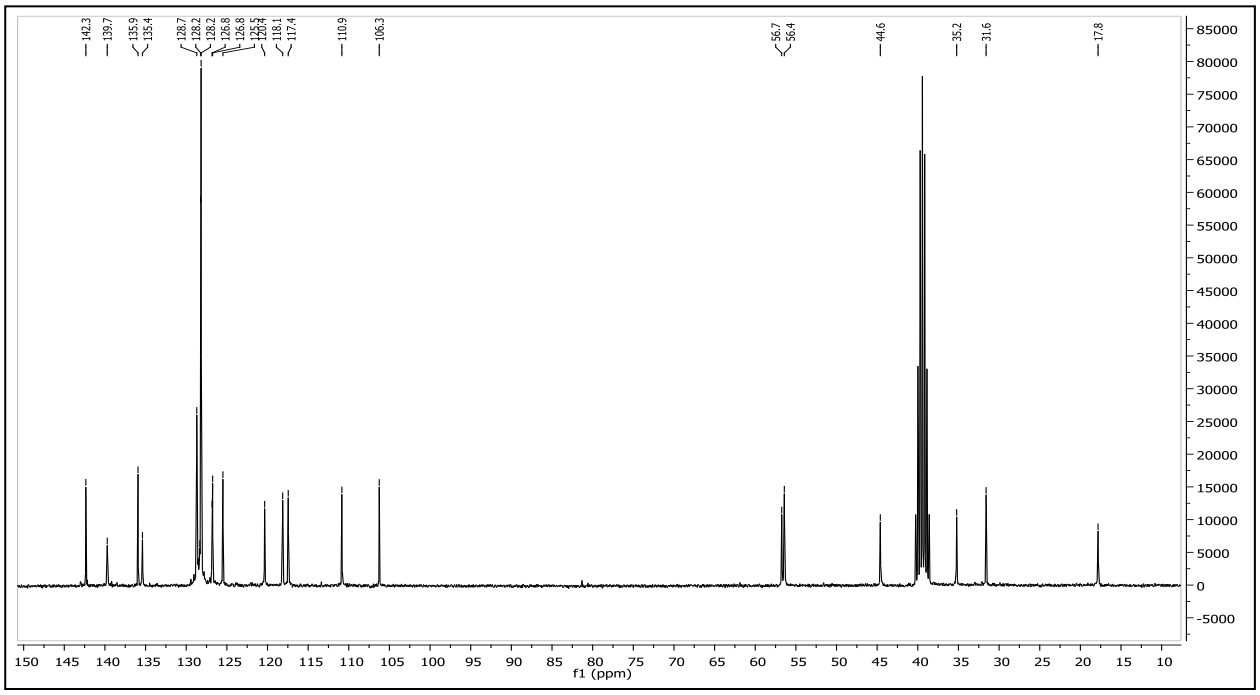
IR of 2q



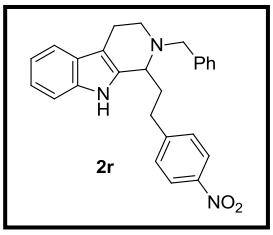
^{1}H NMR of 2q



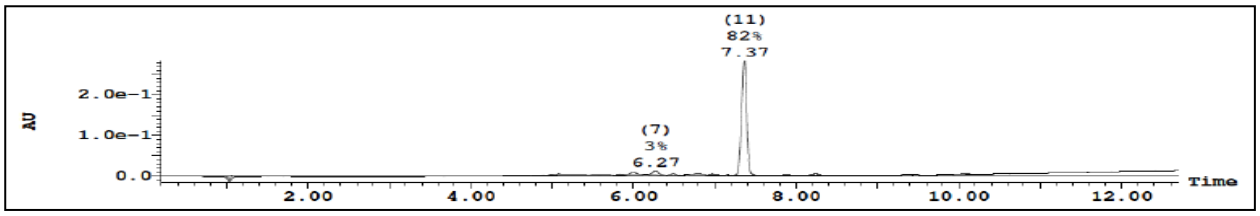
^{13}C NMR of 2q



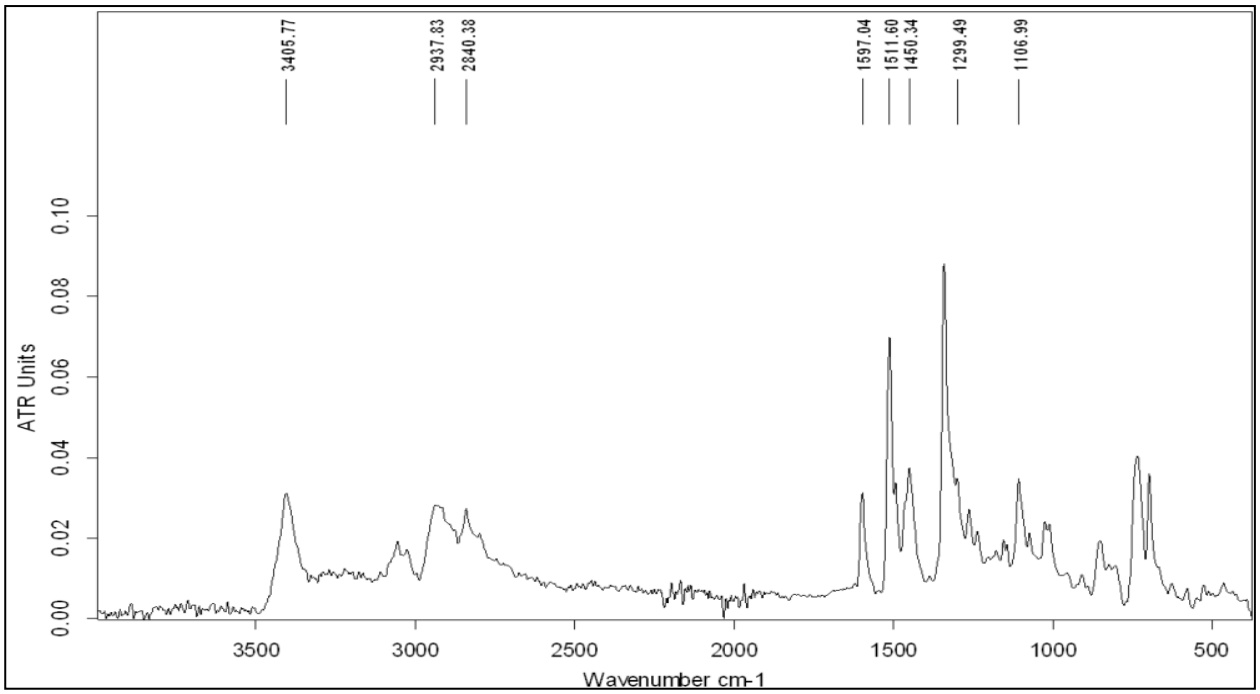
THBC 2r



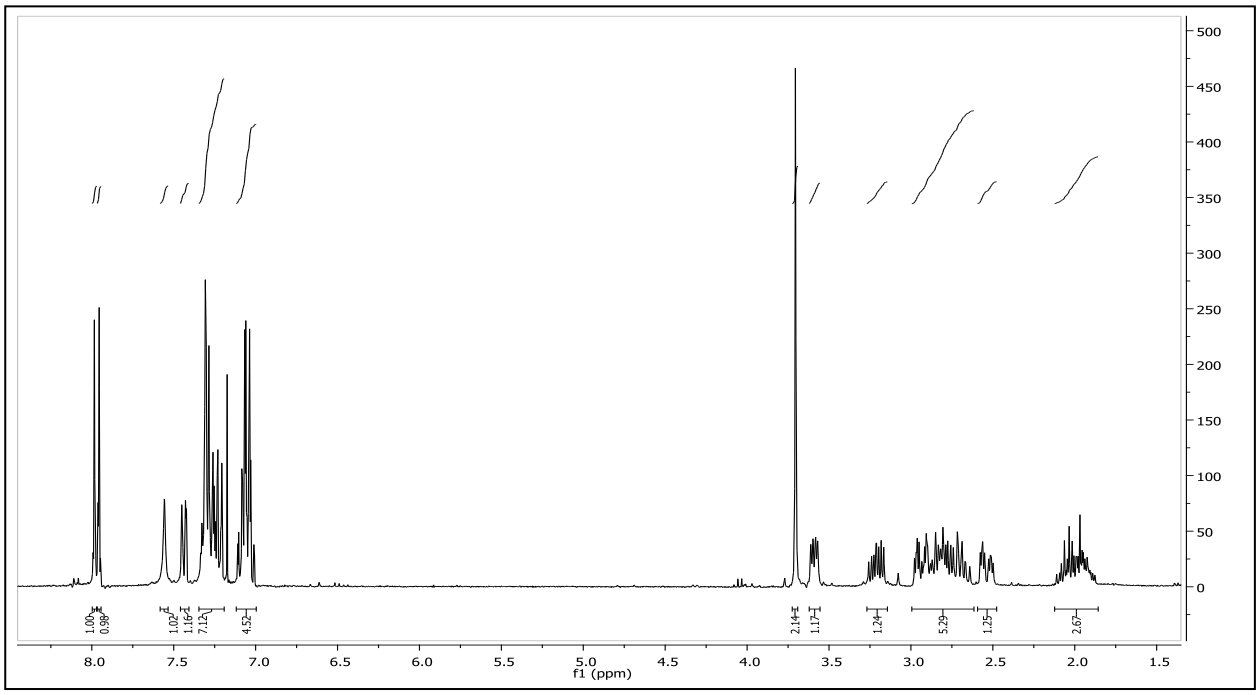
RP-HPLC of 2r



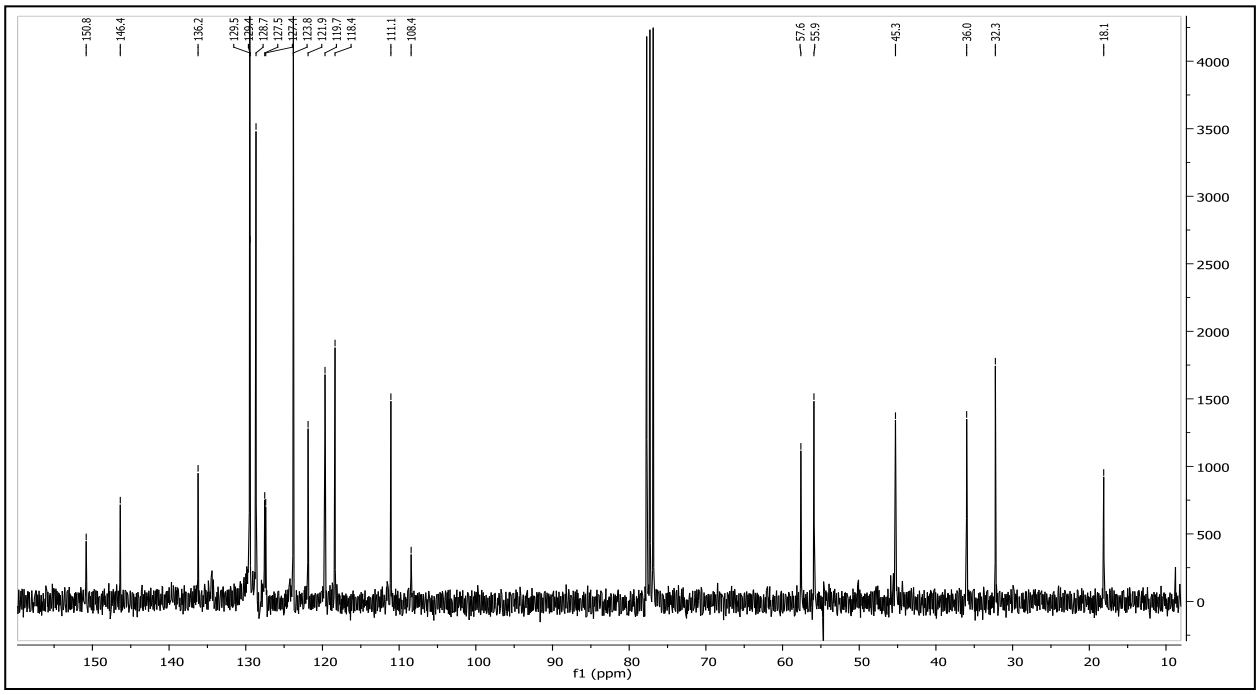
IR of 2r



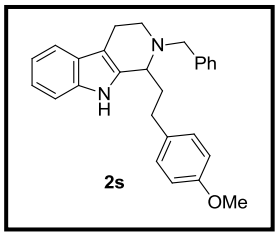
^{1}H NMR of 2r



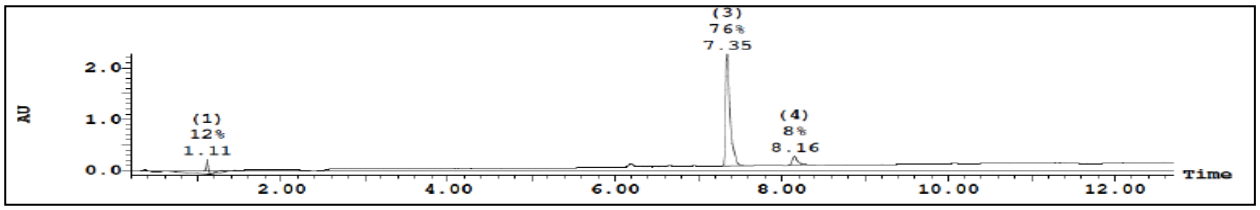
^{13}C NMR of 2r



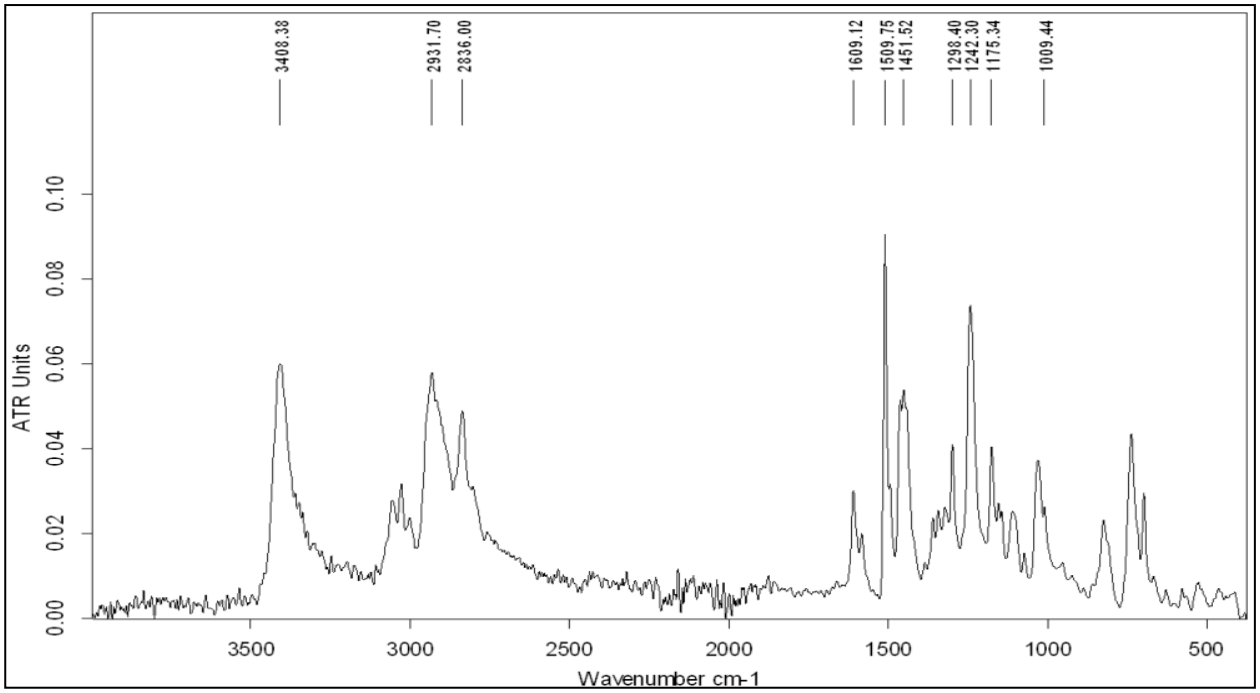
THBC 2s



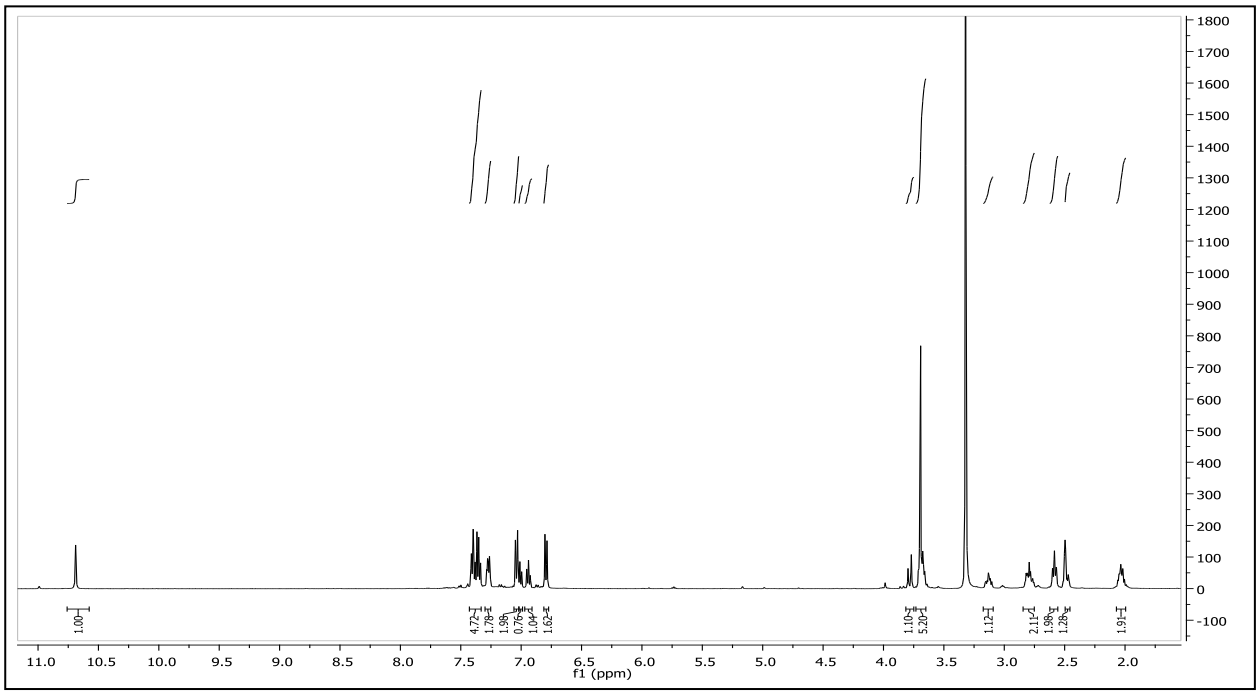
RP-HPLC of 2s



IR of 2s



^{1}H NMR of 2s



^{13}C NMR of 2s