Supporting Information for

NHC Catalysed Addition of Aldehydes to Diazo compounds: Stereoselective Synthesis of *N*-Acylhydrazones

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1. General remarks

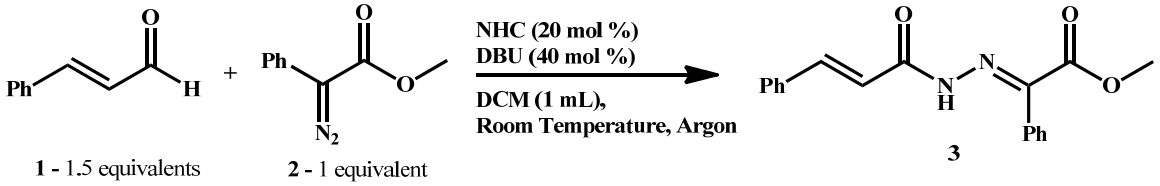
Dichloromethane (DCM) was freshly distilled over calcium hydride. All reactions were performed in oven-dried glassware under argon atmosphere. Preparative thin layer chromatography (TLC) plates were prepared with silica gel 60 GF254 MercK (Ref. 1.07730.1000). Reaction mixtures were analysed by TLC using ALUGRAM® SIL G/UV254 from MN (Ref. 818133, silica gel 60), and visualisation of TLC spots was effected using ultraviolet (UV) and phosphomolybdic acid solution. Nuclear magnetic resonance (NMR) spectra were recorded in a Bruker AMX 400 and in a Bruker Avance II 300 using $CDCl_3$ and $(CD_3)_2SO$ as solvents and $(CH_3)_4Si$ (^{1}H) as internal standard. All coupling constants are expressed in Hz. Electrospray ionization (ESI) mass spectra were recorded in a mass spectrometer (Micromass Quattro Micro API, Waters, Ireland) with a Triple Quadrupole (TQ) and with an electrospray ion source operating in positive mode. Elemental analysis was

performed in a Flash 2000 CHNS-O analyzer (ThermoScientific, UK). Infrared (IR) spectra were recorded on a shimadzu IRAffinity-1 FTIR spectrometer (KBr) and reported in reciprocal centimeters (cm-1). Melting points were measured on a Stuart SMP10 digital melting point apparatus. *N*-heterocyclic carbenes (NHCs) were prepared following reported procedures[1-3], except 1-Mesityl-3,4-dimethyl-4*H*-1,2,4-triazolium tetrafluoroborate which was purchased from Aldrich. All bases were acquired from Sigma-Aldrich. Diazo compounds were prepared according to procedures described in the literarure[4-9]. Aldehydes were obtained from Sigma-Aldrich and were freshly distilled before use. Lewis acids were purchased from Sigma-Aldrich.

2. Optimization of the reaction conditions

NHC (x mol %) and base (x mol %) were dissolved with freshly dry solvent (0.5 mL) in a round bottom flask under argon. The mixture was stirred for 10 minutes at room temperature. Then a solution of 2-diazo-2-phenylacetate **2** (0.477 mmol in 0.5 mL of solvent) was added. Immediately after, cinnamaldehyde **1** (0.715 mmol) was slowly added over an hour. The mixture was left reacting until most of diazo compound was consumed. The final product, (*E*)-*N*-Acylhydrazone **3**, was isolated by preparative thin layer chromatography (eluent: DCM) and recrystallized (DCM/Hexane).

- **NHC scope**

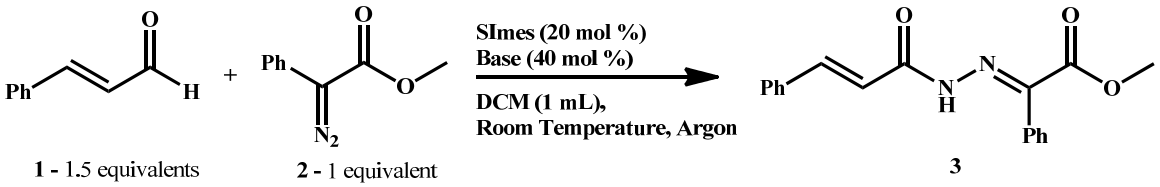


1 - 1.5 equivalents **2** - 1 equivalent **3**

Table 1. NHC scope

NHCs	Yield (%)
NHC **4**	51
NHC **5**	56
NHC **6**	Traces
NHC **7** (SImes)	91
NHC **8**	15
NHC **9**	Traces
NHC **10**	37
NHC **11**	76

- **Base scope**

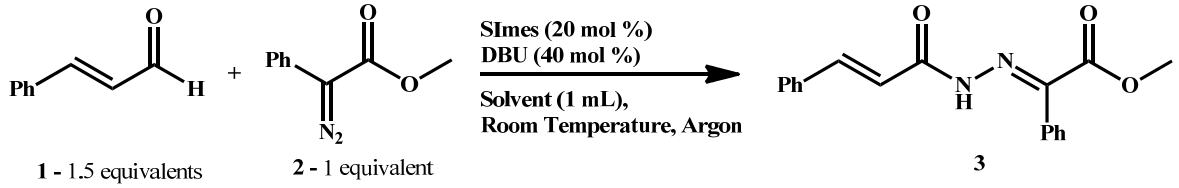


1 - 1.5 equivalents **2** - 1 equivalent **3**

Table 2. Base scope

Base	Yield (%)
1,8-Diazabicyclo[5.4.0]undec-7-ene (DBU)	91
N,*N*-Diisopropylethylamine	Traces
Sodium *tert*-butoxide	NR
Potassium bis(trimethylsilyl)amide	Traces
Triethylamine	Traces

- **Solvent scope**

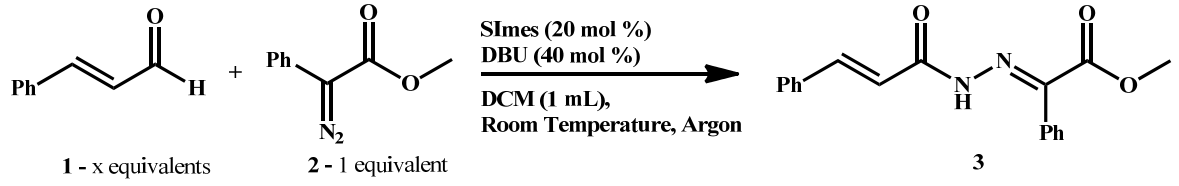


1 - 1.5 equivalents **2** - 1 equivalent **3**

Table 3. Solvent scope

Solvent	Yield (%)
DCM	91
Methanol	70
Acetonitrile	90
Toluene	39
Tetrahydrofuran	65

- **Cinnamaldehyde equivalents scope**

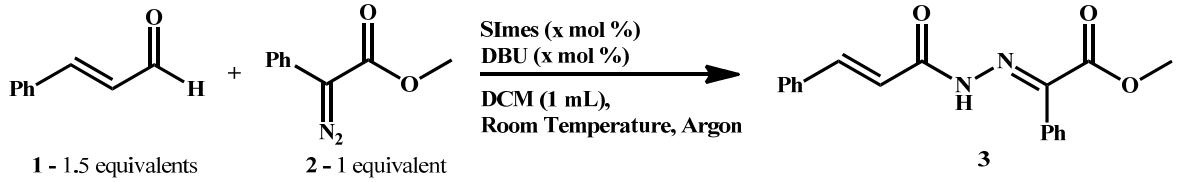


1 - x equivalents **2** - 1 equivalent **3**

Table 4. Cinnamaldehyde equivalents scope

Cinnamaldehyde (equivalents)	Yield (%)
1	75
1.2	82
1.5	91
1.7	87
2	90

- **Scope of the amount of catalysts**



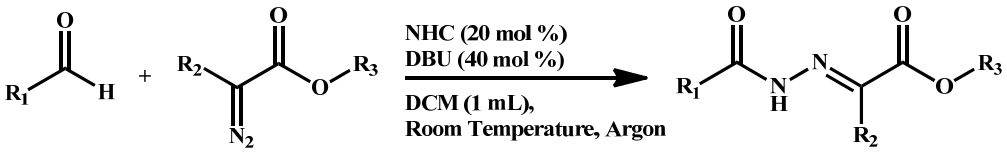
1 - 1.5 equivalents **2** - 1 equivalent **3**

Table 5. Scope of the amount of catalysts

SImes (mol %)	DBU (mol %)	Yield (%)
15	30	70
20	40	91
22.5	45	88

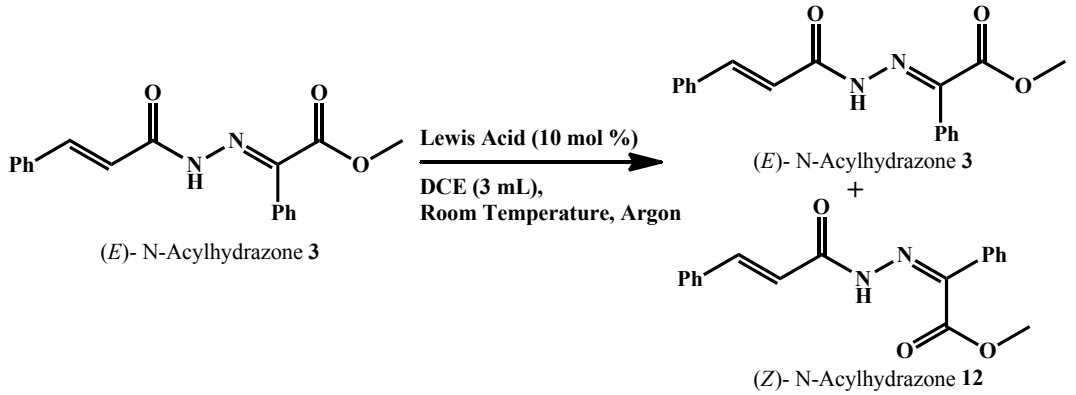
3. General procedure for the synthesis of *N*-Acylhydrazones

To a round bottom flask under argon were added freshly dry DCM over calcium hydride (0.5 mL), SImes (20 mol %) and DBU (40 mol %). The mixture was allowed to react at room temperature for 10 minutes, after which a solution of the diazo compound (1 equivalent, 0.477 mmol in 0.5 mL of dichloromethane) was also added. After that, aldehyde (1.5 equivalents, 0.715 mmol) was slowly added over an hour, neat or in the minimal amount of dry DCM. The mixture was left reacting until most of diazo compound was consumed. The final product, (*E*)-*N*-Acylhydrazone, was isolated by preparative thin layer chromatography (Eluent: DCM or DCM:Methanol) and recrystallized (DCM/Hexane).



4. Isomerization Procedure

To a round bottom flask under argon were added freshly dry 1,2-dichloroethane (DCE) over calcium hydride (3 mL), Lewis acid (10 mol %) and (*E*)- *N*-Acylhydrazone **3** (0.162 mmol). The mixture was refluxed for 20 hours. (*Z*)- *N*-Acylhydrazone **12** was isolated by preparative thin layer chromatography (Eluent: DCM) and recrystallized (DCM/Hexane).



(*E*)- N-Acylhydrazone **3**

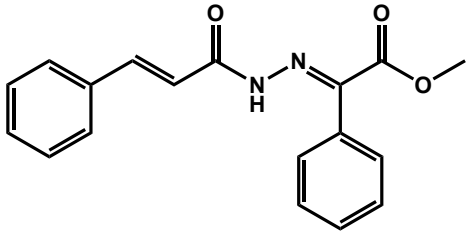
(*E*)- N-Acylhydrazone **3**

+

(*Z*)- N-Acylhydrazone **12**

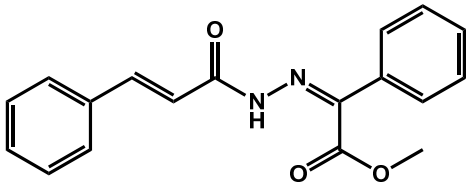
5. Spectra data for *N*-Acylhydrazones 3, 12-30

(*E*)-methyl 2-(2-cinnamoylhydrazono)-2-phenylacetate (3)



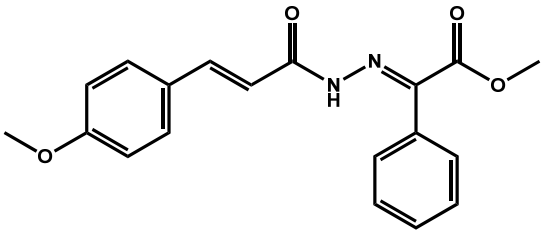
White solid; m.p. 209-211 ºC; ^{1}H NMR (300 MHZ, $(CD_3)_2SO$): δ 10.54 (s, 1H), 7.72 – 7.50 (m, 6H), 7.50 – 7.29 (m, 5H), 7.11 (m, 1H), 3.77 (s, 3H); ^{13}C NMR (75 MHZ, $(CD_3)_2SO$): δ 164.29, 142.43, 134.62, 130.29, 130.05, 129.91, 129.05, 128.99, 128.78, 128.07, 52.56; IR (KBr): υ 3167, 1712, 1666, 1620, 1587; MS (ESI): *m*/*z* ($[M+H]^+$): 309; Elemental analysis calcd (%) for $C_{18}H_{16}N_2O_3$: C 70.12, H 5.23, N 9.09; found (%): C 70.25, H 5.27, N 9.13

(*Z*)-methyl 2-(2-cinnamoylhydrazono)-2-phenylacetate (12)



White solid; m.p. 162-164 ºC; ^{1}H NMR (300 MHZ, $(CD_3)_2SO$): δ 11.59 (s, 1H), 7.82 – 7.59 (m, 5H), 7.56 – 7.40 (m, 6H), 7.04 (m, 1H), 3.95 (s, 3H); ^{13}C NMR (75 MHZ, $(CD_3)_2SO$): δ 163.10, 143.58, 142.60, 134.59, 133.41, 130.29, 130.00, 129.04, 128.67, 128.23, 127.18, 119.82, 116.08, 53.01; IR (KBr): υ 3219, 1694, 1670, 1622, 1599; MS (ESI): *m*/*z* ($[M+H]^+$): 309; Elemental analysis calcd (%) for $C_{18}H_{16}N_2O_3 \cdot {}^1/_4H_2O$: C 68.78, H 5.34, N 8.91; found (%): C 68.89, H 5.17, N 8.97

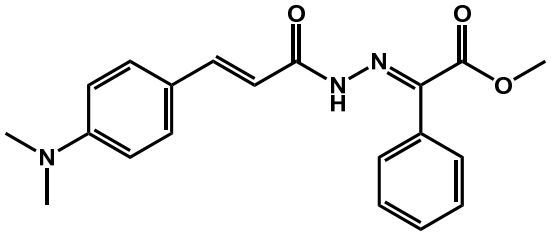
(*E*)-methyl 2-(2-(4-methoxycinnamoyl)-hydrazono)-2-phenylacetate (13)



White solid; m.p. 193-195 ºC; ^{1}H NMR (300 MHZ, $CDCl_3$): δ 8.69 (s, 1H), 7.82 (d, *J* = 15.9 Hz, 1H), 7.61 (d, *J* = 7.8 Hz, 2H), 7.57 – 7.49 (m, 3H), 7.40 – 7.37 (m, 1H), 7.29 (dd, *J* = 7.1, 1.7 Hz, 2H), 6.93 (d, *J* = 8.4 Hz, 2H), 3.90 (s, 3H), 3.86 (s, 3H); ^{13}C NMR (75 MHZ, $CDCl_3$): δ 164.26, 161.69, 145.33, 130.60, 130.45, 129.81, 129.52, 128.82, 128.46, 128.20, 127.60, 114.44, 112.78, 55.71, 53.23; IR (KBr): υ 3153, 1710, 1680, 1618, 1591; MS (ESI): *m*/*z*

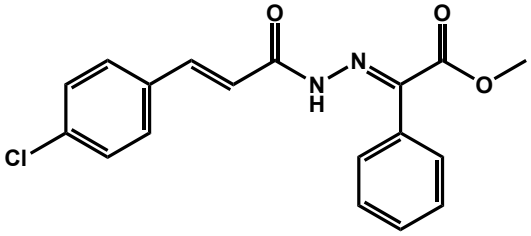
([M+H]$^+$): 339; Elemental analysis calcd (%) for $C_{19}H_{18}N_2O_5$: C 67.44, H 5.36, N 8.28; found (%): C 66.73, H 5.38, N 8.17

(*E*)-methyl 2-(2-(4-dimethylaminocinnamoyl)-hydrazono)-2-phenylacetate (14)



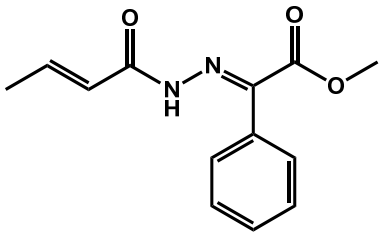
Yellow solid; m.p. 196-198 ºC; ^{1}H NMR (400 MHZ, $CDCl_3$): δ 8.66 (s, 1H), 7.81 (d, *J* = 16.0 Hz, 1H), 7.61 – 7.47 (m, 5H), 7.46 – 7.32 (m, 1H), 7.29 (d, *J* = 7.6 Hz, 2H), 6.71 (d, *J* = 7.6 Hz, 2H), 3.90 (s, 3H), 3.04 (s, 6H); ^{13}C NMR (101 MHZ, $CDCl_3$): δ 168.18, 164.30, 152.13, 146.34, 141.91, 140.46, 130.55, 130.50, 129.77, 128.93, 128.51, 111.99, 109.01, 53.01, 40.39; IR (KBr): υ 3169, 1736, 1707, 1663, 1593; MS (ESI): *m*/*z* ([M+H]$^+$): 352; Elemental analysis calcd (%) for $C_{20}H_{21}N_3O_3$: C 68.36, H 6.02, N 11.96; found (%): C 68.49, H 6.09, N 11.91

(*E*)-methyl 2-(2-(4-chlorocinnamoyl)-hydrazono)-2-phenylacetate (15)



White solid; m.p. 194-196 ºC; ^{1}H NMR (300 MHZ, $(CD_3)_2SO$): δ 10.56 (s, 1H), 7.79 – 7.58 (m, 3H), 7.58 – 7.42 (m, 5H), 7.42 – 7.29 (m, 2H), 7.29 – 6.93 (m, 1H), 3.77 (s, 3H); ^{13}C NMR (75 MHZ, $(CD_3)_2SO$): δ 164.30, 141.02, 134.67, 133.58, 129.98, 129.90, 129.72, 129.07, 128.97, 128.75, 120.79, 52.53; IR (KBr): υ 3157, 1718, 1672, 1620, 1587; MS (ESI): *m*/*z* ([M+H]$^+$): 343, 345; Elemental analysis calcd (%) for $C_{18}H_{15}ClN_2O_3$: C 63.07, H 4.41, N 8.17; found (%): C 63.32, H 4.47, N 8.16

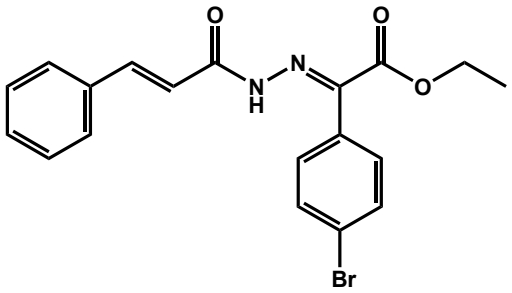
(*E*)-methyl 2-(2-crotonoylhydrazono)-2-phenylacetate (16)



White solid; m.p. 141-143 ºC; ^{1}H NMR (300 MHZ, $(CD_3)_2SO$): δ 10.34 (s, 1H), 7.57 – 7.42 (m, 3H), 7.39 – 7.25 (m, 2H), 6.99 – 6.82 (m, 1H), 6.39 (m, 1H), 3.75 (s, 3H), 1.86 (d, *J* = 2.7 Hz,

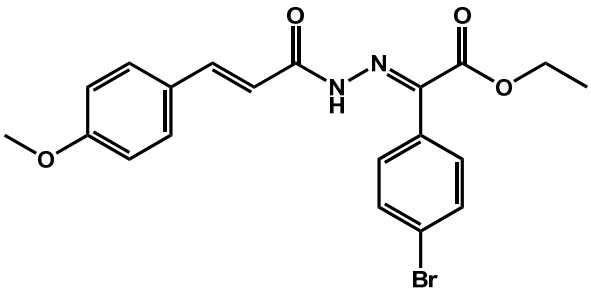
3H); ^{13}C NMR (75 MHZ, $(CD_3)_2SO$): 164.28, 129.98, 129.77, 128.90, 128.70, 52.47, 17.94; IR (KBr): υ 3169, 1720, 1672, 1635, 1587; MS (ESI): *m/z* ($[M+H]^+$): 247; Elemental analysis calcd (%) for $C_{13}H_{14}N_2O_3$: C 63.40, H 5.73, N 11.38; found (%): C 62.86, H 5.68, N 11.24

(*E*)-ethyl 2-(2-cinnamoylhydrazono)-2-(4-bromophenyl)-acetate (17)



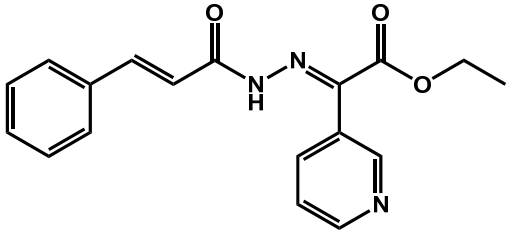
White solid; m.p. 180-182 ºC; ^{1}H NMR (300 MHZ, $CDCl_3$): δ 8.68 (s, 1H), 7.86 (d, *J* = 15.9 Hz, 1H), 7.69 (d, *J* = 8.4 Hz, 2H), 7.66 – 7.45 (m, 3H), 7.45 – 7.29 (m, 3H), 7.19 (d, *J* = 8.4 Hz, 2H), 4.36 (q, *J* = 7.2 Hz, 2H), 1.38 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (75 MHZ, $CDCl_3$): δ 167.28, 163.30, 145.94, 140.29, 134.78, 133.08, 130.71, 130.20, 129.04, 128.67, 127.60, 125.14, 115.32, 62.32, 14.39; IR (KBr): υ 3215, 1719, 1678, 1626, 1609; MS (ESI): *m/z* ($[M+H]^+$): 401, 403; Elemental analysis calcd (%) for $C_{19}H_{17}BrN_2O_3$: C 56.87, H 4.27, N 6.98; found (%): C 56.66, H 4.32, N 6.88

(*E*)-ethyl 2-(2-(4-methoxycinnamoyl)-hydrazono)-2-(4-bromophenyl)-acetate (18)



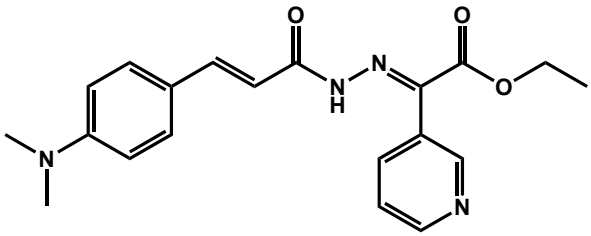
White solid; m.p. 196-198 ºC; ^{1}H NMR (300 MHZ, $CDCl_3$): δ 8.64 (s, 1H), 7.82 (d, *J* = 15.9 Hz, 1H), 7.68 (d, *J* = 8.1 Hz, 2H), 7.58 (d, *J* = 8.1 Hz, 2H), 7.44 (d, *J* = 15.9 Hz, 1H), 7.18 (d, *J* = 8.4 Hz, 2H), 6.93 (d, *J* = 8.4 Hz, 2H), 4.36 (q, *J* = 7.2 Hz, 2H), 3.85 (s, 3H), 1.37 (t, *J* = 7.2 Hz, 3H; ^{13}C NMR (75 MHZ, $CDCl_3$): δ 163.35, 161.79, 145.59, 133.06, 131.48, 130.42, 130.22, 127.67, 127.57, 125.11, 114.47, 112.61, 62.28, 55.54, 14.34; IR (KBr): υ 3177, 1707, 1667, 1620, 1603; MS (ESI): *m/z* ($[M+H]^+$): 431, 433; Elemental analysis calcd (%) for $C_{20}H_{19}BrN_2O_4$: C 55.70, H 4.44, N 6.50; found (%): C 55.86, H 4.51, N 6.44

(*E*)-ethyl 2-(2-cinnamoylhydrazono)-2-(3-pyridinyl)-acetate (19)



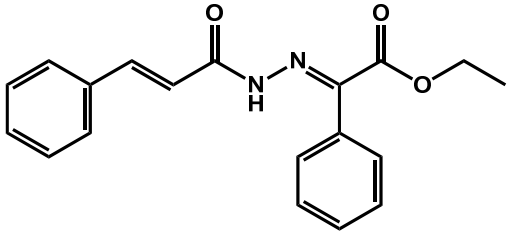
White solid; m.p. 179-181 ºC; ^{1}H NMR (400 MHZ, $(CD_3)_2SO$): δ 10.88 (s, 1H), 8.73 – 8.64 (m, 1H), 8.55 (s, 1H), 7.82 (d, *J* = 7.2 Hz, 1H), 7.73 – 7.50 (m, 4H), 7.47 – 7.38 (m, 3H), 7.38 – 6.75 (m, 1H), 4.25 (q, *J* = 7.2 Hz, 2H), 1.26 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (101 MHZ, $(CD_3)_2SO$): δ 163.58, 150.53, 149.31, 137.00, 134.58, 130.35, 129.10, 128.05, 126.92, 123.93, 61.63, 14.37; IR (KBr): υ 3157, 1709, 1672, 1620, 1576; MS (ESI): *m*/*z* ($[M+H]^+$): 324; Elemental analysis calcd (%) for $C_{18}H_{17}N_3O_3 \cdot {}^1/_4H_2O$: C 65.64, H 5.41, N 12.76; found (%): C 65.94, H 5.23, N 12.99

(*E*)-ethyl 2-(2-(4-dimethylaminocinnamoyl)-hydrazono)-2-(3-pyridinyl)-acetate (20)



Yellow solid; m.p. 189-191 ºC; ^{1}H NMR (400 MHZ, $(CD_3)_2SO$): δ 10.70 (s, 1H), 8.68 (d, *J* = 3.6 Hz, 1H), 8.53 (s, 1H), 7.80 (d, *J* = 7.6 Hz, 1H), 7.62 – 7.52 (m, 3H), 7.43 (d, *J* = 7.6 Hz, 2H), 6.72 (d, *J* = 8.4 Hz, 2H), 4.24 (q, *J* = 7.2 Hz, 2H), 2.96 (s, 6H), 1.26 (d, *J* = 7.2 Hz, 3H); ^{13}C NMR (101 MHZ, $(CD_3)_2SO$): δ 163.84, 151.76, 150.35, 149.26, 137.00, 129.96, 127.02, 124.04, 122.03, 112.01, 61.52, 14.26; IR (KBr): υ 3150, 1734, 1717, 1663, 1585; MS (ESI): *m*/*z* ($[M+H]^+$): 368; Elemental analysis calcd (%) for $C_{20}H_{22}N_4O_3 \cdot {}^1/_4H_2O$: C 64.5, H 6.13, N 15.04; found (%): C 64.45, H 5.95, N 15.08

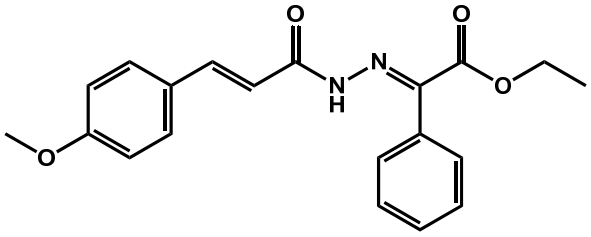
(*E*)-ethyl 2-(2-cinnamoylhydrazono)-2-phenylacetate (21)



White solid; m.p. 177-179 ºC; ^{1}H NMR (400 MHZ, $CDCl_3$): δ 8.73 (s, 1H), 7.86 (d, *J* = 16.0 Hz, 1H), 7.64 (m, 3H), 7.59 – 7.48 (m, 3H), 7.41 (m, 3H), 7.30 (d, *J* = 6.8 Hz, 2H), 4.36 (d, *J* = 7.0 Hz, 2H), 1.38 (d, *J* = 7.0 Hz, 3H); ^{13}C NMR (101 MHZ, $CDCl_3$): δ 167.58, 163.63, 145.50,

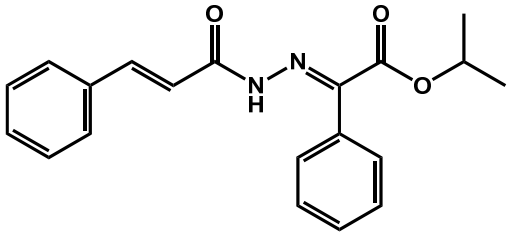
141.37, 134.89, 130.60, 130.57, 129.77, 129.01, 128.84, 128.63, 128.45, 115.58, 62.18, 14.33; IR (KBr): υ 3169, 1708, 1676, 1620, 1585; MS (ESI): *m/z* ($[M+H]^+$): 323; Elemental analysis calcd (%) for $C_{19}H_{18}N_2O_3$: C 70.79, H 5.63, N 8.69; found (%): C 71.17, H 5.75, N 9.07

(*E*)-ethyl 2-(2-(4-methoxycinnamoyl)-hydrazono)-2-phenylacetate (22)



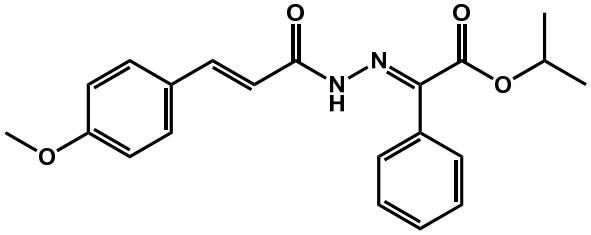
White solid; m.p. 178-180 ºC; ^{1}H NMR (400 MHZ, $CDCl_3$): δ 8.69 (s, 1H), 7.81 (d, *J* = 16.0 Hz, 1H), 7.60 (d, *J* = 7.6 Hz, 2H), 7.57 – 7.40 (m, 4H), 7.29 (d, *J* = 7.6 Hz, 2H), 6.93 (d, *J* = 8.8 Hz, 2H), 4.36 (q, *J* = 7.2 Hz, 2H), 3.85 (s, 3H), 1.38 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (101 MHZ, $CDCl_3$): δ 167.58, 163.70, 161.85, 145.24, 130.51, 130.37, 129.75, 128.92, 128.47, 127.67, 114.46, 112.96, 62.13, 55.53, 14.3; IR (KBr): υ 3154, 1711, 1672, 1618, 1603; MS (ESI): *m/z* ($[M+H]^+$): 353; Elemental analysis calcd (%) for $C_{20}H_{20}N_2O_4$: C 68.17, H 5.72, N 7.95; found (%): C 68.17, H 5.96, N 7.53

(*E*)-isopropyl 2-(2-cinnamoylhydrazono)-2-phenylacetate (23)



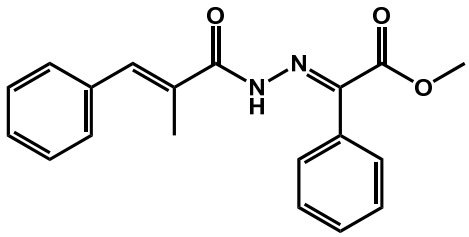
White solid; m.p. 147-149 ºC; ^{1}H NMR (300 MHZ, $(CD_3)_2SO$): δ 10.50 (s, 1H), 7.72 – 7.56 (m, 3H), 7.56 – 7.47 (m, 3H), 7.47 – 7.39 (m, 3H), 7.39 – 7.29 (m, 2H), 7.06 (m, 1H), 5.04 (hept, *J* = 6.3 Hz, 1H), 1.26 (d, *J* = 6.3 Hz, 6H); ^{13}C NMR (75 MHZ, $(CD_3)_2SO$): δ 163.32, 134.62, 130.21, 130.05, 129.81, 129.01, 128.90, 128.71, 127.97, 69.05, 21.73; IR (KBr): υ 3175, 1709, 1670, 1618, 1589; MS (ESI): *m/z* ($[M+H]^+$): 337; Elemental analysis calcd (%) for $C_{20}H_{20}N_2O_3$: C 71.41, H 5.99, N 8.33; found (%): C 70.97, H 5.83, N 8.20

(*E*)-isopropyl 2-(2-(4-methoxycinnamoyl)-hydrazono)-2-phenylacetate (24)



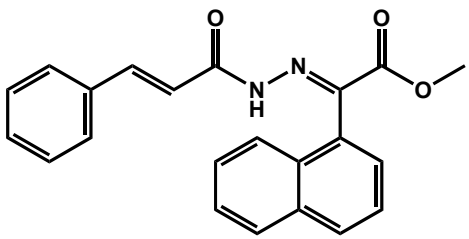
White solid; m.p. 165-167 ºC; ^{1}H NMR (400 MHZ, $CDCl_3$): δ 8.69 (s, 1H), 7.81 (d, *J* = 16.0 Hz, 1H), 7.59 (d, *J* = 8.0 Hz, 2H), 7.56 – 7.43 (m, 4H), 7.29 (d, *J* = 6.8 Hz, 2H), 6.93 (d, *J* = 8.0 Hz, 2H), 5.19 (hept, *J* = 6.0 Hz, 1H), 3.85 (s, 3H), 1.35 (d, *J* = 6.0 Hz, 6H); ^{13}C NMR (101 MHZ, $CDCl_3$): ^{13}C NMR (101 MHz, $CDCl_3$) δ 167.62, 163.45, 161.87, 145.23, 141.31, 130.43, 130.32, 129.69, 129.00, 128.46, 127.72, 114.47, 113.09, 69.94, 55.53, 21.91; IR (KBr): υ 3157, 1705, 1672, 1601, 1591; MS (ESI): *m*/*z* ([M+H]$^{+}$): 367; Elemental analysis calcd (%) for $C_{21}H_{22}N_2O_4$: C 68.84, H 6.05, N 7.65; found (%): C 68.58, H 6.11, N 7.59

(*E*)-methyl 2-(2-((E)-2-methyl-3-phenylacryloyl)hydrazono)-2-phenylacetate (25)



Yellow solid; m.p. 124-126 ºC; ^{1}H NMR (300 MHZ, $(CD_3)_2SO$): δ 10.14 (s, 1H), 7.63 – 7.50 (m, 3H), 7.50 – 7.43 (m, 2H), 7.43 – 7.26 (m, 5H), 7.12 (s, 1H), 3.79 (s, 3H), 1.99 (s, 3H); ^{13}C NMR (75 MHZ, $(CD_3)_2SO$): δ 166.98, 164.23, 143.88, 135.28, 134.81, 130.97, 130.03, 129.69, 129.44, 128.98, 128.66, 128.50, 128.27, 52.67, 14.46; IR (KBr): υ 3348, 1719, 1694, 1624, 1572; MS (ESI): *m*/*z* ([M+H]$^{+}$): 323; Elemental analysis calcd (%) for $C_{19}H_{18}N_2O_3$: C 70.79, H 5.63, N 8.69; found (%): C 70.61, H 5.65, N 8.57

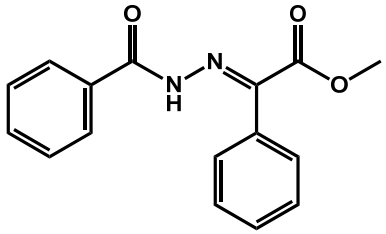
(*E*)-methyl 2-(2-cinnamoylhydrazono)-2-(naphthalen-1-yl)acetate (26)



White solid; m.p. 211-213 ºC; ^{1}H NMR (400 MHZ, $CDCl_3$): δ 8.42 (s, 1H), 8.02 (d, *J* = 8.0 Hz, 1H), 7.96 (d, *J* = 8.0 Hz, 1H), 7.84 (d, *J* = 16.0 Hz, 1H), 7.67 (m, 2H), 7.63 – 7.57 (m, 2H), 7.57 – 7.49 (m, 3H), 7.49 – 7.38 (m, 4H), 3.89 (s, 3H); ^{13}C NMR (101 MHZ, $CDCl_3$): δ 167.20, 164.41, 145.83, 140.79, 134.82, 134.17, 131.12, 130.66, 129.93, 129.18, 129.01, 128.71,

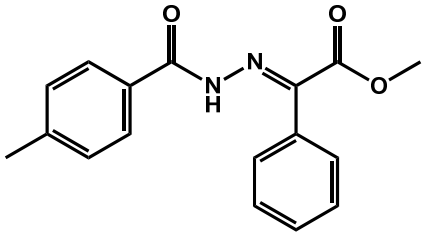
127.98, 127.33, 127.18, 126.48, 125.76, 124.07, 115.43, 53.12; IR (KBr): υ 3223, 1740, 1680, 1634, 1576; MS (ESI): *m*/*z* ([M+H]$^+$): 359; Elemental analysis calcd (%) for $C_{22}H_{18}N_2O_3$. $^1/_4H_2O$: C 72.51, H 5.16, N 7.69; found (%): C 72.66, H 4.94, N 7.71

(*E*)-methyl 2-(2-benzoylhydrazono)-2-phenylacetate (27)



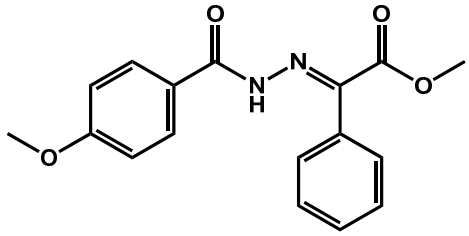
Pale yellow solid; m.p. 145-147 ºC; ^{1}H NMR (300 MHZ, $(CD_3)_2SO$): δ 10.66 (s, 1H), 7.68 (d, *J* = 7.5 Hz, 2H), 7.63 – 7.50 (m, 4H), 7.50 – 7.36 (m, 4H), 3.79 (s, 3H); ^{13}C NMR (75 MHZ, $(CD_3)_2SO$): δ 165.09, 164.34, 144.44, 133.02, 132.16, 130.03, 129.93, 128.96, 128.75, 128.44, 128.19, 52.70; IR (KBr): υ 3057, 1735, 1699, 1678; MS (ESI): *m*/*z* ([M+H]$^+$): 283; Elemental analysis calcd (%) for $C_{16}H_{14}N_2O_3$: C 68.07, H 5.00, N 9.92; found (%): C 67.66, H 5.03, N 9.85

(*E*)-methyl 2-(2-(4-toluoyl)-hydrazono)-2-phenylacetate (28)



White solid; m.p. 132-134 ºC; ^{1}H NMR (300 MHZ, $(CD_3)_2SO$): δ 10.50 (s, 1H), 7.65 – 7.50 (m, 5H), 7.50 – 7.44 (m, 2H), 7.27 (d, *J* = 7.5 Hz, 2H), 3.79 (s, 3H), 2.34 (s, 3H); ^{13}C NMR (75 MHZ, $(CD_3)_2SO$): δ 164.71, 164.28, 144.22, 142.39, 130.04, 129.99, 129.84, 128.95, 128.70, 128.20, 52.68, 21.05; IR (KBr): υ 3179, 1717, 1643, 1609; MS (ESI): *m*/*z* ([M+H]$^+$): 297; Elemental analysis calcd (%) for $C_{17}H_{16}N_2O_3$: C 68.91, H 5.44, N 9.45; found (%): C 68.93, H 5.58, N 9.34

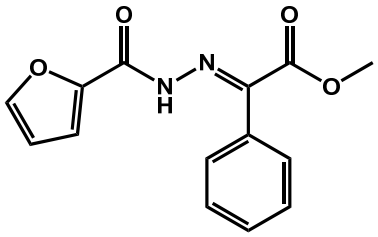
(*E*)-methyl 2-(2-(4-methoxybenzoyl)-hydrazono)-2-phenylacetate (29)



Yellow pale solid; m.p. 151-153 ºC; ^{1}H NMR (300 MHZ, $(CD_3)_2SO$): δ 10.42 (s, 1H), 7.68 (d, *J* = 8.7 Hz, 2H), 7.61 – 7.50 (m, 3H), 7.50 – 7.43 (m, 2H), 7.00 (d, *J* = 8.7 Hz, 2H), 3.80 (s, 3H),

3.79 (s, 3H); ^{13}C NMR (75 MHZ, $(CD_3)_2SO$): δ 164.31, 164.10, 162.41, 143.85, 130.29, 129.99, 129.85, 128.99, 128.71, 124.77, 113.75, 55.51, 52.56; IR (KBr): υ 3167, 1720, 1649, 1600; MS (ESI): *m*/*z* ($[M+H]^+$): 313; Elemental analysis calcd (%) for $C_{17}H_{16}N_2O_4$. $^1/_4H_2O$: C 64.14, H 5.28, N 8.80; found (%): C 64.2, H 5.14, N 8.66

(*E*)-methyl 2-(2-(2-furoyl)-hydrazono)-2-phenylacetate (30)



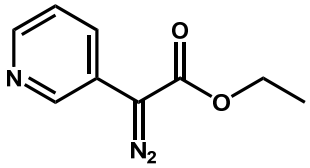
Pale yellow solid; m.p. 146-148 ºC; ^{1}H NMR (400 MHZ, $(CD_3)_2SO$): δ 10.28 (s, 1H), 7.92 (m, 1H), 7.62 – 7.49 (m, 4H), 7.49 – 7.40 (m, 2H), 6.74 – 6.68 (m, 1H), 3.80 (s, 3H); ^{13}C NMR (101 MHZ, $(CD_3)_2SO$): δ 164.00, 146.90, 145.38, 130.26, 129.31, 129.10, 128.70, 112.54, 52.81; IR (KBr): υ 3123, 1697, 1678, 1581; MS (ESI): *m*/*z* ($[M+H]^+$): 273; Elemental analysis calcd (%) for $C_{14}H_{12}N_2O_4$: C 61.76, H 4.44, N 10.29; found (%): C 61.3, H 4.6, N 9.88

6. Spectra data for new diazo compound

All diazo compounds used in this scientific work are described on the literature[4-9], with the exception of:

Ethyl 2-diazo-2-(3-pyridin)acetate

NOTE: This diazo coumpound was synthesized according to this experimental procedure described in the literarure.[6]

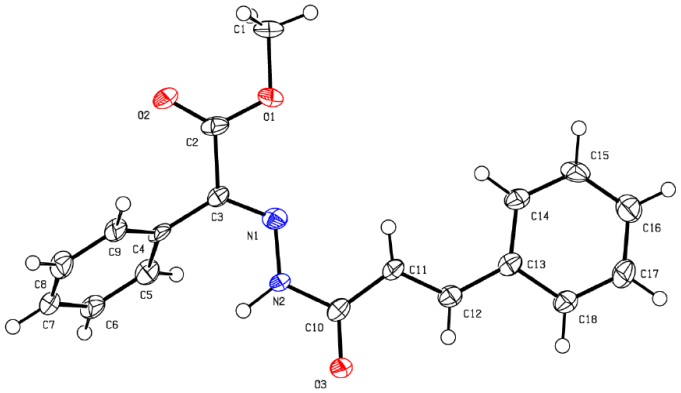


Yield: 91%; Yellow solid; m.p. 34-36 ºC; ^{1}H NMR (400 MHZ, $CDCl_3$): δ 8.66 (d, *J* = 1.6 Hz, 1H), 8.39 (d, *J* = 4.4 Hz, 1H), 7.86 (d, *J* = 8.0 Hz, 1H), 7.28 (dd, *J* = 8.0, 4.4 Hz, 1H), 4.33 (q, *J* = 7.2 Hz, 2H), 1.33 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (101 MHZ, $CDCl_3$): δ 164.68, 146.75, 144.84, 131.32, 123.75, 122.84, 100.21, 61.75, 14.55; IR (KBr): υ 2093, 1701; MS (ESI): *m*/*z* ($[M+H]^+$): 192; Elemental analysis calcd (%) for $C_9H_9N_3O_2$: C 56.54, H 4.74, N 21.98; found (%): C 56.31, H 4.9, N 21.99

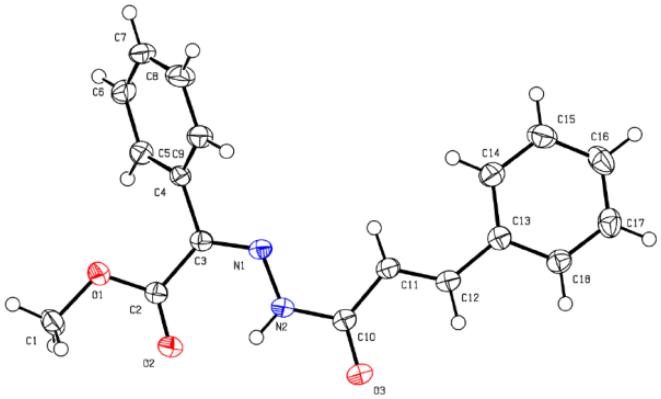
7. X-ray crystal structures of *N*-Acylhydrazones 3 and 12

Crystals of **3** and **12** suitable for X-ray diffraction studies were mounted on a loop with protective oil. X-ray data were collected at 150K on a Bruker AXS-KAPPA APEX II diffractometer using graphite monochromated Mo-Kα radiation (λ=0.71069 Å) and operating at 50kV and 30 mA. Cell parameters were retrieved using Bruker SMART[10] software and refined using Bruker SAINT[11] on all observed reflections. Absorption corrections were applied using SADABS[12]. Structure solution and refinement were performed using direct methods with program SIR97[13] and SHELXL97[14], both included in the package of programs WINGX-Version 1.80.05[15]. A full-matrix least-squares refinement was used for the non-hydrogen atoms with anisotropic thermal parameters. All H_{CH} atoms were inserted in idealized positions and allowed to refine riding in the parent carbon atom; H_{NH} atoms were located from difference Fourier maps and refined.

Crystallographic data for **3** (CCDC 926916): $C_{18}H_{16}N_2O_3$, fw= 308.33, monoclinic, space group $P2_1/n$, a=5.568(2) Å, b=19.571(6) Å, c=14.136(4) Å, β= 100.68(2) °, V =1513.6(8) $Å^3$, Z=4, T=150K, d_{calc}=1.353 $mg.m^{-3}$, μ = 0.093 mm^{-1}, F(000)=648, colourless crystal (0.22 x 0.03 x 0.02 mm). Of 9272 reflections collected, 2770 were independent (R_{int}= 0.1493); 221 variables refined with 2270 reflections to final R indices $R_1(I > 2\sigma(I))$=0.0909, $wR_2(I > 2\sigma(I))$=0.2000, R_1(all data)=0.2211, wR_2(all data)=0.2422, GOF= 0.890.



Crystallographic data for **12** (CCDC 926917): $C_{18}H_{16}N_2O_3$, fw= 308.33, monoclinic, space group $P2_1/c$, a=9.8190(2) Å, b=17.137(1) Å, c=9.3900(8) Å, β= 99.540(5) °, V =1558.2(2) $Å^3$, Z=4, T=150K, d_{calc}=1.314 $mg.m^{-3}$, μ = 0.091 mm^{-1}, F(000)=648, colourless crystal (0.2 x 0.04 x 0.03 mm). Of 25978 reflections collected, 3563 were independent (R_{int}= 0.0481); 212 variables refined with 3563 reflections to final R indices $R_1(I > 2\sigma(I))$=0.0399, $wR_2(I > 2\sigma(I))$=0.0910, R_1(all data)=0.0679, wR_2(all data)=0.0988, GOF= 1.033.



8. Density functional theory (DFT) calculations for the synthesis of *N*-Acylhydrazone 3

Computational details

All calculations were performed using the Gaussian 09 software package,[16] without symmetry constraints. The PBE0 functional was employed in the geometry optimisations. That functional uses a hybrid generalized gradient approximation (GGA), including 25 % mixture of Hartree-Fock[17] exchange with DFT[18] exchange-correlation, given by Perdew, Burke and Ernzerhof functional (PBE).[19] The optimized geometries were obtained with a standard 6-31G(d,p)[20] basis set. Transition state optimizations were performed with the Synchronous Transit-Guided Quasi-Newton Method (STQN) developed by Schlegel *et al*,[21] following extensive searches of the Potential Energy Surface. Frequency calculations were performed to confirm the nature of the stationary points, yielding one imaginary frequency for the transition states and none for the minima. Each transition state was further confirmed by following its vibrational mode downhill on both sides and obtaining the minima presented on the energy profiles. The electronic energies (E_{b1}) obtained at the PBE0/6-31G(d,p) level of theory were converted to free energy at 298.15 K and 1 atm (G_{b1}) by using zero point energy and thermal energy corrections based on structural and vibration frequency data calculated at the same level.

Single point energy calculations were performed using the M06-2X functional and a standard 6-311++G(d,p)[22] basis set. That is a hybrid meta-GGA functional developped by Truhlar and Zhao,[23] and it was shown to perform very well for main-group kinetics, providing a good description of long range effects such as van der Waals interactions or π-π stacking.[24,25] Solvent effects (dichloroethane) were considered in the M06-2X/6-311G(d,p)//PBE0/6-31G(d,p) energy calculations using the Polarizable Continuum Model (PCM) initially devised by Tomasi and coworkers[26] with radii and non-electrostatic terms of the SMD solvation model, developped by Truhler *et al*.[27]

The free energy values presented along the text (G_{b2}^{soln}) were derived from the electronic energy values obtained at the M06-2X/6-311G(d,p)//PBE0/6-31G(d,p) level, including solvent effects (E_{b2}^{soln}), according to the following expression: $G_{b2}^{soln} = E_{b2}^{soln} + G_{b1} - E_{b1}$

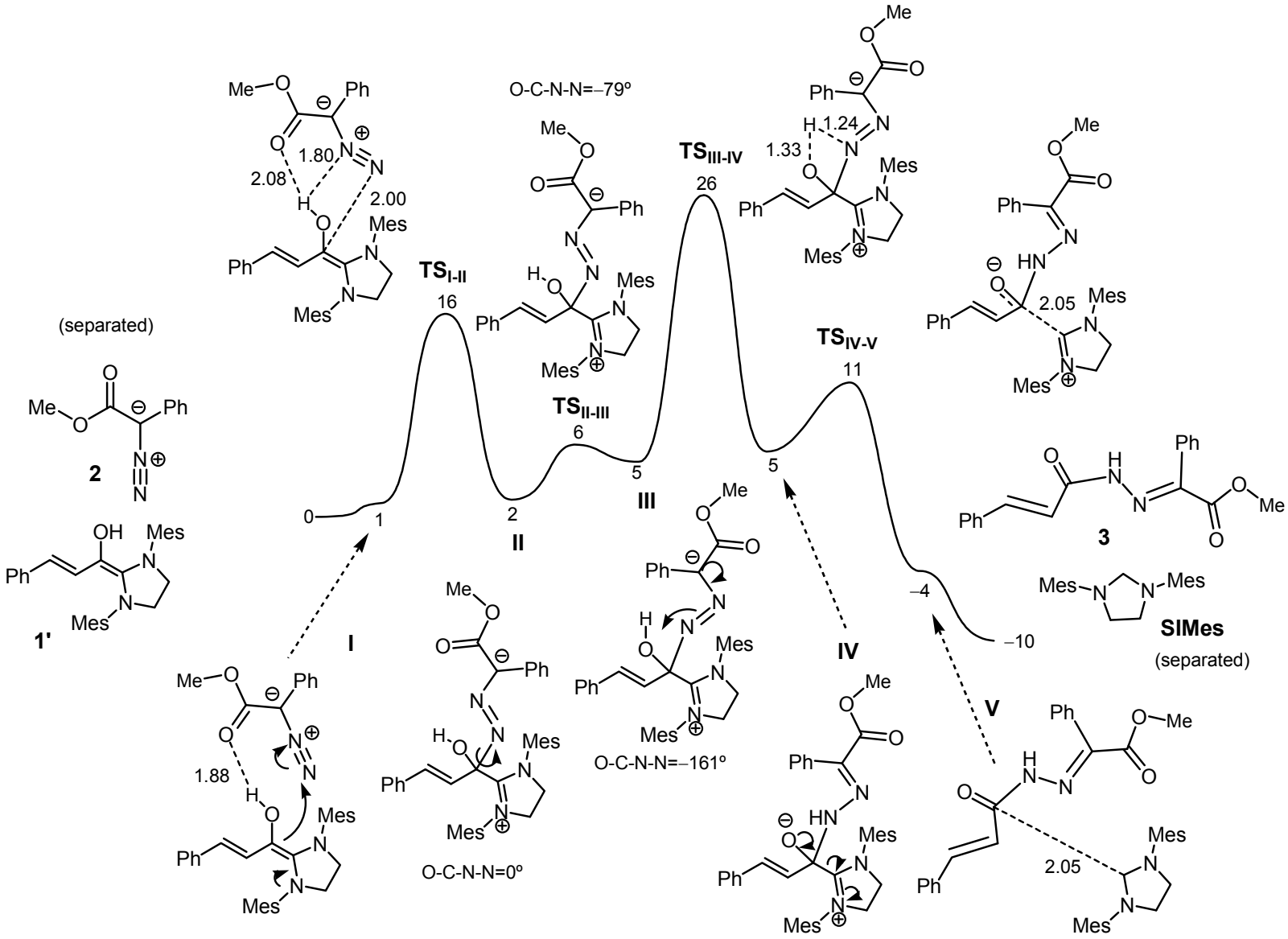


Figure S1. Free energy profile (kcal/mol) calculated for the reaction. Relevant geometric parameters are indicated (distances in Å).

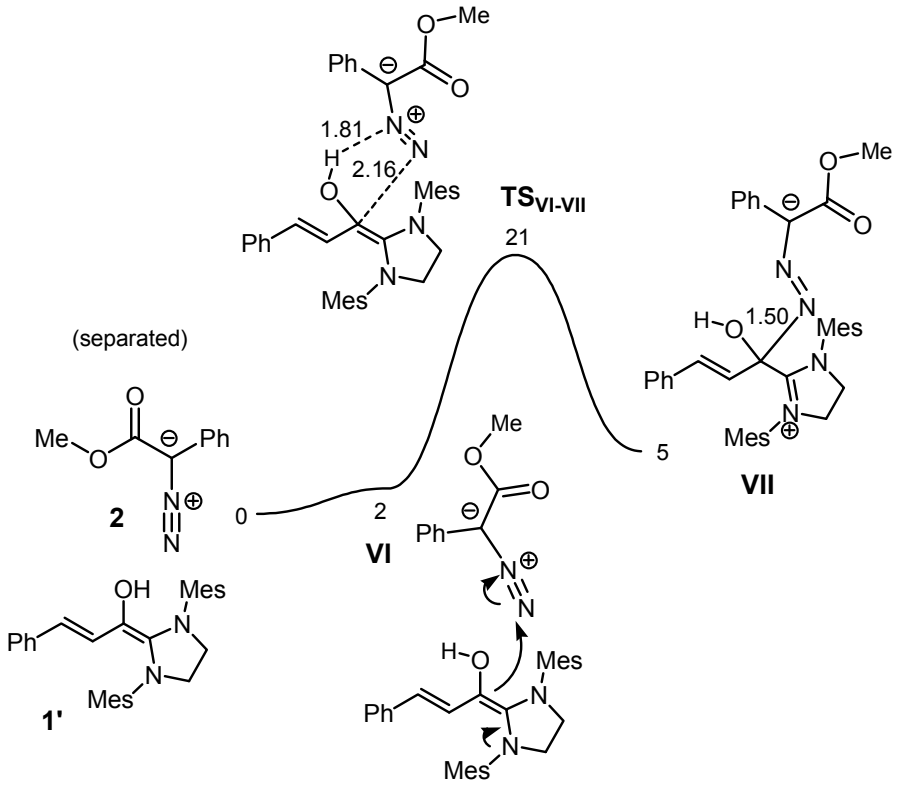


Figure S2. Free energy profile (kcal/mol) calculated for the first step of the reaction with alternative orientation of the reagents. Relevant distances are indicated (Å).

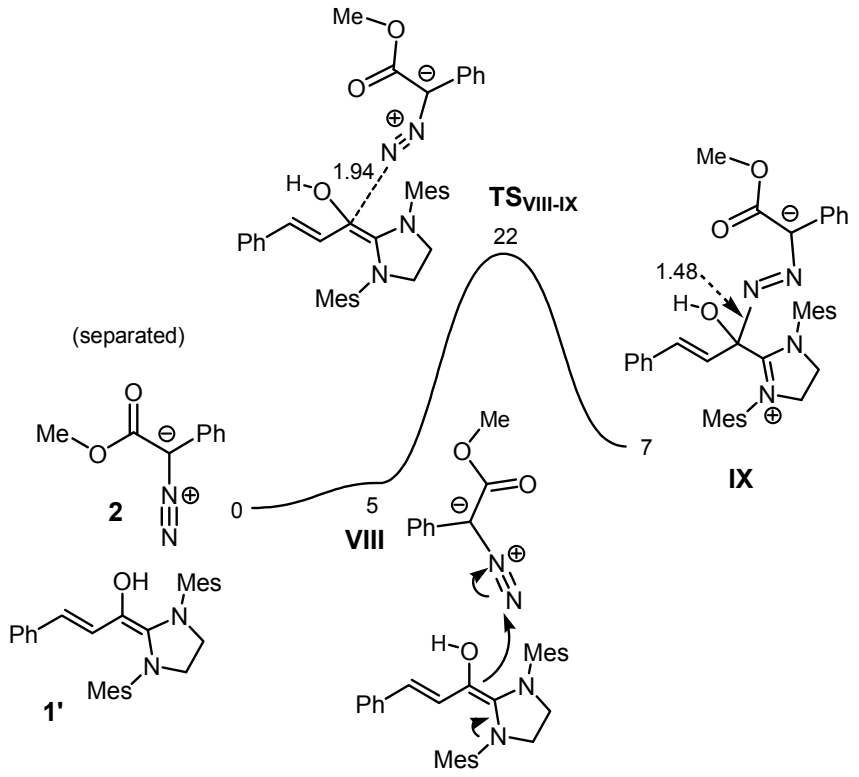


Figure S3. Free energy profile (kcal/mol) calculated for the first step of the reaction with alternative orientation of the reagents. Relevant distances are indicated (Å).

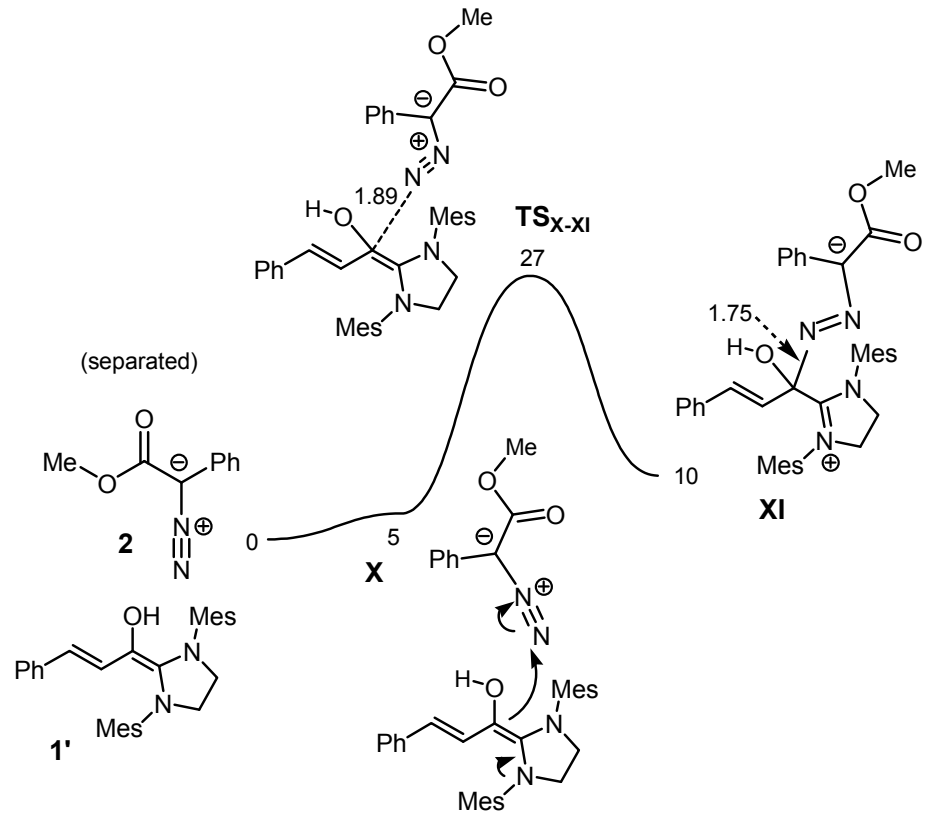


Figure S4. Free energy profile (kcal/mol) calculated for the first step of the reaction with alternative orientation of the reagents. Relevant distances are indicated (Å).

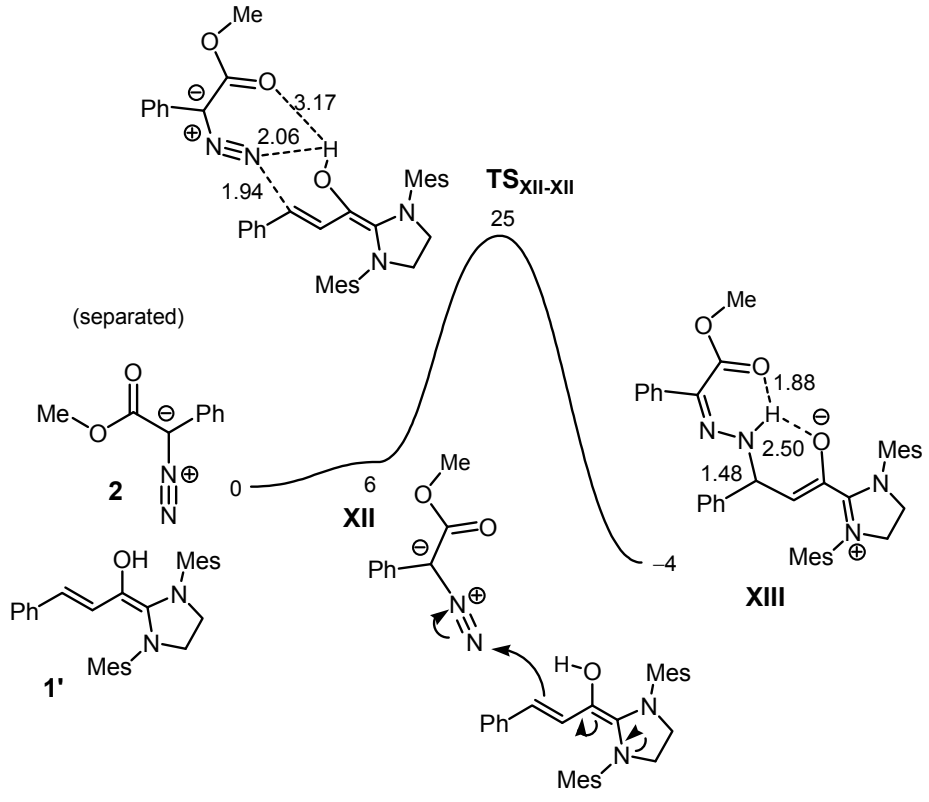


Figure S5. Free energy profile (kcal/mol) calculated for the first step of the reaction of homoenolate attack. Relevant distances are indicated (Å).

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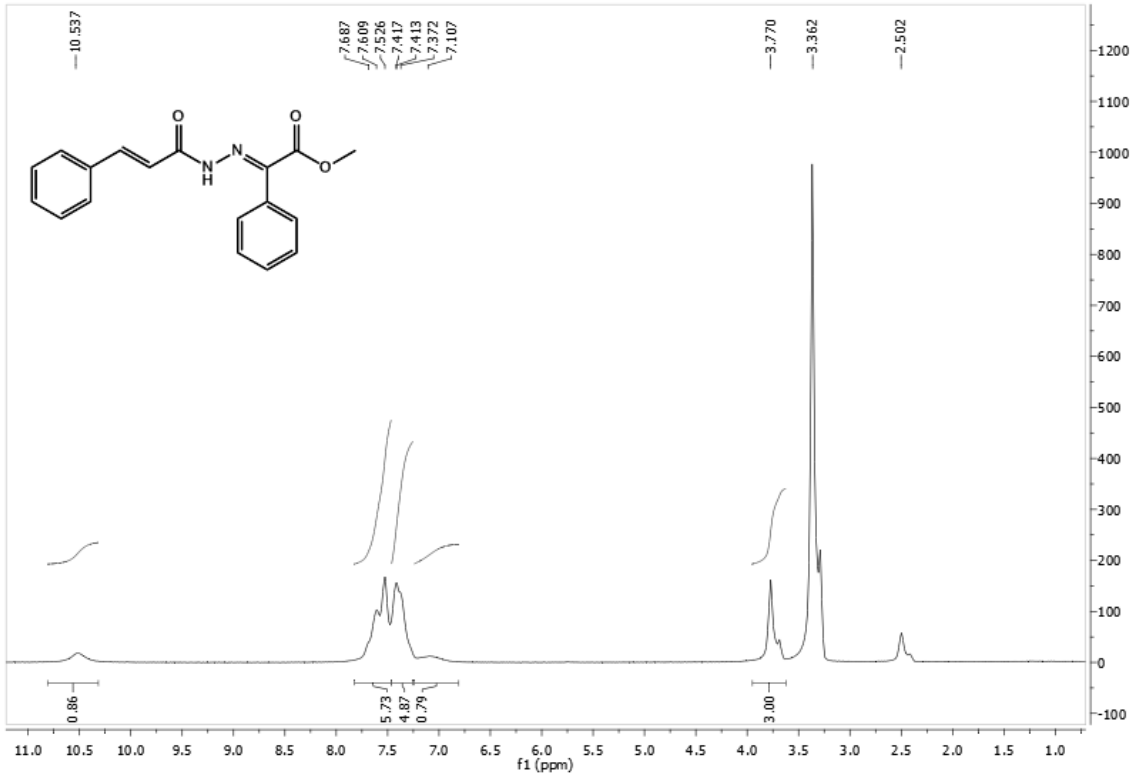
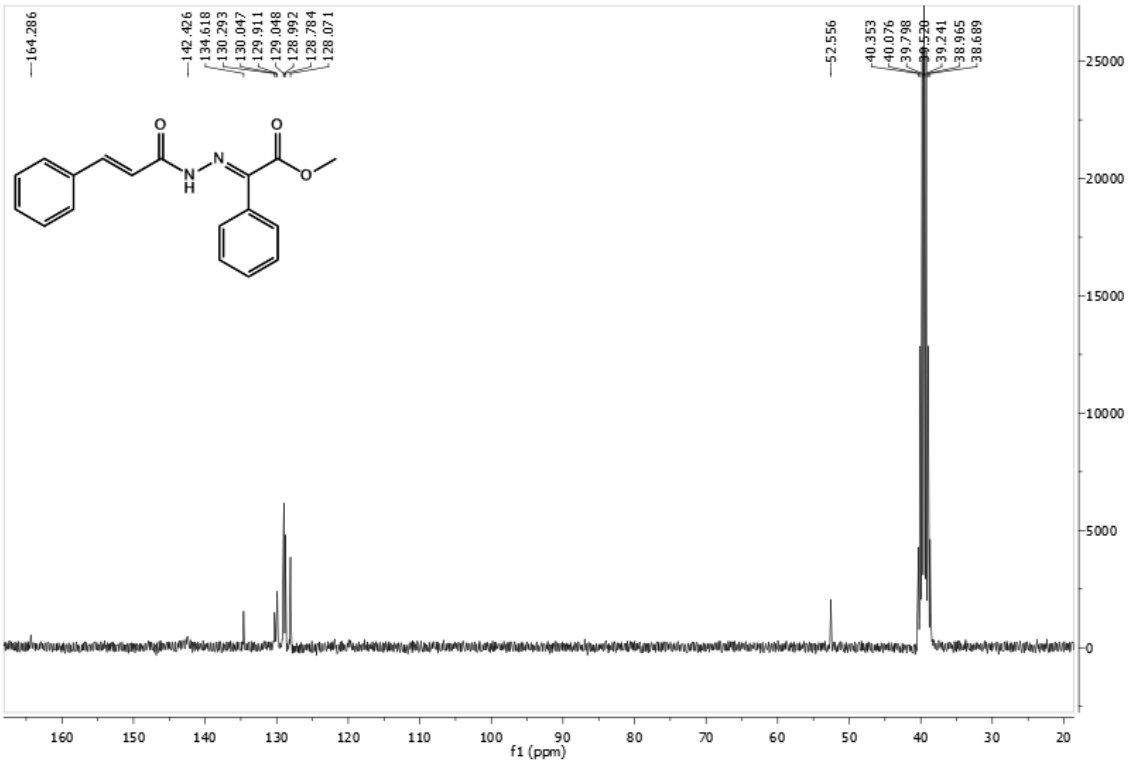
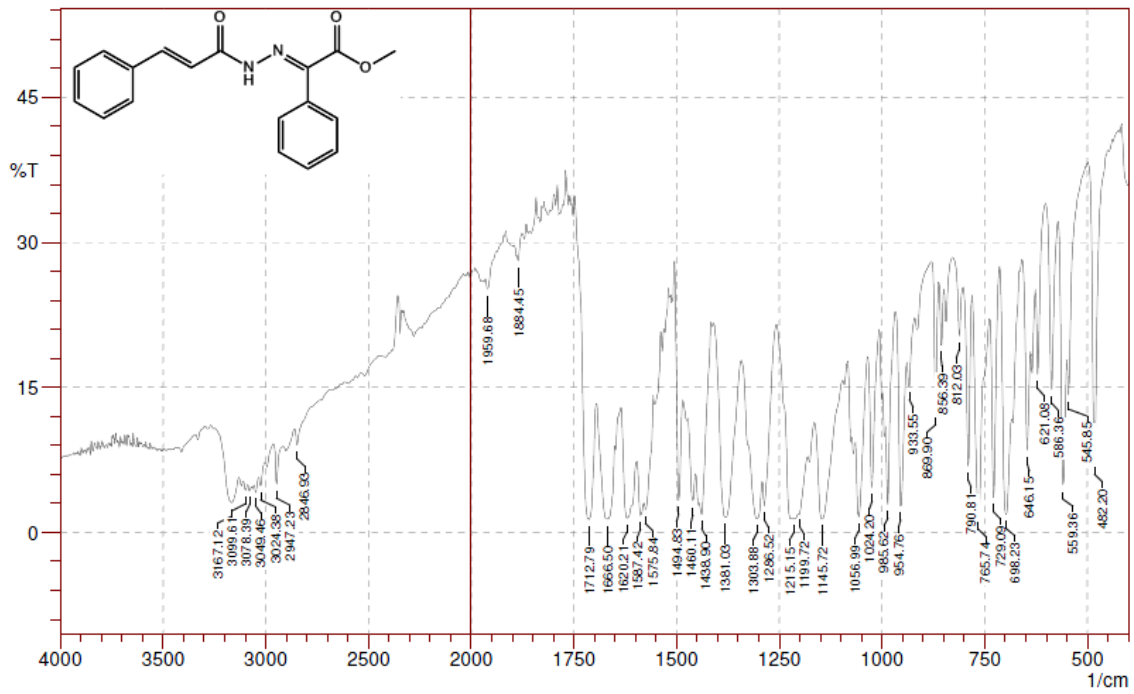
10. Copies of ^{1}H, ^{13}C NMR, infrared and ESI spectra of *N*-Acylhydrazones 3, 12-30 and new diazo compound.

- ***N*-Acylhydrazone (3):**



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3078.39
3049.46
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2947.23
2846.93
1959.68
1884.45
1712.79
1666.50
1620.21
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1494.83
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1381.03
1303.88
1286.52
1215.15
1199.72
1145.72
1056.99
1024.20
985.62
954.76
933.55
869.90
856.39
812.03
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729.09
698.23
646.15
621.08
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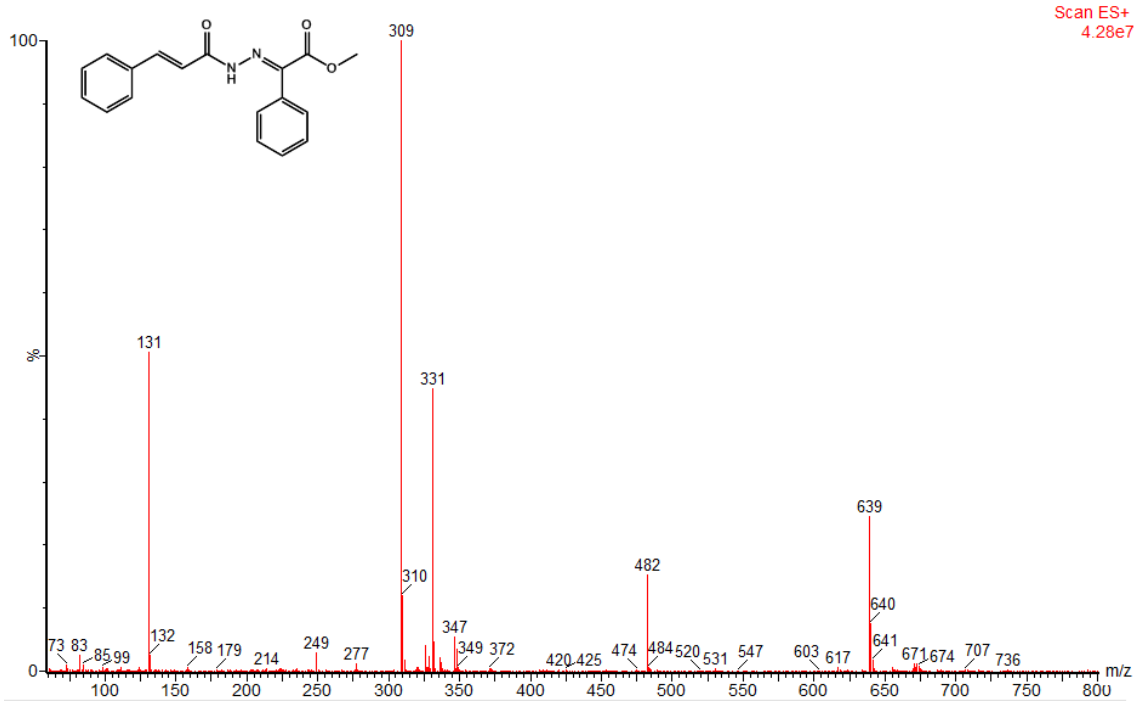
482.20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158
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214
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420
425
474
484
520
531
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603
617
671
674
707
736
m/z
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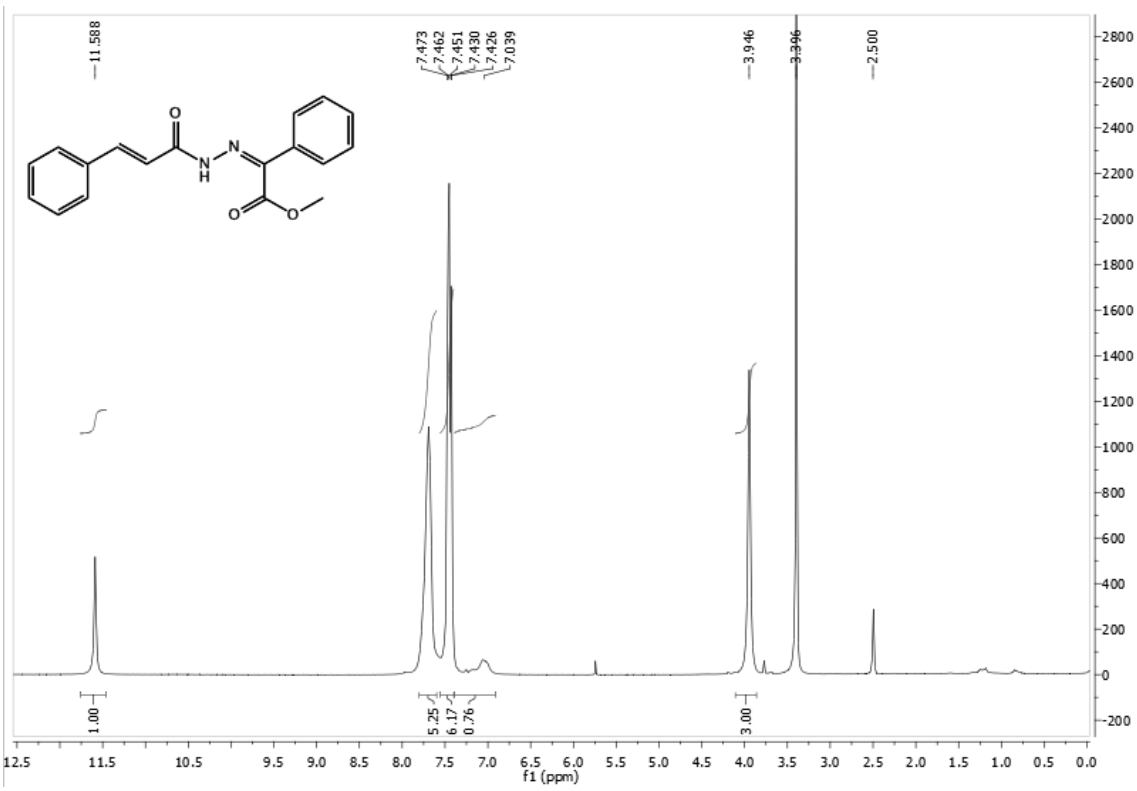
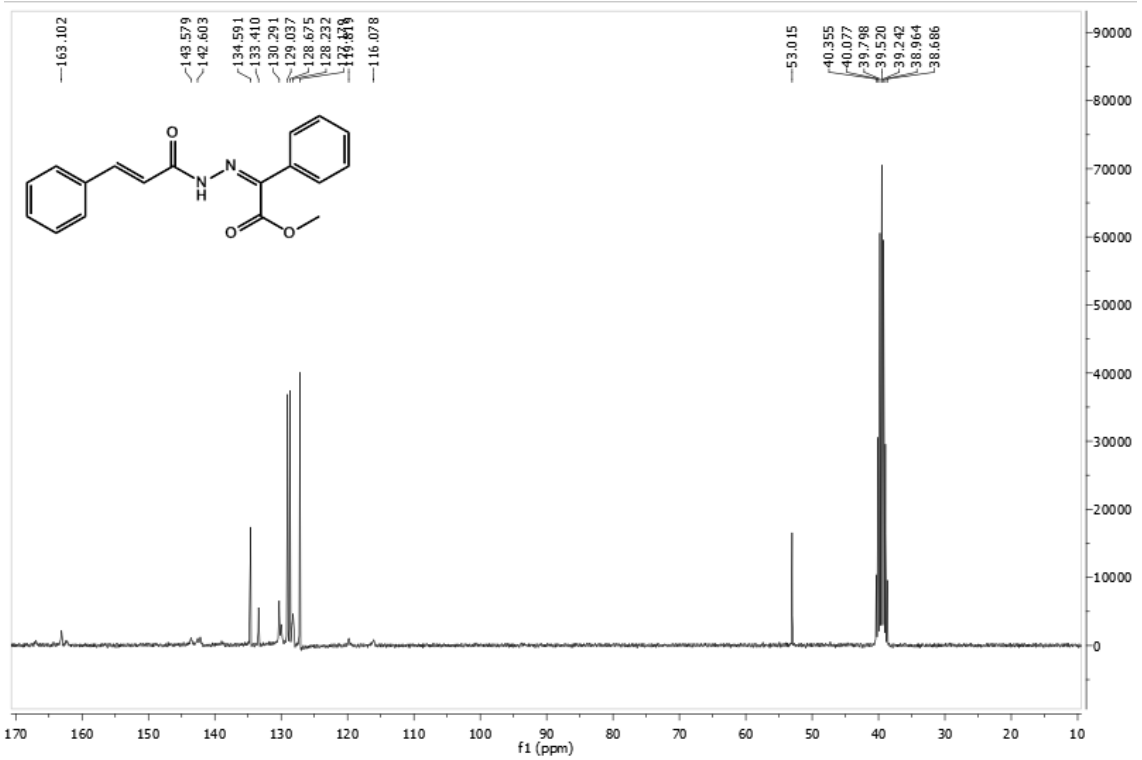
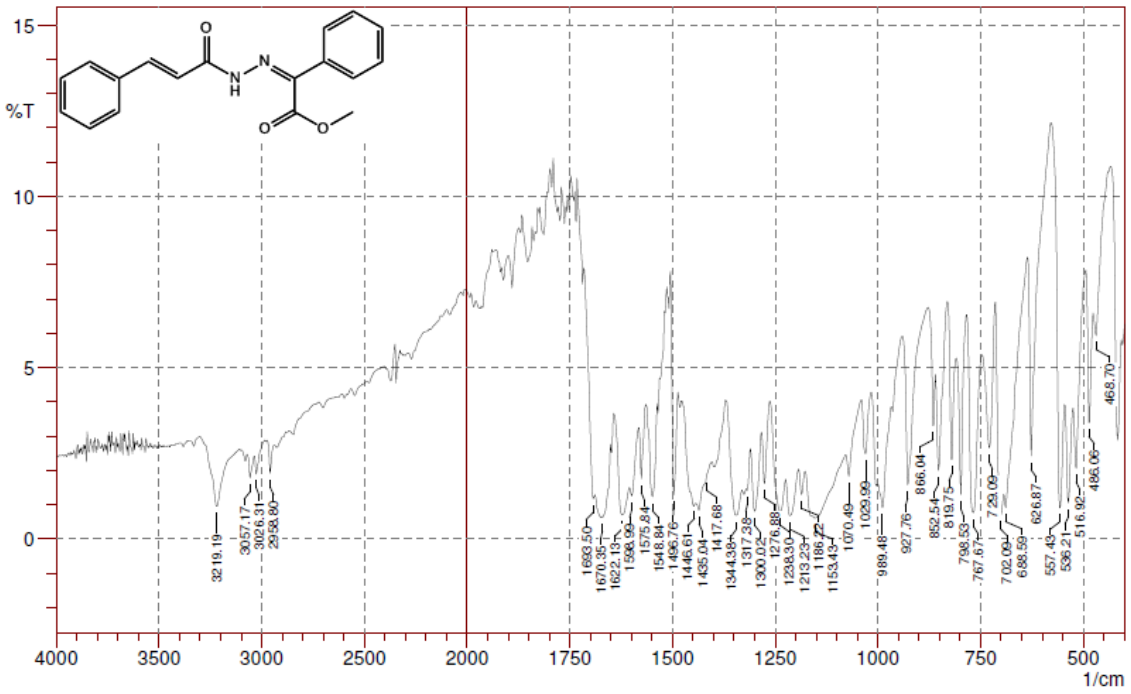
- ***N*-Acylhydrazone (12):**



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750
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3026.31
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1622.13
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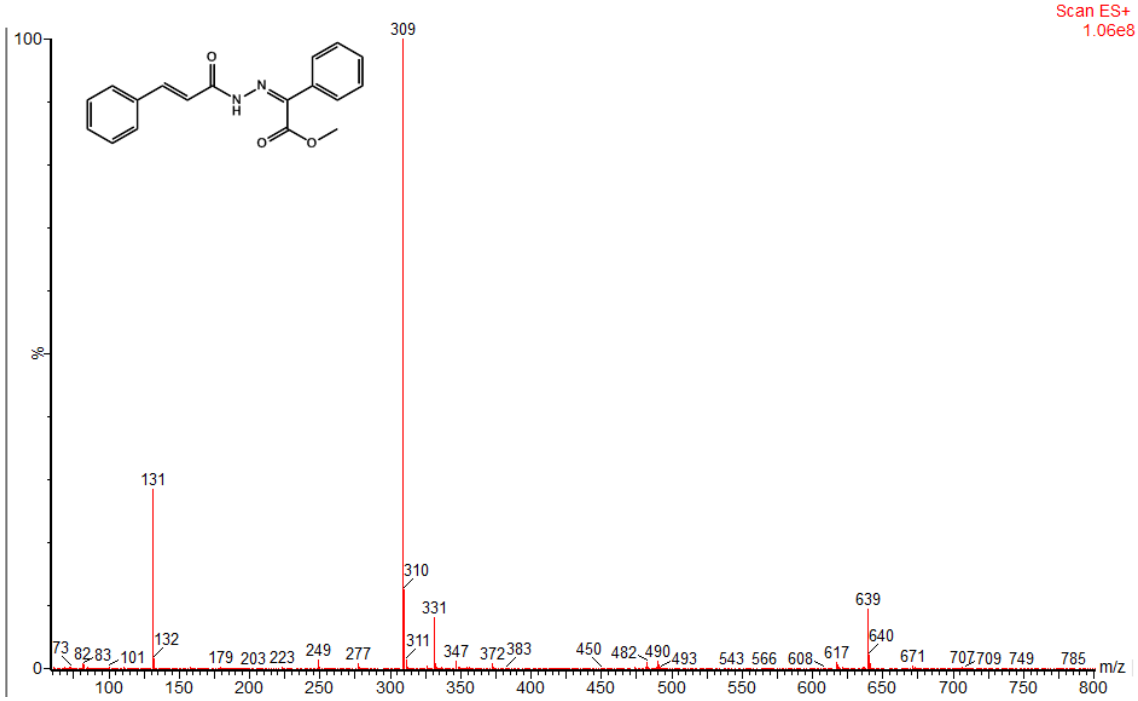
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347
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482
490
493
543
566
608
617
671
707
709
749
785
m/z
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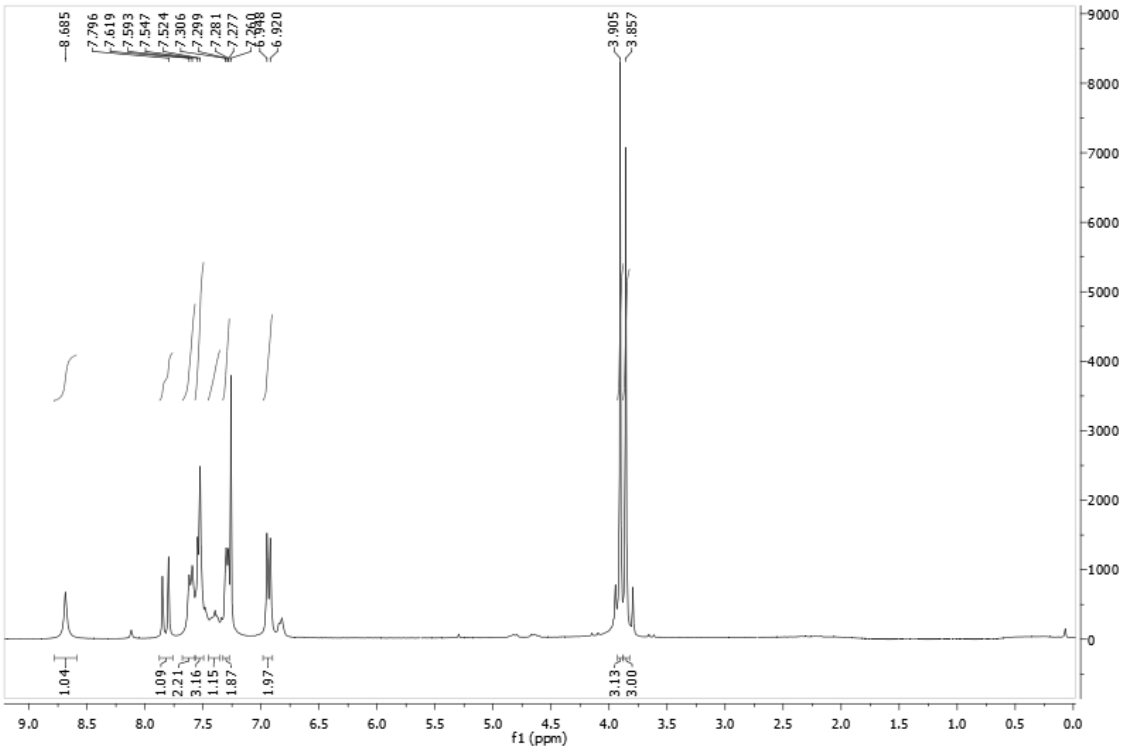
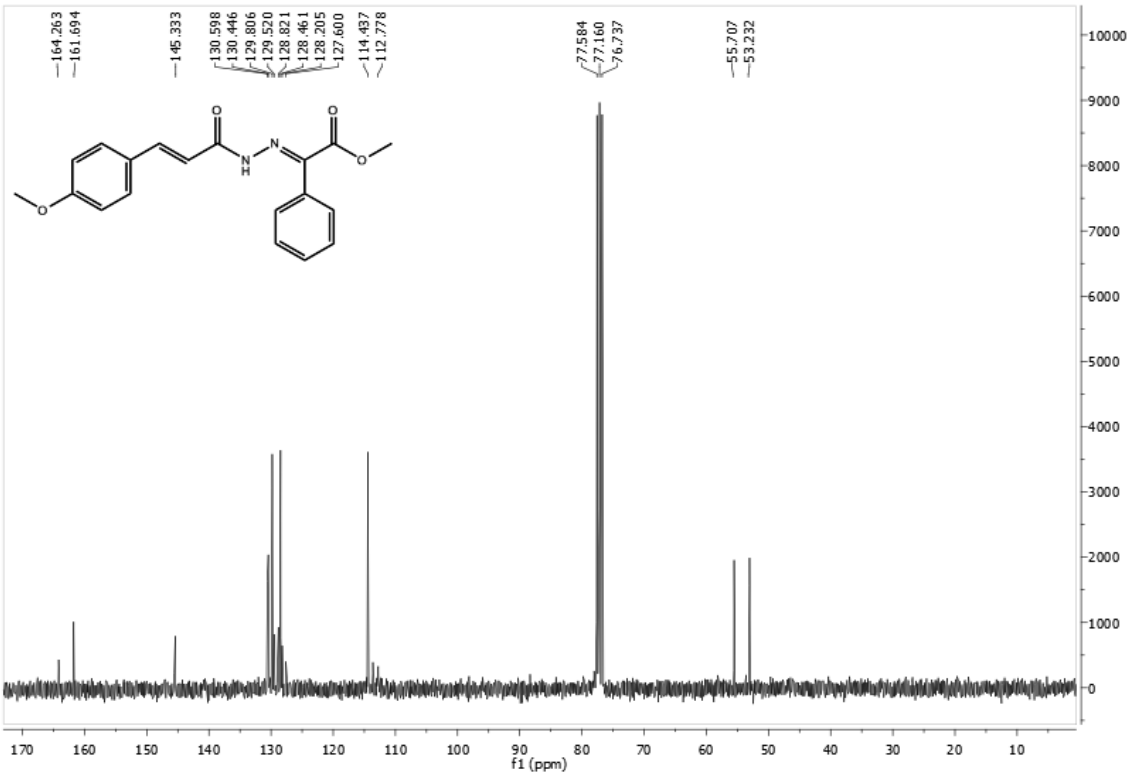
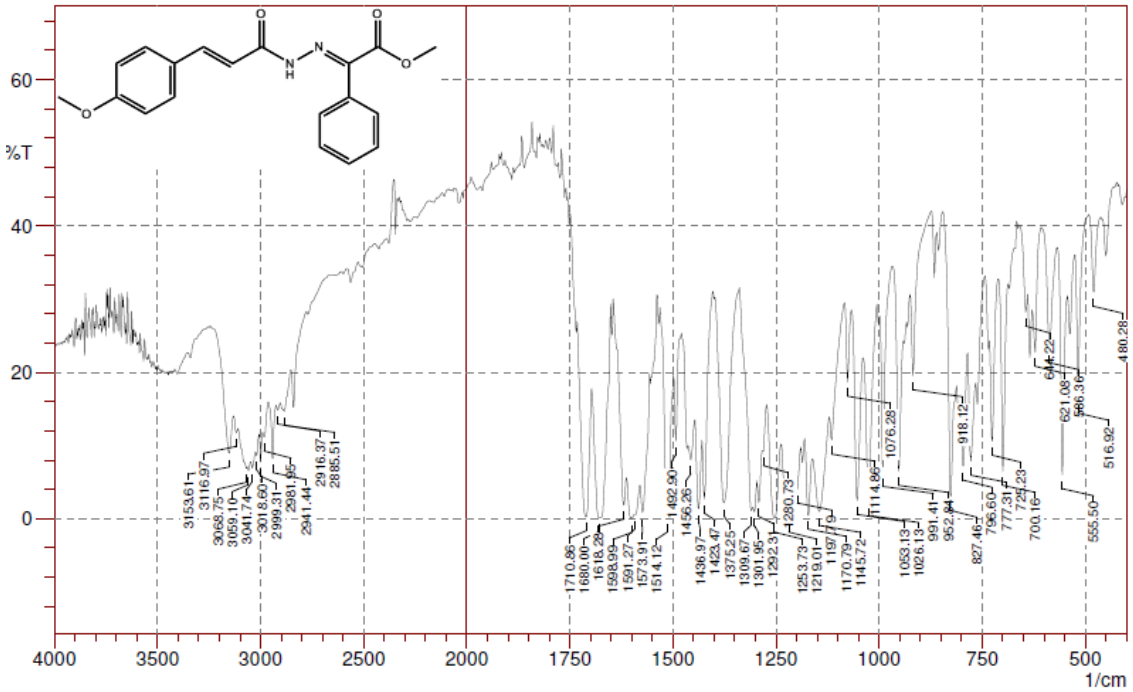
800

- ***N*-Acylhydrazone (13):**



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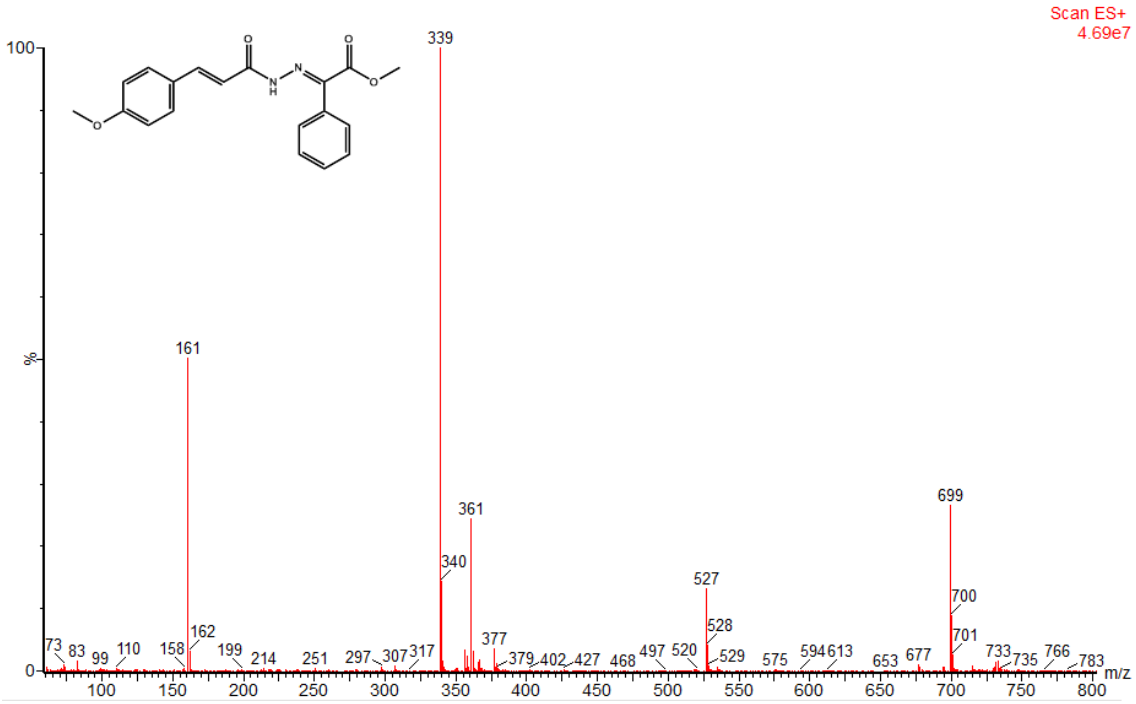
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307
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735
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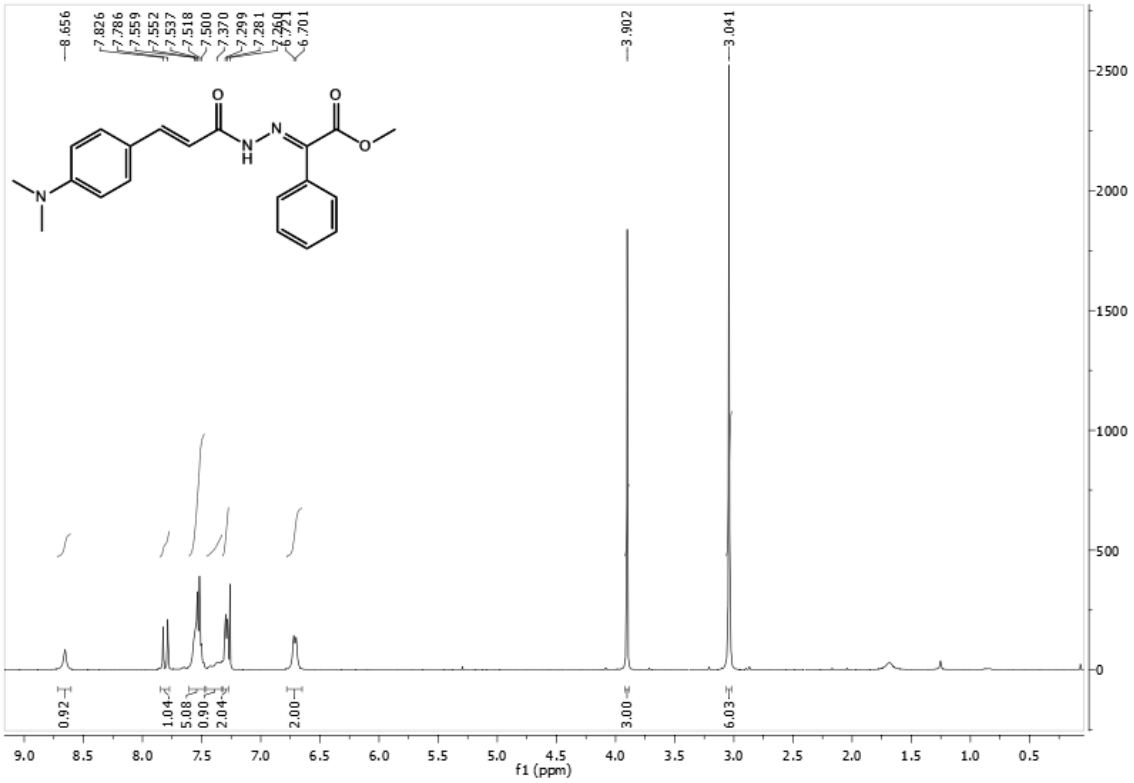
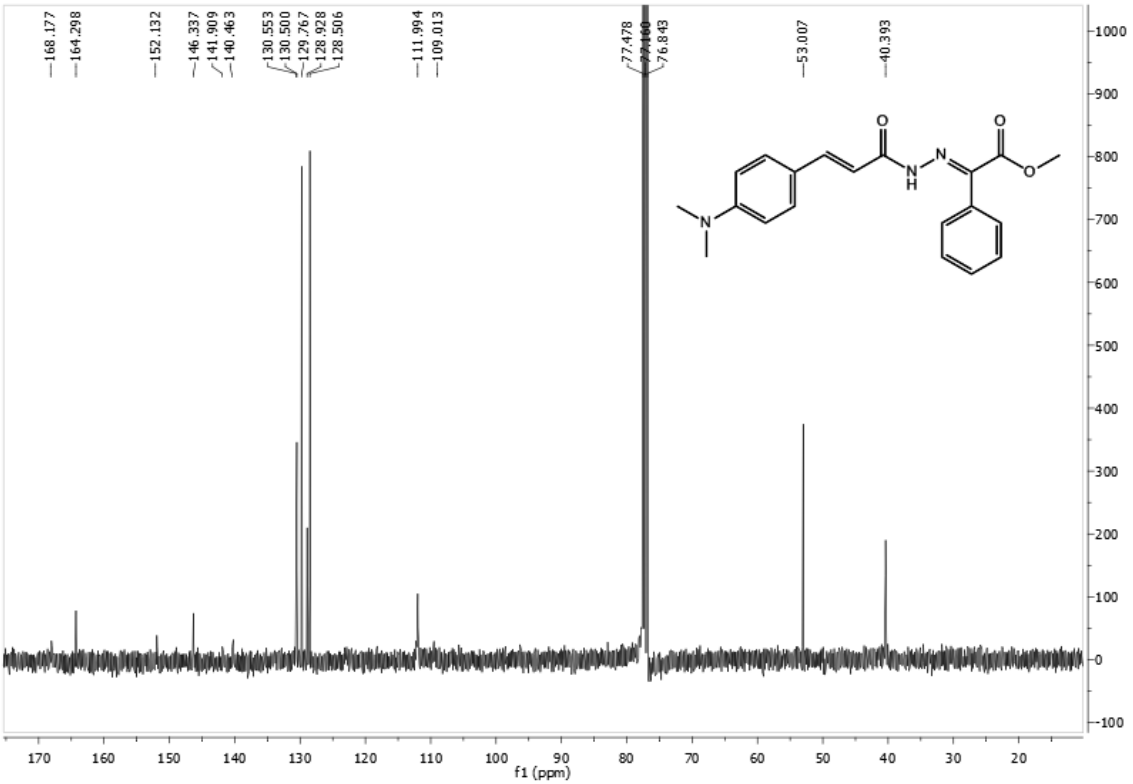
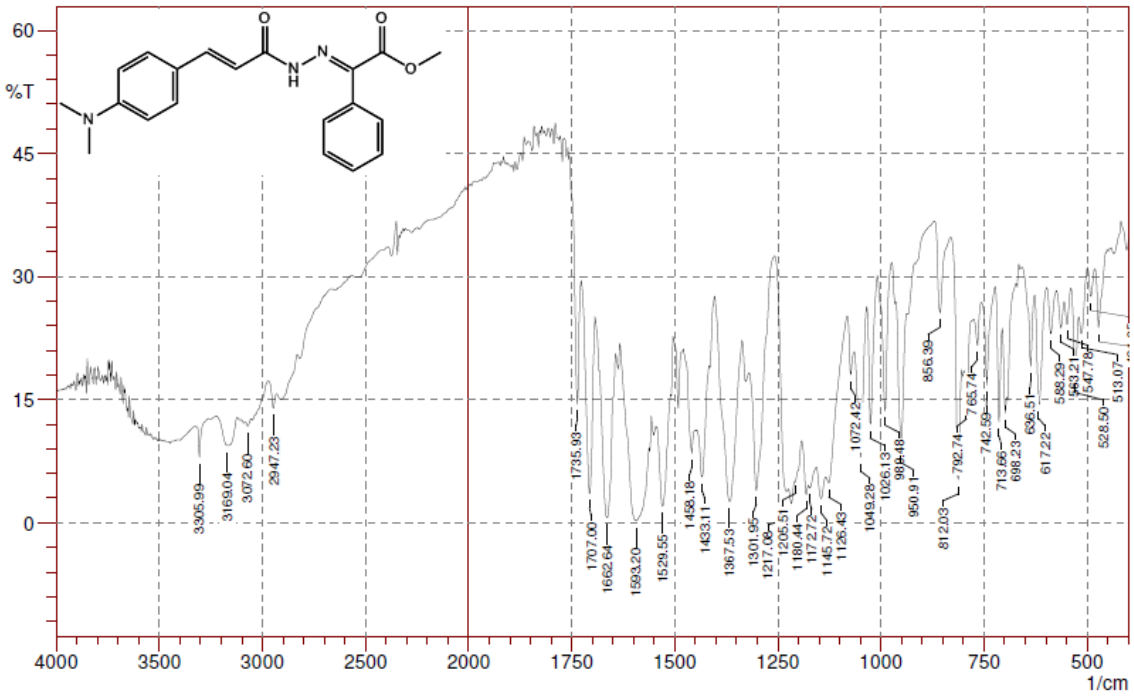
- ***N*-Acylhydrazone (14):**



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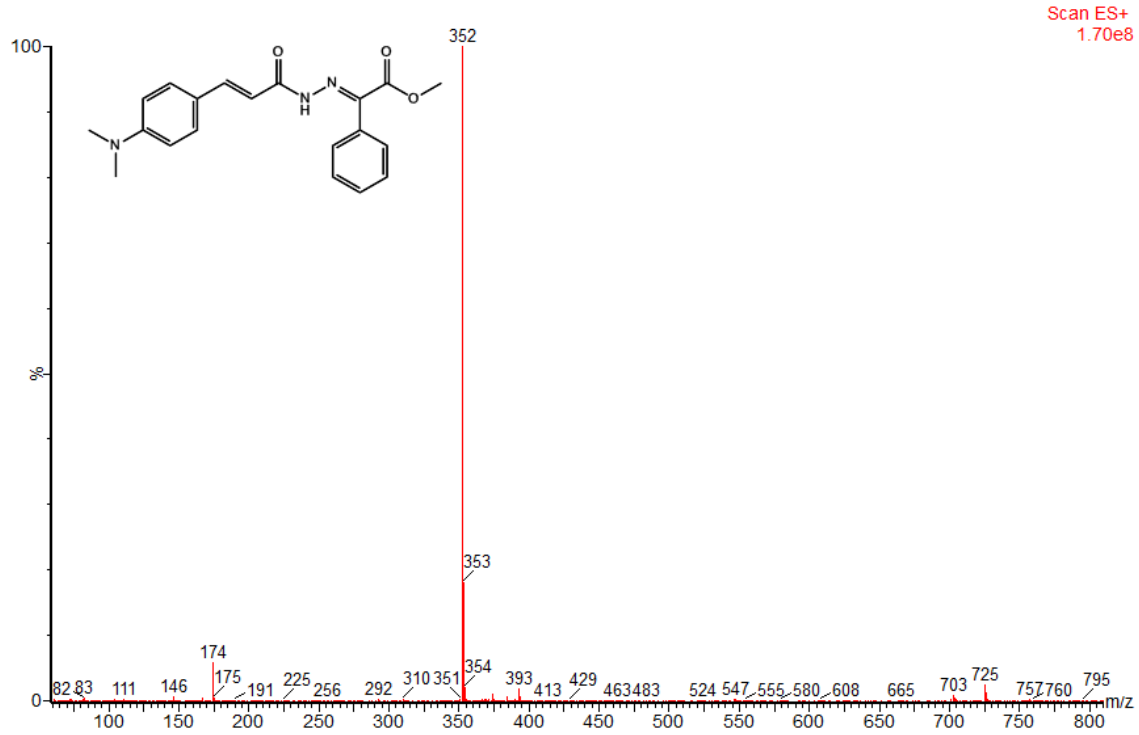
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m/z
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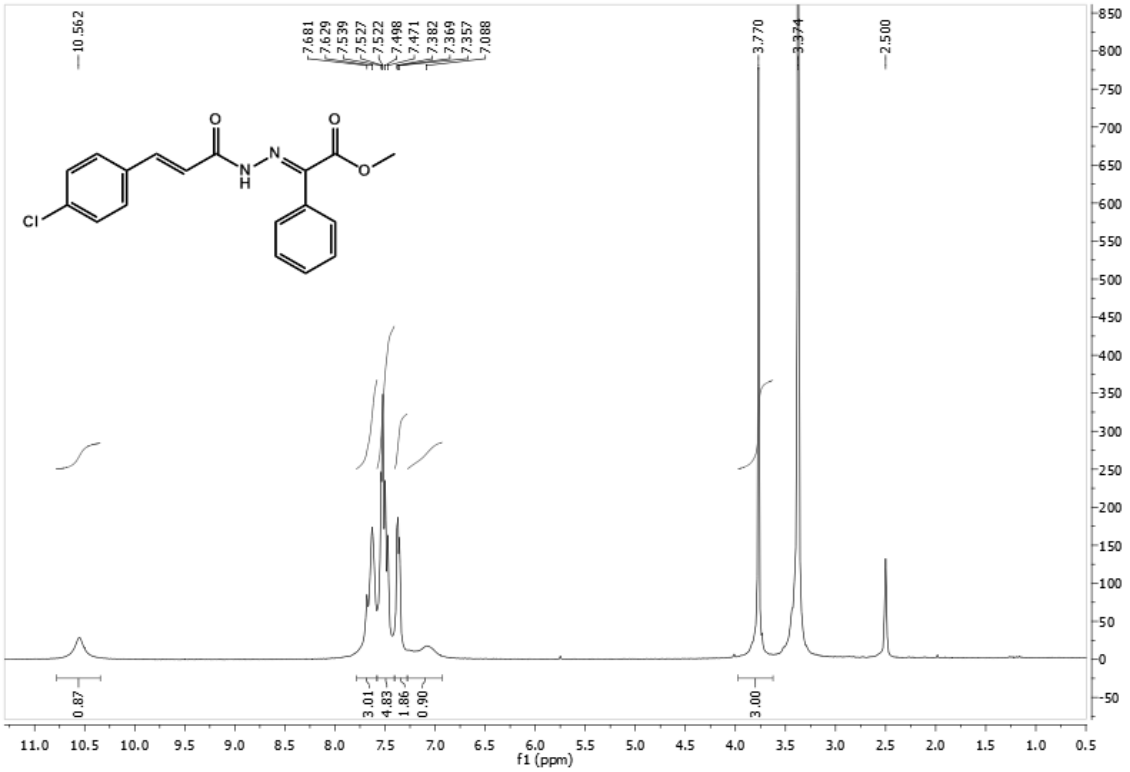
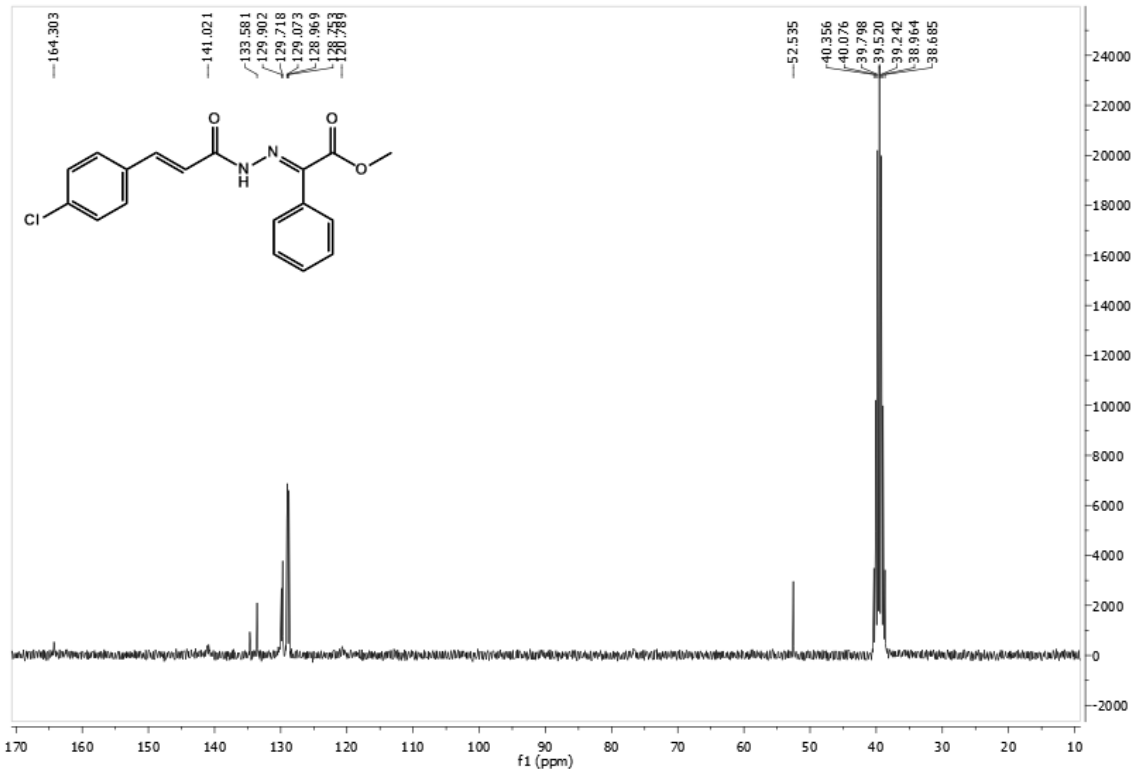
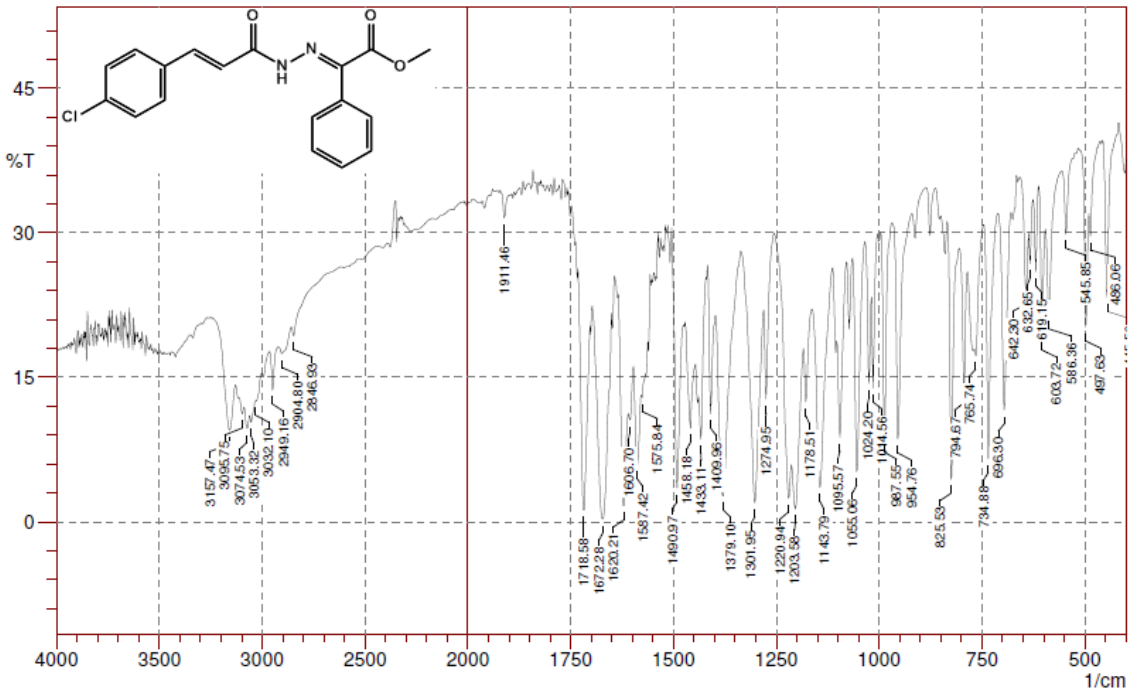
- ***N*-Acylhydrazone (15):**



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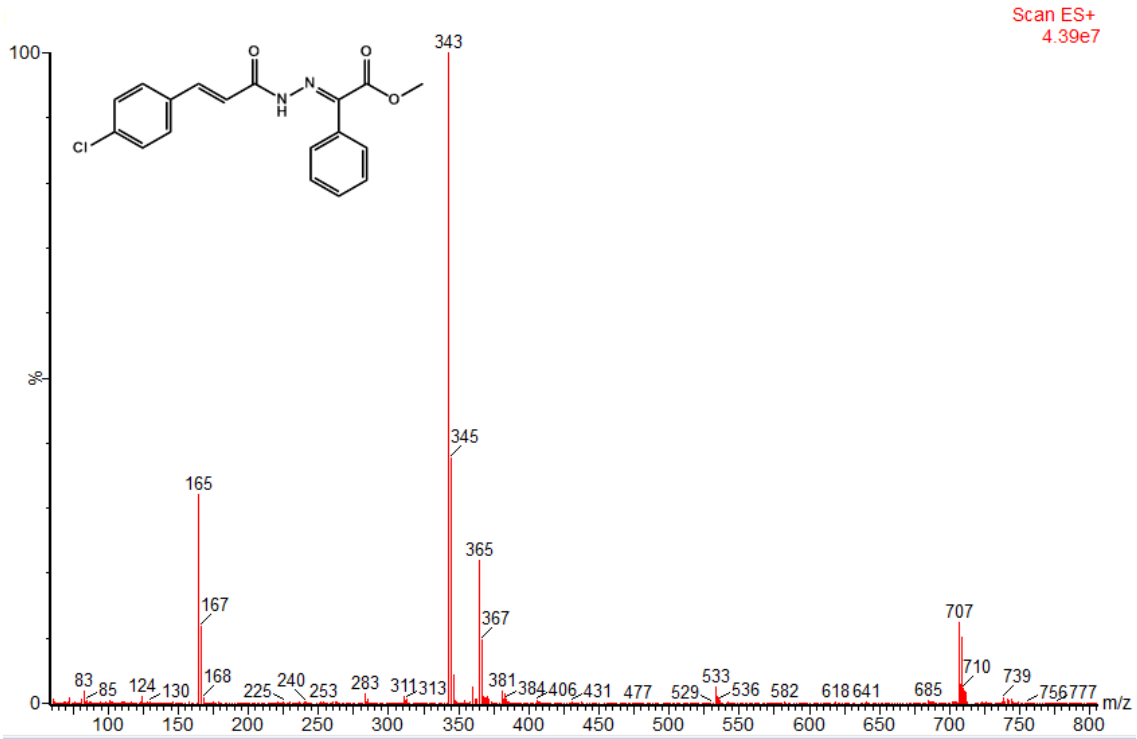
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756
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m/z
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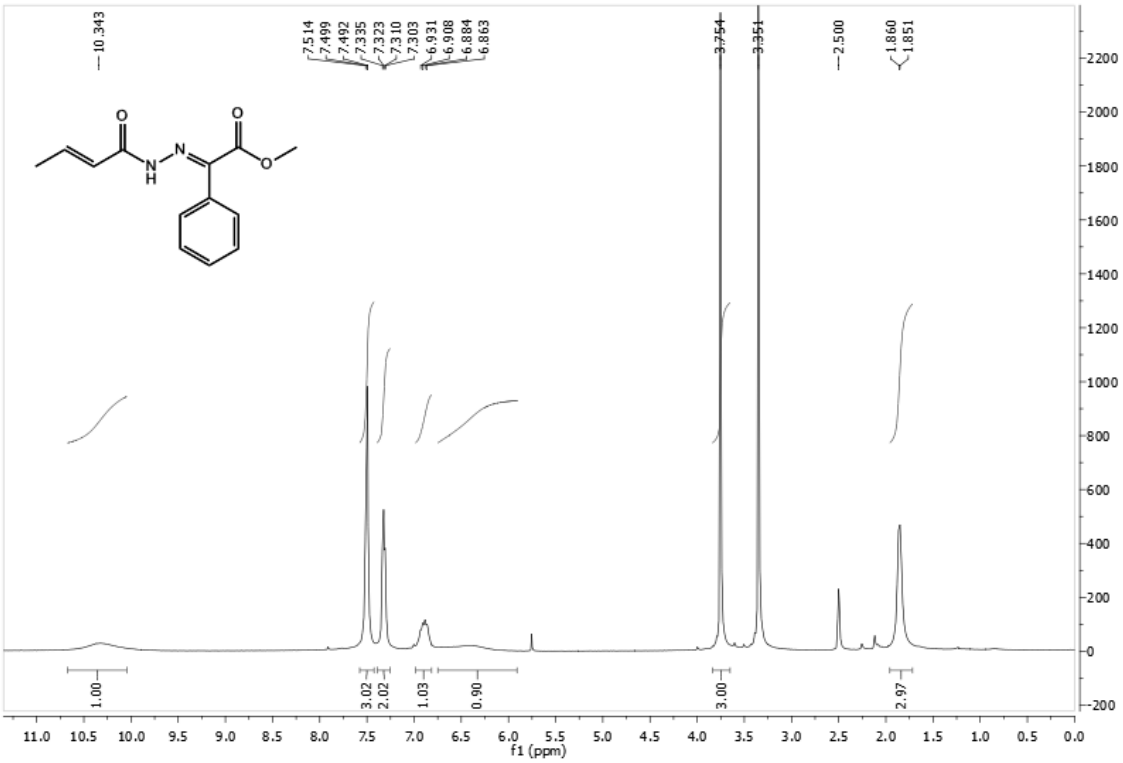
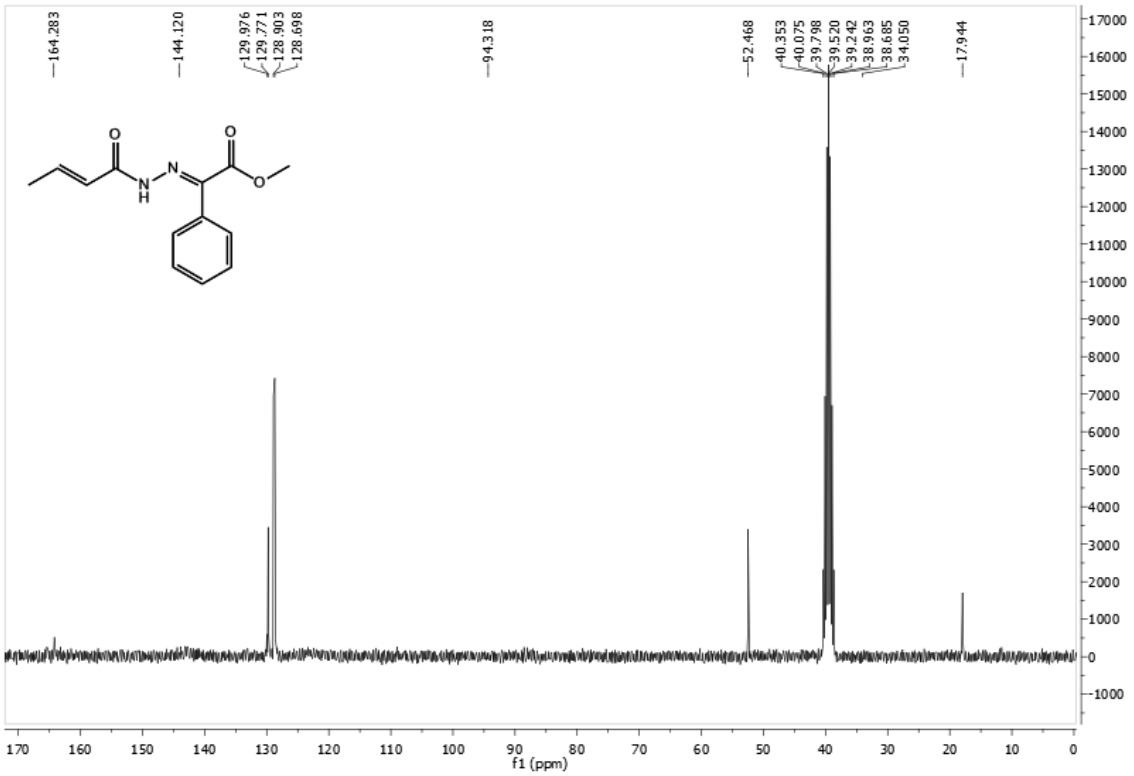
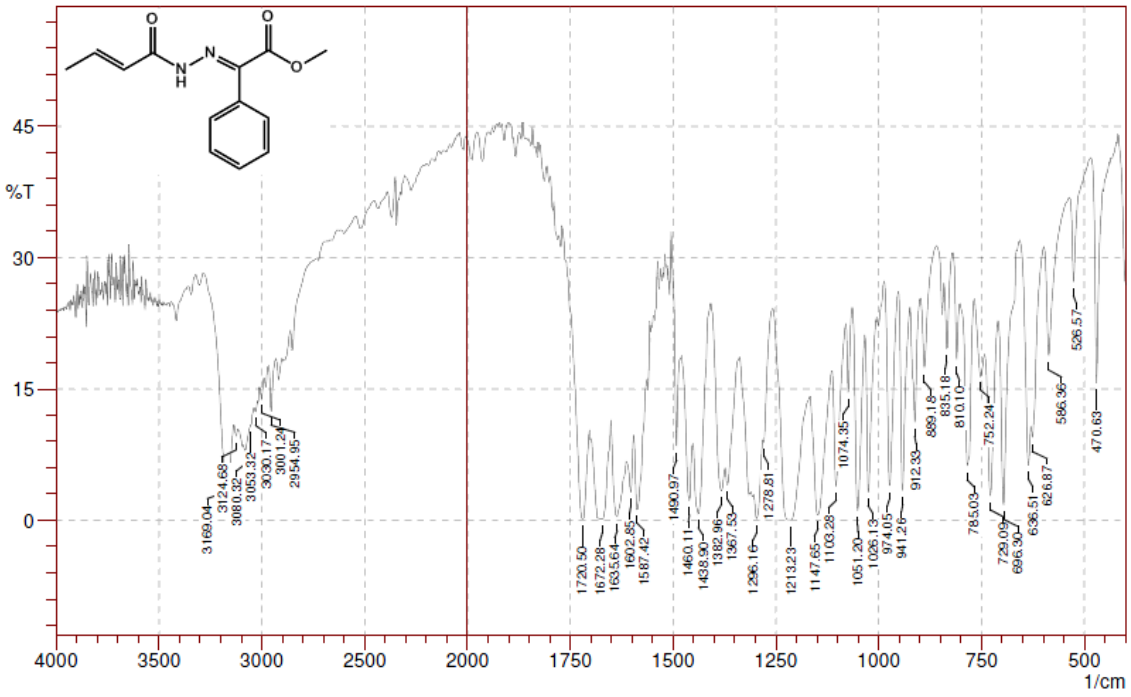
- ***N*-Acylhydrazone (16):**



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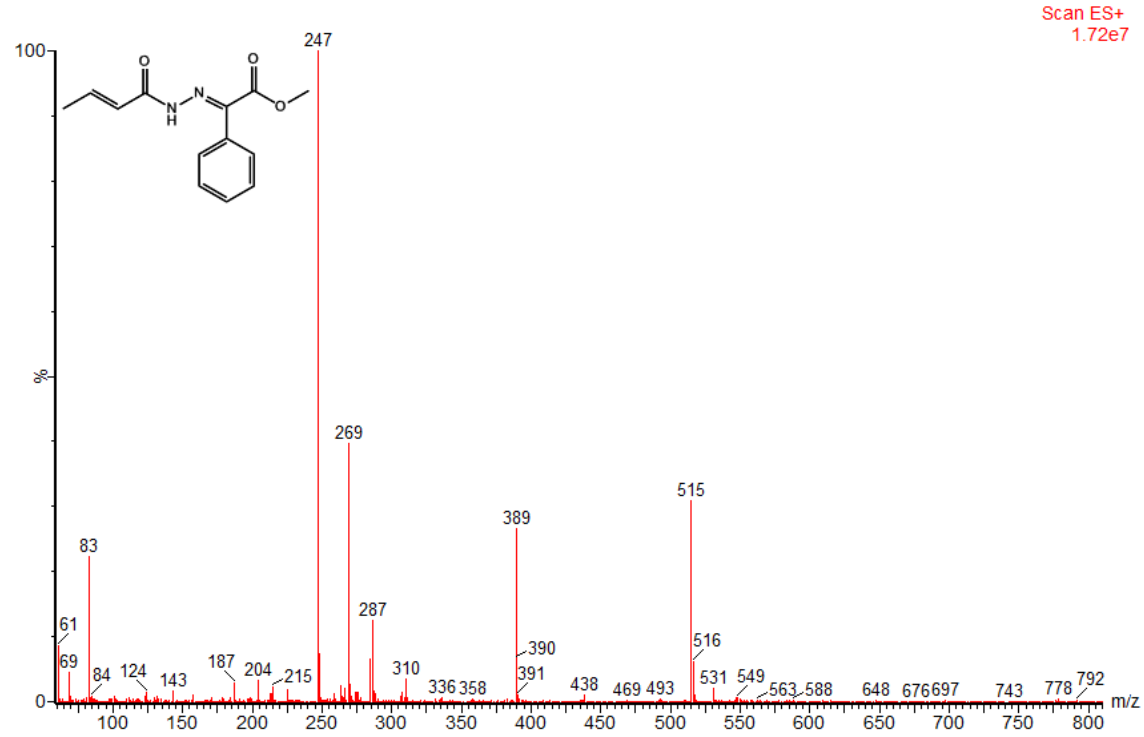
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697
743
778
792
m/z
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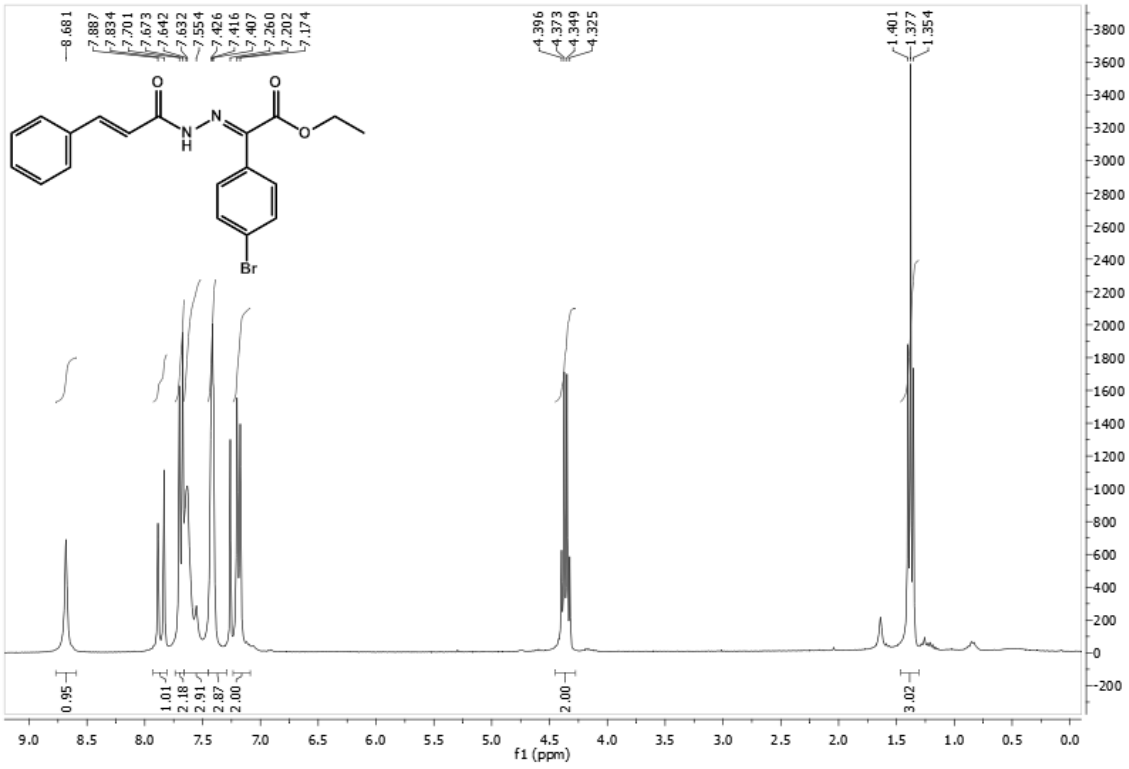
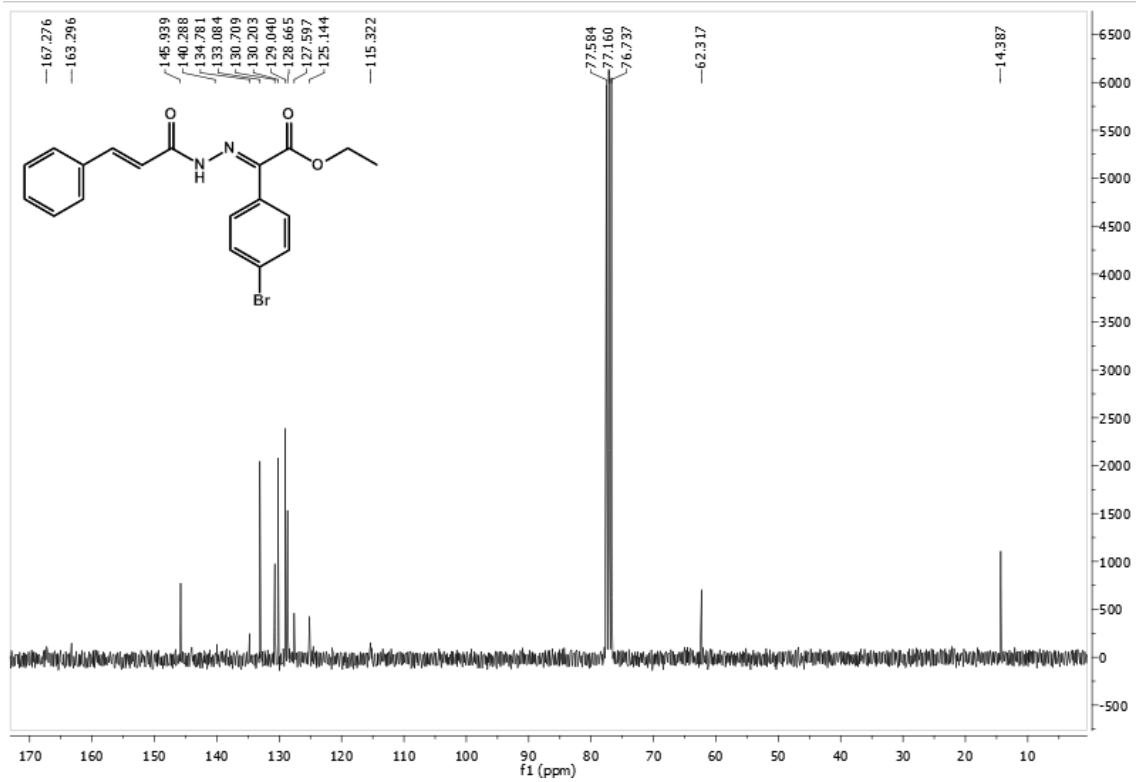
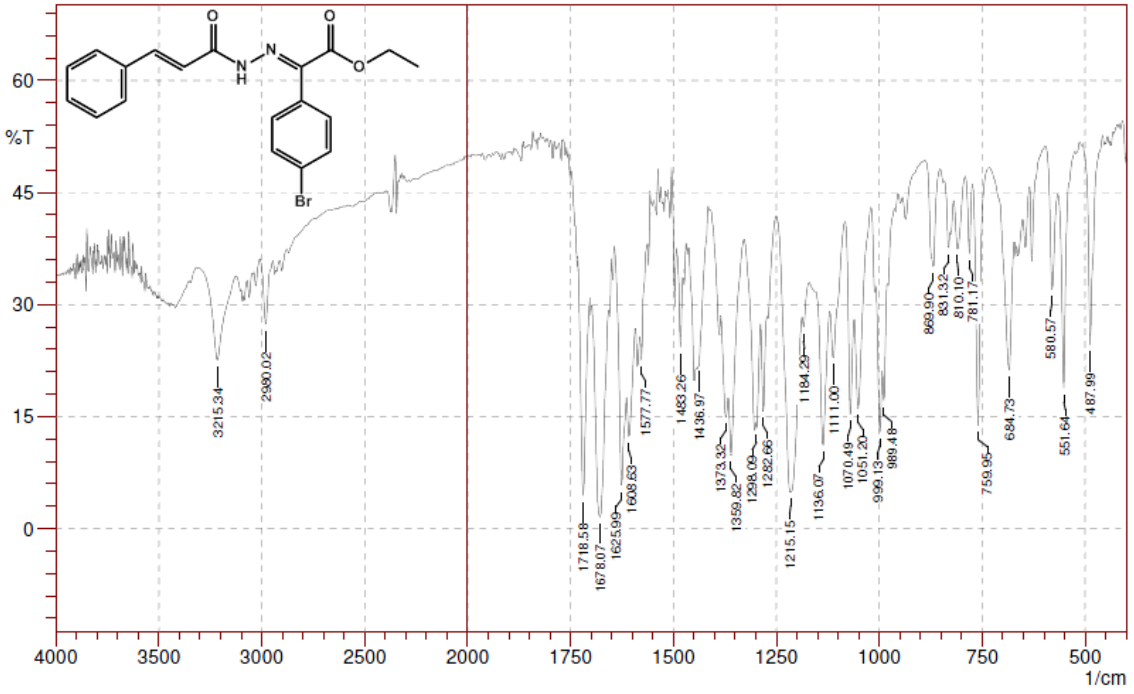
- ***N*-Acylhydrazone (17):**



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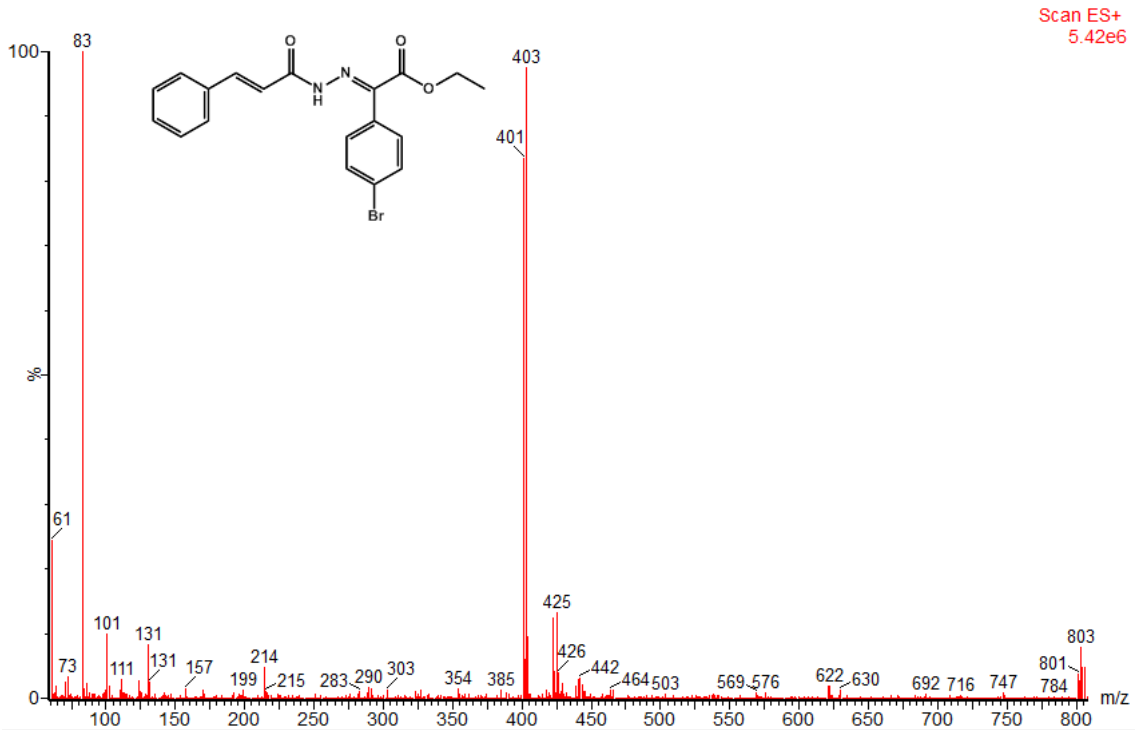
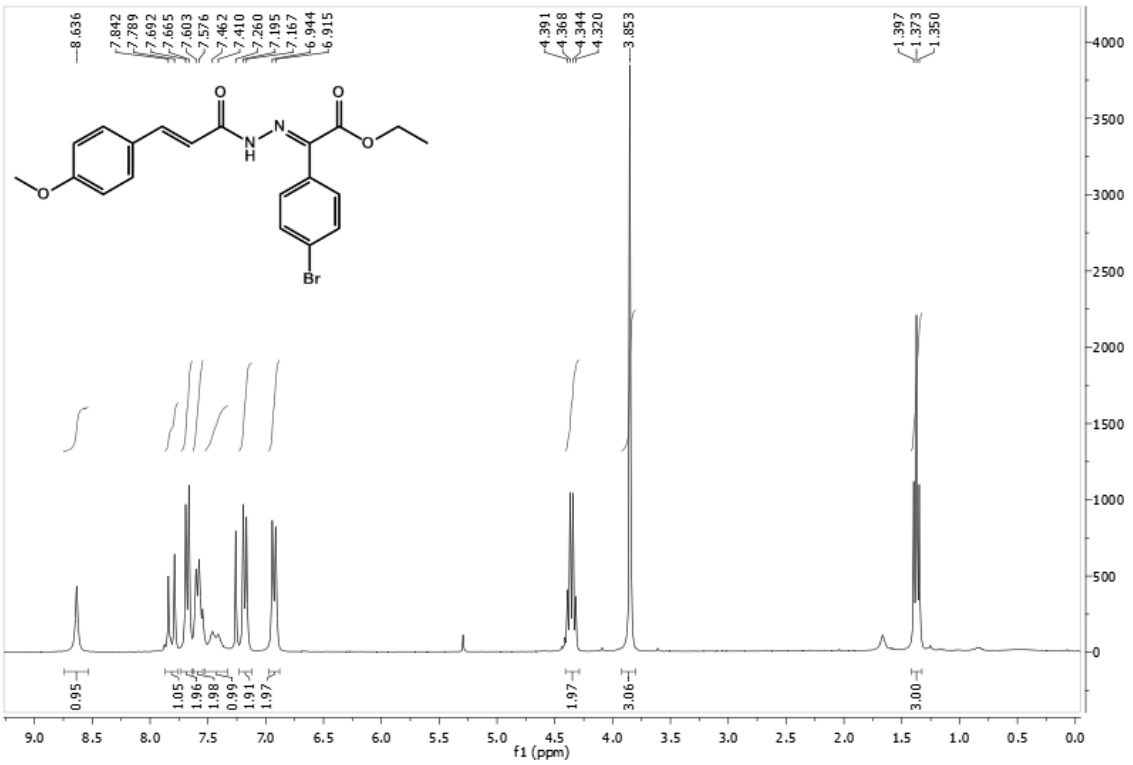
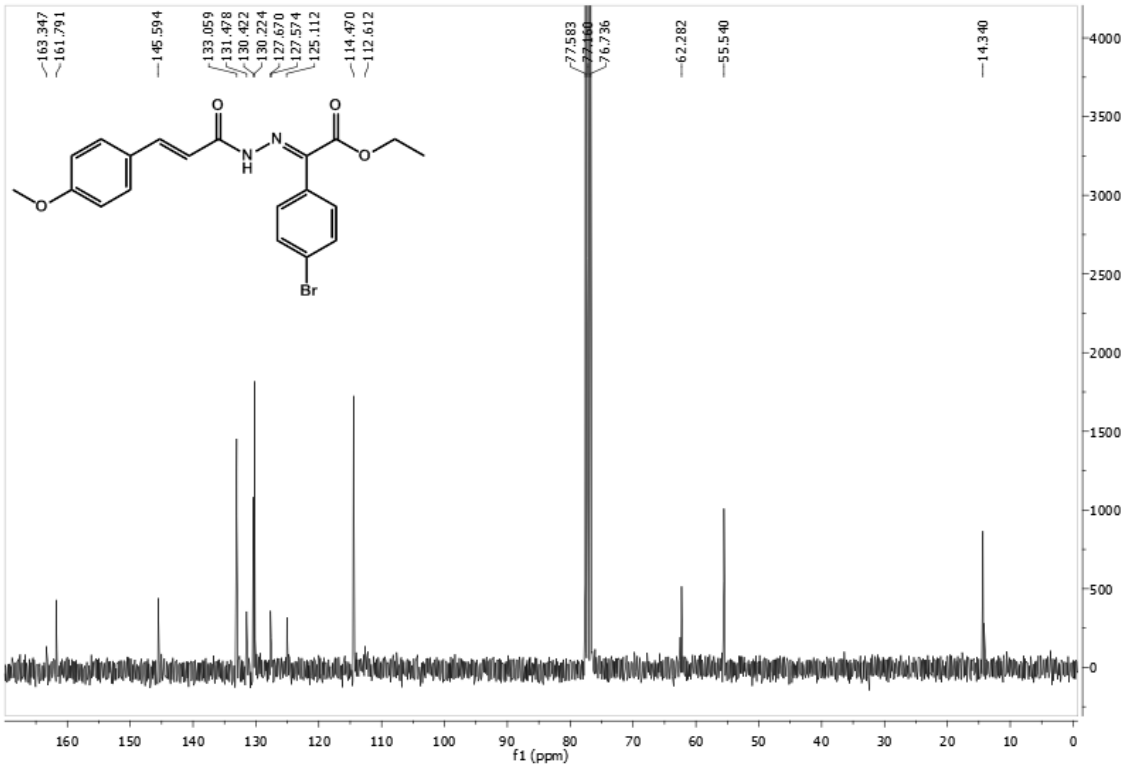
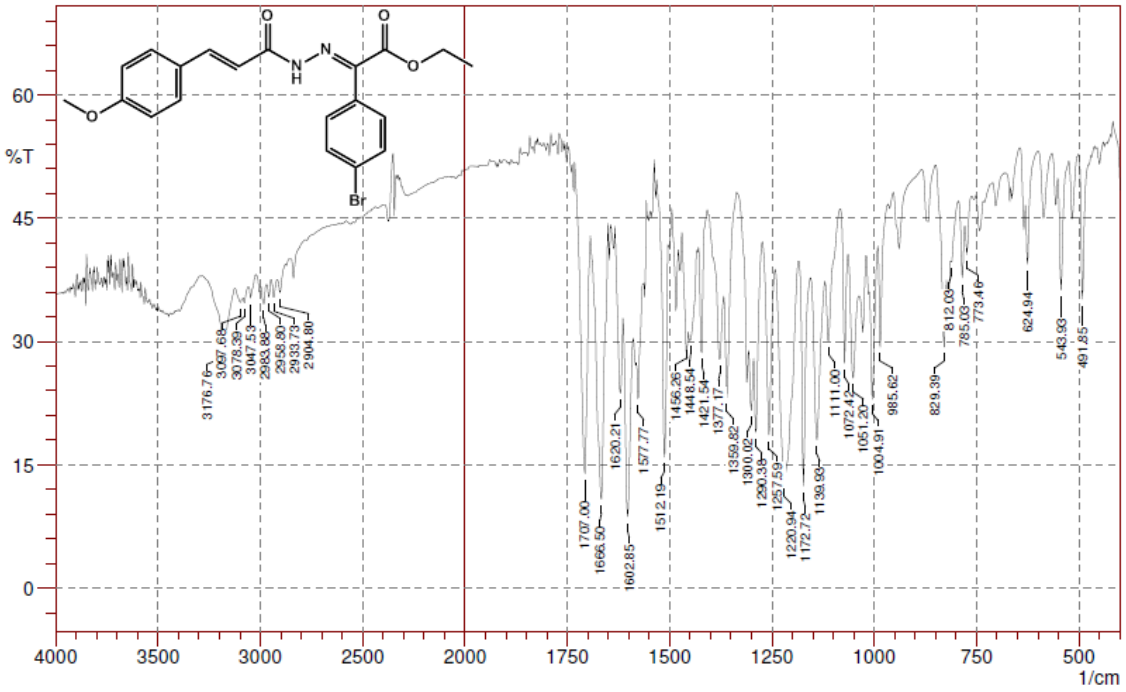
759.95
684.73
580.57
551.64
487.99

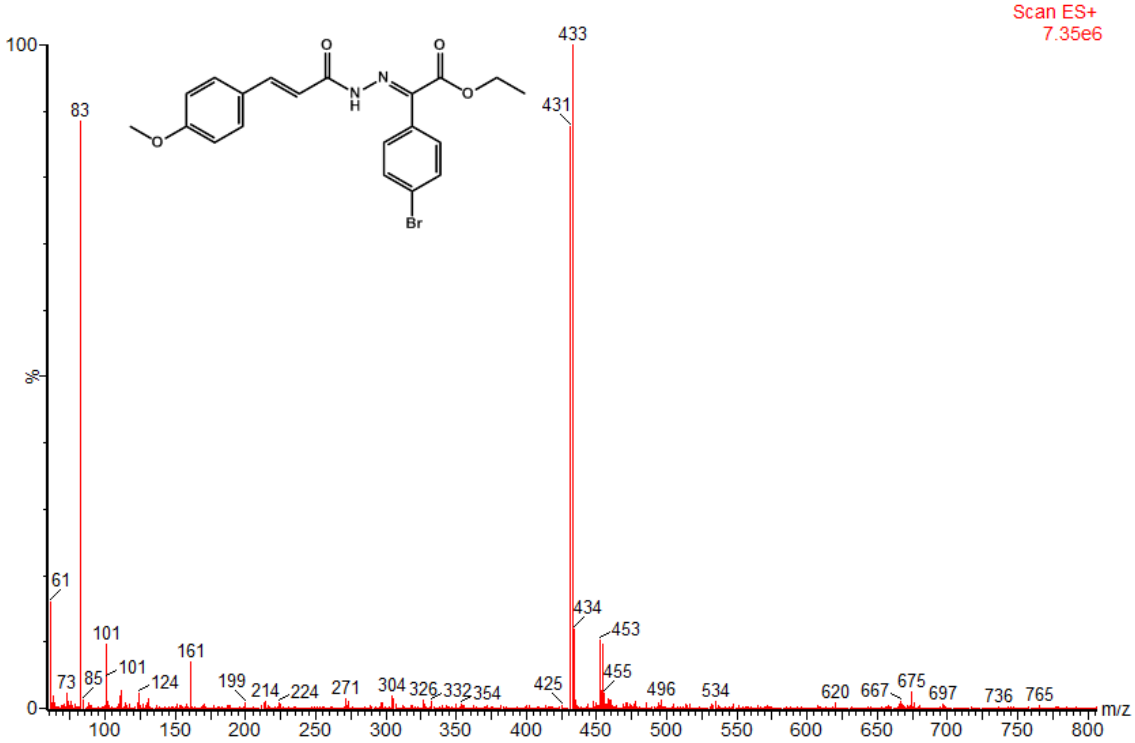

Scan ES+
5.42e6
100
%
0
Br
83
403
401
61
101
131
131
73
111
157
214
199
215
283
290
303
354
385
425
426
442
464
503
569
576
622
630
692
716
747
784
801
803
m/z
100
150
200
250
300
350
400
450
500
550
600
650
700
750
800

- ***N*-Acylhydrazone (18):**

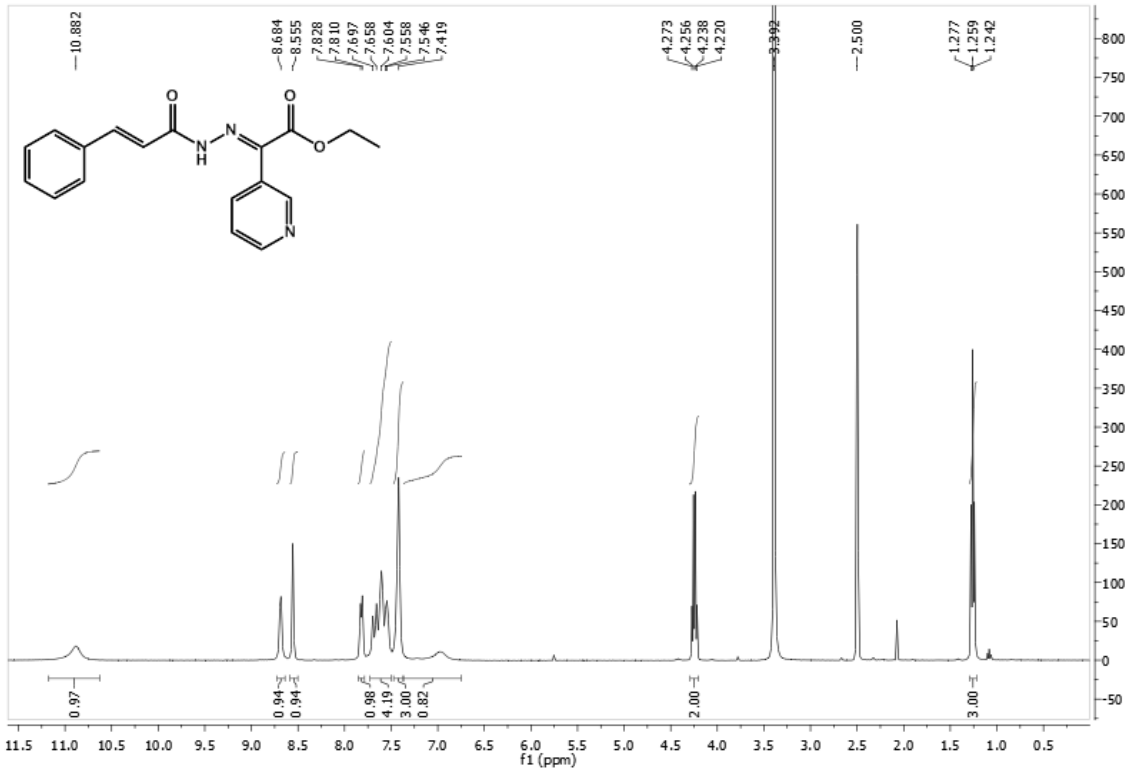


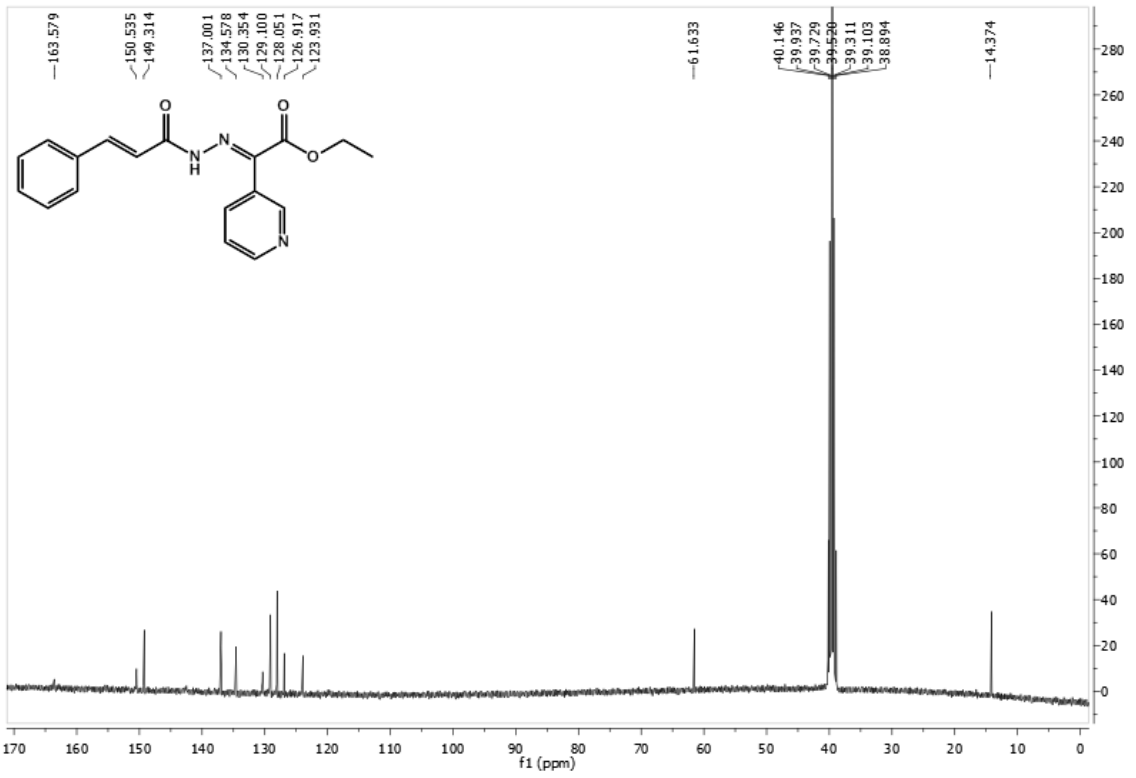


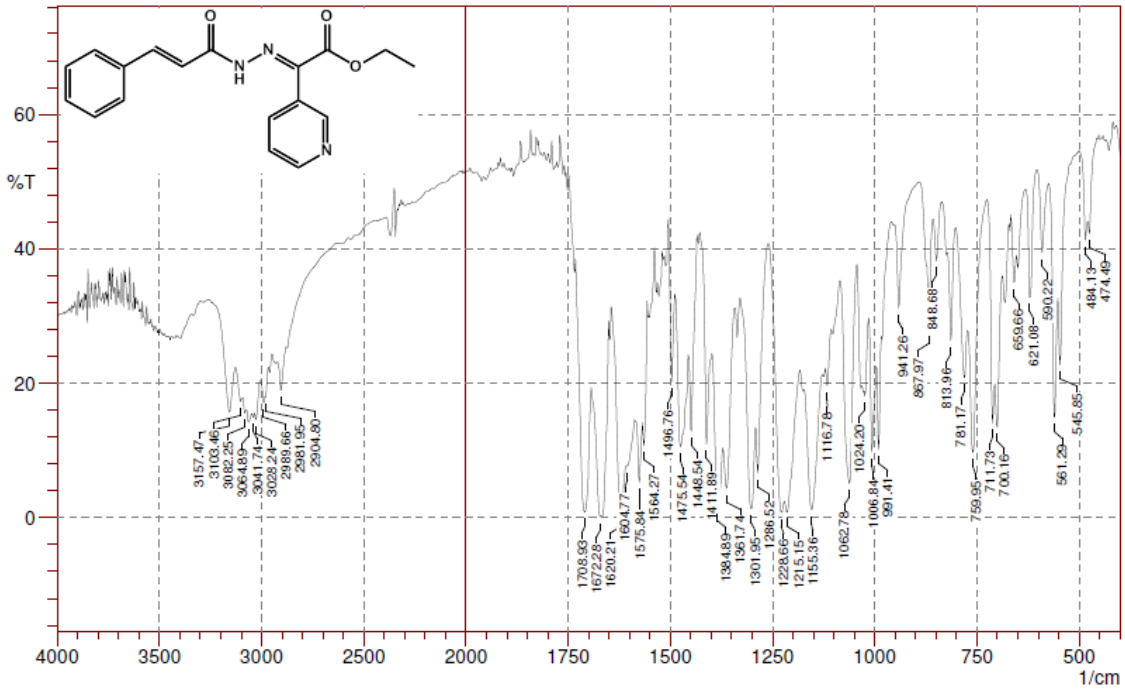

%T
60
45
30
15
0
4000
3500
3000
2500
2000
1750
1500
1250
1000
750
500
1/cm
O
N
H
N
O
O
Br
3176.76
3097.68
3078.39
3047.53
2983.88
2958.80
2933.73
2904.80
1707.00
1666.50
1620.21
1602.85
1577.77
1512.19
1456.26
1448.54
1421.54
1377.17
1359.82
1300.05
1290.38
1257.59
1220.94
1172.72
1139.93
1111.00
1072.42
1051.20
1004.91
985.62
829.39
812.09
785.03
773.46
624.94
543.93
491.85

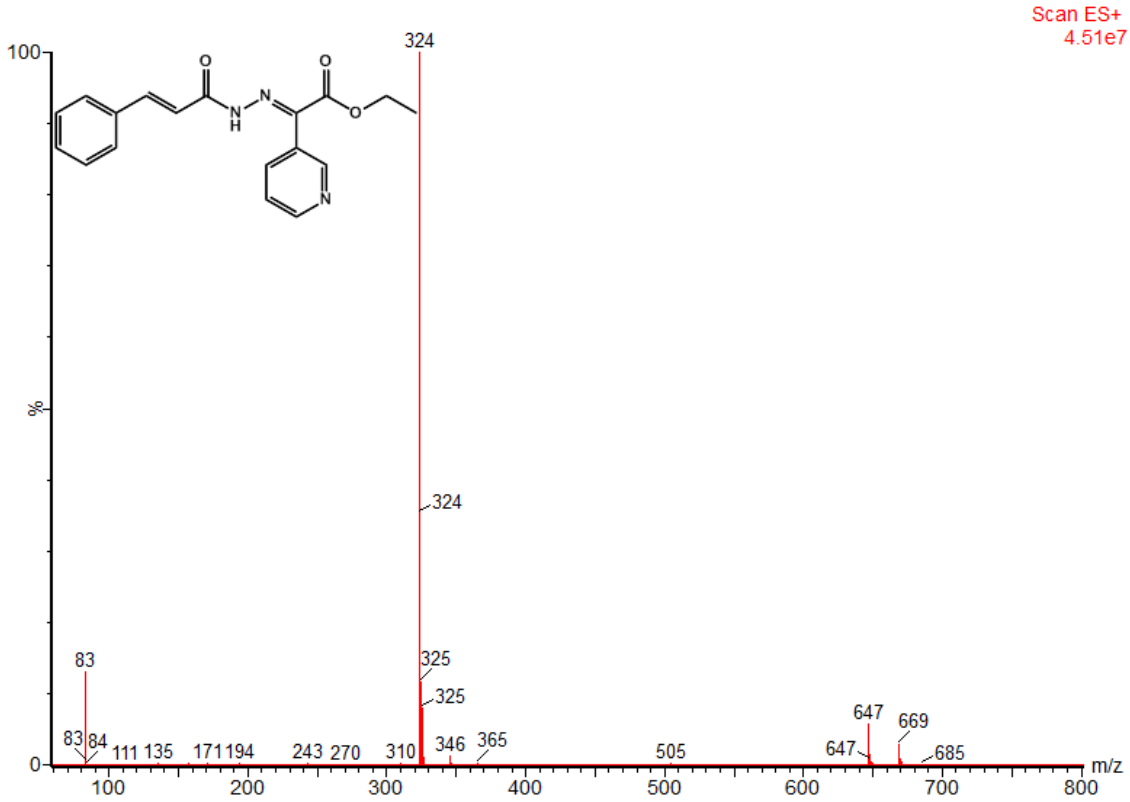

Scan ES+
7.35e6
100
%
0
O
N
H
N
O
O
Br
433
431
83
61
434
453
455
101
161
73
85
101
124
199
214
224
271
304
326
332
354
425
496
534
620
667
675
697
736
765
100
150
200
250
300
350
400
450
500
550
600
650
700
750
800
m/z

- ***N*-Acylhydrazone (19):**

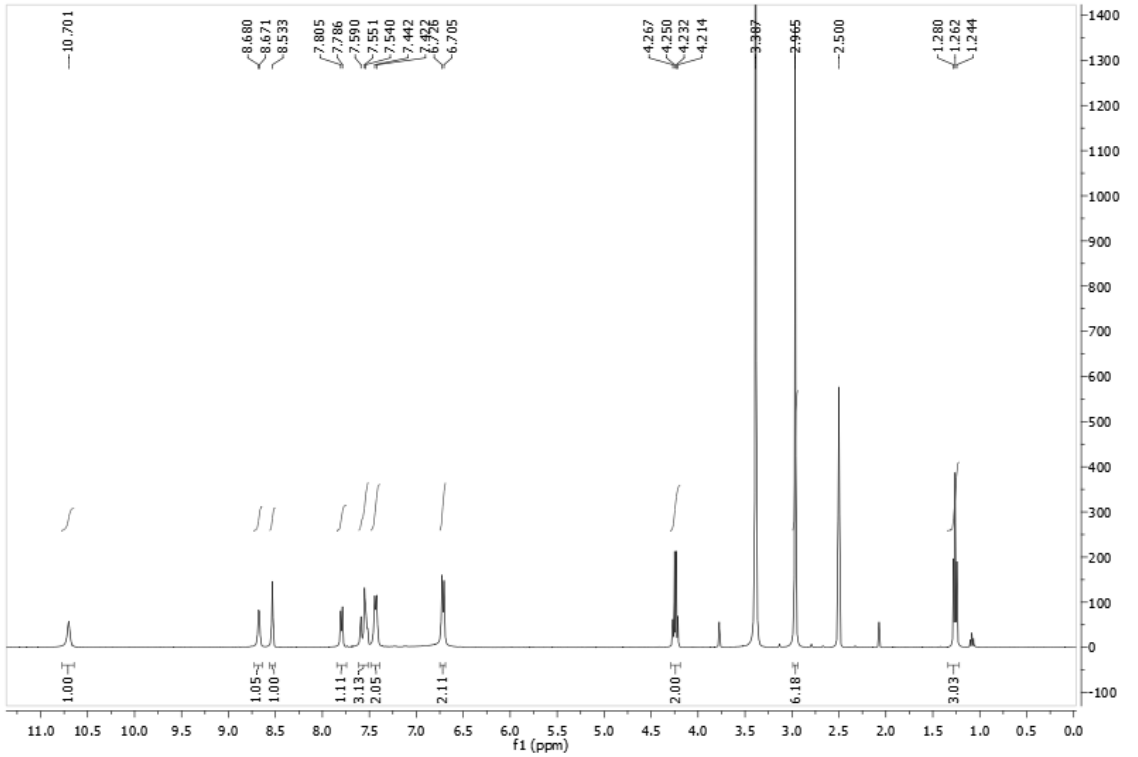


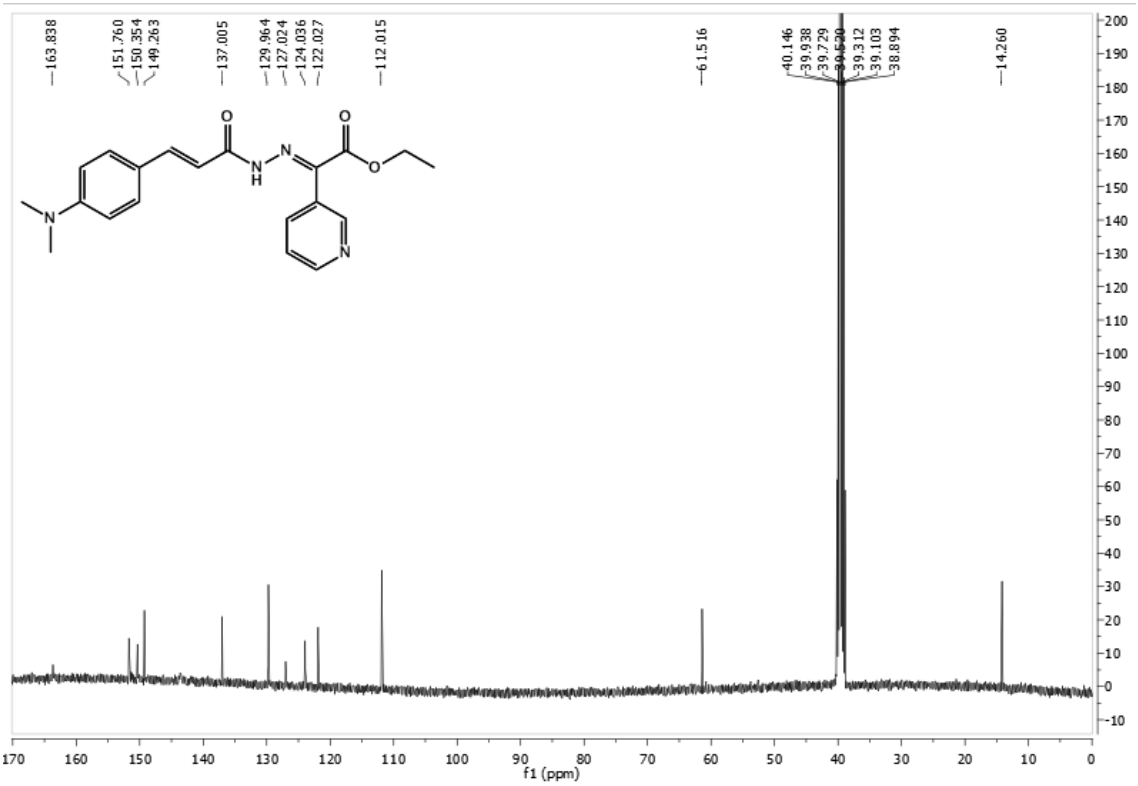


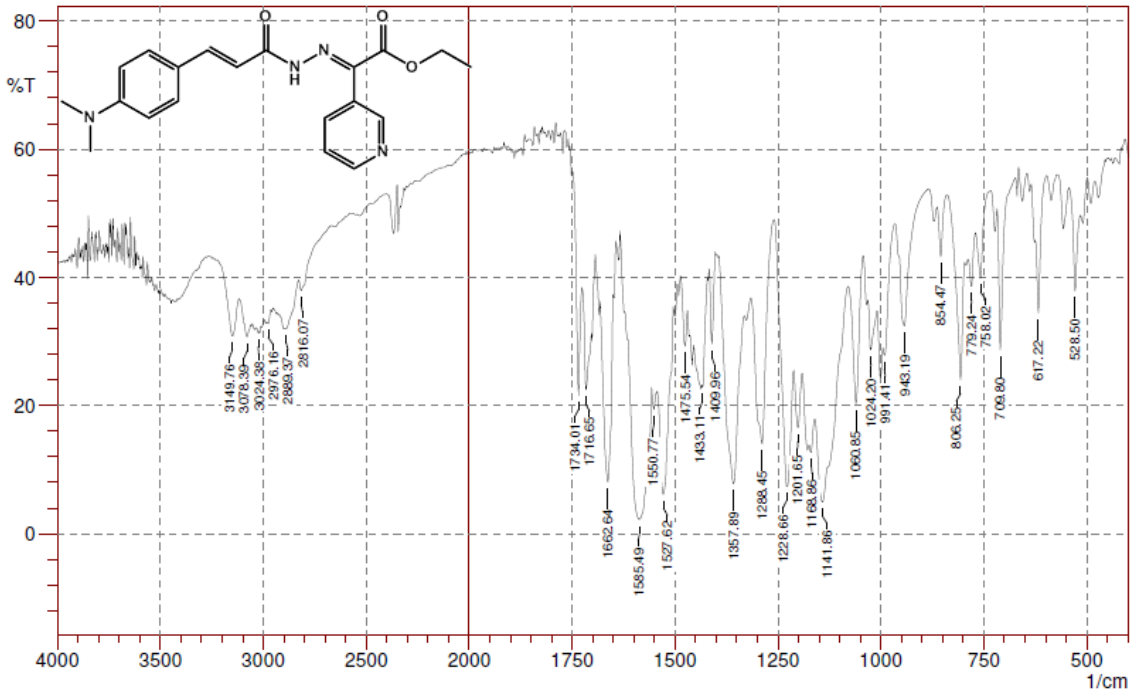

%T
60
40
20
0
4000
3500
3000
2500
2000
1750
1500
1250
1000
750
500
1/cm
3157.47
3103.46
3062.25
3064.89
3041.74
3028.24
2989.66
2981.95
2904.80
1708.93
1672.28
1620.21
1604.77
1575.84
1564.27
1496.76
1475.54
1448.54
1411.89
1384.89
1361.74
1301.95
1286.52
1228.66
1215.15
1155.36
1116.78
1062.78
1024.20
1006.84
991.41
941.26
867.97
848.68
813.96
781.17
759.95
711.73
700.16
659.66
621.08
590.22
561.29
545.85
484.13
474.49

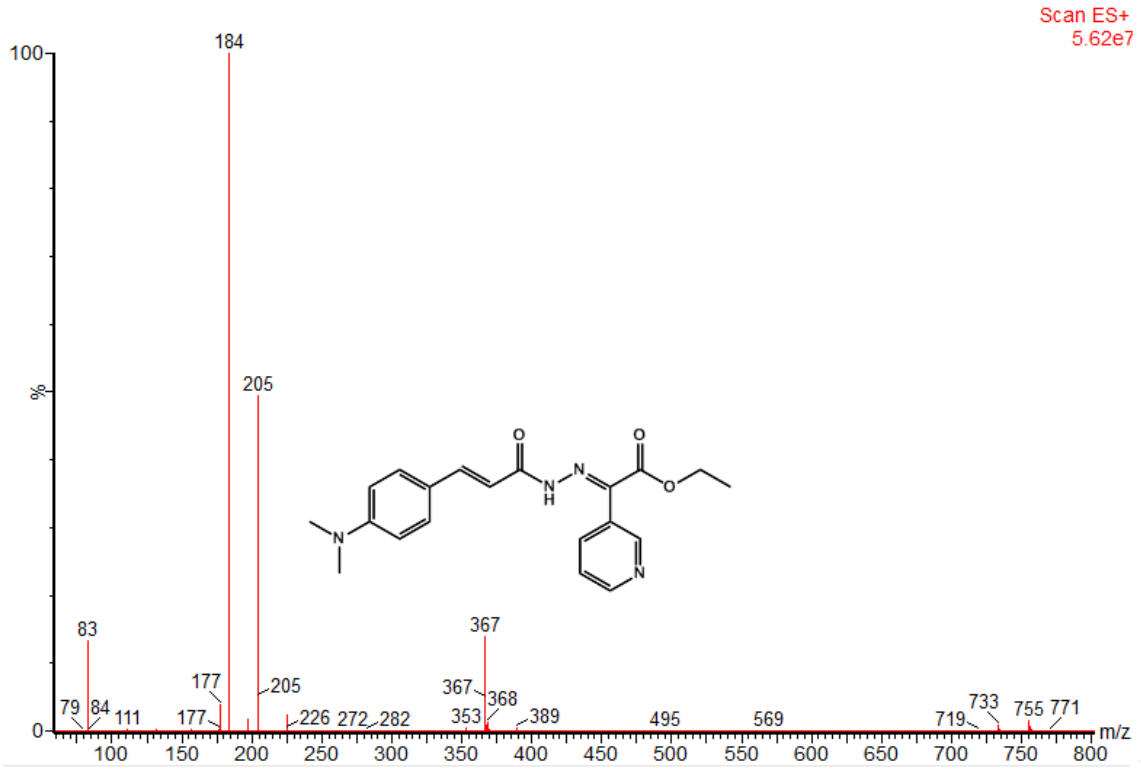

Scan ES+
4.51e7
100
%
0
324
324
325
325
83
83
84
111
135
171
194
243
270
310
346
365
505
647
647
669
685
m/z
100
200
300
400
500
600
700
800

- ***N*-Acylhydrazone (20):**

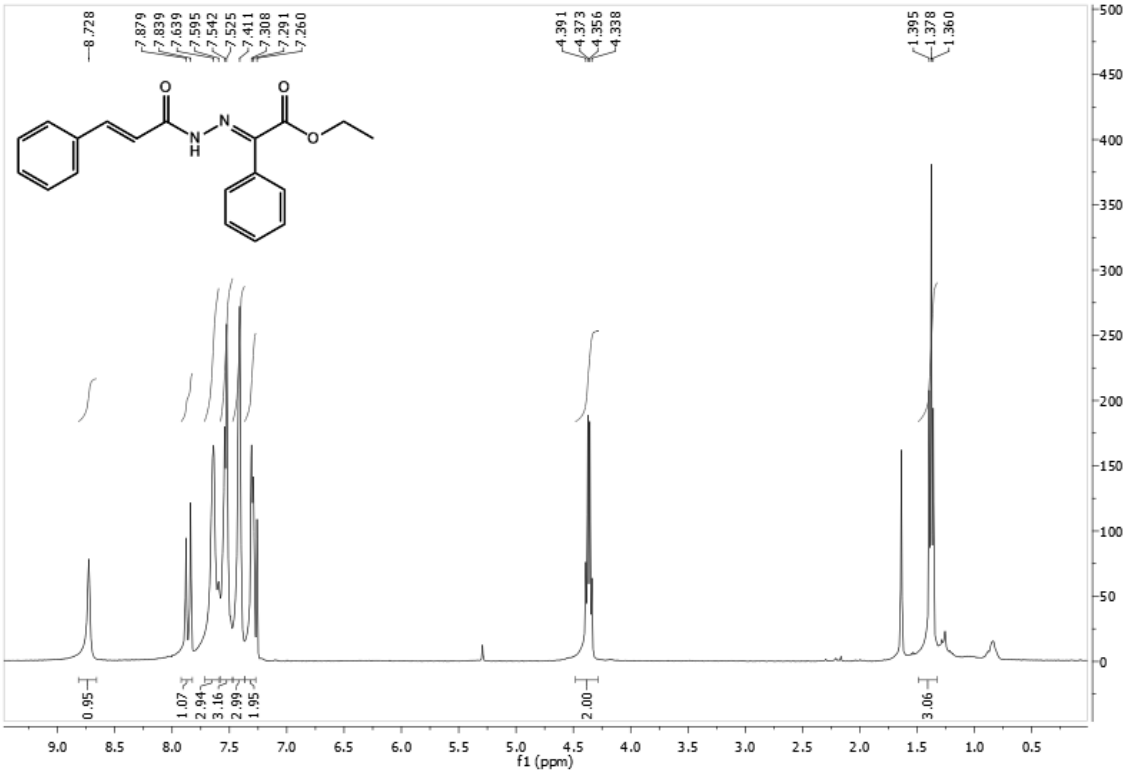


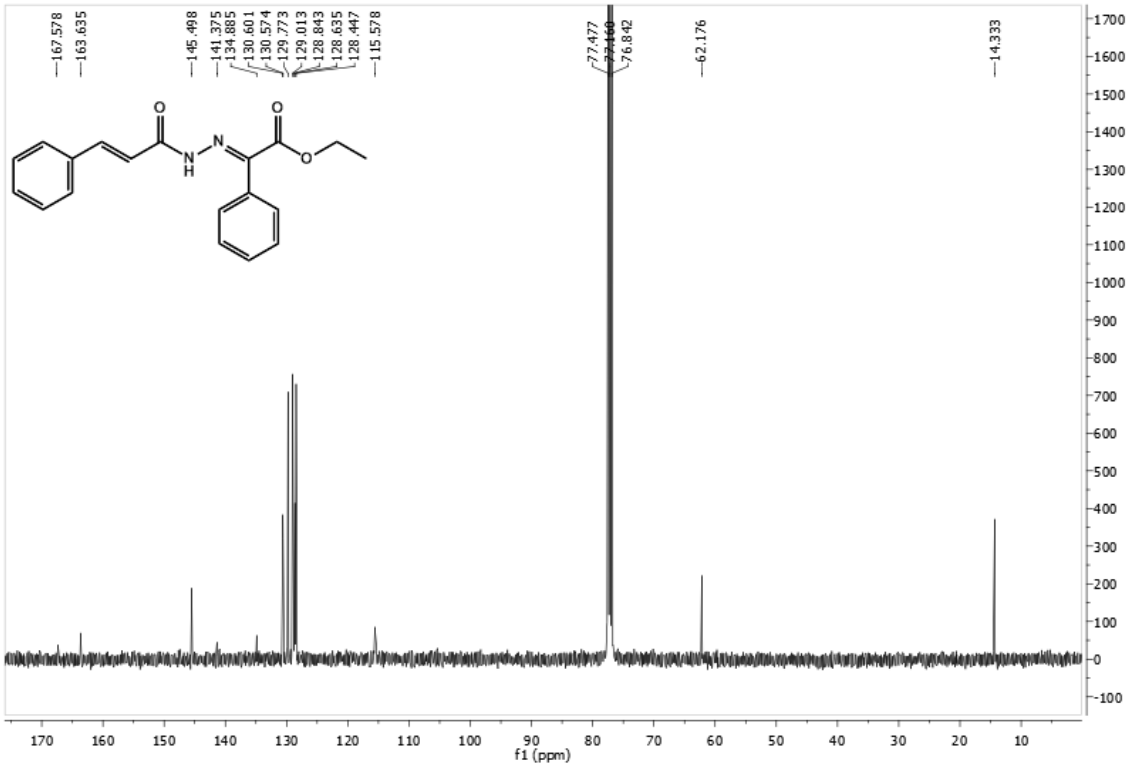


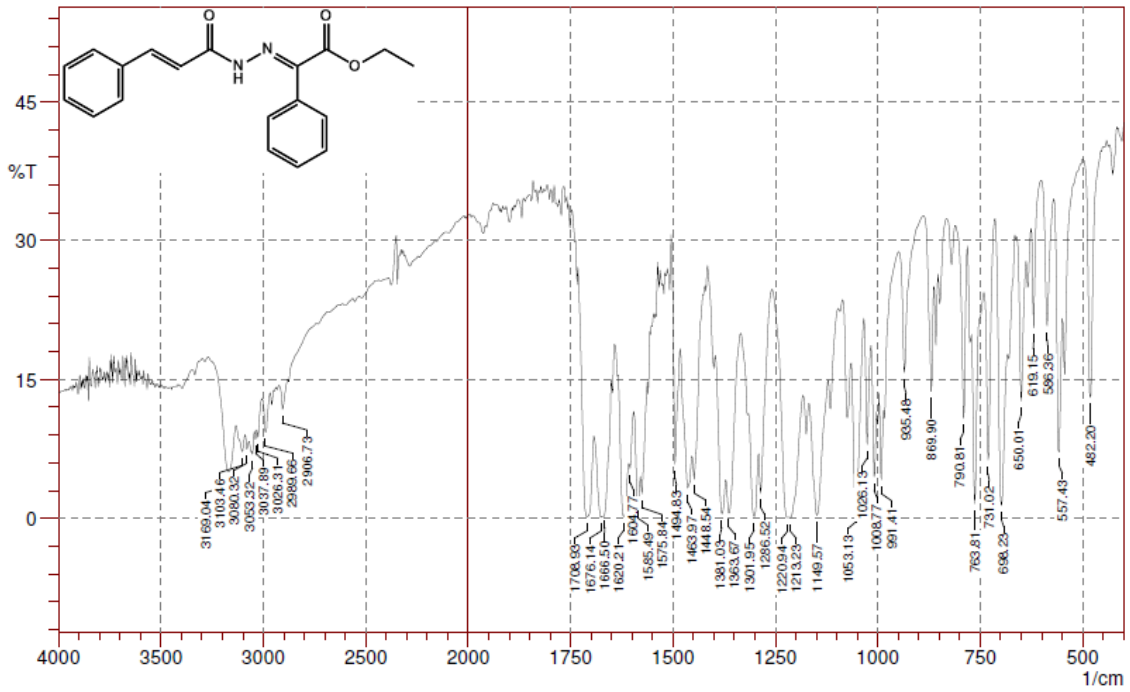

%T
80
60
40
20
0
4000
3500
3000
2500
2000
1750
1500
1250
1000
750
500
1/cm
3149.76
3078.39
3024.38
2976.16
2889.37
2816.07
1734.01
1716.65
1662.64
1585.49
1550.77
1527.62
1475.54
1433.11
1409.96
1357.89
1288.45
1228.66
1201.65
1168.86
1141.86
1060.85
1024.20
991.41
943.19
854.47
806.25
779.24
758.02
709.80
617.22
528.50

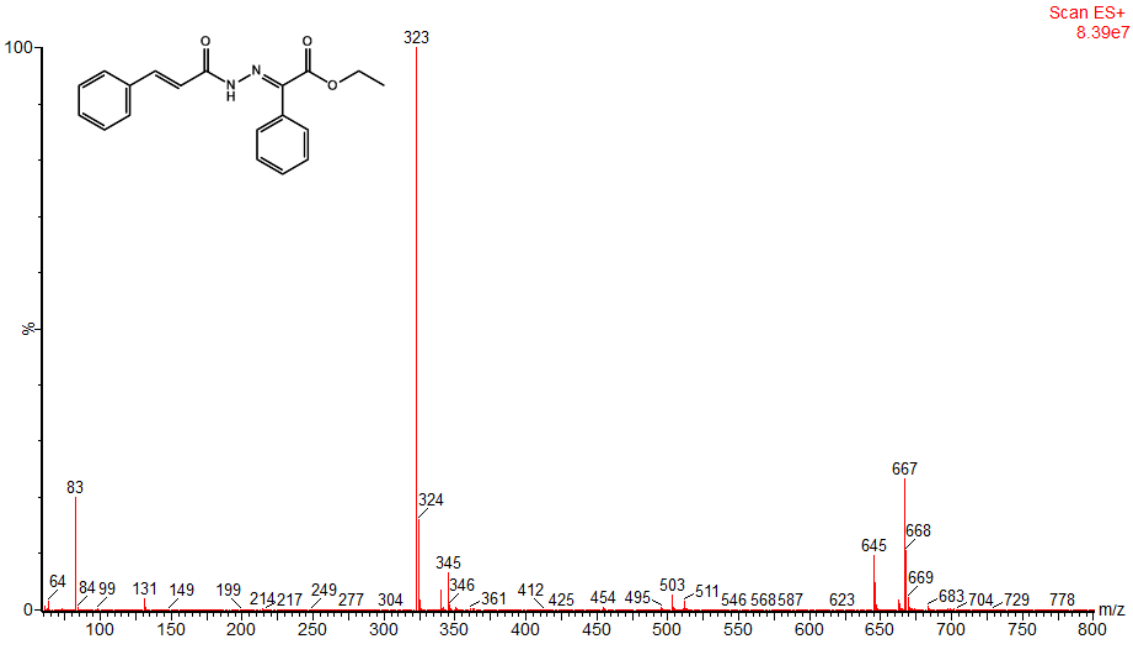

Scan ES+
5.62e7
100
%
0
184
205
83
177
367
79
84
111
177
205
226
272
282
353
367
368
389
495
569
719
733
755
771
100
150
200
250
300
350
400
450
500
550
600
650
700
750
800
m/z

- ***N*-Acylhydrazone (21):**

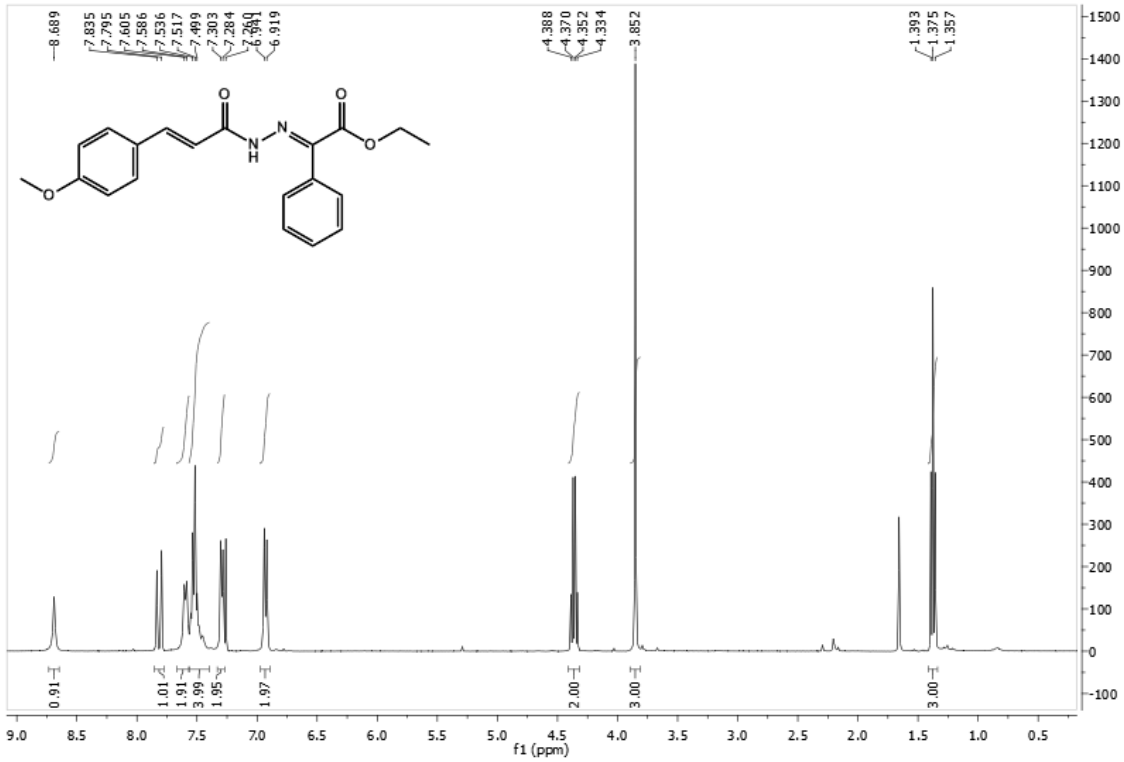


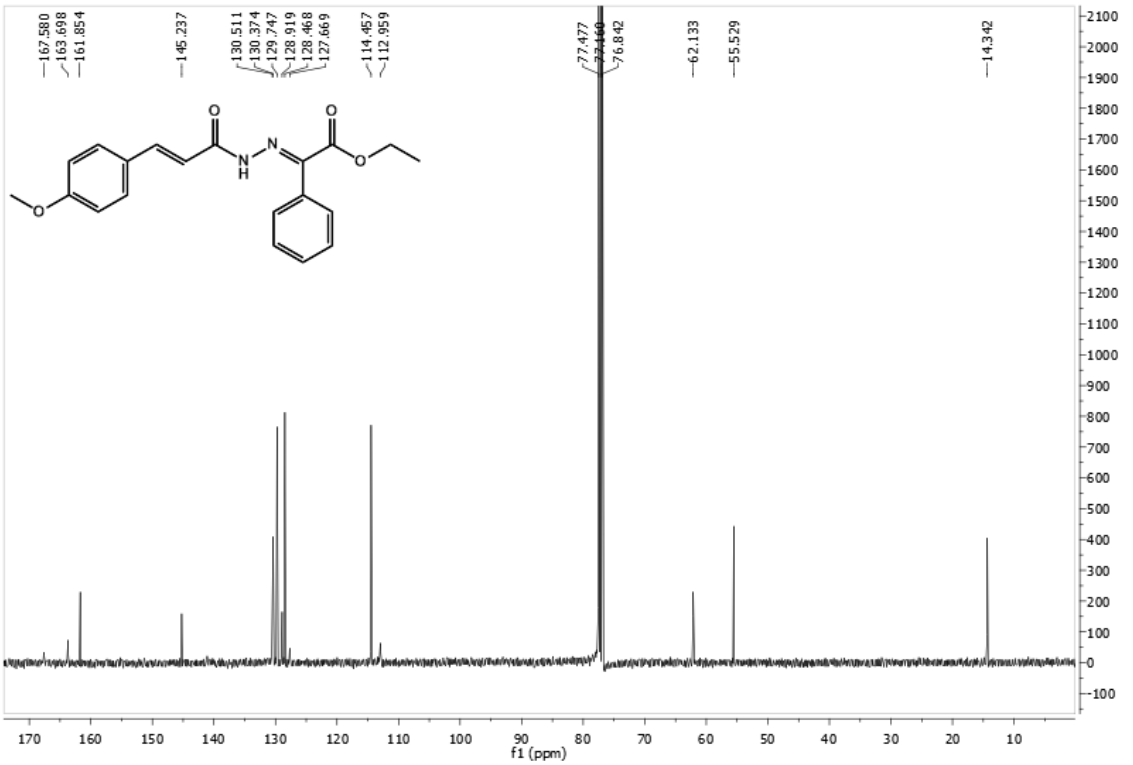


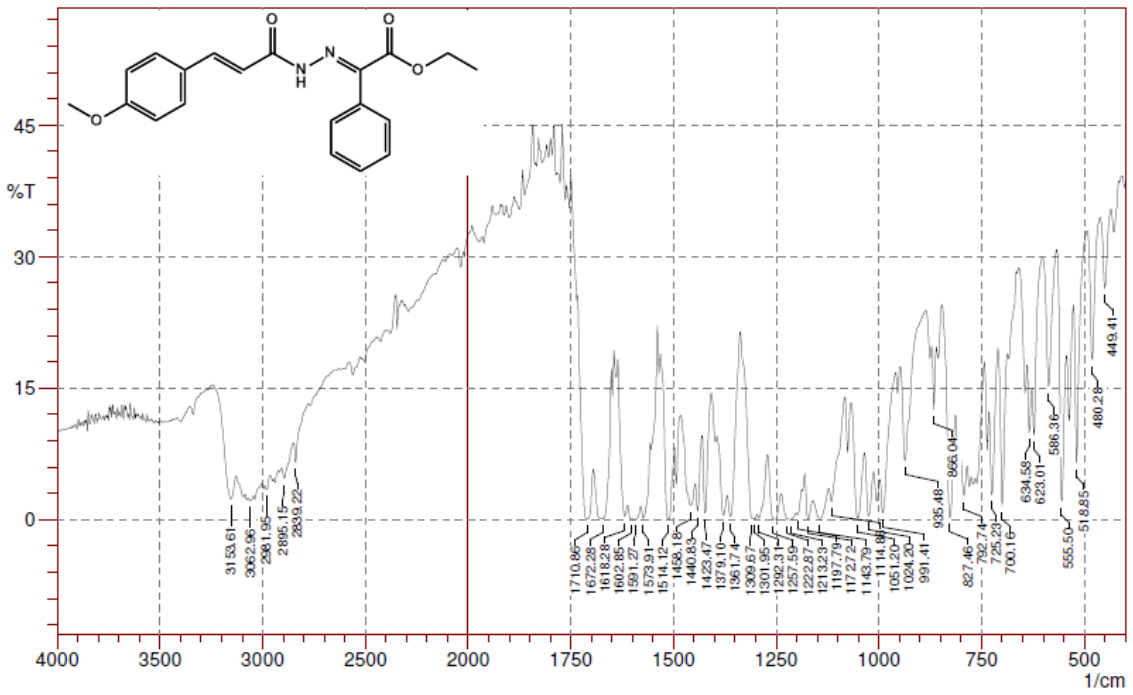

%T
45
30
15
0
4000
3500
3000
2500
2000
1750
1500
1250
1000
750
500
1/cm
3169.04
3103.46
3080.32
3053.32
3037.89
3026.31
2989.66
2906.73
1708.39
1676.14
1666.50
1620.21
1604.77
1585.49
1575.84
1494.83
1463.97
1448.54
1381.03
1363.67
1301.95
1286.52
1220.94
1213.23
1149.57
1053.13
1026.13
1008.77
991.41
935.48
869.90
790.81
763.81
731.02
698.23
650.01
619.15
596.36
557.43
482.20

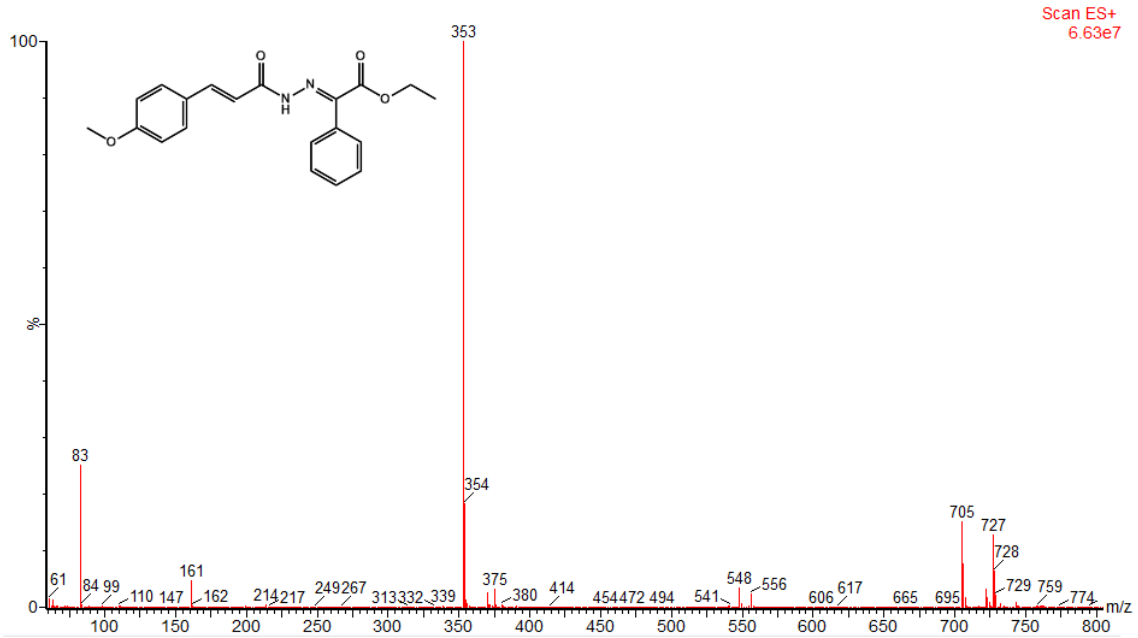

Scan ES+
8.39e7
100
%
0
323
324
83
667
668
645
669
345
346
64
84
99
131
149
199
214
217
249
277
304
361
412
425
454
495
503
511
546
568
587
623
683
704
729
778
m/z
100
150
200
250
300
350
400
450
500
550
600
650
700
750
800

- ***N*-Acylhydrazone (22):**

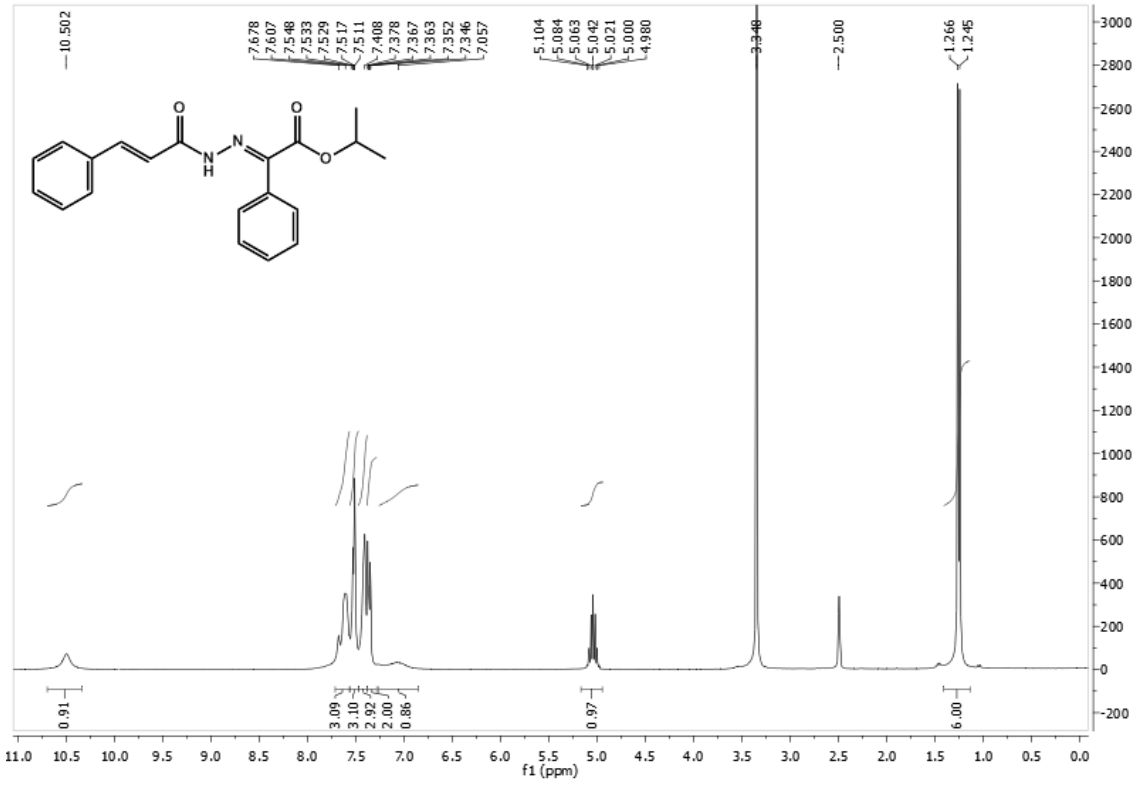


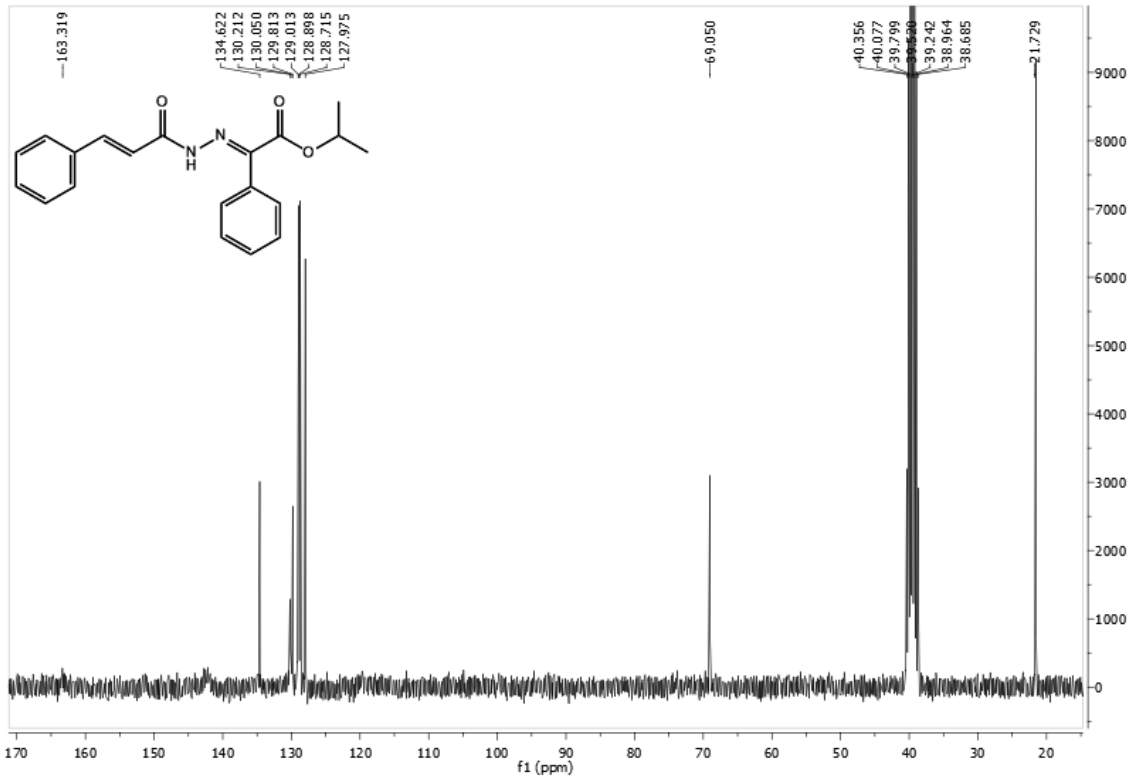


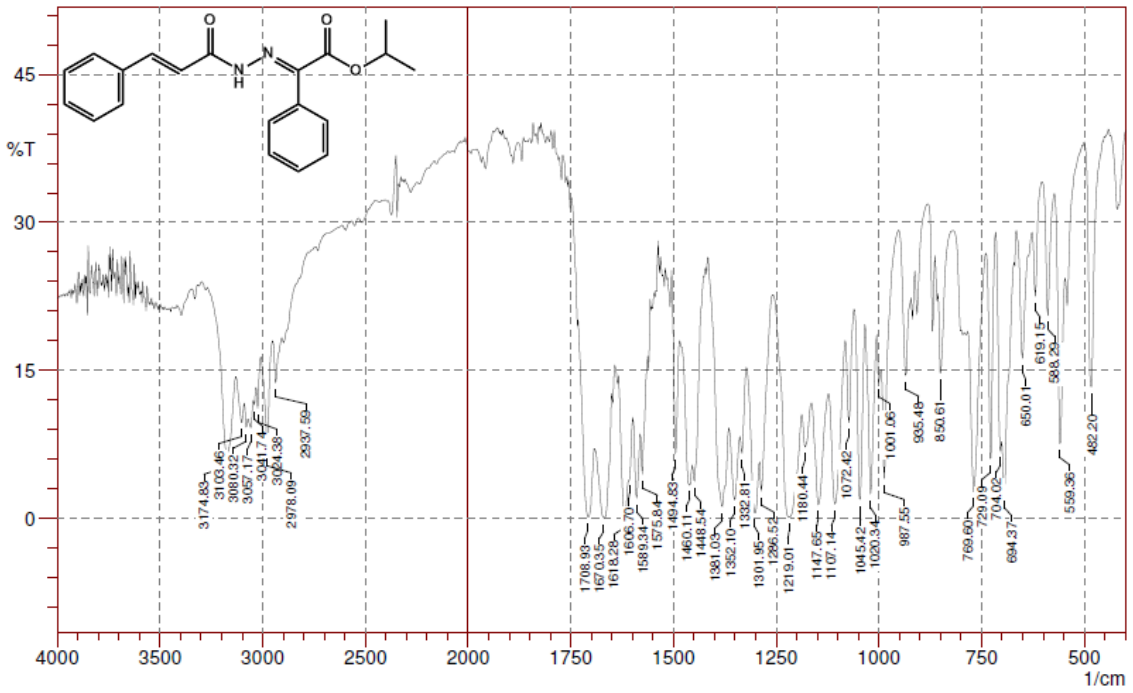

%T
45
30
15
0
4000
3500
3000
2500
2000
1750
1500
1250
1000
750
500
1/cm
3153.61
3062.96
2981.95
2895.15
2839.22
1710.86
1672.28
1618.28
1602.85
1591.27
1573.91
1514.12
1458.18
1440.83
1423.47
1379.10
1361.74
1309.67
1301.95
1292.31
1257.59
1222.87
1213.23
1197.79
1172.72
1143.79
1114.86
1051.20
1024.20
991.41
935.48
866.04
827.46
792.74
725.23
700.16
634.58
623.01
586.36
555.50
518.85
480.28
449.41

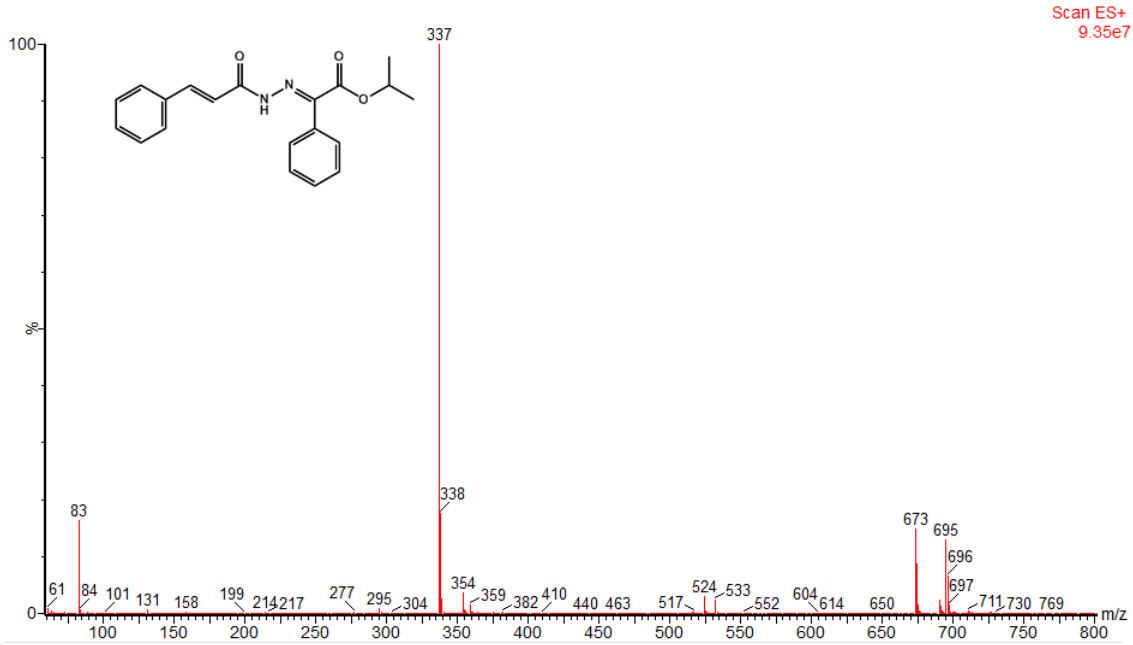

Scan ES+
6.63e7
100
%
0
353
354
83
61
84
99
110
147
161
162
214
217
249
267
313
332
339
375
380
414
454
472
494
541
548
556
606
617
665
695
705
727
728
729
759
774
m/z
100
150
200
250
300
350
400
450
500
550
600
650
700
750
800

- ***N*-Acylhydrazone (23):**

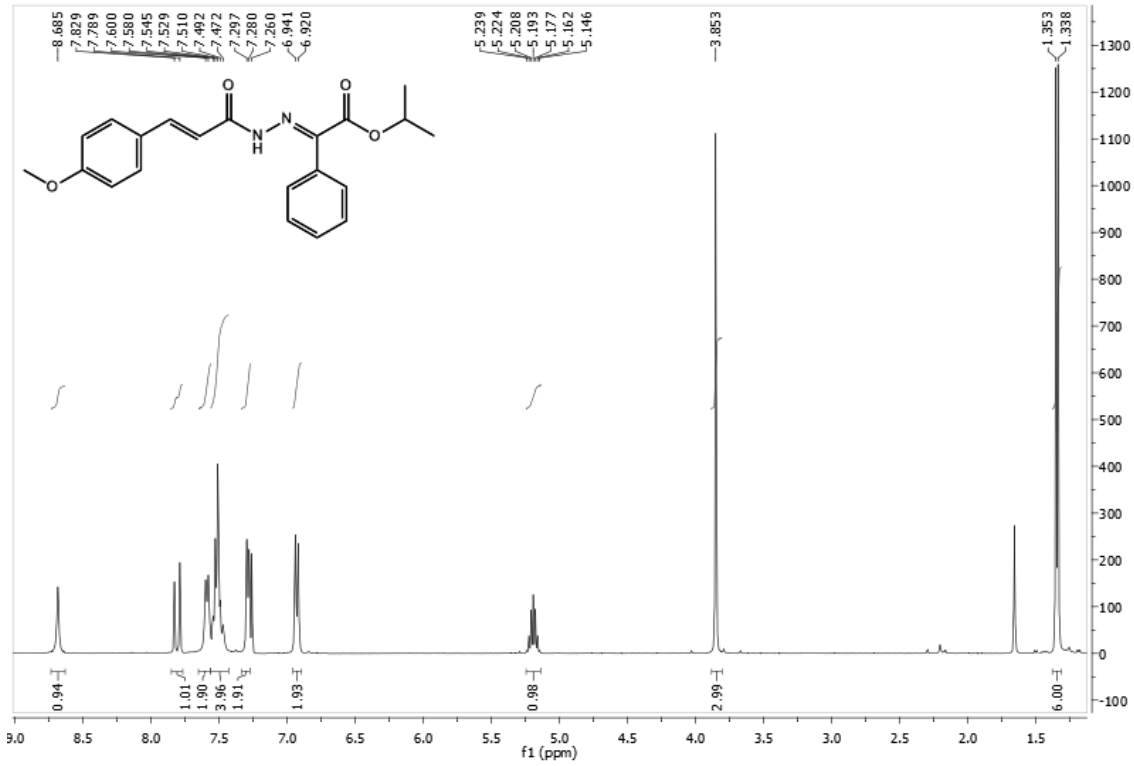


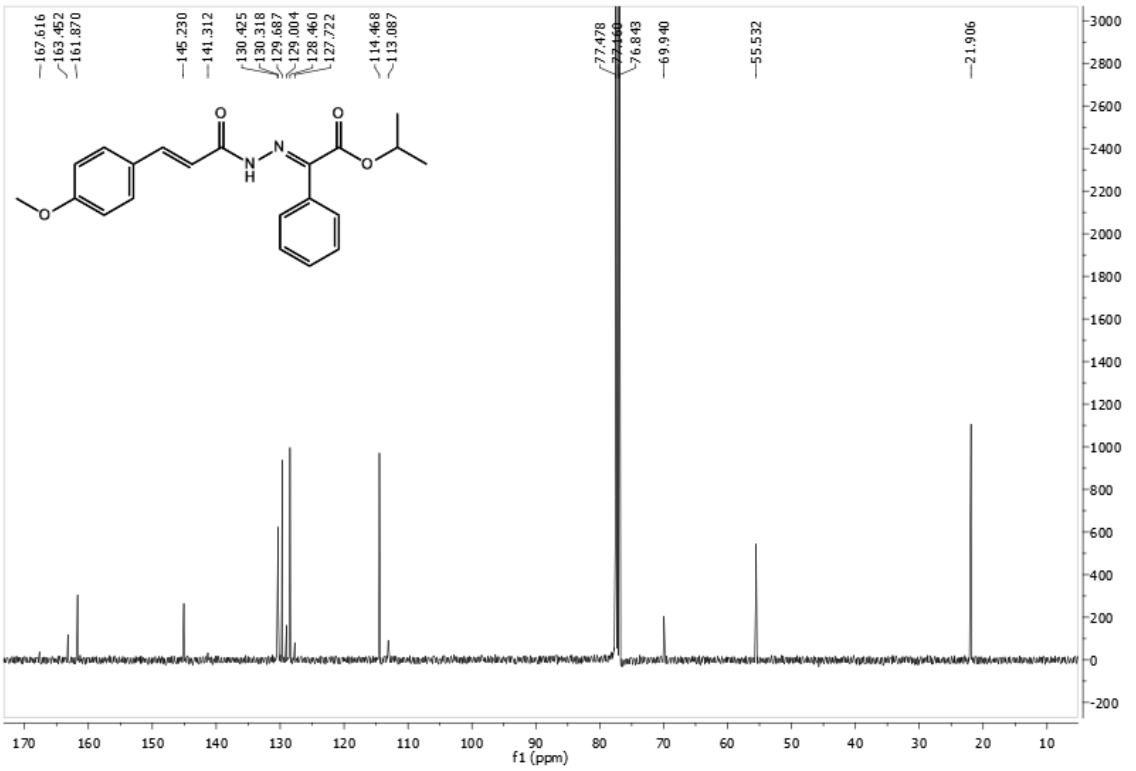


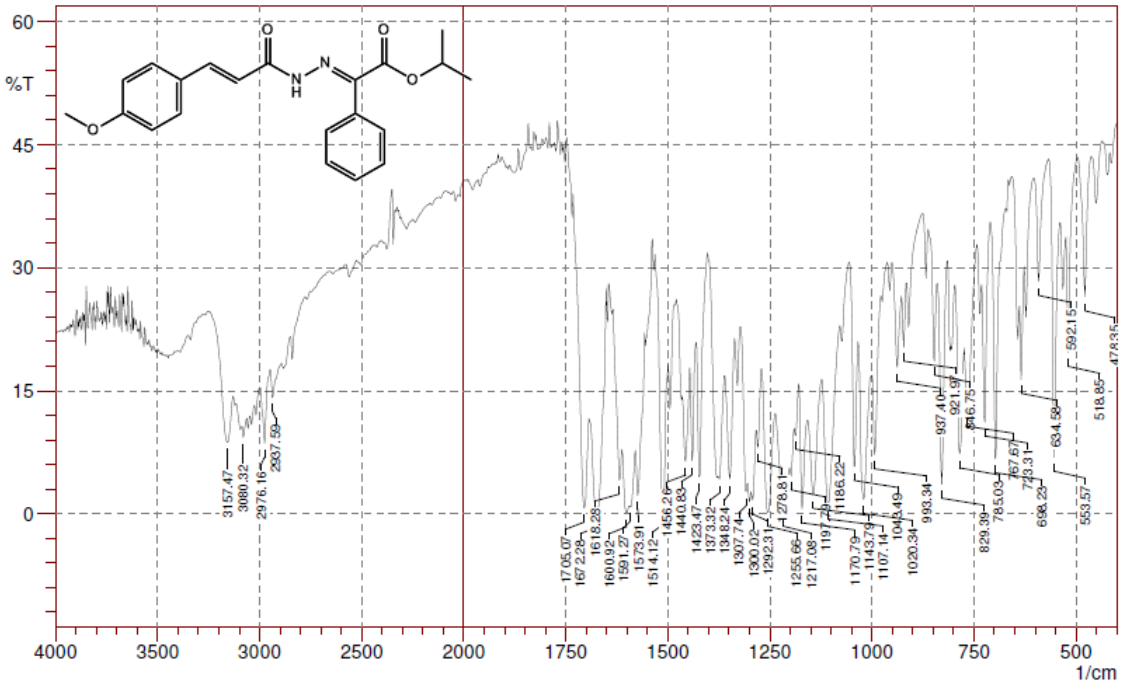

%T
45
30
15
0
4000
3500
3000
2500
2000
1750
1500
1250
1000
750
500
1/cm
3174.83
3103.46
3060.32
3057.17
3031.74
3024.38
2978.09
2937.59
1708.93
1657.35
1618.28
1606.70
1589.34
1575.84
1494.83
1460.11
1448.54
1381.03
1352.10
1332.81
1301.95
1286.52
1219.01
1180.44
1147.65
1107.14
1072.42
1045.42
1020.34
1001.06
987.55
935.48
850.61
769.60
729.09
704.02
694.37
650.01
619.15
588.29
559.36
482.20

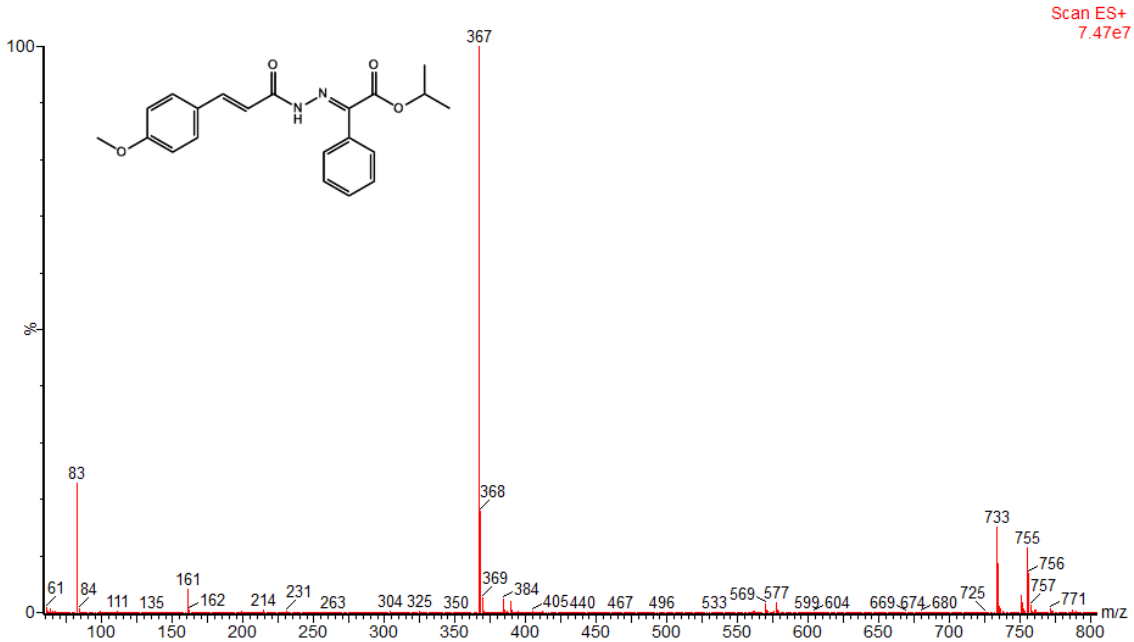

Scan ES+
9.35e7
100
%
0
337
338
83
61
84
101
131
158
199
214
217
277
295
304
354
359
382
410
440
463
517
524
533
552
604
614
650
673
695
696
697
711
730
769
100
150
200
250
300
350
400
450
500
550
600
650
700
750
800
m/z

- ***N*-Acylhydrazone (24):**

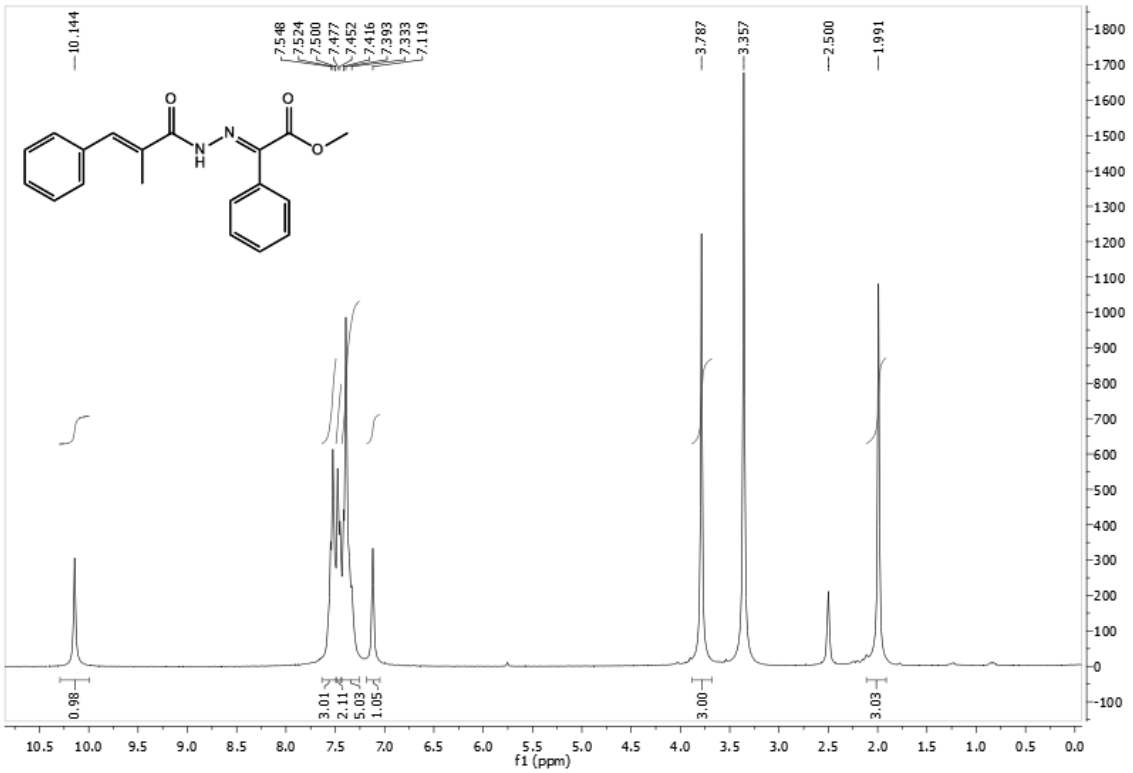


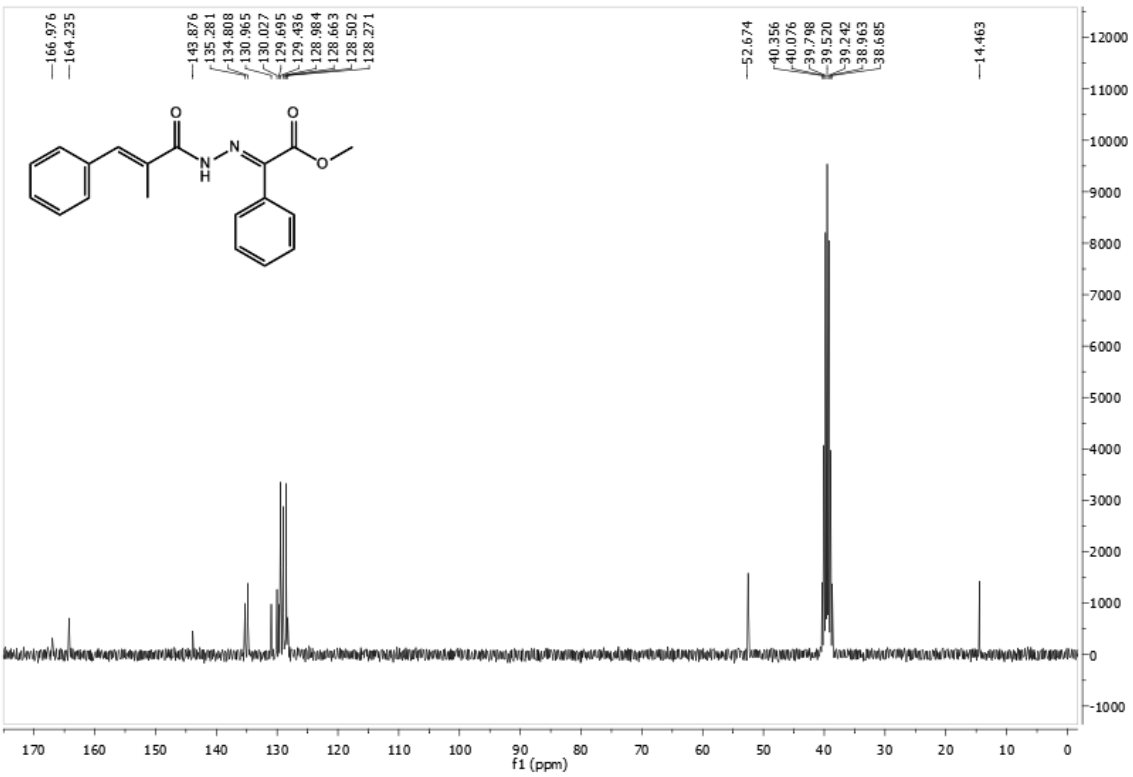


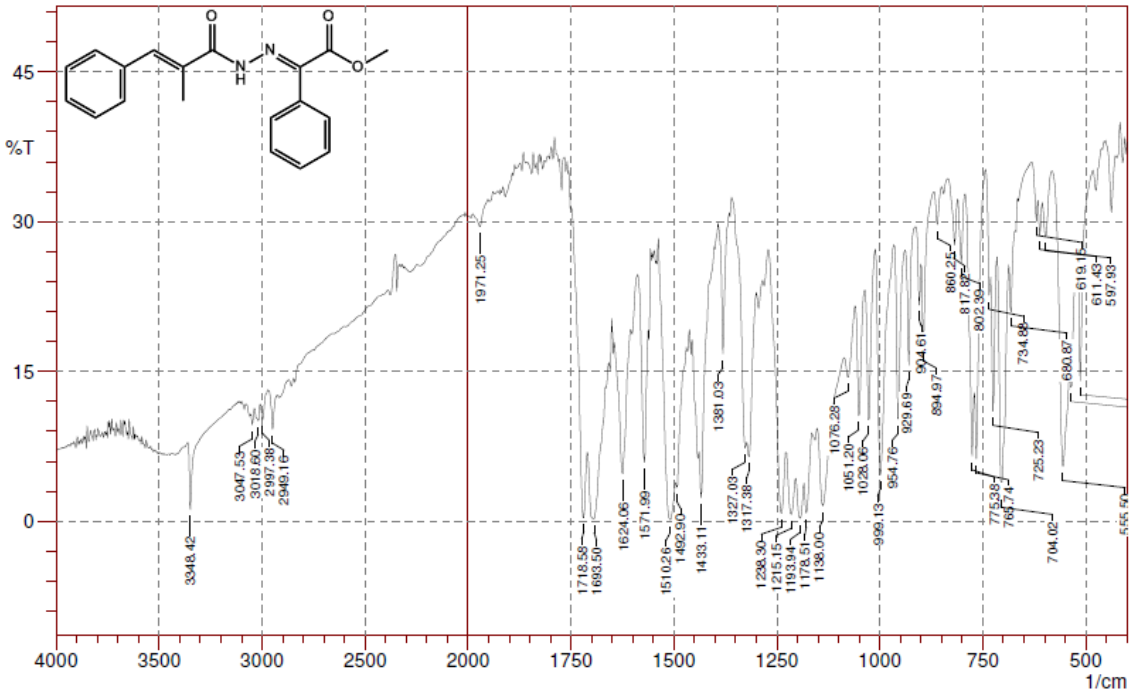

%T
60
45
30
15
0
4000
3500
3000
2500
2000
1750
1500
1250
1000
750
500
1/cm
3157.47
3080.32
2976.16
2937.59
1705.07
1672.28
1618.28
1600.92
1591.27
1573.91
1514.12
1456.26
1440.83
1423.47
1373.32
1341.24
1307.74
1300.02
1292.31
1278.81
1255.66
1217.08
1197.79
1186.22
1170.79
1143.79
1107.14
1045.49
1020.34
993.34
937.40
921.97
876.75
829.39
795.03
767.67
743.31
698.23
634.59
592.15
553.57
518.85

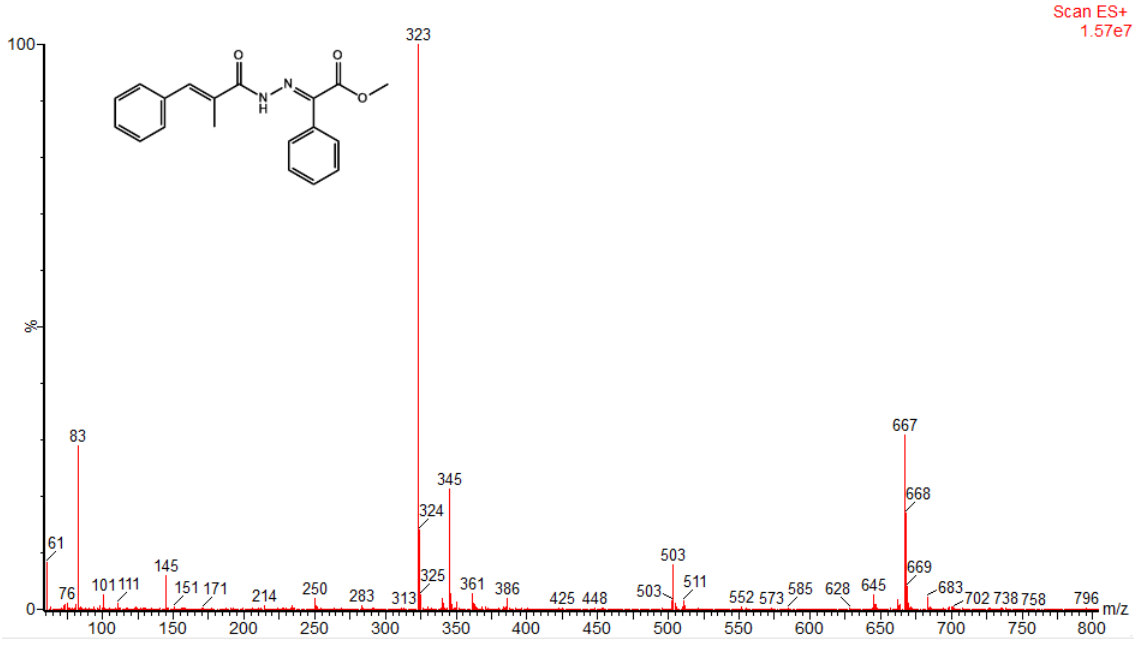

Scan ES+
7.47e7
100
%
0
367
368
369
384
83
61
84
111
135
161
162
214
231
263
304
325
350
405
440
467
496
533
569
577
599
604
669
674
680
725
733
755
756
757
771
m/z
100
150
200
250
300
350
400
450
500
550
600
650
700
750
800

- ***N*-Acylhydrazone (25):**

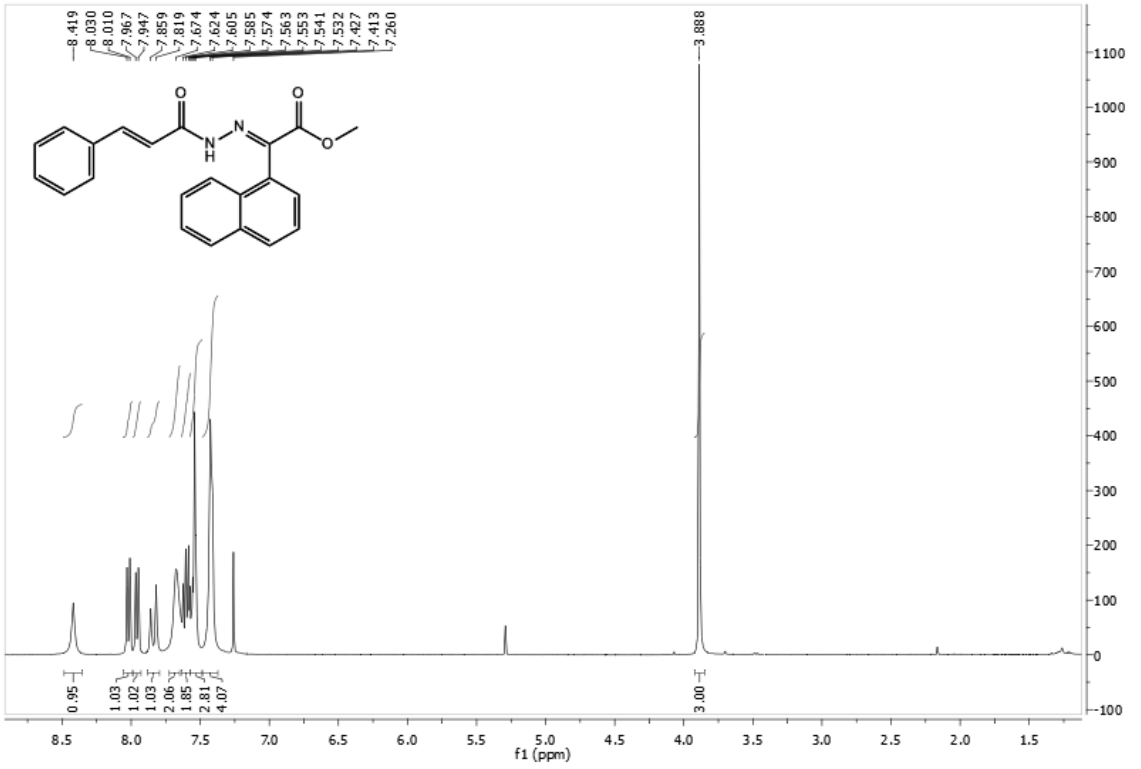


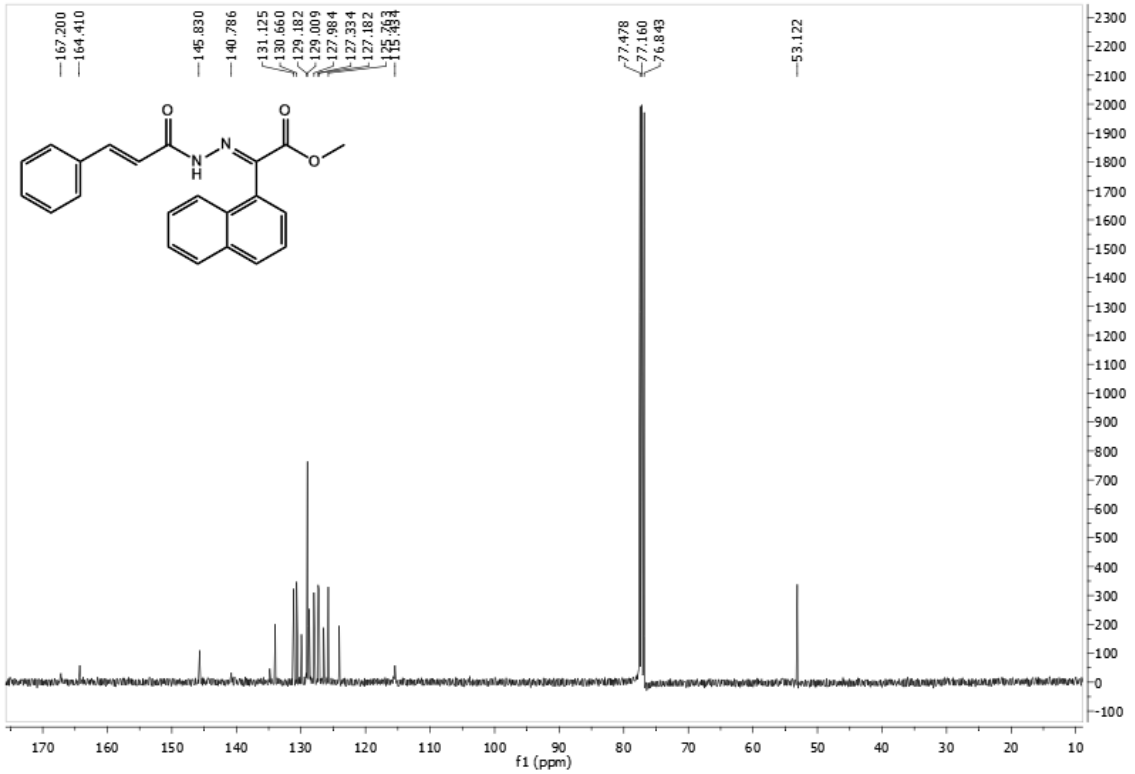


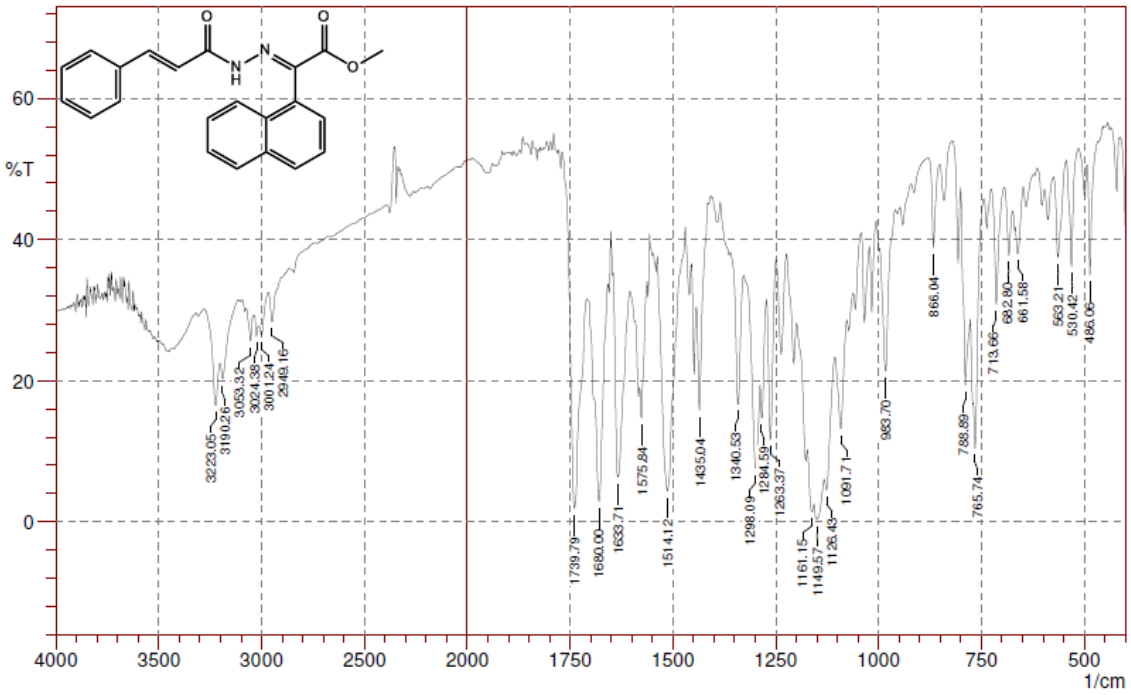

%T
45
30
15
0
4000
3500
3000
2500
2000
1750
1500
1250
1000
750
500
1/cm
3348.42
3047.53
3018.60
2997.38
2949.16
1971.25
1718.58
1693.50
1624.06
1571.99
1510.26
1492.90
1433.11
1381.03
1327.03
1317.36
1238.30
1215.15
1193.94
1178.51
1138.00
1076.28
1051.20
1028.06
999.13
954.76
929.69
904.61
894.97
860.25
817.82
802.39
775.38
765.74
734.88
725.23
704.02
680.87
619.19
611.43
597.93

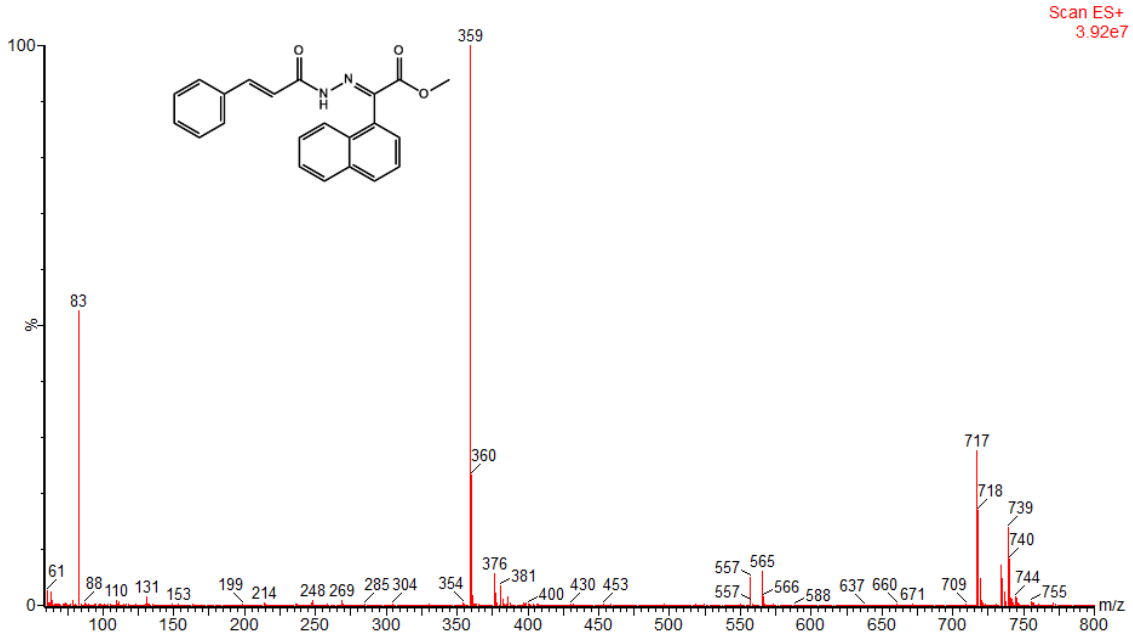

Scan ES+
1.57e7
100
%
0
323
83
61
345
324
667
668
669
145
503
511
325
361
386
425
448
552
573
585
628
645
683
702
738
758
796
m/z
100
150
200
250
300
350
400
450
500
550
600
650
700
750
800

- ***N*-Acylhydrazone (26):**

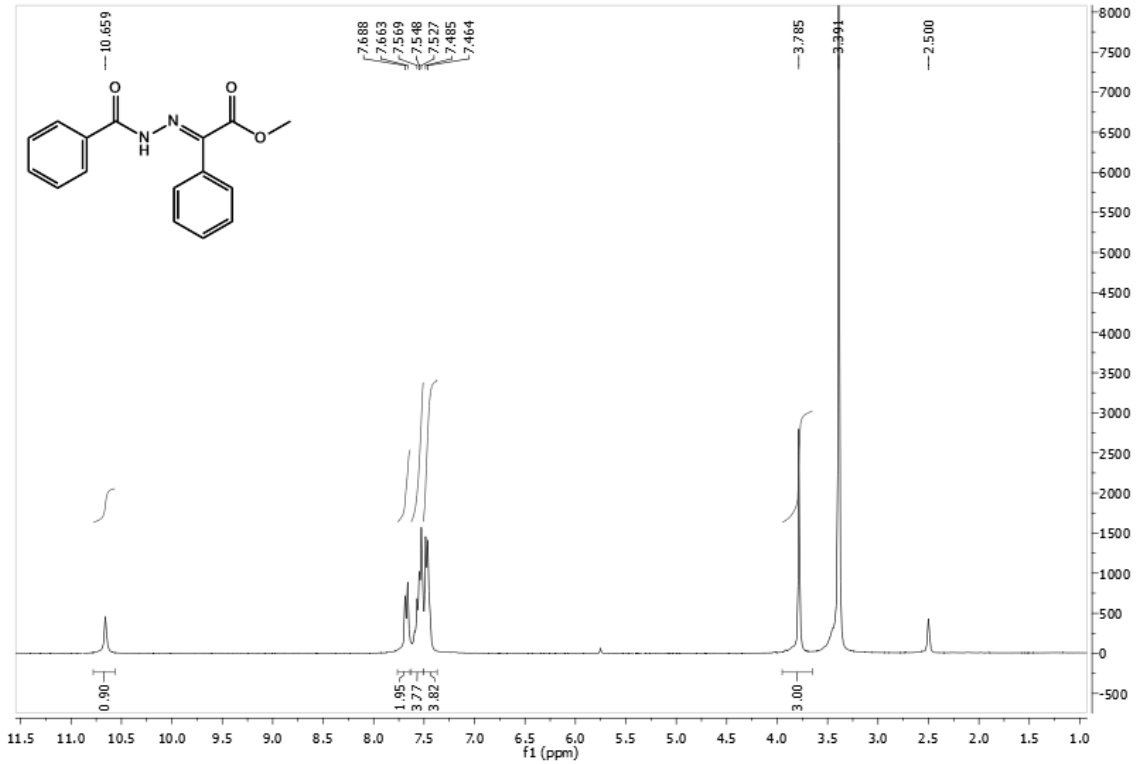


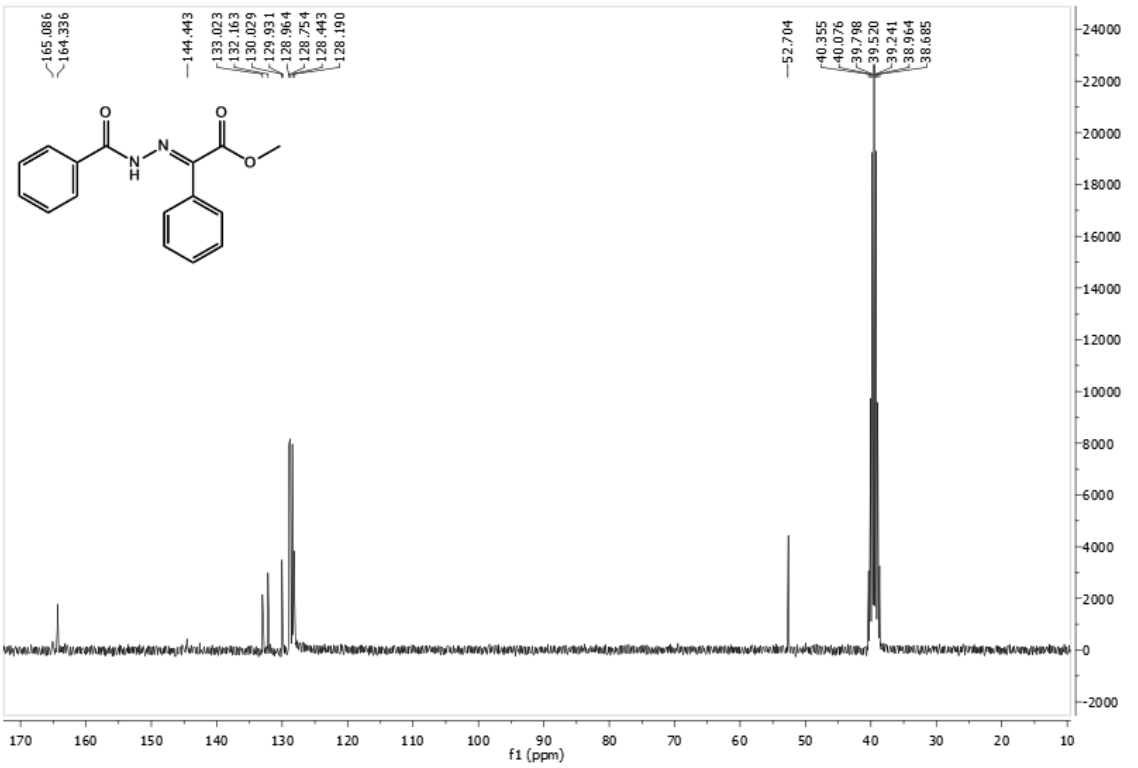


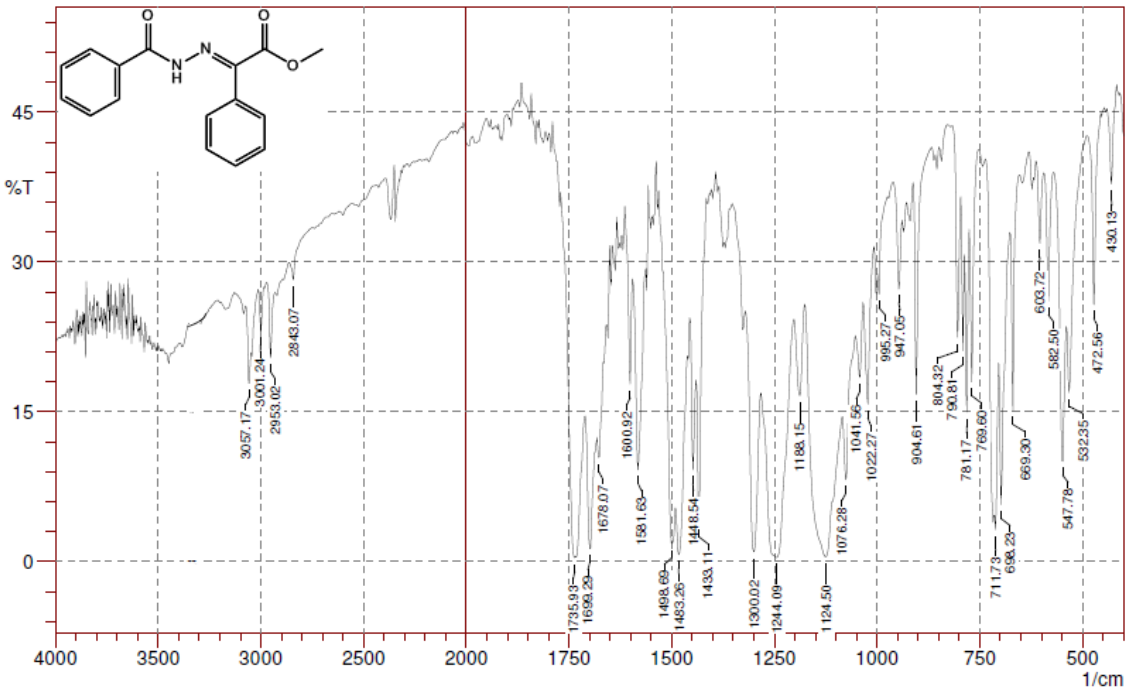

%T
1/cm
3223.05
3190.26
3053.32
3024.38
3001.24
2949.16
1739.79
1680.00
1633.71
1575.84
1514.12
1435.04
1340.53
1298.09
1284.59
1263.37
1161.15
1149.57
1126.43
1091.71
983.70
866.04
788.89
765.74
713.66
682.80
661.58
563.21
530.42
486.06

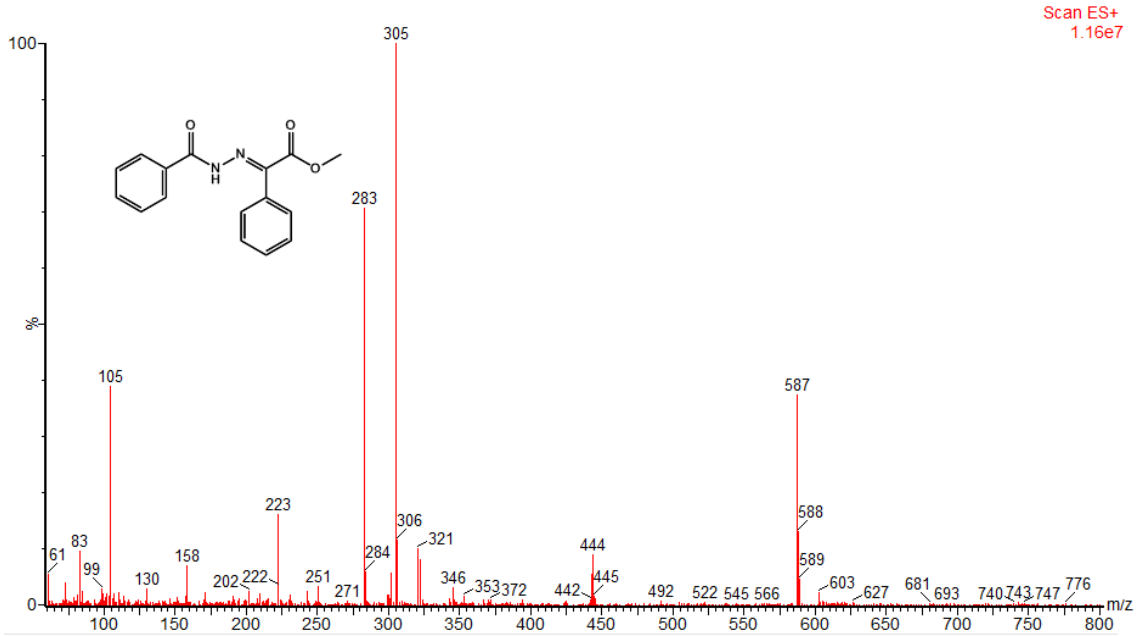

Scan ES+
3.92e7
%
m/z
359
360
83
61
88
110
131
153
199
214
248
269
285
304
354
376
381
400
430
453
557
565
557
566
588
637
660
671
709
717
718
739
740
744
755

- ***N*-Acylhydrazone (27):**

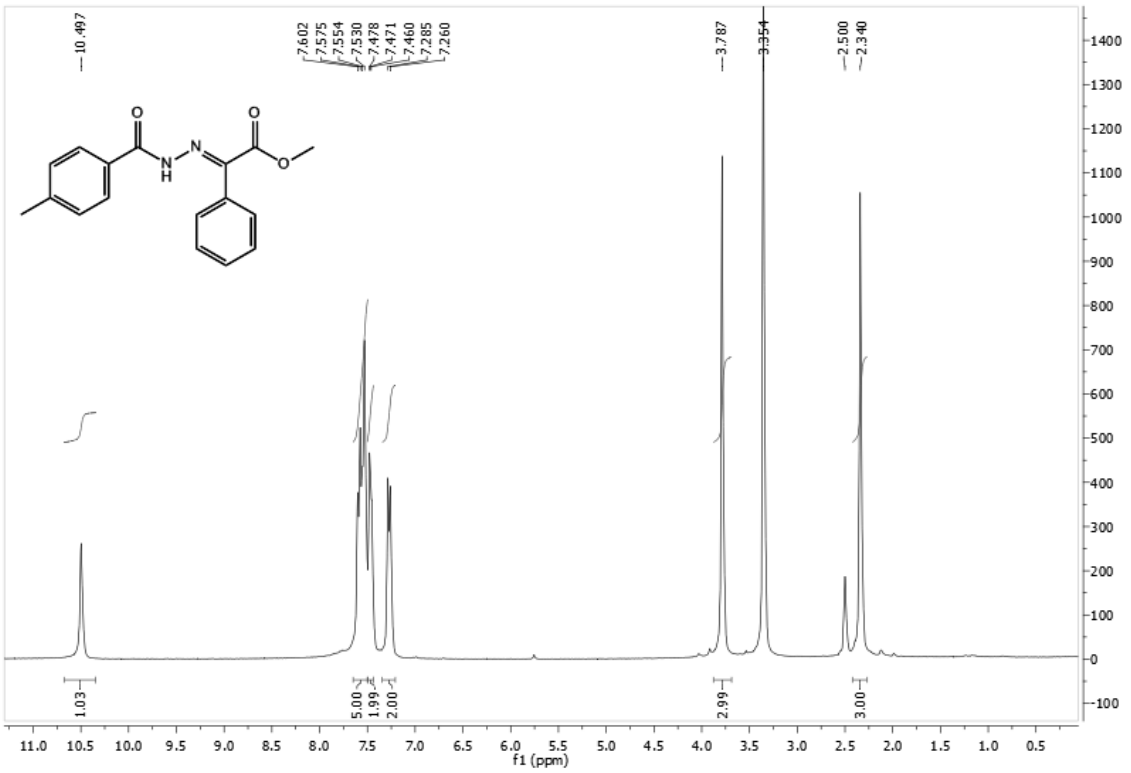


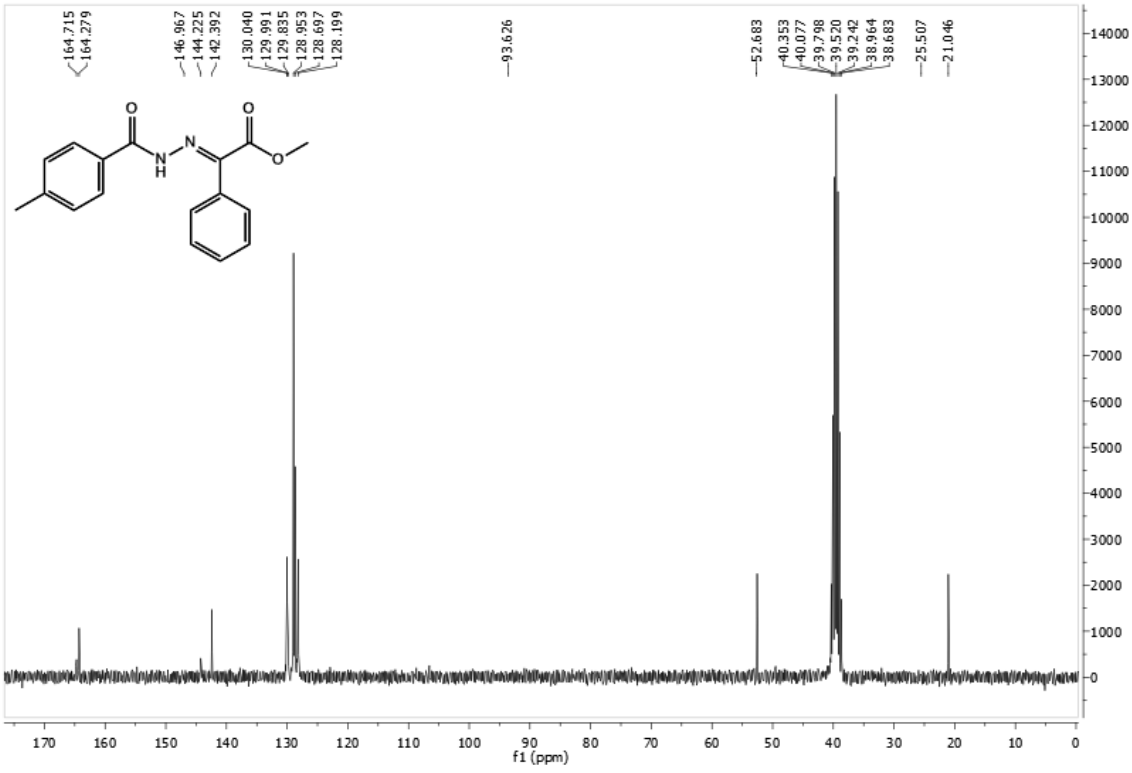


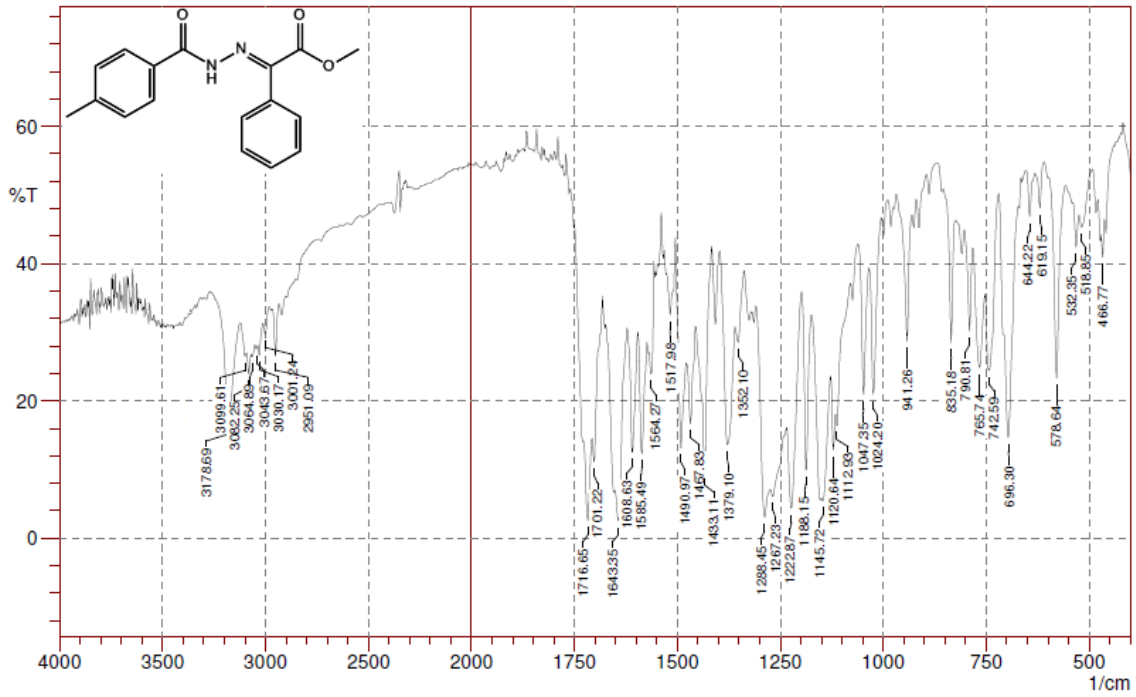

%T
45
30
15
0
4000
3500
3000
2500
2000
1750
1500
1250
1000
750
500
1/cm
3057.17
3001.24
2953.02
2843.07
1735.93
1698.29
1678.07
1600.92
1581.63
1498.69
1483.26
1448.54
1433.11
1300.02
1244.09
1188.15
1124.50
1076.28
1041.56
1022.27
995.27
947.05
904.61
804.32
790.81
781.17
769.60
711.73
698.23
669.30
603.72
582.50
547.78
532.35
472.56
430.13

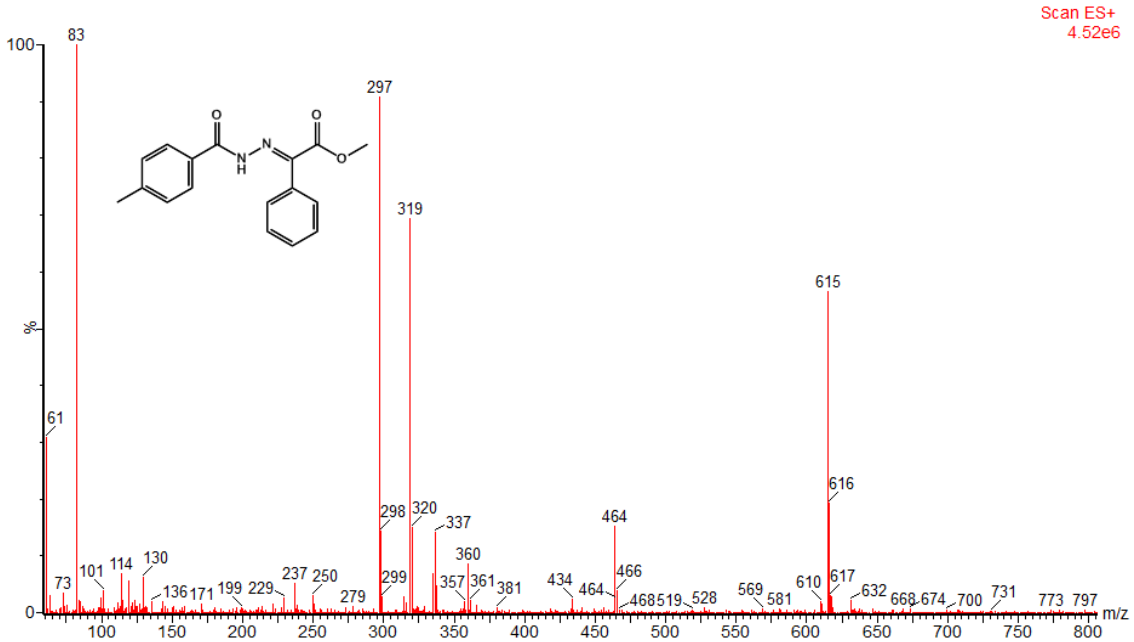

Scan ES+
1.16e7
100
%
0
305
283
105
587
588
589
223
306
321
284
444
445
61
83
99
130
158
202
222
251
271
346
353
372
442
492
522
545
566
603
627
681
693
740
743
747
776
m/z
100
150
200
250
300
350
400
450
500
550
600
650
700
750
800

- ***N*-Acylhydrazone (28):**

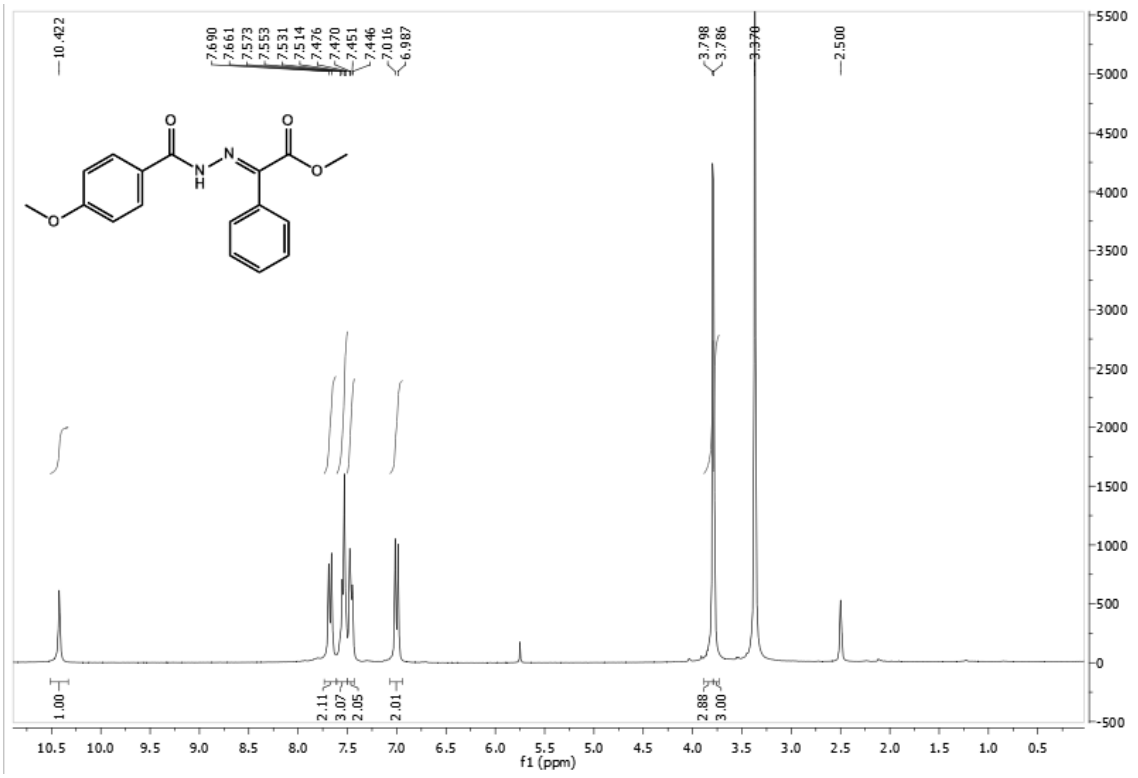


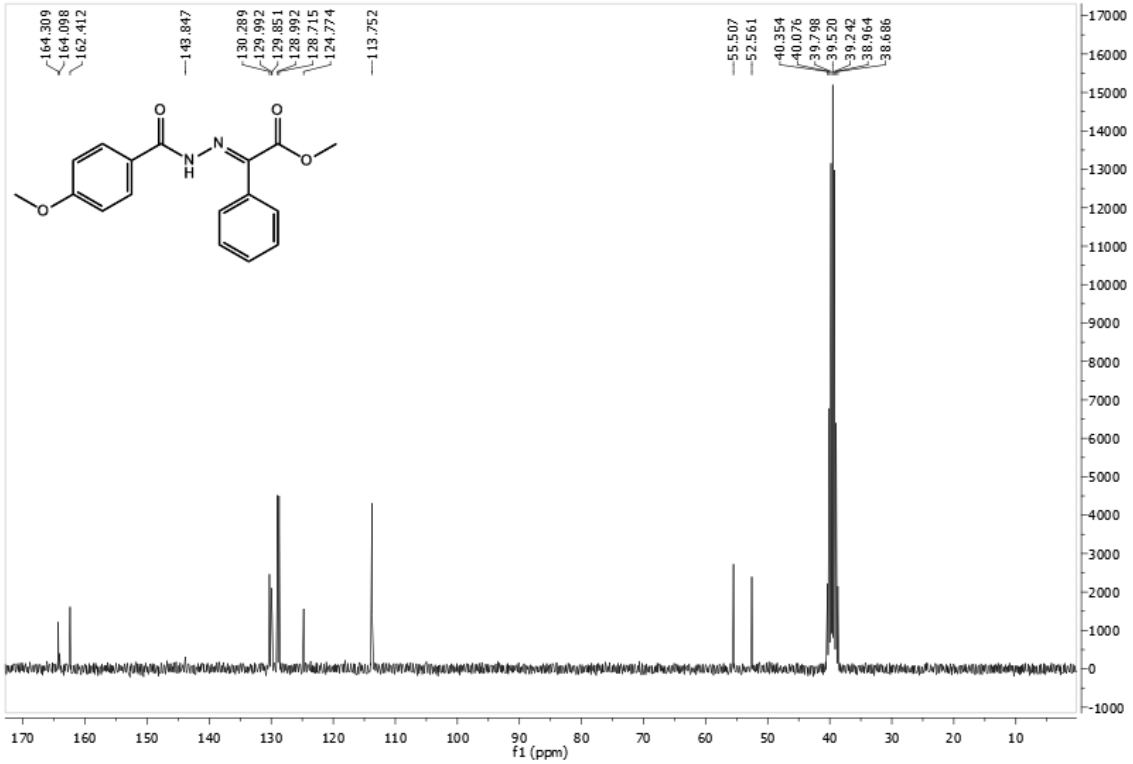


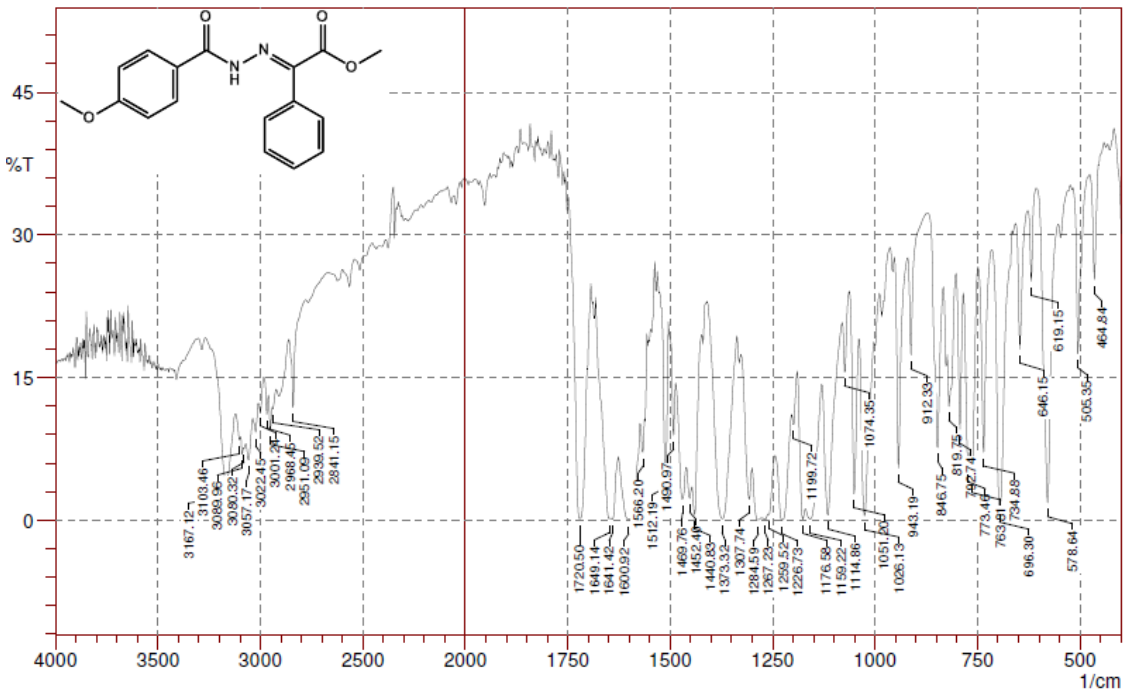

%T
1/cm
3178.69
3099.61
3082.25
3064.89
3043.67
3030.17
3001.24
2951.09
1716.65
1701.22
1643.35
1608.63
1585.49
1564.27
1517.98
1490.97
1467.83
1433.11
1379.10
1352.10
1288.45
1267.23
1222.87
1188.15
1145.72
1120.64
1112.99
1047.35
1024.20
941.26
835.18
790.81
765.74
742.59
696.30
644.22
619.15
578.64
532.35
518.85
466.77

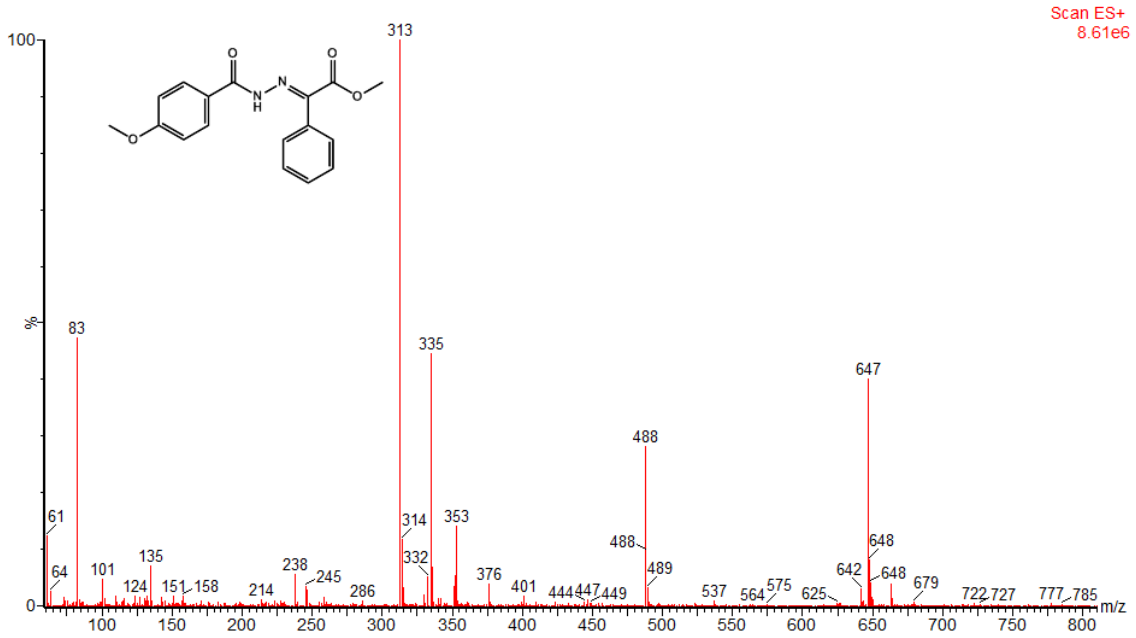

Scan ES+
4.52e6
%
m/z
83
297
319
615
61
616
73
101
114
130
136
171
199
229
237
250
279
298
299
320
337
357
360
361
381
434
464
466
468
519
528
569
581
610
617
632
668
674
700
731
773
797

- ***N*-Acylhydrazone (29):**

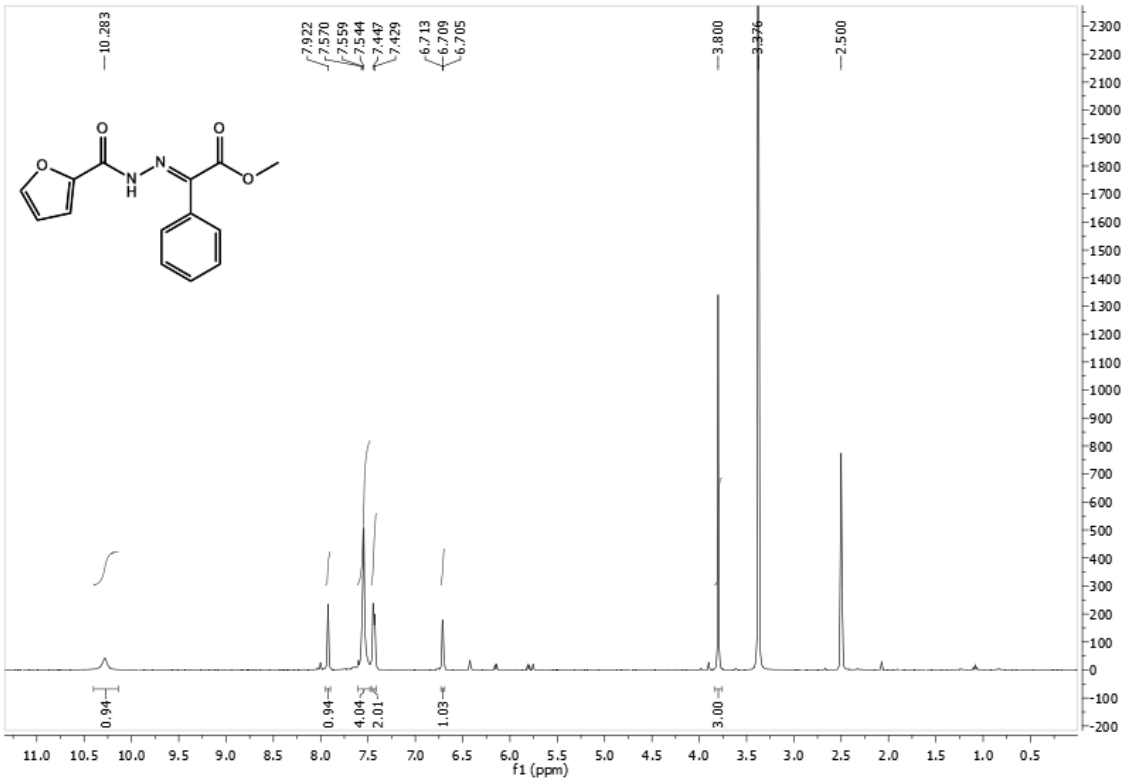


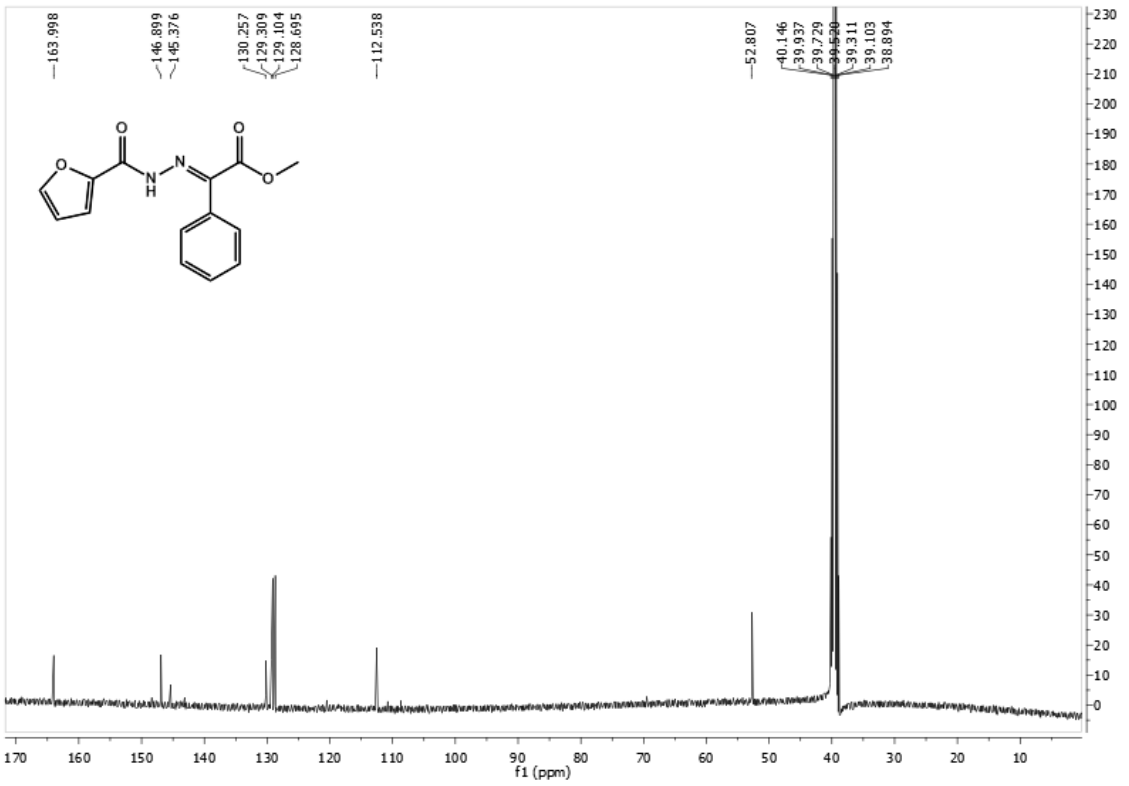


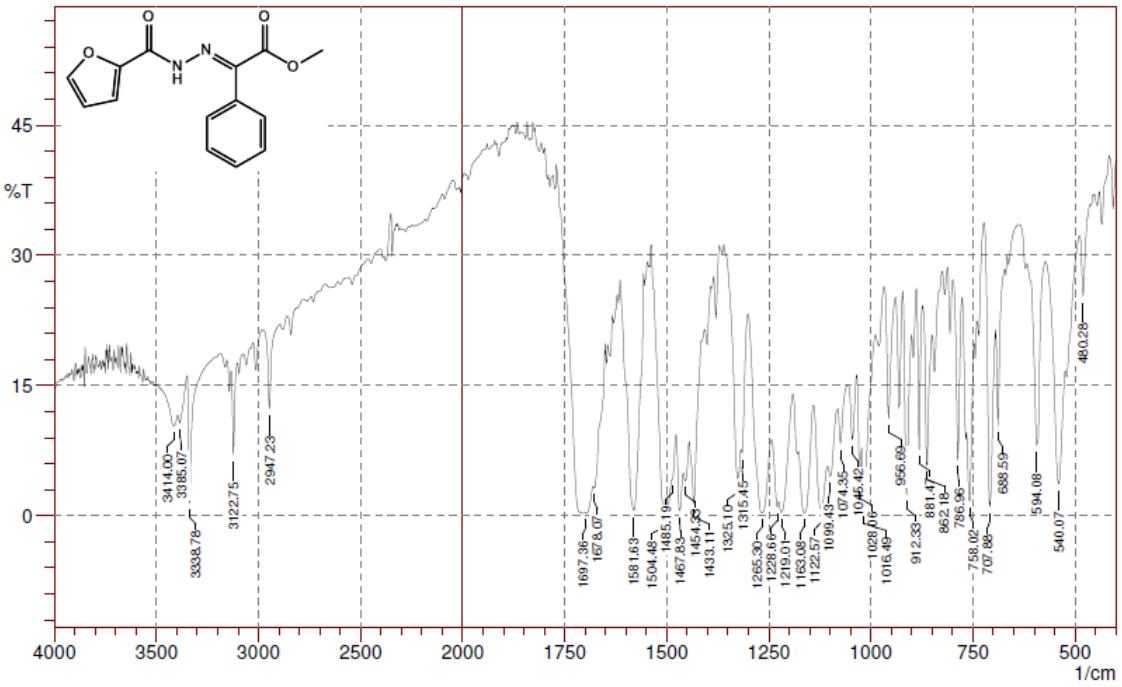

%T
45
30
15
0
4000
3500
3000
2500
2000
1750
1500
1250
1000
750
500
1/cm
3167.12
3103.46
3089.96
3080.32
3057.17
3022.45
3001.24
2968.45
2951.08
2938.52
2841.15
1720.50
1649.14
1641.42
1600.92
1566.20
1512.19
1490.97
1469.76
1452.40
1440.82
1373.32
1307.74
1284.59
1257.23
1259.52
1226.73
1199.72
1176.58
1159.22
1114.86
1074.35
1051.20
1026.13
943.19
912.33
846.75
819.75
792.74
773.48
763.81
734.88
696.30
646.15
619.15
578.64
505.35
464.84

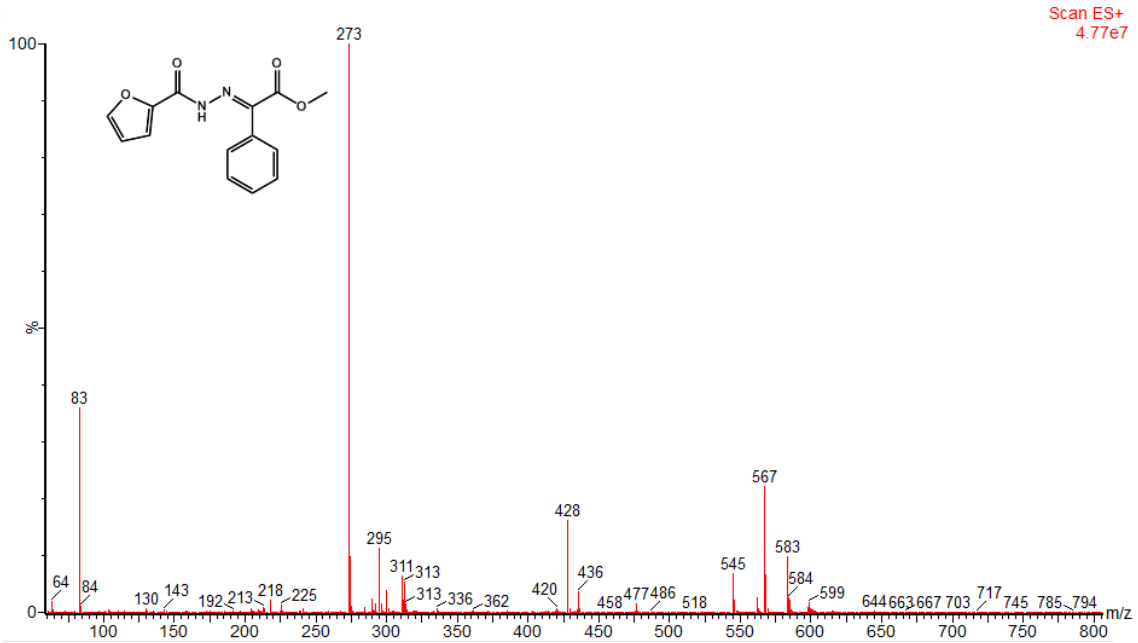

Scan ES+
8.61e6
100
%
0
313
83
335
647
488
61
314
353
648
488
64
101
135
332
489
642
648
679
124
151
158
214
238
245
286
376
401
444
447
449
537
564
575
625
722
727
777
785
m/z
100
150
200
250
300
350
400
450
500
550
600
650
700
750
800

- ***N*-Acylhydrazone (30):**

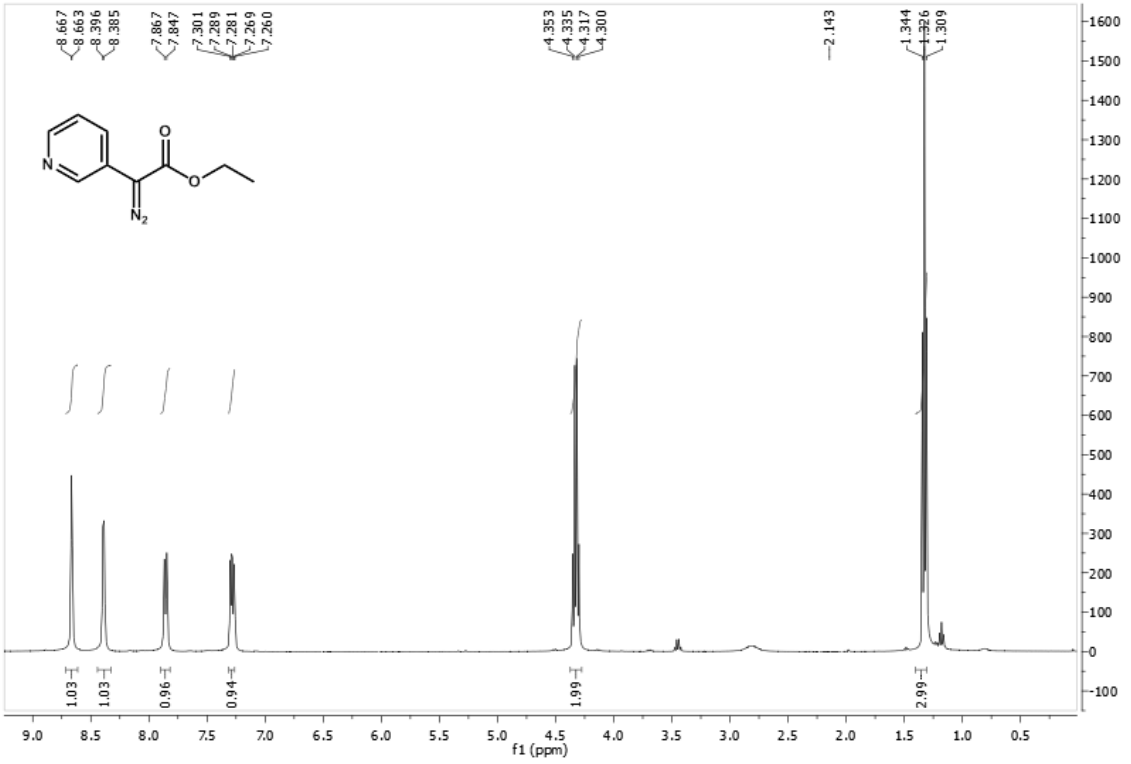


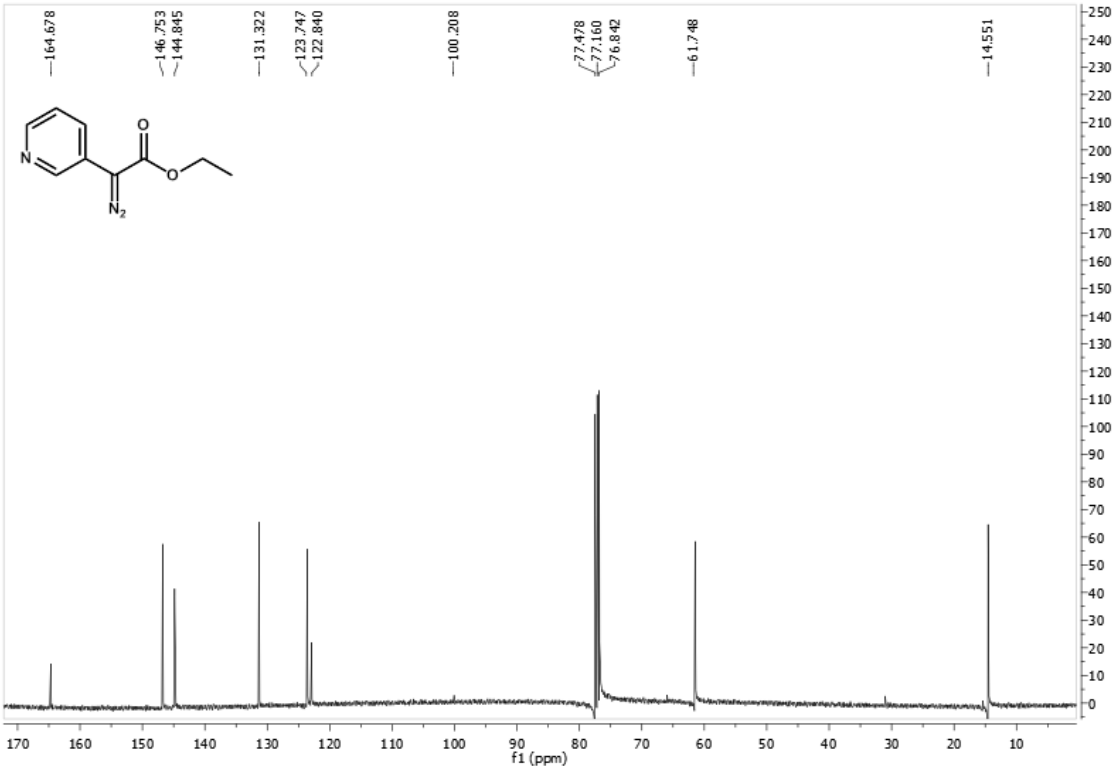


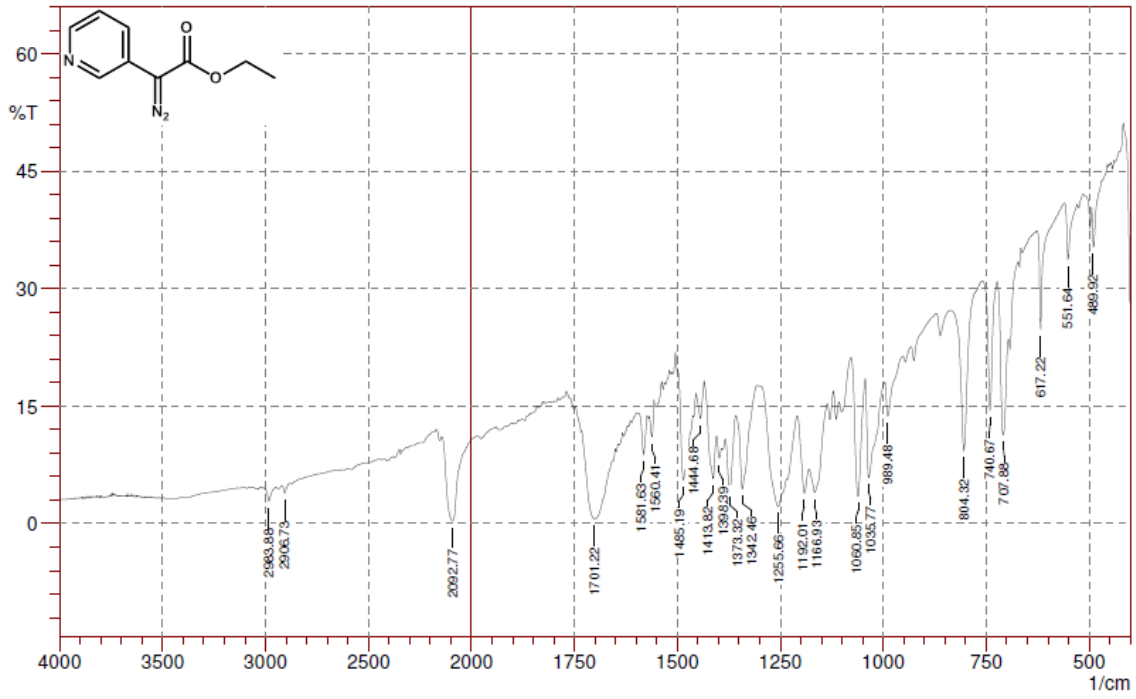

%T
45
30
15
0
4000
3500
3000
2500
2000
1750
1500
1250
1000
750
500
1/cm
3414.00
3385.07
3338.78
3122.75
2947.23
1697.36
1678.07
1581.63
1504.48
1485.19
1467.83
1454.33
1433.11
1325.10
1315.45
1265.30
1228.66
1219.01
1163.08
1122.57
1099.43
1074.35
1046.42
1028.06
1016.49
956.69
912.33
881.47
862.18
786.96
758.02
707.88
688.59
594.08
540.07
480.28

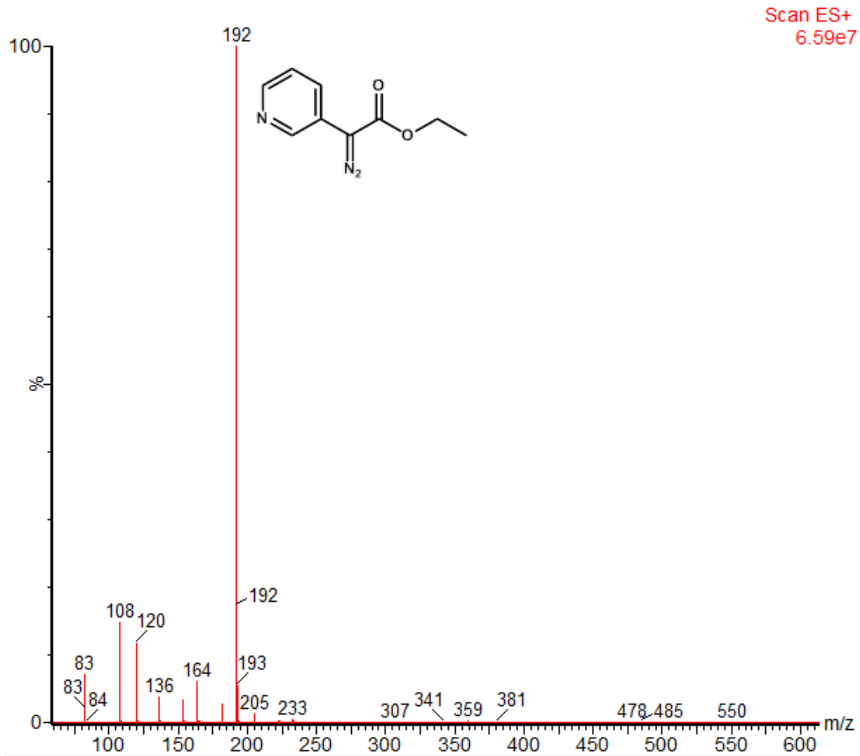

Scan ES+
4.77e7
100
%
0
273
83
64
84
130
143
192
213
218
225
295
311
313
313
336
362
420
428
436
458
477
486
518
545
567
583
584
599
644
663
667
703
717
745
785
794
100
150
200
250
300
350
400
450
500
550
600
650
700
750
800
m/z

- **Ethyl 2-diazo-2-(3-pyridin)acetate:**






%T
60
45
30
15
0
4000
3500
3000
2500
2000
1750
1500
1250
1000
750
500
1/cm
2963.88
2906.73
2092.77
1701.22
1581.63
1560.41
1485.19
1444.68
1413.82
1398.39
1373.32
1342.46
1255.66
1192.01
1166.93
1060.85
1035.77
989.48
804.32
740.67
707.88
617.22
551.64
499.92


Scan ES+
6.59e7
100
%
0
192
108
120
83
83
84
136
164
193
205
233
307
341
359
381
478.485
550
m/z
100
150
200
250
300
350
400
450
500
550
600

11. DFT- Atomic coordinates for all the optimized molecules (PBE0/6-31G*

1′

O	1.199321	1.693822	-0.939290
C	0.421696	0.612170	-0.550780
C	1.032252	-0.322925	0.249436
N	2.348984	-0.266117	0.691340
N	0.456162	-1.475165	0.790506
C	2.565816	-1.257682	1.738268
H	2.450956	-0.807122	2.735697
C	1.477992	-2.276108	1.458003
H	3.572736	-1.681499	1.674609
C	-0.953004	0.614289	-0.946798
C	-1.549836	1.631917	-1.617760
H	-1.541790	-0.259223	-0.689702
H	-0.976810	2.539297	-1.802725
H	1.839563	-3.079933	0.799339
H	1.081826	-2.738829	2.367604
C	-2.931079	1.658456	-2.076851
C	-0.601148	-2.218022	0.184884
C	3.179453	0.894792	0.765148
C	-3.771943	0.529434	-2.074292
C	-3.470758	2.863857	-2.558936
C	-5.086131	0.614415	-2.511644
C	2.842091	1.990756	1.573442
H	-3.387470	-0.430291	-1.739461
C	-0.470672	-2.770938	-1.100544
H	3.491173	3.899418	2.291387
C	-4.785223	2.946702	-3.000279
H	-1.438339	-3.946801	-2.605849
C	3.751292	3.043415	1.671532
C	-1.530563	-3.523849	-1.607391
H	-2.840248	3.750007	-2.576366
C	-5.605604	1.822030	-2.977061
C	4.973728	3.034020	1.001084
H	-5.711505	-0.274619	-2.498013
C	-2.696727	-3.750143	-0.877608
C	-3.808405	-4.592077	-1.438205
H	-5.171425	3.895434	-3.363548
C	5.947473	4.168986	1.154823
H	-6.633545	1.882292	-3.322351
H	6.217633	1.910066	-0.342766
H	-3.697385	-3.349349	0.982140
H	1.094792	1.782525	-1.894327
C	5.275697	1.932628	0.201732
C	-2.792547	-3.193692	0.398284
C	4.397017	0.858249	0.072248
C	-1.761571	-2.432226	0.946006
C	0.743046	-2.530656	-1.952054
C	1.519498	2.074162	2.278944
C	-1.899184	-1.824427	2.312439
C	4.735851	-0.304376	-0.816404
H	6.596221	4.259939	0.279035
H	-4.782909	-4.268710	-1.061516
H	-3.683971	-5.644995	-1.158182
H	6.595411	4.019222	2.026923
H	-3.833614	-4.545693	-2.530395
H	5.430958	5.123030	1.294527
H	0.840662	-3.310043	-2.712363
H	1.554584	2.817584	3.079639
H	1.665887	-2.503564	-1.366736
H	1.216932	1.117740	2.715444
H	0.732709	2.365980	1.574824
H	0.666852	-1.564265	-2.462835
H	5.642976	-0.102277	-1.391836
H	-2.915099	-1.952918	2.693807
H	-1.665351	-0.756106	2.291752
H	3.919232	-0.512824	-1.514068
H	4.906541	-1.223825	-0.243927
H	-1.213357	-2.286145	3.032319

2

N	2.606511	-1.156392	-1.735162
O	-1.256178	-1.782926	0.569211
O	-0.013011	-2.959670	-0.899973
N	1.706446	-0.981573	-1.071770
C	-0.213773	-1.947720	-0.260499
C	0.585689	0.523701	0.397375
C	0.664564	-0.772815	-0.298425
C	1.750187	1.276510	0.610837
H	2.714495	0.888985	0.292782
C	-0.685355	2.282318	1.471728
H	-1.644216	2.669383	1.804563
C	-0.638684	1.048106	0.834133
H	-1.549323	0.484701	0.676251
C	0.473892	3.024573	1.675346
H	0.428797	3.989936	2.170087
C	-2.124058	-2.912711	0.652220
H	-2.909788	-2.627349	1.350987
H	-1.582517	-3.787211	1.020167
H	-2.546333	-3.148422	-0.327468
C	1.692506	2.514337	1.237532
H	2.608448	3.077239	1.391779

3

N	-0.446779	-2.361453	0.864517
O	-3.761703	0.485464	2.321717
O	-1.784117	1.354560	1.689243
O	1.219715	-3.706341	0.199549
N	-0.930189	-1.156774	1.130255
C	-2.502882	0.398913	1.857371
C	-3.082917	-2.140886	1.811060
C	3.878387	-0.435021	-0.562930
C	1.660183	-1.351529	0.176827
H	1.204140	-0.393254	0.397778
C	5.140886	-0.791235	-1.058825
H	5.366926	-1.842468	-1.218743
C	2.915167	-1.492808	-0.281315
H	3.250478	-2.513689	-0.464048
C	-2.131661	-1.022813	1.581453
C	0.851967	-2.559925	0.395971
C	-3.470255	-2.960957	0.743441
H	-3.105487	-2.745856	-0.257837
C	3.600946	0.926702	-0.360369
H	2.632194	1.230130	0.024788
C	-4.439104	-3.486025	3.297220
H	-4.815871	-3.688982	4.295362
C	-3.579437	-2.413984	3.090438
H	-3.290878	-1.777581	3.921086
C	-4.817405	-4.297954	2.230219
H	-5.489831	-5.134735	2.394439
C	-4.197414	1.812286	2.604122
H	-5.218563	1.717253	2.972134
H	-4.170673	2.426437	1.700480
H	-3.557598	2.277019	3.358654
C	6.096623	0.175935	-1.345933
H	7.068352	-0.120470	-1.729744
C	-4.333813	-4.032205	0.952912
H	-4.630727	-4.656286	0.115274
C	4.554922	1.891787	-0.646349
H	4.324498	2.940582	-0.483569
C	5.805972	1.521146	-1.140328
H	6.550021	2.280446	-1.362799
H	-0.991176	-3.207429	1.023781

13

N	-0.949493	-1.945227	0.156655
O	-3.650729	-1.743650	3.248238
O	-2.935453	-2.976581	1.521406
O	0.108176	-3.045583	-1.485498
N	-1.112398	-0.867281	0.901135
C	-2.900250	-1.937204	2.161763
C	-2.035005	0.477641	2.605346
C	2.700490	0.229814	-2.393904
C	0.835446	-0.807106	-1.066601
H	0.637205	0.061077	-0.449312
C	3.647983	-0.020305	-3.397135
H	3.673592	-1.001368	-3.864591
C	1.785268	-0.840751	-2.015885
H	1.883072	-1.776919	-2.565424

C	-2.006353	-0.792818	1.841470
C	0.013116	-2.008271	-0.851444
C	-0.827343	1.134956	2.872524
H	0.101281	0.671607	2.554231
C	2.678723	1.502656	-1.801108
H	1.952369	1.725066	-1.025319
C	-3.214003	2.297716	3.685330
H	-4.151345	2.751170	3.994449
C	-3.230295	1.076256	3.021348
H	-4.177059	0.588921	2.818193
C	-2.008019	2.940720	3.948331
H	-1.998633	3.892265	4.471859
C	-4.491689	-2.841768	3.605292
H	-5.025390	-2.521755	4.499044
H	-3.891844	-3.731012	3.812020
H	-5.191079	-3.069460	2.797443
C	4.546350	0.962205	-3.795794
H	5.272486	0.747635	-4.574277
C	-0.813601	2.354158	3.537900
H	0.133732	2.844227	3.743652
C	3.574540	2.483598	-2.199078
H	3.543317	3.463209	-1.731037
C	4.512417	2.217893	-3.197199
H	5.212057	2.989083	-3.505912
H	-1.549137	-2.760314	0.296889

SIMes

C	0.040493	0.378773	0.191820
N	1.281746	0.023122	0.582467
N	-0.760230	-0.632745	0.586625
C	1.380874	-1.333555	1.155749
H	1.974221	-1.342007	2.073925
C	-0.087512	-1.670767	1.392095
H	1.858022	-2.011810	0.436006
H	-0.353767	-2.677240	1.058521
H	-0.377107	-1.574114	2.446901
C	-2.179099	-0.590688	0.496432
C	2.453069	0.750571	0.232923
C	3.227710	1.334192	1.244151
C	-2.844794	-1.518589	-0.315267
H	4.989193	2.480470	1.668551
H	-4.758125	-2.193357	-1.008483
C	4.391042	2.018442	0.885549
C	-4.239581	-1.480297	-0.370461
C	4.793244	2.139874	-0.441463
C	-4.978809	-0.547652	0.351411
C	-6.480942	-0.532822	0.294307
C	6.057917	2.864728	-0.808903
H	4.282262	1.654421	-2.471975
H	-4.844573	1.117274	1.704127
C	3.991798	1.560791	-1.427307
C	-4.285869	0.372383	1.140756
C	2.828327	0.861304	-1.117051
C	-2.896436	0.367669	1.233164
C	-2.085282	-2.523262	-1.134417
C	2.812769	1.256683	2.686067
C	-2.183076	1.375188	2.087706
C	1.988170	0.253954	-2.203152
H	6.853091	2.160537	-1.080947
H	-6.854469	-1.120865	-0.548352
H	-6.866795	0.486352	0.192760
H	6.426351	3.472236	0.022038
H	-6.916266	-0.953262	1.208601
H	5.904354	3.524823	-1.668341
H	-1.138222	-2.106135	-1.487909
H	3.244726	2.082061	3.257980
H	-2.671272	-2.837898	-2.001958
H	3.150295	0.326106	3.159770
H	1.724353	1.299071	2.783857
H	-1.853136	-3.427928	-0.558288
H	2.434248	0.431296	-3.184945
H	-2.896623	2.019152	2.607864
H	-1.517593	1.993915	1.478015
H	0.977110	0.672015	-2.185658
H	1.884331	-0.829319	-2.069725
H	-1.555236	0.886706	2.841958

I

O	0.712117	1.380801	2.013784
N	2.433639	-0.648888	-1.904146
C	0.632742	0.031992	1.724504
O	2.082390	3.838420	-1.298603
C	1.135767	-0.839294	2.660787
O	2.578485	2.065122	0.001666
N	1.933643	-0.477408	3.730907
N	2.316276	0.459509	-2.089599
N	0.921263	-2.209814	2.733489
C	2.304486	2.535662	-1.093870
C	2.118743	-1.604181	4.636704
C	1.869399	2.183875	-3.685254
C	2.181669	1.748364	-2.310433
H	1.437027	-1.546881	5.498678
C	1.791115	-2.800675	3.745566
C	1.033560	1.404856	-4.494817
H	3.145019	-1.625293	5.012254
H	0.570728	0.506325	-4.094865
C	0.010427	-0.370217	0.502148
C	2.127901	3.752856	-5.506922
C	-0.601510	0.483642	-0.358070
H	2.556814	4.671634	-5.896679
C	2.418363	3.362507	-4.205351
H	0.054499	-1.429136	0.262990
H	-0.680538	1.527048	-0.059060
H	3.065605	3.972053	-3.585042
C	1.305118	2.969433	-6.312397
H	2.701627	-3.226914	3.299162
H	1.085064	3.276467	-7.330624
H	1.263876	-3.596905	4.277084
C	-1.188560	0.141494	-1.643122
C	2.142044	4.646423	-0.122653
C	-0.208438	-2.915638	2.246144
H	2.045043	5.674283	-0.470262
C	2.812803	0.640081	3.773924
H	3.088532	4.499306	0.402127
C	-1.071451	-1.128514	-2.244372
H	1.320637	4.396827	0.554156
C	-1.904396	1.122945	-2.354574
C	0.762051	1.794469	-5.800996
C	-1.647049	-1.395074	-3.479909
H	0.104546	1.181956	-6.410682
C	2.569621	1.644864	4.723712
H	-0.521997	-1.916293	-1.737054
C	0.009700	-3.995396	1.373574
H	3.273281	3.489909	5.552121
C	-2.479807	0.855014	-3.589783
H	-0.917359	-5.558026	0.237659
C	3.463860	2.707106	4.820276
C	-1.087456	-4.724420	0.916244
H	-2.005491	2.113702	-1.917984
C	-2.356390	-0.407831	-4.165015
C	4.582613	2.802343	3.990349
H	-1.540551	-2.385774	-3.914817
C	-2.390560	-4.401918	1.290144
C	-3.565367	-5.166072	0.747480
H	-3.025365	1.638852	-4.108432
C	5.549111	3.945420	4.131715
H	-2.806039	-0.621978	-5.130244
H	5.649635	1.859556	2.384369
H	-3.584344	-3.072564	2.479998
H	1.386216	1.761279	1.423714
C	4.787312	1.800178	3.045439
C	-2.575560	-3.330425	2.163550
C	3.925295	0.707962	2.922811
C	-1.510774	-2.581196	2.661427
C	1.399123	-4.344061	0.921210
C	1.332603	1.593222	5.570697
C	-1.770045	-1.451545	3.613793
C	4.189641	-0.344567	1.885701
H	6.248922	3.772609	4.958174
H	-3.982529	-4.668660	-0.136203
H	-4.369170	-5.241745	1.485855
H	5.029097	4.885234	4.341946
H	-3.281618	-6.179325	0.449529
H	6.143254	4.081994	3.223885

H	1.371395	-4.981244	0.033670
H	1.227698	2.504009	6.165853
H	1.958241	-4.885617	1.694172
H	1.338868	0.743157	6.262575
H	0.451505	1.488014	4.929864
H	1.971083	-3.440853	0.684674
H	5.222248	-0.286850	1.531669
H	-2.773056	-1.531077	4.040715
H	-1.685238	-0.483286	3.108405
H	3.528545	-0.210583	1.023006
H	4.018176	-1.352589	2.276108
H	-1.046507	-1.442846	4.435381

TSI-II

O	0.481952	1.418252	1.548601
N	1.576545	0.045994	-0.433408
C	0.366923	0.136911	1.150508
O	3.061651	4.335819	-1.574625
C	1.170039	-0.790361	1.903785
O	1.735472	3.732642	0.128901
N	2.272549	-0.450571	2.609565
N	1.848576	1.211333	-0.551383
N	1.029846	-2.138686	1.920148
C	2.407605	3.408864	-0.841379
C	2.860189	-1.619011	3.260769
C	3.355891	1.531115	-2.444450
C	2.564190	2.037191	-1.315109
H	2.634469	-1.602918	4.335845
C	2.191133	-2.780619	2.536996
C	3.148257	0.217114	-2.904949
H	3.945624	-1.615177	3.140899
H	2.380758	-0.394633	-2.441539
C	-0.892082	-0.237630	0.507687
C	5.101050	1.750652	-4.128709
C	-1.909941	0.631138	0.369289
H	5.867377	2.362389	-4.598080
C	4.357352	2.286636	-3.085203
H	-0.949741	-1.226085	0.068868
H	-1.788704	1.618016	0.811394
H	4.548860	3.300195	-2.759855
C	4.880516	0.449886	-4.573492
H	2.841082	-3.215378	1.768199
H	5.465799	0.037102	-5.390060
H	1.866724	-3.577643	3.210323
C	-3.173055	0.384073	-0.321848
C	2.886766	5.672943	-1.126303
C	-0.077996	-2.931780	1.500686
H	3.468034	6.292660	-1.810021
C	2.874001	0.828623	2.840695
H	3.247639	5.792527	-0.101019
C	-3.501078	-0.841189	-0.927625
H	1.832428	5.959703	-1.155386
C	-4.122109	1.416072	-0.381901
C	3.895827	-0.310179	-3.951026
C	-4.721771	-1.017882	-1.563518
H	3.700849	-1.326825	-4.282854
C	2.369391	1.654278	3.856586
H	-2.794494	-1.665814	-0.899617
C	0.026577	-3.688245	0.325173
H	2.636738	3.505520	4.892805
C	-5.344978	1.239135	-1.018548
H	-0.996633	-5.068010	-0.954849
C	3.028347	2.851476	4.116670
C	-1.060849	-4.485277	-0.038609
H	-3.886324	2.372171	0.079033
C	-5.652417	0.019705	-1.614005
C	4.161719	3.240450	3.400873
H	-4.950578	-1.973530	-2.028090
C	-2.224427	-4.542649	0.726499
C	-3.397069	-5.377534	0.295857
H	-6.058791	2.057581	-1.051302
C	4.816395	4.566950	3.663001
H	-6.605769	-0.122771	-2.114476
H	5.538413	2.661745	1.859193
H	-3.187432	-3.812533	2.504212
H	0.976541	1.936629	0.842195
C	4.650079	2.381314	2.420864
C	-2.286670	-3.781196	1.895306
C	4.031978	1.164344	2.127007
C	-1.228962	-2.974181	2.304843
C	1.247521	-3.618769	-0.546836
C	1.124775	1.289288	4.609568
C	-1.338950	-2.138099	3.545938
C	4.625367	0.254282	1.089069
H	4.768473	4.836424	4.722220
H	-4.212609	-4.743355	-0.070428
H	-3.795133	-5.965540	1.128663
H	4.312636	5.362668	3.101529
H	-3.125222	-6.067010	-0.507359
H	5.866509	4.563834	3.358481
H	1.021988	-3.986553	-1.550627
H	1.006313	1.920098	5.493827
H	2.061981	-4.238873	-0.152678
H	1.129485	0.244331	4.937983
H	0.252258	1.429445	3.963144
H	1.618390	-2.592035	-0.631493
H	5.216325	0.825231	0.369249
H	-2.198163	-2.445544	4.146289
H	-1.470648	-1.080761	3.288417
H	3.855523	-0.286038	0.532651
H	5.297625	-0.484454	1.545374
H	-0.441827	-2.212711	4.169179

II

O	0.284034	1.588881	1.635235
N	1.344677	0.463280	-0.194248
C	0.402807	0.391384	0.969924
O	3.750819	4.088260	-1.840692
C	1.096353	-0.609033	1.913208
O	2.577012	4.222978	0.070001
N	2.057670	-0.258745	2.769030
N	1.792639	1.669915	-0.226306
N	0.875051	-1.926054	1.969922
C	2.969761	3.548982	-0.866512
C	2.524519	-1.408659	3.548891
C	3.269731	1.329049	-2.186963
C	2.670822	2.131178	-1.101617
H	2.240255	-1.278392	4.599031
C	1.815318	-2.587083	2.883323
C	2.509993	0.359418	-2.863075
H	3.613283	-1.479423	3.496515
H	1.470827	0.223836	-2.587314
C	-0.927856	-0.087617	0.443534
C	5.175070	0.690074	-3.562647
C	-2.081528	0.494683	0.792743
H	6.220722	0.825363	-3.827308
C	4.616962	1.473298	-2.559691
H	-0.881076	-0.862539	-0.313808
H	-2.025702	1.312279	1.509321
H	5.226295	2.218316	-2.060293
C	4.406083	-0.262855	-4.226146
H	2.494837	-3.227964	2.311113
H	4.843182	-0.873740	-5.011216
H	1.268055	-3.216109	3.590146
C	-3.418066	0.170614	0.287798
C	4.037132	5.465141	-1.666573
C	-0.024532	-2.746385	1.216222
H	4.646221	5.754551	-2.524247
C	2.730913	1.000141	2.913256
H	4.585681	5.642171	-0.735989
C	-3.677602	-0.910525	-0.569427
H	3.118246	6.057359	-1.636042
C	-4.500056	0.968306	0.686040
C	3.069590	-0.419713	-3.869867
C	-4.966740	-1.172606	-1.012512
H	2.452238	-1.152667	-4.383564
C	2.272667	1.920472	3.862837
H	-2.863932	-1.555955	-0.886523
C	0.403028	-3.274461	-0.009861
H	2.598728	3.867542	4.687968
C	-5.791574	0.706054	0.243219
H	-0.165403	-4.535194	-1.644247
C	2.960737	3.125376	3.980147
C	-0.473195	-4.126966	-0.684467

H	-4.316274	1.810229	1.349079
C	-6.031167	-0.366826	-0.609738
C	4.072112	3.418591	3.190354
H	-5.144781	-2.012284	-1.679093
C	-1.723040	-4.465619	-0.167623
C	-2.644190	-5.394733	-0.906530
H	-6.611666	1.342398	0.563682
C	4.721179	4.770430	3.238920
H	-7.038245	-0.575286	-0.959059
H	5.410601	2.651228	1.697052
H	-3.079201	-4.169306	1.475172
H	0.909290	2.165208	1.085063
C	4.534535	2.445294	2.307362
C	-2.102664	-3.925772	1.063051
C	3.885758	1.222759	2.151282
C	-1.269612	-3.067726	1.776193
C	1.728350	-2.900757	-0.607227
C	1.041990	1.653311	4.677707
C	-1.720658	-2.461091	3.072118
C	4.407381	0.195543	1.187557
H	4.508853	5.290775	4.176735
H	-3.655122	-4.979653	-0.970768
H	-2.724039	-6.359895	-0.393621
H	4.334413	5.384453	2.417248
H	-2.290361	-5.586239	-1.922420
H	5.806775	4.703306	3.120132
H	1.863680	-3.385397	-1.576662
H	0.903425	2.427582	5.435936
H	2.565318	-3.208481	0.030770
H	1.085173	0.687276	5.193581
H	0.166472	1.643913	4.021400
H	1.806504	-1.814635	-0.748372
H	5.237425	0.600780	0.605703
H	-2.657156	-2.913195	3.405393
H	-1.888888	-1.385217	2.948592
H	3.630145	-0.119661	0.483426
H	4.778591	-0.697733	1.706627
H	-0.982708	-2.587584	3.871406

TSII-III

O	0.643772	1.653454	1.893652
N	1.654305	0.613050	-0.005010
C	0.665035	0.513038	1.043817
O	2.102589	2.970877	-3.933716
C	1.226142	-0.614275	1.920385
O	0.107269	3.046478	-2.890590
N	2.216775	-0.436426	2.788596
N	1.152962	1.384693	-0.945243
N	0.846101	-1.892002	1.882254
C	1.248998	2.632925	-2.924671
C	2.578014	-1.697793	3.447555
C	3.325098	1.337554	-2.131731
C	1.903047	1.743810	-1.960132
H	2.370384	-1.621522	4.519864
C	1.696140	-2.726188	2.738113
C	3.664272	0.026543	-2.483595
H	3.646613	-1.887178	3.319715
H	2.868285	-0.688958	-2.667685
C	-0.740239	0.240164	0.539672
C	5.694121	1.871947	-2.057792
C	-1.836234	0.770848	1.093319
H	6.483803	2.602065	-1.899164
C	4.362517	2.253190	-1.923795
H	-0.803374	-0.386146	-0.342907
H	-1.704756	1.412085	1.963549
H	4.113835	3.277514	-1.660880
C	6.015953	0.560631	-2.400190
H	2.268596	-3.422393	2.116704
H	7.055186	0.262063	-2.509102
H	1.076845	-3.311322	3.423240
C	-3.217095	0.559876	0.648512
C	1.537500	3.830160	-4.907317
C	-0.121280	-2.531581	1.041275
H	2.324790	4.013080	-5.640483
C	2.972821	0.734626	3.140025
H	1.208757	4.773564	-4.460663
C	-3.541967	0.026247	-0.608181
H	0.671392	3.366426	-5.389298
C	-4.267677	0.894991	1.513903
C	4.994461	-0.361516	-2.614452
C	-4.866090	-0.181536	-0.970311
H	5.235046	-1.383963	-2.894931
C	2.564992	1.495671	4.244241
H	-2.750204	-0.199950	-1.315581
C	0.269025	-2.965453	-0.232164
H	3.070859	3.158466	5.490875
C	-5.593993	0.684342	1.153193
H	-0.407896	-3.949371	-2.009180
C	3.379573	2.552031	4.642084
C	-0.685871	-3.621892	-1.010190
H	-4.033618	1.325349	2.484984
C	-5.899231	0.140951	-0.090887
C	4.570682	2.854674	3.979398
H	-5.096380	-0.583149	-1.953442
C	-1.979768	-3.858198	-0.548892
C	-3.006756	-4.523853	-1.419582
H	-6.390297	0.951113	1.842521
C	5.409324	4.026119	4.406383
H	-6.933976	-0.017808	-0.380591
H	5.877087	2.272381	2.377429
H	-3.320417	-3.612545	1.114340
H	0.869539	2.380252	1.296922
C	4.948635	2.057894	2.901397
C	-2.314592	-3.437716	0.739853
C	4.173790	0.981789	2.463816
C	-1.401611	-2.777891	1.557142
C	1.648744	-2.698855	-0.758286
C	1.266855	1.224535	4.946085
C	-1.801292	-2.294108	2.919375
C	4.604964	0.145071	1.297958
H	5.383240	4.163801	5.491314
H	-3.770760	-3.802669	-1.731650
H	-3.521969	-5.328666	-0.885768
H	5.042983	4.954166	3.951915
H	-2.557311	-4.946309	-2.321524
H	6.452365	3.903342	4.102798
H	1.725145	-3.006509	-1.803810
H	1.173672	1.844521	5.840765
H	2.411989	-3.255420	-0.200431
H	1.166863	0.178227	5.256384
H	0.433126	1.450902	4.274083
H	1.897652	-1.631190	-0.685379
H	5.532408	0.525471	0.865471
H	-2.798533	-2.654972	3.179356
H	-1.822164	-1.198678	2.939924
H	3.824729	0.162995	0.526282
H	4.777909	-0.899885	1.586287
H	-1.109328	-2.625886	3.701167

III

O	0.638291	1.461510	2.254689
N	1.654068	1.048619	0.250795
C	0.651314	0.544661	1.193035
O	2.694739	0.885261	-4.237087
C	1.251850	-0.754488	1.738520
O	1.204758	-0.566565	-3.400424
N	2.365710	-0.776705	2.483128
N	1.526436	0.559022	-0.942781
N	0.866974	-1.998100	1.435710
C	2.002813	0.336754	-3.205347
C	2.882541	-2.140701	2.621079
C	3.387143	1.983789	-1.779854
C	2.317153	0.969272	-1.921347
H	3.112048	-2.351390	3.669180
C	1.743115	-2.992637	2.066836
C	4.650303	1.800083	-2.364899
H	3.803844	-2.244717	2.037829
H	4.827812	0.917335	-2.970174
C	-0.709203	0.405573	0.570939
C	4.208142	4.069667	-0.832807
C	-1.788697	1.039388	1.042998
H	4.023086	4.960192	-0.237472
C	3.188068	3.141347	-1.012356

H	-0.718174	-0.138273	-0.367775
H	-1.671316	1.629482	1.950411
H	2.221376	3.303483	-0.550860
C	5.457385	3.867530	-1.413047
H	2.072353	-3.729545	1.330207
H	6.254235	4.592660	-1.271566
H	1.183804	-3.519744	2.848502
C	-3.127355	1.040254	0.446499
C	2.401414	0.326481	-5.506498
C	-0.384069	-2.459397	0.908881
H	3.034863	0.856647	-6.219093
C	3.152444	0.305571	2.999362
H	1.346841	0.464010	-5.762155
C	-3.473790	0.253796	-0.663797
H	2.619154	-0.745526	-5.528028
C	-4.118218	1.855825	1.010012
C	5.670687	2.727023	-2.184556
C	-4.757576	0.295202	-1.190166
H	6.638625	2.556914	-2.649228
C	2.841680	0.798273	4.277277
H	-2.733062	-0.399070	-1.115286
C	-0.415517	-2.978757	-0.390913
H	3.421649	2.185836	5.799036
C	-5.405055	1.896614	0.484309
H	-1.677525	-3.888983	-1.860677
C	3.657472	1.790126	4.813496
C	-1.631654	-3.493149	-0.848802
H	-3.866939	2.470530	1.871217
C	-5.730676	1.116315	-0.620386
C	4.762828	2.288966	4.120633
H	-5.001448	-0.315174	-2.055633
C	-2.777607	-3.504122	-0.057574
C	-4.086072	-4.011790	-0.592333
H	-6.153393	2.540852	0.937395
C	5.599286	3.392686	4.703692
H	-6.733598	1.146133	-1.036412
H	5.914459	2.122382	2.315933
H	-3.576439	-3.010932	1.877316
H	1.302267	2.112321	1.972225
C	5.055568	1.751594	2.870388
C	-2.692784	-3.003250	1.243396
C	4.276623	0.747328	2.290439
C	-1.507274	-2.483237	1.752358
C	0.777011	-2.938059	-1.297322
C	1.648412	0.296062	5.035590
C	-1.459484	-1.920833	3.142807
C	4.679333	0.162772	0.968906
H	5.684073	3.299529	5.790422
H	-4.758911	-3.174422	-0.811801
H	-4.594531	-4.653444	0.133950
H	5.153131	4.372211	4.495116
H	-3.949417	-4.581258	-1.515092
H	6.607472	3.396454	4.281213
H	0.866398	-1.958960	-1.789510
H	1.640508	0.693510	6.053203
H	0.685538	-3.694183	-2.081126
H	1.634604	-0.797718	5.102092
H	0.729051	0.607391	4.530190
H	1.715126	-3.114653	-0.763478
H	5.209957	0.904212	0.367557
H	-2.348558	-2.211936	3.706632
H	-1.427395	-0.825458	3.110942
H	3.811990	-0.156298	0.389760
H	5.354487	-0.691772	1.110261
H	-0.581680	-2.258011	3.703996

TSIII-IV

O	0.820172	1.447131	2.075178
N	1.664714	0.878512	0.226626
C	0.650045	0.408203	1.218400
O	2.960601	0.961043	-4.206963
C	1.209455	-0.883899	1.821347
O	1.717035	-0.739245	-3.427491
N	2.324067	-0.898548	2.554647
N	1.679315	0.455901	-0.991584
N	0.735612	-2.122253	1.664780
C	2.306526	0.305120	-3.219207
C	2.720612	-2.266065	2.899357
C	3.244742	2.217034	-1.741248
C	2.404624	1.011055	-1.931083
H	2.874908	-2.347386	3.979145
C	1.547184	-3.105324	2.391378
C	4.587307	2.242254	-2.143434
H	3.663578	-2.511841	2.399417
H	5.005714	1.374058	-2.643181
C	-0.715663	0.286462	0.594578
C	3.509931	4.480164	-0.899969
C	-1.729856	1.036899	1.039634
H	3.079395	5.354148	-0.419064
C	2.719548	3.356832	-1.117848
H	-0.796394	-0.336877	-0.290769
H	-1.512184	1.683289	1.889442
H	1.678068	3.362362	-0.811263
C	4.843546	4.488537	-1.298914
H	1.850779	-3.910944	1.717716
H	5.460844	5.366153	-1.128529
H	0.951931	-3.543598	3.199921
C	-3.086920	1.098754	0.492292
C	2.890616	0.333597	-5.478151
C	-0.470407	-2.566486	1.033389
H	3.465923	0.966313	-6.154901
C	3.192338	0.173273	2.948606
H	1.854520	0.256144	-5.819394
C	-3.529305	0.279812	-0.559153
H	3.315203	-0.673889	-5.444133
C	-3.998056	2.011112	1.042276
C	5.378209	3.364630	-1.923896
C	-4.826958	0.380528	-1.041557
H	6.416480	3.362443	-2.245138
C	2.934036	0.827293	4.163546
H	-2.851338	-0.445027	-0.999628
C	-0.405679	-3.064646	-0.273610
H	3.654849	2.299448	5.534436
C	-5.299120	2.111056	0.561377
H	-1.563294	-3.927185	-1.854972
C	3.849583	1.777016	4.600289
C	-1.590815	-3.546347	-0.836720
H	-3.671389	2.652705	1.857109
C	-5.719904	1.295870	-0.484654
C	4.997893	2.087802	3.866604
H	-5.145456	-0.257411	-1.861854
C	-2.797026	-3.543200	-0.140292
C	-4.066495	-4.030389	-0.778930
H	-5.984439	2.828943	1.003399
C	5.945740	3.151048	4.345164
H	-6.734451	1.371808	-0.865168
H	6.108469	1.639188	2.086227
H	-3.745332	-3.039400	1.723659
H	1.632692	1.786845	1.073646
C	5.223134	1.408151	2.674442
C	-2.810708	-3.052570	1.167803
C	4.340856	0.435177	2.196025
C	-1.660487	-2.564024	1.778252
C	0.858067	-3.032090	-1.082294
C	1.675065	0.555995	4.928727
C	-1.710581	-1.994782	3.165854
C	4.659383	-0.292124	0.920521
H	6.113152	3.081242	5.424485
H	-4.759871	-3.197226	-0.941444
H	-4.580247	-4.757377	-0.141661
H	5.544083	4.150869	4.143557
H	-3.875072	-4.501488	-1.746128
H	6.914820	3.078832	3.844607
H	1.023668	-2.044603	-1.535273
H	1.680677	1.075026	5.890089
H	0.808203	-3.759216	-1.896257
H	1.527486	-0.512913	5.123310
H	0.829985	0.910552	4.327989
H	1.743026	-3.260749	-0.480392
H	5.107959	0.394494	0.197635
H	-2.684292	-2.181231	3.624034
H	-1.553430	-0.910355	3.137878
H	3.768378	-0.711932	0.450911
H	5.380050	-1.101278	1.096288

H	-0.944729	-2.421017	3.822849

IV

O	0.033730	0.820149	2.446100
N	1.510072	1.097896	0.697215
C	0.442094	0.263265	1.331793
O	3.930030	1.939434	-3.138978
C	1.098787	-1.063950	1.816334
O	3.213982	-0.149934	-2.713561
N	2.329343	-1.169542	2.327563
N	2.016308	0.782361	-0.456972
N	0.407267	-2.184873	2.047229
C	3.296828	1.016259	-2.383593
C	2.476791	-2.400457	3.111741
C	3.010762	3.019824	-0.764521
C	2.746556	1.610201	-1.148664
H	2.555113	-2.150278	4.175639
C	1.199672	-3.173000	2.782446
C	4.316103	3.495176	-0.593447
H	3.388106	-2.926977	2.816484
H	5.150173	2.822571	-0.766789
C	-0.610849	0.053445	0.246021
C	2.174439	5.216611	-0.156662
C	-1.846889	0.527128	0.417393
H	1.334067	5.885164	0.006533
C	1.942943	3.899803	-0.543612
H	-0.278825	-0.405264	-0.683228
H	-2.054548	0.964451	1.394139
H	0.924023	3.550855	-0.693118
C	3.477152	5.676509	0.009862
H	1.382716	-4.048069	2.149024
H	3.659145	6.704987	0.308166
H	0.658483	-3.503782	3.673276
C	-2.948411	0.479110	-0.546293
C	4.483372	1.435582	-4.346993
C	-0.928032	-2.504712	1.648712
H	4.969117	2.284341	-4.828849
C	3.438777	-0.263364	2.285020
H	3.701401	1.027279	-4.992999
C	-2.763884	0.192422	-1.907857
H	5.209222	0.643158	-4.144338
C	-4.254823	0.723784	-0.098923
C	4.546880	4.812397	-0.213911
C	-3.844489	0.132626	-2.777672
H	5.566733	5.168357	-0.094318
C	3.578833	0.703967	3.292730
H	-1.759917	0.029288	-2.289198
C	-1.133329	-3.157164	0.426489
H	4.827396	2.277133	4.025449
C	-5.338766	0.663371	-0.968501
H	-2.624523	-3.945816	-0.893426
C	4.714259	1.510145	3.262271
C	-2.444088	-3.462135	0.063878
H	-4.413724	0.957366	0.950943
C	-5.138808	0.364066	-2.313493
C	5.702970	1.362123	2.288228
H	-3.676416	-0.087305	-3.828497
C	-3.526155	-3.141900	0.882862
C	-4.935059	-3.399716	0.431996
H	-6.341174	0.857032	-0.596164
C	6.892944	2.278956	2.263150
H	-5.981608	0.321913	-2.997483
H	6.317472	0.213943	0.579672
H	-4.106436	-2.281786	2.763828
H	1.545167	2.042203	1.079528
C	5.546469	0.359713	1.333491
C	-3.272549	-2.529684	2.110700
C	4.424397	-0.470896	1.310440
C	-1.981926	-2.201506	2.519793
C	0.012274	-3.499180	-0.484428
C	2.531674	0.880242	4.352725
C	-1.729060	-1.488888	3.815420
C	4.283921	-1.526124	0.250700
H	7.261181	2.486266	3.272465
H	-5.332871	-2.515280	-0.080112
H	-5.594616	-3.616013	1.277349
H	6.626064	3.241595	1.810821
H	-4.987715	-4.238165	-0.267972
H	7.715470	1.855031	1.680675
H	0.666729	-2.640552	-0.664701
H	2.741727	1.768217	4.954236
H	-0.357033	-3.846352	-1.452048
H	2.507237	0.023131	5.038042
H	1.537952	0.974337	3.892128
H	0.636688	-4.299639	-0.069383
H	5.250184	-1.725773	-0.219446
H	-2.669873	-1.279827	4.330487
H	-1.200508	-0.545449	3.620535
H	3.591556	-1.205801	-0.537267
H	3.908080	-2.471821	0.654534
H	-1.109037	-2.088021	4.493860

TSIV-V

O	-0.078147	1.197281	2.425401
N	1.345181	1.456894	0.677596
C	0.243311	0.764319	1.301189
O	3.883007	1.970319	-3.142907
C	1.097310	-1.047527	1.753599
O	2.863943	0.009647	-2.730844
N	2.278078	-1.131453	2.376767
N	1.812294	1.091949	-0.484963
N	0.392881	-2.141584	2.058292
C	3.136084	1.140293	-2.386877
C	2.429428	-2.353257	3.186863
C	3.235607	3.106620	-0.695100
C	2.710359	1.784374	-1.118398
H	2.577758	-2.093283	4.240216
C	1.110619	-3.083656	2.933419
C	4.609100	3.377393	-0.670125
H	3.305186	-2.919632	2.853126
H	5.307913	2.601295	-0.963359
C	-0.774784	0.349998	0.283894
C	2.818788	5.376903	0.061444
C	-2.065762	0.627730	0.493901
H	2.113400	6.155335	0.337471
C	2.347101	4.126918	-0.326742
H	-0.396471	-0.091195	-0.632754
H	-2.309612	1.098610	1.445779
H	1.276710	3.943112	-0.364035
C	4.186506	5.631705	0.083594
H	1.243266	-4.043850	2.422874
H	4.555740	6.608581	0.382166
H	0.539521	-3.265256	3.849223
C	-3.188349	0.373836	-0.410362
C	4.318232	1.413903	-4.377310
C	-0.897256	-2.497624	1.565158
H	4.927707	2.183064	-4.851772
C	3.384733	-0.233195	2.298348
H	3.464094	1.160018	-5.010645
C	-3.039558	-0.208794	-1.678765
H	4.904919	0.506441	-4.210787
C	-4.479952	0.732693	-0.000071
C	5.078900	4.628745	-0.288377
C	-4.139402	-0.421766	-2.498189
H	6.147800	4.824430	-0.287080
C	3.553654	0.735818	3.300410
H	-2.052061	-0.498923	-2.024386
C	-0.997469	-3.135321	0.322648
H	4.837192	2.287988	4.024337
C	-5.583491	0.520150	-0.819307
H	-2.359512	-4.000764	-1.088204
C	4.698268	1.529377	3.256884
C	-2.264497	-3.514456	-0.119690
H	-4.612430	1.186548	0.979041
C	-5.418129	-0.058074	-2.074580
C	5.668695	1.373476	2.265749
H	-4.000140	-0.871613	-3.477445
C	-3.409353	-3.276343	0.639557
C	-4.769582	-3.632476	0.111184
H	-6.573470	0.809939	-0.478029
C	6.881785	2.259231	2.239844
H	-6.275919	-0.221706	-2.720650
H	6.221355	0.251275	0.519562
H	-4.152077	-2.441981	2.474436

H	1.756850	2.208930	1.225882
C	5.470337	0.394606	1.294038
C	-3.266627	-2.646614	1.876321
C	4.336466	-0.420277	1.286795
C	-2.022867	-2.243769	2.358588
C	0.220299	-3.377756	-0.523828
C	2.521767	0.928689	4.374480
C	-1.895229	-1.495096	3.654101
C	4.142517	-1.451447	0.211849
H	7.272145	2.432963	3.247210
H	-5.194911	-2.786013	-0.441023
H	-5.462704	-3.881176	0.919976
H	6.633406	3.237594	1.812072
H	-4.723829	-4.484003	-0.573796
H	7.682828	1.825429	1.634938
H	0.707919	-2.438505	-0.806895
H	2.799070	1.760461	5.027094
H	-0.044983	-3.910250	-1.440322
H	2.421472	0.037209	5.004904
H	1.538374	1.133130	3.933853
H	0.971250	-3.977138	0.003446
H	5.073756	-1.615517	-0.336418
H	-2.879333	-1.319462	4.095937
H	-1.404377	-0.528101	3.489481
H	3.382696	-1.130660	-0.510188
H	3.818464	-2.414080	0.620386
H	-1.298865	-2.045443	4.391597

V

O	-0.338289	1.952321	2.159961
N	1.183613	2.078524	0.518608
C	-0.024877	1.611878	1.027562
O	4.024632	2.429465	-3.093570
C	1.086903	-1.235813	1.668806
O	2.702620	0.619901	-2.908529
N	2.277914	-1.355463	2.284091
N	1.650117	1.701906	-0.661873
N	0.406397	-2.350819	1.992362
C	3.111826	1.667114	-2.464369
C	2.474094	-2.606729	3.042368
C	3.367064	3.482734	-0.621082
C	2.684620	2.283753	-1.171362
H	2.745269	-2.393914	4.082107
C	1.107904	-3.275812	2.903853
C	4.755597	3.529011	-0.456185
H	3.285927	-3.198117	2.601399
H	5.351016	2.661212	-0.717956
C	-0.880163	0.874040	0.086395
C	3.227555	5.759910	0.207303
C	-2.203828	0.841193	0.302875
H	2.626878	6.629965	0.455485
C	2.611031	4.614994	-0.286169
H	-0.403365	0.454419	-0.791030
H	-2.567366	1.335666	1.203157
H	1.534430	4.603014	-0.433234
C	4.609128	5.792101	0.370804
H	1.165792	-4.281375	2.473696
H	5.092395	6.686591	0.752913
H	0.571647	-3.351525	3.857523
C	-3.219885	0.252402	-0.564900
C	4.472963	1.906130	-4.339582
C	-0.941085	-2.623792	1.624597
H	5.217783	2.611593	-4.707185
C	3.356026	-0.432809	2.196240
H	3.641949	1.824913	-5.044923
C	-2.906608	-0.540077	-1.679920
H	4.912920	0.914187	-4.207769
C	-4.571342	0.504624	-0.289131
C	5.370126	4.674895	0.035009
C	-3.909887	-1.044523	-2.494683
H	6.449605	4.696635	0.153363
C	3.510525	0.535271	3.201105
H	-1.869089	-0.769862	-1.901248
C	-1.194910	-3.466278	0.534522
H	4.769920	2.098332	3.950137
C	-5.577369	0.003421	-1.107231
H	-2.723463	-4.439009	-0.612370
C	4.641411	1.349172	3.171237
C	-2.518659	-3.787522	0.234883
H	-4.828075	1.112372	0.575013
C	-5.249518	-0.771334	-2.216730
C	5.614326	1.219415	2.178404
H	-3.647836	-1.655891	-3.353530
C	-3.582215	-3.290529	0.986672
C	-5.002940	-3.620725	0.625199
H	-6.617497	0.219724	-0.880202
C	6.855232	2.067131	2.211407
H	-6.031655	-1.162927	-2.860906
H	6.145856	0.177626	0.376653
H	-4.114343	-2.037974	2.648402
H	1.714067	2.693994	1.131931
C	5.408075	0.278997	1.170779
C	-3.295528	-2.443666	2.057413
C	4.284289	-0.550439	1.153902
C	-1.987752	-2.094472	2.392628
C	-0.065345	-3.994971	-0.303034
C	2.458380	0.715041	4.258359
C	-1.708405	-1.148939	3.525304
C	4.053905	-1.507311	0.019784
H	7.522864	1.756918	3.023633
H	-5.413896	-2.862698	-0.051646
H	-5.644019	-3.653803	1.511169
H	6.611626	3.121520	2.375461
H	-5.072576	-4.588024	0.119133
H	7.417607	1.990220	1.276509
H	0.613556	-3.188694	-0.596778
H	2.769384	1.464561	4.990631
H	-0.444231	-4.478379	-1.207096
H	2.253868	-0.216521	4.796662
H	1.512024	1.040546	3.811675
H	0.533749	-4.736580	0.239148
H	4.957555	-1.620933	-0.584935
H	-2.626834	-0.918602	4.071730
H	-1.282094	-0.209220	3.155427
H	3.253313	-1.138590	-0.632023
H	3.750322	-2.498251	0.370481
H	-0.989758	-1.566759	4.239009

VI

O	0.458554	1.732413	2.219237
N	2.895902	-0.027454	-1.802323
C	0.435060	0.506849	1.579332
O	0.822390	3.233990	-4.166284
C	1.027230	-0.542418	2.237352
O	1.479788	1.103808	-4.503676
N	1.898950	-0.420316	3.310274
N	2.419180	0.962168	-2.077062
N	0.834378	-1.893263	1.984145
C	1.376428	2.075821	-3.784761
C	2.196971	-1.736197	3.869419
C	1.816796	3.146667	-1.357497
C	1.869713	2.109332	-2.399211
H	1.616165	-1.916940	4.785298
C	1.787158	-2.691939	2.748753
C	2.597511	3.015482	-0.196936
H	3.258273	-1.811565	4.121058
H	3.271601	2.171873	-0.078985
C	-0.263038	0.394506	0.334627
C	0.914326	5.201728	-0.442982
C	-0.982771	1.400072	-0.222655
H	0.249386	6.054262	-0.549612
C	0.972944	4.261611	-1.465958
H	-0.170090	-0.555471	-0.184184
H	-1.083337	2.324093	0.343303
H	0.354253	4.378016	-2.345238
C	1.677985	5.055531	0.710912
H	2.650521	-2.988793	2.136378
H	1.617965	5.788578	1.509476
H	1.302801	-3.598573	3.120131
C	-1.646032	1.383444	-1.517241
C	0.272518	3.217213	-5.483998
C	-0.335850	-2.485562	1.440870
H	-0.087775	4.230152	-5.661593
C	2.845199	0.638793	3.449305

H	-0.552015	2.502835	-5.537951
C	-1.601318	0.293919	-2.407984
H	1.036182	2.945453	-6.215982
C	-2.370321	2.518916	-1.925009
C	2.523762	3.953775	0.827314
C	-2.247816	0.342701	-3.634984
H	3.131900	3.812348	1.716677
C	2.667725	1.574699	4.477248
H	-1.054265	-0.604433	-2.136871
C	-0.197738	-3.321938	0.320335
H	3.496355	3.295525	5.448566
C	-3.019563	2.566678	-3.152083
H	-1.225193	-4.584001	-1.072646
C	3.630417	2.569693	4.649042
C	-1.333494	-3.939729	-0.202383
H	-2.418766	3.374304	-1.255225
C	-2.963957	1.477275	-4.018790
C	4.753004	2.660336	3.825984
H	-2.191082	-0.513626	-4.301524
C	-2.597882	-3.739883	0.347829
C	-3.817830	-4.374274	-0.258461
H	-3.575545	3.457886	-3.431851
C	5.764543	3.757408	4.011336
H	-3.474937	1.507250	-4.976961
H	5.776169	1.761402	2.162591
H	-3.678557	-2.754446	1.919268
H	0.884734	2.375193	1.632815
C	4.901747	1.715696	2.809242
C	-2.702275	-2.911159	1.464694
C	3.967763	0.698401	2.607403
C	-1.595924	-2.282776	2.033984
C	1.144104	-3.533214	-0.321796
C	1.447257	1.521596	5.346692
C	-1.770337	-1.415804	3.246036
C	4.184862	-0.323357	1.526772
H	6.782275	3.396948	3.834355
H	-4.315533	-3.684598	-0.950462
H	-4.549105	-4.647840	0.507990
H	5.722408	4.172589	5.021873
H	-3.562705	-5.276133	-0.821836
H	5.587910	4.582107	3.310360
H	1.033024	-3.966733	-1.318830
H	1.478904	2.298515	6.114869
H	1.775634	-4.214854	0.261109
H	1.345203	0.552355	5.845553
H	0.555432	1.666291	4.729170
H	1.691586	-2.589491	-0.415835
H	4.441073	-1.304230	1.945817
H	-2.728054	-1.622052	3.730746
H	-1.741449	-0.353597	2.979272
H	5.008988	-0.028808	0.871651
H	3.290352	-0.458239	0.911287
H	-0.973409	-1.578792	3.978606

TSVI-VII

O	0.408410	1.627738	1.544562
N	1.514612	0.409751	-0.624924
C	0.203178	0.367762	1.095484
O	3.769668	2.705492	-3.329062
C	1.013611	-0.639725	1.685801
O	3.091783	0.625512	-2.778434
N	2.154161	-0.420117	2.394868
N	1.735769	1.578786	-0.671783
N	0.821922	-1.983830	1.582911
C	3.088363	1.824954	-2.556954
C	2.672561	-1.669456	2.944415
C	2.399273	3.869620	-1.059070
C	2.392291	2.451017	-1.442436
H	2.409296	-1.754498	4.008479
C	1.978722	-2.718735	2.090229
C	2.368122	4.234225	0.297509
H	3.760405	-1.703330	2.858754
H	2.410274	3.462704	1.061433
C	-1.037016	0.119277	0.384948
C	2.385107	6.233285	-1.621749
C	-1.995056	1.058545	0.250172
H	2.390839	7.009934	-2.381960
C	2.410403	4.899730	-2.012445
H	-1.148391	-0.841909	-0.099621
H	-1.845643	2.010257	0.755917
H	2.436523	4.646420	-3.065579
C	2.334348	6.579877	-0.273967
H	2.614827	-3.060109	1.263890
H	2.306918	7.623544	0.025757
H	1.649883	-3.590224	2.661395
C	-3.239265	0.920418	-0.500253
C	4.482254	2.110250	-4.404261
C	-0.301543	-2.694993	1.070740
H	4.962167	2.933961	-4.933877
C	2.840115	0.795535	2.703340
H	3.805956	1.569608	-5.072061
C	-3.576791	-0.225065	-1.242609
H	5.234382	1.407624	-4.034497
C	-4.161155	1.978943	-0.480687
C	2.323157	5.569131	0.683076
C	-4.782242	-0.302770	-1.925361
H	2.292527	5.816563	1.741170
C	2.408843	1.586136	3.777965
H	-2.887875	-1.063662	-1.289522
C	-0.221721	-3.291623	-0.196443
H	2.814141	3.348986	4.923271
C	-5.368351	1.900992	-1.164868
H	-1.286005	-4.467008	-1.636280
C	3.149858	2.722487	4.099650
C	-1.330876	-4.008663	-0.650836
H	-3.917689	2.875760	0.083939
C	-5.687254	0.757948	-1.891598
C	4.301445	3.076129	3.397165
H	-5.017778	-1.197688	-2.495484
C	-2.491275	-4.139798	0.110073
C	-3.687948	-4.878105	-0.419507
H	-6.061231	2.737272	-1.131754
C	5.055076	4.334529	3.722191
H	-6.628338	0.693470	-2.429943
H	5.621325	2.499953	1.804231
H	-3.424906	-3.633361	1.979038
H	0.818096	2.124944	0.784964
C	4.721493	2.245148	2.359431
C	-2.527839	-3.540968	1.370718
C	4.016190	1.097631	1.996748
C	-1.448118	-2.819604	1.872460
C	0.991873	-3.137079	-1.068223
C	1.162135	1.250691	4.541789
C	-1.530037	-2.151488	3.213745
C	4.526616	0.223896	0.885949
H	6.136846	4.172172	3.696034
H	-4.472200	-4.176159	-0.725864
H	-4.121508	-5.534201	0.341517
H	4.791167	4.717088	4.711757
H	-3.430518	-5.488812	-1.288538
H	4.827462	5.117680	2.989407
H	0.762161	-3.426527	-2.096214
H	1.128233	1.794734	5.488868
H	1.815792	-3.777515	-0.731072
H	1.090677	0.180734	4.762292
H	0.280337	1.523513	3.953386
H	1.355480	-2.104336	-1.080573
H	4.988954	-0.692457	1.275327
H	-2.396509	-2.510186	3.773912
H	-1.629116	-1.065718	3.099273
H	5.293863	0.747637	0.311225
H	3.730752	-0.072966	0.197230
H	-0.633151	-2.333811	3.814605

VII

O	0.227658	1.791558	1.553664
N	1.167855	0.699102	-0.367764
C	0.249293	0.629528	0.812462
O	3.937449	2.076546	-3.162957
C	0.919612	-0.468581	1.648213
O	2.861381	0.253175	-2.418900
N	1.912903	-0.236721	2.508100
N	1.601634	1.905278	-0.438951
N	0.651967	-1.773601	1.576756

C	3.047627	1.457307	-2.335536
C	2.363601	-1.478099	3.146915
C	2.758493	3.805047	-1.265463
C	2.443824	2.362094	-1.363978
H	2.126343	-1.446060	4.216123
C	1.583946	-2.556689	2.395559
C	2.770342	4.429381	-0.005835
H	3.446029	-1.581040	3.041287
H	2.603152	3.824900	0.879803
C	-1.123835	0.268557	0.299783
C	3.246180	5.977722	-2.250100
C	-2.232200	0.872348	0.745938
H	3.424277	6.576507	-3.139781
C	2.999508	4.615936	-2.386298
H	-1.141370	-0.437109	-0.522998
H	-2.111261	1.612857	1.534781
H	2.988271	4.172193	-3.374258
C	3.251785	6.579152	-0.994986
H	2.217381	-3.169047	1.745373
H	3.442038	7.643925	-0.893271
H	1.026524	-3.225374	3.056842
C	-3.601340	0.662964	0.268386
C	4.581428	1.210591	-4.081529
C	-0.279889	-2.477654	0.746235
H	5.236212	1.845365	-4.680428
C	2.641733	0.968132	2.780715
H	3.855780	0.700983	-4.722160
C	-3.938991	-0.273862	-0.721353
H	5.168363	0.447586	-3.561038
C	-4.634039	1.425424	0.832139
C	3.007011	5.792016	0.127510
C	-5.256488	-0.433298	-1.128158
H	3.004920	6.240383	1.118386
C	2.241976	1.783749	3.845248
H	-3.163721	-0.884405	-1.174268
C	0.119922	-2.880965	-0.535926
H	2.722108	3.549336	4.956814
C	-5.954032	1.265173	0.426218
H	-0.515821	-3.927593	-2.290844
C	3.028774	2.895343	4.143722
C	-0.799586	-3.616851	-1.288230
H	-4.389218	2.157531	1.597976
C	-6.271656	0.333798	-0.557298
C	4.184734	3.195155	3.423528
H	-5.495483	-1.160547	-1.899490
C	-2.058170	-3.959948	-0.798319
C	-3.025861	-4.755389	-1.628349
H	-6.734980	1.870966	0.877143
C	4.998139	4.420714	3.729219
H	-7.301018	0.206118	-0.879492
H	5.458987	2.558783	1.814651
H	-3.385512	-3.804246	0.888516
H	0.773159	2.383301	0.949064
C	4.562245	2.338897	2.388926
C	-2.404653	-3.552083	0.492004
C	3.814805	1.211979	2.050776
C	-1.530603	-2.814758	1.285228
C	1.451596	-2.502582	-1.113721
C	0.979065	1.508931	4.605879
C	-1.945550	-2.342694	2.647913
C	4.263326	0.302051	0.943105
H	6.053365	4.171664	3.881612
H	-3.995063	-4.250151	-1.695851
H	-3.207298	-5.741415	-1.186323
H	4.636556	4.929327	4.626398
H	-2.652161	-4.907558	-2.643701
H	4.951468	5.130457	2.895591
H	1.607157	-3.003672	-2.071707
H	0.900699	2.161001	5.478960
H	2.279253	-2.792178	-0.455899
H	0.922235	0.472505	4.956567
H	0.116890	1.685395	3.955302
H	1.535638	-1.418073	-1.273472
H	4.609584	-0.664582	1.332006
H	-2.882243	-2.815014	2.951573
H	-2.100083	-1.257597	2.641132
H	5.100119	0.748416	0.402040
H	3.461197	0.105442	0.223467
H	-1.194095	-2.562161	3.413790

VIII

O	0.289882	1.125018	1.945669
N	1.762987	2.167036	-0.710665
C	0.127751	-0.189900	1.540138
O	4.223456	0.738584	-4.259187
C	0.902772	-1.137549	2.168015
O	4.664091	1.388187	-2.146558
N	2.027216	-0.861089	2.920830
N	2.074159	1.811123	-1.740005
N	0.700489	-2.509265	2.176632
C	3.869103	1.188043	-3.046706
C	2.520292	-2.071682	3.568846
C	1.345747	1.164039	-3.915727
C	2.424292	1.393833	-2.933220
H	2.217715	-2.110686	4.625524
C	1.859926	-3.184049	2.753779
C	0.074568	0.773710	-3.472850
H	3.611892	-2.107881	3.524641
H	-0.113043	0.606992	-2.414361
C	-0.866397	-0.478804	0.555395
C	0.520340	1.151629	-6.187608
C	-1.688532	0.449984	0.002920
H	0.700261	1.302482	-7.248360
C	1.558106	1.358623	-5.286591
H	-0.936969	-1.514478	0.234494
H	-1.601716	1.474802	0.358574
H	2.534202	1.665721	-5.641878
C	-0.741390	0.768596	-5.740792
H	2.534396	-3.562567	1.972606
H	-1.549132	0.614709	-6.450259
H	1.535747	-4.027450	3.368357
C	-2.704262	0.210378	-1.011686
C	5.620392	0.497291	-4.415860
C	-0.551386	-3.169354	2.070558
H	5.743323	0.147140	-5.440162
C	2.892650	0.247624	2.688305
H	5.961904	-0.261909	-3.708138
C	-3.031736	-1.067849	-1.505701
H	6.192343	1.413438	-4.250676
C	-3.413572	1.304418	-1.540887
C	-0.962338	0.584319	-4.378716
C	-4.005578	-1.233022	-2.480919
H	-1.939247	0.284617	-4.011039
C	2.996073	1.239567	3.673737
H	-2.527753	-1.945465	-1.110460
C	-0.699076	-4.161085	1.086380
H	3.939744	3.084145	4.215023
C	-4.390186	1.137874	-2.514953
H	-2.029574	-5.601128	0.222024
C	3.862991	2.308090	3.455844
C	-1.915871	-4.835663	0.987148
H	-3.183807	2.302203	-1.174515
C	-4.692636	-0.133486	-2.997089
C	4.608033	2.422770	2.281194
H	-4.236312	-2.232689	-2.840115
C	-2.987867	-4.544234	1.828488
C	-4.308285	-5.245463	1.675952
H	-4.916918	2.006580	-2.900929
C	5.542941	3.581040	2.071374
H	-5.456073	-0.268468	-3.757626
H	5.027117	1.506894	0.379016
H	-3.626569	-3.332585	3.481730
H	0.804322	1.593519	1.274782
C	4.476431	1.427670	1.313263
C	-2.807455	-3.563039	2.803456
C	3.639953	0.325294	1.503709
C	-1.606751	-2.871182	2.952945
C	0.426337	-4.480009	0.143757
C	2.137528	1.173709	4.902135
C	-1.465944	-1.839518	4.033072
C	3.556869	-0.745863	0.451918
H	6.525024	3.380635	2.516568
H	-4.997957	-4.653590	1.062573
H	-4.791334	-5.403532	2.644781

H	5.158240	4.495026	2.533534
H	-4.191849	-6.219050	1.191884
H	5.700736	3.776391	1.007271
H	0.056808	-5.004709	-0.740884
H	2.312061	2.037721	5.548256
H	1.181786	-5.123266	0.611798
H	2.328399	0.269565	5.490722
H	1.082152	1.158652	4.611655
H	0.937951	-3.567982	-0.180087
H	3.897355	-1.713843	0.839280
H	-2.245018	-1.965704	4.789171
H	-1.543634	-0.826234	3.624157
H	4.182243	-0.485707	-0.404786
H	2.529021	-0.886172	0.099631
H	-0.492350	-1.905279	4.529083

TSVIII-IX

O	0.772890	1.547453	1.592502
N	1.780739	0.544456	-0.427084
C	0.529907	0.315600	1.031394
O	3.420889	0.722207	-4.298818
C	1.220078	-0.775567	1.653615
O	3.629159	1.466485	-2.183012
N	2.378556	-0.647943	2.346070
N	1.488521	-0.053997	-1.427289
N	0.923090	-2.098304	1.526101
C	3.054867	0.756613	-2.994929
C	2.829786	-1.941989	2.851653
C	1.202958	-0.991151	-3.609610
C	1.930107	-0.110457	-2.681111
H	2.604448	-2.030630	3.923786
C	2.035353	-2.923691	2.001776
C	-0.173898	-1.199068	-3.422432
H	3.909760	-2.043870	2.721473
H	-0.682065	-0.650534	-2.634248
C	-0.762504	0.139191	0.389591
C	1.108129	-2.538998	-5.480343
C	-1.692473	1.109151	0.319371
H	1.619522	-3.059091	-6.286284
C	1.828995	-1.675297	-4.662782
H	-0.914835	-0.800679	-0.128518
H	-1.482269	2.046569	0.830539
H	2.888473	-1.527468	-4.836971
C	-0.252409	-2.749645	-5.270755
H	2.623173	-3.300236	1.155792
H	-0.810785	-3.423868	-5.913980
H	1.653777	-3.775552	2.568926
C	-2.968912	1.027466	-0.386783
C	4.503047	1.581376	-4.628168
C	-0.311779	-2.710758	1.161559
H	4.675416	1.445431	-5.696402
C	3.114147	0.518096	2.735061
H	5.400867	1.319377	-4.061092
C	-3.438175	-0.146779	-1.001549
H	4.253708	2.624136	-4.413634
C	-3.780049	2.170222	-0.454857
C	-0.889355	-2.070235	-4.234427
C	-4.657955	-0.165574	-1.662993
H	-1.955686	-2.201074	-4.067810
C	2.725741	1.219015	3.889755
H	-2.848363	-1.057983	-0.952926
C	-0.379125	-3.462268	-0.021690
H	3.218169	2.832415	5.204250
C	-5.002369	2.150645	-1.116525
H	-1.659101	-4.638153	-1.270499
C	3.516812	2.280549	4.315322
C	-1.594576	-4.069938	-0.345395
H	-3.435915	3.087258	0.017219
C	-5.447895	0.982145	-1.726621
C	4.679379	2.651766	3.635136
H	-4.998321	-1.084422	-2.133273
C	-2.719646	-3.955070	0.467624
C	-4.028886	-4.582911	0.081140
H	-5.607766	3.051882	-1.156925
C	5.499400	3.820972	4.102747
H	-6.401671	0.963025	-2.245710
H	5.952402	2.187160	1.972595
H	-3.471698	-3.126650	2.303133
H	1.394141	1.975737	0.974269
C	5.045309	1.920138	2.510408
C	-2.607059	-3.220216	1.649626
C	4.284811	0.845487	2.038895
C	-1.418761	-2.597664	2.021471
C	0.799690	-3.604193	-0.940216
C	1.466133	0.866579	4.624278
C	-1.347482	-1.803687	3.293070
C	4.730508	0.116575	0.804934
H	5.581368	3.841367	5.193837
H	-4.755877	-3.817543	-0.214160
H	-4.467278	-5.137576	0.916847
H	5.041402	4.768192	3.794780
H	-3.910714	-5.272046	-0.758700
H	6.509437	3.793852	3.685749
H	0.474873	-3.874780	-1.946953
H	1.410942	1.398251	5.577193
H	1.486201	-4.386006	-0.591887
H	1.393742	-0.205989	4.833812
H	0.595604	1.145153	4.021608
H	1.361801	-2.669415	-1.017744
H	5.822256	0.112472	0.738556
H	-2.205036	-2.024707	3.932696
H	-1.353812	-0.727850	3.083727
H	4.332722	0.604688	-0.092700
H	4.379669	-0.918044	0.780122
H	-0.435280	-2.020884	3.858397

IX

O	0.807185	1.595645	1.386595
N	1.628149	0.531491	-0.459242
C	0.662597	0.413871	0.654142
O	3.435830	0.668635	-4.204211
C	1.222256	-0.728527	1.498723
O	3.641332	1.422594	-2.099831
N	2.311083	-0.594891	2.264263
N	1.344375	-0.257690	-1.439208
N	0.834910	-2.011177	1.457405
C	3.086061	0.675815	-2.888768
C	2.713208	-1.875035	2.852459
C	1.489815	-1.224970	-3.590777
C	1.999249	-0.257449	-2.592579
H	2.584781	-1.836460	3.940632
C	1.781838	-2.876280	2.171776
C	0.112219	-1.486374	-3.662782
H	3.769133	-2.065379	2.643287
H	-0.555097	-0.913720	-3.026123
C	-0.754929	0.225568	0.195117
C	1.822468	-2.915419	-5.309224
C	-1.745438	1.054797	0.543789
H	2.502039	-3.471713	-5.949882
C	2.333045	-1.957667	-4.440130
H	-0.892161	-0.570065	-0.527834
H	-1.507139	1.862090	1.234157
H	3.401642	-1.774164	-4.412845
C	0.454096	-3.171526	-5.358122
H	2.305506	-3.520258	1.458130
H	0.057381	-3.917812	-6.040854
H	1.239879	-3.511211	2.877552
C	-3.133872	1.000055	0.077862
C	4.469574	1.578770	-4.541516
C	-0.389778	-2.578961	0.981166
H	4.644308	1.448366	-5.610356
C	3.086148	0.561709	2.610453
H	5.383603	1.367880	-3.978130
C	-3.615449	0.014680	-0.798950
H	4.170699	2.609479	-4.329731
C	-4.035335	1.972886	0.531588
C	-0.398815	-2.446422	-4.528755
C	-4.942910	0.011913	-1.204797
H	-1.471915	-2.617989	-4.567120
C	2.715407	1.301529	3.745048
H	-2.945058	-0.757378	-1.164479
C	-0.379160	-3.354178	-0.185982
H	3.260559	2.932287	5.016692
C	-5.365864	1.969501	0.127610

H	-1.601894	-4.489743	-1.524516
C	3.542129	2.345956	4.144637
C	-1.590501	-3.911073	-0.603919
H	-3.678604	2.744770	1.209422
C	-5.826361	0.987977	-0.744005
C	4.716958	2.659126	3.456209
H	-5.292341	-0.754953	-1.891082
C	-2.771941	-3.741454	0.114017
C	-4.070855	-4.318802	-0.371810
H	-6.042784	2.737053	0.492147
C	5.574062	3.814585	3.889988
H	-6.863832	0.982781	-1.065452
H	5.974954	2.110386	1.806729
H	-3.636039	-2.877077	1.883757
H	1.461745	2.085652	0.859241
C	5.059855	1.887301	2.350569
C	-2.726867	-3.007127	1.301230
C	4.266124	0.825684	1.905810
C	-1.549567	-2.423940	1.759537
C	0.875784	-3.596960	-0.971509
C	1.437356	1.015118	4.476640
C	-1.539034	-1.635816	3.036802
C	4.669200	0.051215	0.688253
H	5.591908	3.913592	4.979387
H	-4.773628	-3.520857	-0.637439
H	-4.551575	-4.925661	0.402499
H	5.191073	4.758204	3.483939
H	-3.926103	-4.947277	-1.253875
H	6.603727	3.702471	3.540361
H	0.639177	-3.897816	-1.993906
H	1.372522	1.608838	5.391446
H	1.471951	-4.400476	-0.520270
H	1.341698	-0.039939	4.756887
H	0.584430	1.265756	3.837810
H	1.486763	-2.693056	-1.031604
H	5.754317	0.080556	0.557943
H	-2.453363	-1.815677	3.606673
H	-1.479770	-0.561302	2.829763
H	4.195790	0.488155	-0.200268
H	4.358013	-0.996399	0.734215
H	-0.687331	-1.896416	3.674126

X

O	1.154518	1.033752	0.927825
N	3.316712	-0.926715	-0.965797
C	0.132337	0.277617	1.481432
O	-0.451187	-0.153781	-3.359539
C	0.447794	-0.403454	2.633307
O	0.541997	-1.927167	-2.383752
N	1.616485	-0.213869	3.360106
N	2.518513	-0.403976	-1.573328
N	-0.287704	-1.408699	3.252338
C	0.531238	-0.745249	-2.671259
C	1.574892	-1.005515	4.585987
C	1.722368	1.642183	-2.498172
C	1.596135	0.190429	-2.292859
H	1.269874	-0.384051	5.440813
C	0.532976	-2.063937	4.266678
C	2.485971	2.415243	-1.608402
H	2.556105	-1.433148	4.815002
H	2.948827	1.946000	-0.744937
C	-1.143927	0.290675	0.841063
C	1.251056	3.654813	-3.762161
C	-1.428804	0.986185	-0.289911
H	0.765389	4.131502	-4.609036
C	1.108466	2.283082	-3.584408
H	-1.936633	-0.259275	1.337892
H	-0.626763	1.532589	-0.782221
H	0.517469	1.704003	-4.282586
C	2.014045	4.413260	-2.879284
H	0.995570	-2.976950	3.863843
H	2.124420	5.483258	-3.027262
H	-0.067681	-2.344850	5.137287
C	-2.726736	1.072689	-0.943225
C	-1.567368	-0.998001	-3.648623
C	-1.256177	-2.223669	2.592241
H	-2.298337	-0.355095	-4.136518
C	2.298696	1.039130	3.447599
H	-1.982812	-1.401712	-2.723472
C	-3.852560	0.324046	-0.549194
H	-1.265944	-1.820183	-4.302270
C	-2.878637	1.935354	-2.044609
C	2.632708	3.783002	-1.803146
C	-5.062796	0.443046	-1.218543
H	3.227506	4.359228	-1.100043
C	1.651976	2.191099	3.921944
H	-3.776644	-0.370679	0.283117
C	-0.910741	-3.053151	1.514207
H	1.897728	4.264404	4.401053
C	-4.091007	2.052379	-2.713343
H	-1.654179	-4.481577	0.103946
C	2.395464	3.367266	4.037395
C	-1.914159	-3.841573	0.944883
H	-2.020560	2.516233	-2.374776
C	-5.194934	1.307649	-2.304947
C	3.749314	3.423815	3.712251
H	-5.913806	-0.149024	-0.891458
C	-3.224558	-3.833453	1.414824
C	-4.288505	-4.665171	0.754941
H	-4.175045	2.731828	-3.557719
C	4.533692	4.694437	3.885462
H	-6.144149	1.397230	-2.825056
H	5.416233	2.282853	2.978588
H	-4.546316	-2.998534	2.892742
H	0.842050	1.941801	0.822241
C	4.362115	2.259713	3.248022
C	-3.530662	-3.012437	2.502445
C	3.659395	1.064583	3.109259
C	-2.566377	-2.206080	3.101854
C	0.473572	-3.107943	0.932715
C	0.191560	2.198719	4.281413
C	-2.920968	-1.322828	4.264571
C	4.329936	-0.164556	2.568690
H	5.349385	4.763210	3.159847
H	-4.829876	-4.081857	0.000571
H	-5.025526	-5.022558	1.480080
H	4.982746	4.748252	4.884532
H	-3.859578	-5.534172	0.248590
H	3.898413	5.576821	3.766926
H	0.757337	-4.145533	0.730311
H	-0.044196	3.063286	4.907463
H	1.227707	-2.668008	1.587073
H	-0.108144	1.296462	4.822682
H	-0.440730	2.244736	3.387373
H	0.510949	-2.571426	-0.021778
H	5.357338	0.053768	2.266070
H	-4.002005	-1.306804	4.424463
H	-2.577048	-0.296939	4.102126
H	3.784439	-0.550566	1.702527
H	4.367297	-0.971207	3.309708
H	-2.454432	-1.669362	5.194414

TSX-XI

O	0.651440	2.356978	2.782569
N	1.513685	1.065034	0.865637
C	0.341983	1.081948	2.344984
O	0.450941	-0.764806	-3.290166
C	0.992074	0.021280	3.070503
O	-0.691051	-1.089926	-1.387391
N	2.134480	0.193597	3.787677
N	1.037353	0.436837	-0.046418
N	0.712296	-1.306826	2.988703
C	0.278815	-0.603513	-1.955487
C	2.614145	-1.079807	4.318768
C	2.515730	0.776087	-1.966580
C	1.321718	0.197445	-1.324330
H	2.399605	-1.149030	5.394105
C	1.833965	-2.098268	3.498408
C	3.138421	1.900475	-1.395830
H	3.694825	-1.167469	4.182371
H	2.708409	2.355635	-0.508685
C	-0.968411	0.883717	1.734720
C	4.257420	0.778067	-3.667160
C	-1.912101	1.835904	1.648624

H	4.691157	0.324128	-4.554672
C	3.108042	0.224552	-3.117488
H	-1.109444	-0.061869	1.220955
H	-1.749836	2.792482	2.144966
H	2.660352	-0.644613	-3.581774
C	4.858295	1.895153	-3.092631
H	2.432070	-2.492076	2.668796
H	5.757444	2.323407	-3.526434
H	1.461524	-2.937037	4.090640
C	-3.179503	1.702974	0.929344
C	-0.580668	-1.493605	-3.936231
C	-0.508021	-1.952155	2.623000
H	-0.306406	-1.523970	-4.991492
C	2.735022	1.391036	4.293777
H	-1.547856	-0.999429	-3.809923
C	-3.383465	0.728031	-0.061956
H	-0.659507	-2.508345	-3.535256
C	-4.232396	2.579192	1.228724
C	4.287645	2.450748	-1.952108
C	-4.612833	0.624103	-0.699502
H	4.735976	3.325715	-1.488379
C	2.214868	1.984169	5.453733
H	-2.567858	0.072976	-0.359978
C	-0.528703	-2.793932	1.500607
H	2.467398	3.563375	6.878118
C	-5.461147	2.472097	0.587523
H	-1.757671	-4.057539	0.291495
C	2.869379	3.094087	5.982568
C	-1.728557	-3.428288	1.177555
H	-4.081932	3.349847	1.981622
C	-5.658649	1.488433	-0.377114
C	4.025540	3.612594	5.399129
H	-4.750413	-0.130454	-1.469348
C	-2.886143	-3.255428	1.930808
C	-4.182495	-3.893733	1.521184
H	-6.263720	3.159960	0.839054
C	4.696568	4.831831	5.965729
H	-6.615428	1.404133	-0.884664
H	5.433564	3.364655	3.797980
H	-3.706063	-2.309620	3.677575
H	0.032284	2.603561	3.479199
C	4.528124	2.981368	4.263415
C	-2.818318	-2.443486	3.063184
C	3.906761	1.869538	3.692866
C	-1.645955	-1.791148	3.433592
C	0.685352	-3.018192	0.649021
C	0.979419	1.449401	6.120701
C	-1.631836	-0.921434	4.656105
C	4.477006	1.224453	2.464851
H	4.315596	5.743754	5.490973
H	-4.792586	-3.187222	0.946171
H	-4.771748	-4.200188	2.390542
H	5.777254	4.806964	5.800038
H	-4.016616	-4.772904	0.892965
H	4.518735	4.924549	7.040786
H	1.325358	-3.806150	1.065988
H	0.700105	2.069936	6.975389
H	1.277476	-2.105378	0.550768
H	1.121497	0.427292	6.490301
H	0.124040	1.415012	5.438098
H	0.387106	-3.322000	-0.355075
H	5.347157	1.779423	2.106945
H	-2.485006	-1.149384	5.299453
H	-1.699333	0.137366	4.378682
H	3.730097	1.183457	1.665588
H	4.801479	0.194790	2.658337
H	-0.717024	-1.053815	5.241965

XI

O	0.408885	2.258597	2.640047
N	1.227650	1.024604	0.911658
C	0.265525	1.012963	2.005024
O	1.535839	-0.431200	-3.446023
C	0.854127	-0.077410	2.910332
O	-0.039316	-1.299697	-2.105291
N	1.993405	0.088591	3.602311
N	0.827893	0.300242	-0.091557
N	0.458103	-1.358990	2.970260
C	0.925623	-0.561232	-2.240778
C	2.528609	-1.199921	4.049641
C	2.778661	1.050989	-1.440205
C	1.537650	0.276865	-1.206234
H	2.828863	-1.139368	5.099130
C	1.362843	-2.154023	3.807118
C	2.890809	2.380015	-1.002243
H	3.409829	-1.459897	3.452866
H	2.051574	2.838395	-0.492489
C	-1.143240	0.752683	1.547561
C	5.067575	1.189979	-2.255345
C	-2.155760	1.614622	1.690830
H	5.914469	0.715966	-2.744991
C	3.891448	0.472549	-2.069253
H	-1.271122	-0.149465	0.964637
H	-2.002105	2.549746	2.229736
H	3.826291	-0.552459	-2.419366
C	5.162411	2.509094	-1.817923
H	1.656082	-3.069298	3.286589
H	6.080180	3.072114	-1.965583
H	0.843690	-2.438675	4.730489
C	-3.508458	1.418669	1.156354
C	0.960100	-1.204192	-4.485383
C	-0.821253	-1.925904	2.661619
H	1.564482	-1.008551	-5.372239
C	2.764197	1.270164	3.862804
H	-0.078776	-0.911761	-4.663575
C	-3.787735	0.498913	0.133482
H	0.975714	-2.270610	-4.241402
C	-4.567614	2.172395	1.678707
C	4.065858	3.098766	-1.192996
C	-5.087391	0.325464	-0.323923
H	4.123641	4.128888	-0.850674
C	2.446134	2.018116	5.006555
H	-2.977866	-0.061707	-0.324734
C	-0.933930	-2.787165	1.563097
H	2.991216	3.711535	6.196731
C	-5.868907	1.997556	1.220718
H	-2.290084	-4.017754	0.456853
C	3.236155	3.120014	5.317101
C	-2.183503	-3.362507	1.318286
H	-4.363799	2.901286	2.459993
C	-6.134993	1.068517	0.219667
C	4.332385	3.480585	4.531342
H	-5.282290	-0.383473	-1.123892
C	-3.289751	-3.107029	2.123685
C	-4.637997	-3.680564	1.794343
H	-6.674815	2.591090	1.643261
C	5.144018	4.701994	4.858244
H	-7.148794	0.933339	-0.146105
H	5.500401	2.942051	2.813199
H	-3.975444	-2.070908	3.878804
H	-0.287305	2.324155	3.304075
C	4.640927	2.688126	3.429520
C	-3.125410	-2.272045	3.230741
C	3.883247	1.568714	3.076701
C	-1.902982	-1.676482	3.523162
C	0.200040	-3.041784	0.616964
C	1.291572	1.640198	5.889640
C	-1.780257	-0.752950	4.700458
C	4.292350	0.716843	1.912145
H	4.712192	5.593546	4.388451
H	-5.246510	-2.937372	1.265576
H	-5.185248	-3.966411	2.697523
H	6.171593	4.608568	4.496587
H	-4.554680	-4.559783	1.150317
H	5.176646	4.885427	5.936160
H	0.150416	-4.062742	0.227970
H	1.214715	2.321538	6.740189
H	1.178092	-2.893150	1.079642
H	1.395823	0.623855	6.287592
H	0.338694	1.669494	5.351427
H	0.134921	-2.350708	-0.235456
H	4.899319	1.290187	1.207860
H	-2.612874	-0.898158	5.392650
H	-1.807299	0.292183	4.368353

H	3.413996	0.364060	1.367935
H	4.893715	-0.140243	2.242971
H	-0.849790	-0.898154	5.258275

XII

O	1.051166	2.192888	3.306173
N	2.643178	1.895250	0.584309
C	0.415772	1.054058	2.833250
O	2.492754	-1.726214	-2.159620
C	0.831655	-0.156094	3.346071
O	3.305857	-1.299419	-0.098999
N	1.959184	-0.370335	4.119743
N	2.431660	1.209422	-0.291801
N	0.236746	-1.395805	3.150329
C	2.726406	-0.931169	-1.104482
C	2.016022	-1.748894	4.579886
C	1.374482	0.946075	-2.416254
C	2.189546	0.414031	-1.304942
H	1.615684	-1.847350	5.601770
C	1.143730	-2.460426	3.557523
C	0.304196	1.803955	-2.136459
H	3.046669	-2.113415	4.581924
H	0.055609	2.044761	-1.106102
C	-0.624287	1.240462	1.870146
C	0.878050	1.138303	-4.772054
C	-1.045915	2.456985	1.435169
H	1.105844	0.876109	-5.801426
C	1.660793	0.619813	-3.747265
H	-1.078521	0.345374	1.458254
H	-0.581375	3.339867	1.869500
H	2.488142	-0.043282	-3.972461
C	-0.183499	1.994730	-4.488584
H	1.746937	-2.827171	2.714410
H	-0.789727	2.396364	-5.295322
H	0.581852	-3.297359	3.979567
C	-2.088344	2.706752	0.449948
C	2.971151	-3.061212	-2.012488
C	-1.077624	-1.674015	2.702880
H	2.727921	-3.563665	-2.948177
C	2.881428	0.571033	4.660530
H	2.477543	-3.557586	-1.173214
C	-2.894236	1.697008	-0.112657
H	4.049997	-3.069552	-1.839966
C	-2.317888	4.026507	0.018168
C	-0.467125	2.328074	-3.167113
C	-3.863461	1.996595	-1.059383
H	-1.301724	2.979246	-2.923904
C	2.530279	1.349612	5.776732
H	-2.767707	0.665124	0.203388
C	-1.263277	-2.337325	1.479489
H	3.221486	2.795691	7.193615
C	-3.291093	4.325552	-0.927796
H	-2.708624	-3.139668	0.114113
C	3.491729	2.188854	6.331457
C	-2.564396	-2.634208	1.066943
H	-1.714101	4.826632	0.440302
C	-4.071493	3.311190	-1.477969
C	4.786062	2.273840	5.814370
H	-4.469142	1.194671	-1.473598
C	-3.676062	-2.282525	1.827976
C	-5.071052	-2.598983	1.366778
H	-3.442019	5.357176	-1.235111
C	5.793563	3.211494	6.418853
H	-4.834977	3.540462	-2.215577
H	6.111531	1.529244	4.299696
H	-4.315085	-1.346760	3.654533
H	1.658972	2.493565	2.617603
C	5.107286	1.481490	4.716143
C	-3.460134	-1.625852	3.041842
C	4.176998	0.621334	4.127021
C	-2.182608	-1.323041	3.503393
C	-0.093328	-2.696518	0.608733
C	1.140539	1.311097	6.337441
C	-1.995410	-0.626343	4.817362
C	4.576694	-0.231695	2.957163
H	6.809577	2.970167	6.095116
H	-5.690898	-1.696930	1.330375
H	-5.564341	-3.301560	2.047895
H	5.768481	3.174082	7.512537
H	-5.070451	-3.046692	0.369613
H	5.592016	4.249010	6.127224
H	-0.390232	-2.737923	-0.442865
H	1.104078	1.780080	7.324036
H	0.317493	-3.679837	0.871570
H	0.765340	0.287386	6.431226
H	0.457513	1.850231	5.672619
H	0.716746	-1.969974	0.713662
H	5.467099	0.174377	2.469941
H	-2.927002	-0.615505	5.388147
H	-1.669001	0.409001	4.669750
H	3.786028	-0.317148	2.208643
H	4.825114	-1.253657	3.272039
H	-1.225145	-1.118909	5.420005

TSXII-XIII

O	2.273692	1.542288	2.687154
N	1.103069	1.557984	0.088100
C	1.029959	0.990126	2.890468
O	2.478138	-0.846320	-2.992846
C	0.986100	-0.140791	3.745961
O	3.003175	0.184705	-1.060379
N	1.962370	-0.452562	4.629681
N	0.446764	1.100637	-0.812084
N	-0.000401	-1.080687	3.789695
C	2.159869	-0.104753	-1.899158
C	1.597222	-1.626878	5.420510
C	-0.322006	-0.103609	-2.739844
C	0.765997	0.293578	-1.835229
H	1.352986	-1.321332	6.445533
C	0.384239	-2.181365	4.675848
C	-1.456445	0.719425	-2.857785
H	2.428736	-2.336180	5.470765
H	-1.477826	1.658622	-2.315197
C	-0.077029	1.512594	2.258287
C	-1.399905	-1.664511	-4.266954
C	0.022498	2.580004	1.328848
H	-1.364402	-2.601778	-4.816831
C	-0.318135	-1.305926	-3.468780
H	-1.033615	1.018038	2.387150
H	0.818961	3.297098	1.515529
H	0.543245	-1.960372	-3.410792
C	-2.520753	-0.844458	-4.363028
H	0.638025	-3.061225	4.071628
H	-3.361205	-1.127305	-4.990515
H	-0.437582	-2.453816	5.344396
C	-1.164713	3.115546	0.668129
C	3.844618	-1.221970	-3.068390
C	-0.898433	-1.366814	2.711558
H	3.943184	-1.800890	-3.987682
C	2.948122	0.441210	5.157870
H	4.137493	-1.826933	-2.205116
C	-2.236255	2.285657	0.304598
H	4.492432	-0.341668	-3.103853
C	-1.223358	4.470452	0.306525
C	-2.537450	0.352641	-3.648923
C	-3.343517	2.805565	-0.359831
H	-3.393943	1.018806	-3.719136
C	2.568376	1.452982	6.047755
H	-2.198742	1.223404	0.529629
C	-0.399184	-1.773128	1.461625
H	3.293267	3.032241	7.300250
C	-2.326812	4.986767	-0.358009
H	-0.943941	-2.275999	-0.545508
C	3.573813	2.242819	6.606295
C	-1.317158	-2.001525	0.438420
H	-0.390361	5.121296	0.561343
C	-3.396917	4.156066	-0.690645
C	4.919471	2.049550	6.300184
H	-4.162121	2.145018	-0.632676
C	-2.693143	-1.860885	0.628153
C	-3.642089	-2.098108	-0.511786
H	-2.354679	6.041063	-0.619152
C	5.980878	2.932860	6.892927
H	-4.260965	4.559227	-1.210961

H	6.300012	0.878110	5.141738
H	-4.220559	-1.385902	2.063354
H	2.370156	1.572658	1.718640
C	5.255669	1.035105	5.402505
C	-3.151651	-1.495315	1.893817
C	4.288268	0.224260	4.815367
C	-2.274114	-1.242389	2.948760
C	1.069473	-1.926582	1.186400
C	1.125785	1.715251	6.378352
C	-2.794005	-0.822779	4.294865
C	4.658293	-0.812358	3.796160
H	6.900212	2.374889	7.093020
H	-4.666858	-1.830425	-0.241059
H	-3.639664	-3.152092	-0.811447
H	5.647202	3.387201	7.829674
H	-3.351403	-1.513321	-1.390863
H	6.238139	3.747558	6.205952
H	1.229392	-2.673129	0.404454
H	1.043125	2.421338	7.207817
H	1.631868	-2.241881	2.070461
H	0.588490	0.804209	6.663545
H	0.597577	2.143086	5.518917
H	1.512613	-0.987481	0.834266
H	5.741832	-0.864127	3.667730
H	-3.828236	-0.478462	4.221187
H	-2.191177	-0.016019	4.722399
H	4.208085	-0.561720	2.829892
H	4.304893	-1.812431	4.070380
H	-2.778735	-1.653227	5.011799

XIII

O	2.546815	0.636020	2.237013
N	1.005070	1.613644	-0.139940
C	1.338689	0.622106	2.632197
O	2.061219	-0.809201	-3.307911
C	1.073850	-0.369830	3.726925
O	2.785244	0.203761	-1.445361
N	1.812966	-0.442451	4.830758
N	0.148595	1.098172	-0.953864
N	0.186284	-1.364998	3.677764
C	1.852440	-0.100921	-2.179095
C	1.392771	-1.556839	5.683006
C	-0.681321	-0.139672	-2.789211
C	0.458980	0.284193	-1.942175
H	0.962099	-1.169756	6.613277
C	0.359005	-2.282792	4.810140
C	-1.815171	0.687033	-2.862947
H	2.249961	-2.184906	5.942403
H	-1.807220	1.626409	-2.319482
C	0.274507	1.356317	2.186154
C	-1.827582	-1.714966	-4.246650
C	0.532908	2.325639	1.068767
H	-1.821453	-2.660154	-4.783395
C	-0.714216	-1.352914	-3.493452
H	-0.733241	1.183098	2.545345
H	1.403366	2.936797	1.341220
H	0.141081	-2.016758	-3.458838
C	-2.941544	-0.884161	-4.312488
H	0.721204	-3.248399	4.440496
H	-3.806703	-1.167040	-4.905451
H	-0.591685	-2.447861	5.323640
C	-0.625540	3.246321	0.767254
C	3.422465	-1.139690	-3.557680
C	-0.655636	-1.695947	2.569038
H	3.421099	-1.712909	-4.484972
C	2.732108	0.545899	5.305632
H	3.838165	-1.733387	-2.739167
C	-1.920319	2.751778	0.578106
H	4.027521	-0.236186	-3.669063
C	-0.417131	4.623072	0.676801
C	-2.927148	0.319443	-3.609385
C	-2.975264	3.616270	0.304191
H	-3.784767	0.985820	-3.652738
C	2.236118	1.659192	5.993087
H	-2.093149	1.681376	0.631661
C	-0.084327	-2.220350	1.399028
H	2.791364	3.432192	7.059623
C	-1.471780	5.491757	0.408155
H	-0.514827	-2.910503	-0.579332
C	3.159010	2.560748	6.522419
C	-0.940241	-2.525703	0.344299
H	0.585717	5.018756	0.818996
C	-2.755228	4.989460	0.219807
C	4.533235	2.378080	6.372830
H	-3.974527	3.216042	0.154787
C	-2.321021	-2.332851	0.426182
C	-3.204151	-2.626069	-0.751541
H	-1.289032	6.560959	0.345596
C	5.507533	3.380190	6.925144
H	-3.580723	5.663472	0.008251
H	6.051957	1.118982	5.519372
H	-3.921538	-1.676084	1.697841
H	1.958900	1.244373	-0.116019
C	4.983589	1.264093	5.663080
C	-2.848172	-1.831971	1.614813
C	4.102362	0.336189	5.113039
C	-2.035399	-1.503515	2.699920
C	1.398273	-2.425858	1.268144
C	0.758982	1.905683	6.118638
C	-2.637771	-0.942508	3.957597
C	4.586374	-0.810263	4.278294
H	6.428112	2.897533	7.265635
H	-4.255918	-2.682145	-0.458161
H	-2.931017	-3.572319	-1.228082
H	5.080555	3.932999	7.766280
H	-3.104477	-1.844122	-1.512803
H	5.788275	4.112590	6.159230
H	1.624613	-2.977253	0.352764
H	0.565377	2.787989	6.732840
H	1.803246	-3.000237	2.109875
H	0.231683	1.061338	6.577858
H	0.314675	2.074318	5.130495
H	1.941878	-1.474135	1.236010
H	5.676284	-0.807837	4.205485
H	-3.627581	-0.525776	3.756973
H	-2.017001	-0.148679	4.384027
H	4.153807	-0.706160	3.276033
H	4.280878	-1.781196	4.686243
H	-2.764096	-1.712823	4.729032