Electronic Supplementary Material (ESI) for Green Chemistry.

Base Mediated Benzannulation of α-Cyano Crotonates with Ynones: Facile Synthesis of Benzonitriles and Fluorenes

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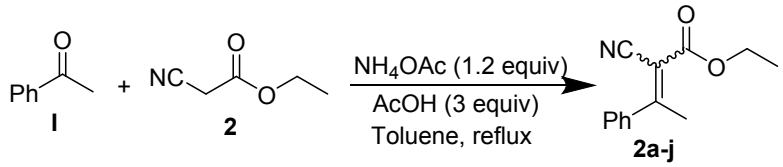
I. General Information and methods.

All reagents and solvents were purchased from commercial sources and used without purification. NMR spectra were recorded with a 300, 400 or 500 MHz spectrometer for ^{1}H NMR, 100 or 125 MHz for ^{13}C NMR spectroscopy. Chemical shifts are reported relative to the residual signals of tetramethylsilane in $CDCl_3$ or deuterated solvent $CDCl_3$ for ^{1}H and ^{13}C NMR spectroscopy. Multiplicities are reported as follows: singlet (s), doublet (d), doublet of doublets (dd), doublet of triplets (dt), triplet (t), quartet (q), multiplet (m). HRMS were recorded by using QTof mass spectrometer. Column chromatography was performed with silica gel (100–200 mesh) as the stationary phase. All reactions were monitored by using TLC.

Ynones **1** were prepared following literature procedures.[1] Starting materials **2a-j** were prepared from literature procedures.[3]

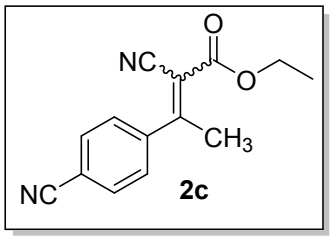
II. General Procedure A for the preparation of starting materials:

Starting materials **2a-j** were prepared from literature procedures.[3]

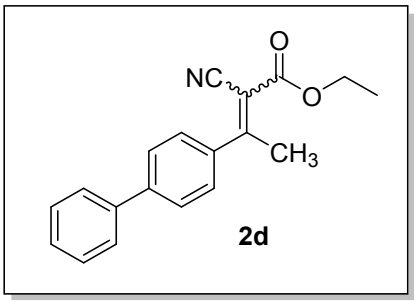


To a mixture of acetophenone **I** (1 g, 8.33 mmol, 1 equiv), ethyl cyano acetate **2** (1.13 g, 10 mmol, 1.2 equiv) and ammonium acetate (770 mg, 10 mmol, 1.2 equiv) in toluene (10 mL) was added acetic acid (1.43 mL, 25 mmol, 3 equiv) under N_2 atmosphere. The reaction contents were refluxed for 6-10 hours. Upon completion, reaction mixture was concentrated under reduced pressure and the crude material was purified on silica gel using 1-15% EtOAc/hexane.

Methyl 2-cyano-3-(4-cyanophenyl)but-2-enoate (2c): 911 mg of **2c** was obtained from 1g (6.9 mmol) of **Ic** following general procedure **A**. Yield 55%; brownish oil; R_f = 0.4 (SiO_2, EtOAc:Hexane, 1:99); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.78 – 7.74 (m, 2H), 7.73 – 7.68 (m, 1H), 7.60 – 7.44 (m, 3H), 7.29 – 7.25 (m, 1H), 4.36 (q, *J* = 7.1 Hz, 2H), 4.12 (q, *J* = 7.1 Hz, 1H), 2.69 (s, 3H), 2.54 (s, 1H), 1.41 – 1.37 (t, 2H), 1.18 (t, *J* = 9.0, 5.3 Hz, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 169.5, 167.9, 161.6, 144.5, 143.6, 132.6, 132.2, 128.6, 128.3, 127.8, 126.8, 126.38, 118.1, 117.9, 115.3, 114.8, 114.0, 113.0, 107.6, 106.9, 63.0, 62.5, 24.8, 22.9, 14.1, 13.8; **HRMS** (QToF) calcd for $C_{14}H_{13}N_2O_2$ $[M+H]^+$ 241.0977 found 241.0956.

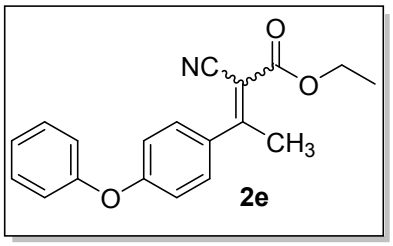


Ethyl 3-([1,1'-biphenyl]-4-yl)-2-cyanobut-2-enoate (2d): 742 mg of **2d** was obtained from 1g (5.1 mmol) of **Id** following general procedure **A**. Yield 50%; colourless solid; R_f = 0.5 (SiO_2, EtOAc:Hexane, 2:98); **^{1}H NMR** (400 MHz, CDCl3) δ 7.69 – 7.65 (m, 2H), 7.61 (ddd, *J* = 6.0, 3.7, 1.6 Hz, 4H), 7.57 – 7.53 (m, 2H), 7.49 – 7.42 (m, 3H), 7.41 – 7.35 (m, 1H), 7.28 – 7.24 (m, 1H), 4.35 (q, *J* = 7.1 Hz, 2H), 4.13 (q, *J* = 7.1 Hz, 1H), 2.73 (s, 3H), 2.58 (s, 1H), 1.39 (t, *J* = 7.1 Hz, 3H), 1.15 (t, *J* = 7.1 Hz, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 171.8, 169.3, 162.3, 161.4, 143.3, 142.4, 139.9, 139.8, 138.8, 137.6, 128.8, 127.9, 127.8, 127.2, 127.0, 127.0, 126.9, 126.8, 116.3, 115.6, 105.8, 104.7, 62.0, 61.9, 26.7, 23.1, 14.0, 13.7; **HRMS** (QToF) calcd for $C_{19}H_{18}NO_2$ $[M+H]^+$ 292.1338 found 292.1328.



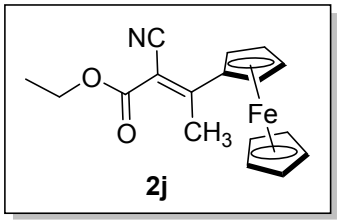
2d

Methyl 2-cyano-3-(4-phenoxyphenyl)but-2-enoate (2e): 652 mg of **2e** was obtained from 1g (4.7 mmol) of **Ie** following general procedure **A**. Yield 45%; brownish oil; R_f = 0.5 (SiO_2, EtOAc:Hexane, 8:92); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.48 – 7.43 (m, 2H), 7.41 – 7.35 (m, 3H), 7.21 – 7.13 (m, 2H), 7.09 – 6.95 (m, 6H), 4.33 (q, *J* = 7.1 Hz, 2H), 4.14 (d, *J* = 7.1 Hz, 1H), 2.68 (s, 3H), 2.54 (s, 1H), 1.38 (t, *J* = 7.1 Hz, 3H), 1.19 (t, *J* = 7.1 Hz, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 171.6, 168.9, 162.5, 161.7, 159.9, 159.2, 155.6, 134.2, 132.8, 130.0, 129.4, 128.5, 124.4, 120.1, 119.9, 117.7, 117.6, 116.6, 115.9, 105.4, 104.2, 62.0, 61.9, 26.75, 23.2, 14.1, 13.8; **HRMS** (QToF) calcd for $C_{19}H_{18}NO_3$ $[M+H]^+$ 308.1287 found 308.1278.



2e

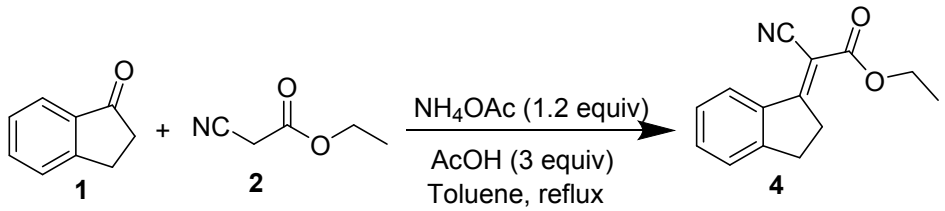
(E)-(2-(3-cyano-4-ethoxy-4-oxobut-2-en-2-yl)cyclopenta-2,4-dien-1-yl)(cyclopenta-2,4-dien-1-yl)iron (2j): 850 mg was obtained from 1g (4.4 mmol) of **1j** following general procedure **A**. Yield 60%; pink solid; R_f= 0.45 (SiO_2, EtOAc:Hexane, 2:98); **^{1}HNMR** (400 MHz, $CDCl_3$) δ 5.04 (dd, *J* = 4.1, 2.1 Hz, 2H), 4.63 (dd, *J* = 4.8, 2.8 Hz, 2H), 4.32 – 4.25 (q, 2H), 4.24(s, 4H), 2.68(s, 6H), 1.39 – 1.33 (t, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 172.3, 163.3, 118.5, 98.0, 81.3, 72.6, 70.7, 70.5, 61.5, 21.8, 14.2; **HRMS** (QToF) calcd for $C_{17}H_{18}NO_2Fe$ $[M+H]^+$ 324.0687 found 324.0677.



2j

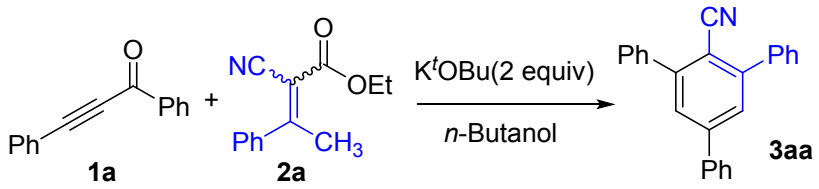
Ethyl (E)-2-cyano-2-(2,3-dihydro-1H-inden-1-ylidene)acetate(4) was prepared following literature procedures.[3]

To a mixture of indanone **1** (1g, 7.6 mmol, 1 equiv), ethyl cyano acetate **2** (0.97 ml, 9.1 mmol, 1.2 equiv) and ammonium acetate (702 mg, 9.1 mmol, 1.2 equiv) in toluene (10 mL) was added acetic acid (1.3 mL, 23 mmol, 3 equiv) under N_2 atmosphere. The reaction contents were refluxed for 6-10hours. Upon completion, reaction mixture was concentrated under reduced pressure and the crude material was purified on silica gel using 3% EtOAc/hexaneto get **4** as sticky white solid (850 mg).

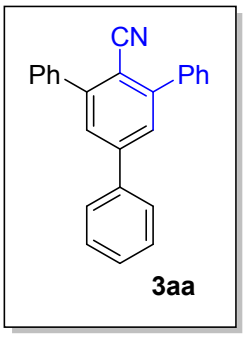


III. General procedure and chareteristic data of final compounds

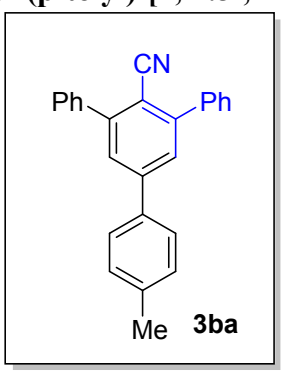
(A). General procedure B for the synthesis of final compounds (3) taking Synthesis of 3aa as an Example.



To a 15 mL Schlenk tube was added ynone **1a** (103 mg, 0.5 mmol, 1 equiv), α-cyano crotonates **2a** (129 mg, 0.6 mmol, 2 equiv) and KO^{t}Bu (112 mg, 1 mmol, 2 equiv) in 1-butanol (3 mL) and the reaction mixture was stirred at room temperature under open air until the complete conversion of starting material (60-90 min). The reaction mixture was concentrated under reduced pressure, washed with hexane (2 times) and the remaining solid was dissolved in 20% EtOAc/Hexane and filtered through a small silica bed. Filtrate was concentrated to get the desired solids in purified form. In case of **3ea, 3i-3la, 3sa, 3ua** and **3aj**, the reaction contents were concentrated under reduced pressure and the crude material was purified on silica gel using EtOAc/hexane to get the desired product.



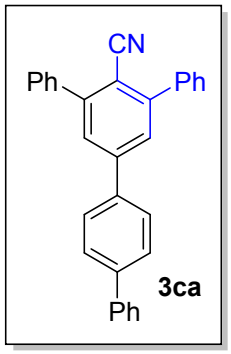
5'-phenyl-[1,1':3',1''-terphenyl]-2'-carbonitrile (3aa)[2]: 149 mg was obtained from **1a** (103 mg, 0.5 mmol) and **2a** following general procedure **B**. Yield 90%; greyish white solid; mp 163−166 °C; R_f = 0.53 (SiO_2, EtOAc:Hexane, 1:99); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.70 – 7.68 (m, 3H), 7.66 (q, J = 2.3 Hz, 3H), 7.64 (q, J = 2.0 Hz, 2H), 7.54 (t, J = 1.8 Hz, 1H), 7.53 – 7.47 (m, 7H), 7.47 – 7.43 (m, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 147.3, 145.1, 139.0, 138.7, 129.1, 129.0, 128.7, 128.6, 127.5, 127.3, 118.0, 109.0; **IR** (KBr) ν 3049, 2431, 2223, 1962, 1595, 1498, 891, 768, 702 cm^{-1}; **HRMS** (QToF) calcd for $C_{25}H_{18}N$ $[M+H]^+$ 332.1439 found 332.1440.



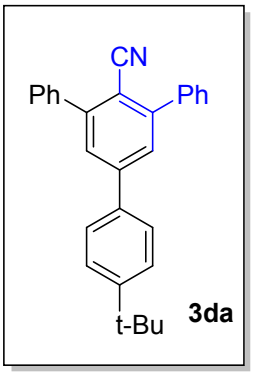
5'-(p-tolyl)-[1,1':3',1''-terphenyl]-2'-carbonitrile (3ba)[2]: 152 mg was obtained from **1b** (110 mg, 0.5 mmol) and **2a** following general procedure **B.** Yield 88%; pale yellow solid; mp 132−135 °C; R_f = 0.55 (SiO_2, EtOAc:Hexane, 1:99); **^{1}H NMR** (300 MHz, $CDCl_3$) δ 7.69 (d, J = 5.6 Hz, 4H), 7.66 (s, 2H), 7.61 (s, 1H), 7.59 – 7.55 (m, 2H), 7.54 (s, 2H), 7.50 (d, J = 8.5 Hz, 3H), 7.31 (d, J = 7.9 Hz, 2H), 2.44 (s, 3H);

^{13}C NMR (75 MHz, $CDCl_3$) δ 147.2, 144.9, 138.8, 138.7, 136.0, 129.8, 128.9, 128.6, 128.5, 127.2, 127.1, 118.1, 108.6, 21.1; **IR** (KBr) *v* 3033, 2917, 2309,2222, 2130, 1596, 769, 703 cm^{-1}; **HRMS** (QToF) calcd for $C_{26}H_{20}N$ $[M+H]^+$ 346.1596 found 346.1597.

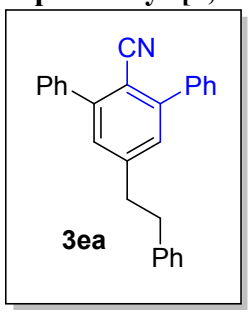
5'-phenyl-[1,1':3',1'':4'',1'''-quaterphenyl]-6'-carbonitrile (3ca): 165 mg was obtained from **1c** (141 mg, 0.5 mmol) and **2a** following general procedure **B**. Yield 81%; colourless solid; mp 193−195 °C; R_f = 0.45(SiO_2, EtOAc:Hexane, 1:99); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.79 – 7.74 (m, 2H), 7.73 (d, *J* = 8.5 Hz, 2H), 7.68 (d, *J* = 1.5 Hz, 2H), 7.66 (s, 2H), 7.65 (s, 3H), 7.57 – 7.55 (m, 1H), 7.54 (s, 1H), 7.52 (s, 2H), 7.51 – 7.49 (m, 1H), 7.49 (d, *J* = 3.0 Hz, 3H), 7.47 (d, *J* = 3.4 Hz, 1H), 7.39 (t, *J* = 7.3 Hz, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 147.4, 144.5, 141.6, 140.1, 138.6, 137.7, 129.0, 128.8, 128.7, 128.6, 127.7, 127.7, 127.3, 127.0, 118.0, 109.0; **IR** (KBr) *v* 2928, 2308, 2223, 1597, 1505, 770, 703 cm^{-1}; **HRMS** (QToF) calcd for $C_{31}H_{22}N$ $[M+H]^+$ 408.1752 found 408.1760.



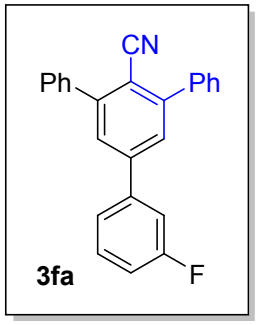
5'-(4-(tert-butyl)phenyl)-[1,1':3',1''-terphenyl]-2'-carbonitrile (3da): 159 mg was obtained from **1d** (131 mg, 0.5 mmol) and **2a** following general procedure **B**. Yield 82%; brownish solid; mp 135−138 °C; R_f = 0.55 (SiO_2, EtOAc:Hexane, 1:99); **^{1}H NMR** (300 MHz, $CDCl_3$) δ 7.71 (s, 2H), 7.68 (d, *J* = 1.4 Hz, 2H), 7.65 (d, *J* = 1.1 Hz, 3H), 7.62 (s, 1H), 7.56 (d, *J* = 2.0 Hz, 1H), 7.54 (s, 3H), 7.51 (s, 3H), 7.49 – 7.45 (m, 1H), 1.39 (s, 9H); **^{13}C NMR** (75 MHz, $CDCl_3$) δ 152.0, 147.2, 144.9, 138.7, 136.0, 129.0, 128.6, 128.6, 127.2, 127.0, 126.0, 118.1, 108.6, 34.6, 31.2; **IR** (KBr) *v* 2966, 2307, 2223, 1595, 1510, 1381, 771, 703 cm^{-1}; **HRMS** (QToF) calcd for $C_{29}H_{26}N$ $[M+H]^+$ 388.2065 found 388.2072.



5'-phenethyl-[1,1':3',1''-terphenyl]-2'-carbonitrile (3ea): 129 mg was obtained from **1e** (155 mg, 0.5 mmol) and **2a** following general procedure **B**. Yield 72%; colourless gum; R_f = 0.6 (SiO_2, EtOAc:Hexane, 1:99); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.57 – 7.53 (m, 4H), 7.51 – 7.50 (m, 1H), 7.49 (q, *J* = 1.5 Hz, 2H), 7.48 – 7.42 (m, 3H), 7.32 (ddd, *J* = 7.5, 4.4, 1.2 Hz, 2H), 7.27 – 7.25 (m, 1H), 7.24 (s, 2H), 7.18 (dd, *J* = 5.2, 3.1 Hz, 2H), 3.09 – 3.03 (m, 2H), 3.02 – 2.97 (m, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 146.8, 146.5, 140.6, 138.7, 129.1, 128.9, 128.5, 126.2, 118.1, 107.9, 37.9, 37.3; **IR** (neat) *v* 2926, 2300, 2221, 1597, 1502, 1291, 770, 704 cm^{-1}; **HRMS** (QToF) calcd for $C_{27}H_{22}N$ $[M+H]^+$ 360.1752 found 360.1745

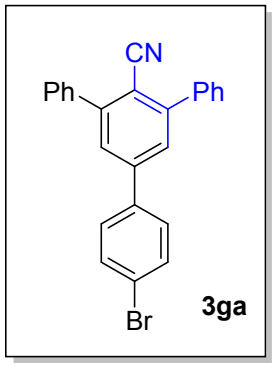


5'-(3-fluorophenyl)-[1,1':3',1''-terphenyl]-2'-carbonitrile (3fa): 136 mg was obtained from **1f** (224mg, 0.5 mmol) and **2a** following general procedure **B**. Yield 78%; brownish solid; mp 195−198 °C; R_f = 0.55 (SiO_2, EtOAc:Hexane, 1:99); **^{1}H NMR** (300 MHz, $CDCl_3$) δ 7.66 (d, *J* = 3.4 Hz, 4H), 7.63 (s, 2H), 7.56 (d, *J* = 2.3 Hz, 1H), 7.53 (s, 2H), 7.49 (d, *J* = 7.9 Hz, 3H), 7.46 (s, 2H), 7.37 (d, *J* = 9.9 Hz, 1H), 7.14 (ddd, *J* = 11.4, 7.1, 4.5 Hz,

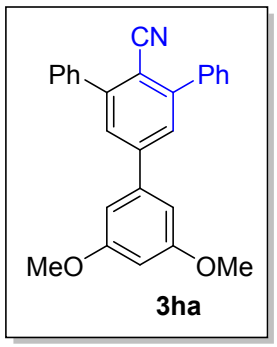


1H); **^{13}C NMR** (75 MHz, $CDCl_3$) δ 147.5, 143.8, 141.3, 141.2, 130.7, 130.6, 129.0, 128.9, 128.7, 127.5, 123.0, 117.9, 115.7, 115.5, 114.4, 114.2, 109.6; **IR** (KBr) *v* 3108, 3051, 2301, 2222, 1593, 1499, 771, 700 cm^{-1}; **HRMS** (QToF) calcd for $C_{25}H_{17}NF$ $[M+H]^+$ 350.1345 found 350.1346.

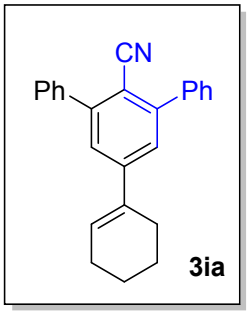
5'-(4-bromophenyl)-[1,1':3',1''-terphenyl]-2'-carbonitrile (3ga)[2]: 157 mg was obtained from **1g** (142 mg, 0.5 mmol) and **2a** following general procedure **B**. Yield 77%; puffy white solid; mp 167−170 °C; R_f = 0.55 (SiO_2, EtOAc:Hexane, 2:98); **^{1}H NMR** (300 MHz, $CDCl_3$) δ 7.65 (s, 4H), 7.62 (d, *J* = 5.8 Hz, 4H), 7.55 (s, 2H), 7.53 (s, 3H), 7.50 (s, 2H), 7.47 (d, *J* = 7.4 Hz, 1H); **^{13}C NMR** (75 MHz, $CDCl_3$) δ 147.5, 143.8, 138.4, 137.9, 132.2, 129.0, 128.8, 128.7, 127.2, 123.2, 117.8, 109.4; **IR** (KBr) *v* 3047, 2308, 2222, 1597, 1497, 769, 706 cm^{-1}; **HRMS** (TOF) calcd for $C_{25}H_{17}NBr$ $[M+H]^+$ 410.0544 found 410.0546.



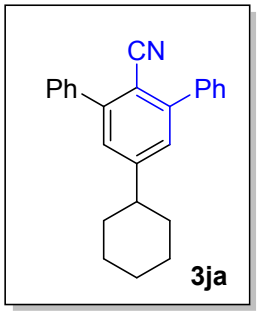
5'-(3,5-dimethoxyphenyl)-[1,1':3',1''-terphenyl]-2'-carbonitrile (3ha): 162 mg was obtained from **1h** (133mg, 0.5 mmol) and **2a** following general procedure **B**. Yield 83%; pale white solid; mp 213−216 °C; R_f = 0.5 (SiO_2, EtOAc:Hexane, 9:91); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.67 (s, 2H), 7.66 (d, *J* = 1.4 Hz, 2H), 7.64 (s, 2H), 7.55 (d, *J* = 1.5 Hz, 1H), 7.53 (s, 1H), 7.51 (s, 1H), 7.50 (s, 2H), 7.48 (dd, *J* = 6.6, 3.2 Hz, 1H), 6.79 (d, *J* = 2.2 Hz, 2H), 6.54 (t, *J* = 2.1 Hz, 1H), 3.85 (s, 6H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 161.3, 147.2, 145.0, 141.1, 138.6, 129.0, 128.7, 128.6, 127.5, 117.9, 109.2, 105.6, 100.5, 55.5; **IR** (KBr) *v* 3009, 2304, 2223, 1598, 1499, 771, 702 cm^{-1}; **HRMS** (QToF) calcd for $C_{27}H_{22}NO_2$ $[M+H]^+$ 392.1651 found 392.1648.



5'-(cyclohex-1-en-1-yl)-[1,1':3',1''-terphenyl]-2'-carbonitrile (3ia): 117 mg was obtained from **1i** (105 mg, 0.5 mmol) and **2a** following general procedure **B**. Yield 70%; colourless gel; R_f = 0.55 (SiO_2, EtOAc:Hexane, 1:99); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.61 (t, *J* = 1.8 Hz, 4H), 7.60 – 7.58 (m, 1H), 7.52 (t, *J* = 1.8 Hz, 2H), 7.50 (q, *J* = 1.6 Hz, 1H), 7.48 (d, *J* = 1.4 Hz, 1H), 7.48 – 7.46 (m, 2H), 7.46 – 7.43 (m, 1H), 6.38 – 6.34 (m, 1H), 2.46 (dtd, *J* = 8.5, 4.2, 2.3 Hz, 2H), 2.29 – 2.23 (m, 2H), 1.85 – 1.78 (m, 2H), 1.72 – 1.66 (m, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 146.7, 146.4, 139.0, 135.3, 128.9, 128.7, 128.5, 125.3, 118.2, 107.9, 27.1, 26.0, 22.7, 21.8; **IR** (neat) *v* 2991, 2304, 2226, 1598, 1495, 771, 703 cm^{-1}; **HRMS** (QToF) calcd for $C_{25}H_{22}N$ $[M+H]^+$ 336.1752 found 336.1753.

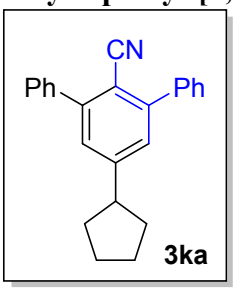


5'-cyclohexyl-[1,1':3',1''-terphenyl]-2'-carbonitrile (3ja): 111 mg was obtained from **1j** (106 mg, 0.5 mmol) and **2a** following general procedure **B.** Yield 66%; colourless liquid; R_f = 0.6 (SiO_2, EtOAc:Hexane, 1:99); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.62 – 7.58 (m, 4H), 7.51 (t, *J* = 1.8 Hz, 1H), 7.50 (t, *J*= 1.9 Hz, 2H), 7.48 (t, *J* = 1.9 Hz, 1H), 7.46 (t, *J* = 1.5 Hz, 1H), 7.44

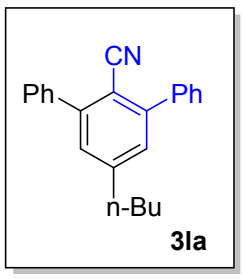


(dt, *J* = 2.7, 2.0 Hz, 1H), 7.31 (s, 2H), 2.65 (tt, *J* = 11.6, 3.1 Hz, 1H), 1.96 (d, *J* = 11.9 Hz, 2H), 1.88 (d, *J* = 12.5 Hz, 2H), 1.82 – 1.75 (m, 1H), 1.52 (dd, *J* = 12.5, 2.8 Hz, 1H), 1.45 (dd, *J* = 14.6, 6.3 Hz, 2H), 1.39 (dt, *J* = 12.6, 3.0 Hz, 1H), 1.28 (tt, *J* = 10.7, 3.3 Hz, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 153.0, 146.9, 139.0, 129.0, 128.5, 127.6, 118.3, 107.7, 44.8, 34.0, 26.6, 25.9; **IR** (neat) *ν* 2995, 2224, 1595, 1498, 771, 704 cm^{-1}; **HRMS** (QToF) calcd for $C_{25}H_{24}N$ $[M+H]^+$ 338.1909 found 338.1917.

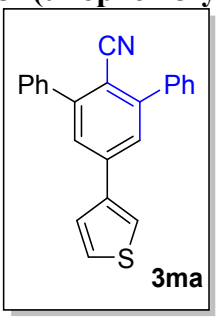
5'-cyclopentyl-[1,1':3',1''-terphenyl]-2'-carbonitrile (3ka): 94 mg was obtained from **1k** (99 mg, 0.5mmol) and **2a** following general procedure **B**. Yield 58%; colourless liquid; R_f = 0.6 (SiO_2, EtOAc:Hexane, 1:99); **^{1}H NMR** (300 MHz, $CDCl_3$) δ 7.62 – 7.58 (m, 4H), 7.54 – 7.52 (m, 1H), 7.50 (s, 2H), 7.49 – 7.42 (m, 3H), 7.34 (s, 2H), 3.18 – 3.05 (m, 1H), 2.20 – 2.10 (m, 2H), 1.85 (dd, *J* = 8.0, 5.3 Hz, 2H), 1.80 – 1.63 (m, 4H); **^{13}C NMR** (75 MHz, $CDCl_3$) δ 151.8, 146.7, 138.9, 129.0, 128.5, 127.8, 118.2, 107.6, 46.0, 34.5, 25.5; **IR** (neat) *ν* 2958, 2226, 1595, 1498, 771, 703 cm^{-1}; **HRMS** (QToF) calcd for $C_{24}H_{22}N$ $[M+H]^+$ 324.1752 found 324.1756.



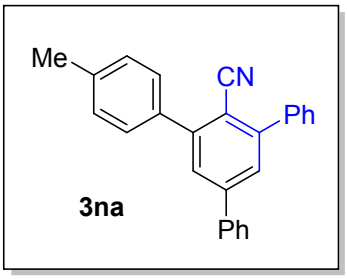
5'-butyl-[1,1':3',1''-terphenyl]-2'-carbonitrile (3la): 81 mg was obtained from **1l** (93 mg, 0.5 mmol) and **2a** following general procedure **B**. Yield 52%; colorless liquid; R_f = 0.6 (SiO_2, EtOAc:Hexane, 1:99); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.64 (d, *J* = 1.6 Hz, 1H), 7.62 (q, *J* = 1.9 Hz, 2H), 7.54 (t, *J* = 1.7 Hz, 1H), 7.52 (d, *J* = 1.6 Hz, 2H), 7.50 (t, *J* = 1.8 Hz, 1H), 7.49 (t, *J* = 1.4 Hz, 1H), 7.46 (dt, *J* = 2.6, 1.9 Hz, 1H), 7.33 (s, 2H), 2.80 – 2.74 (m, 2H), 1.72 (dq, *J* = 12.8, 7.6 Hz, 2H), 1.44 (dt, *J* = 14.6, 7.4 Hz, 2H), 0.99 (t, *J* = 7.3 Hz, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 147.9, 146.7, 138.8, 129.0, 128.9, 128.4, 118.2, 107.5, 35.7, 33.0, 22.3, 13.8; **IR** (neat) *ν* 2950, 2224,1597, 1500, 771, 704 cm^{-1}; **HRMS** (QToF) calcd for $C_{23}H_{22}N$ $[M+H]^+$ 312.1752 found 312.1757.



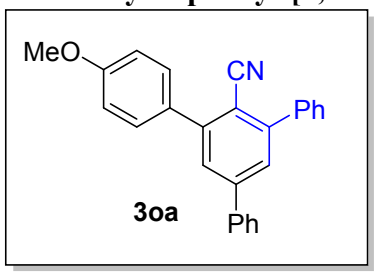
5'-(thiophen-3-yl)-[1,1':3',1''-terphenyl]-2'-carbonitrile (3ma): 133 mg was obtained from **1m** (106 mg, 0.5 mmol) and **2a** following general procedure **B**. Yield 79%; amorphous powder; mp 152−155 °C; R_f = 0.5 (SiO_2, EtOAc:Hexane, 2:98); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.69 (s, 2H), 7.65 (d, *J* = 1.4 Hz, 5H), 7.63 (s, 1H), 7.55 – 7.54 (m, 2H), 7.53 (s, 1H), 7.51 (s, 1H), 7.49 (dd, *J* = 6.4, 2.1 Hz, 1H), 7.46 (d, *J* = 2.6 Hz, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 147.4, 140.2, 139.4, 138.6, 128.9, 128.7, 128.6, 127.1, 126.6, 126.0, 122.8, 118.0, 108.6; **IR** (KBr) *ν* 3109, 2965, 2303, 2224,1597, 1505,773, 704 cm^{-1}; **HRMS** (QToF) calcd for $C_{23}H_{16}NS$ $[M+H]^+$ 338.1003 found 338.1003.



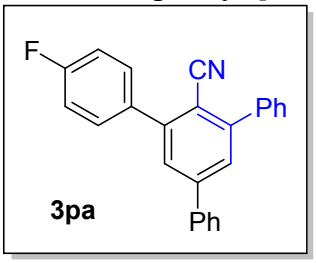
4-methyl-5'-phenyl-[1,1':3',1''-terphenyl]-2'-carbonitrile (3na): 143 mg was obtained from **1n** (110 mg, 0.5 mmol) and **2a** following general procedure **B**. Yield 83%; greyish white solid; mp 145−148 °C; R_f = 0.53 (SiO_2, EtOAc:Hexane, 1:99); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.69 – 7.65 (m, 4H), 7.64 (s, 1H), 7.56 – 7.47 (m, 7H), 7.43 (dd, *J* = 8.3, 6.3 Hz, 1H), 7.33 (d, *J* = 7.9 Hz, 2H), 2.44 (s, 3H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 147.4, 147.3, 145.0, 139.1, 138.7, 135.8, 129.3, 129.0, 129.0, 128.9, 128.7, 128.6, 127.4, 127.3, 118.2, 108.9, 21.2; **IR** (KBr) *v* 2962, 2917, 2223, 1517,769, 703 cm^{-1}; **HRMS** (QToF) calcd for $C_{26}H_{20}N$ $[M+H]^+$ 346.1596 found 346.1598.



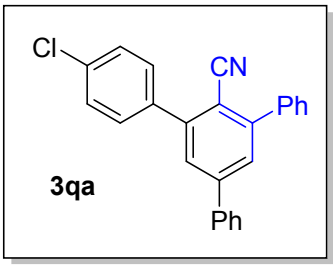
4-methoxy-5'-phenyl-[1,1':3',1''-terphenyl]-2'-carbonitrile (3oa)[2]: 153 mg was obtained from **1o** (118 mg, 0.5 mmol) and **2a** following general procedure **B**. Yield 85%; white solid; mp 179−181 °C; R_f = 0.45 (SiO_2, EtOAc:Hexane, 3:97); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.69 – 7.65 (m, 5H), 7.64 (d, *J* = 1.2 Hz, 1H), 7.61 (d, *J* = 2.1 Hz, 1H), 7.60 – 7.58 (m, 1H), 7.55 – 7.48 (m, 4H), 7.48 – 7.43 (m, 2H), 7.07 – 7.02 (m, 2H), 3.88 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 160.0, 147.3, 147.0, 145.0, 139.1, 138.7, 132.9, 131.9, 131.0, 130.5, 130.2, 129.0, 129.0, 128.6, 128.6, 127.3, 127.3, 127.1, 118.3, 114.1, 113.8, 108.8, 55.3; **IR** (KBr) *v* 3048, 2217, 1603, 1512, 768, 701 cm^{-1}; **HRMS** (QToF) calcd for $C_{26}H_{20}NO$ $[M+H]^+$ 362.1545 found 362.1547.



4-fluoro-5'-phenyl-[1,1':3',1''-terphenyl]-2'-carbonitrile (3pa)[2]: 138 mg was obtained from **1p** (112 mg, 0.5 mmol) and **2a** following general procedure **B**. Yield 79%; pale brown solid; mp 195−198 °C; R_f = 0.50 (SiO_2, EtOAc:Hexane, 1:99); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.70 (d, *J* = 1.8 Hz, 1H), 7.68 (t, *J* = 1.8 Hz, 1H), 7.66 – 7.60 (m, 6H), 7.56 – 7.49 (m, 4H), 7.48 – 7.41 (m, 2H), 7.22 (ddd, *J* = 10.6, 5.9, 2.5 Hz, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 161.8, 147.4, 146.3, 145.2, 138.9, 138.5, 134.7, 130.9, 130.8, 129.1, 129.0, 128.8, 128.6, 127.6, 127.4, 127.3, 117.9, 115.8, 115.6, 109.0; **IR** (KBr) *v* 2925, 2299, 2227, 1510, 770, 705 cm^{-1}; **HRMS** (QToF) calcd for $C_{25}H_{17}NF$ $[M+H]^+$ 350.1345 found 350.1335.

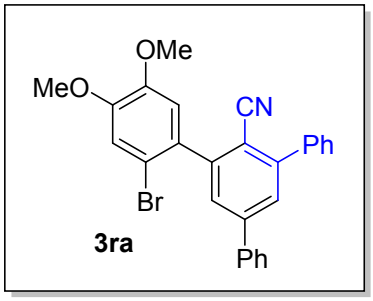


4-chloro-5'-phenyl-[1,1':3',1''-terphenyl]-2'-carbonitrile (3qa)[2]: 141 mg was obtained from **1q** (120 mg, 0.5mmol) and **2a** following general procedure **B**. Yield 77%; pale yellowish solid; mp 205−210 °C; R_f = 0.55 (SiO_2, EtOAc:Hexane, 1:99); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.71 (d, *J* = 1.7 Hz, 1H), 7.68 (d, *J* = 1.5 Hz, 1H), 7.65 (d, *J* = 1.5 Hz, 3H), 7.63 (d, *J* = 1.1 Hz, 1H), 7.60 – 7.57 (m, 2H), 7.55 – 7.47 (m, 7H), 7.47 – 7.42 (m, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 147.5, 146.1, 145.3, 138.9, 138.5, 137.1, 135.1, 130.4, 129.2,

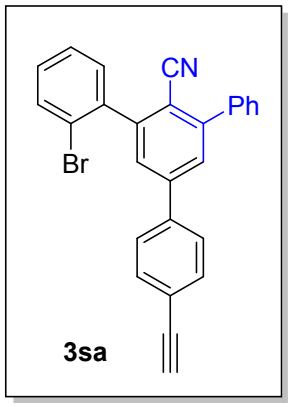


129.0, 128.9, 128.9, 128.7, 127.8, 127.3, 117.9, 108.9; **IR** (KBr) *v* 2893, 2316, 2218, 1592, 1496, 769, 698 cm^{-1}; **HRMS** (TOF) calcd for $C_{25}H_{17}NCl$ $[M+H]^+$ 366.1050 found 366.1053.

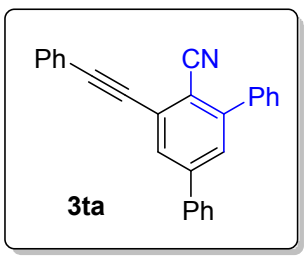
2-bromo-4,5-dimethoxy-5'-phenyl-[1,1':3',1''-terphenyl]-2'-carbonitrile (3ra): 157 mg was obtained from **1t** (172 mg, 0.5 mmol) and **2a** following general procedure **B**; Yield 67%; white solid; mp 189−193 °C; R_f = 0.53 (SiO_2, EtOAc:Hexane, 7:93); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.74 (d, *J* = 1.6 Hz, 1H), 7.68 (t, *J* = 6.8 Hz, 4H), 7.64 (d, *J* = 1.6 Hz, 1H), 7.54 (s, 1H), 7.50 (dd, *J* = 12.7, 7.6 Hz, 4H), 7.46 – 7.41 (m, 1H), 7.19 (s, 1H), 6.95 (s, 1H), 3.95 (s, 3H), 3.90 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 149.9, 148.3, 146.7, 146.4, 144.8, 138.9, 138.4, 131.4, 129.1, 129.0, 128.8, 128.7, 128.2, 127.8, 127.4, 117.5, 115.7, 113.6, 113.3, 110.6, 56.2, 56.2; **IR** (KBr) *v* 2961, 2307, 2223, 1511, 1460, 767, 699 cm^{-1}; **HRMS** (QToF) calcd for $C_{27}H_{21}NO_2Br$ $[M+H]^+$ 470.0756 found 470.0761.



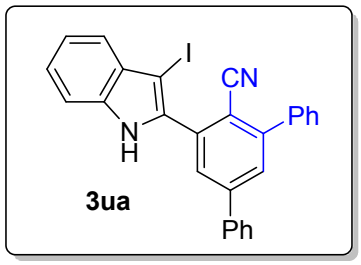
2-bromo-5'-(4-ethynylphenyl)-[1,1':3',1''-terphenyl]-2'-carbonitrile (3sa): 136 mg was obtained from **1s** (154 mg, 0.5 mmol) and **2a** following general procedure **B**. Yield 63%; pale yellow solid; mp 167−170 °C; R_f = 0.55 (SiO_2, EtOAc:Hexane, 8:92); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.75 (dd, *J* = 7.0, 4.9 Hz, 2H), 7.67 (d, *J* = 1.6 Hz, 1H), 7.66 – 7.65 (m, 2H), 7.64 (d, *J* = 2.2 Hz, 1H), 7.61 (t, *J* = 1.8 Hz, 2H), 7.59 (d, *J* = 2.0 Hz, 1H), 7.55 – 7.52 (m, 2H), 7.51 (d, *J* = 1.3 Hz, 1H), 7.50 – 7.48 (m, 1H), 7.46 (t, *J* = 3.4 Hz, 2H), 7.34 (dt, *J* = 8.1, 4.7 Hz, 1H), 3.18 (s, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 146.7, 146.5, 143.7, 139.3, 139.0, 138.2, 133.1, 132.8, 131.0, 130.3, 128.9, 128.9, 128.7, 127.8, 127.7, 127.5, 127.2, 122.9, 122.6, 117.1, 110.7, 83.0, 78.7; **IR** (KBr) *v* 3025, 2995, 2316, 2223,2159, 1595, 1389, 767, 703 cm^{-1}; **HRMS** (QToF) calcd for C_{27} $H_{17}NBr$ $[M+H]^+$ 434.0544 found 434.0541.



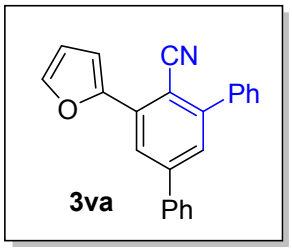
5'-(phenylethynyl)-[1,1':3',1''-terphenyl]-4'-carbonitrile (3ta): 140 mg was obtained from **1r** (115 mg, 0.5 mmol) and **2a** following general procedure **B**. Yield 79%; off white solid; mp 118−121 °C; R_f = 0.53 (SiO_2, EtOAc:Hexane, 1:99); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.85 (d, *J* = 1.7 Hz, 1H), 7.69 – 7.64 (m, 6H), 7.63 (d, *J* = 1.3 Hz, 1H), 7.56 – 7.49 (m, 4H), 7.49 – 7.44(m, 2H), 7.41 – 7.38 (m, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 146.6, 145.0, 138.5, 138.0, 132.0, 129.2, 129.1, 128.9, 128.9, 128.7, 128.4, 128.1, 127.2, 122.1, 117.2, 112.5, 95.8, 86.2; **IR** (KBr) *v* 3050, 2962, 2223, 1595, 1494,766, 701 cm^{-1}; **HRMS**(QToF) calcd for $C_{27}H_{18}N$ $[M+H]^+$ 356.1439 found 356.1429.



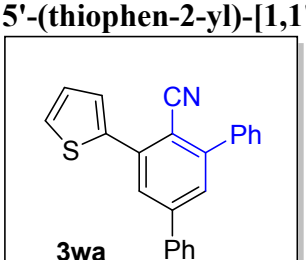
5'-(3-iodo-1H-indol-2-yl)-[1,1':3',1''-terphenyl]-4'-carbonitrile (3ua): 176 mg was obtained from **1u** (186 mg, 0.5 mmol) and **2a** following general procedure **B**. Yield 71%; yellow solid; mp 182−185 °C; R_f = 0.55 (SiO_2, EtOAc:Hexane, 10:90); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.29 (d, *J* = 1.5 Hz, 1H), 8.23 (s, 1H), 7.97 (d, *J* = 8.0 Hz, 1H), 7.72 (d, *J* = 1.4 Hz, 1H), 7.71 (s, 1H), 7.54 (dd, *J* = 5.2, 1.3 Hz, 5H), 7.52 – 7.49 (m, 2H), 7.47 – 7.42 (m, 2H), 7.39 (d, *J* = 7.9 Hz, 1H), 7.36 – 7.30 (m, 1H), 7.25 – 7.21 (m, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 157.2, 144.8, 141.1, 139.7, 139.6, 136.8, 135.8, 134.0, 133.5, 129.8, 129.2, 129.0, 128.9, 128.5, 128.4, 127.7, 127.3, 126.2, 123.0, 121.9, 118.6, 113.4, 57.4; **IR** (KBr) *v* 3670, 2962, 2367, 2223, 1650, 1509, 766, 701 cm^{-1}; **HRMS** (QToF) calcd for $C_{27}H_{18}N_2I$ $[M+H]^+$ 497.0515 found 497.0516.



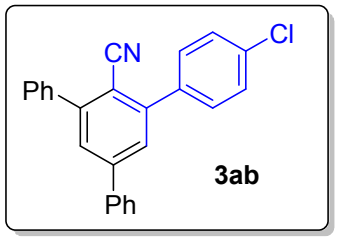
5'-(furan-2-yl)-[1,1':3',1''-terphenyl]-4'-carbonitrile (3va)[2]: 112 mg was obtained from **1v** (98 mg, 0.5 mmol) and **2a** following general procedure **B**. Yield 70%; grey solid; mp 105−110 °C; R_f =0.55 (SiO_2, EtOAc:Hexane, 2:98); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.13 (d, *J* = 1.8 Hz, 1H), 7.70 (t, *J* = 1.7 Hz, 1H), 7.69 – 7.68 (m, 1H), 7.62 (t, *J* = 1.8 Hz, 1H), 7.60 (dt, *J* = 1.7, 1.1 Hz, 1H), 7.58 (d, *J* = 1.8 Hz, 1H), 7.54 (t, *J* = 1.8 Hz, 1H), 7.52 (dd, *J* = 2.2, 1.5 Hz, 1H), 7.51 (d, *J* = 1.5 Hz, 1H), 7.50 (dd, *J* = 2.9, 1.5 Hz, 1H), 7.49 (t, *J* = 1.9 Hz, 1H), 7.46 (dd, *J* = 2.5, 0.9 Hz, 1H), 7.44 (t, *J* = 2.3 Hz, 1H), 7.43 (t, *J* = 1.2 Hz, 1H), 6.60 (dd, *J* = 3.6, 1.8 Hz, 1H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 149.9, 147.8, 145.3, 143.3, 139.0, 138.6, 134.8, 129.0, 129.0, 128.7, 128.6, 127.3, 127.2, 123.5, 118.4, 112.3, 111.2, 104.6; **IR** (KBr) *v* 3012, 2998, 2304, 2223, 1542, 1265, 767, 703 cm^{-1}; **HRMS** (QToF) calcd for $C_{23}H_{16}NO$ $[M+H]^+$ 322.1232 found 322.1234.



5'-(thiophen-2-yl)-[1,1':3',1''-terphenyl]-4'-carbonitrile (3wa)[2]: 123 mg was obtained from **1w** (106 mg, 0.5 mmol) and **2a** following general procedure **B**. Yield 73%; greyish white solid; mp 149−152 °C; R_f = 0.55 (SiO_2, EtOAc:Hexane, 2:98); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.80 (d, *J* = 1.7 Hz, 1H), 7.69 – 7.67 (m, 2H), 7.66 – 7.65 (m, 1H), 7.64 (d, *J* = 1.6 Hz, 2H), 7.63 – 7.62 (m, 1H), 7.55 – 7.52 (m, 2H), 7.50 (dd, *J* = 3.9, 1.5 Hz, 2H), 7.47 (ddd, *J* = 7.1, 6.4, 2.2 Hz, 3H), 7.19 (dd, *J* = 5.1, 3.7 Hz, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 147.9, 145.3, 139.6, 139.3, 138.8, 138.5, 129.1, 128.9, 128.8, 128.6, 128.1, 128.1, 127.7, 127.4, 127.3, 118.1, 108.1; **IR** (KBr) *v* 3013, 2959, 2302, 2228, 1542, 766, 710 cm^{-1}; **HRMS** (QToF) calcd for $C_{23}H_{16}NS$ $[M+H]^+$ 338.1003 found 338.1010.

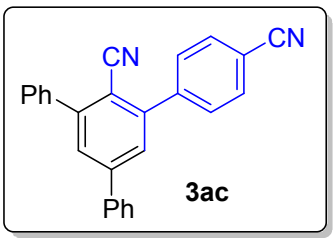


4-chloro-5'-phenyl-[1,1':3',1''-terphenyl]-2'-carbonitrile (3ab)[2]: 142 mg was obtained from**1a** (106 mg, 0.5 mmol) and **2b** following general procedure **B**. Yield 78%; puffy white solid; mp 205−208 °C; R_f = 0.55 (SiO_2, EtOAc:Hexane, 1:99); **^{1}H NMR** (500 MHz, $CDCl_3$) δ

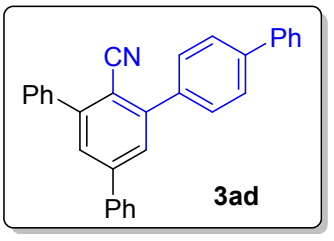


7.71 (d, J = 1.8 Hz, 1H), 7.67 (t, J = 1.7 Hz, 1H), 7.66 – 7.64 (m, 3H), 7.64 – 7.63 (m, 1H), 7.61 – 7.59 (m, 1H), 7.59 – 7.57 (m, 1H), 7.54 (t, J = 1.7 Hz, 1H), 7.53 (d, J = 1.6 Hz, 1H), 7.51 (dd, J = 4.0, 1.7 Hz, 2H), 7.49 (dd, J = 4.8, 2.7 Hz, 3H), 7.47 – 7.43 (m, 1H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 147.5, 146.0, 145.3, 138.8, 138.4, 137.0, 135.0, 130.3, 129.1, 128.9, 128.9, 128.8, 128.7, 127., 127.3, 117.8, 108.9; **IR** (KBr) ν 2962, 2306, 2221, 1597, 1495, 768, 701 cm^{-1}; **HRMS** (QToF) calcd for $C_{25}H_{17}ClN$ $[M+H]^+$ 366.1050 found 366.1043.

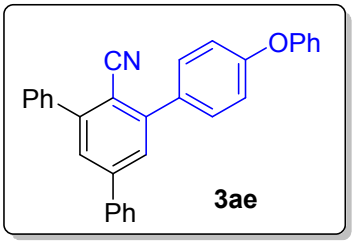
5'-phenyl-[1,1':3',1''-terphenyl]-2',4-dicarbonitrile (3ac): 139 mg was obtained from **1a** (106 mg, 0.5 mmol) and **2c** following general procedure **B**. Yield 78%; colourless solid; mp 228−232 °C; R_f = 0.53 (SiO_2, EtOAc:Hexane, 1:99); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.84 – 7.81 (m, 2H), 7.78 – 7.75 (m, 3H), 7.67 (t, J = 1.8 Hz, 1H), 7.66 (d, J = 1.7 Hz, 2H), 7.64 (q, J = 2.0 Hz, 1H), 7.63 – 7.62 (m, 1H), 7.56 – 7.50 (m, 4H), 7.50 – 7.45 (m, 2H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 147.7, 145.6, 145.2, 143.1, 138.5, 138.1, 132.4, 129.8, 129.2, 129.0, 129.0, 128.9, 128.7, 128.5, 127.3, 127.2, 118.4, 117.5, 112.6, 108.7; **IR** (KBr) ν 3022, 2359, 2223, 1595, 1251, 740, 670 cm^{-1}; **HRMS** (QToF) calcd for $C_{26}H_{17}N_2$ $[M+H]^+$ 357.1392 found 357.1386.



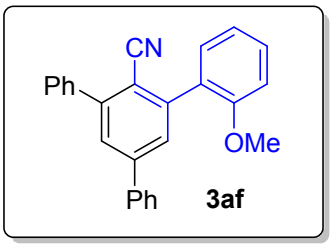
5'-phenyl-[1,1':3',1'':4'',1'''-quaterphenyl]-2'-carbonitrile (3ad): 163 mg was obtained from **1a** (106 mg, 0.5 mmol) and **2d** following general procedure **B**. Yield 80%; colourless solid; mp 193−196 °C; R_f = 0.55 (SiO_2, EtOAc:Hexane, 1:99); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.75 (d, J = 2.0 Hz, 5H), 7.72 – 7.70 (m, 2H), 7.69 (s, 2H), 7.67 – 7.66 (m, 2H), 7.57 – 7.53 (m, 2H), 7.51 (t, J = 3.9 Hz, 3H), 7.49 – 7.43 (m, 4H), 7.41 – 7.37 (m, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 147.4, 146.95, 145.1, 141.6, 140.4, 139.0, 138.7, 137.5, 129.4, 129.1, 129.0, 128.8, 128.7, 128.6, 127.6, 127.5, 127.4, 127.3, 127.3, 127.1, 118.1, 108.8; **IR** (KBr) ν 3037, 2221, 1696, 1595, 1222, 765, 700 cm^{-1}; **HRMS** (QToF) calcd for $C_{31}H_{22}N$ $[M+H]^+$ 408.1752 found 408.1747.



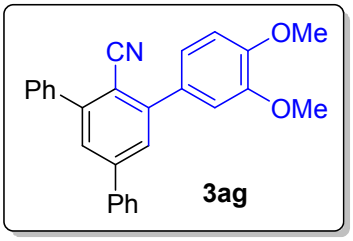
4-phenoxy-5'-phenyl-[1,1':3',1''-terphenyl]-2'-carbonitrile (3ae): 171 mg was obtained from **1a** (106 mg, 0.5 mmol) and **2e** following general procedure **B**. Yield 81%; greyish white solid; mp 150−153 °C; R_f = 0.55 (SiO_2, EtOAc:Hexane, 2:98); **^{1}H NMR** (300 MHz, $CDCl_3$) δ 7.69 (s, 3H), 7.68 (d, J = 1.5 Hz, 2H), 7.66 – 7.64 (m, 2H), 7.62 (s, 1H), 7.57 – 7.50 (m, 4H), 7.49 – 7.44 (m, 2H), 7.40 (t, J = 7.9 Hz, 2H), 7.19 (d, J = 7.4 Hz, 1H), 7.16 – 7.14 (m, 2H), 7.12 (t, J = 2.1 Hz, 2H); **^{13}C NMR** (75 MHz, $CDCl_3$) δ 158.1, 156.4, 147.4, 146.7, 145.1, 139.0, 138.6, 133.2, 130.5, 129.8, 129.0, 129.0, 128.7, 128.6, 127.4, 127.3, 127.3, 123.8, 119.6, 118.3, 118.1, 108.8; **IR** (KBr) ν 3029, 2223, 1593, 1495, 1223, 840, 758 cm^{-1}; **HRMS** (QToF) calcd for $C_{31}H_{22}NO$ $[M+H]^+$ 424.1701 found 424.1701.



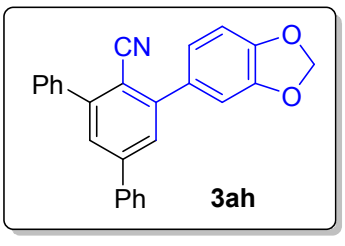
2-methoxy-5'-phenyl-[1,1':3',1''-terphenyl]-2'-carbonitrile (3af)[2]: 143 mg was obtained from **1a** (106 mg, 0.5 mmol) and **2f** following general procedure **B**. Yield 79%; brownish white solid; mp 178-181 °C; R_f = 0.45 (SiO_2, EtOAc:Hexane, 3:97); **^{1}H NMR** (300 MHz, $CDCl_3$) δ 7.68 (s, 3H), 7.66 (s, 3H), 7.53 (d, *J* = 6.7 Hz, 1H), 7.49 (d, *J* = 3.4 Hz, 3H), 7.44 (dd, *J* = 8.6, 2.3 Hz, 3H), 7.37 (dd, *J* = 7.5, 1.3 Hz, 1H), 7.12 – 7.04 (m, 2H), 3.89 (s, 3H); **^{13}C NMR** (75 MHz, $CDCl_3$) δ 156.6, 146.4, 144.8, 144.3, 139.2, 138.8, 130.9, 130.3, 129.0, 129.0, 128.6, 128.1, 127.7, 127.3, 120.7, 117.9, 111.3, 110.9, 55.6; **IR** (KBr) *v* 3017, 2924, 2225, 1598, 1496, 1253, 763, 702 cm^{-1}; **HRMS** (QToF) calcd for $C_{26}H_{20}NO$ $[M+H]^+$ 362.1545 found 362.1541.



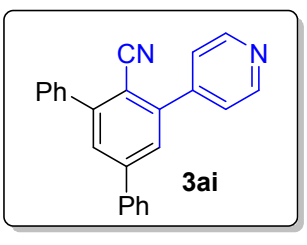
3,4-dimethoxy-5'-phenyl-[1,1':3',1''-terphenyl]-2'-carbonitrile (3ag): 152 mg was obtained from **1a** (106 mg, 0.5 mmol) and **2g** following general procedure **B**. Yield 78%; white solid; mp 208−211 °C; R_f = 0.45 (SiO_2, EtOAc:Hexane, 6:94); **^{1}H NMR** (300 MHz, $CDCl_3$) δ 7.66 (t, *J* = 7.9 Hz, 2H), 7.53 (d, *J* = 6.5 Hz, 2H), 7.50 (s, 2H), 7.47 (d, *J* = 3.6 Hz, 2H), 7.43 (t, *J* = 4.9 Hz, 3H), 7.24 (d, *J* = 1.9 Hz, 1H), 7.22 – 7.17 (m, 2H), 7.01 (d, *J* = 8.2 Hz, 1H), 3.96 (d, *J* = 2.8 Hz, 6H); **^{13}C NMR** (75 MHz, $CDCl_3$) δ 149.5, 148.8, 147.4, 147.1, 145.0, 139.1, 138.7, 131.2, 129.1, 129.0, 128.7, 128.6, 127.3, 127.2, 121.6, 118.3, 112.3, 111.2, 108.9, 56.0, 55.9; **IR** (KBr) *v* 3016, 2312, 2222, 1596, 1516, 1259, 766, 703 cm^{-1}; **HRMS** (QToF) calcd for $C_{27}H_{22}NO_2$ $[M+H]^+$ 392.1651 found 392.1649.



5'-(benzo[d][1,3]dioxol-5-yl)-[1,1':3',1''-terphenyl]-4'-carbonitrile (3ah)[2]: 139 mg was obtained from **1a** (106 mg, 0.5 mmol) and **2h** following general procedure **B**. Yield 74%; greyish white solid; mp 188-191 °C; R_f = 0.45 (SiO_2, EtOAc:Hexane, 5:95); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.66 (ddd, *J* = 7.3, 5.4, 1.5 Hz, 5H), 7.63 (s, 1H), 7.54 – 7.46 (m, 5H), 7.46 – 7.41 (m, 1H), 7.12 (dd, *J* = 7.0, 1.6 Hz, 2H), 6.96 – 6.93 (m, 1H), 6.05 (s, 2H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 148.1, 147.8, 147.3, 147.0, 145.0, 139.0, 138.6, 132.5, 129.1, 129.0, 128.7, 128.6, 127.4, 127.3, 123.0, 118.1, 109.5, 108.9, 108.5, 101.4; **IR** (KBr) *v* 2966, 2920, 2223, 1599, 1498, 767, 702 cm^{-1}; **HRMS** (QToF) calcd for $C_{26}H_{18}NO_2$ $[M+H]^+$ 376.1338 found 376.1336.

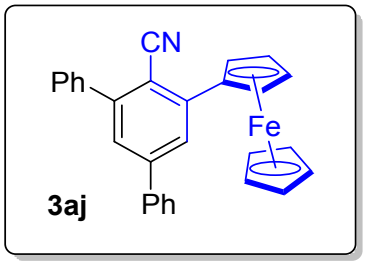


5'-(pyridin-4-yl)-[1,1':3',1''-terphenyl]-4'-carbonitrile (3ai): 125 mg was obtained from **1a** (106 mg, 0.5 mmol) and **2i** following general procedure **B**. Yield 75%; pale yellow solid; mp 193−196 °C; R_f = 0.53 (SiO_2, EtOAc:Hexane, 2:98); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.78 (dd, *J* =

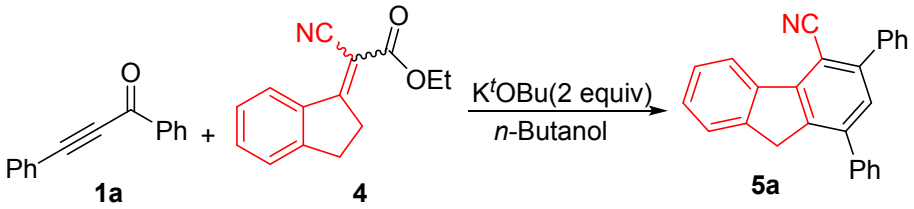


4.5, 1.6 Hz, 2H), 7.77 (d, *J* = 1.8 Hz, 1H), 7.68 (d, *J* = 1.7 Hz, 2H), 7.67 – 7.64 (m, 2H), 7.64 – 7.63 (m, 1H), 7.58 (dd, *J* = 4.4, 1.7 Hz, 2H), 7.56 – 7.50 (m, 4H), 7.47 (ddd, *J* = 8.9, 5.8, 2.4 Hz, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 150.2, 147.7, 146.2, 145.6, 144.3, 138.5, 138.1, 129.2, 129.0, 129.0, 128.9, 128.7, 128.7, 127.3, 127.1, 123.6, 117.4, 108.6; **IR** (KBr) *v* 3031, 2219, 1594, 1550, 764, 699 cm^{-1}; **HRMS** (QToF) calcd for $C_{24}H_{17}N_2$ $[M+H]^+$ 333.1392 found 333.1396.

(2-(4'-cyano-[1,1':3',1''-terphenyl]-5'-yl)cyclopenta-2,4-dien-1-yl)(cyclopenta-2,4-dien-1-yl)iron (3aj): 167 mg was obtained from **1a** (106 mg, 0.5 mmol) and **2j** following general procedure **B**. Yield 76%; pink solid; mp 140−145 °C; R_f = 0.55 (SiO_2, EtOAc:Hexane, 3:97); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.89 (d, *J* = 1.8 Hz, 1H), 7.69 (d, *J* = 1.5 Hz, 1H), 7.66 (d, *J* = 3.0 Hz, 1H), 7.63 (d, *J* = 1.6 Hz, 1H), 7.61 (t, *J* = 1.7 Hz, 1H), 7.55 – 7.53 (m, 1H), 7.52 (d, *J* = 1.1 Hz, 1H), 7.52 – 7.50 (m, 1H), 7.49 (d, *J* = 1.6 Hz, 1H), 7.47 (s, 1H), 7.46 (s, 1H), 5.02 – 5.00 (m, 1H), 4.48 – 4.46 (m, 1H), 4.23 (s, 5H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 147.7, 145.2, 144.4, 139.3, 138.8, 129.1, 129.0, 128.6, 128.5, 128.5, 127.2, 126.9, 126.4, 118.9, 107.5, 82.8, 70.0, 69.7, 69.1; **IR** (KBr) *v* 3040, 2923, 2220, 1596, 1554, 840, 768, 701 cm^{-1}; **HRMS** (QToF) calcd for $C_{29}H_{22}NFe$ $[M+H]^+$ 440.1102 found 440.1087.

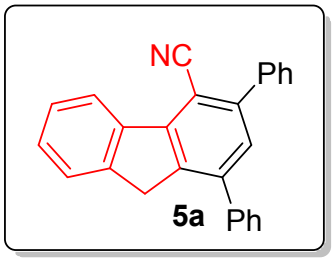


(B). General procedure C for the synthesis of final compounds (5) taking Synthesis of 4a as an Example.



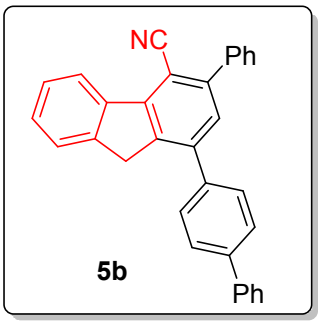
To a 15 mL Schlenk tube was added ynone **1a** (103 mg, 0.5 mmol, 1 equiv), ethyl (E)-2-cyano-2-(2,3-dihydro-1H-inden-1-ylidene)acetate **4** (136 mg, 0.6 mmol, 2 equiv), KO^{t}Bu (112 mg, 1 mmol, 2 equiv) in 1-butanol (3 mL) and the reaction mixture was stirred at room temperature under open air until the complete conversion of starting material (30-60 min). The reaction mixture was concentrated under reduced pressure, washed with hexane (2 times) and the remaining solid was dissolved in 20% EtOAc/Hexane and filtered through a small silica bed. Filtrate was concentrated to get the desired solids in purified form **5a.**

1,3-diphenyl-9H-fluorene-4-carbonitrile (5a): 146 mg was obtained from **4** (136 mg, 0.6 mmol) and **1a** following general procedure **B**. Yield 71%; colourless solid; mp 165−168 °C; R_f = 0.55 (SiO_2, EtOAc:Hexane, 1:99); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.67 (d, *J* = 7.7 Hz, 1H), 7.67 (t, *J* = 1.8 Hz, 1H), 7.66 – 7.65 (m, 1H), 7.59 (d, *J* = 1.5 Hz, 1H), 7.57 (d, *J* = 1.0 Hz, 2H), 7.55 – 7.48 (m,

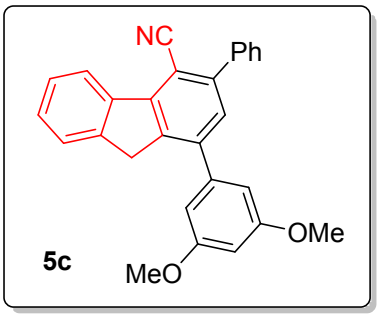


5H), 7.48 – 7.47 (m, 1H), 7.46 (t, *J* = 1.9 Hz, 1H), 7.44 – 7.42 (m, 2H), 4.00 (s, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 145.6, 144.6, 144.2, 142.9, 140.9, 139.4, 139.0, 138.4, 129.1, 128.7, 128.7, 128.6, 128.5, 128.4, 128.3, 127.4, 124.7, 122.8, 118.1, 102.2, 36.3; **IR** (KBr) *v* 3031, 2925, 2221, 2158, 1509, 1387, 769, 704 cm^{-1}; **HRMS** (QToF) calcd for $C_{26}H_{18}N$ $[M+H]^+$ 344.1439 found 344.1432

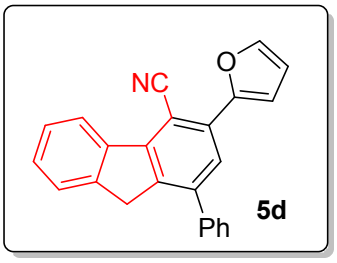
1-([1,1'-biphenyl]-4-yl)-3-phenyl-9H-fluorene-4-carbonitrile (5b): 176 mg was obtained from **4** (136 mg, 0.6 mmol) and **1c** following general procedure **B**. Yield 70%; grey solid; mp 199–203 °C; R_f = 0.55 (SiO_2, EtOAc:Hexane, 1:99); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.68 (d, *J* = 7.7 Hz, 1H), 7.76 (d, *J* = 1.8 Hz, 1H), 7.74 (d, *J* = 1.9 Hz, 1H), 7.67 (ddd, *J* = 6.2, 4.4, 3.0 Hz, 6H), 7.60 (d, *J* = 7.2 Hz, 1H), 7.56 – 7.51 (m, 3H), 7.48 (dd, *J* = 8.3, 4.0 Hz, 4H), 7.46 – 7.38 (m, 2H), 4.07 (s, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 145.7, 144.2, 142.5, 141.2, 140.9, 140.3, 139.0, 138.4, 138.2, 129.1, 128.9, 128.6, 127.6, 127.4, 127.4, 127.1, 124.8, 122.8, 118.1, 102.2, 36.4; **IR** (KBr) *v* 3043, 2917, 2220, 1581, 1486, 840, 742, 702 cm^{-1}; **HRMS** (QToF) calcd for $C_{32}H_{22}N$ $[M+H]^+$ 420.1752 found 420.1747.



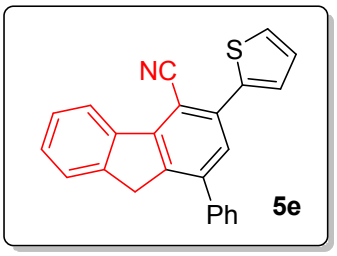
1-(3,5-dimethoxyphenyl)-3-phenyl-9H-fluorene-4-carbonitrile (5c): 177 mg was obtained from **4** (136 mg, 0.6 mmol) and **1h** following general procedure **B**. Yield 73%; white solid; mp 213-215 °C; R_f = 0.45 (SiO_2, EtOAc:Hexane, 6:94); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.66 (d, *J* = 7.7 Hz, 1H), 7.66 (dt, *J* = 3.4, 2.0 Hz, 2H), 7.58 (d, *J* = 7.3 Hz, 1H), 7.56 – 7.47 (m, 4H), 7.46 – 7.42 (m, 2H), 6.69 (d, *J* = 2.3 Hz, 2H), 6.55 (t, *J* = 2.2 Hz, 1H), 4.01 (s, 2H), 3.86 (s, 6H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 160.9, 145.5, 144.6, 144.2, 142.8, 141.3, 140.9, 139.0, 138.4, 129.1, 128.6, 128.6, 128.4, 127.3, 124.7, 122.7, 118.1, 106.7, 102.3, 99.9, 55.4, 36.3; **IR** (KBr) ν 3055, 2308, 2222, 1590, 1493, 1303, 751 cm^{-1}; **HRMS** (QToF) calcd for $C_{28}H_{22}NO_2$ $[M+H]^+$ 404.1651 found 404.1646.



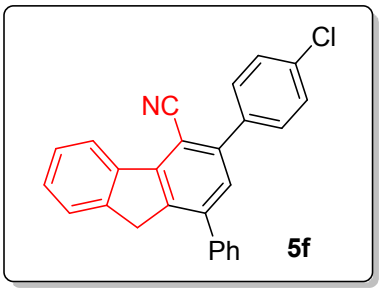
3-(furan-2-yl)-1-phenyl-9H-fluorene-4-carbonitrile (5d): 124 mg was obtained from **4** (136 mg, 0.6 mmol) and **1v** following general procedure **B**. Yield 62%; brownish white solid; mp 203-206 °C; R_f = 0.53 (SiO_2, EtOAc:Hexane, 2:98); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.69 (d, *J* = 7.8 Hz, 1H), 7.84 (s, 1H), 7.58 (ddd, *J* = 6.5, 3.7, 1.4 Hz, 3H), 7.55 – 7.46 (m, 5H), 7.46 – 7.41 (m, 2H), 6.60 (dd, *J* = 3.5, 1.8 Hz, 1H), 3.96 (s, 2H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 150.2, 144.7, 144.2, 143.2, 143.0, 140.8, 139.40, 138.9, 133.2, 128.7, 128.6, 128.3, 127.3, 124.9, 124.7, 122.8, 118.5, 112.2, 110.4, 98.1, 36.3; **IR** (KBr) *v* 2923, 1540, 1471, 1378, 756, 636 cm^{-1}; **HRMS** (QToF) calcd for $C_{24}H_{16}NO[M+H]^+$ 334.1232 found 334.1224.



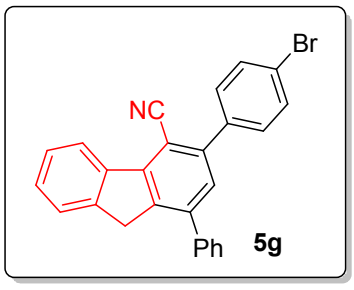
1-phenyl-3-(thiophen-2-yl)-9H-fluorene-4-carbonitrile (5e): 126 mg was obtained from **4** (136 mg, 0.6 mmol) and **1w** following general procedure **B**. Yield 60%; greyish white solid; mp 216–219 °C; R_f = 0.55 (SiO_2, EtOAc:Hexane, 2:98); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.68 (d, *J* = 7.7 Hz, 1H), 7.69 (dd, *J* = 3.6, 1.1 Hz, 1H), 7.58 – 7.55 (m, 3H), 7.55 – 7.52 (m, 3H), 7.51 – 7.46 (m, 3H), 7.45 – 7.42 (m, 1H), 7.20 (dd, *J* = 5.1, 3.7 Hz, 1H), 3.98 (s, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 145.0, 144.3, 143.1, 141.3, 139.6, 139.1, 138.8, 137.6, 128.8, 128.7, 128.6, 128.4, 128.1, 127.8, 127.4, 127.0, 124.8, 122.9, 118.2, 101.3, 36.3; **IR** (KBr) *v* 3045, 2899, 2222, 1581, 1500, 769, 707 cm^{-1}; **HRMS** (QToF) calcd for $C_{24}H_{16}NS$ $[M+H]^+$ 350.1003 found 350.0996.



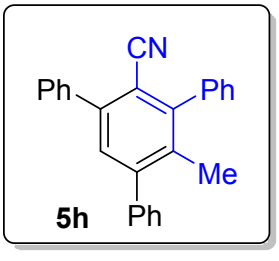
3-(4-chlorophenyl)-1-phenyl-9H-fluorene-4-carbonitrile (5f): 156 mg was obtained from **4** (136 mg, 0.6 mmol) and **1q** following general procedure **B**. Yield 69%; greyish white solid; mp 223–226 °C; R_f = 0.53 (SiO_2, EtOAc:Hexane, 2:98); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.65 (d, *J* = 7.8 Hz, 1H), 7.61 – 7.55 (m, 5H), 7.54 – 7.50 (m, 3H), 7.50 – 7.48 (m, 2H), 7.45 (ddd, *J* = 12.4, 6.1, 2.4 Hz, 2H), 7.38 (s, 1H), 4.00 (s, 2H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 144.8, 144.3, 143.1, 141.4, 139.2, 138.9, 136.9, 134.9, 130.4, 128.9, 128.8, 128.7, 128.5, 128.4, 128.4, 127.5, 124.8, 122.8, 118.0, 102.1, 36.3; **IR** (KBr) *v* 2960, 2222, 1572, 1516, 1382, 762, 672 cm^{-1}; **HRMS** (QToF) calcd for $C_{26}H_{17}ClN$ $[M+H]^+$ 378.1050 found 378.1044.



3-(4-bromophenyl)-1-phenyl-9H-fluorene-4-carbonitrile (5g): 164 mg was obtained from **4** (136 mg, 0.6mmol) following general procedure **B**. Yield 65%; brownish white solid; mp 195–198 °C; R_f = 0.55 (SiO_2, EtOAc:Hexane, 2:98); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.64 (d, *J* = 7.5 Hz, 1H), 7.68 – 7.63 (m, 2H), 7.58 – 7.55 (m, 3H), 7.53 (dt, *J* = 11.8, 3.6 Hz, 4H), 7.49 – 7.41 (m, 3H), 7.38 (s, 1H), 3.98 (s, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 144.8, 144.3, 143.1, 141.4, 139.2, 138.9, 137.3, 131.9, 130.7, 128.8, 128.8, 128.4, 127.5, 124.8, 123.1, 122.8, 118.0, 102.0, 36.3; **IR** (KBr) *v* 3050, 2311, 2215, 1582, 1485,747, 698 cm^{-1}; **HRMS** (QToF) calcd for $C_{26}H_{17}BrN$ $[M+H]^+$ 422.0544 found 422.0540.



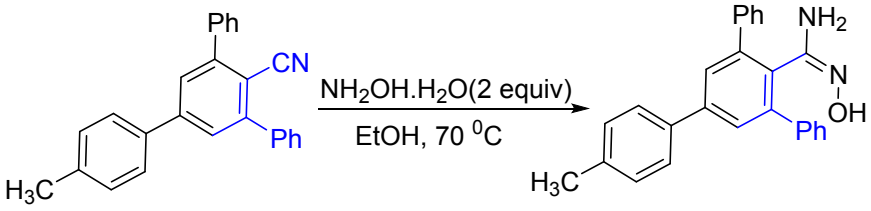
4'-methyl-5'-phenyl-[1,1':3',1''-terphenyl]-2'-carbonitrile (5h): 122 mg was obtained from **1a** (106 mg, 0.5 mmol) and **2j** following general procedure **A**. Yield 71%; white solid; mp 168–171 °C; R_f = 0.55 (SiO_2, EtOAc:Hexane, 1:99); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.62 (d, *J* = 1.5 Hz, 1H), 7.60 (s, 1H), 7.54 – 7.50 (m, 2H), 7.49 – 7.43 (m, 6H), 7.42 (d, *J* = 1.6 Hz, 1H), 7.39 (ddd, *J* = 6.5, 4.0, 1.7 Hz, 5H), 2.04 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 147.4, 146.8, 143.1, 140.7, 138.8, 138.42,



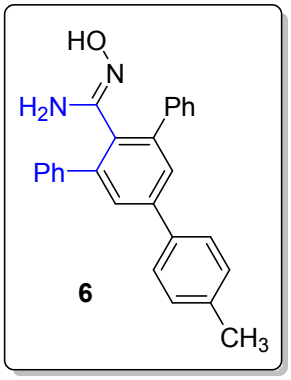
133.9, 130.6, 129.1, 128.9, 128.9, 128.7, 128.6, 128.5, 128.4, 128.3, 127.8, 117.9, 110.9, 18.6; **IR** (KBr) *v* 3049, 2431, 2223, 1962, 1595, 1498, 891, 768, 702 cm^{-1}; **HRMS** (QToF) calcd for $C_{26}H_{20}N$ $[M+H]^+$ 346.1596 found 346.1592.

IV. General Procedure and Characteristic data of derivatives:

(A). General procedure D for the synthesis of derivative (6):

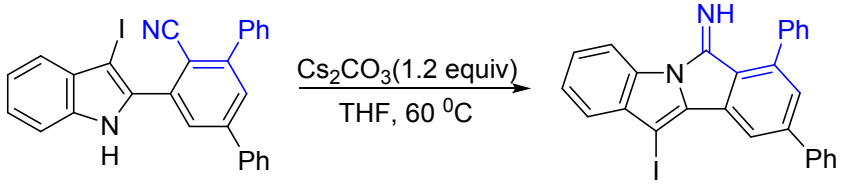


Benzonitrile **3ba** (0.41 mmol) and 50% hydroxylamine in water (0.3 mL) were added to ethanol at room temperature. The reaction mixture was stirred at reflux for 3 to 4 hours until the complete consumption of starting materials (monitored by TLC). The mixture was concentrated to give the crude product, which was further purified by column chromatography to afford compound **6** as a colourless solid.



(Z)-N'-hydroxy-5'-(p-tolyl)-[1,1':3',1''-terphenyl]-2'-carboximidamide (6): 110 mg was obtained from **3ba** (140 mg, 0.6 mmol) following general procedure **D**. Yield 72%; colourless solid; R_f = 0.55 (SiO_2, EtOAc:Hexane, 35:65); **^{1}H NMR** (400 MHz, DMSO) δ 7.68 (d, *J* = 7.2 Hz, 2H), 7.50 (d, *J* = 6.6 Hz, 3H), 7.45 (s, 2H), 7.43 – 7.36 (m, 4H), 7.32 (dd, *J* = 9.3, 7.4 Hz, 4H), 7.15 (d, *J* = 7.9 Hz, 2H), 7.07 (s, 1H), 2.27 (s, 3H); **^{13}C NMR** (100 MHz, DMSO) δ 170.1, 140.8, 140.2, 139.8, 139.8, 139.6, 137.8, 136.7, 136.1, 129.2, 129.0, 128.9, 128.8, 128.2, 128.0, 127.5, 127.2, 12.16, 20.9; **HRMS** (QToF) calcd for $C_{26}H_{21}N_2$ $[M-OH]^+$ 361.1705 found 361.1700.

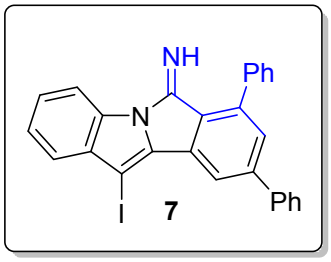
(B). General procedure E for the synthesis of derivative (7):



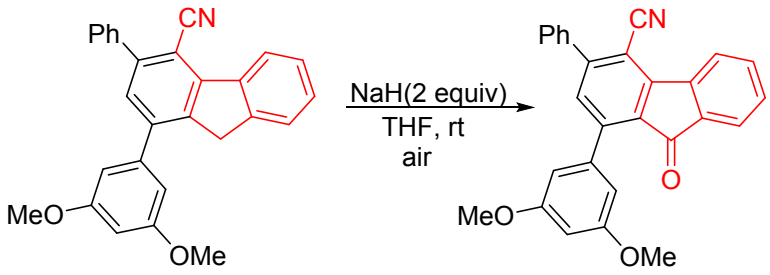
To a round bottomed flask, nitrile **3ua** (0.30 mmol) and caesium carbonate (0.6 mmol) were added in THF and the reaction mixture was stirred at reflux at 60 °C for 4-6 hours until the complete consumption of starting materials (monitored by TLC). The mixture was

concentrated to give the crude product, which was further purified by column chromatography to afford compound **7**.

11-iodo-7,9-diphenyl-6H-isoindolo[2,1-a]indol-6-imine (7): 126 mg was obtained from **3ua** (150 mg, 0.30 mmol) following general procedure **E**. Yield 85%; yellow solid; R_f = 0.55 (SiO_2, EtOAc:Hexane, 15:85); **^{1}H NMR** (400 MHz, DMSO) δ 12.27 (s, 1H), 8.02 (d, *J* = 1.7 Hz, 1H), 7.97 (d, *J* = 1.7 Hz, 1H), 7.94 – 7.90 (m, 2H), 7.76 (dd, *J* = 8.1, 1.3 Hz, 2H), 7.58 (ddd, *J* = 20.7, 9.2, 4.7 Hz, 6H), 7.49 (dt, *J* = 7.2, 3.1 Hz, 2H), 7.41 (d, *J* = 7.9 Hz, 1H), 7.31 – 7.26 (m, 1H), 7.23 – 7.18 (m, 1H); **^{13}C NMR** (100 MHz, DMSO) δ 146.8, 144.4, 138.1, 137.9, 136.9, 136.4, 130.6, 129.5, 129.4, 129.3, 129.0, 128.4, 127.7, 123.8, 121.0, 120.9, 117.7, 112.3, 110.1, 61.7; **IR** (KBr) *ν* 3454, 2258, 1664, 1032, 770 cm^{-1}; **HRMS** (QToF) calcd for $C_{27}H_{18}N_2I$ $[M+H]^+$ 497.0515 found 497.0513.

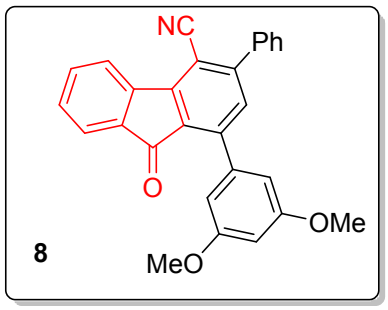


(C). General procedure F for the synthesis of derivative (8):



To a round bottomed flask, nitrile **4c** (0.44 mmol) and sodium hydride (0.88 mmol) were added to THF, the reaction mixture was stirred under open air at room temperature until the complete consumption of nitrile (monitored by TLC). The mixture was concentrated to give the crude product, which was further purified by column chromatography to afford compound **8** as a yellow solid.

1-(3-hydroxy-5-methoxyphenyl)-9-oxo-3-phenyl-9H-fluorene-4-carbonitrile (8): 142 mg was obtained from **4c** (177 mg, 0.44 mmol) following general procedure **F**. Yield 80%; yellow solid; mp 189−193 °C; R_f = 0.55 (SiO_2, EtOAc:Hexane, 10:90); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.46 (d, *J* = 7.7 Hz, 1H), 7.70 (d, *J* = 7.2 Hz, 1H), 7.65 – 7.60 (m, 3H), 7.57 – 7.51 (m, 3H), 7.45 (td, *J* = 7.5, 0.8 Hz, 1H), 7.37 (s, 1H), 6.67 (d, *J* = 2.3 Hz, 2H), 6.57 (t, *J* = 2.3 Hz, 1H), 3.84 (s, 6H; **^{13}C NMR** (100 MHz, $CDCl_3$) δ 190.0, 160.4, 150.4, 149.0, 145.4, 140.6, 137.8, 137.1, 135.2, 134.3, 132.7, 130.8, 129.5, 129.0, 128.8, 128.7, 124.4, 122.7, 117.0, 107.2, 103.4, 101.1, 55.4; **IR** (KBr) *ν* 3055, 2308, 2222, 1590, 1493, 751 cm^{-1}; **HRMS** (QToF) calcd for $C_{28}H_{20}NO_3$ $[M+H]^+$ 418.1443 found 418.1436.



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1.(a) S. Cai, K. Yang, D. Z. Wang, *Org. Lett.*, 2014,**16**, 2606; (b) K. Okamoto, T. Shimbayashi, E. Tamura, K. Ohe, *Org. Lett*., 2015, **17**, 5843; (c) C. E. Song, D. Jung, S. Y. Choung, E. J. S. G. RohLee, *Angew. Chem., Int. Ed*., 2004, **43**, 6183; (d) D. Qiana, J. Zhang, *Chem. Commun*., 2012, **48**, 7082; (e) J. Meesin, P. Katrun, C. Pareseecharoen, M. Pohmakotr, V. Reutrakul, D. Soorukram, C. Kuhakarn*, J. Org. Chem*., 2016, **81**, 2744; (f) R. Samineni, J. Madapal, S. Pabbaraja, G. Mehta, *Org. Lett*., 2017, **19**, 6152; (g) S. Singh, R. Samineni, S. Pabbaraja, G. Mehta, *Angew. Chem., Int. Ed*., 2018, **57**, 16847.

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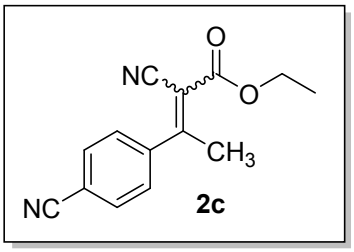
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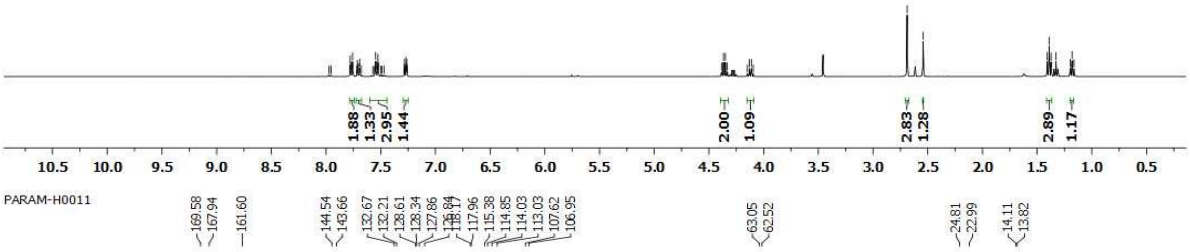
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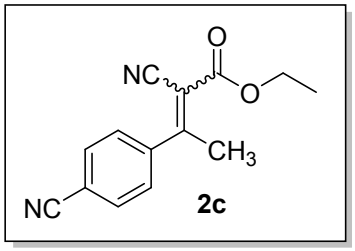
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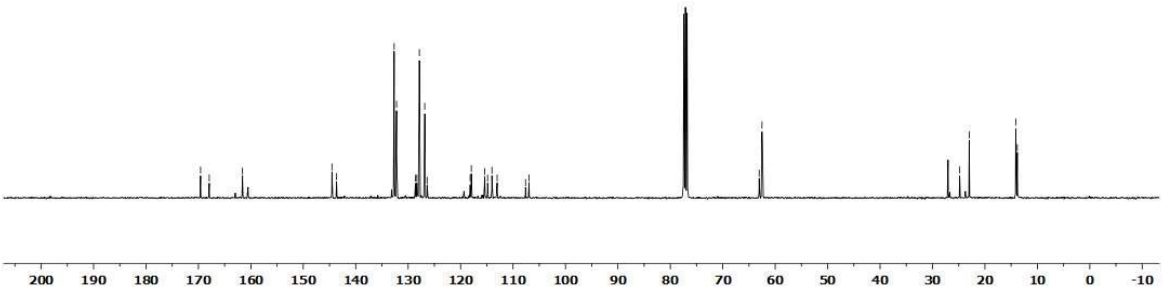
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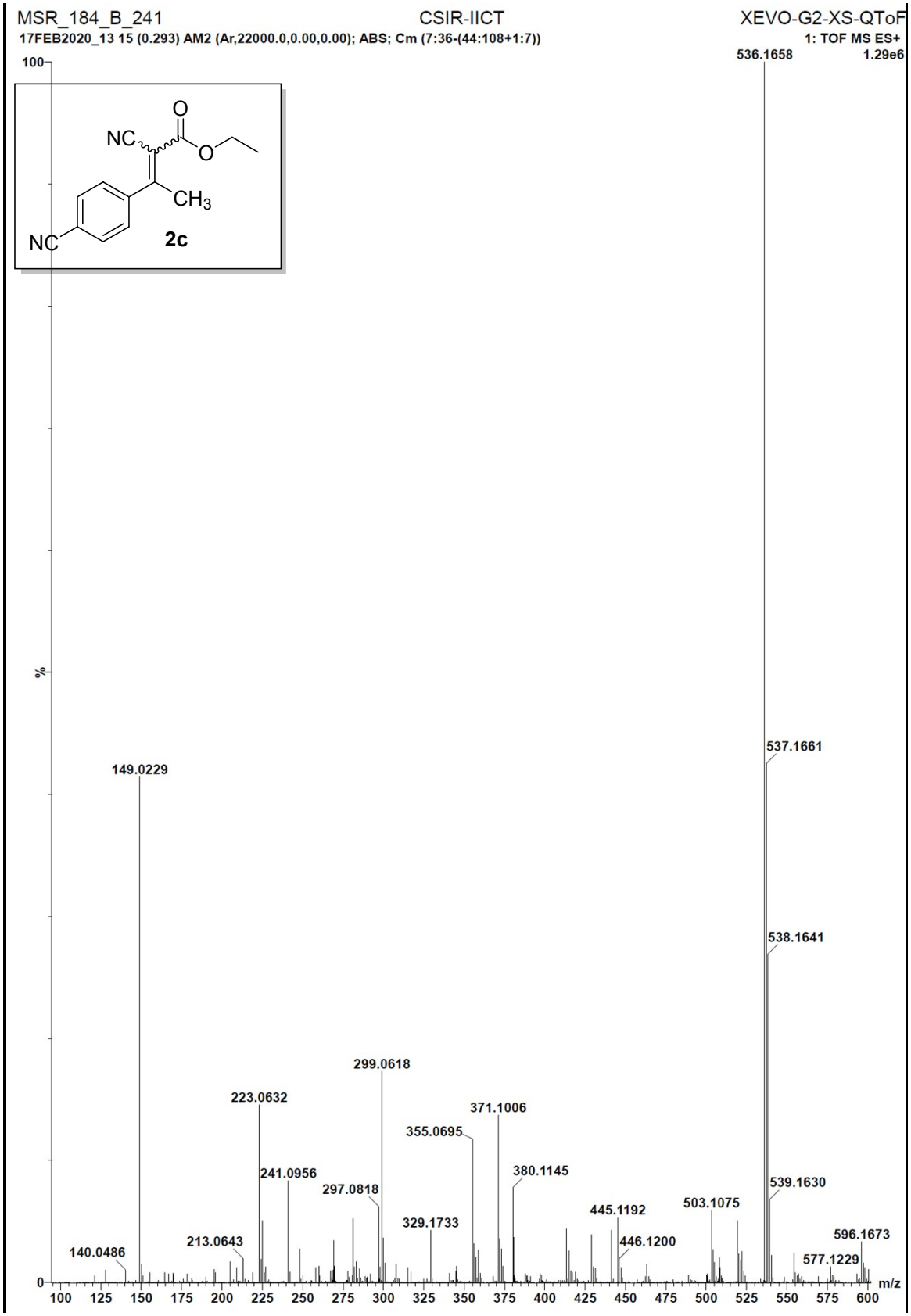
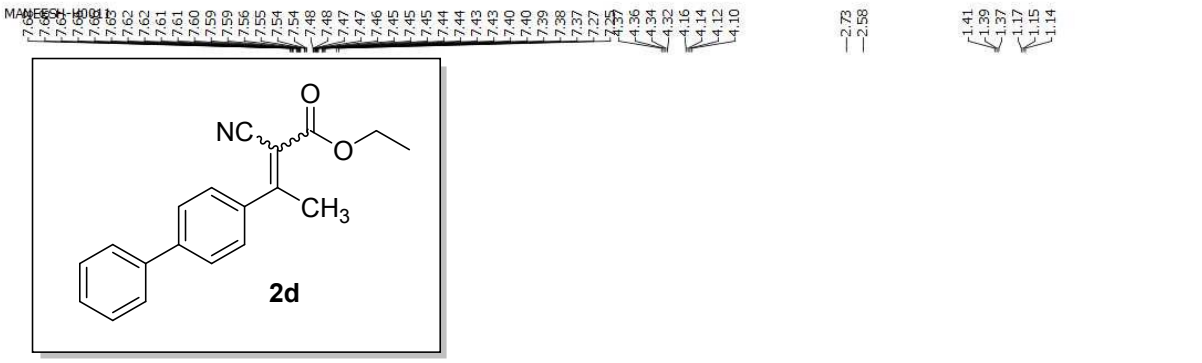
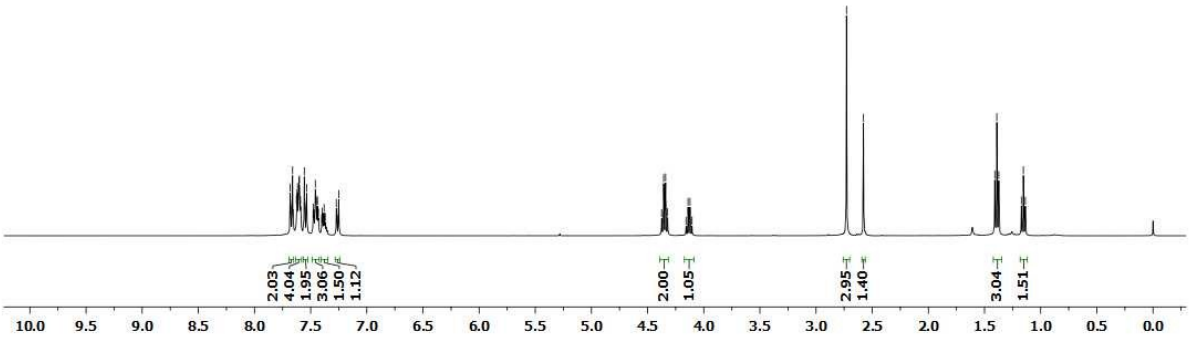
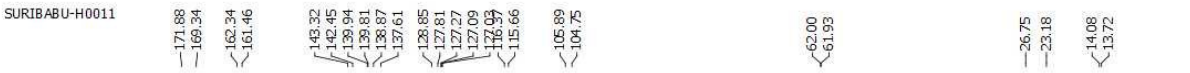
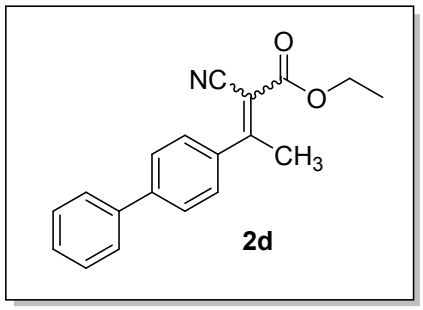
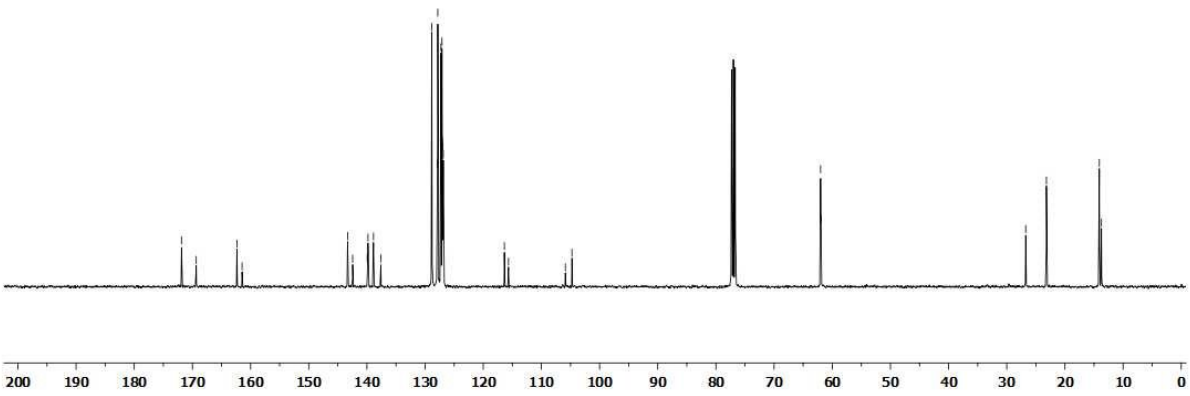

MSR_184_B_241
CSIR-IICT
XEVO-G2-XS-QToF
17FEB2020_13 15 (0.293) AM2 (Ar,22000.0,0.00,0.00); ABS; Cm (7:36-(44:108+1:7))
1: TOF MS ES+
536.1658
1.29e6
NC
O
O
CH3
NC
2c
%
m/z
537.1661
149.0229
538.1641
299.0618
223.0632
371.1006
355.0695
241.0956
380.1145
297.0818
539.1630
445.1192
503.1075
329.1733
596.1673
213.0643
446.1200
140.0486
577.1229

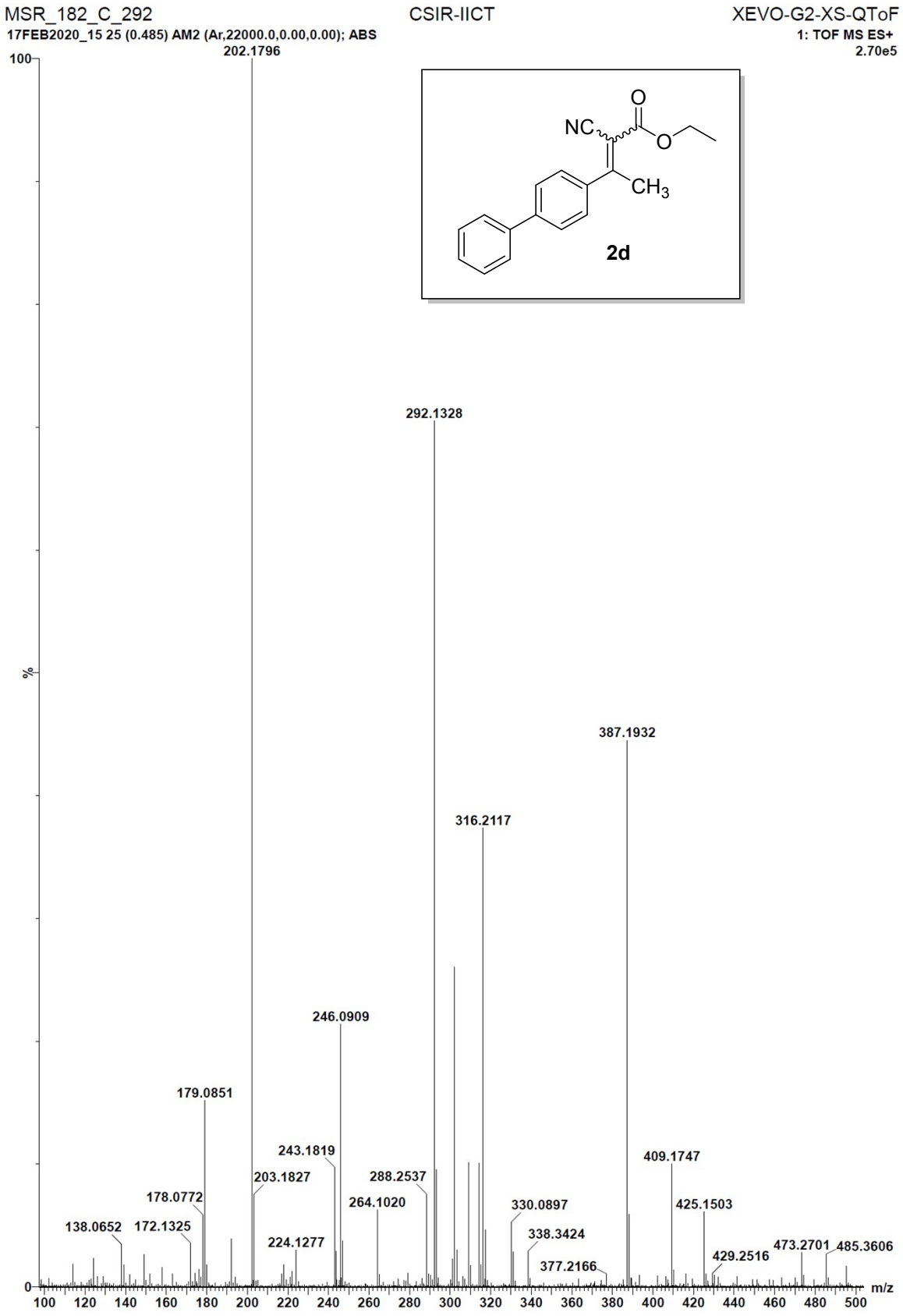

NC
O
O
CH3
2d

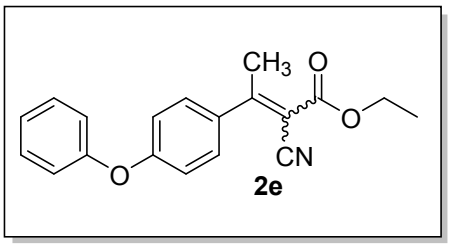

2.03
4.04
1.95
3.06
1.50
1.12
2.00
1.05
2.95
1.40
3.04
1.51


SURIBABU-H0011

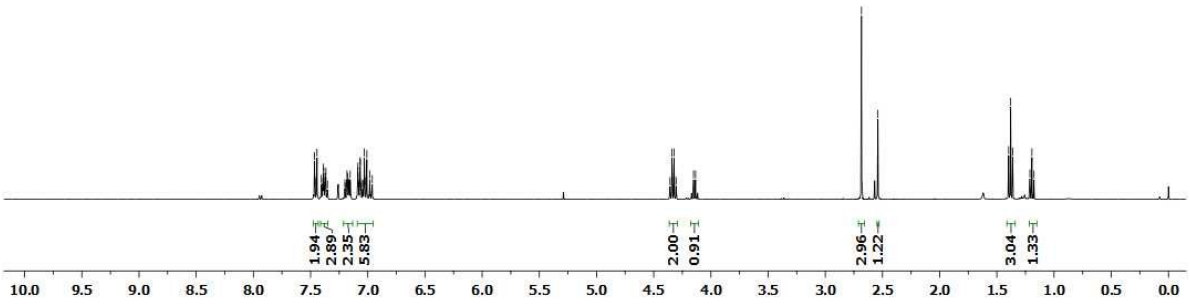

NC
O
O
CH3
2d



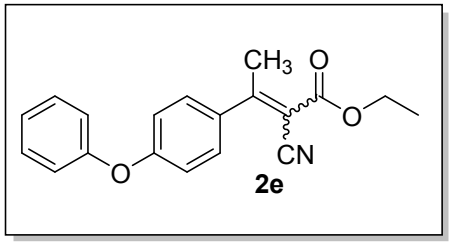

MSR_182_C_292
CSIR-IICT
XEVO-G2-XS-QToF
17FEB2020_15 25 (0.485) AM2 (Ar,22000.0,0.00,0.00); ABS
1: TOF MS ES+
2.70e5
NC
O
O
CH3
2d
%
m/z
202.1796
292.1328
387.1932
316.2117
246.0909
179.0851
243.1819
203.1827
288.2537
409.1747
178.0772
264.1020
330.0897
425.1503
138.0652
172.1325
338.3424
224.1277
473.2701
485.3606
429.2516
377.2166


CH3
O
O
CN
O

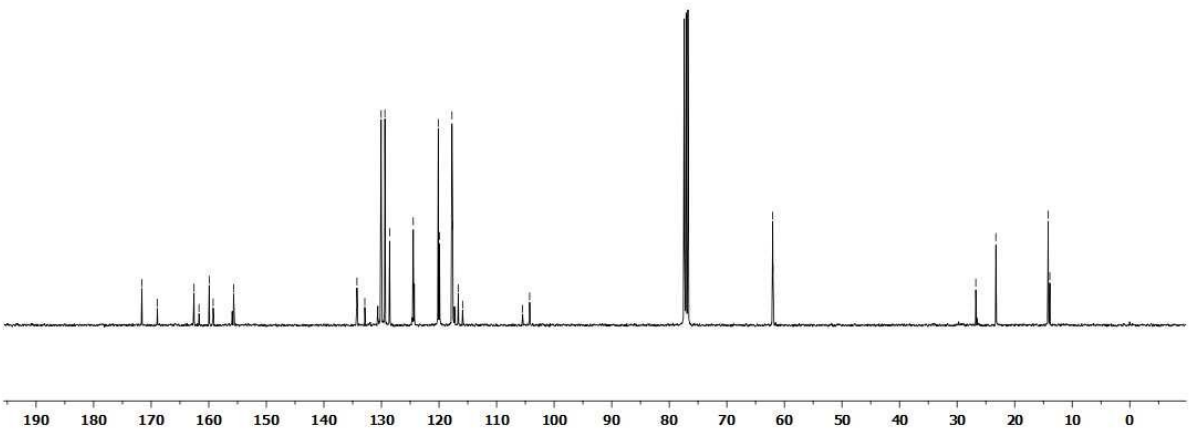
2e

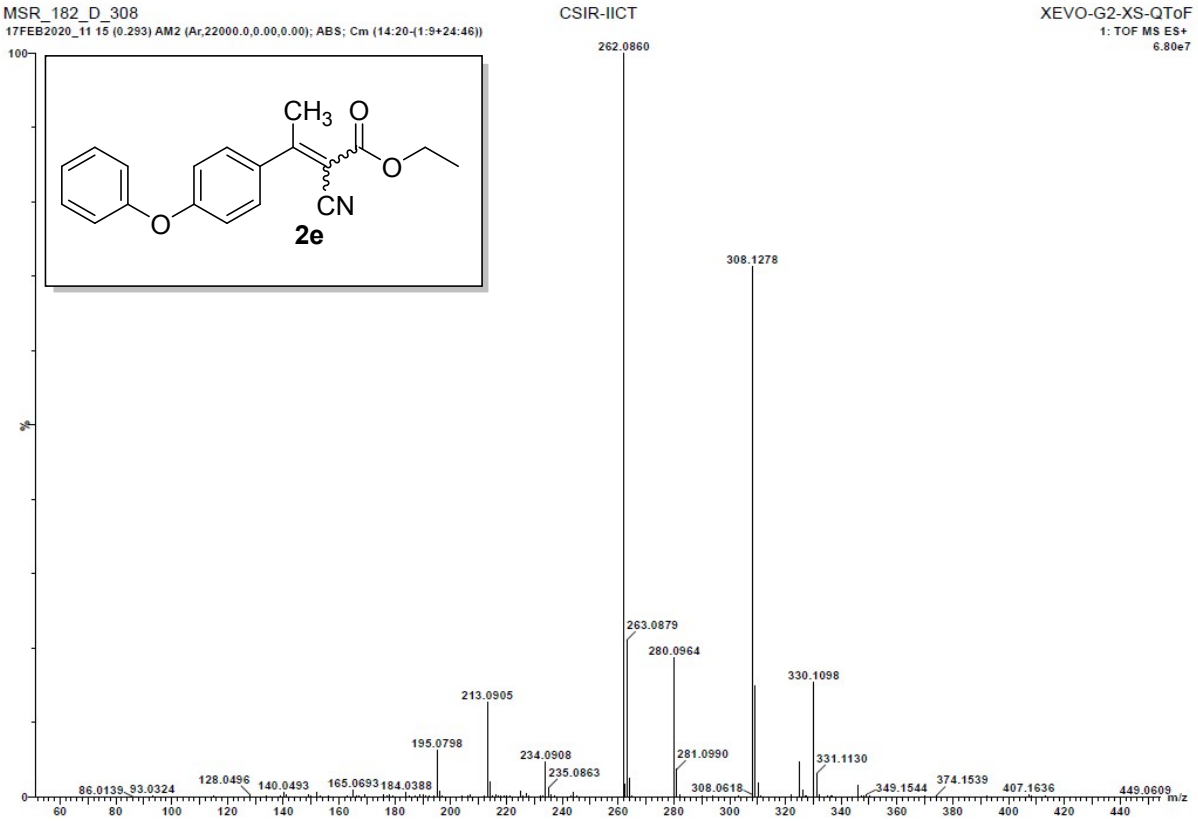

1.94
2.89
2.35
5.83
2.00
0.91
2.96
1.22
3.04
1.33
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0

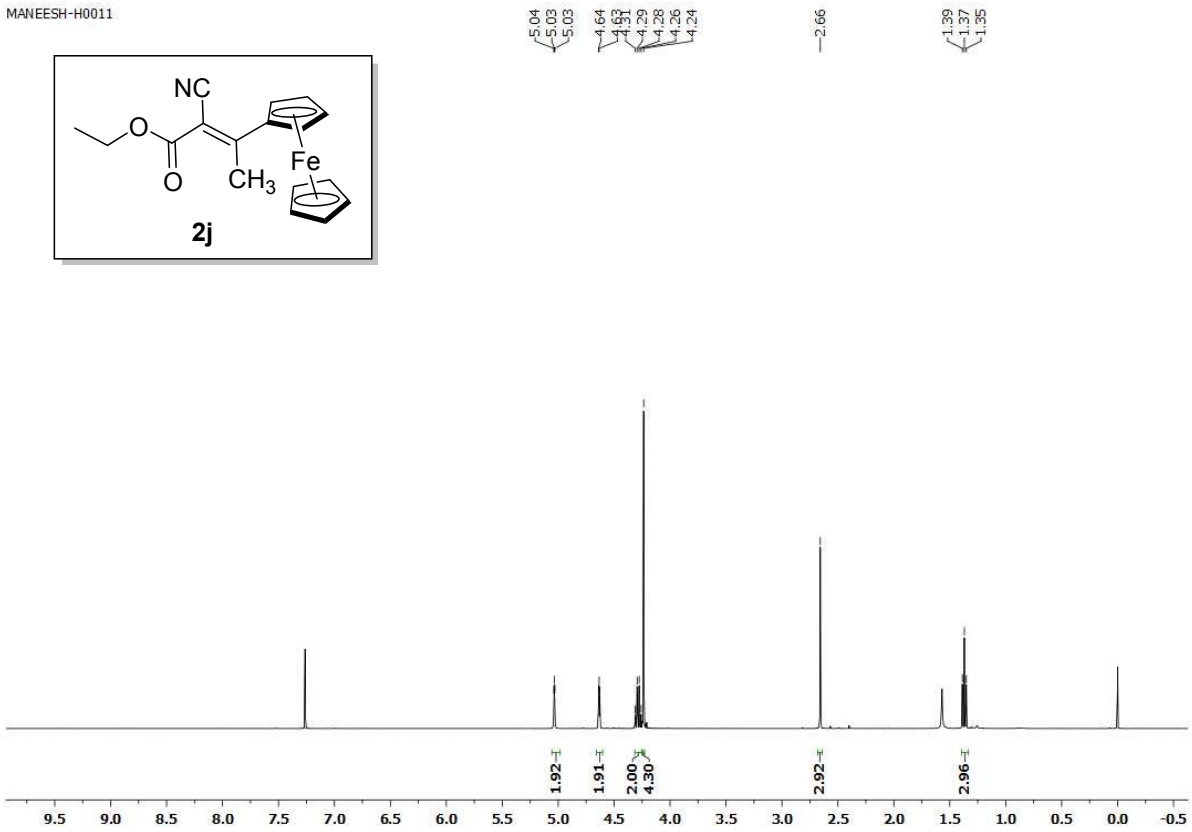

PARAM-H0011

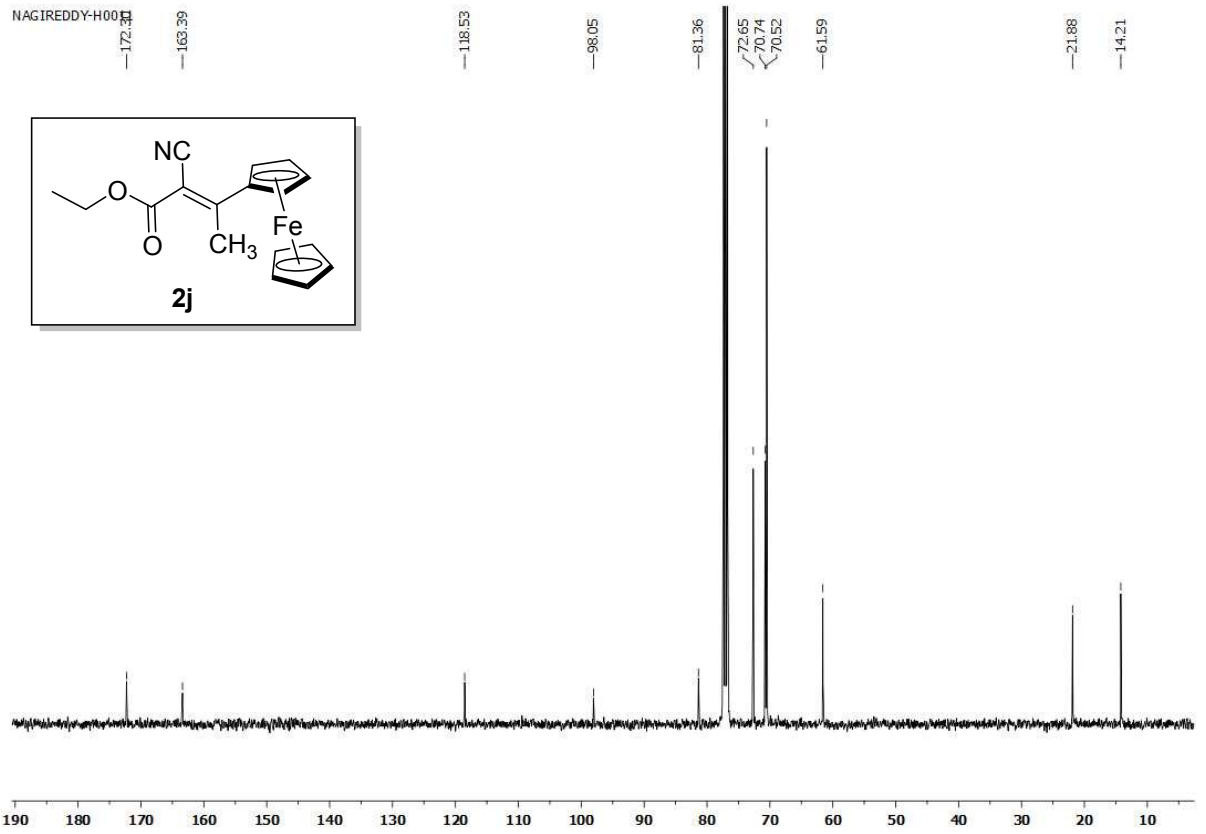

CH3
O
O
CN
O

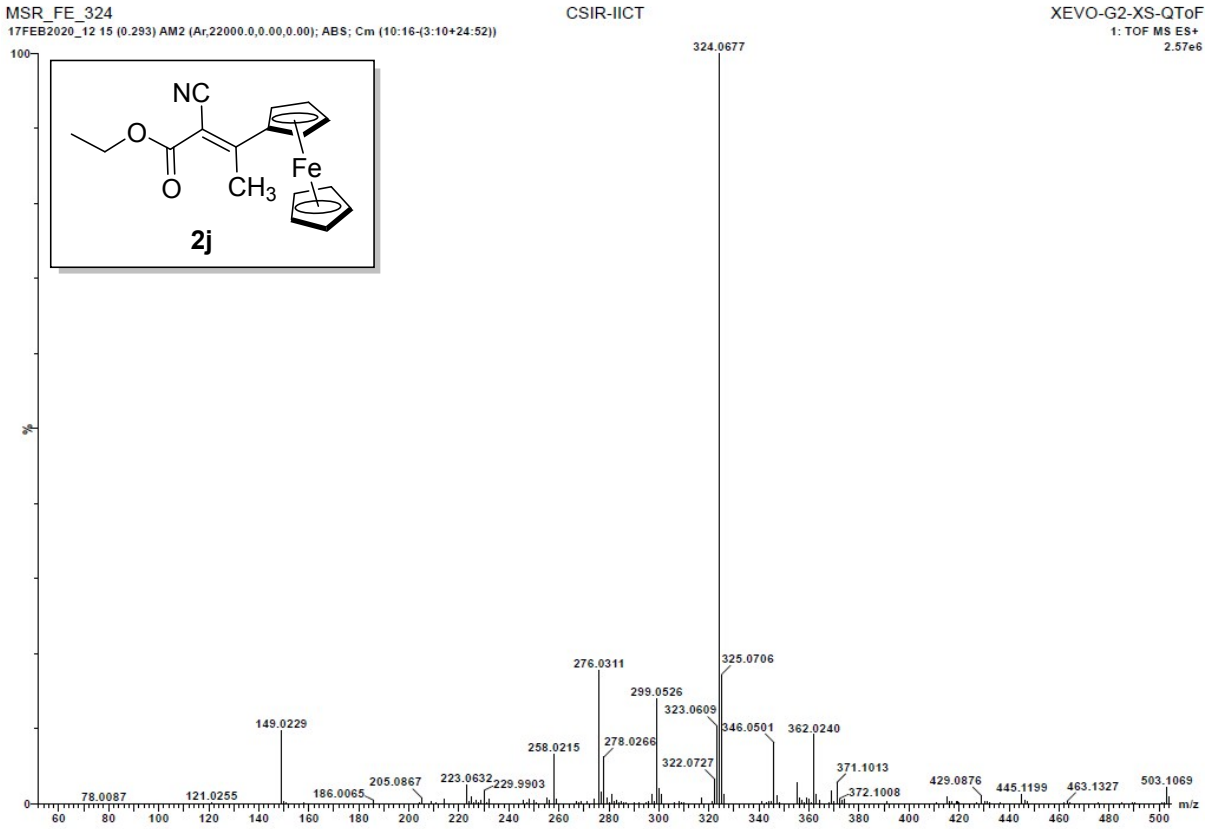
2e

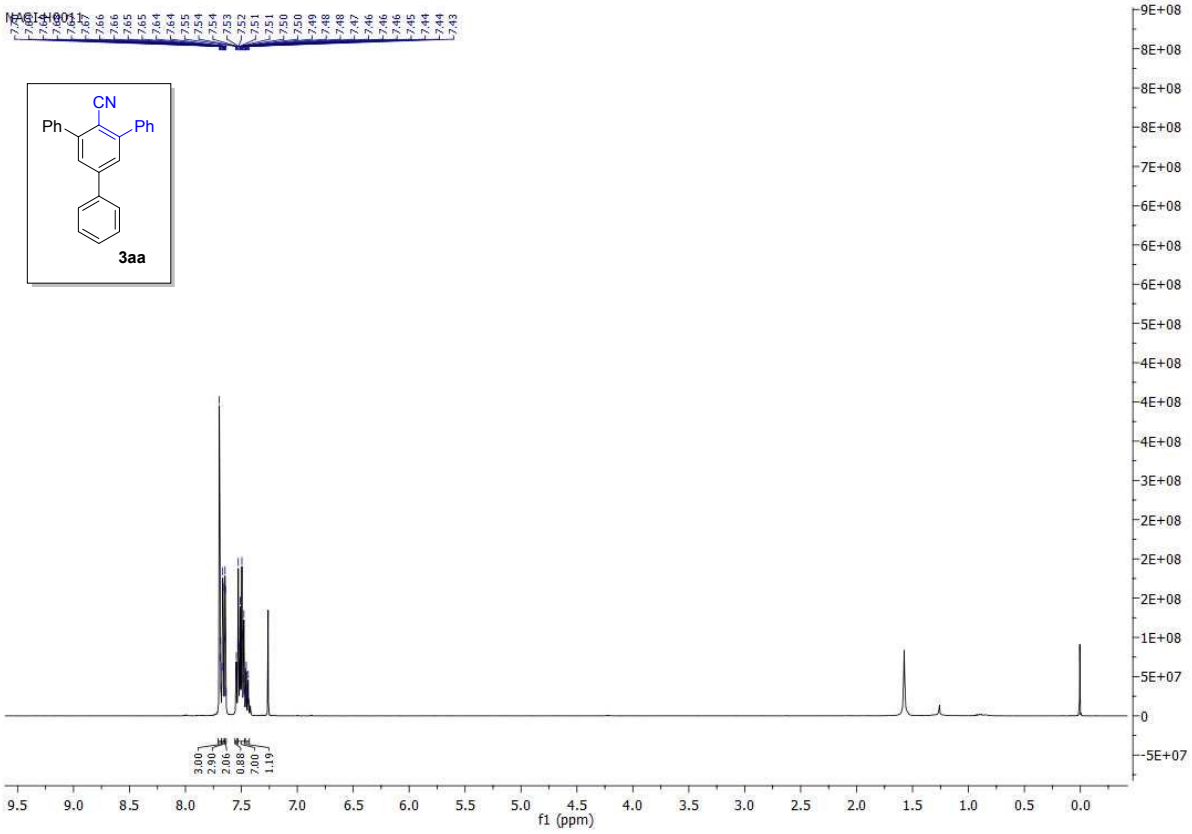

190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

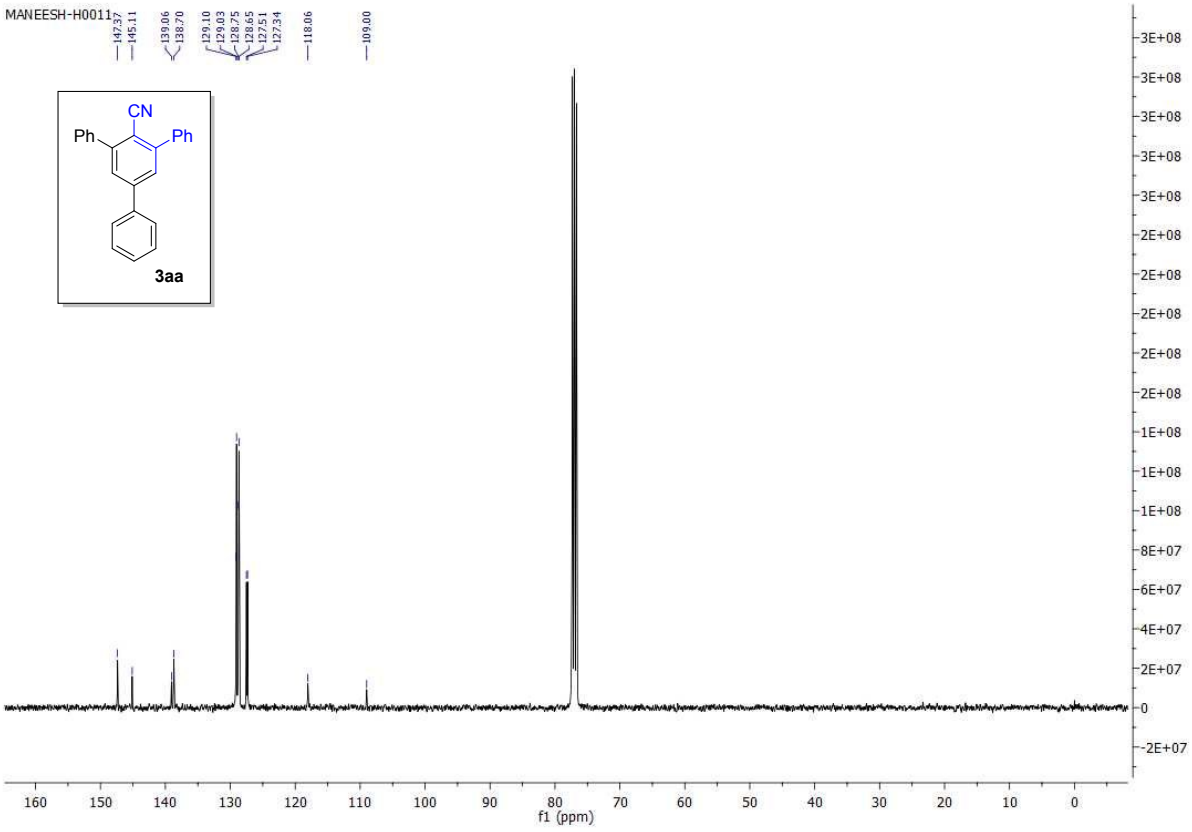

MSR_182_D_308
17FEB2020_11 15 (0.293) AM2 (Ar,22000.0,0.00,0.00); ABS; Cm (14:20-(1:9+24:46))
CSIR-IICT
XEVO-G2-XS-QToF
1: TOF MS ES+
6.80e7
CH3 O
O
CN
O
2e
262.0860
308.1278
263.0879
280.0964
330.1098
213.0905
195.0798
234.0908
235.0863
281.0990
331.1130
86.0139 93.0324
128.0496
140.0493
165.0693
184.0388
308.0618
349.1544
374.1539
407.1636
449.0609
m/z

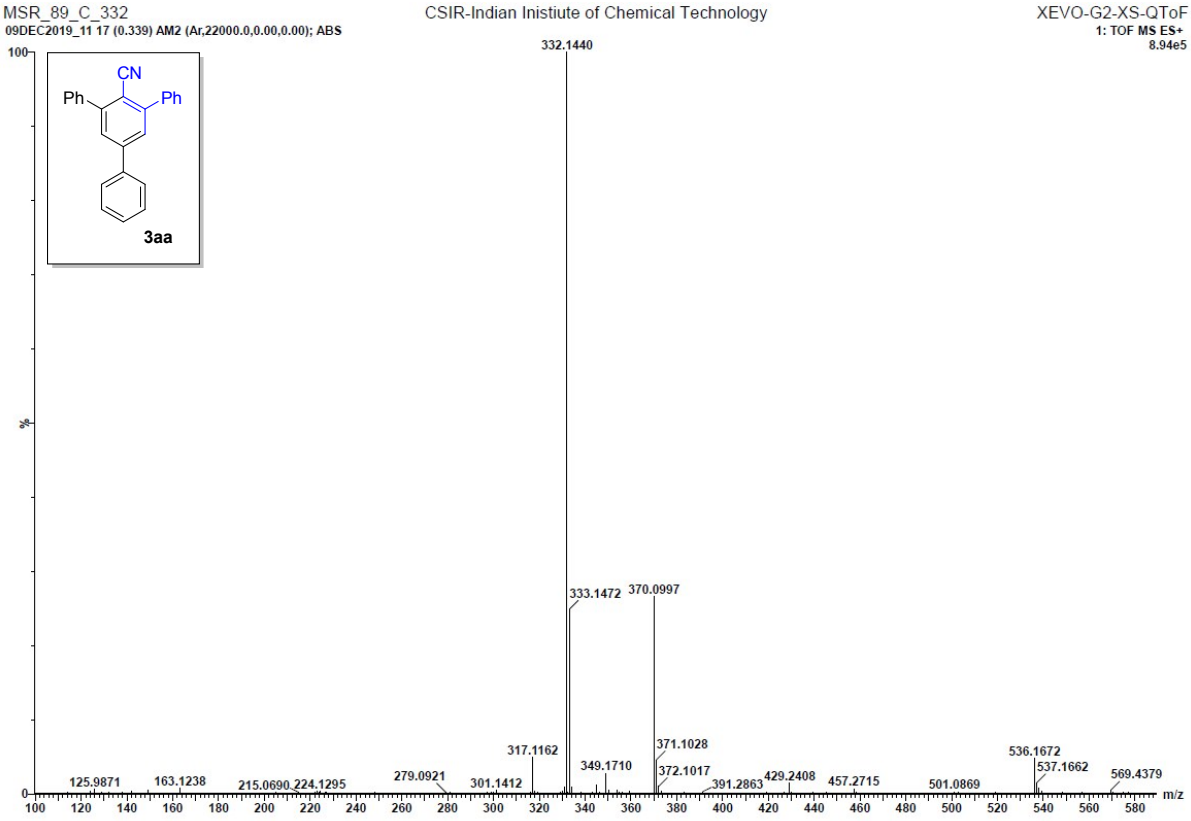

MANEESH-H0011
5.04
5.03
5.03
4.64
4.63
4.31
4.29
4.28
4.26
4.24
2.66
1.39
1.37
1.35
NC
O
O
CH3
Fe
2j
1.92
1.91
2.00
4.30
2.92
2.96

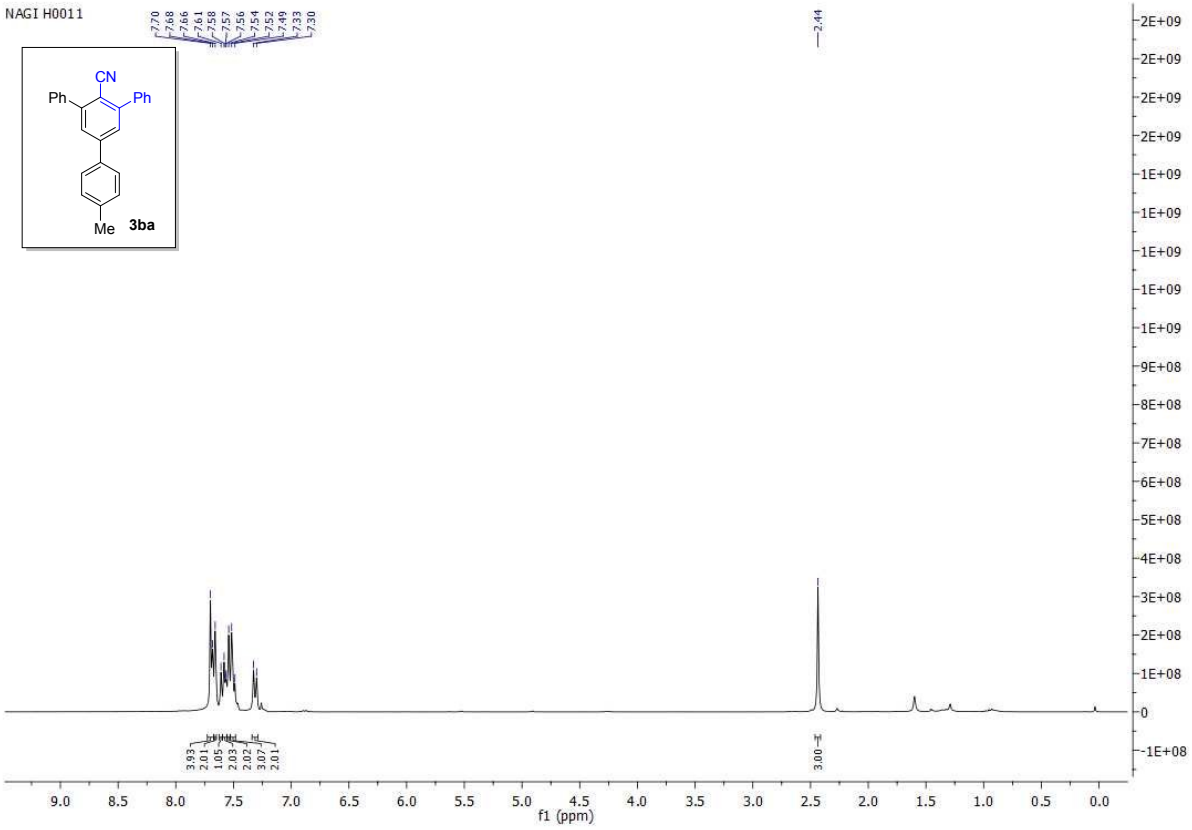

NAGIREDDY-H001
172.41
163.39
118.53
98.05
81.36
72.65
70.74
70.52
61.59
21.88
14.21
NC
O
O
CH3
Fe
2j
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10

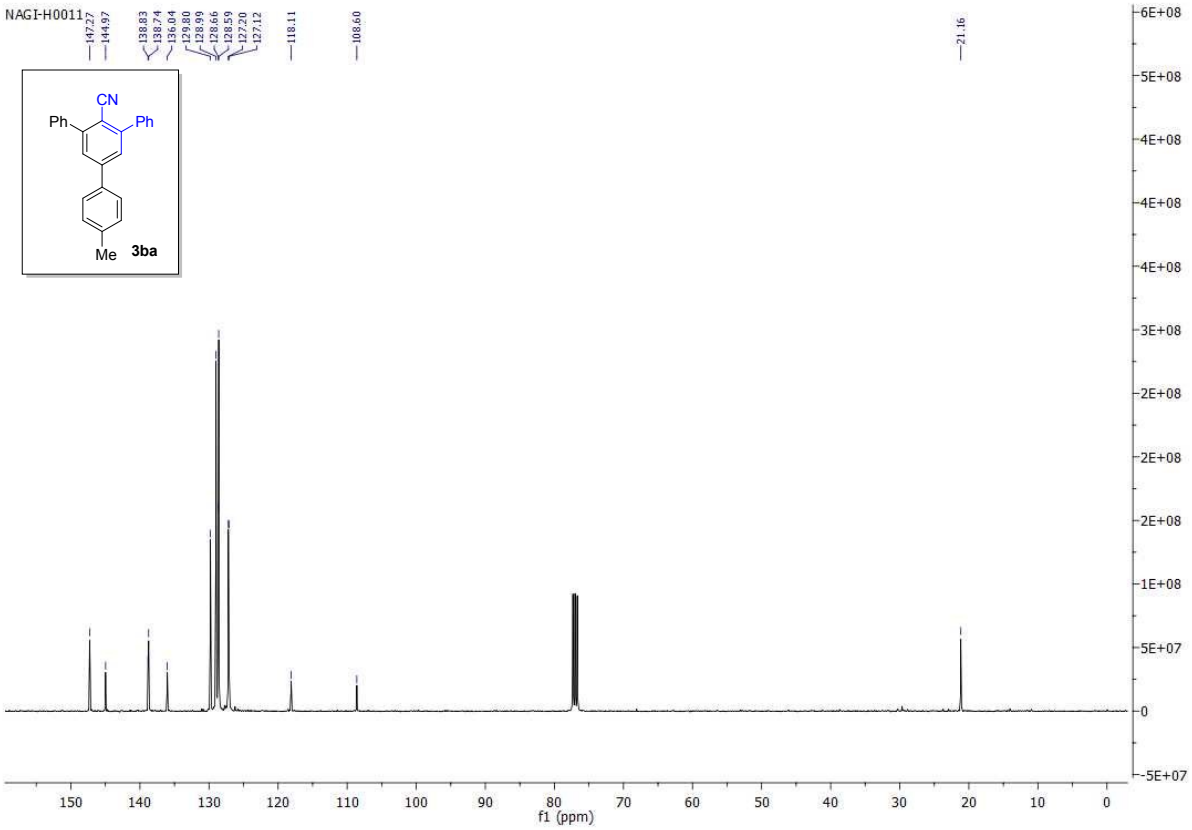

MSR_FE_324
CSIR-IICT
XEVO-G2-XS-QToF
17FEB2020_12 15 (0.293) AM2 (Ar,22000.0,0.00,0.00); ABS; Cm (10:16-(3:10+24:52))
1: TOF MS ES+
2.57e6
100
%
NC
O
O
CH3
Fe
2j
324.0677
325.0706
276.0311
299.0526
323.0609
346.0501
362.0240
149.0229
258.0215
278.0266
322.0727
371.1013
372.1008
429.0876
445.1199
463.1327
503.1069
78.0087
121.0255
186.0065
205.0867
223.0632
229.9903
0
60 80 100 120 140 160 180 200 220 240 260 280 300 320 340 360 380 400 420 440 460 480 500
m/z

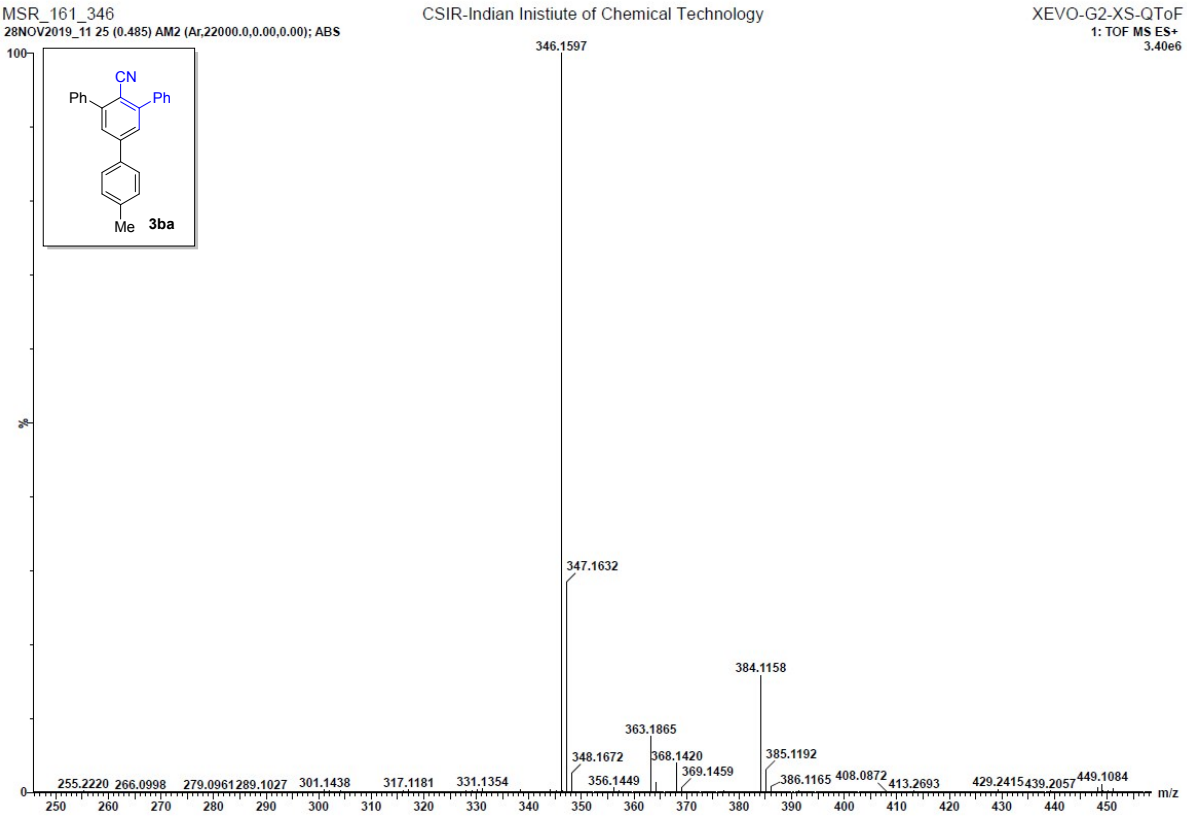

CN
Ph
Ph
3aa
f1 (ppm)

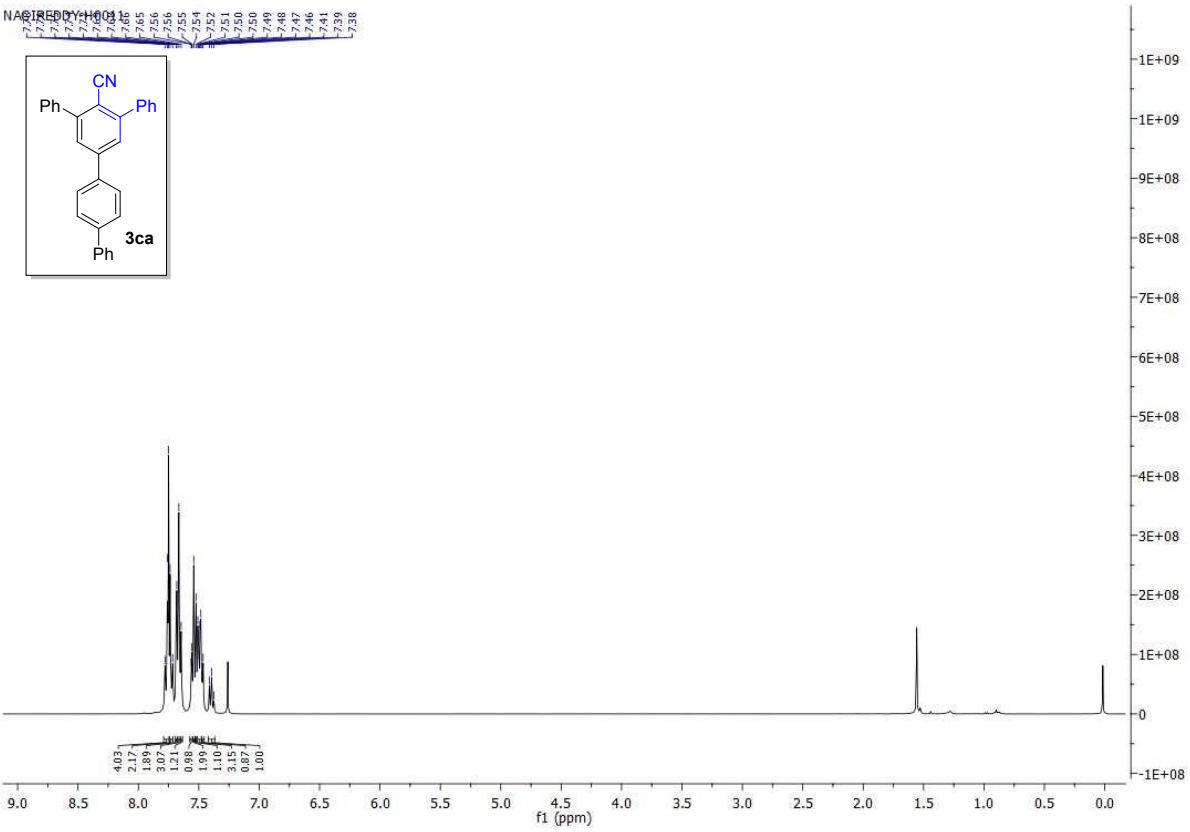

MANEESH-H0011
CN
Ph
Ph
3aa
f1 (ppm)

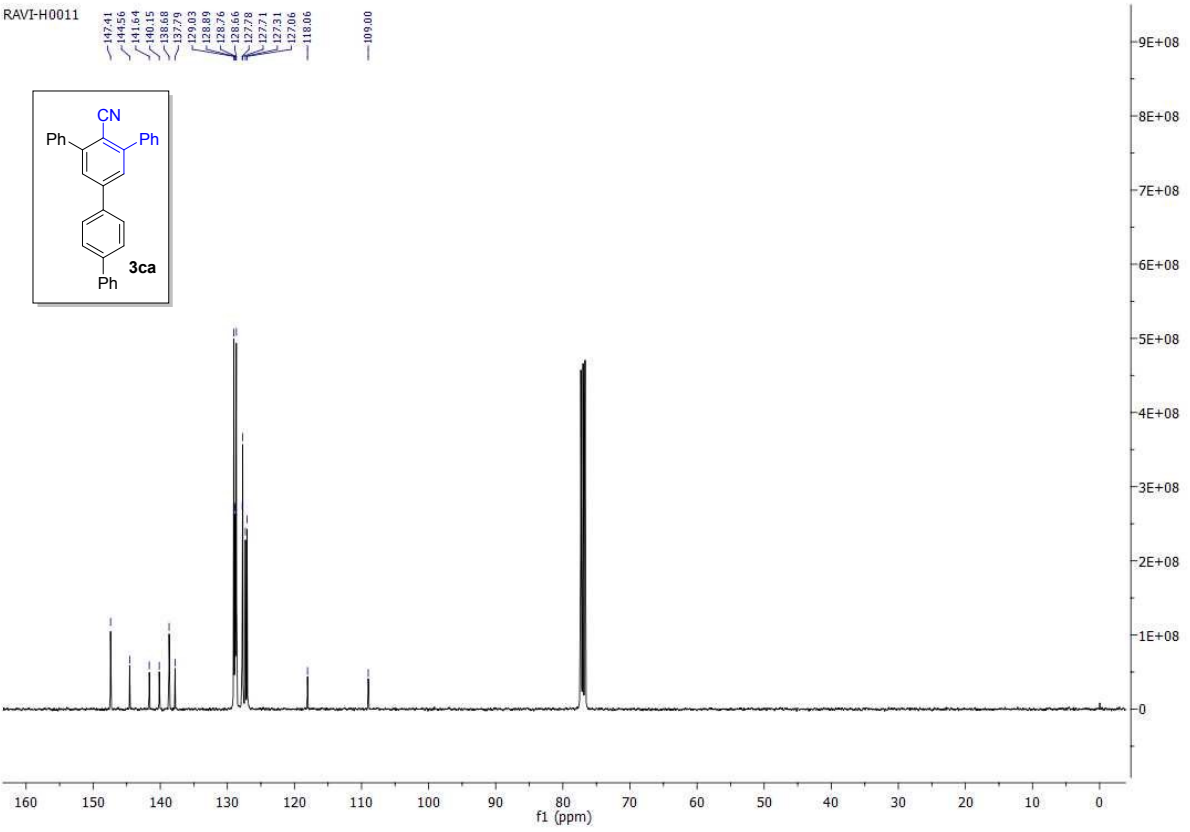

MSR_89_C_332
09DEC2019_11 17 (0.339) AM2 (Ar,22000.0,0.00,0.00); ABS
CSIR-Indian Inistiute of Chemical Technology
XEVO-G2-XS-QToF
1: TOF MS ES+
8.94e5
CN
Ph
Ph
3aa
332.1440
333.1472
370.0997
317.1162
371.1028
372.1017
349.1710
536.1672
537.1662
569.4379
125.9871
163.1238
215.0690
224.1295
279.0921
301.1412
391.2863
429.2408
457.2715
501.0869
%
m/z

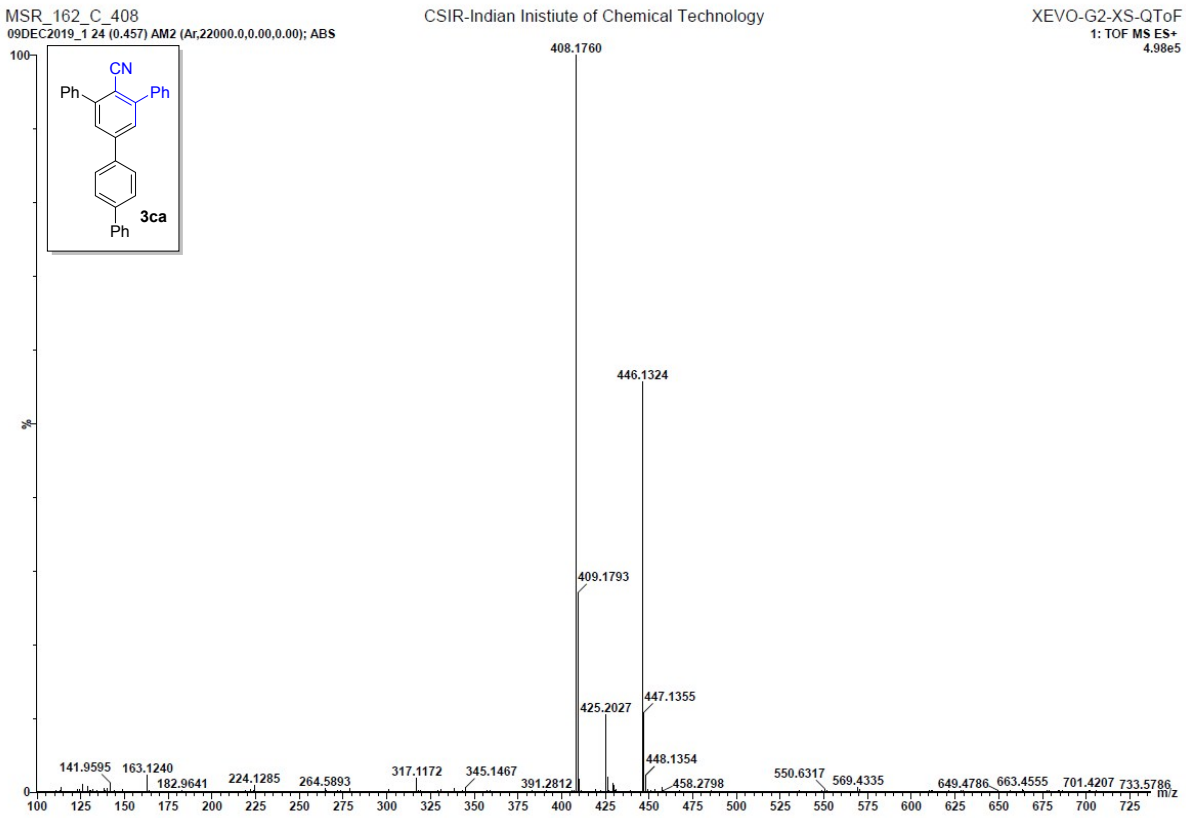

NAGI H0011
7.70
7.68
7.66
7.61
7.58
7.57
7.56
7.54
7.52
7.49
7.33
7.30
2.44
CN
Ph
Ph
Me
3ba
3.93
2.01
1.05
2.03
2.02
3.07
2.01
3.00
f1 (ppm)

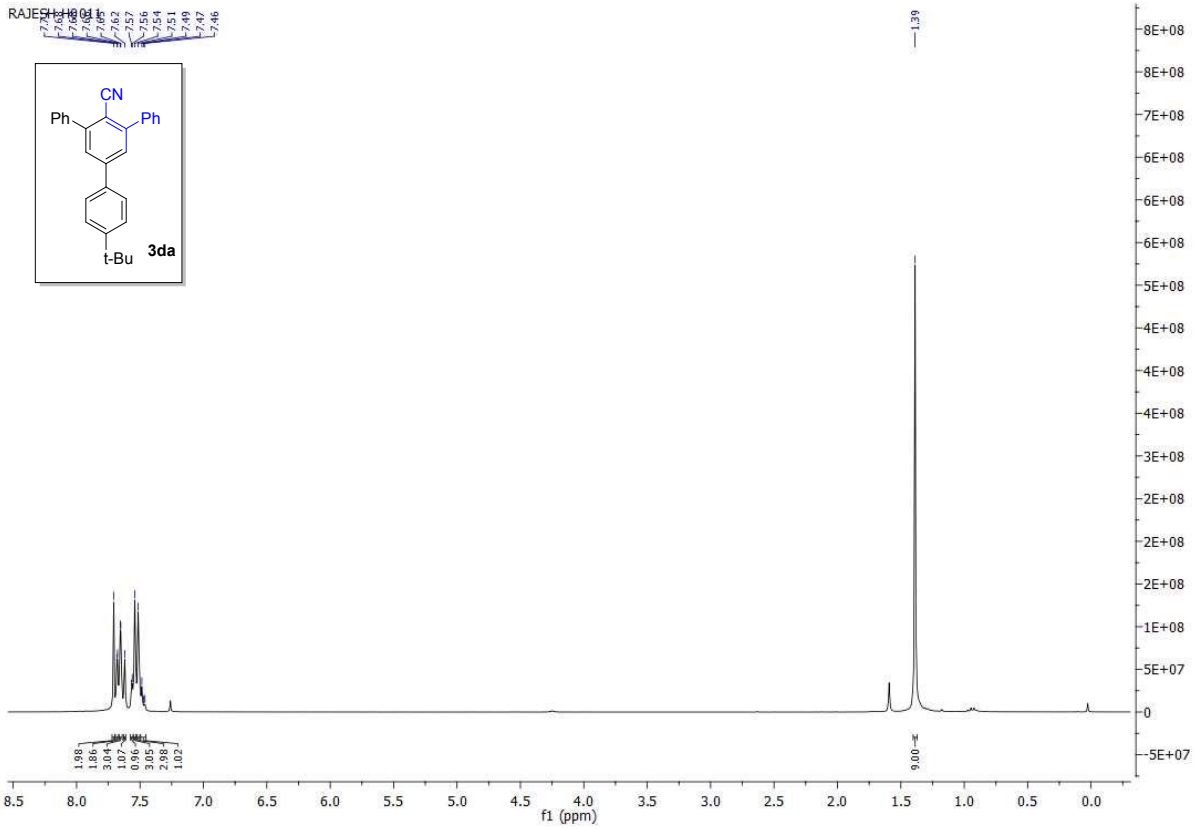

NAGI-H0011
147.27
144.97
138.83
138.74
136.04
129.80
128.99
128.66
128.59
127.20
127.12
118.11
108.60
21.16
CN
Ph
Ph
Me
3ba
f1 (ppm)

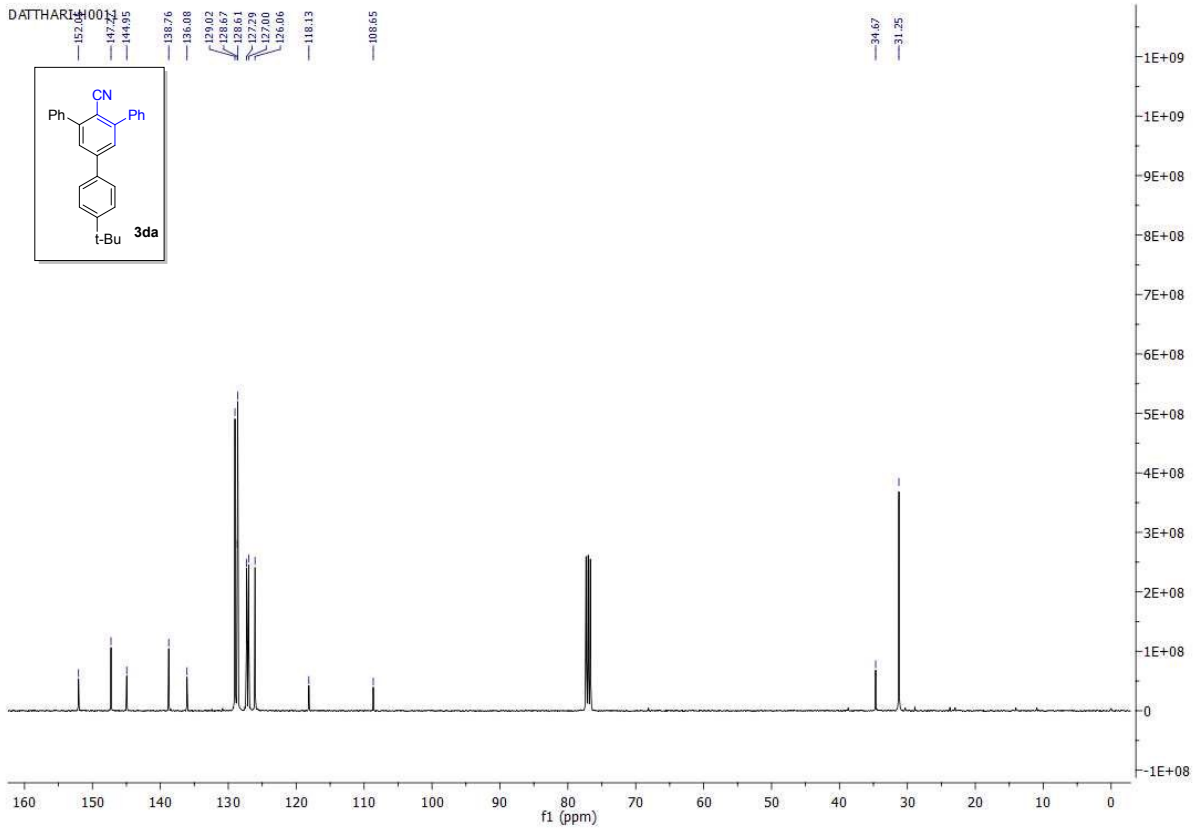

MSR_161_346
CSIR-Indian Inistiute of Chemical Technology
XEVO-G2-XS-QToF
28NOV2019_11 25 (0.485) AM2 (Ar,22000.0,0.00,0.00); ABS
1: TOF MS ES+
3.40e6
CN
Ph
Ph
Me
3ba
346.1597
347.1632
384.1158
363.1865
348.1672
368.1420
385.1192
356.1449
369.1459
386.1165
408.0872
413.2693
429.2415
439.2057
449.1084
255.2220
266.0998
279.0961
289.1027
301.1438
317.1181
331.1354
%
m/z

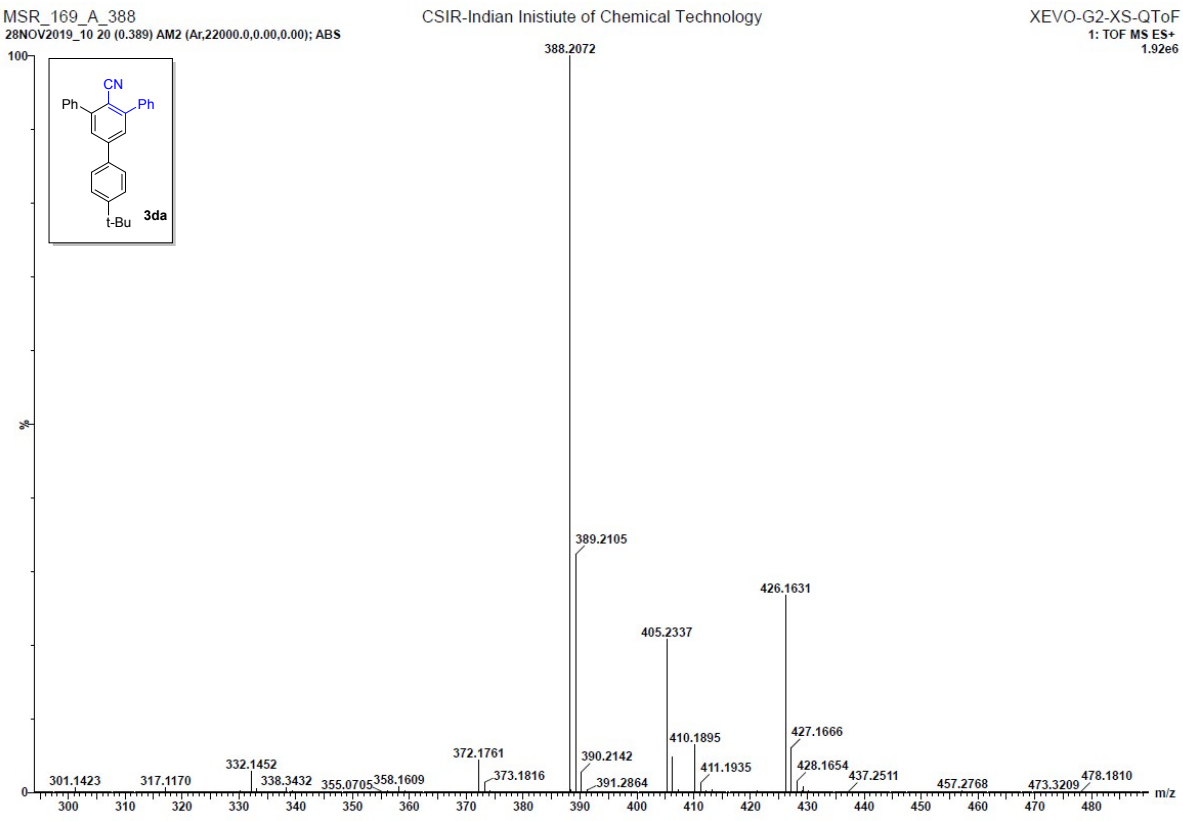

NAGIREDDY-H0011
CN
Ph
Ph
3ca
Ph
4.03
2.17
1.89
3.07
1.21
0.98
1.99
1.10
3.15
0.87
1.00
f1 (ppm)

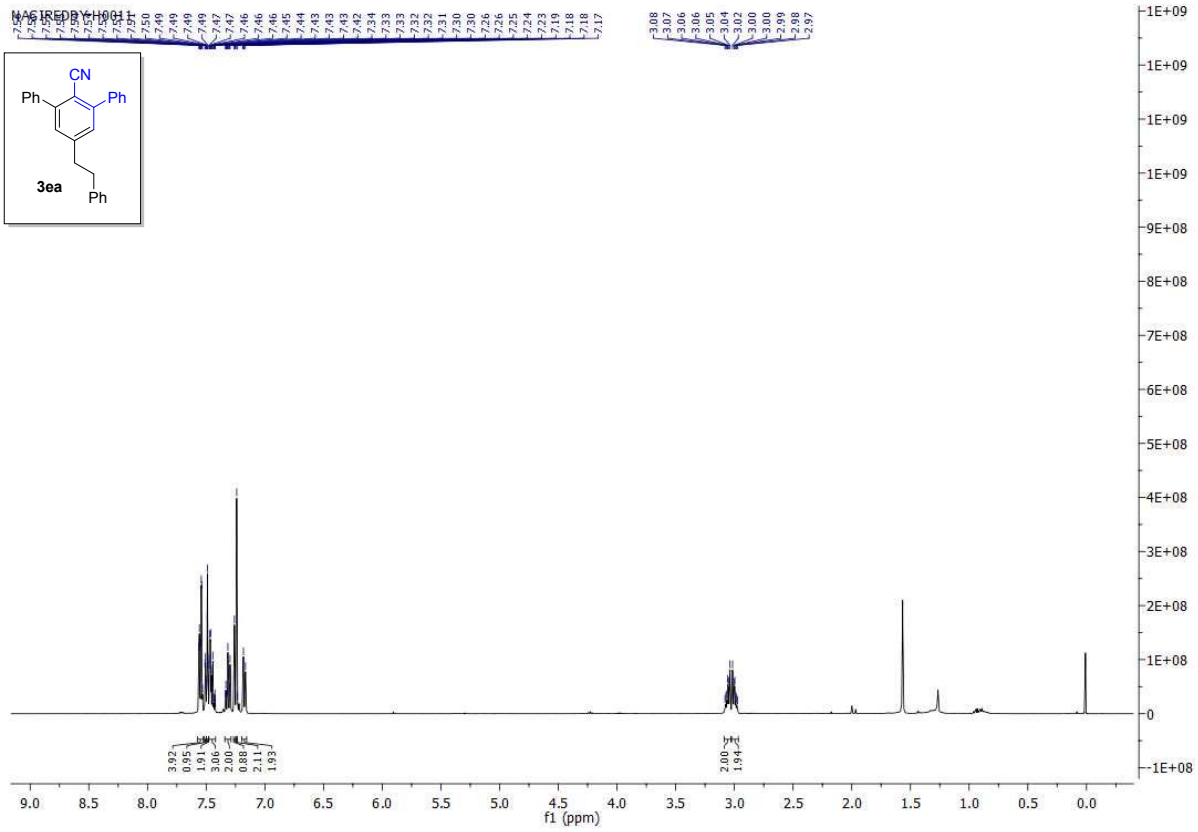

RAVI-H0011
147.41
144.56
141.64
140.15
138.68
132.79
129.03
128.89
128.76
128.66
127.78
127.71
127.31
127.06
118.06
109.00
CN
Ph
Ph
3ca
Ph
f1 (ppm)

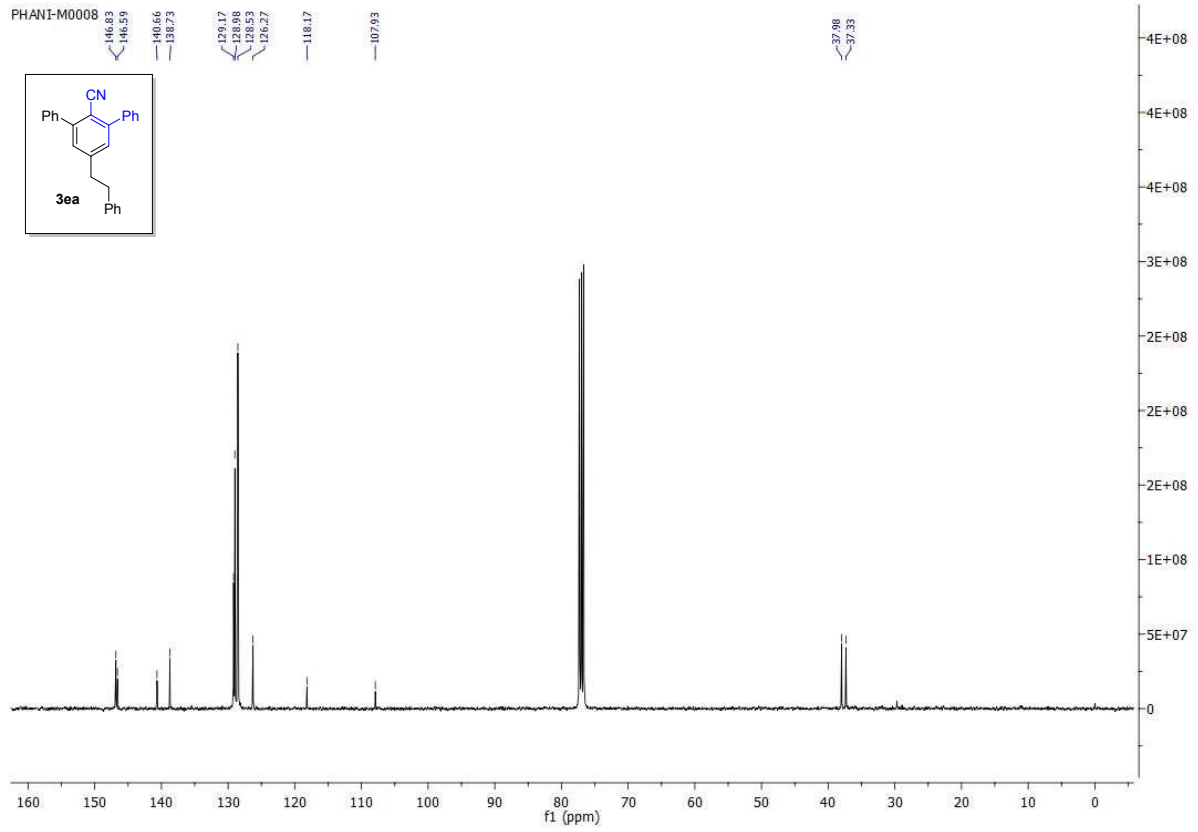

MSR_162_C_408
CSIR-Indian Inistiute of Chemical Technology
XEVO-G2-XS-QToF
09DEC2019_1 24 (0.457) AM2 (Ar,22000.0,0.00,0.00); ABS
1: TOF MS ES+
4.98e5
CN
Ph
Ph
Ph
3ca
408.1760
446.1324
409.1793
425.2027
447.1355
448.1354
141.9595
163.1240
182.9641
224.1285
264.5893
317.1172
345.1467
391.2812
458.2798
550.6317
569.4335
649.4786
663.4555
701.4207
733.5786
%
m/z

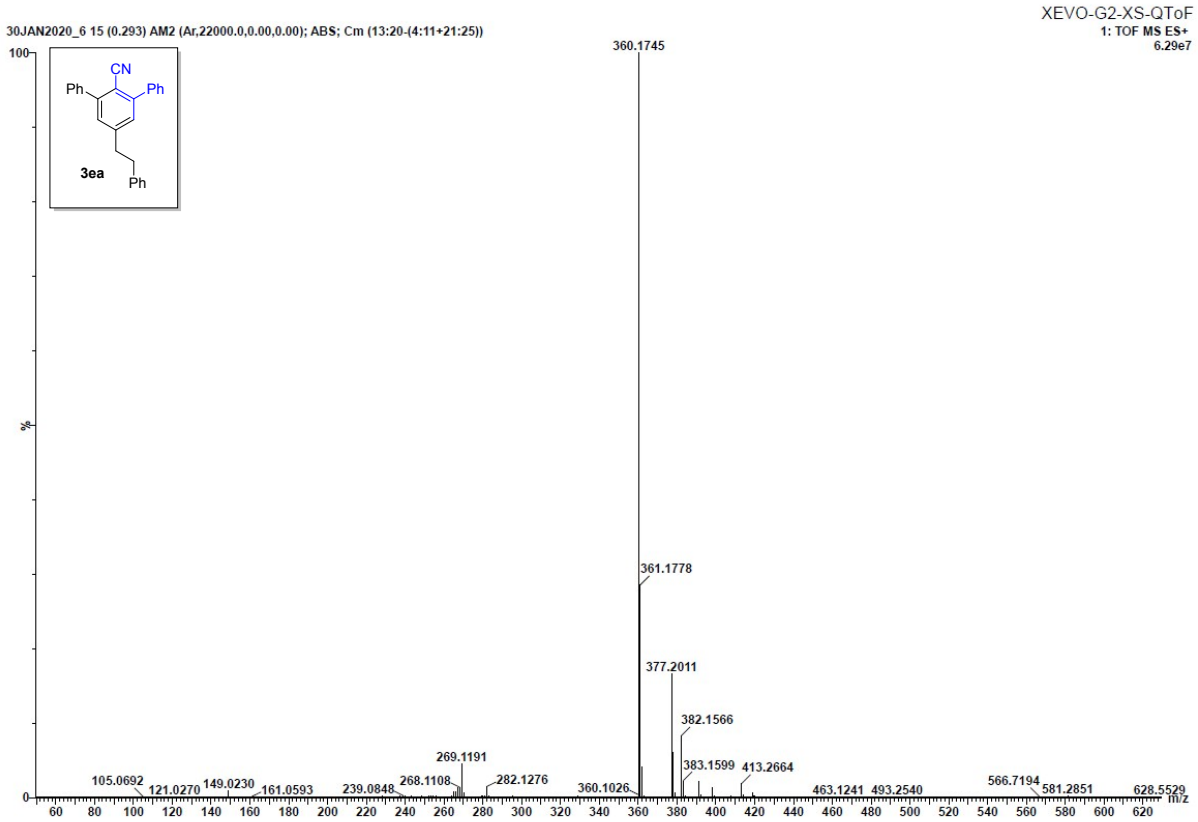

CN
Ph
Ph
t-Bu
3da
1.39
9.00
f1 (ppm)

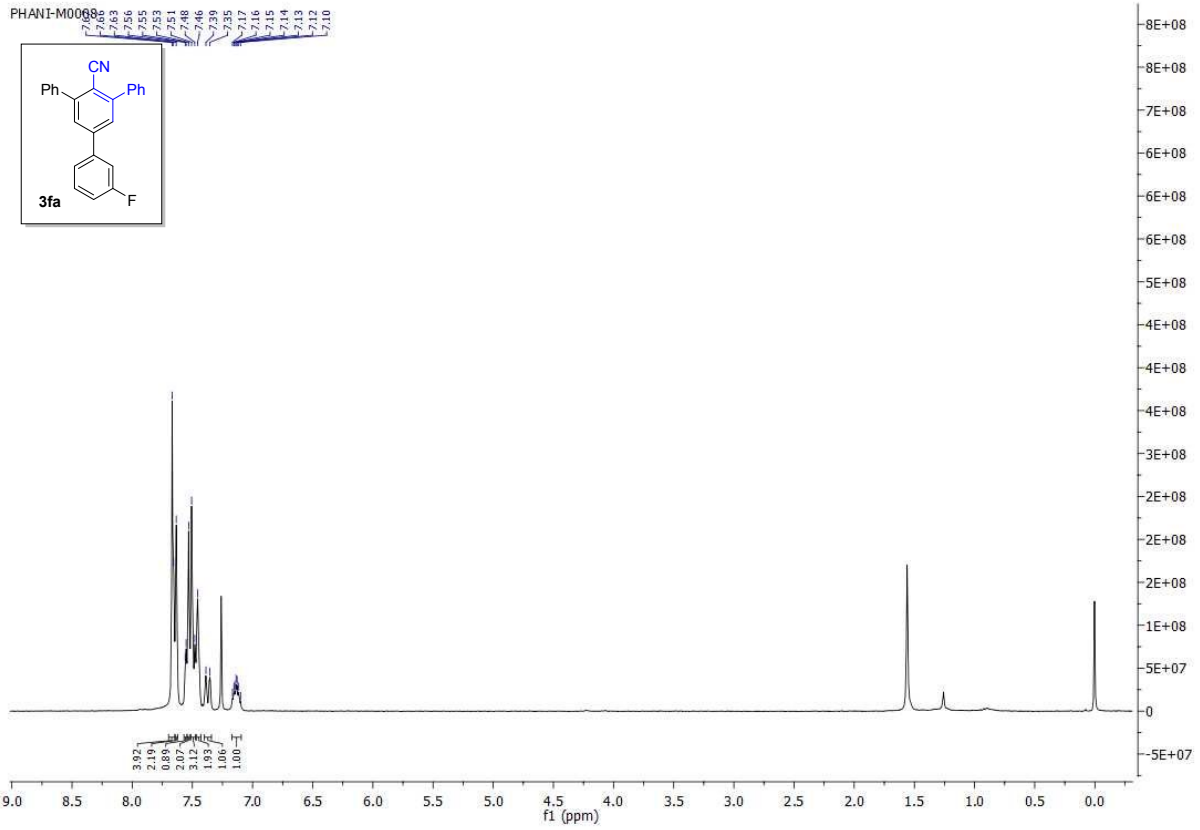

CN
Ph
Ph
t-Bu
3da
152.04
147.21
144.95
138.76
136.08
129.02
128.67
128.61
127.29
127.00
126.06
118.13
108.65
34.67
31.25
f1 (ppm)

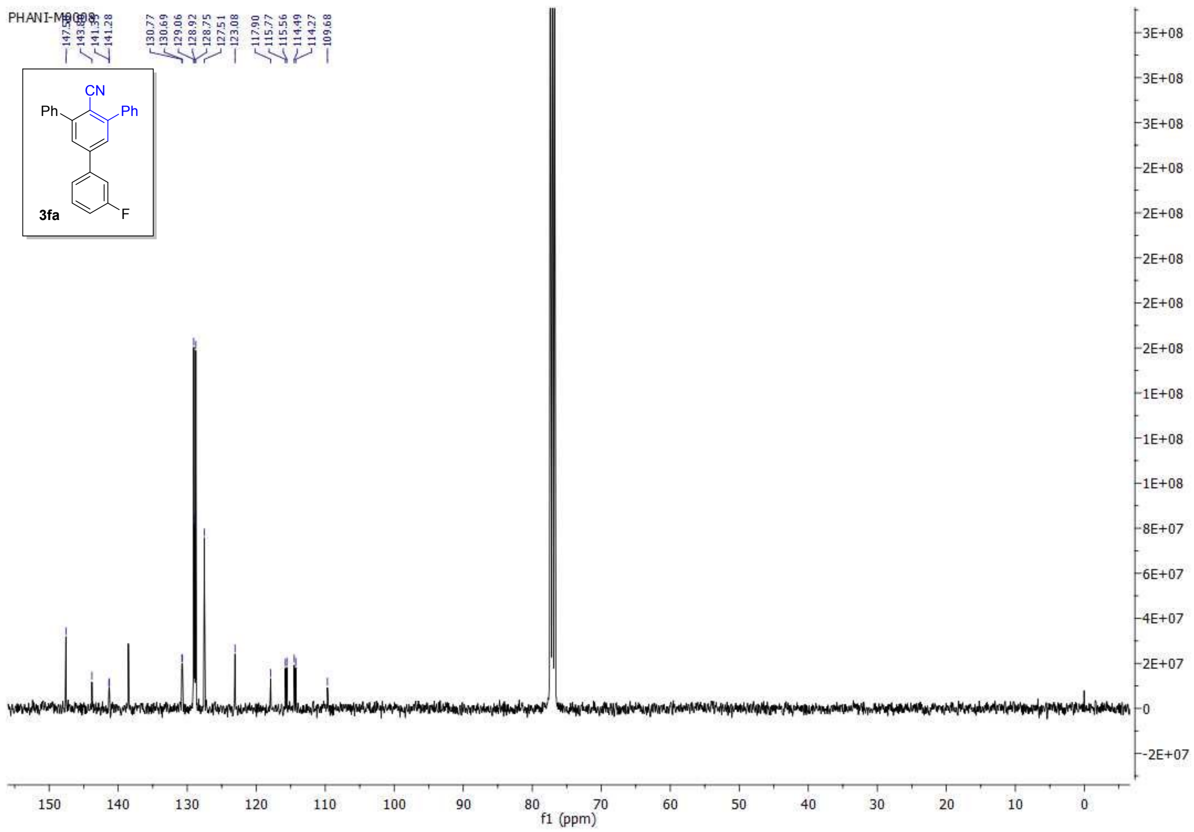

MSR_169_A_388
28NOV2019_10 20 (0.389) AM2 (Ar,22000.0,0.00,0.00); ABS
CSIR-Indian Inistiute of Chemical Technology
XEVO-G2-XS-QToF
1: TOF MS ES+
1.92e6
CN
Ph
Ph
t-Bu
3da
%
m/z
388.2072
389.2105
426.1631
405.2337
410.1895
427.1666
372.1761
390.2142
332.1452
373.1816
411.1935
428.1654
301.1423
317.1170
338.3432
355.0705
358.1609
391.2864
437.2511
457.2768
473.3209
478.1810

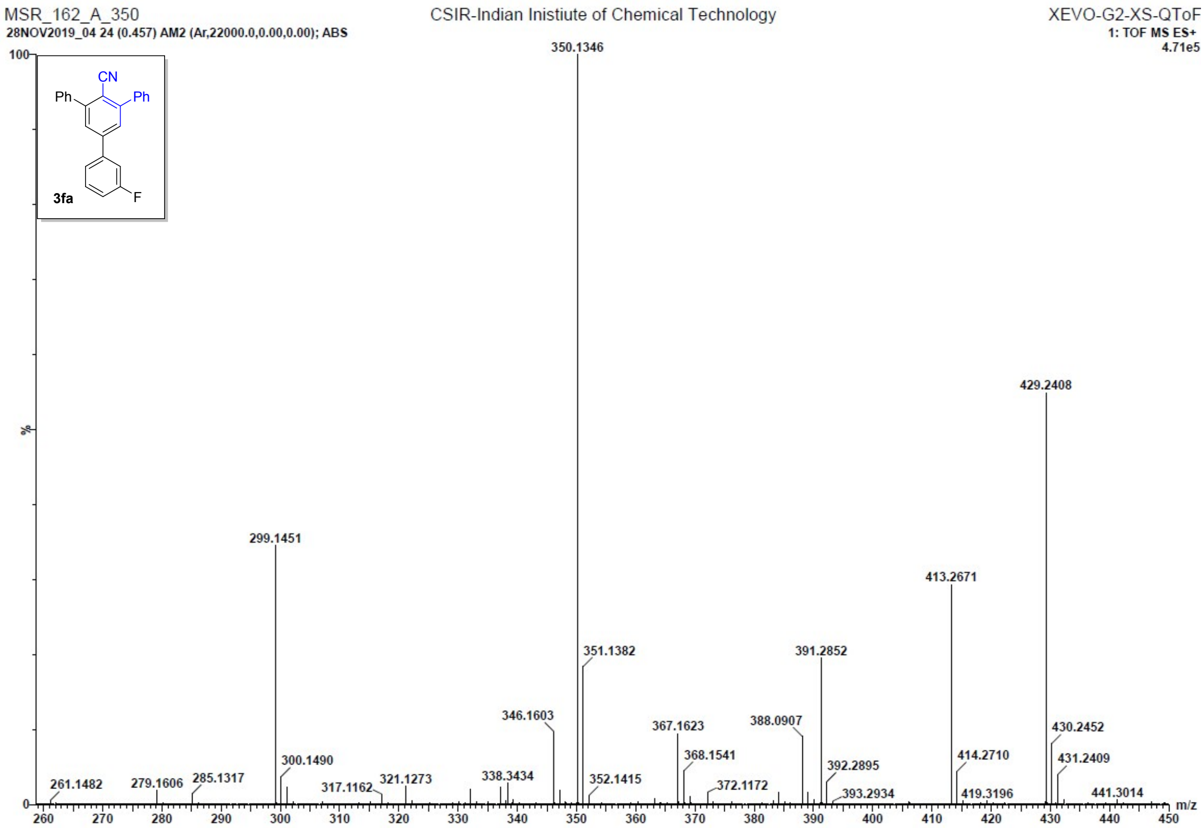

CN
Ph
Ph
3ea
Ph
f1 (ppm)

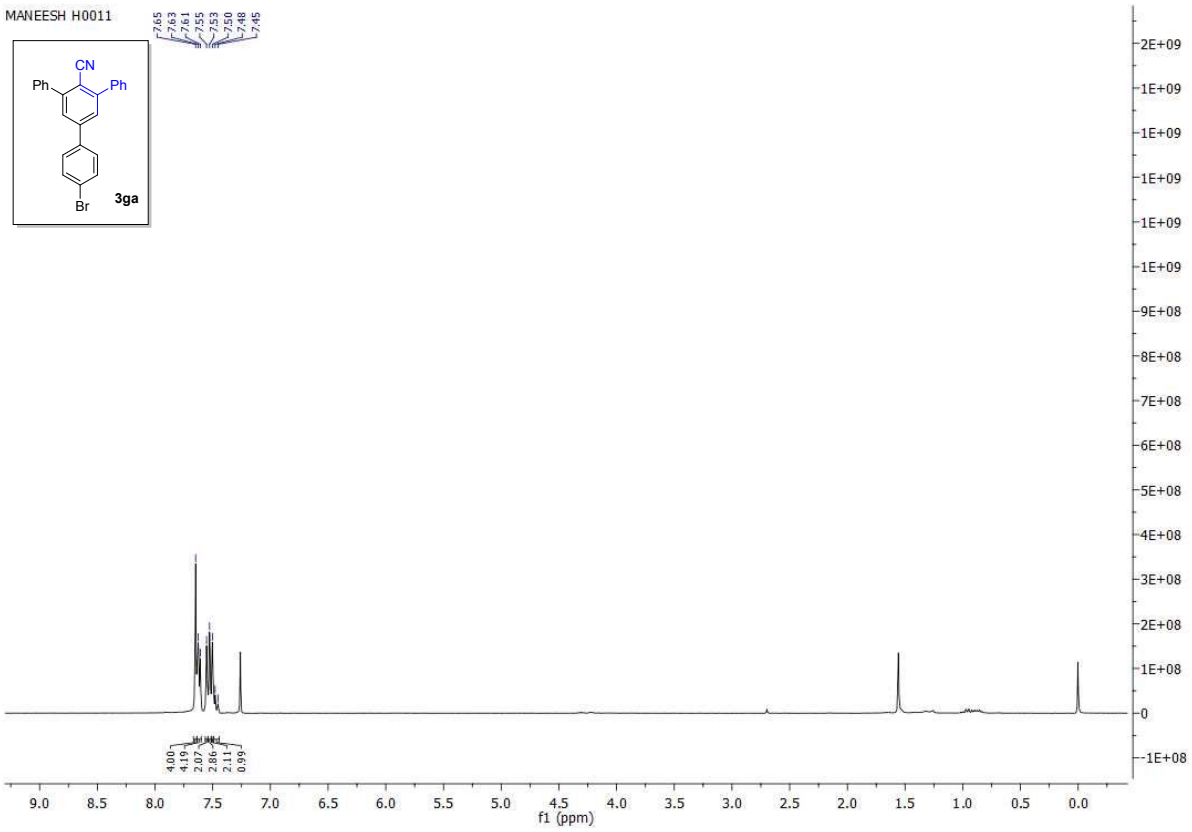

PHANI-M0008
CN
Ph
Ph
3ea
Ph
f1 (ppm)

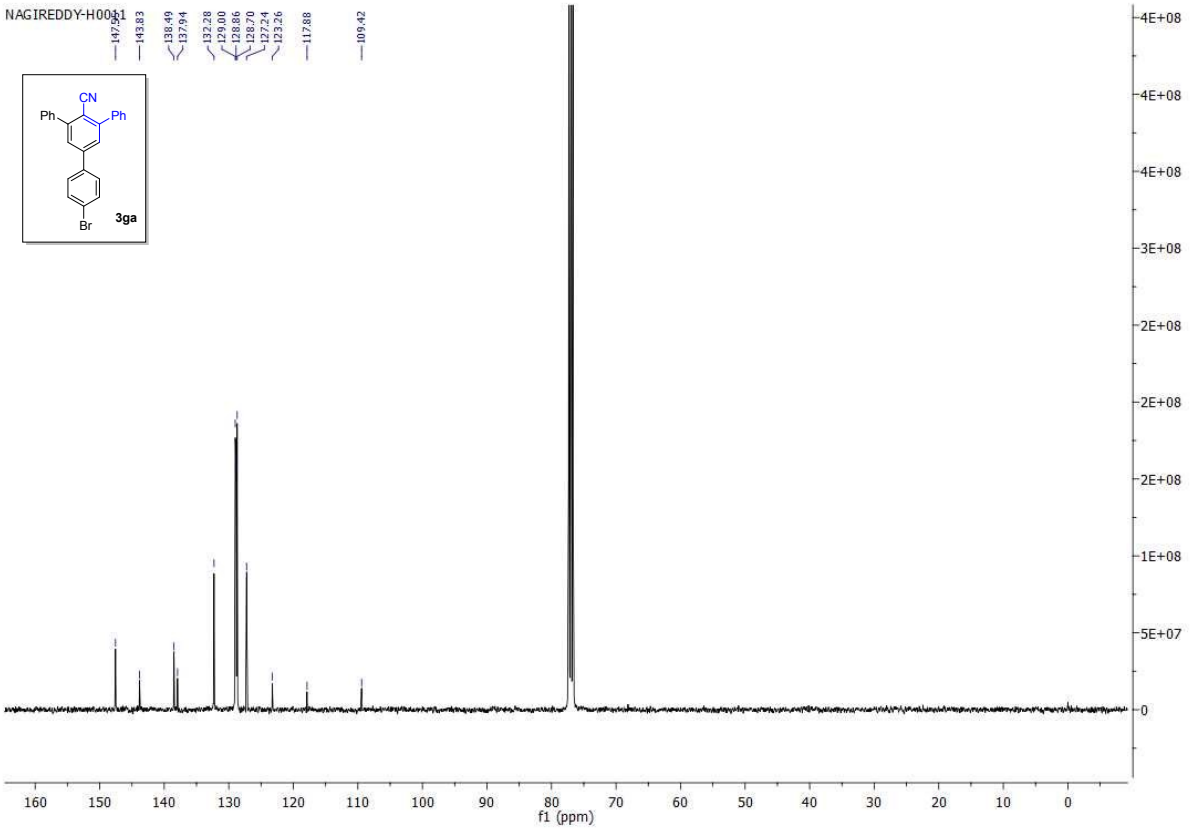

XEVO-G2-XS-QToF
1: TOF MS ES+
6.29e7
30JAN2020_6 15 (0.293) AM2 (Ar,22000.0,0.00,0.00); ABS; Cm (13:20-(4:11+21:25))
3ea
360.1745
361.1778
377.2011
382.1566
269.1191
383.1599
413.2664
105.0692
121.0270
149.0230
161.0593
239.0848
268.1108
282.1276
360.1026
463.1241
493.2540
566.7194
581.2851
628.5529
m/z

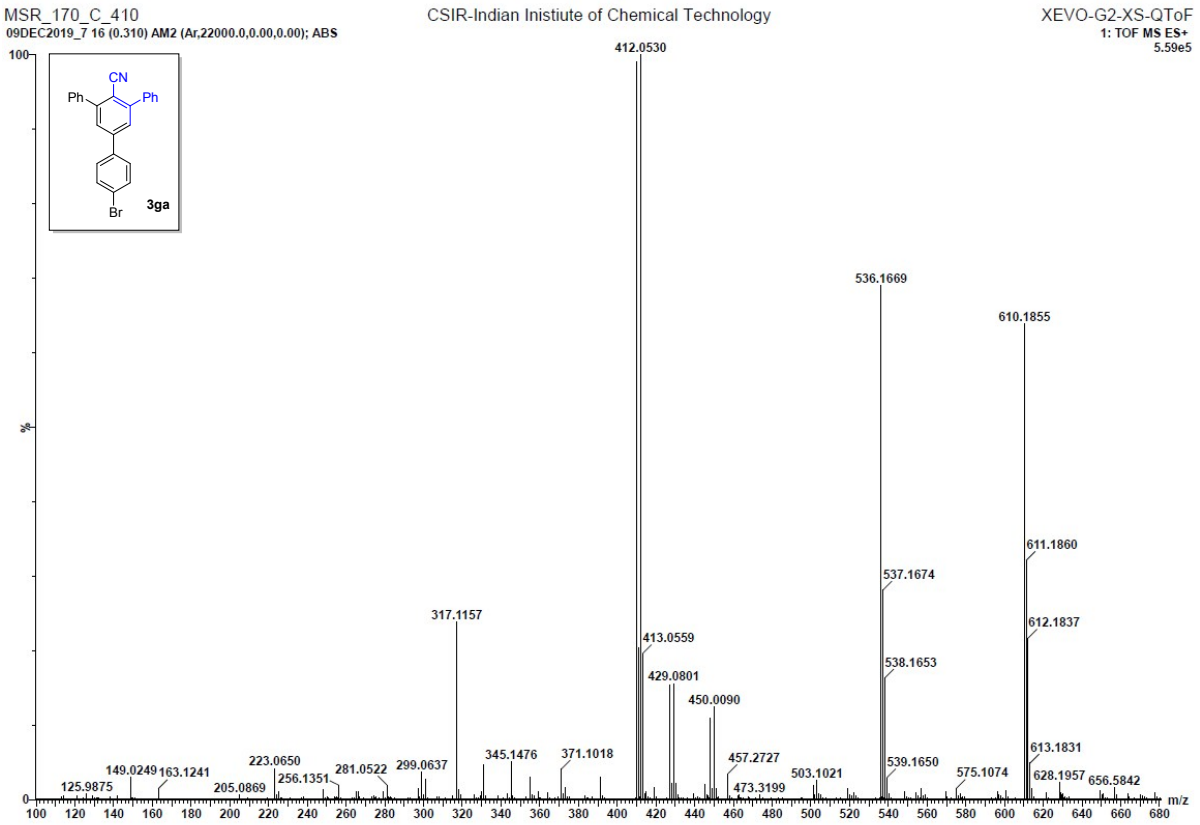

PHANI-M0008
3fa
f1 (ppm)

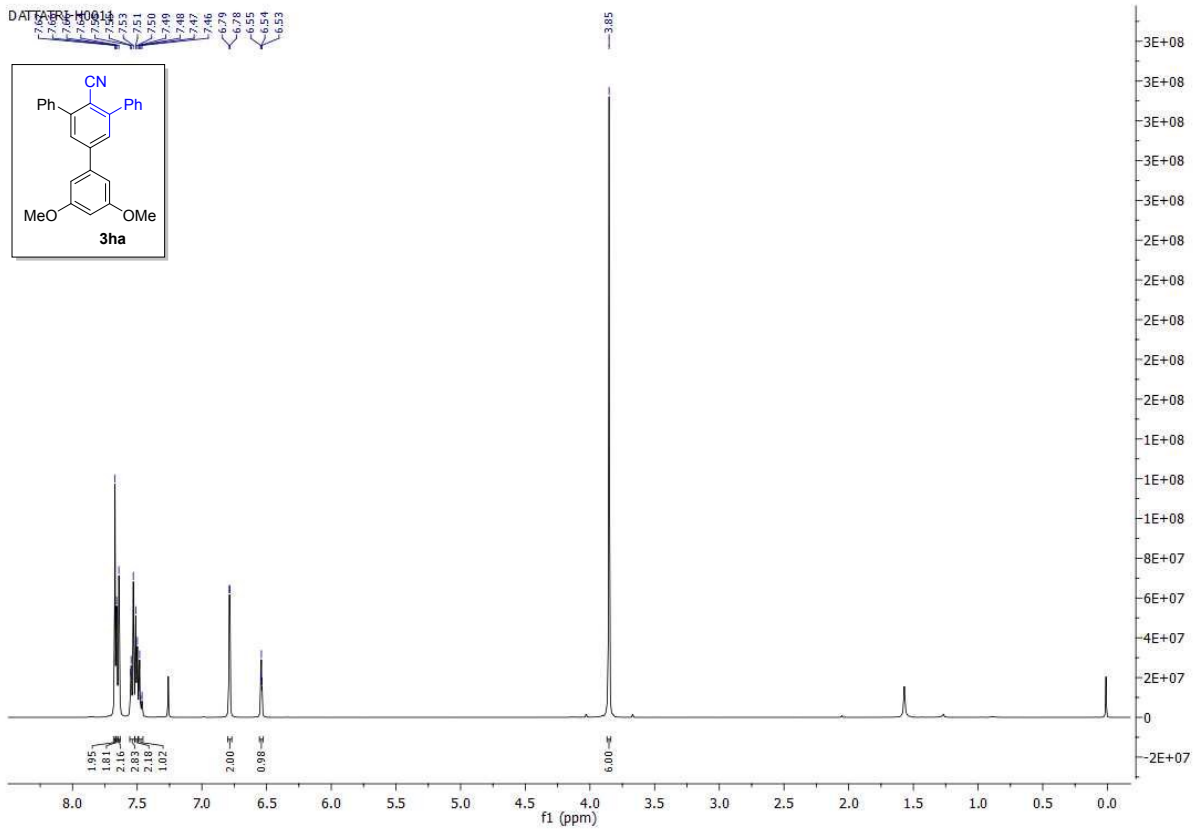

PHANI-M9008
147.58
143.88
141.39
141.28
130.77
130.69
129.06
128.92
128.75
127.51
123.08
117.90
115.77
115.56
114.49
114.27
109.68
CN
Ph
Ph
F
3fa
f1 (ppm)

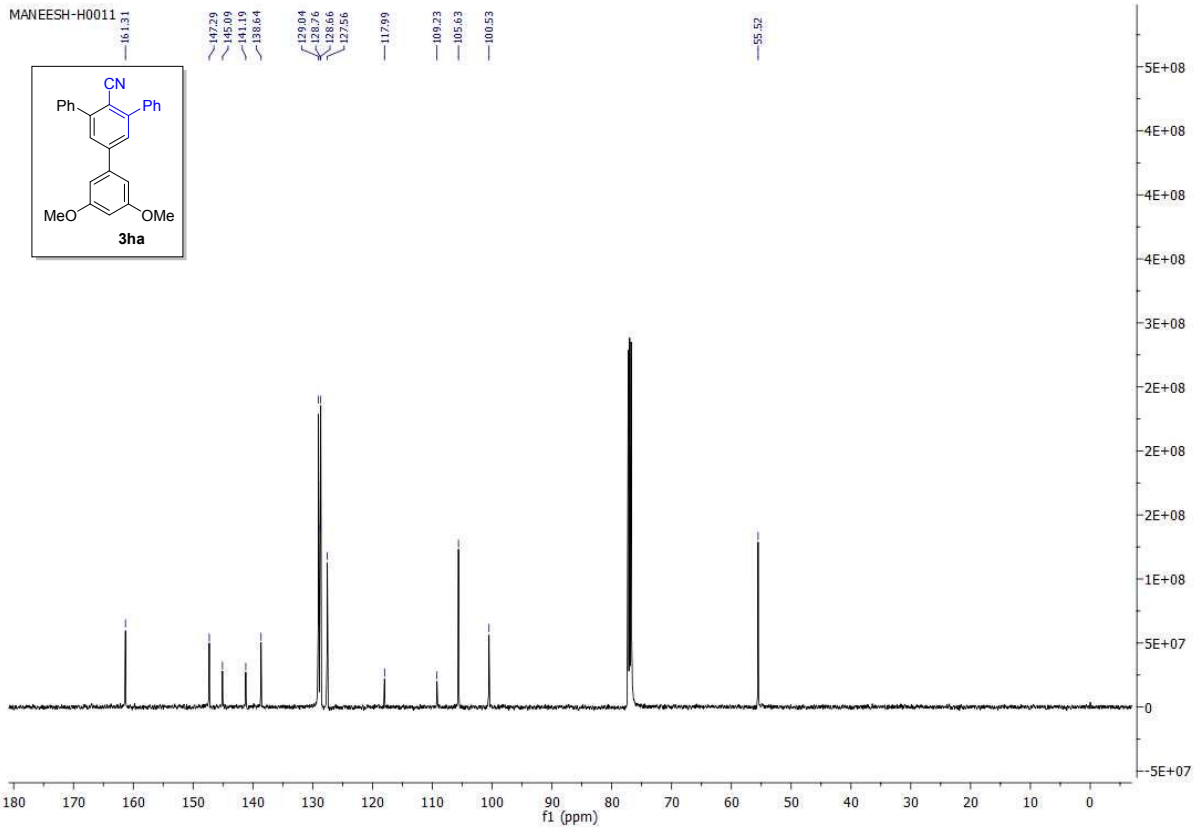

MSR_162_A_350
28NOV2019_04 24 (0.457) AM2 (Ar,22000.0,0.00,0.00); ABS
CSIR-Indian Inistiute of Chemical Technology
XEVO-G2-XS-QToF
1: TOF MS ES+
4.71e5
350.1346
429.2408
299.1451
413.2671
351.1382
391.2852
346.1603
367.1623
388.0907
430.2452
368.1541
300.1490
392.2895
414.2710
431.2409
261.1482
279.1606
285.1317
317.1162
321.1273
338.3434
352.1415
372.1172
393.2934
419.3196
441.3014
CN
Ph
Ph
F
3fa
m/z

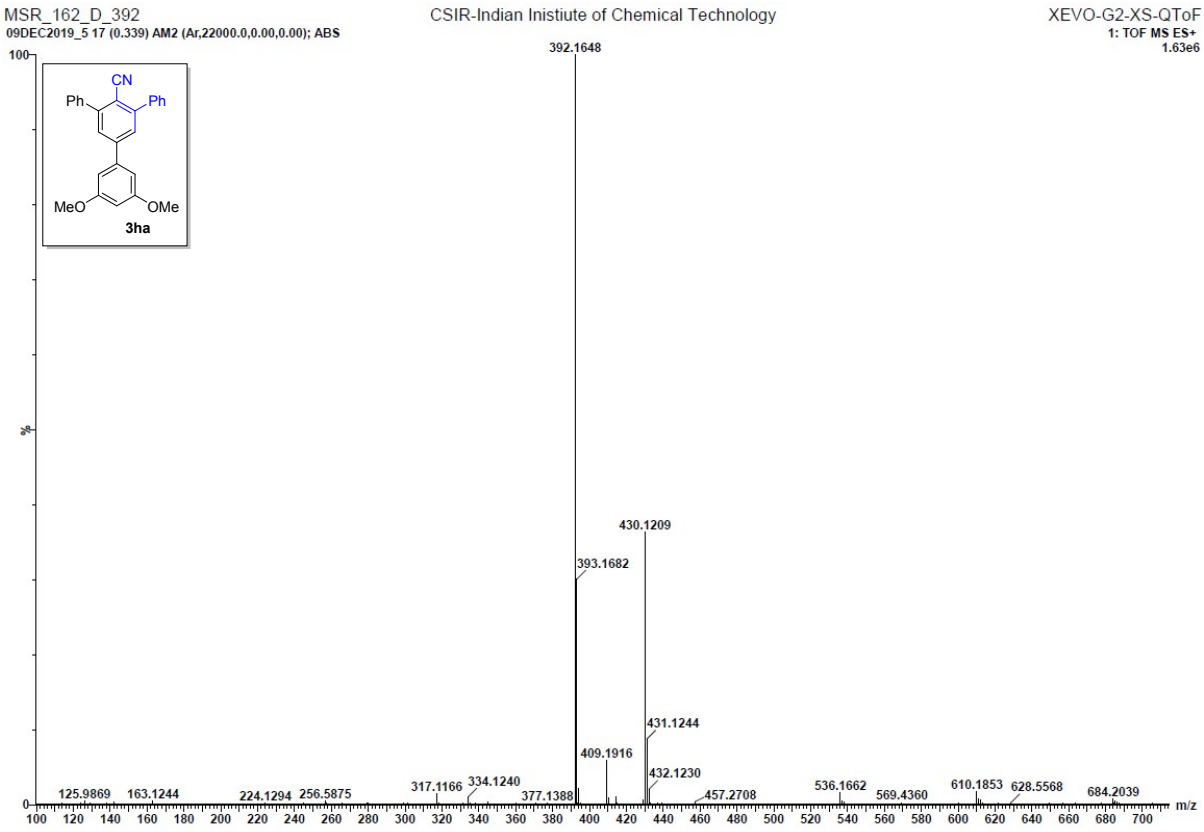

MANEESH H0011
7.65
7.63
7.61
7.55
7.53
7.50
7.48
7.45
CN
Ph
Ph
Br
3ga
4.00
4.19
2.07
2.86
2.11
0.99
f1 (ppm)

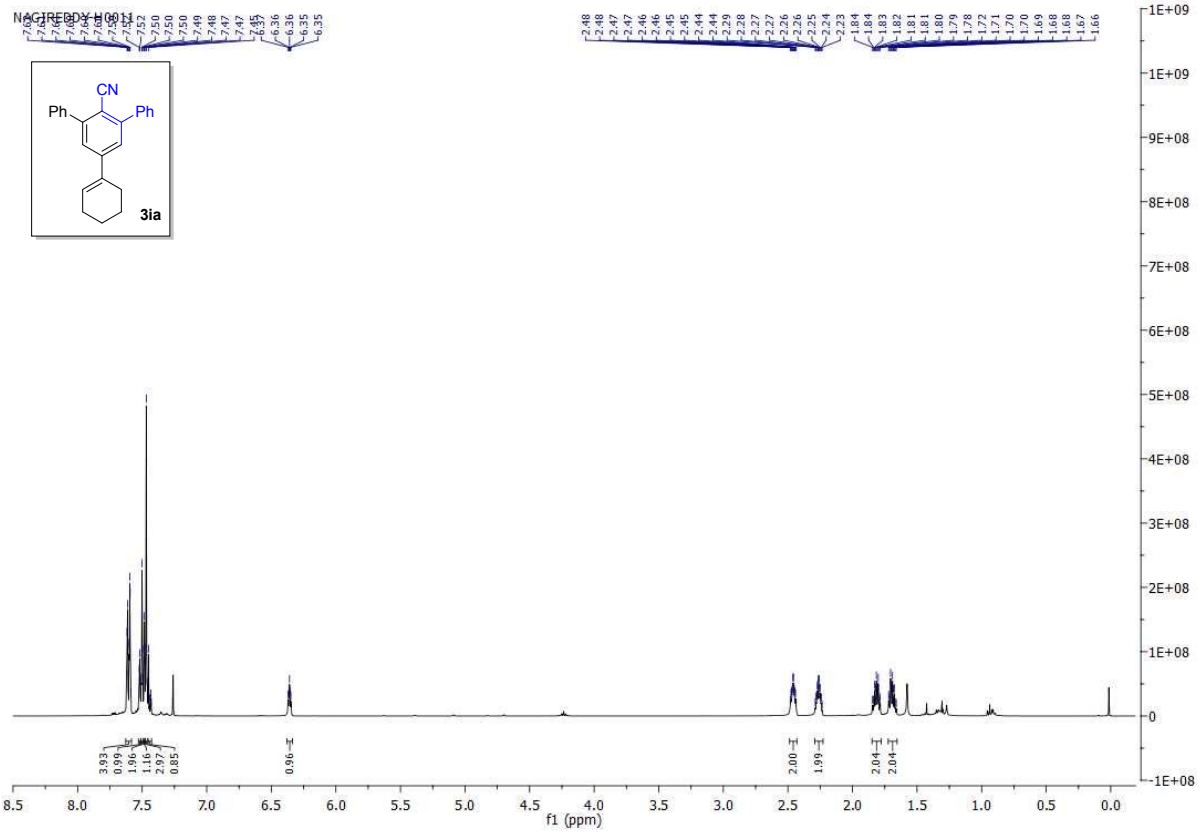

NAGIREDDY-H0011
147.51
143.83
138.49
137.94
132.28
129.60
128.86
128.70
127.24
123.26
117.88
109.42
CN
Ph
Ph
Br
3ga
f1 (ppm)


MSR_170_C_410
09DEC2019_7 16 (0.310) AM2 (Ar,22000.0,0.00,0.00); ABS
CSIR-Indian Inistiute of Chemical Technology
XEVO-G2-XS-QToF
1: TOF MS ES+
5.59e5
CN
Ph
Ph
Br
3ga
%
m/z
412.0530
536.1669
610.1855
611.1860
537.1674
612.1837
317.1157
413.0559
538.1653
429.0801
450.0090
613.1831
539.1650
345.1476
371.1018
457.2727
503.1021
575.1074
628.1957
656.5842
223.0650
281.0522
299.0637
149.0249
163.1241
256.1351
205.0869
125.9875
473.3199

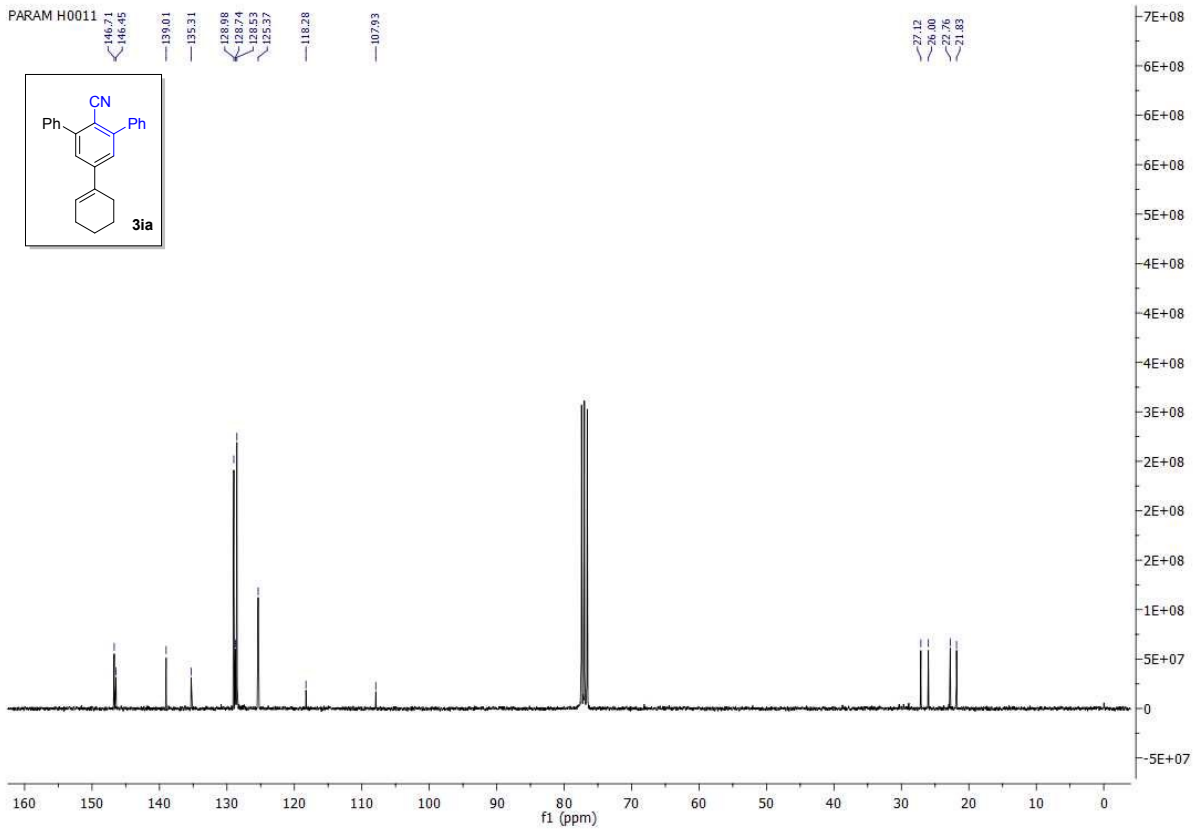

DATTATRI-H0014
CN
Ph
Ph
MeO
OMe
3ha
3.85
f1 (ppm)

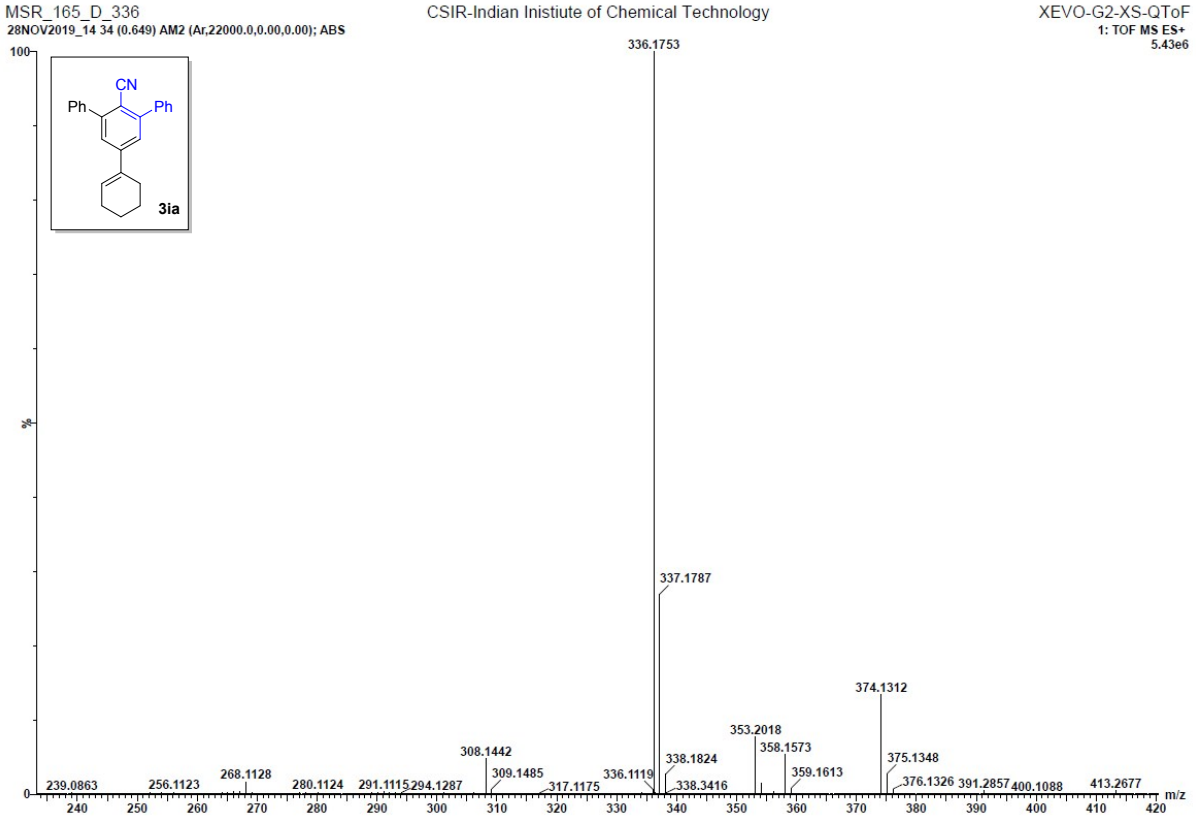

MANEESH-H0011
CN
Ph
Ph
MeO
OMe
3ha
161.31
147.29
145.09
141.19
138.64
129.04
128.76
128.66
127.56
117.99
109.23
105.63
100.53
55.52
f1 (ppm)

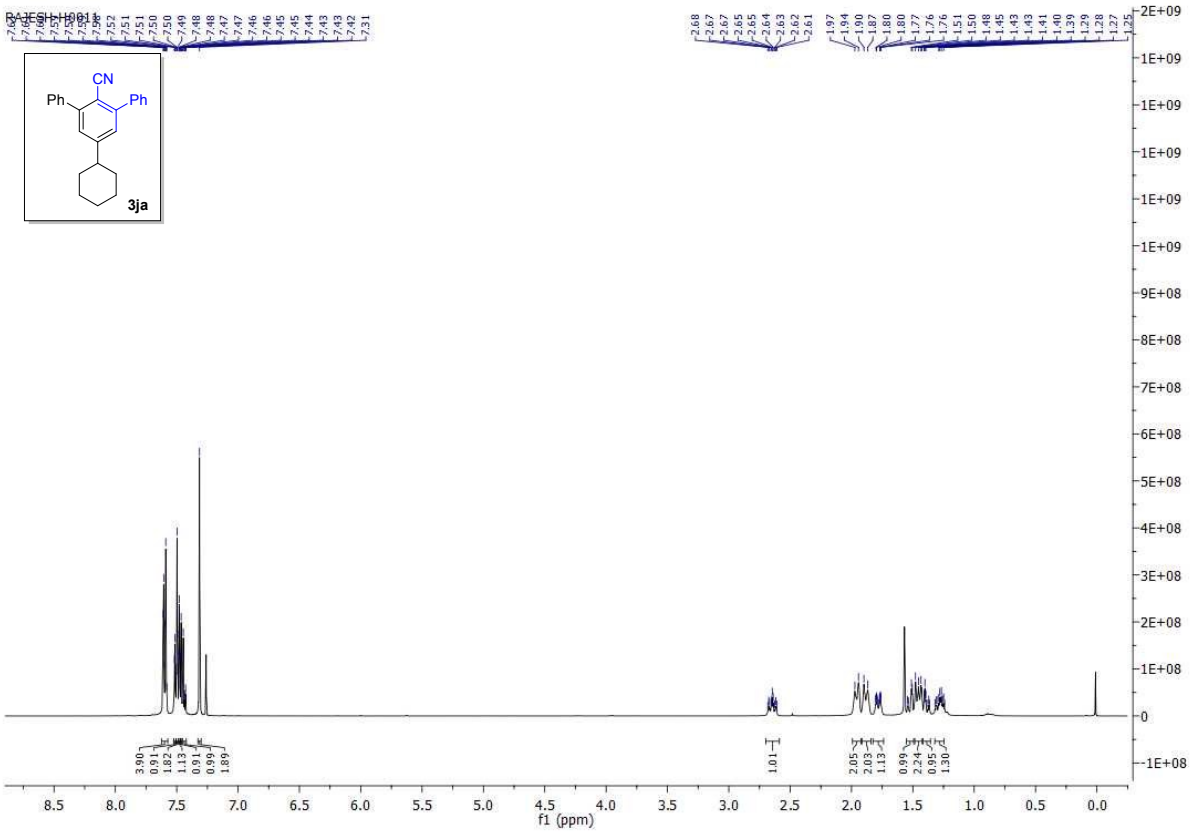

MSR_162_D_392
CSIR-Indian Institute of Chemical Technology
XEVO-G2-XS-QToF
09DEC2019_5 17 (0.339) AM2 (Ar,22000.0,0.00,0.00); ABS
1: TOF MS ES+
1.63e6
CN
Ph
Ph
MeO
OMe
3ha
392.1648
430.1209
393.1682
431.1244
409.1916
432.1230
125.9869
163.1244
224.1294
256.5875
317.1166
334.1240
377.1388
457.2708
536.1662
569.4360
610.1853
628.5568
684.2039
%
m/z

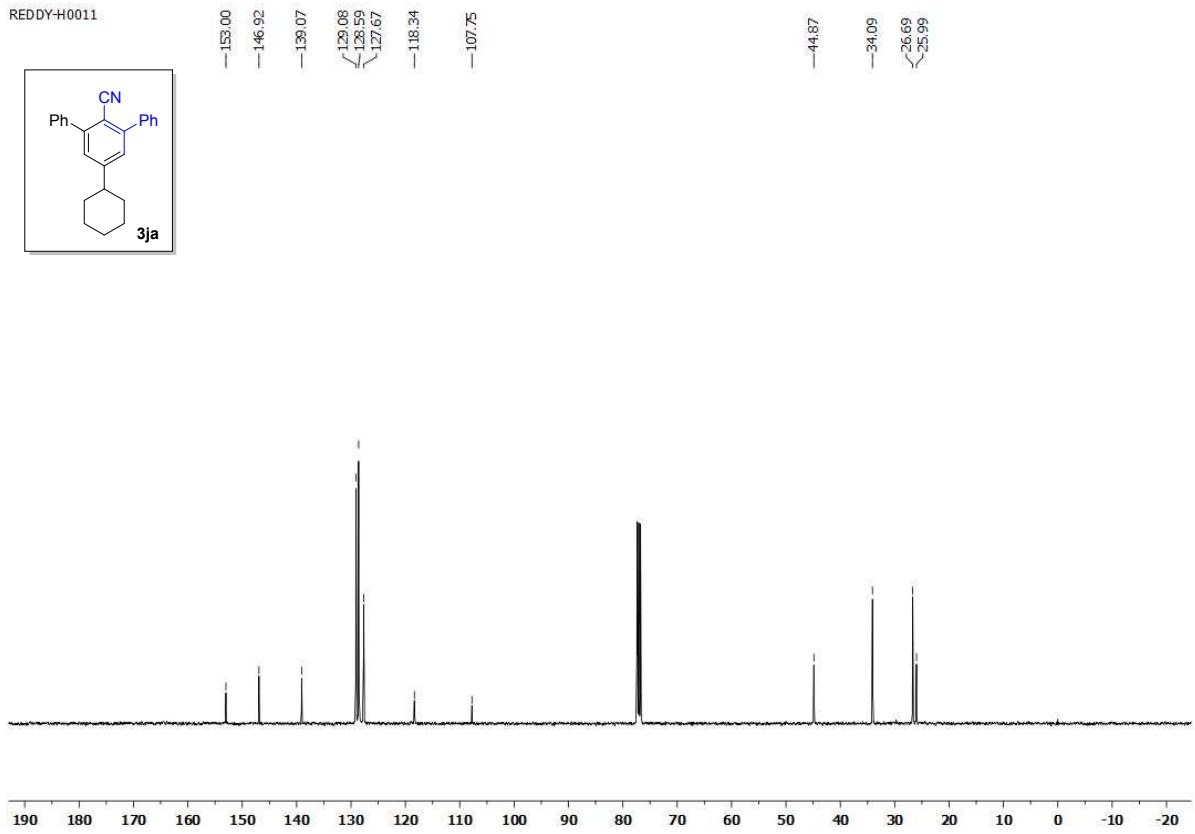

CN
Ph
Ph
3ia
f1 (ppm)

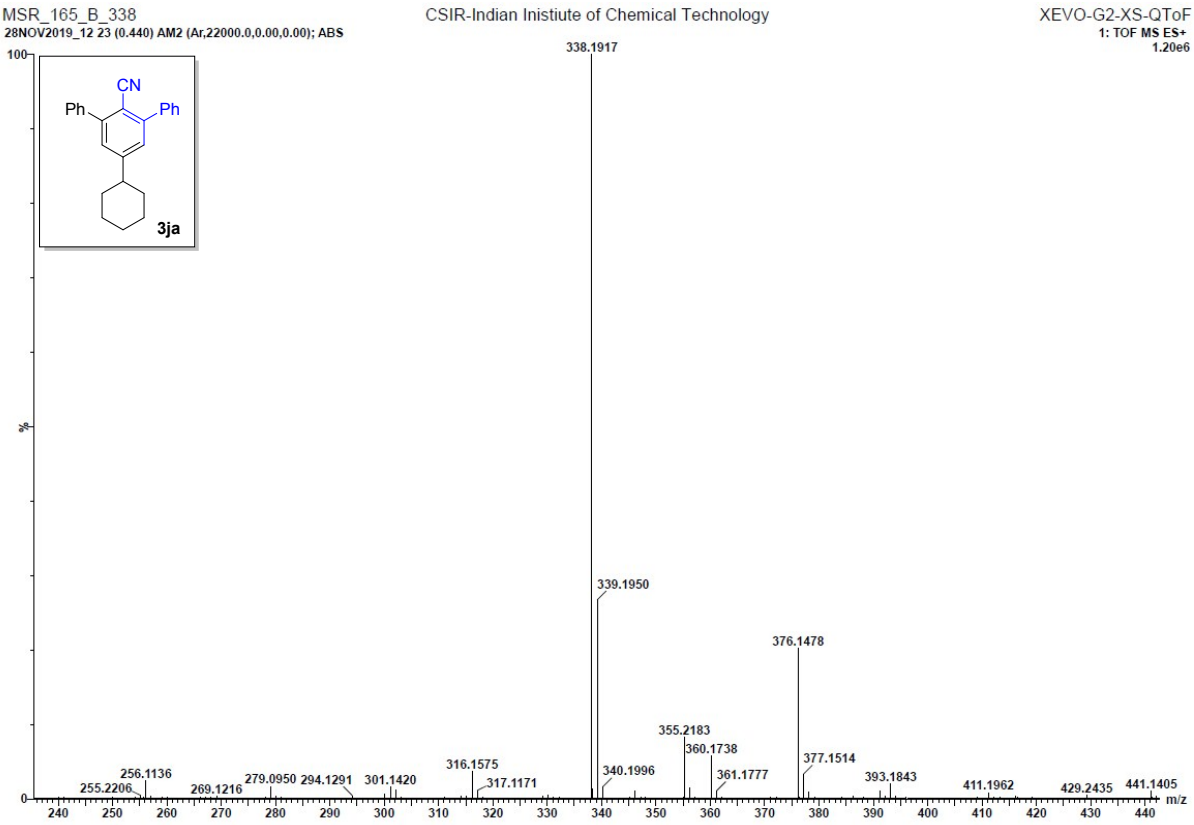
S

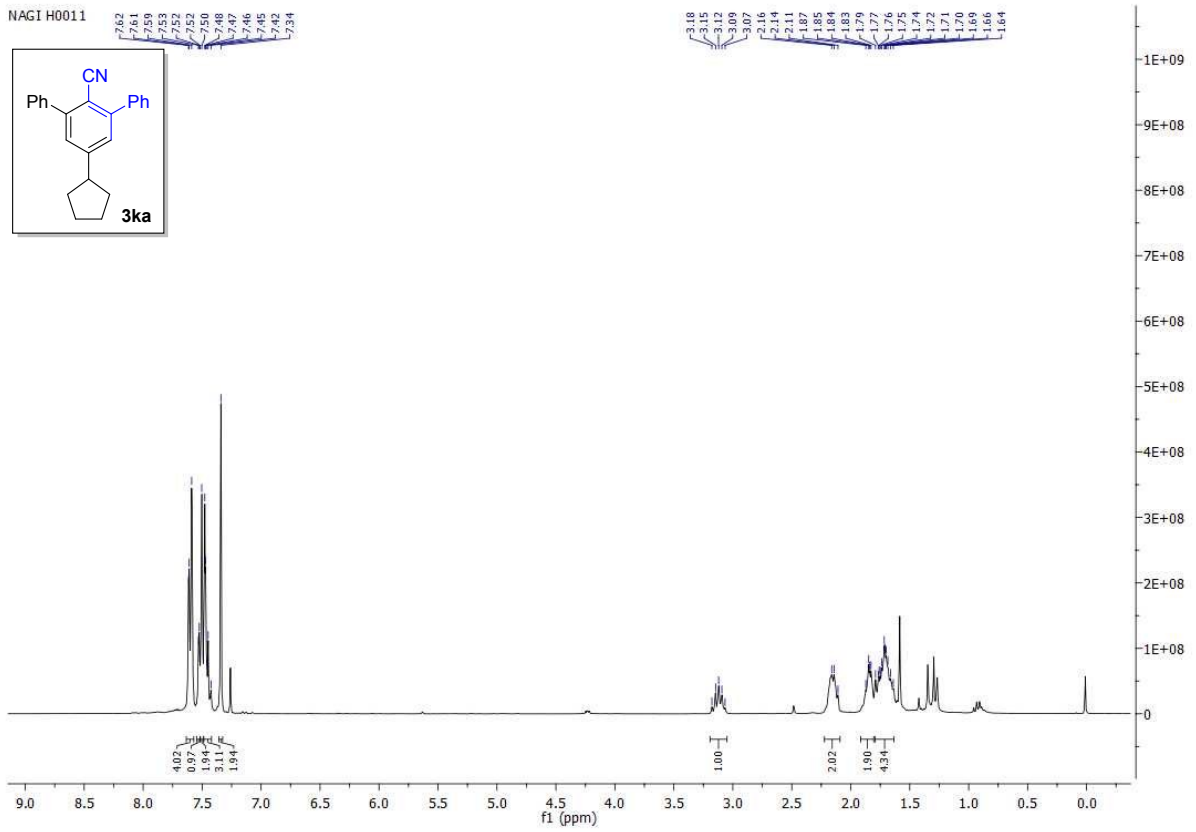

PARAM H0011
146.71
146.45
139.01
135.31
128.98
128.74
128.53
125.37
118.28
107.93
27.12
26.00
22.76
21.83
CN
Ph
Ph
3ia
f1 (ppm)

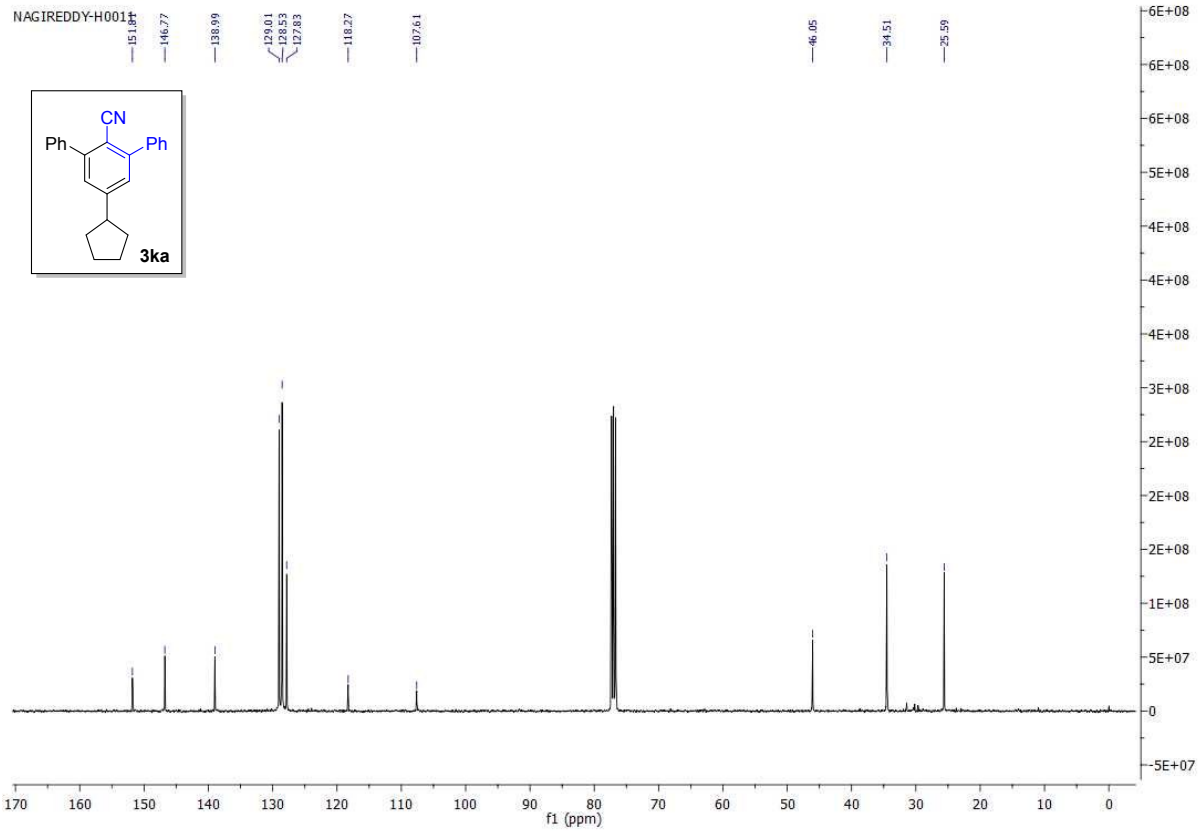

MSR_165_D_336
CSIR-Indian Inistiute of Chemical Technology
XEVO-G2-XS-QToF
28NOV2019_14 34 (0.649) AM2 (Ar,22000.0,0.00,0.00); ABS
1: TOF MS ES+
5.43e6
CN
Ph
Ph
3ia
336.1753
337.1787
374.1312
353.2018
358.1573
308.1442
309.1485
338.1824
375.1348
359.1613
336.1119
338.3416
376.1326
391.2857
400.1088
413.2677
239.0863
256.1123
268.1128
280.1124
291.1115
294.1287
317.1175
%
m/z

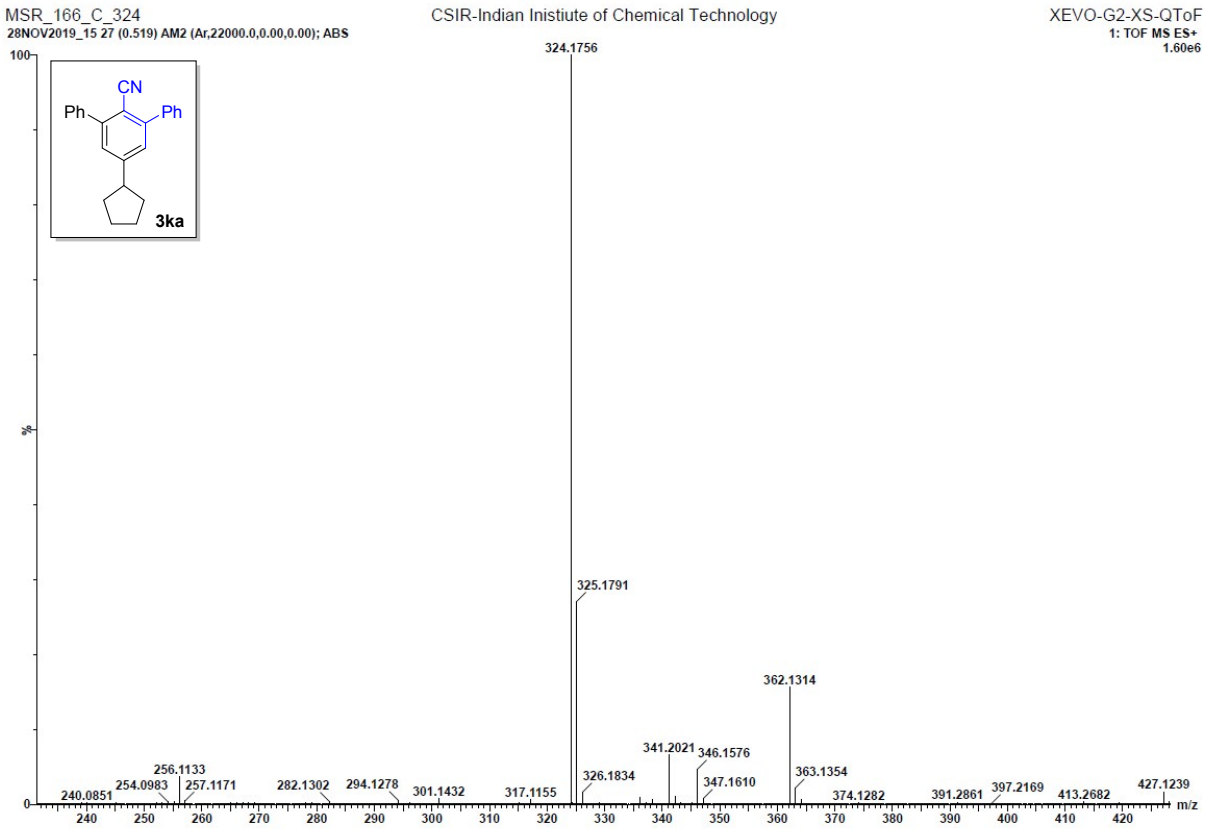

CN
Ph
Ph
3ja
f1 (ppm)

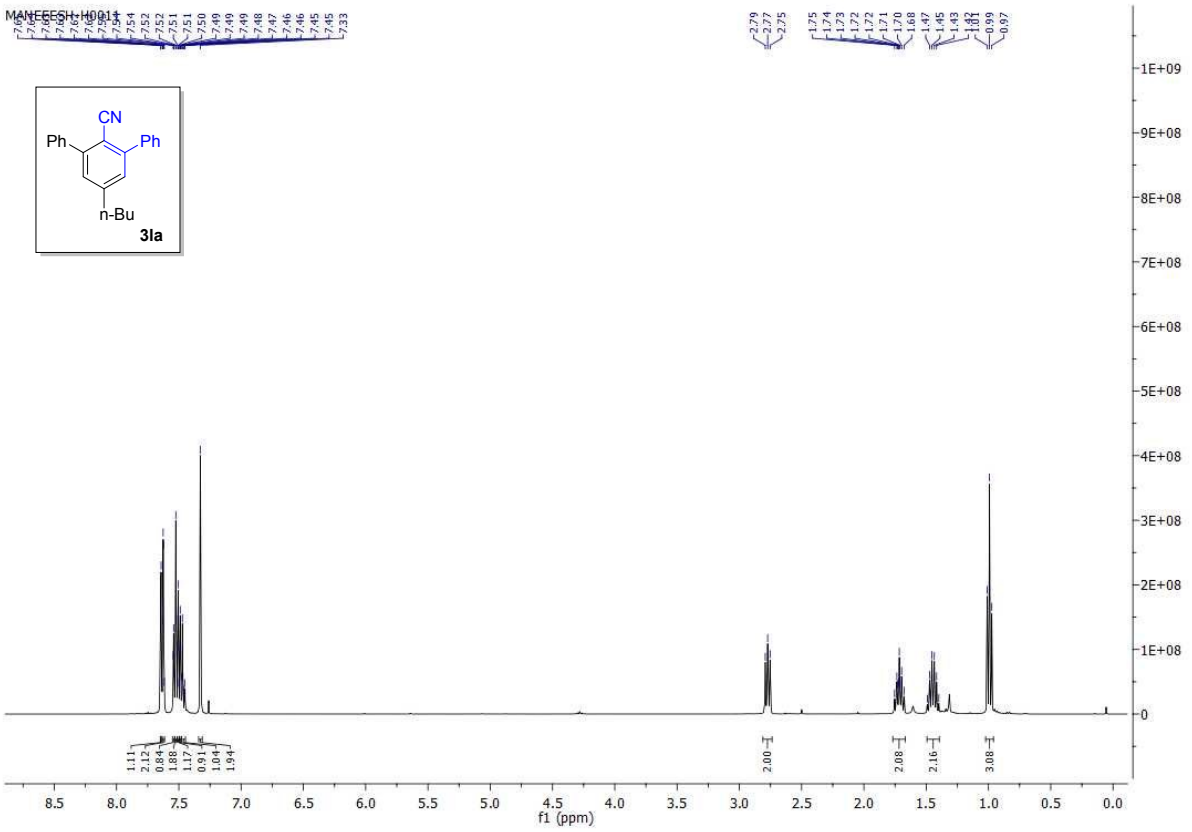

REDDY-H0011
153.00
146.92
139.07
129.08
128.59
127.67
118.34
107.75
44.87
34.09
26.69
25.99
CN
Ph
Ph
3ja

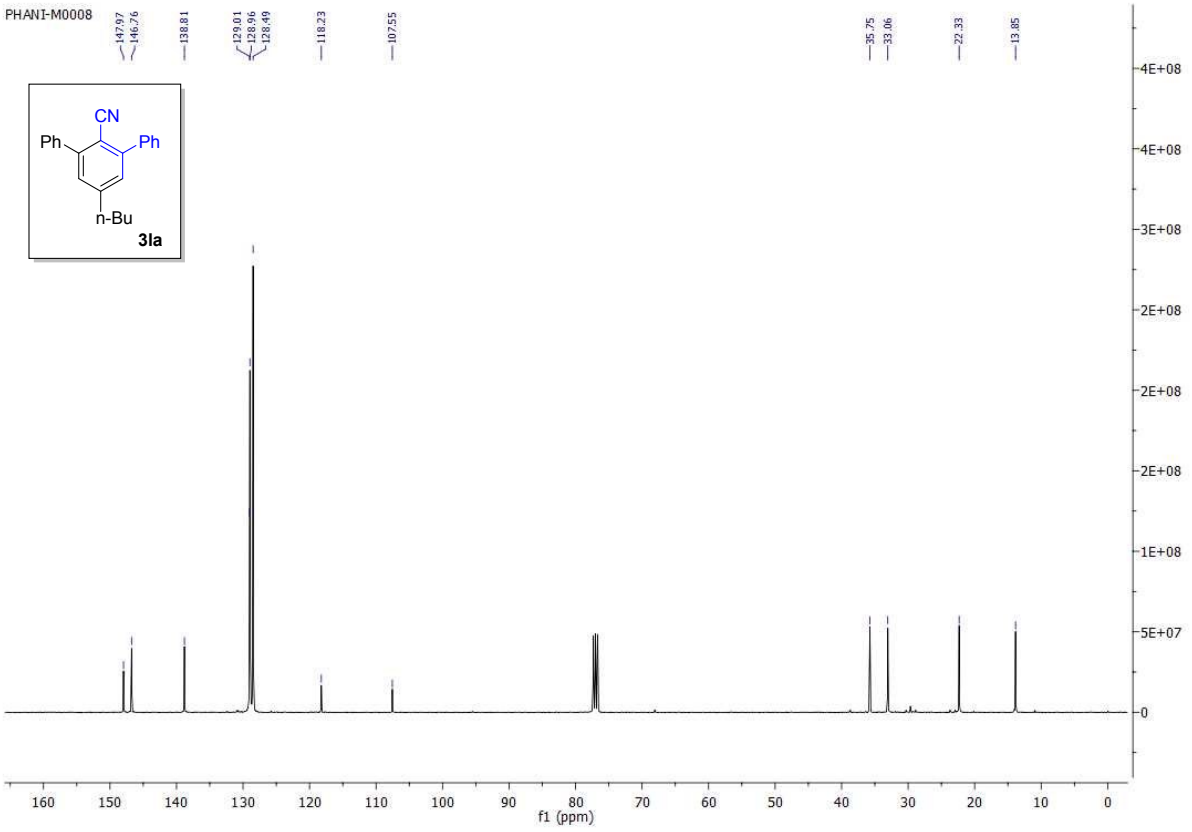

MSR_165_B_338
CSIR-Indian Institute of Chemical Technology
XEVO-G2-XS-QToF
28NOV2019_12 23 (0.440) AM2 (Ar,22000.0,0.00,0.00); ABS
1: TOF MS ES+
1.20e6
CN
Ph
Ph
3ja
338.1917
339.1950
376.1478
355.2183
360.1738
377.1514
316.1575
317.1171
340.1996
361.1777
393.1843
256.1136
255.2206
269.1216
279.0950
294.1291
301.1420
411.1962
429.2435
441.1405
%
m/z

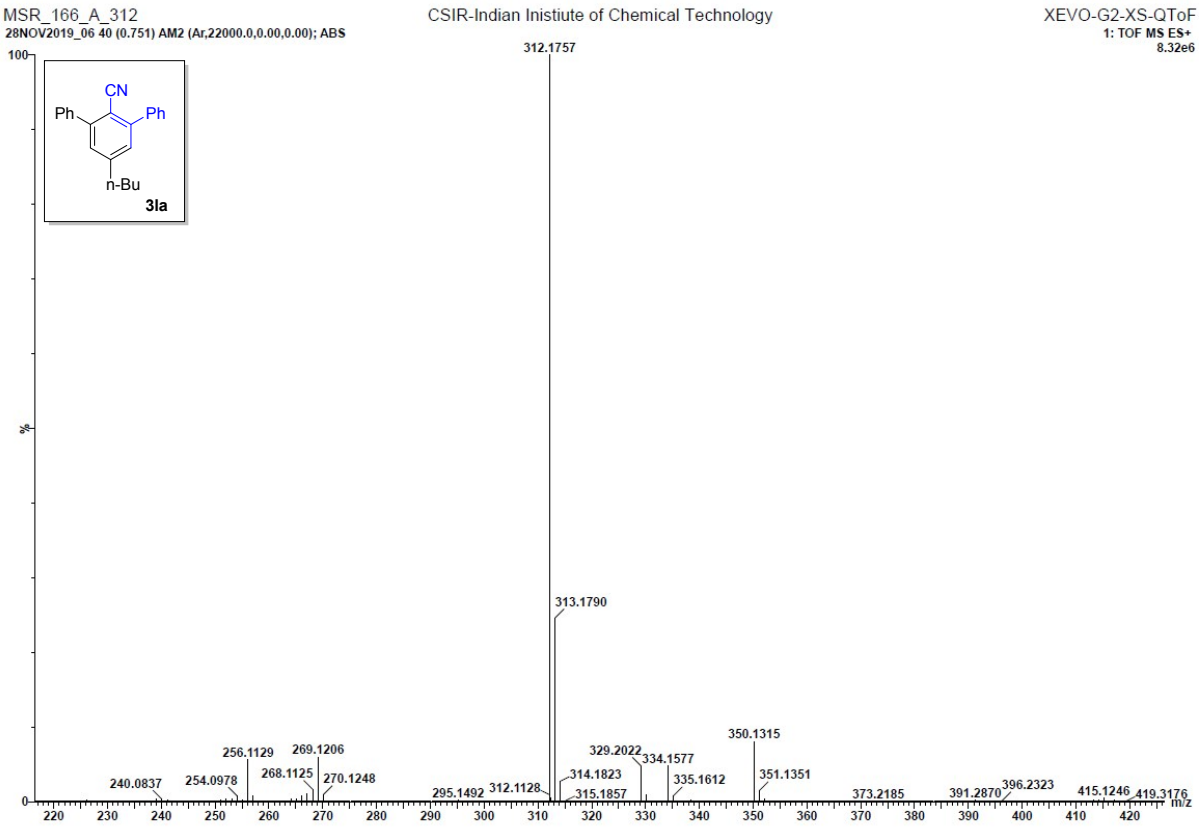

NAGI H0011
CN
Ph
Ph
3ka
f1 (ppm)

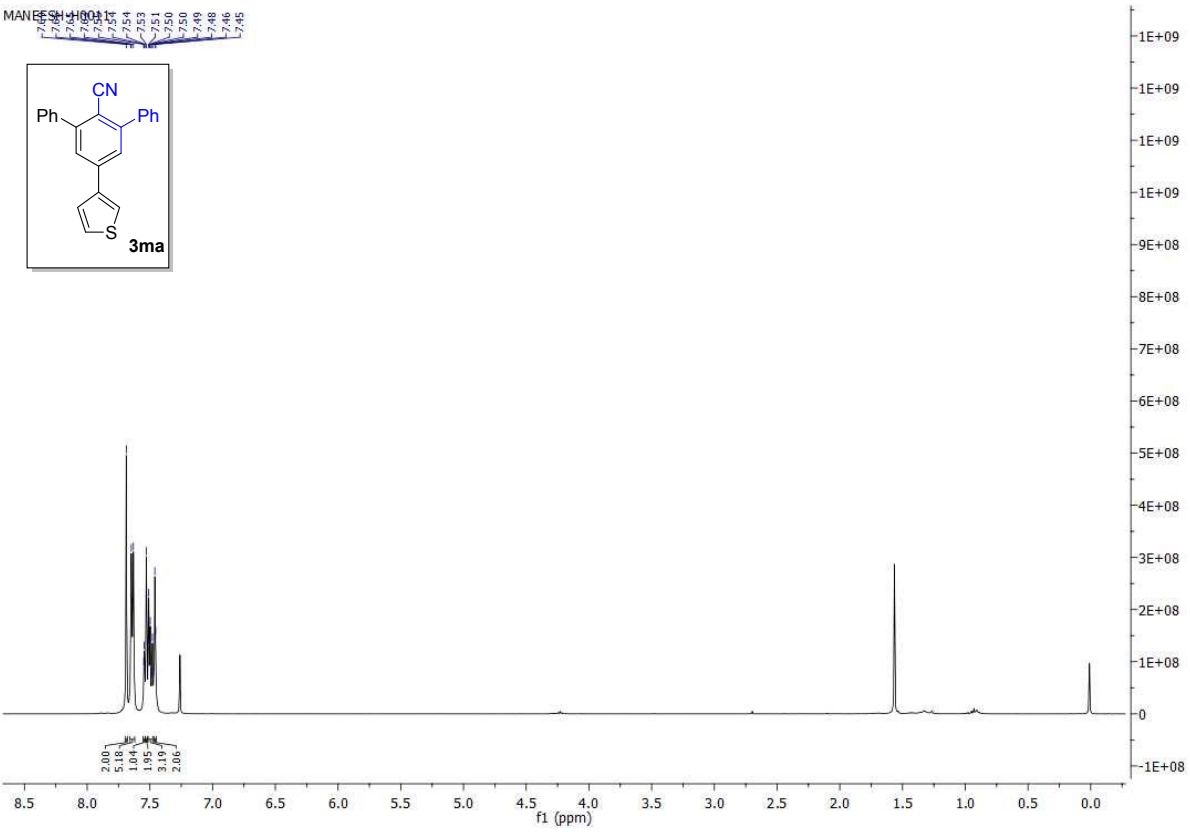

NAGIREDDY-H0011
CN
Ph
Ph
3ka
f1 (ppm)

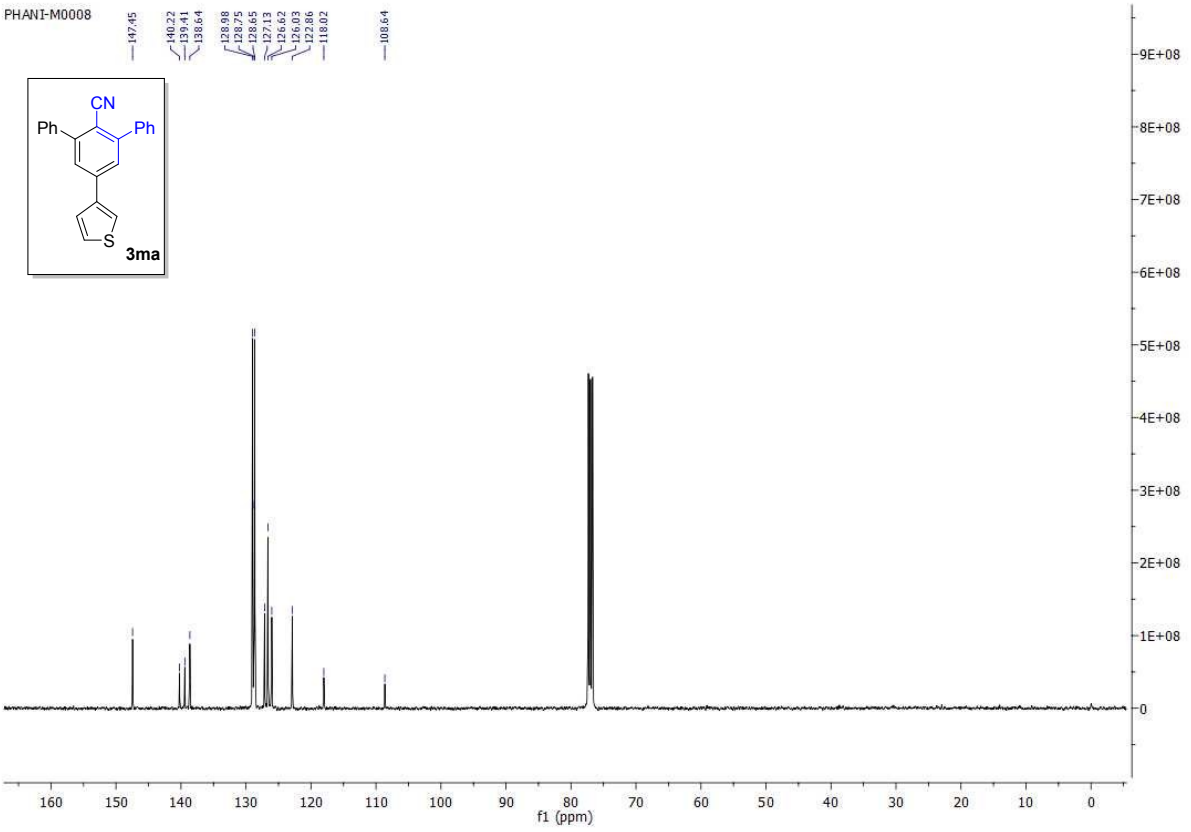

MSR_166_C_324
28NOV2019_15 27 (0.519) AM2 (Ar,22000.0,0.00,0.00); ABS
CSIR-Indian Inistiute of Chemical Technology
XEVO-G2-XS-QToF
1: TOF MS ES+
1.60e6
CN
Ph
Ph
3ka
324.1756
325.1791
362.1314
341.2021
346.1576
326.1834
347.1610
363.1354
256.1133
254.0983
257.1171
240.0851
282.1302
294.1278
301.1432
317.1155
374.1282
391.2861
397.2169
413.2682
427.1239
%
m/z

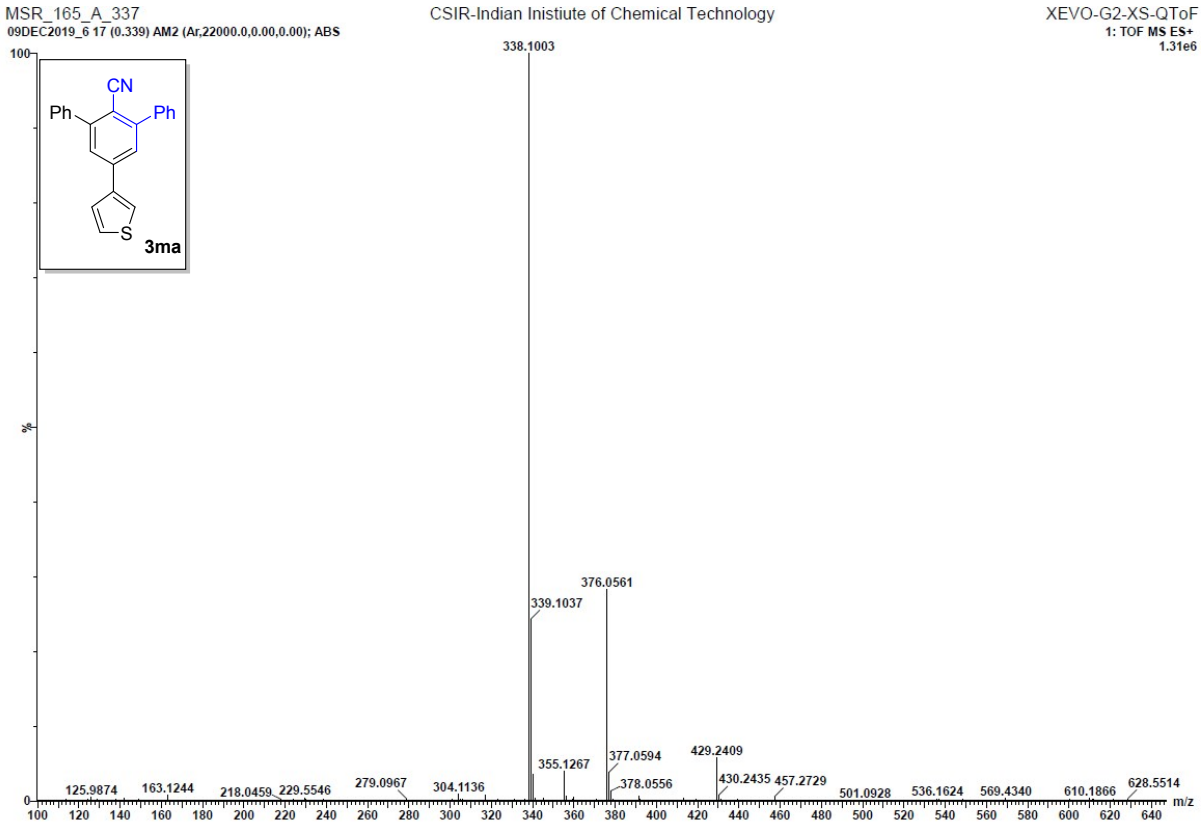

MANEEESH-H0011
CN
Ph
Ph
n-Bu
3la
f1 (ppm)

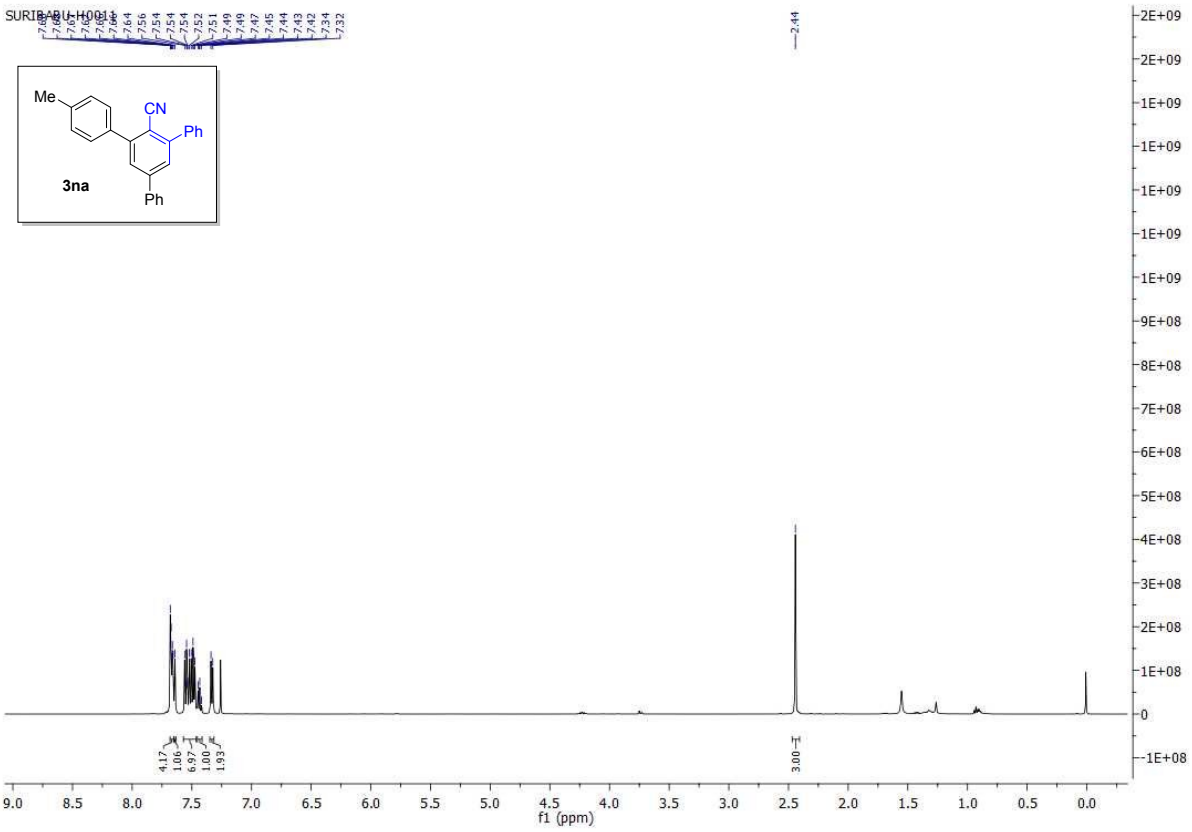

PHANI-M0008
CN
Ph
Ph
n-Bu
3la
f1 (ppm)

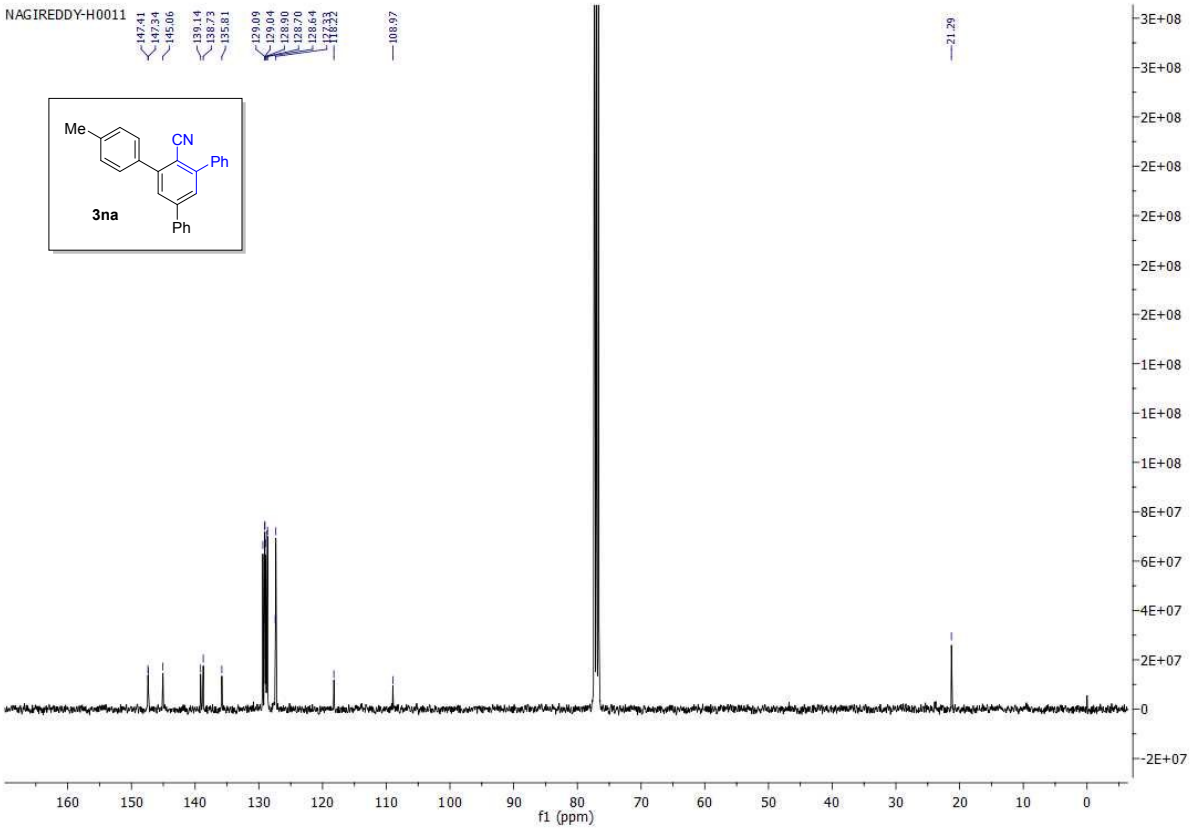

MSR_166_A_312
28NOV2019_06 40 (0.751) AM2 (Ar,22000.0,0.00,0.00); ABS
CSIR-Indian Inistiute of Chemical Technology
XEVO-G2-XS-QToF
1: TOF MS ES+
8.32e6
CN
Ph
Ph
n-Bu
3la
312.1757
313.1790
350.1315
329.2022
334.1577
256.1129
269.1206
268.1125
270.1248
254.0978
240.0837
314.1823
335.1612
351.1351
295.1492
312.1128
315.1857
373.2185
391.2870
396.2323
415.1246
419.3176
%
m/z

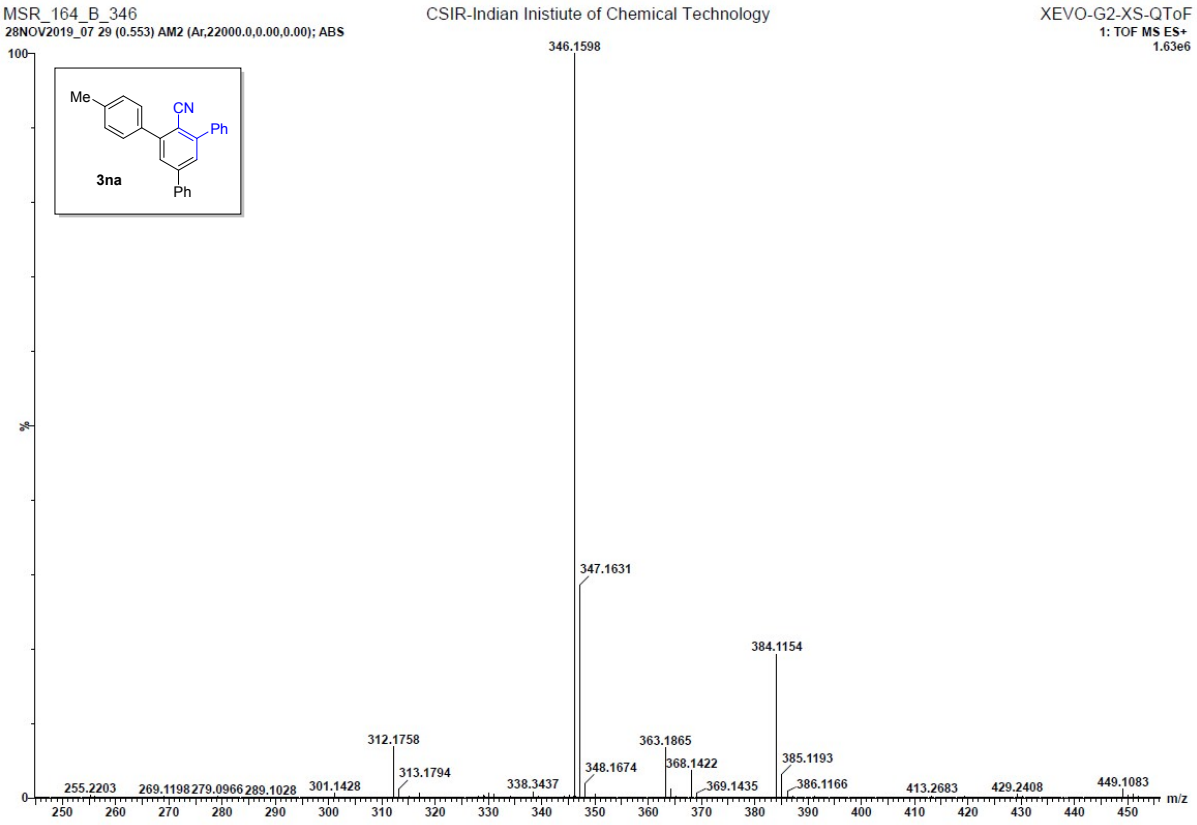

MANEESH-H0011
CN
Ph
Ph
S
3ma
f1 (ppm)

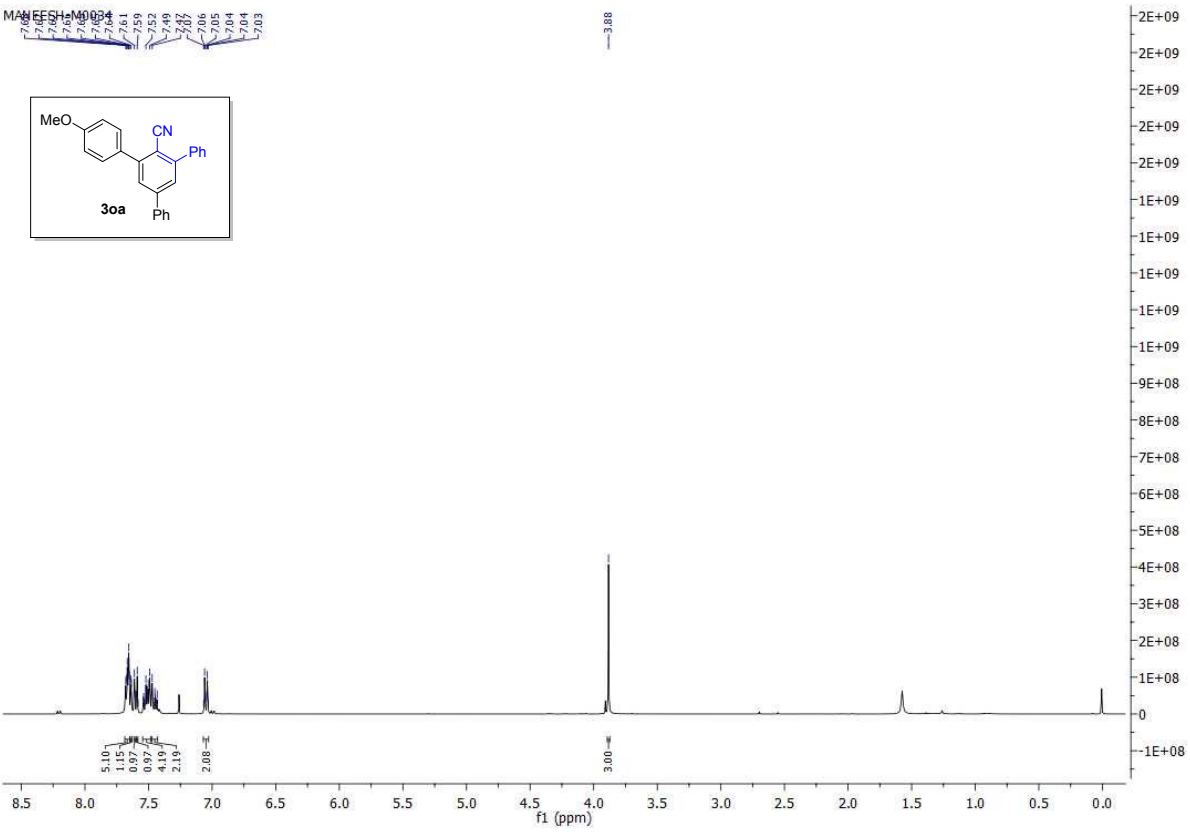

PHANI-M0008
147.45
140.22
139.41
138.64
128.98
128.75
128.65
127.13
126.62
126.03
122.86
118.02
108.64
CN
Ph
Ph
S
3ma
f1 (ppm)

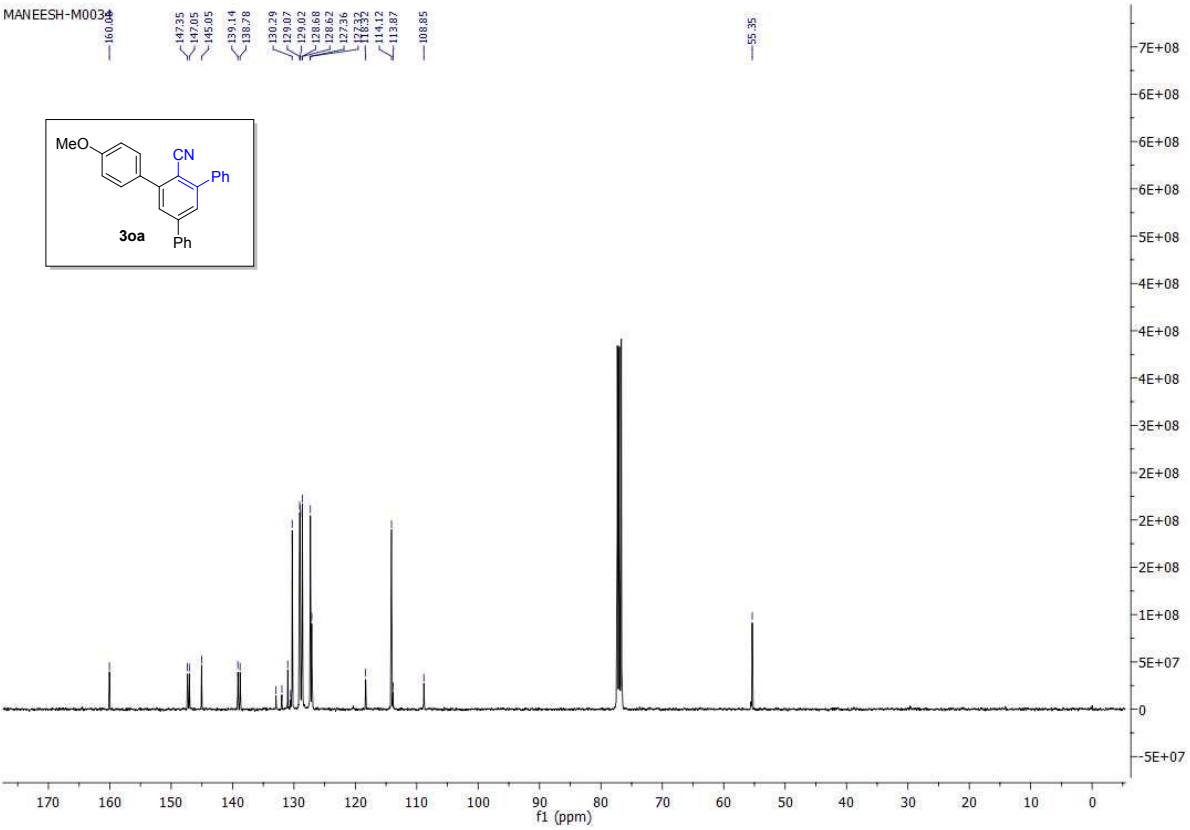

MSR_165_A_337
09DEC2019_6 17 (0.339) AM2 (Ar,22000.0,0.00,0.00); ABS
CSIR-Indian Inistiute of Chemical Technology
XEVO-G2-XS-QToF
1: TOF MS ES+
1.31e6
CN
Ph
Ph
S
3ma
338.1003
376.0561
339.1037
429.2409
377.0594
355.1267
378.0556
430.2435
457.2729
125.9874
163.1244
218.0459
229.5546
279.0967
304.1136
501.0928
536.1624
569.4340
610.1866
628.5514
%
m/z

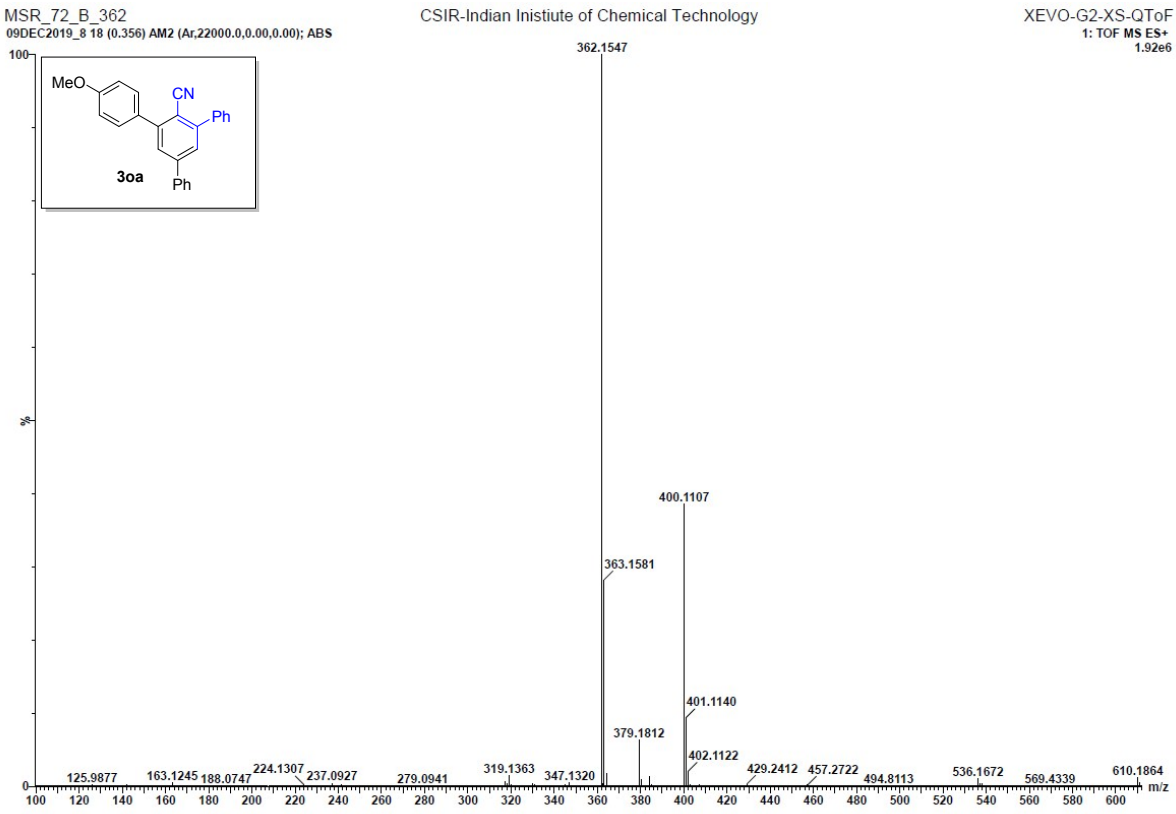

Me
CN
Ph
3na
Ph
f1 (ppm)

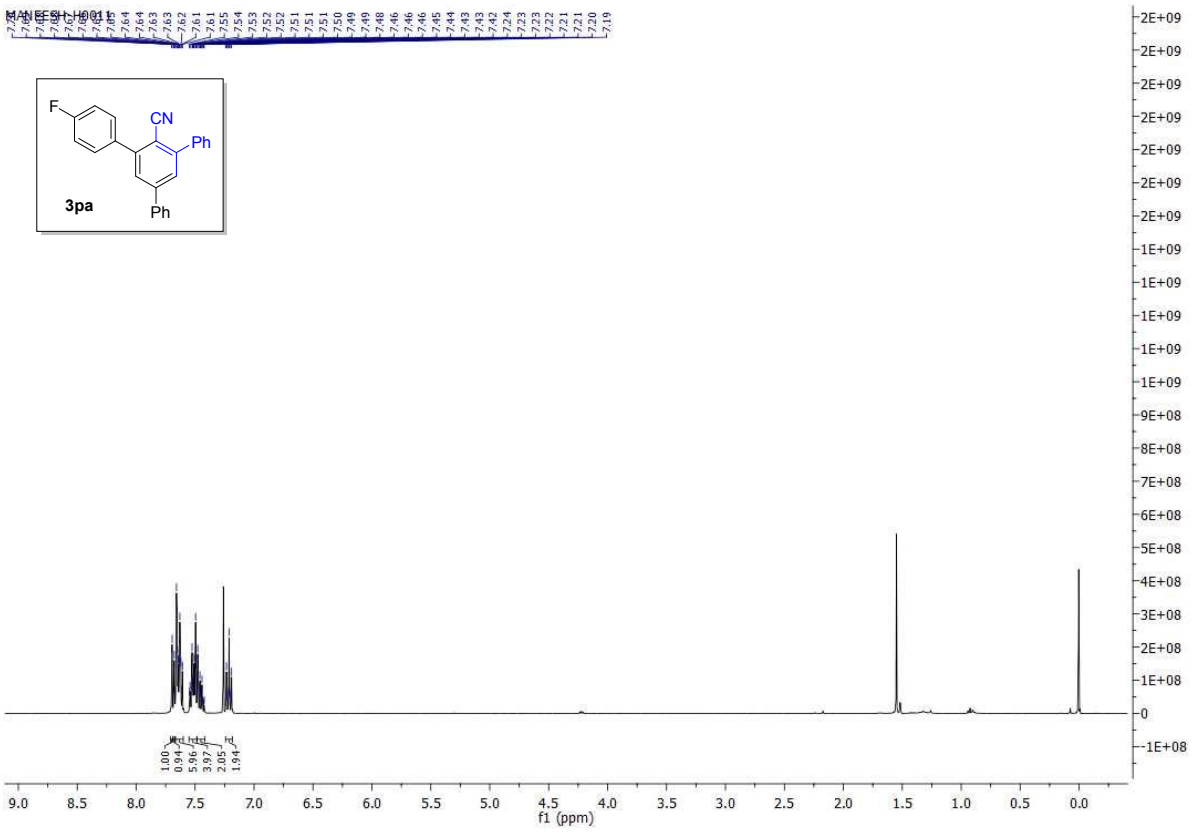

NAGIREDDY-H0011
Me
CN
Ph
3na
Ph
f1 (ppm)

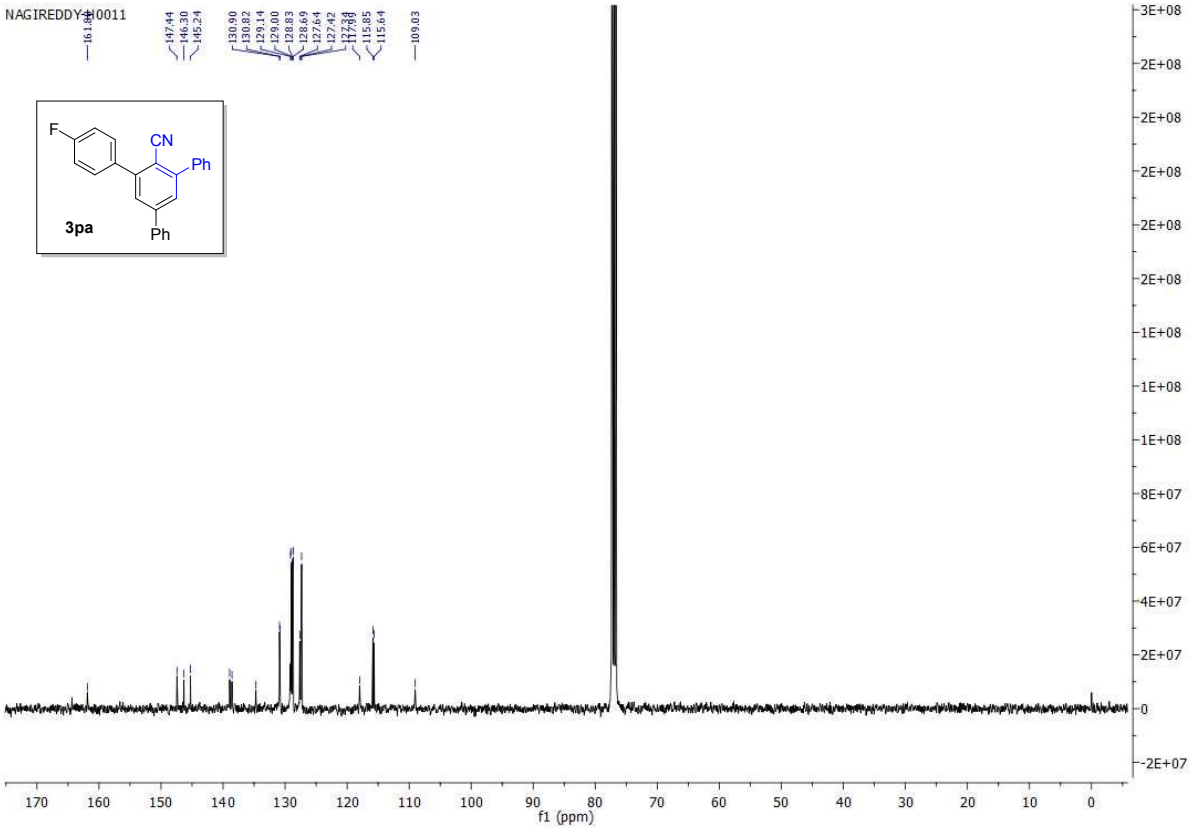

MSR_164_B_346
CSIR-Indian Inistiute of Chemical Technology
XEVO-G2-XS-QToF
28NOV2019_07 29 (0.553) AM2 (Ar,22000.0,0.00,0.00); ABS
1: TOF MS ES+
1.63e6
Me
CN
Ph
Ph
3na
346.1598
347.1631
384.1154
312.1758
363.1865
313.1794
348.1674
368.1422
385.1193
255.2203
269.1198
279.0966
289.1028
301.1428
338.3437
369.1435
386.1166
413.2683
429.2408
449.1083
%
m/z

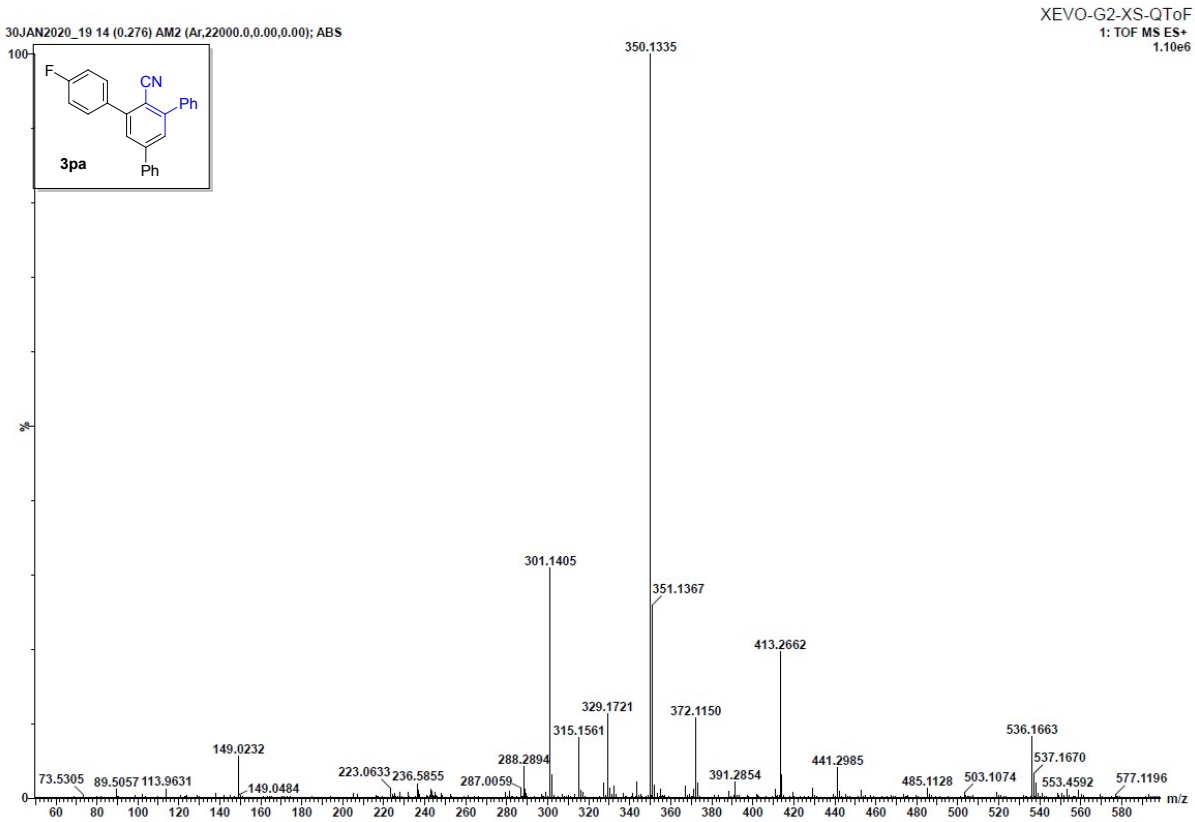

MANEESH-M0034
MeO
CN
Ph
3oa
Ph
3.88
5.10
1.15
0.97
0.97
4.19
2.19
2.08
3.00
f1 (ppm)

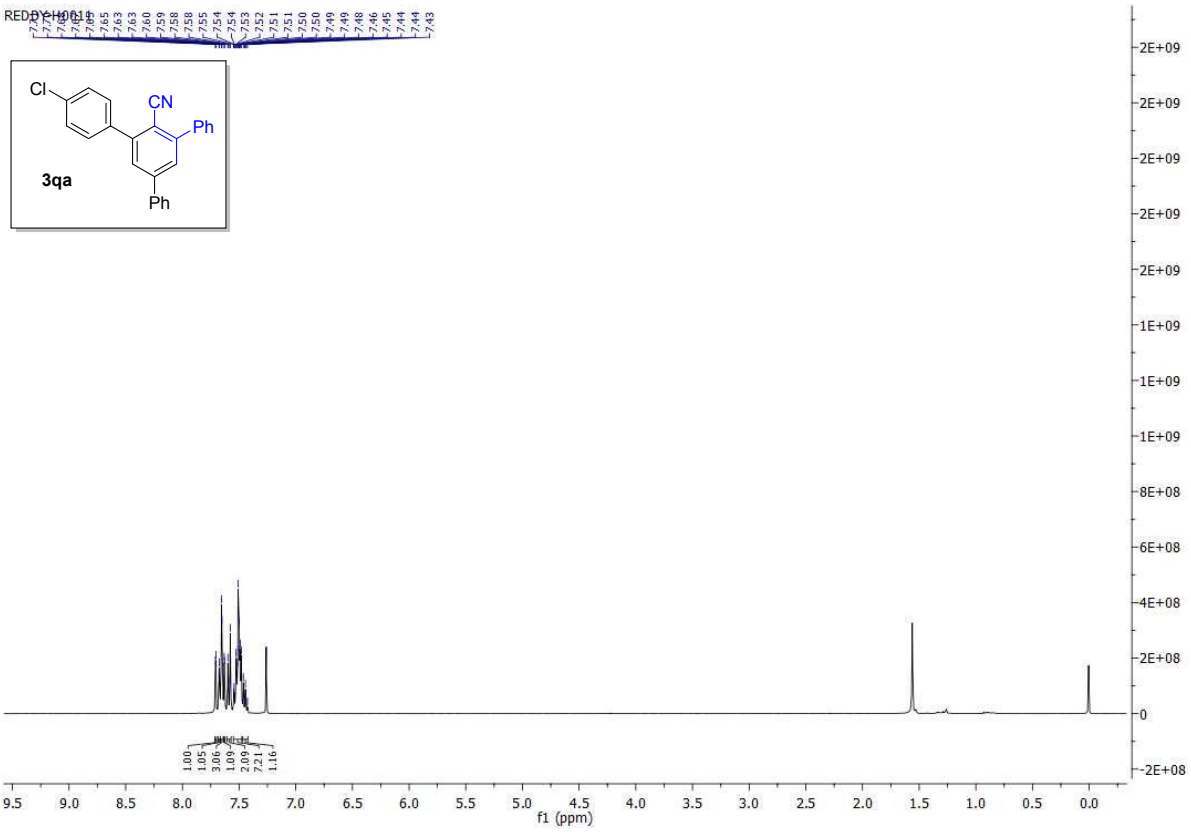

MANEESH-M0034
160.04
147.35
147.05
145.05
139.14
138.78
130.29
129.07
129.02
128.68
128.62
127.36
127.33
118.32
114.12
113.87
108.85
55.35
MeO
CN
Ph
3oa
Ph
f1 (ppm)

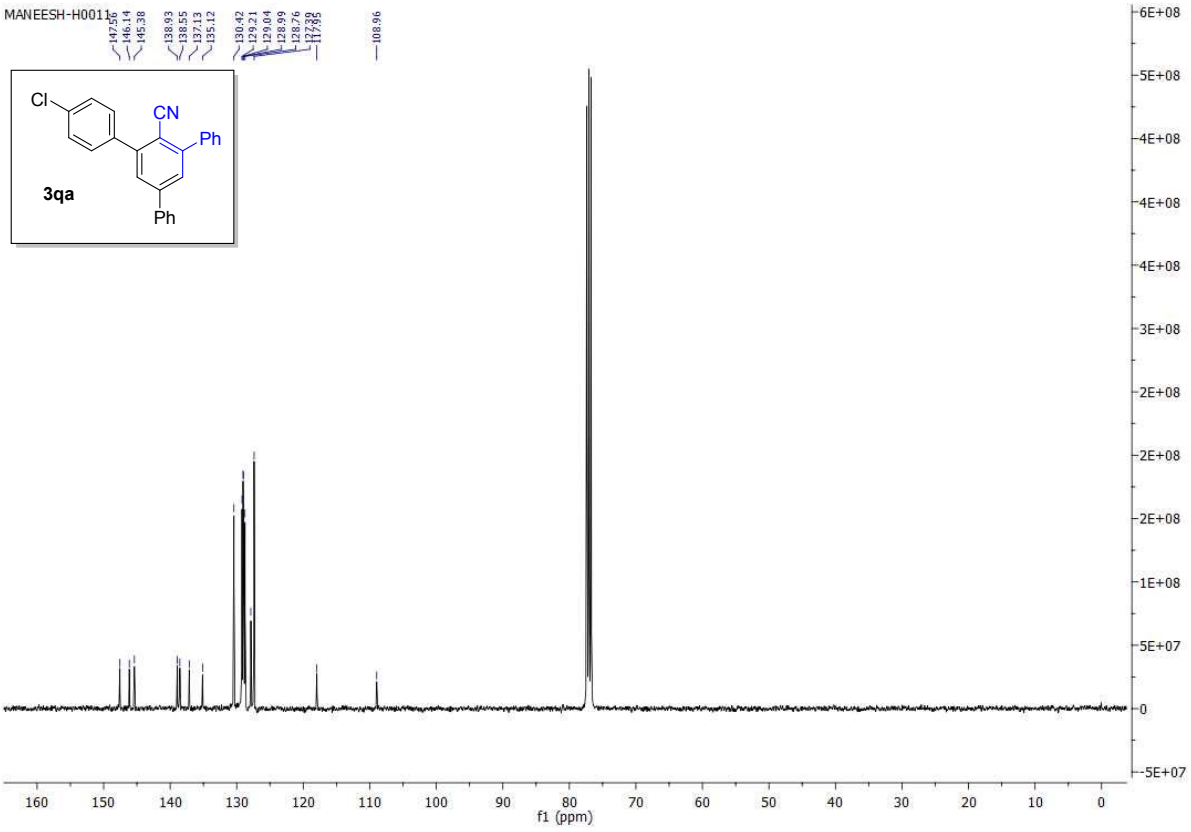

MSR_72_B_362
CSIR-Indian Inistiute of Chemical Technology
XEVO-G2-XS-QToF
09DEC2019_8 18 (0.356) AM2 (Ar,22000.0,0.00,0.00); ABS
1: TOF MS ES+
1.92e6
MeO
CN
Ph
3oa
Ph
362.1547
400.1107
363.1581
401.1140
379.1812
402.1122
125.9877
163.1245
188.0747
224.1307
237.0927
279.0941
319.1363
347.1320
429.2412
457.2722
494.8113
536.1672
569.4339
610.1864
%
m/z

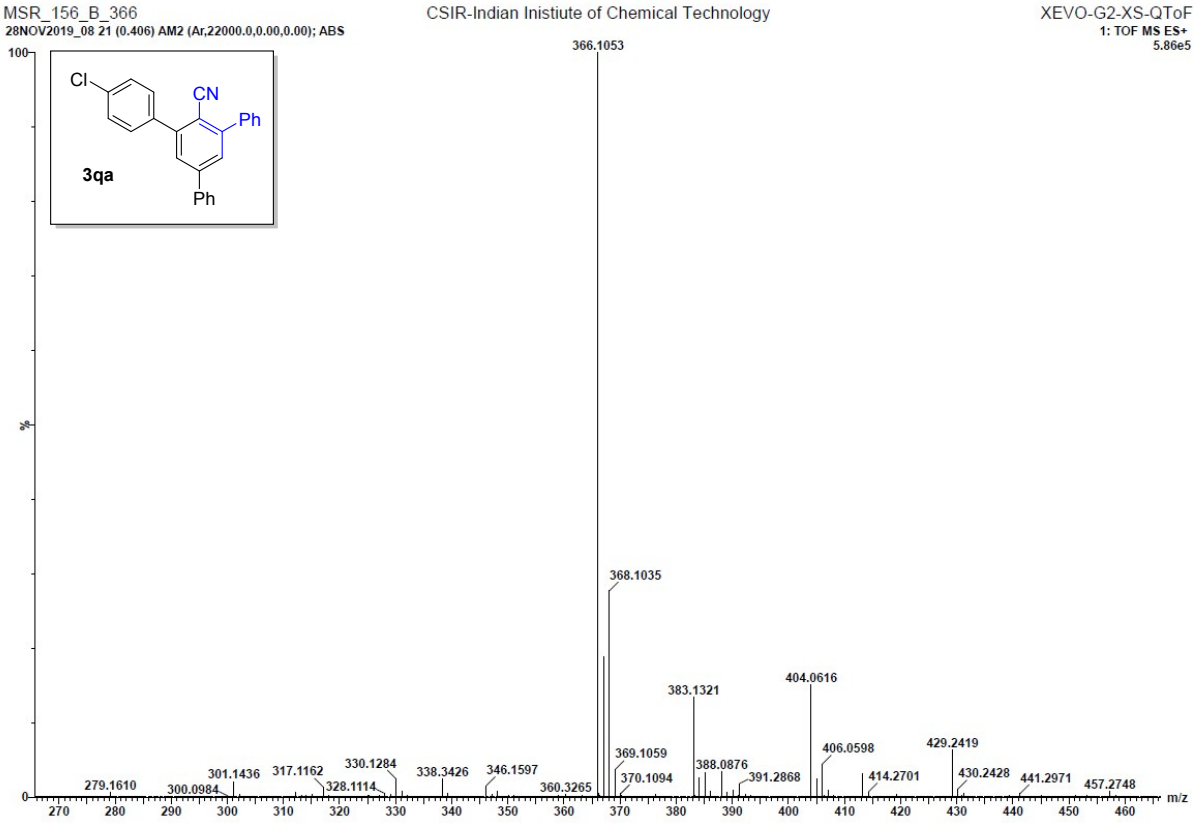

F
CN
Ph
Ph
3pa
f1 (ppm)

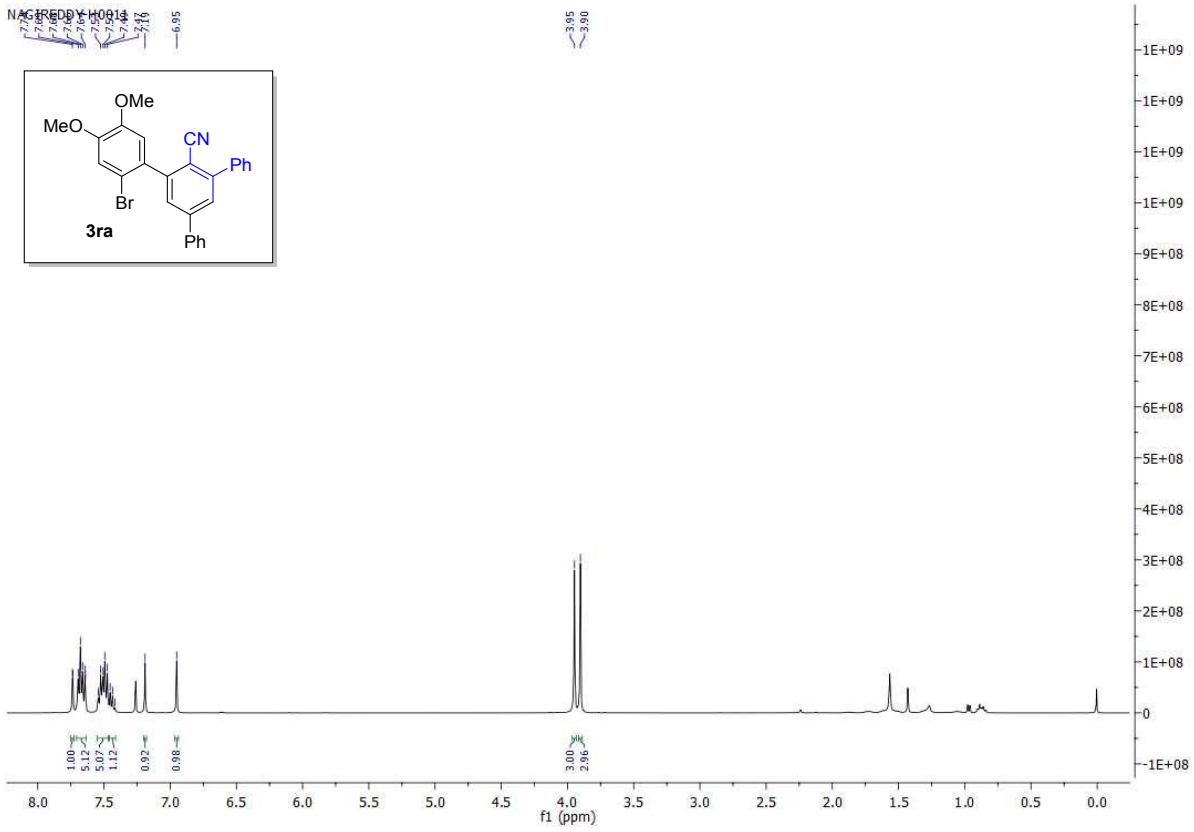

NAGIREDDY-H0011
F
CN
Ph
Ph
3pa
f1 (ppm)

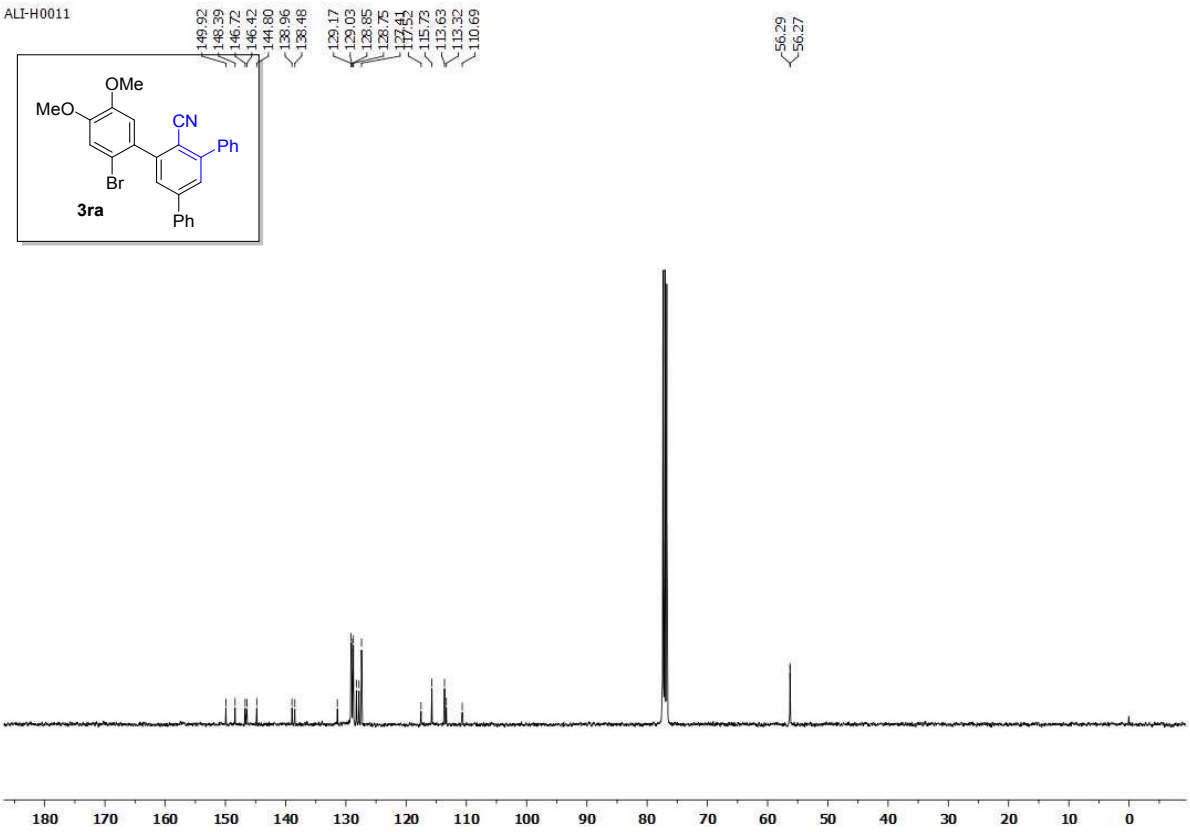

30JAN2020_19 14 (0.276) AM2 (Ar,22000.0,0.00,0.00); ABS
XEVO-G2-XS-QToF
1: TOF MS ES+
1.10e6
3pa
F
CN
Ph
Ph
350.1335
301.1405
351.1367
413.2662
329.1721
372.1150
315.1561
536.1663
537.1670
149.0232
288.2894
441.2985
73.5305
89.5057
113.9631
149.0484
223.0633
236.5855
287.0059
391.2854
485.1128
503.1074
553.4592
577.1196
%
m/z

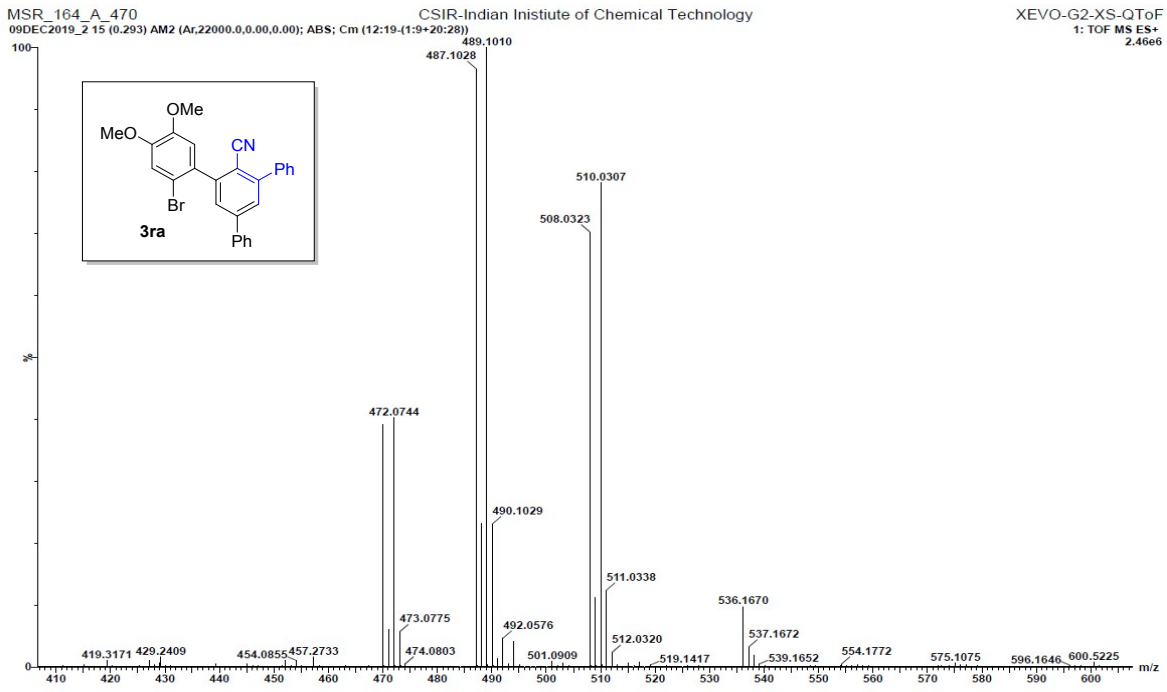

REDDY-H0011
Cl
CN
Ph
3qa
Ph
f1 (ppm)

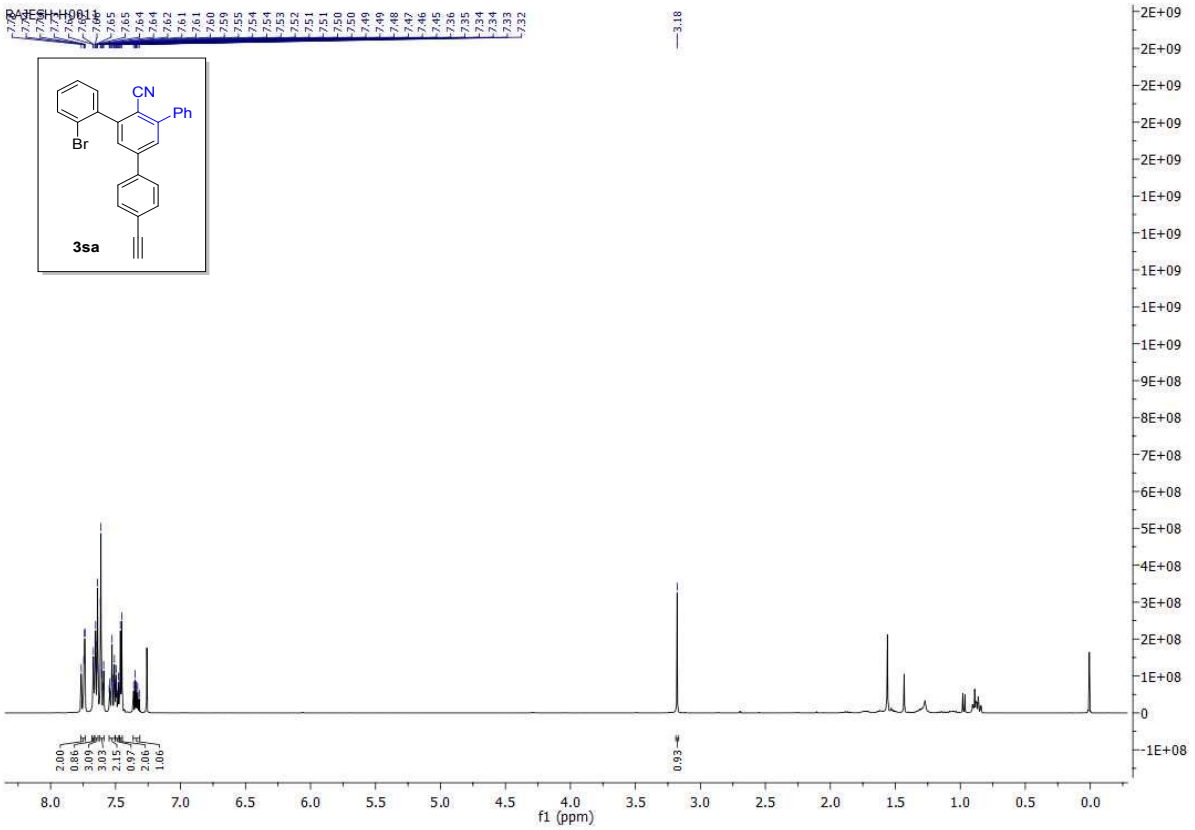

MANEESH-H0011
Cl
CN
Ph
3qa
Ph
f1 (ppm)

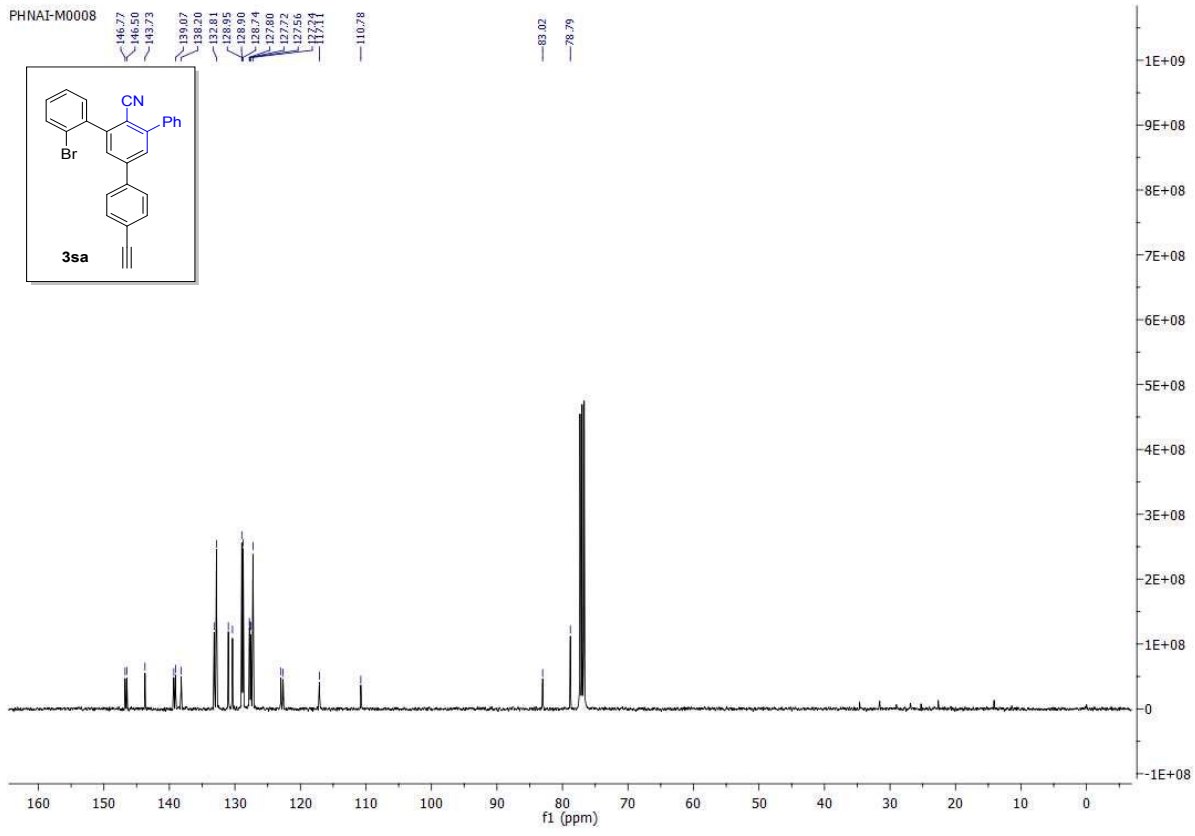

MSR_156_B_366
CSIR-Indian Institute of Chemical Technology
XEVO-G2-XS-QToF
28NOV2019_08 21 (0.406) AM2 (Ar,22000.0,0.00,0.00); ABS
1: TOF MS ES+
5.86e5
Cl
CN
Ph
3qa
Ph
366.1053
368.1035
383.1321
404.0616
369.1059
388.0876
406.0598
429.2419
370.1094
391.2868
414.2701
430.2428
441.2971
457.2748
279.1610
300.0984
301.1436
317.1162
328.1114
330.1284
338.3426
346.1597
360.3265
%
m/z

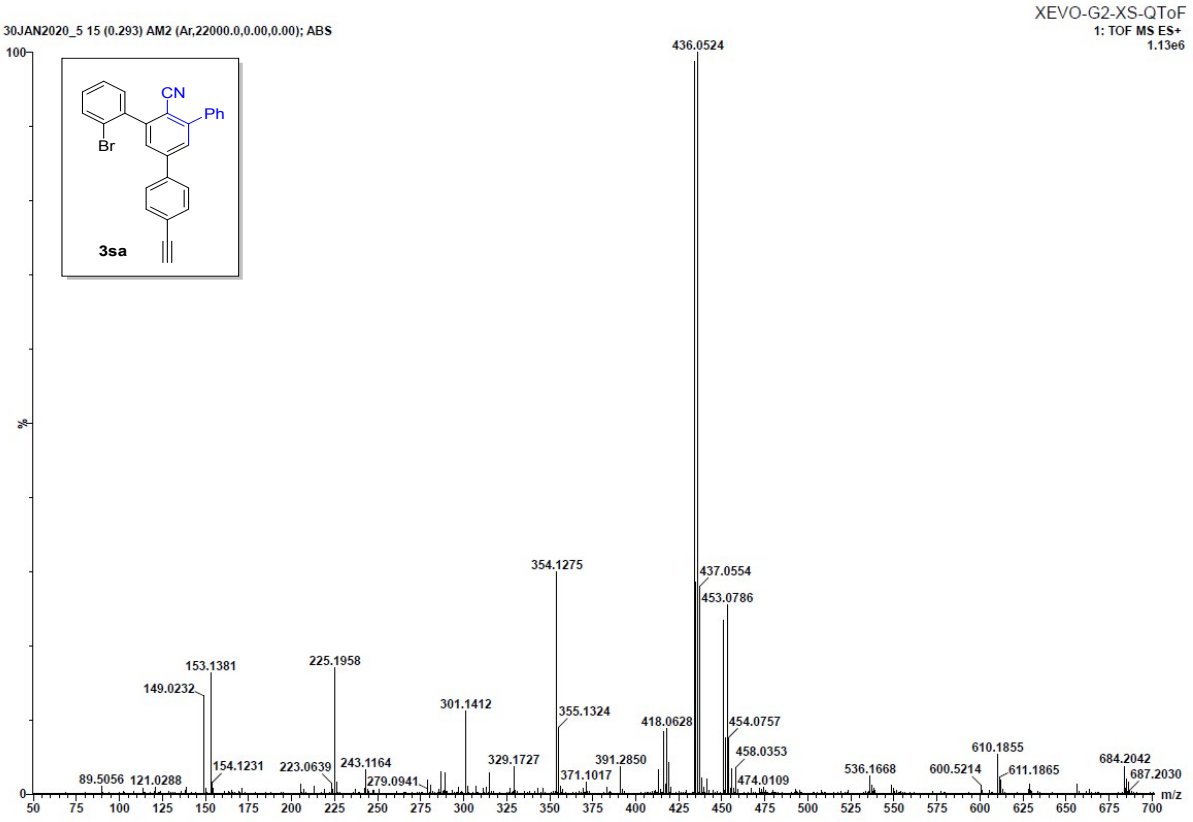

NAGAREDDY H061
OMe
MeO
CN
Ph
Br
3ra
Ph
f1 (ppm)

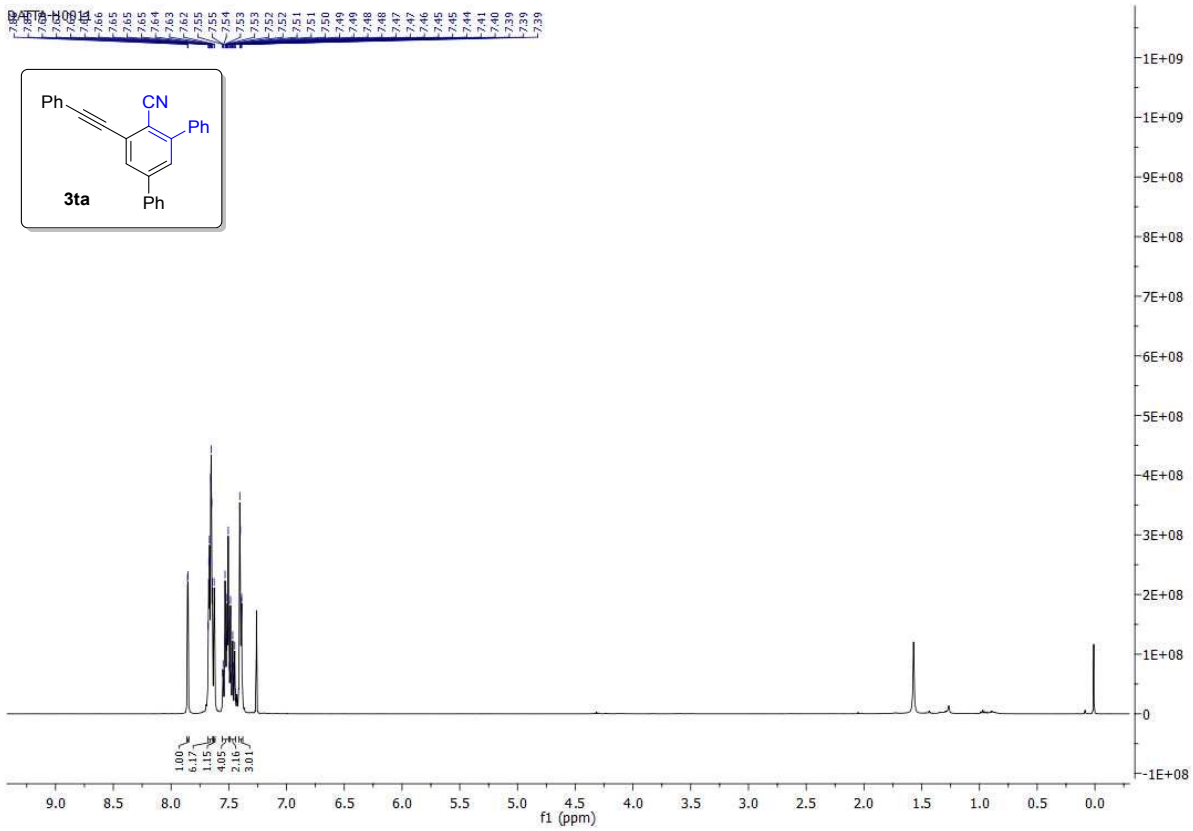

ALI-H0011
149.92
148.39
146.72
146.42
144.80
138.96
138.48
129.17
129.03
128.85
128.75
127.44
127.32
115.73
113.63
113.32
110.69
56.29
56.27
OMe
MeO
CN
Ph
Br
3ra
Ph
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

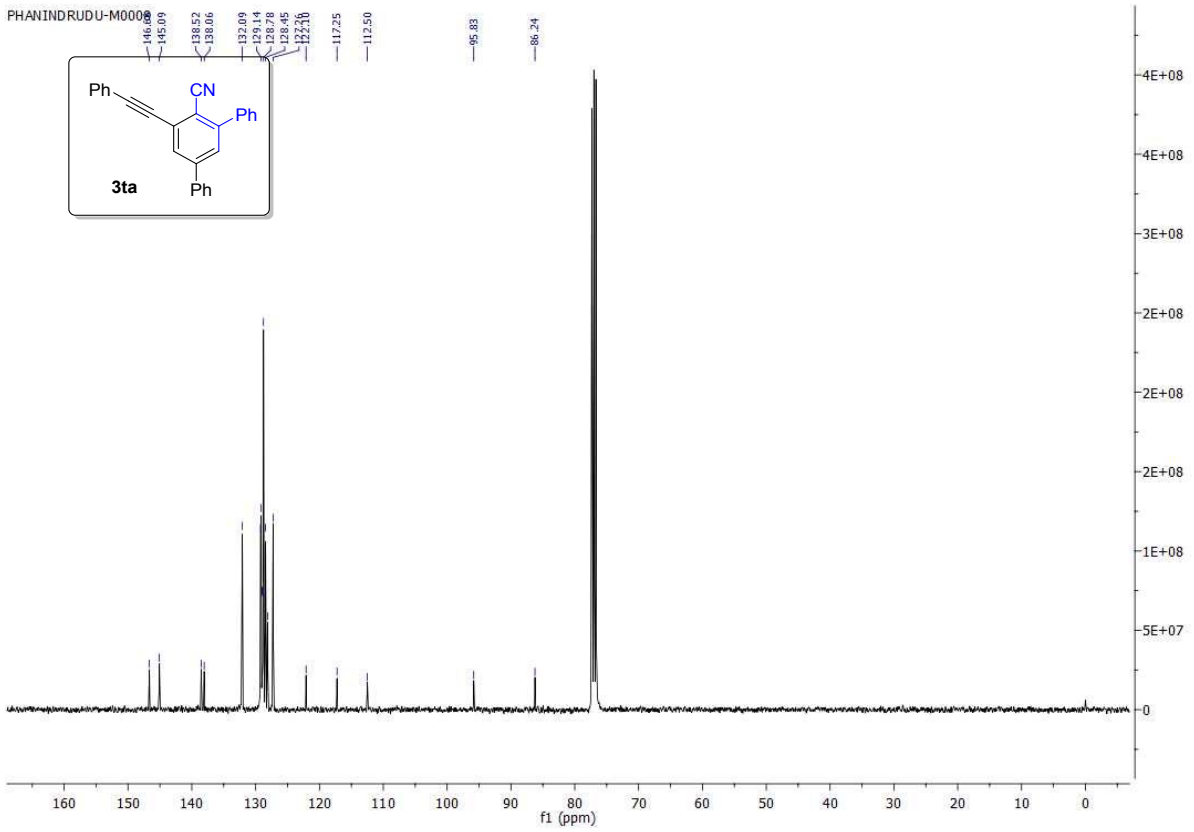

MSR_164_A_470
CSIR-Indian Inistiute of Chemical Technology
XEVO-G2-XS-QToF
09DEC2019_2 15 (0.293) AM2 (Ar,22000.0,0.00,0.00); ABS; Cm (12:19-(1:9+20:28))
1: TOF MS ES+
2.46e6
100
%
0
OMe
MeO
CN
Ph
Br
3ra
Ph
489.1010
487.1028
510.0307
508.0323
472.0744
490.1029
511.0338
536.1670
537.1672
473.0775
492.0576
512.0320
419.3171
429.2409
454.0855
457.2733
474.0803
501.0909
519.1417
539.1652
554.1772
575.1075
596.1646
600.5225
410
420
430
440
450
460
470
480
490
500
510
520
530
540
550
560
570
580
590
600
m/z

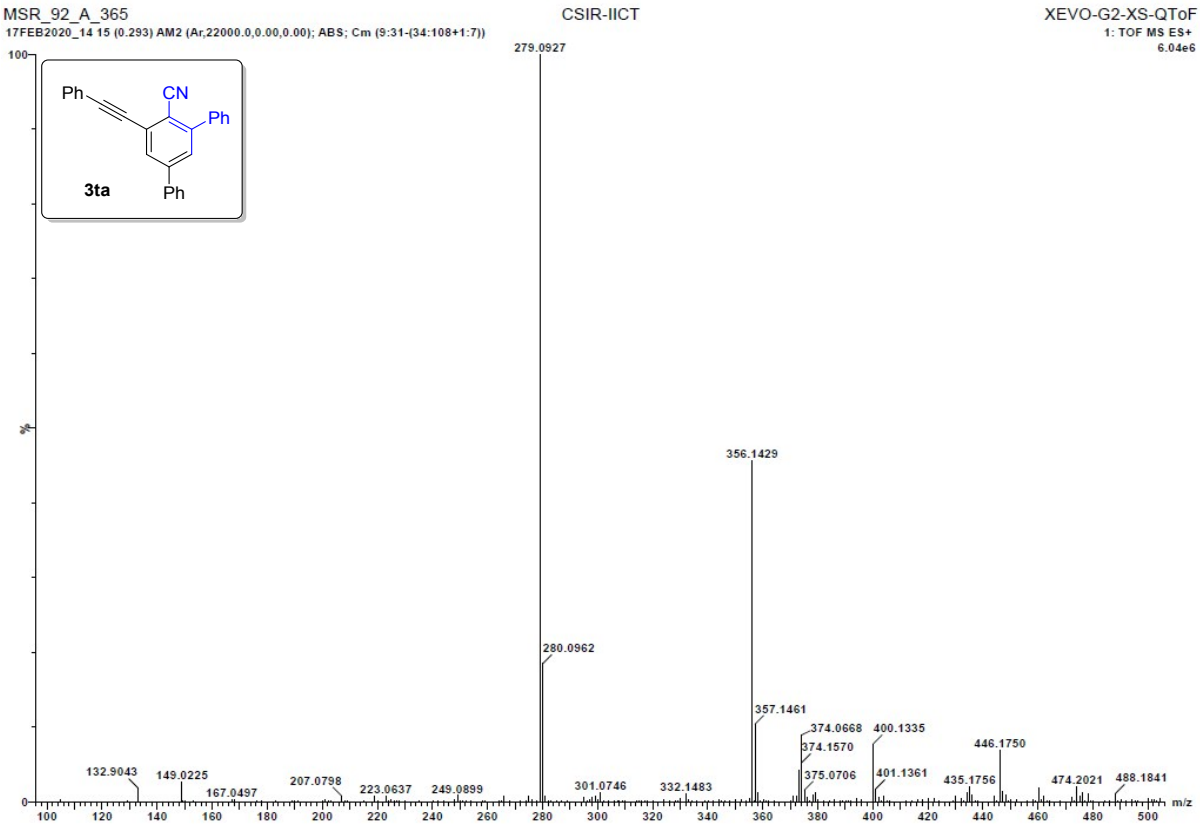

CN
Ph
Br
3sa
f1 (ppm)

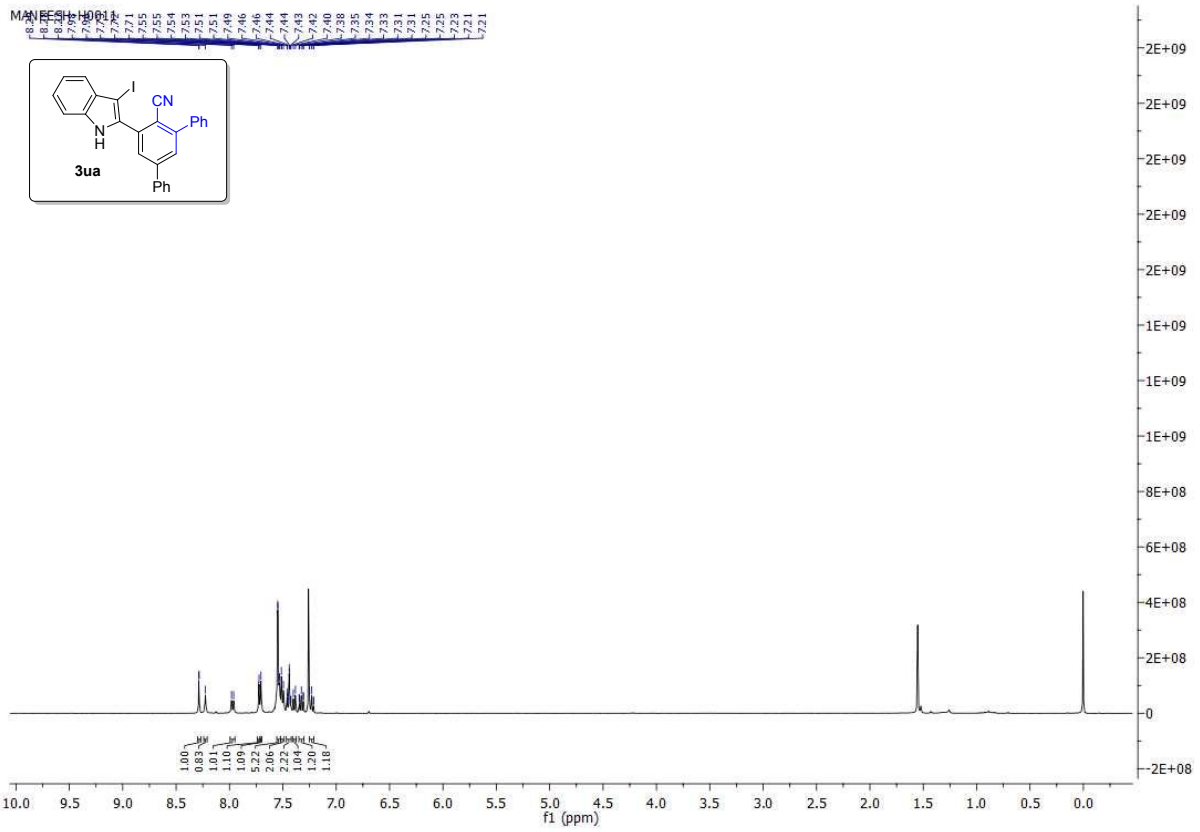

PHNAI-M0008
CN
Ph
Br
3sa
f1 (ppm)

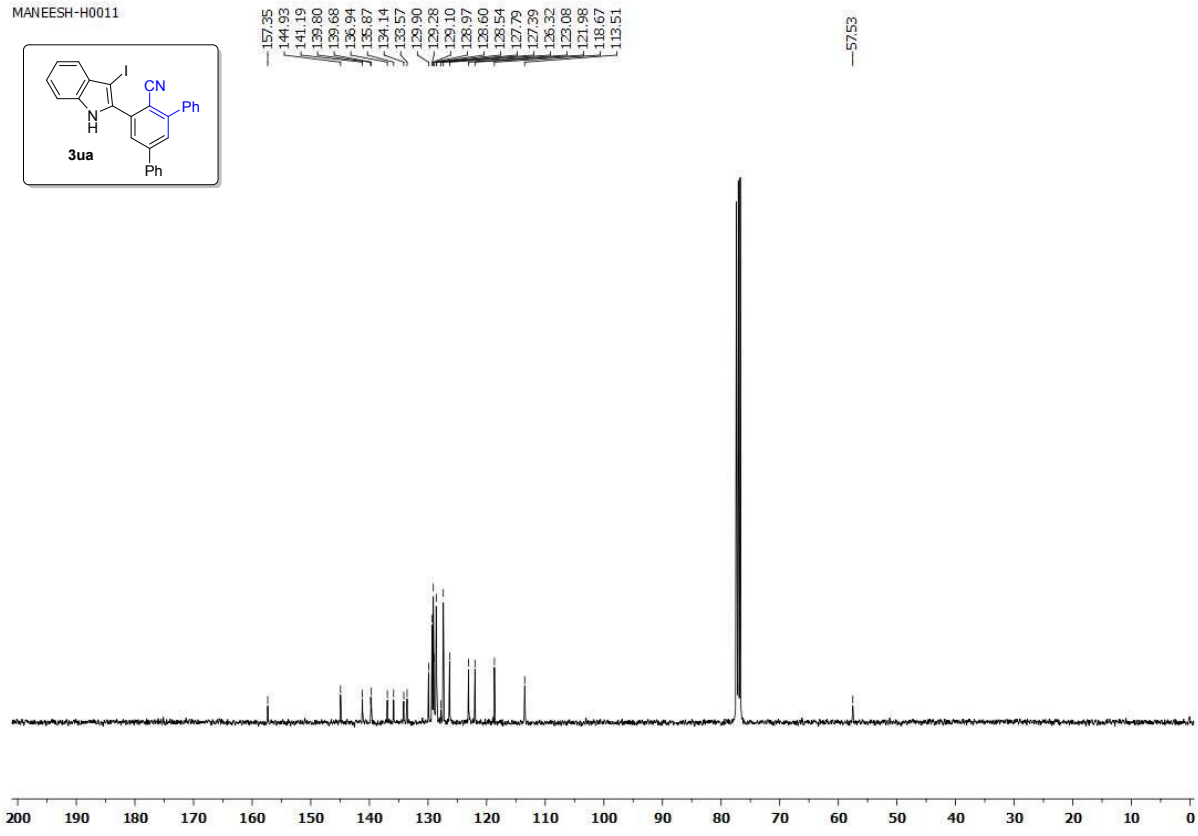

30JAN2020_5 15 (0.293) AM2 (Ar,22000.0,0.00,0.00); ABS
XEVO-G2-XS-QTOF
1: TOF MS ES+
1.13e6
CN
Ph
Br
3sa
436.0524
437.0554
453.0786
354.1275
225.1958
153.1381
149.0232
301.1412
355.1324
418.0628
454.0757
458.0353
474.0109
610.1855
611.1865
684.2042
687.2030
536.1668
600.5214
391.2850
371.1017
329.1727
243.1164
223.0639
154.1231
121.0288
89.5056
279.0941
%
m/z

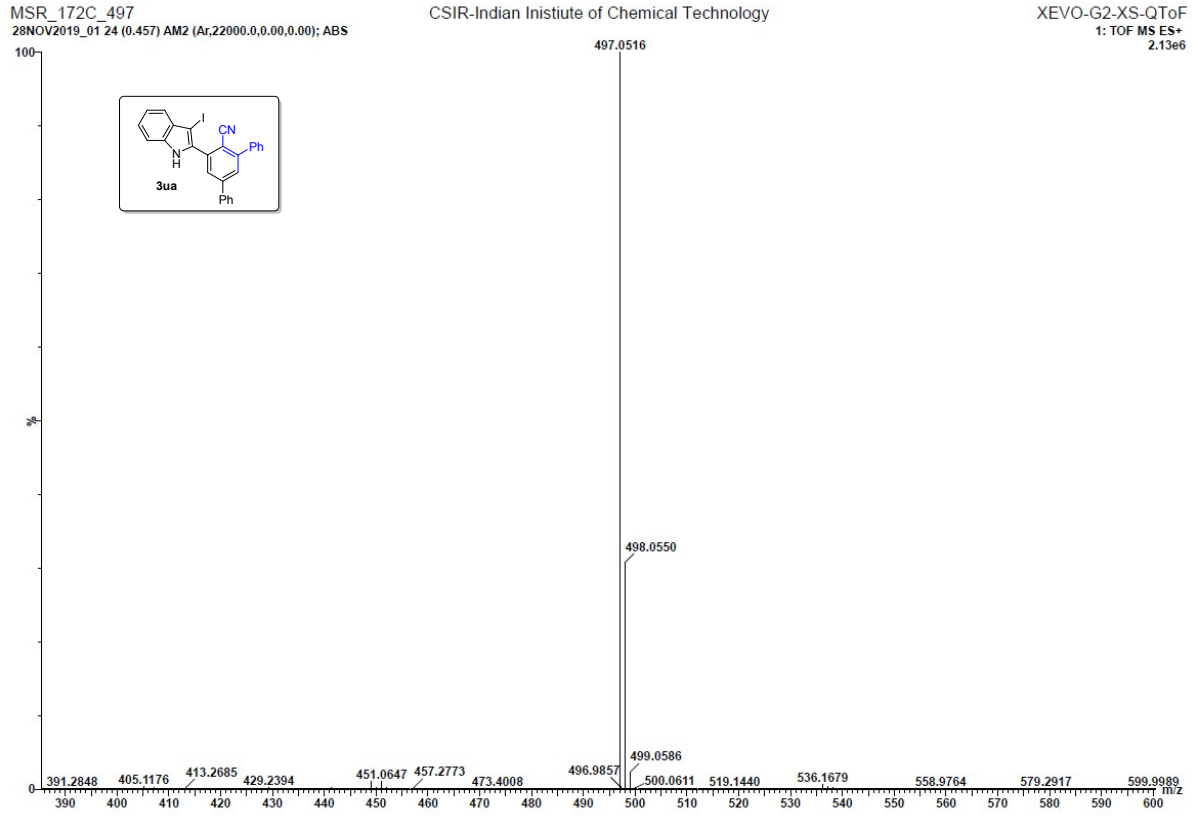

Ph
CN
Ph
3ta
Ph
f1 (ppm)

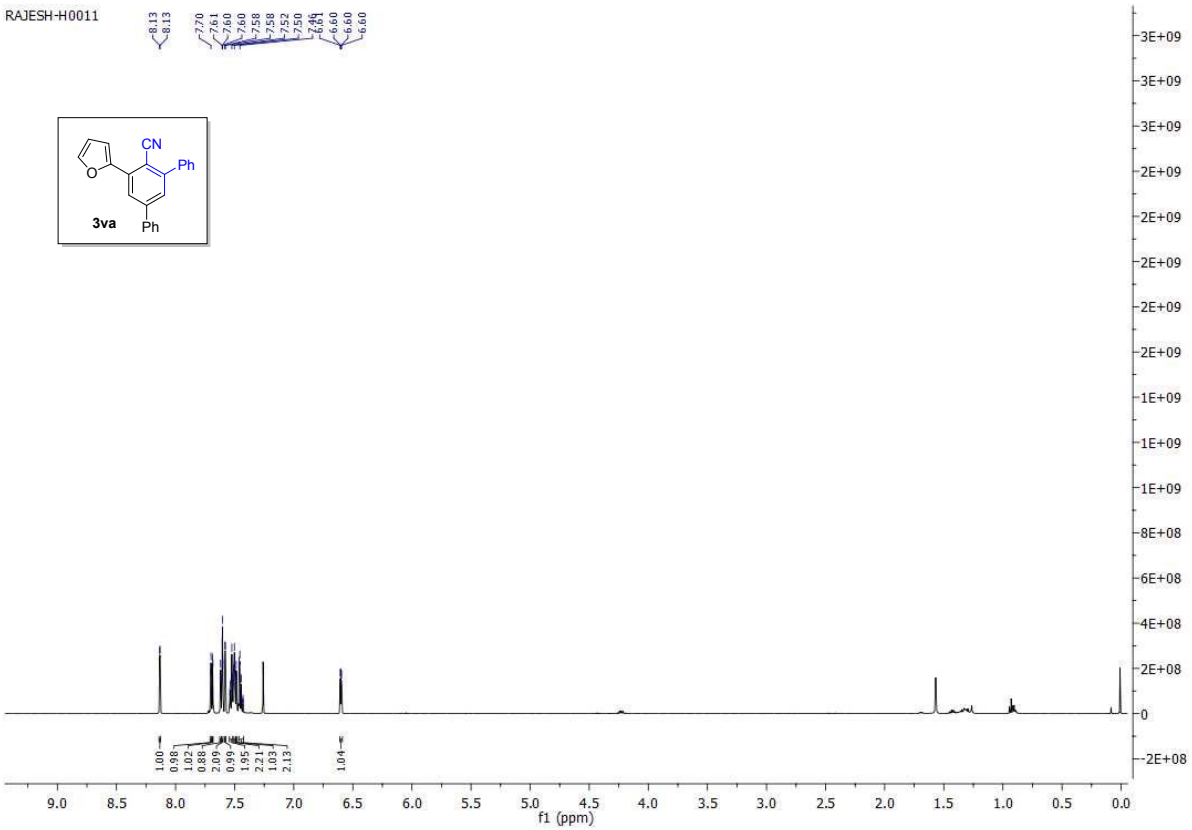

PHANINDRUDU-M0008
146.08
145.09
138.52
138.06
132.09
129.14
128.78
128.45
127.26
122.10
117.25
112.50
95.83
86.24
Ph
CN
Ph
3ta
Ph
4E+08
4E+08
3E+08
2E+08
2E+08
2E+08
1E+08
5E+07
0
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

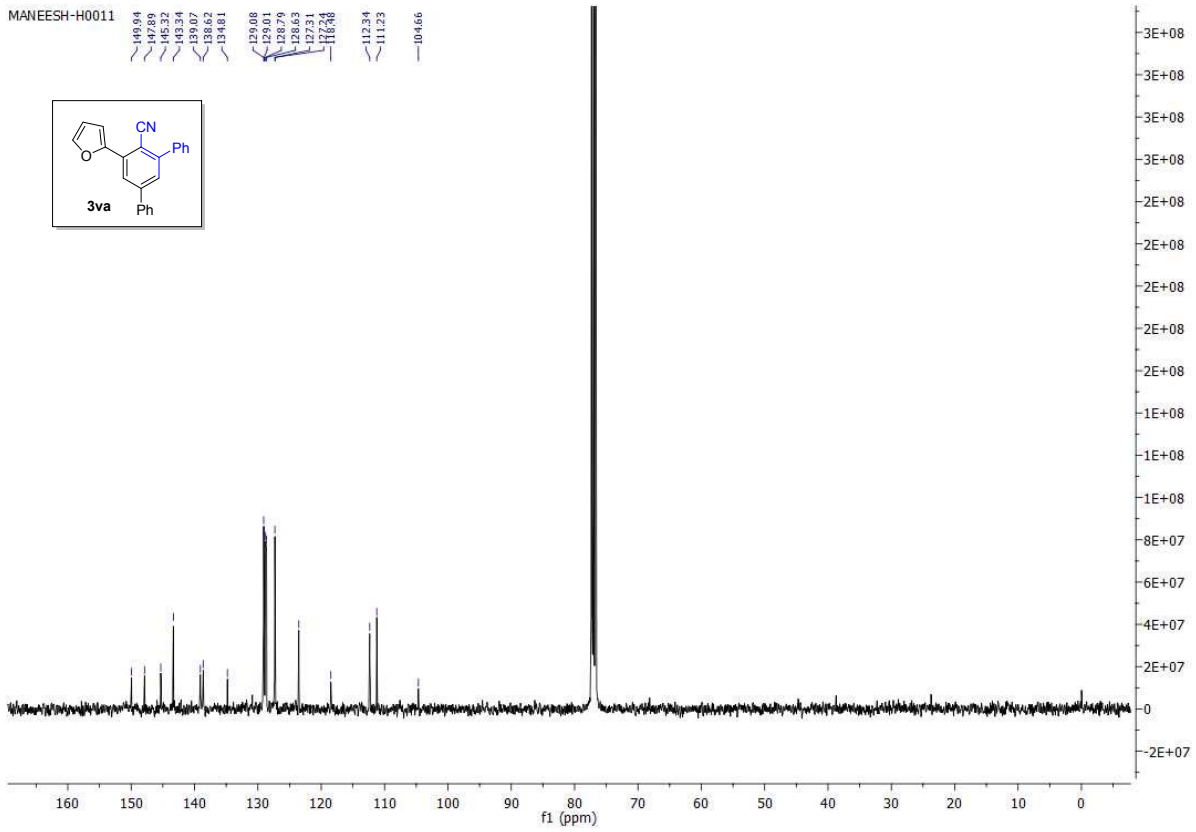

MSR_92_A_365
CSIR-IICT
XEVO-G2-XS-QToF
17FEB2020_14 15 (0.293) AM2 (Ar,22000.0,0.00,0.00); ABS; Cm (9:31-(34:108+1:7))
1: TOF MS ES+
6.04e6
100
%
Ph
CN
Ph
3ta
Ph
279.0927
356.1429
280.0962
357.1461
374.0668
374.1570
375.0706
400.1335
401.1361
446.1750
435.1756
474.2021
488.1841
132.9043
149.0225
167.0497
207.0798
223.0637
249.0899
301.0746
332.1483
0
100
120
140
160
180
200
220
240
260
280
300
320
340
360
380
400
420
440
460
480
500
m/z

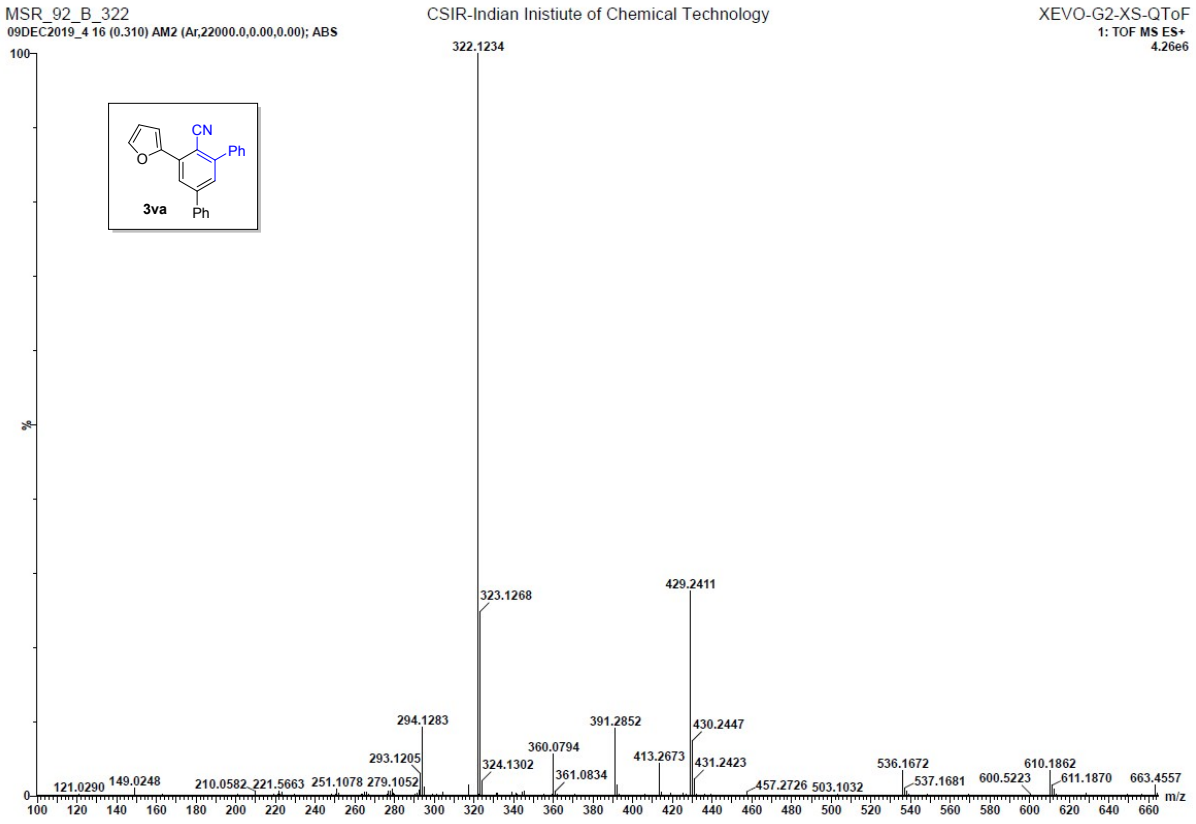

MANEESH-H0011
I
CN
Ph
N
H
3ua
Ph
f1 (ppm)

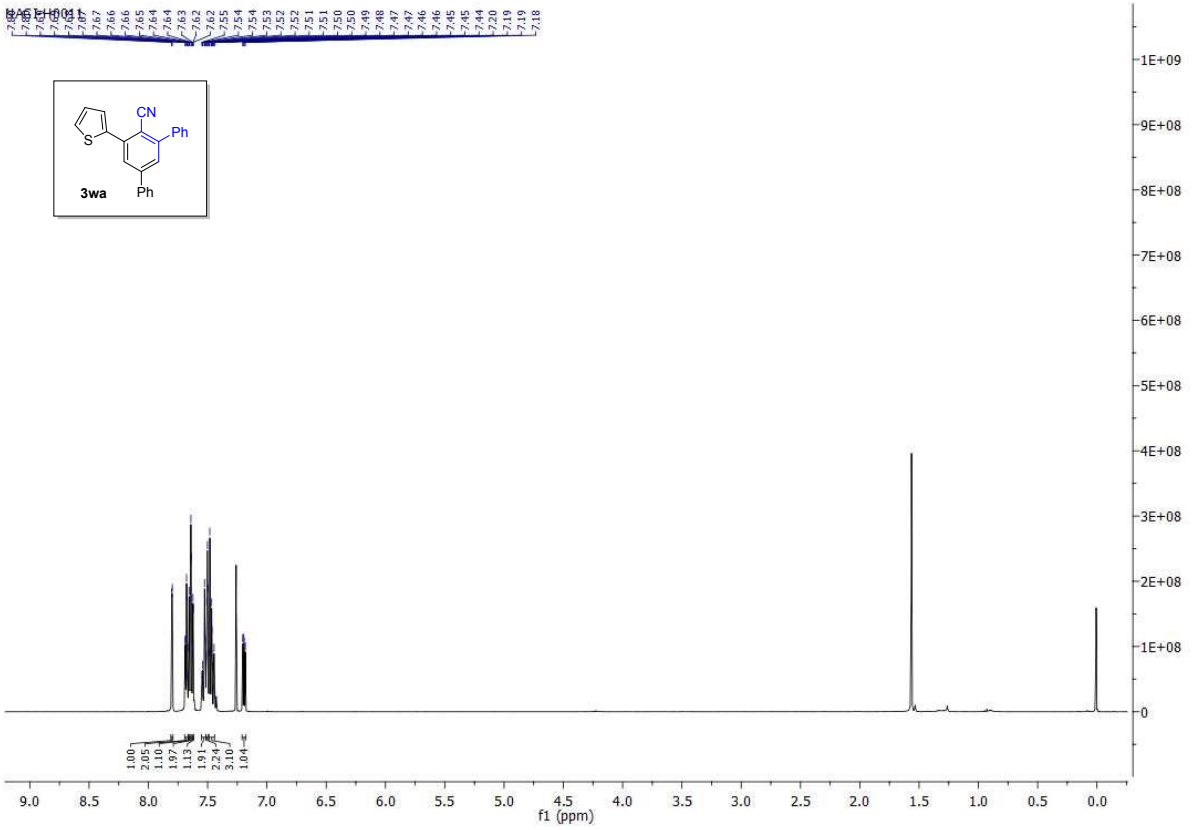

MANEESH-H0011
157.35
144.93
141.19
139.80
139.68
136.94
135.87
134.14
133.57
129.90
129.28
129.10
128.97
128.60
128.54
127.79
127.39
126.32
123.08
121.98
118.67
113.51
57.53
I
CN
Ph
N
H
3ua
Ph

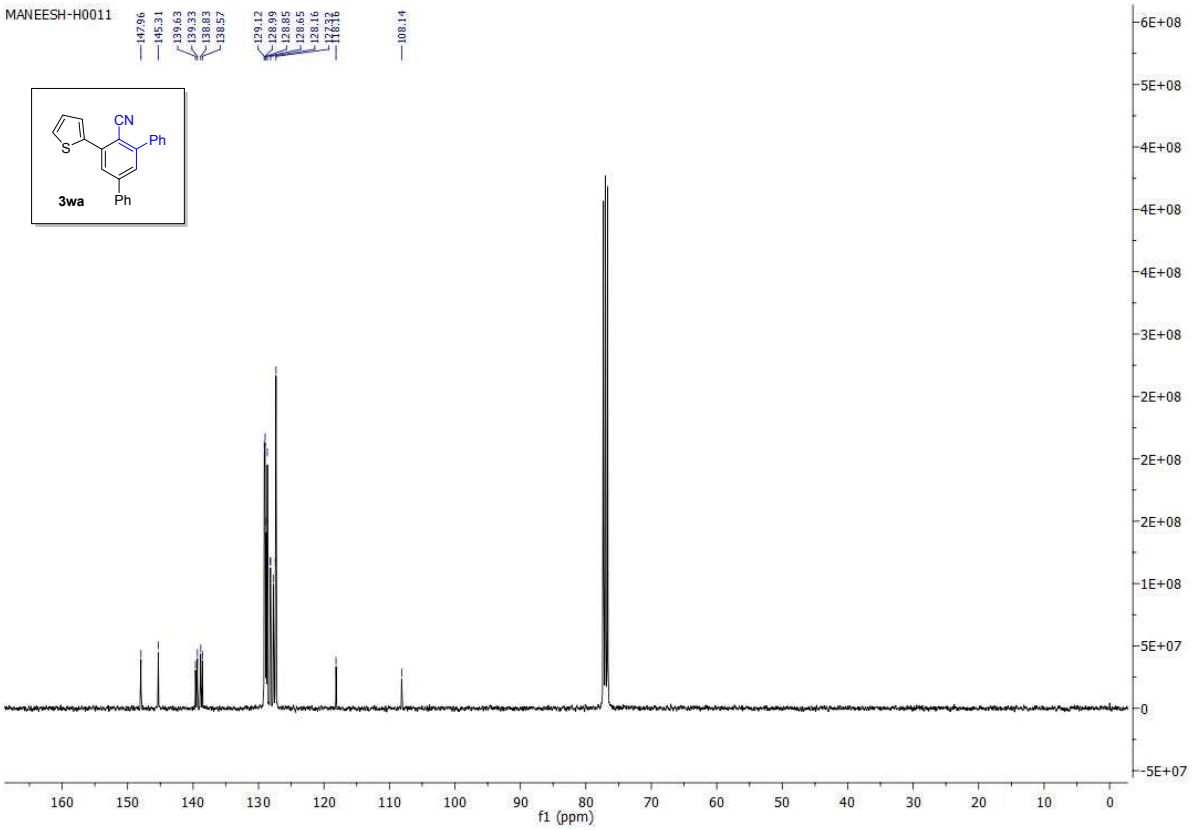

MSR_172C_497
CSIR-Indian Institute of Chemical Technology
XEVO-G2-XS-QToF
28NOV2019_01 24 (0.457) AM2 (Ar,22000.0,0.00,0.00); ABS
1: TOF MS ES+
2.13e6
497.0516
498.0550
499.0586
3ua
m/z

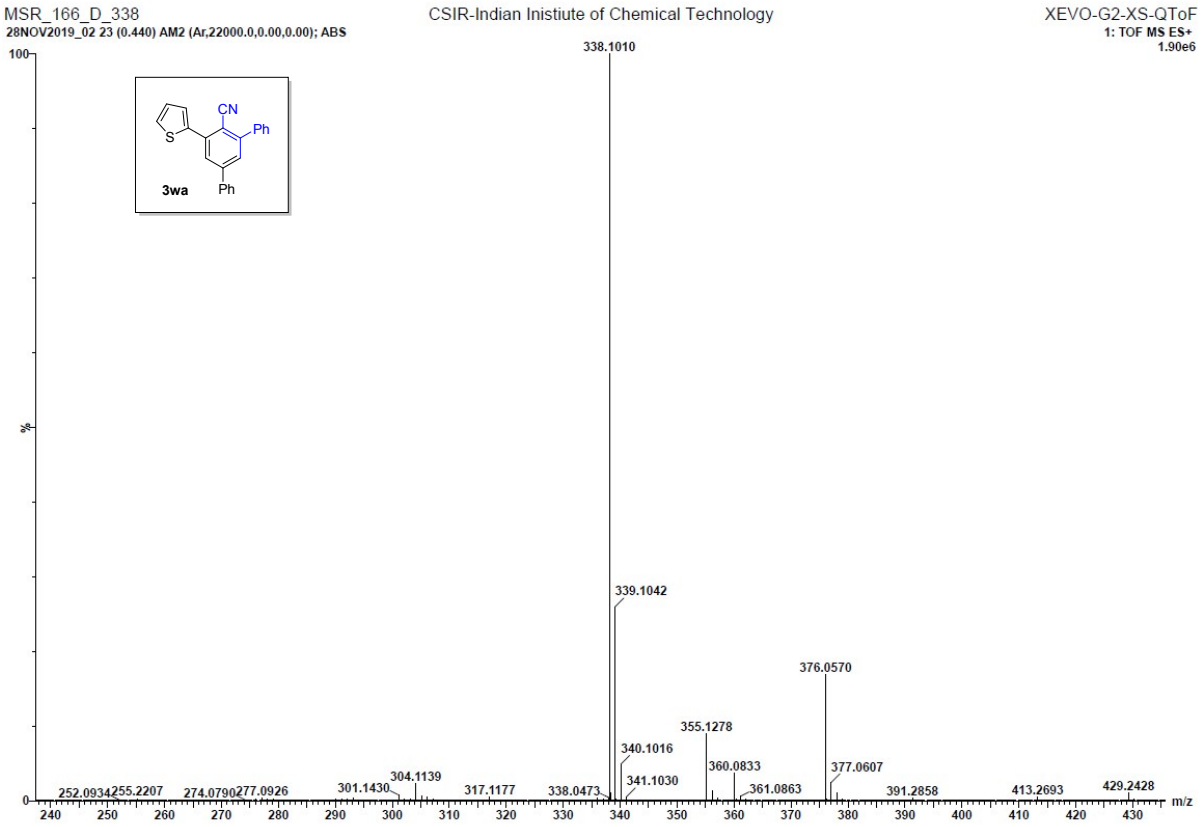

RAJESH-H0011
3va
f1 (ppm)

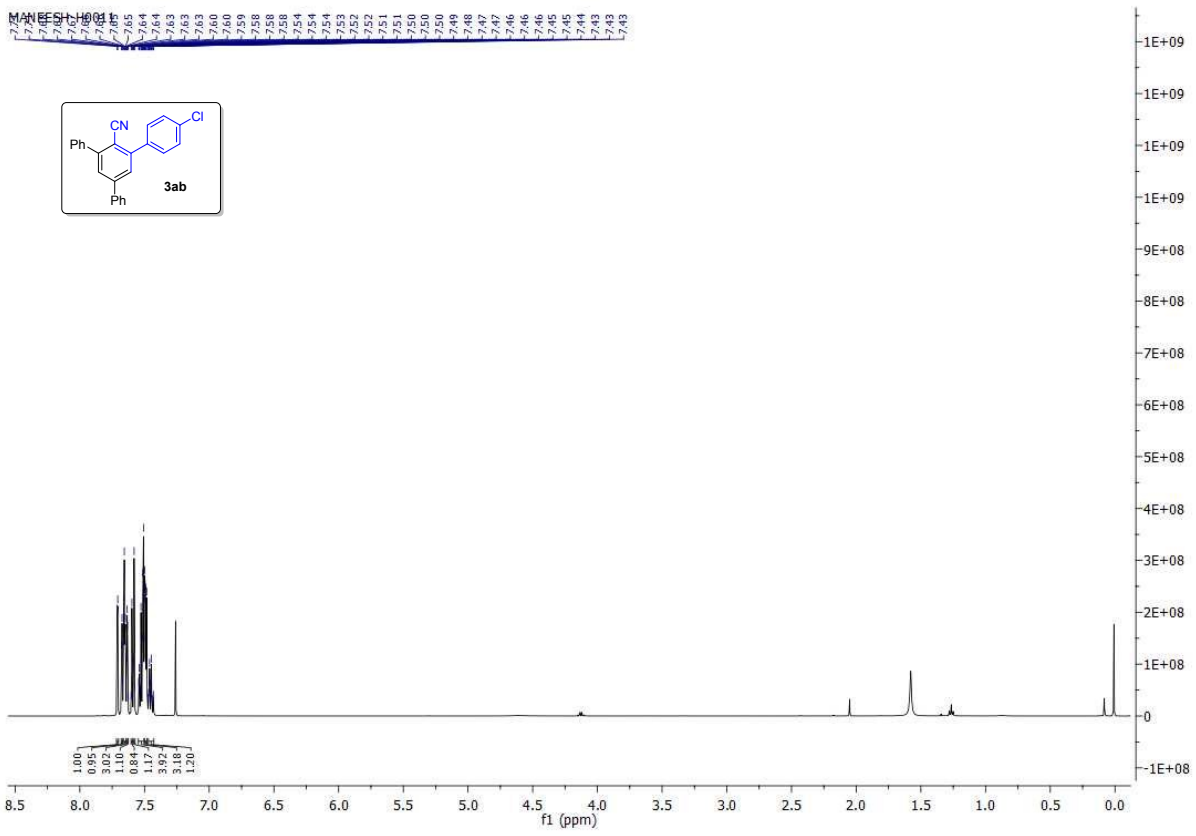

MANEESH-H0011
149.94
147.89
145.32
143.34
139.07
138.62
134.81
129.08
129.01
128.79
128.63
127.31
127.24
118.48
112.34
111.23
104.66
CN
Ph
3va
Ph
f1 (ppm)

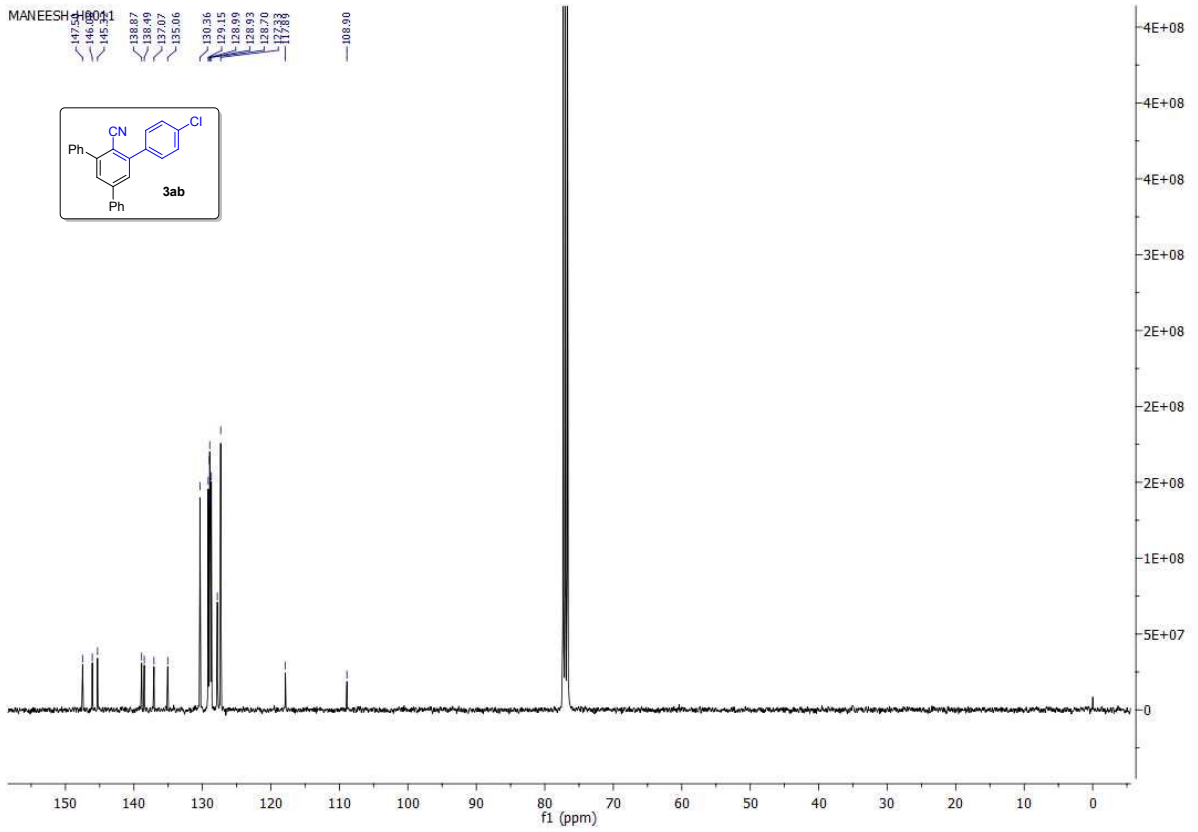

MSR_92_B_322
09DEC2019_4 16 (0.310) AM2 (Ar,22000.0,0.00,0.00); ABS
CSIR-Indian Inistiute of Chemical Technology
XEVO-G2-XS-QToF
1: TOF MS ES+
4.26e6
CN
Ph
3va
Ph
%
m/z
322.1234
323.1268
429.2411
294.1283
391.2852
430.2447
360.0794
293.1205
324.1302
413.2673
431.2423
361.0834
121.0290
149.0248
210.0582
221.5663
251.1078
279.1052
457.2726
503.1032
536.1672
537.1681
600.5223
610.1862
611.1870
663.4557

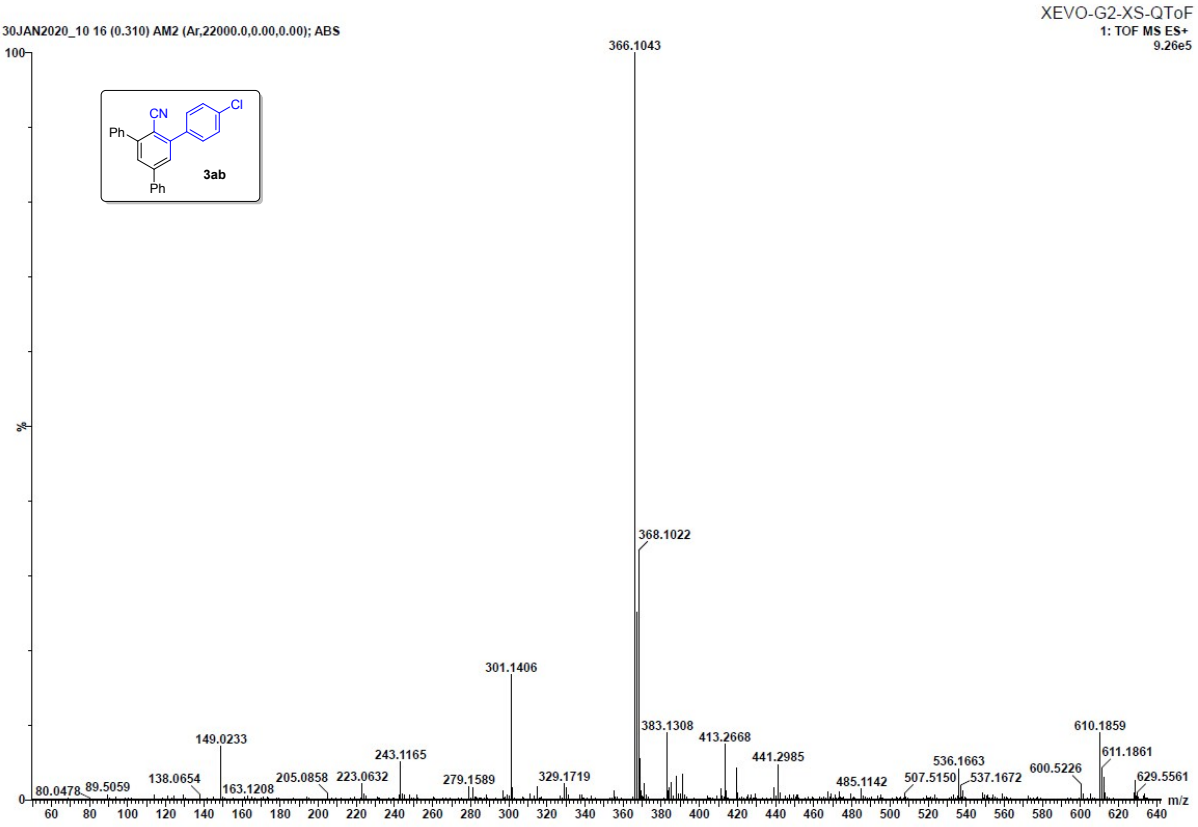

MANEESH-H0011
CN
Ph
S
3wa
Ph
1.00
2.05
1.10
1.97
1.13
1.91
2.24
3.10
1.04
f1 (ppm)

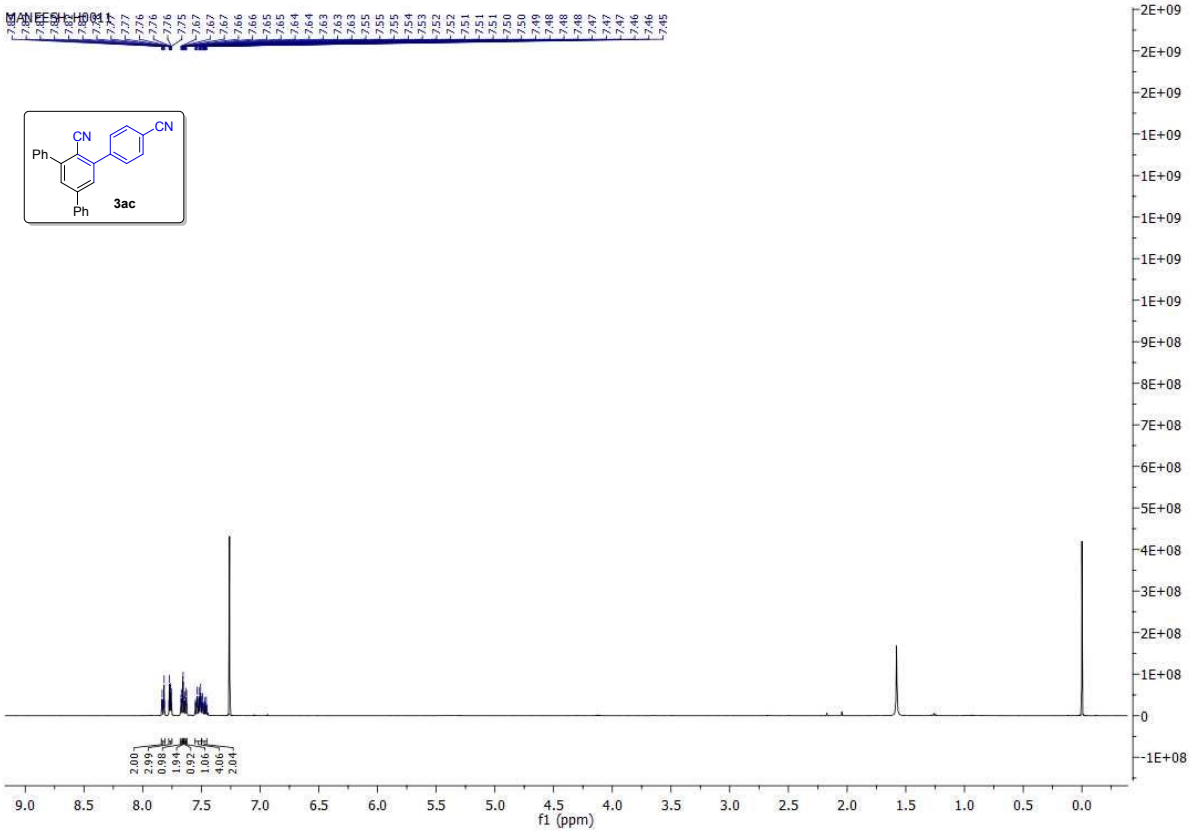

MANEESH-H0011
147.96
145.31
139.63
139.33
138.83
138.57
129.12
128.99
128.85
128.65
128.16
127.32
118.16
108.14
CN
Ph
S
3wa
Ph
f1 (ppm)

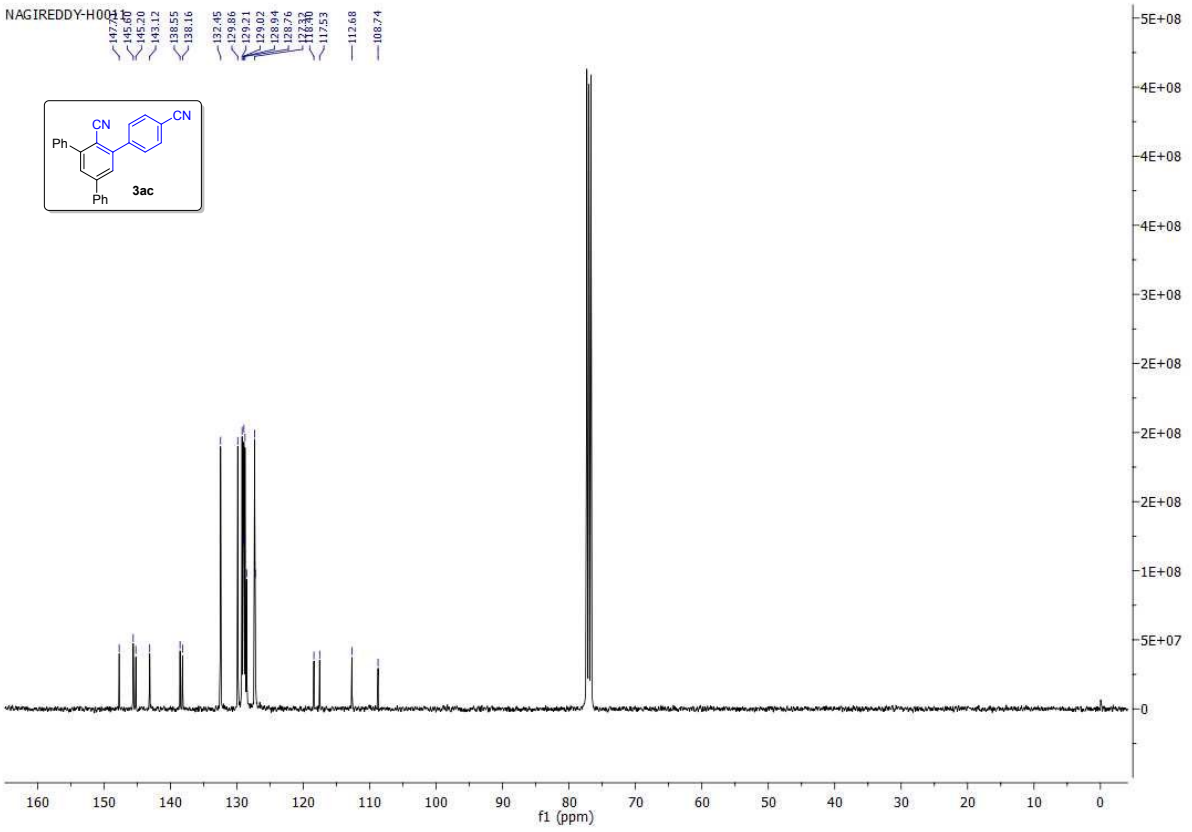

MSR_166_D_338
CSIR-Indian Inistiute of Chemical Technology
XEVO-G2-XS-QToF
28NOV2019_02 23 (0.440) AM2 (Ar,22000.0,0.00,0.00); ABS
1: TOF MS ES+
1.90e6
3wa
338.1010
339.1042
376.0570
355.1278
340.1016
360.0833
377.0607
341.1030
304.1139
252.0934
255.2207
274.0790
277.0926
301.1430
317.1177
338.0473
361.0863
391.2858
413.2693
429.2428
m/z

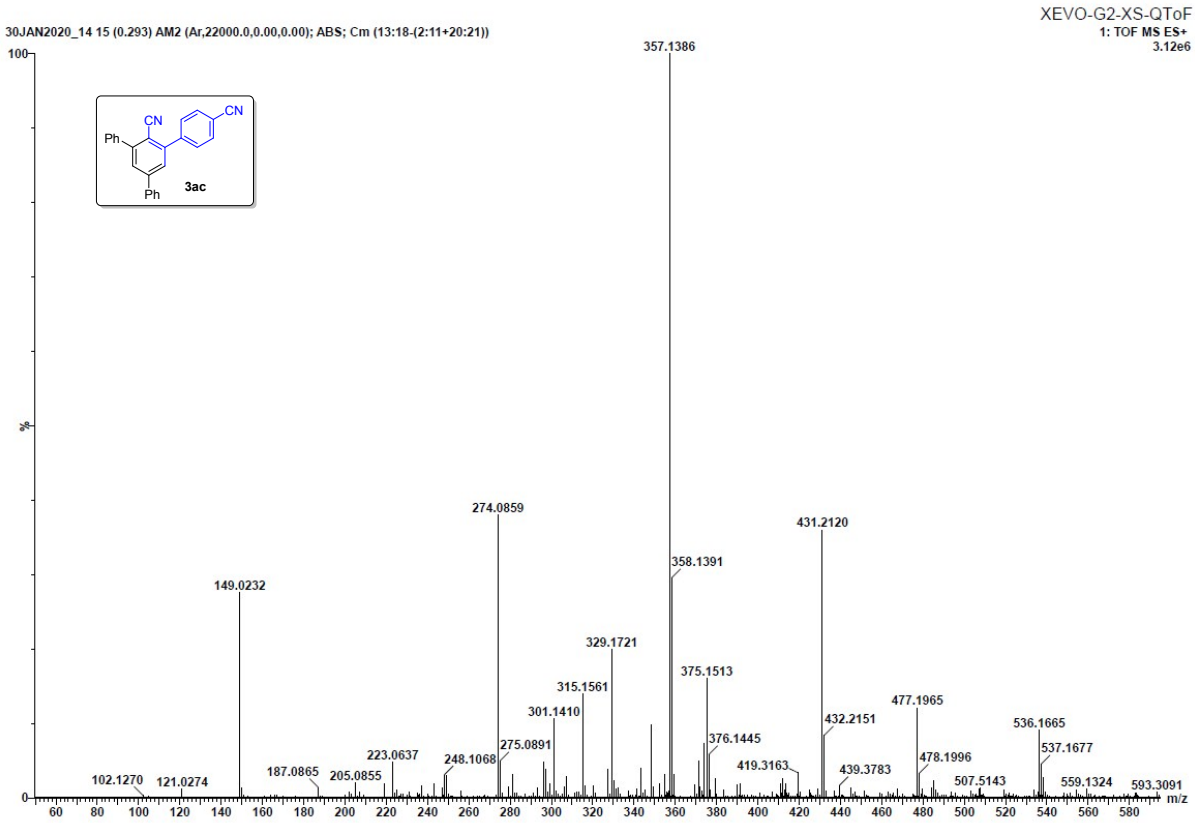

MANEESH_H001
3ab
f1 (ppm)

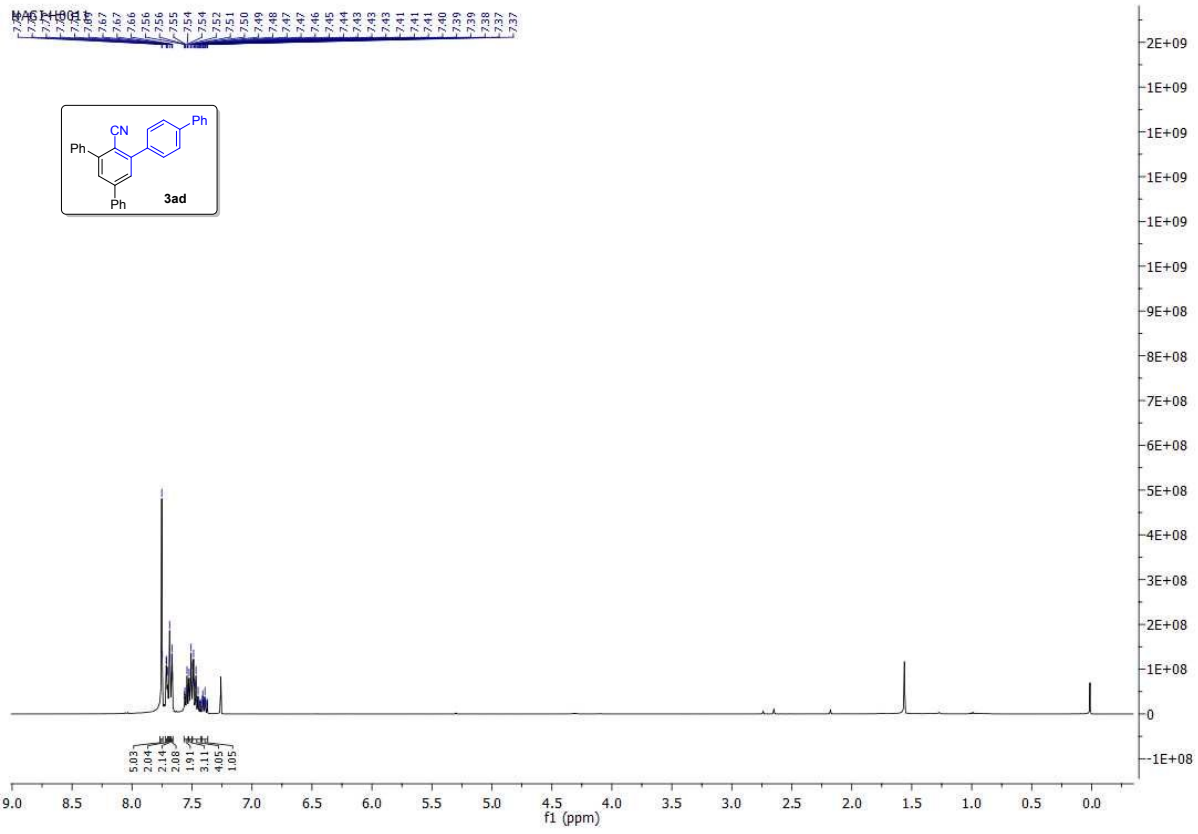

MANEESH-JH011
147.54
146.01
145.11
138.87
138.49
137.07
135.06
130.36
129.15
128.99
128.93
128.70
127.33
117.89
108.90
CN
Cl
Ph
Ph
3ab
4E+08
4E+08
4E+08
3E+08
2E+08
2E+08
2E+08
1E+08
5E+07
0
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

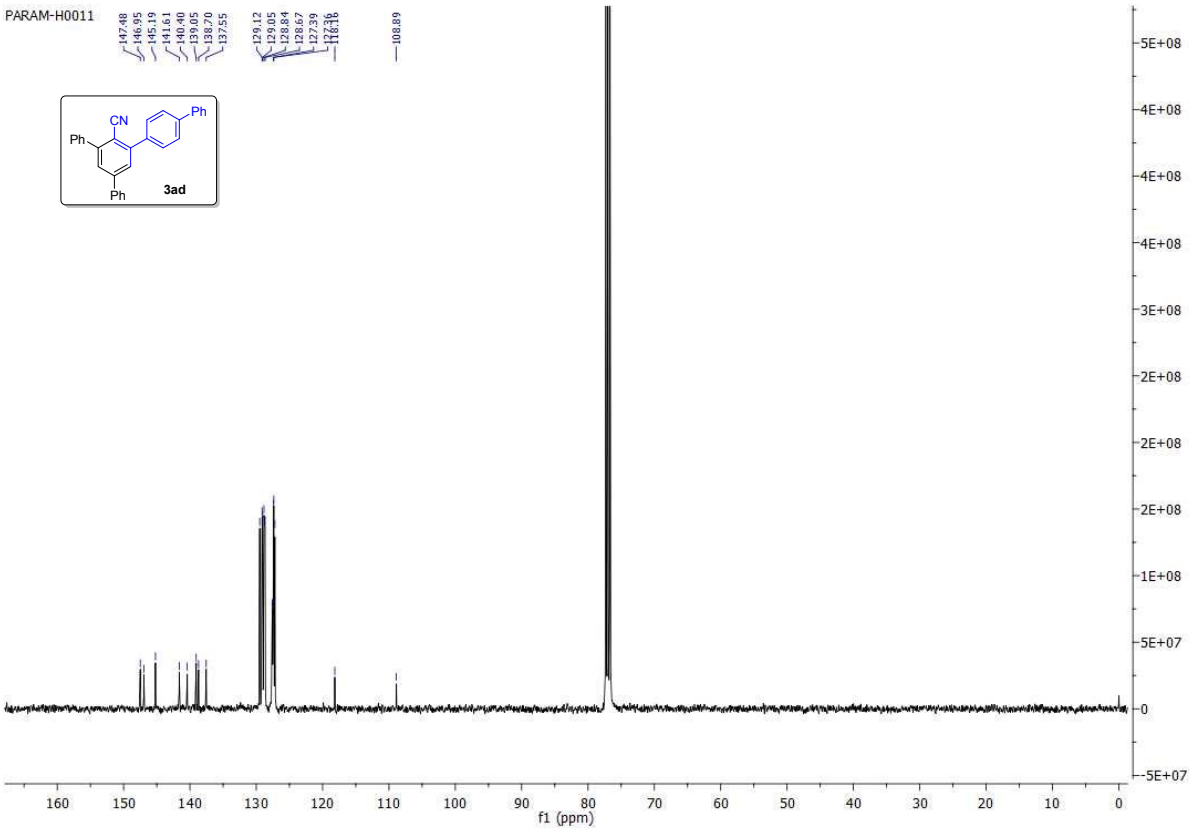

30JAN2020_10 16 (0.310) AM2 (Ar,22000.0,0.00,0.00); ABS
XEVO-G2-XS-QToF
1: TOF MS ES+
9.26e5
100
%
0
CN
Cl
Ph
Ph
3ab
366.1043
368.1022
301.1406
383.1308
413.2668
441.2985
610.1859
611.1861
629.5561
149.0233
243.1165
138.0654
163.1208
205.0858
223.0632
279.1589
329.1719
485.1142
507.5150
536.1663
537.1672
600.5226
80.0478
89.5059
m/z
60
80
100
120
140
160
180
200
220
240
260
280
300
320
340
360
380
400
420
440
460
480
500
520
540
560
580
600
620
640

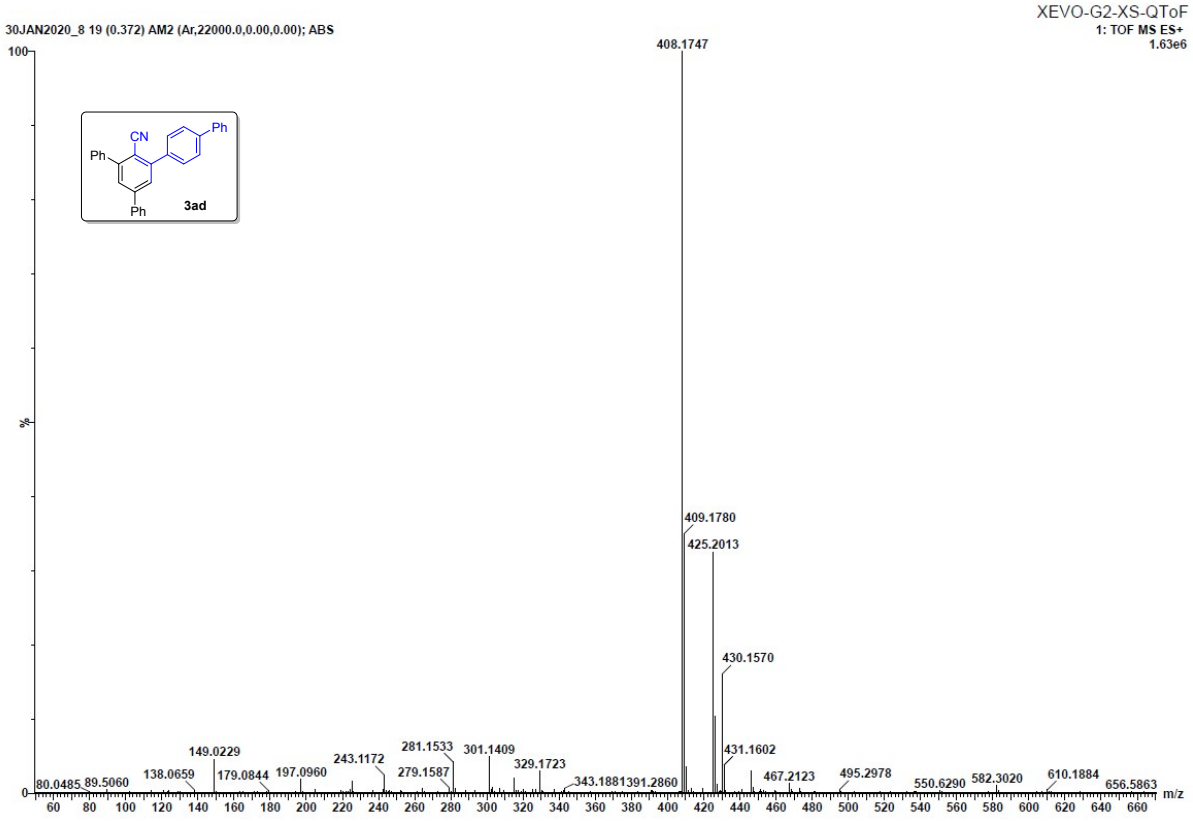

MANEESH-H0041
CN
CN
Ph
Ph
3ac
f1 (ppm)

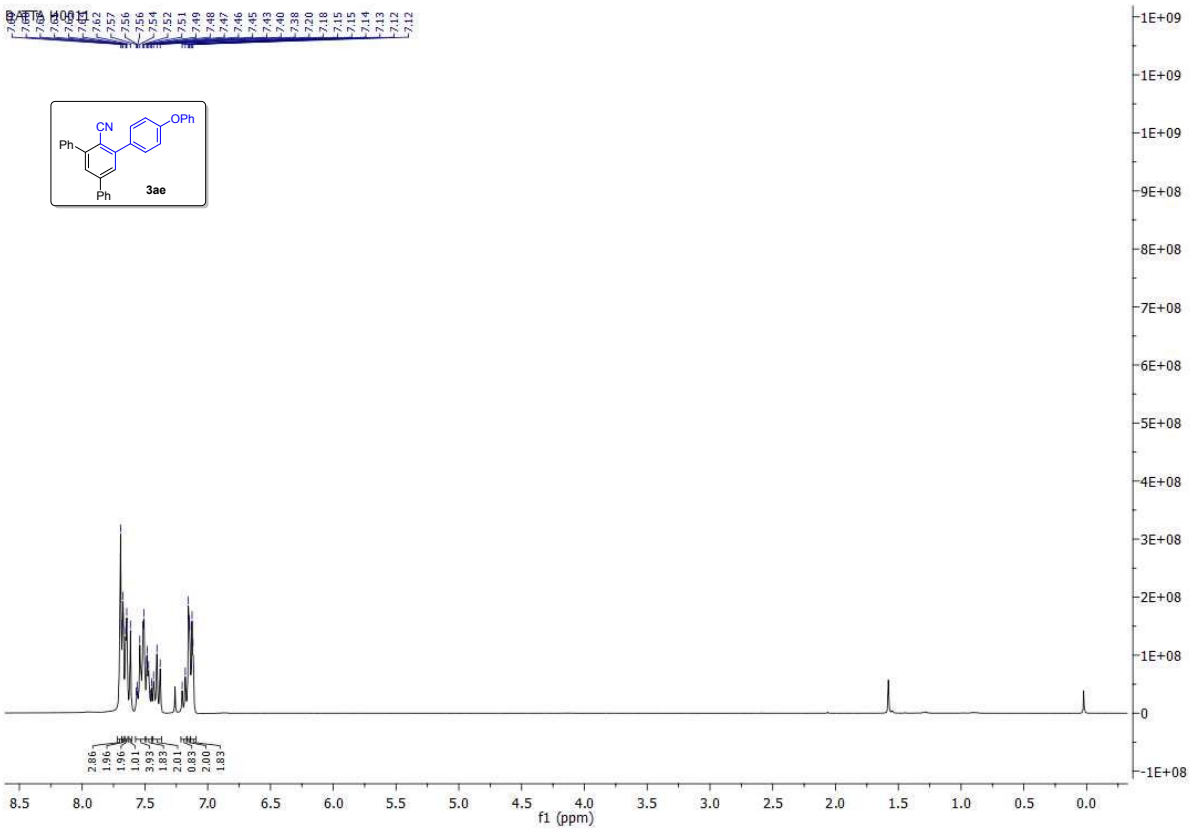

NAGIREDDY-H0011
147.71
145.60
145.20
143.12
138.55
138.16
132.45
129.86
129.21
129.02
128.94
128.76
127.32
118.30
117.53
112.68
108.74
CN
CN
Ph
Ph
3ac
f1 (ppm)

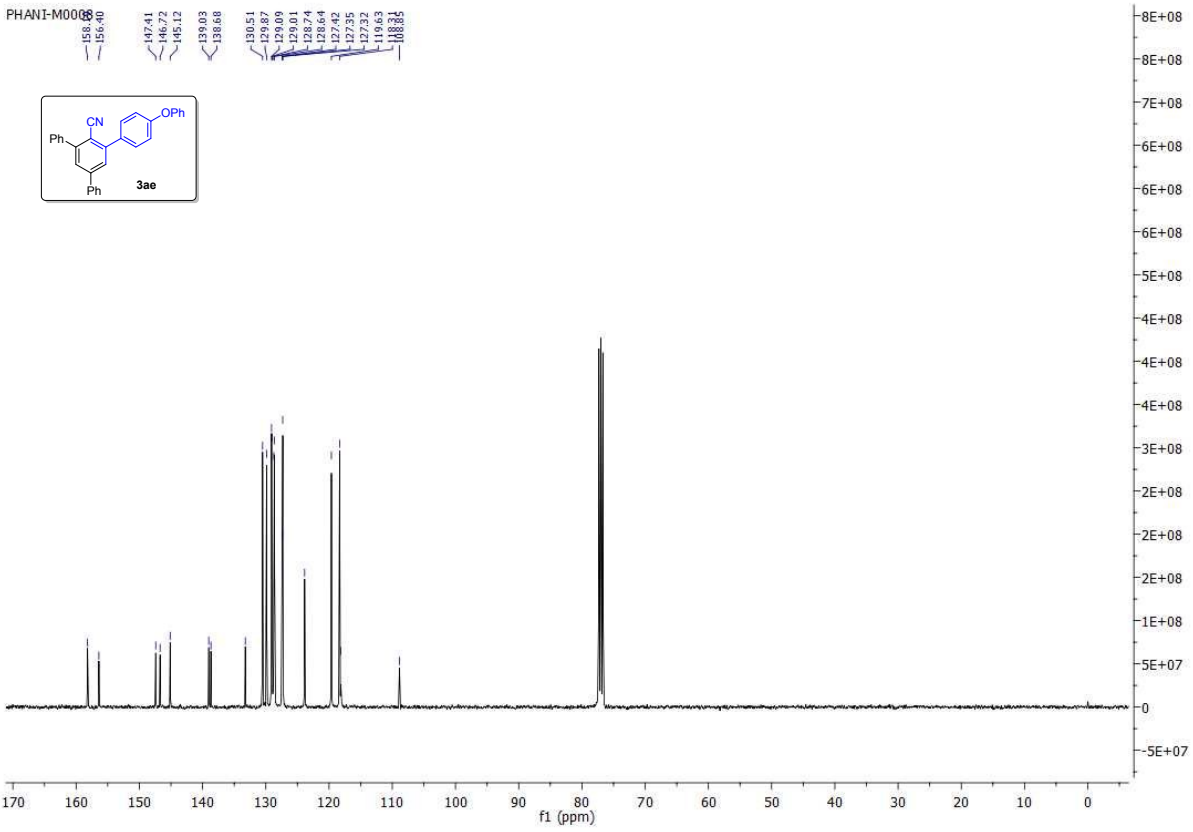

XEVO-G2-XS-QToF
1: TOF MS ES+
3.12e6
30JAN2020_14 15 (0.293) AM2 (Ar,22000.0,0.00,0.00); ABS; Cm (13:18-(2:11+20:21))
100
%
0
CN
CN
Ph
Ph
3ac
357.1386
274.0859
431.2120
358.1391
149.0232
329.1721
375.1513
315.1561
477.1965
301.1410
432.2151
536.1665
376.1445
275.0891
537.1677
223.0637
248.1068
478.1996
419.3163
439.3783
187.0865
205.0855
102.1270
121.0274
507.5143
559.1324
593.3091
m/z
60
80
100
120
140
160
180
200
220
240
260
280
300
320
340
360
380
400
420
440
460
480
500
520
540
560
580

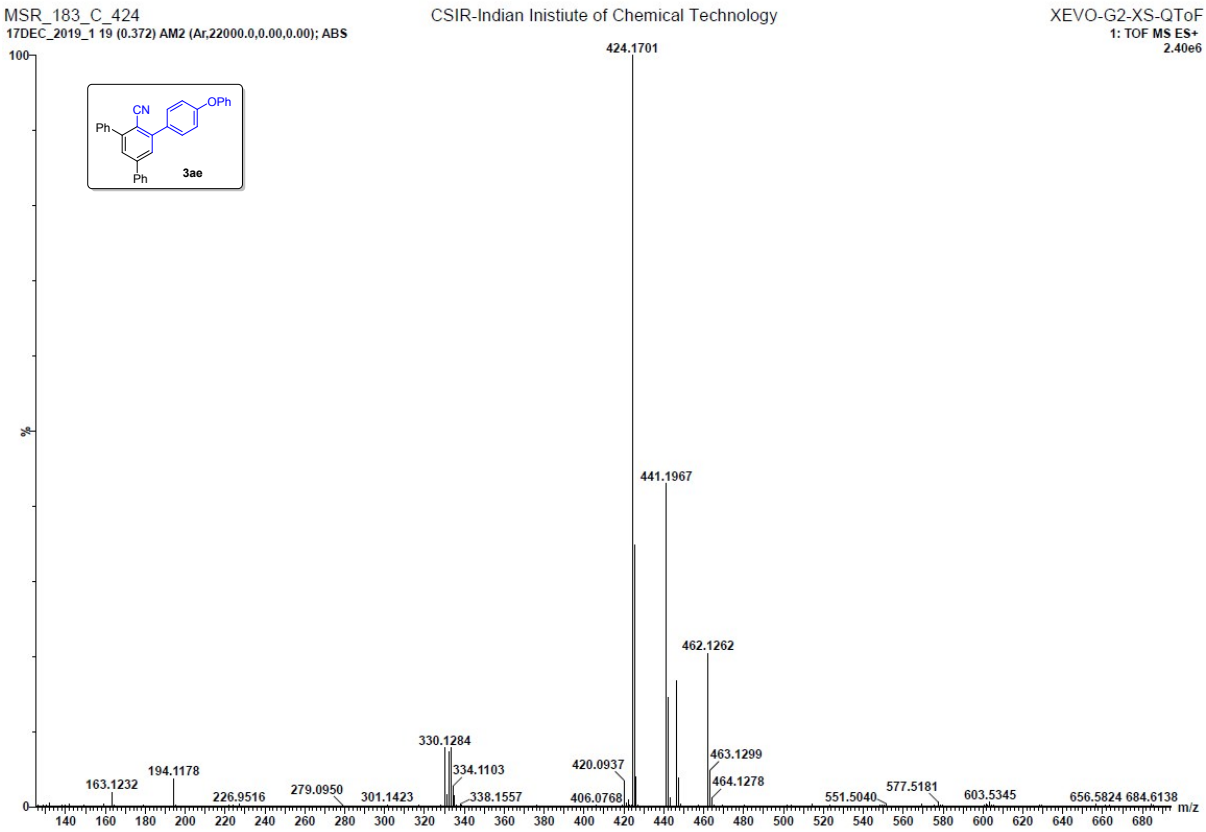

MAG1-H-001-1
CN
Ph
Ph
Ph
3ad
2E+09
1E+09
1E+09
1E+09
1E+09
1E+09
1E+09
9E+08
8E+08
7E+08
6E+08
5E+08
4E+08
3E+08
2E+08
1E+08
0
-1E+08
5.03
2.04
2.14
2.08
1.91
3.11
4.05
1.05
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

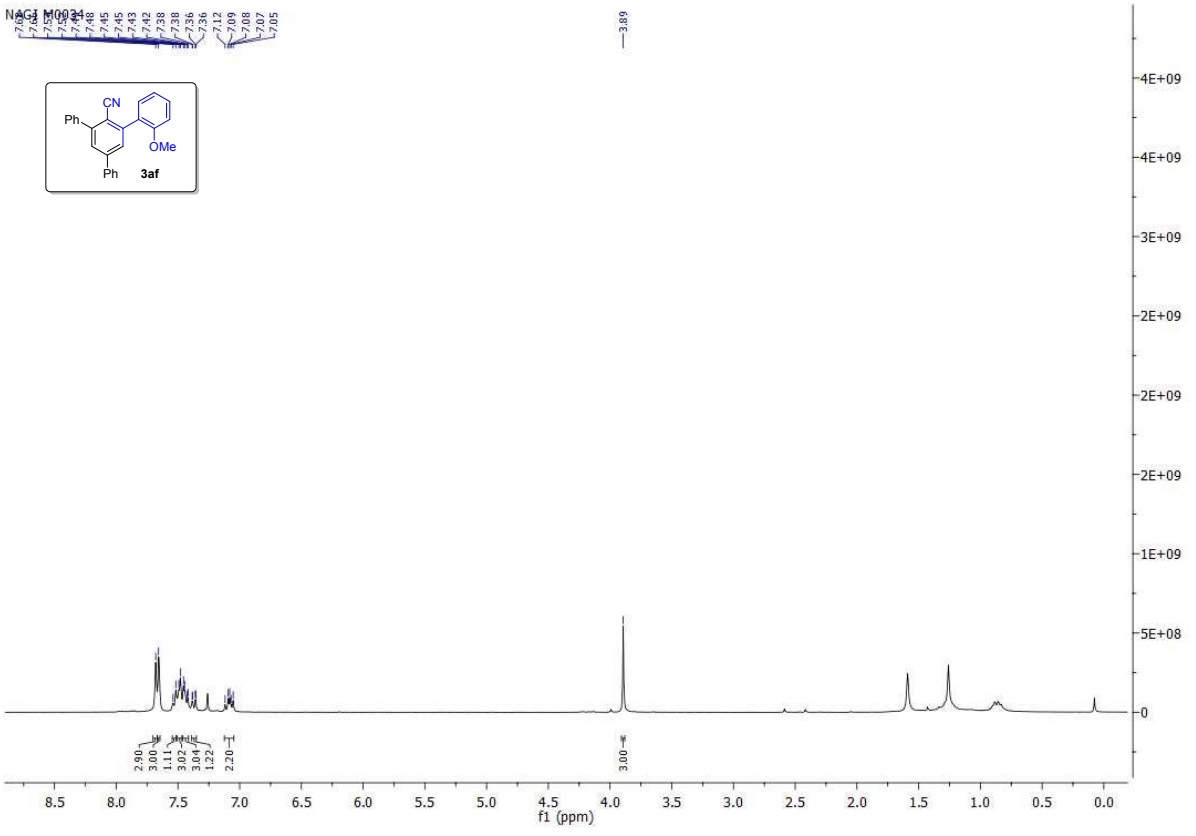

PARAM-H0011
147.48
146.95
145.19
141.61
140.40
139.05
138.70
137.55
129.12
129.05
128.84
128.67
127.39
118.16
108.89
CN
Ph
Ph
Ph
3ad
f1 (ppm)

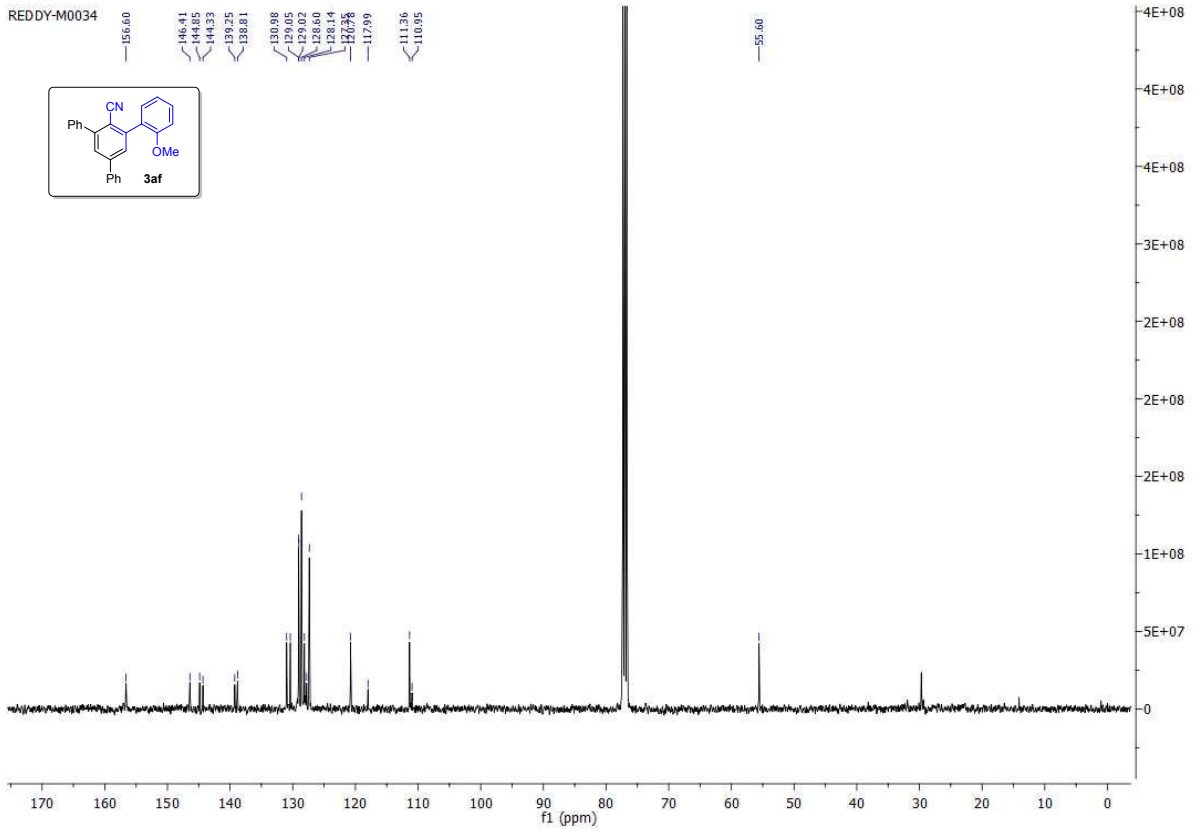

30JAN2020_8 19 (0.372) AM2 (Ar,22000.0,0.00,0.00); ABS
XEVO-G2-XS-QToF
1: TOF MS ES+
1.63e6
408.1747
409.1780
425.2013
430.1570
431.1602
CN
Ph
Ph
Ph
3ad
m/z

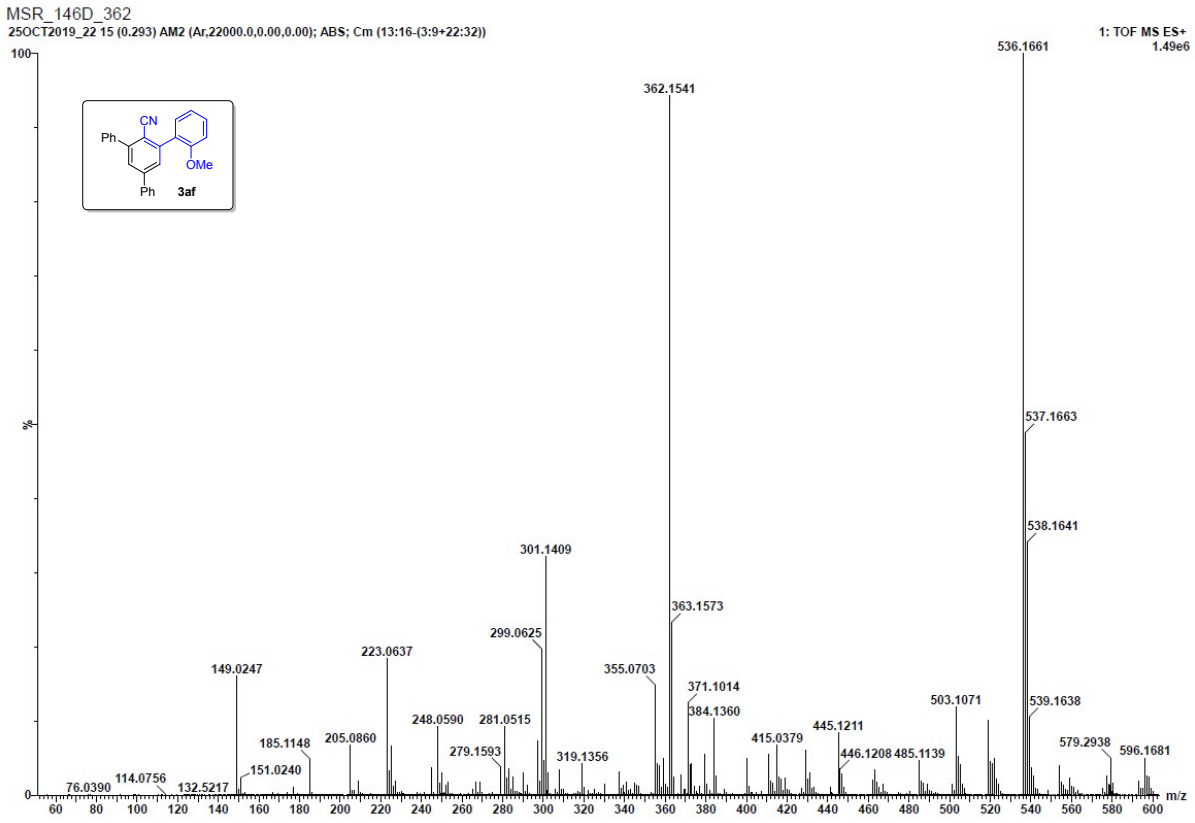

CN
OPh
Ph
Ph
3ae
f1 (ppm)

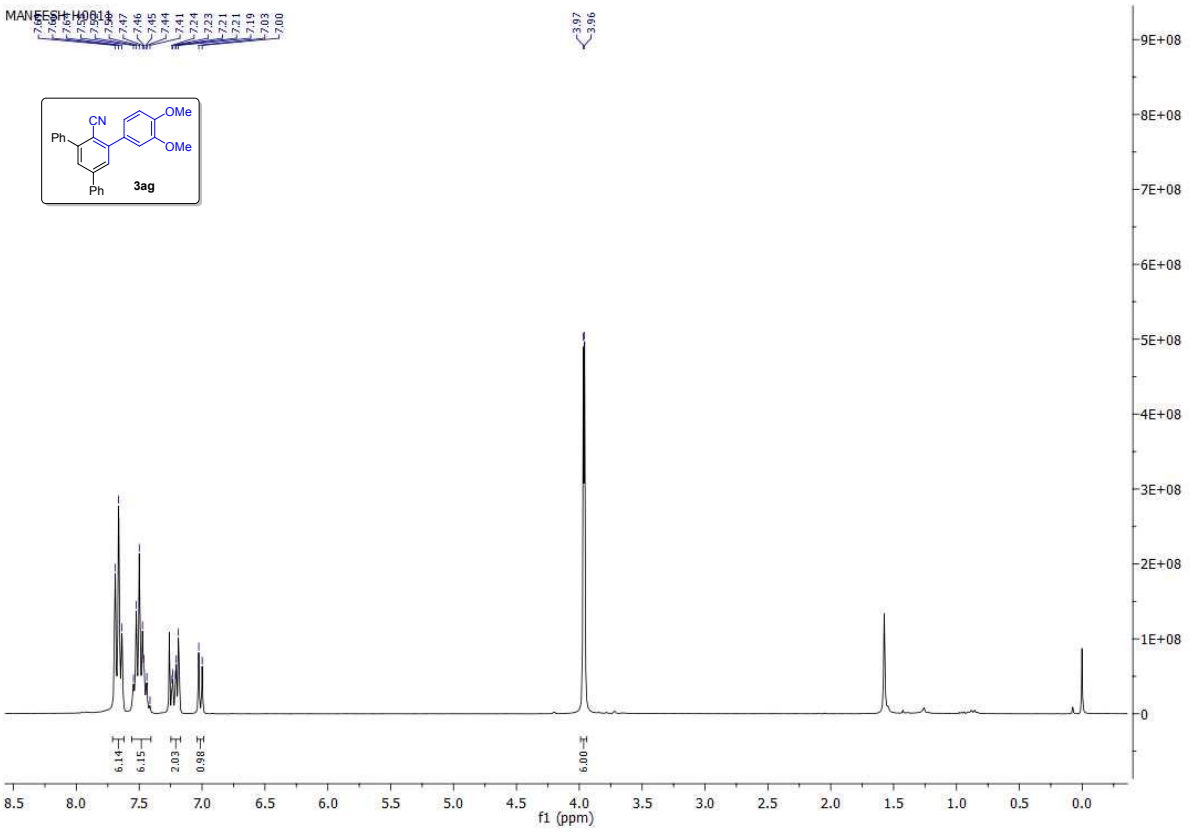

CN
OPh
Ph
Ph
3ae
f1 (ppm)

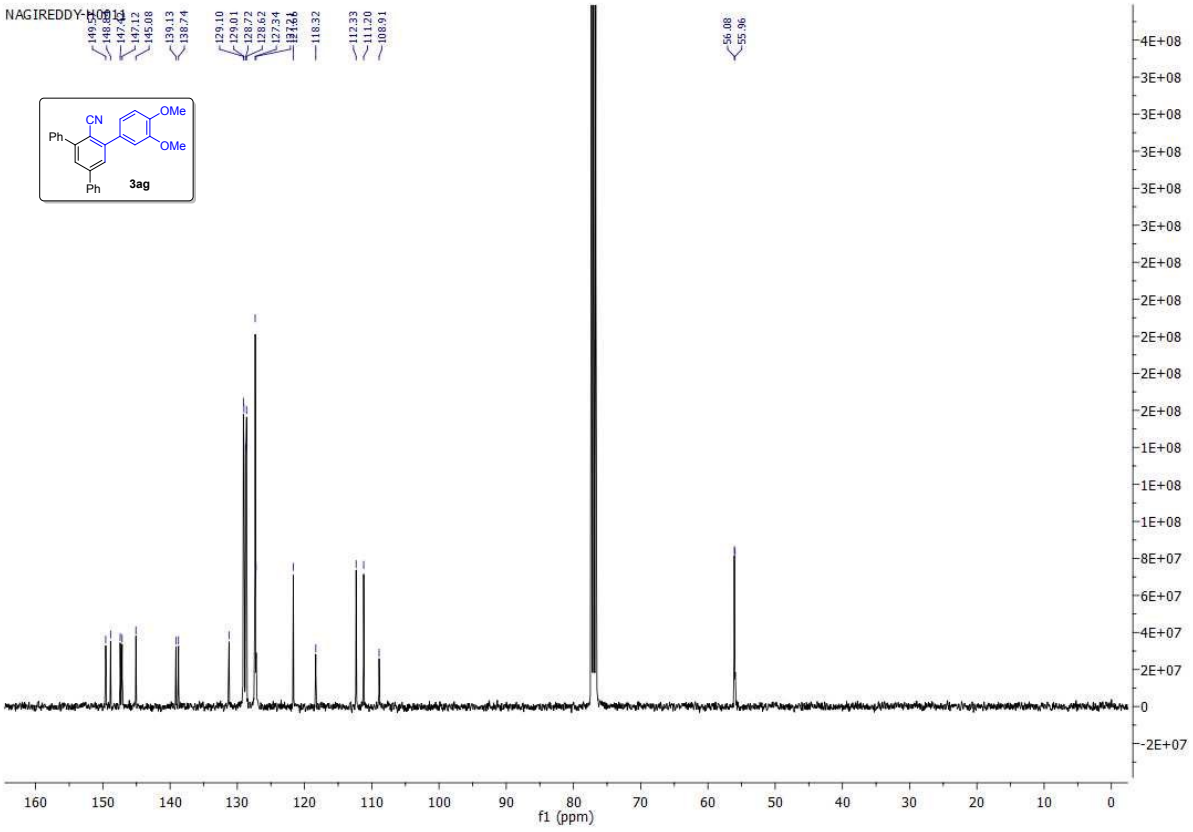

MSR_183_C_424
CSIR-Indian Inistiute of Chemical Technology
XEVO-G2-XS-QToF
17DEC_2019_1 19 (0.372) AM2 (Ar,22000.0,0.00,0.00); ABS
1: TOF MS ES+
2.40e6
424.1701
441.1967
462.1262
330.1284
334.1103
420.0937
463.1299
464.1278
194.1178
163.1232
226.9516
279.0950
301.1423
338.1557
406.0768
551.5040
577.5181
603.5345
656.5824 684.6138
m/z
%
CN
OPh
Ph
Ph
3ae

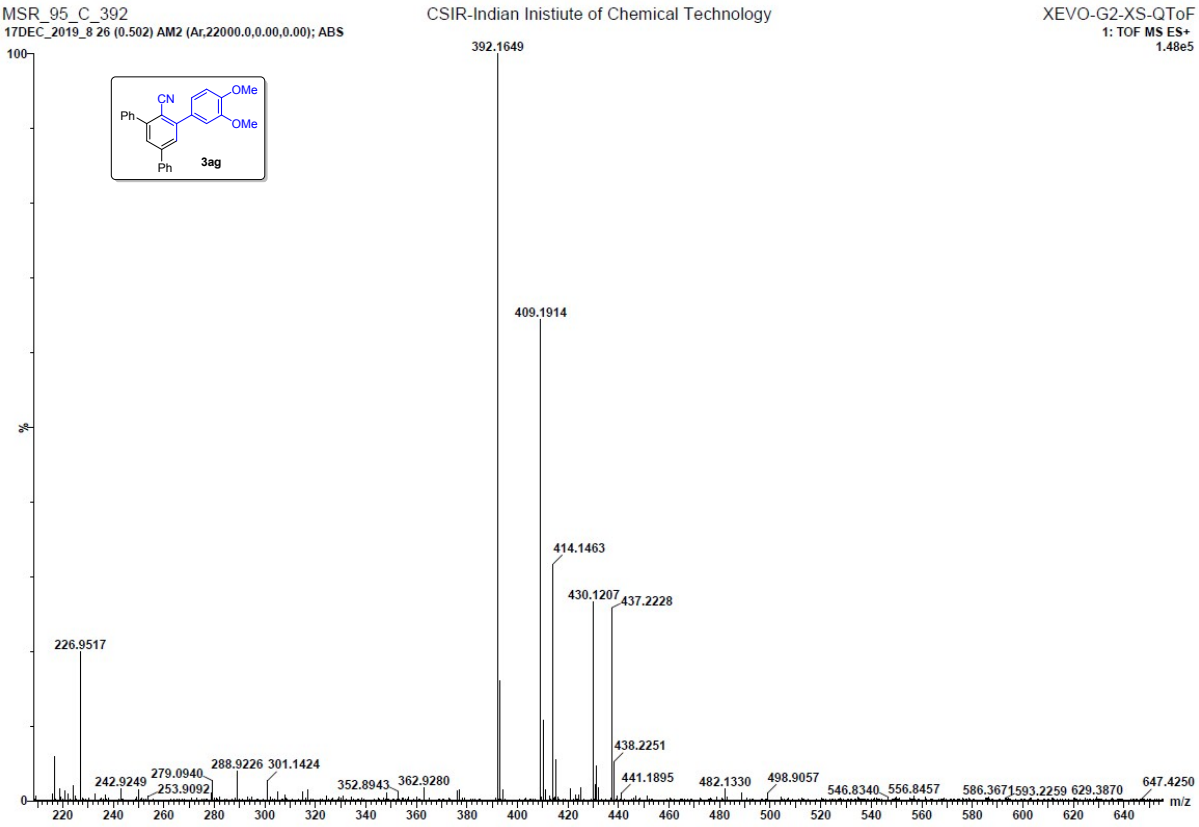

NAG1 M0034
3.89
CN
Ph
OMe
Ph
3af
2.90
3.00
1.11
3.02
3.04
1.22
2.20
3.00
f1 (ppm)

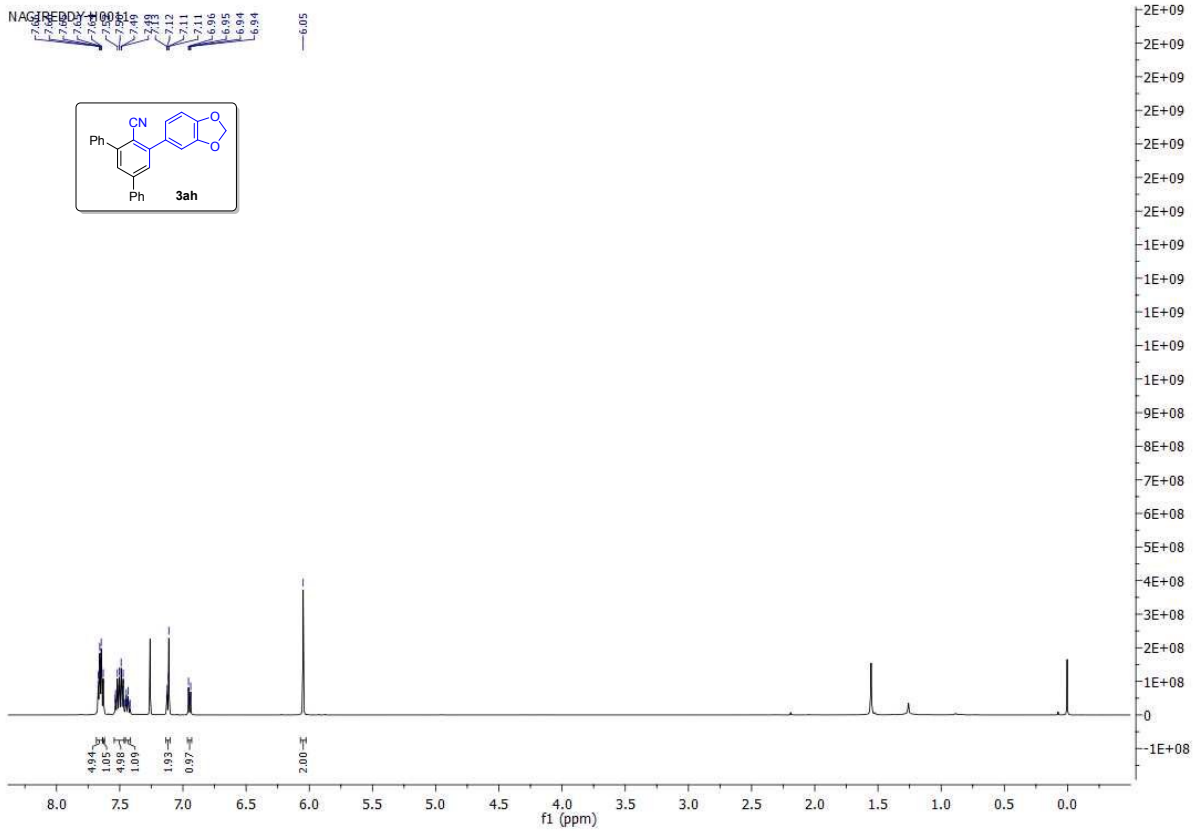

REDDY-M0034
156.60
146.41
144.85
144.33
139.25
138.81
130.98
129.05
129.02
128.60
128.14
120.78
117.99
111.36
110.95
55.60
CN
Ph
OMe
Ph
3af
f1 (ppm)

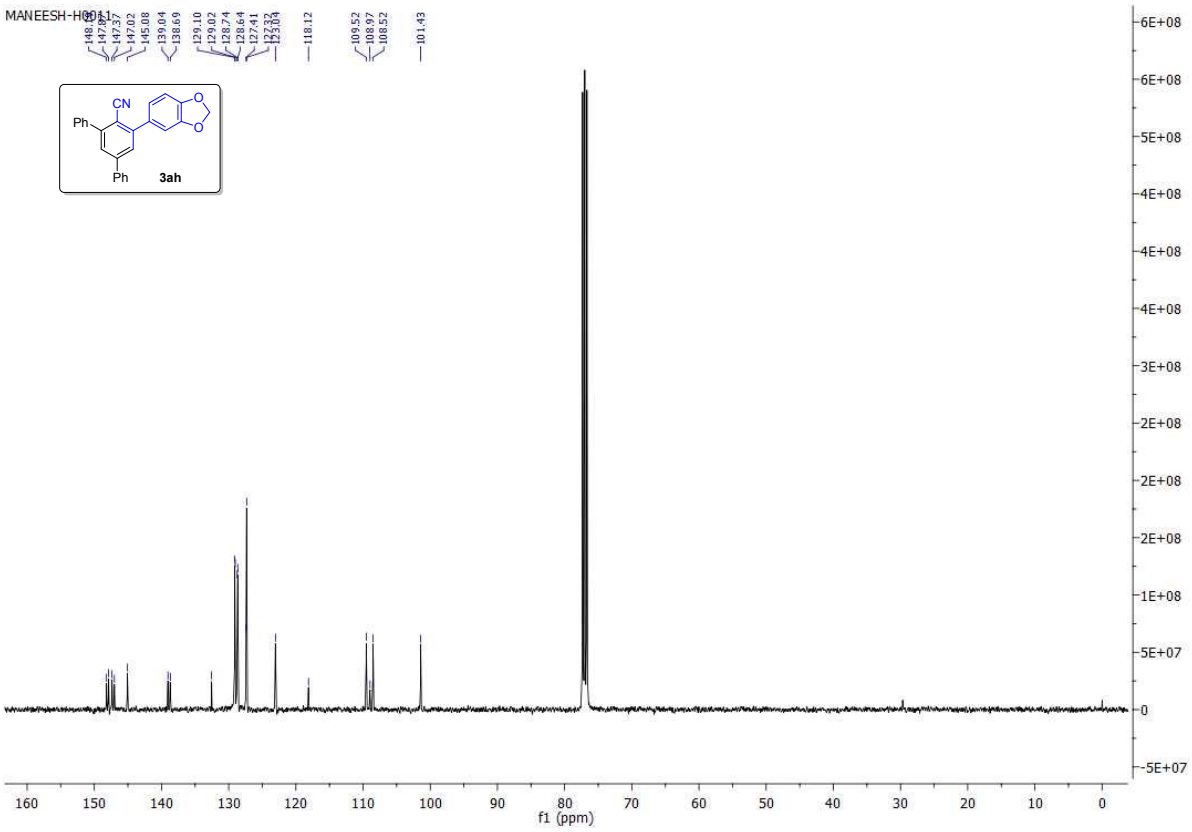

MSR_146D_362
25OCT2019_22 15 (0.293) AM2 (Ar,22000.0,0.00,0.00); ABS; Cm (13:16-(3:9+22:32))
1: TOF MS ES+
1.49e6
536.1661
362.1541
537.1663
538.1641
301.1409
363.1573
299.0625
223.0637
149.0247
355.0703
371.1014
384.1360
503.1071
539.1638
248.0590
281.0515
445.1211
205.0860
185.1148
279.1593
415.0379
579.2938
596.1681
319.1356
446.1208
485.1139
151.0240
114.0756
76.0390
132.5217
CN
Ph
OMe
Ph
3af
%
m/z

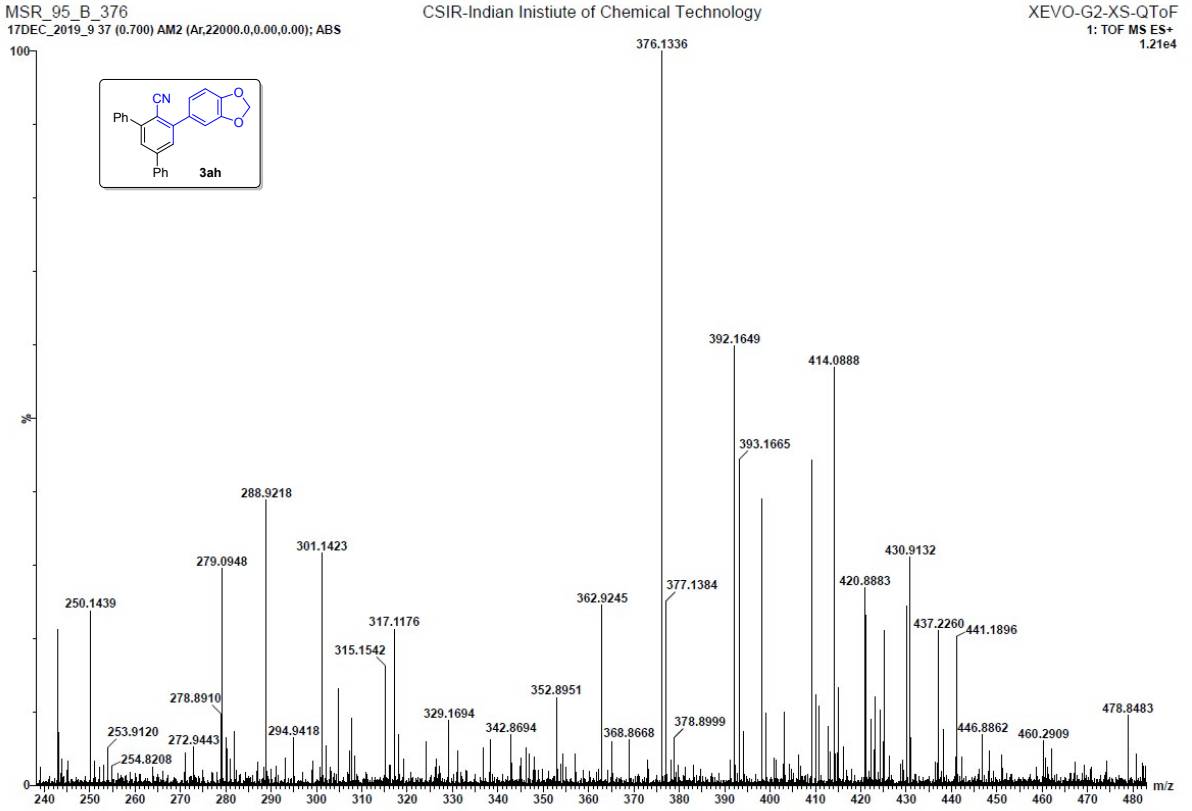

MANEESH-H001a
CN
OMe
OMe
Ph
Ph
3ag
3.97
3.96
6.14
6.15
2.03
0.98
6.00
f1 (ppm)

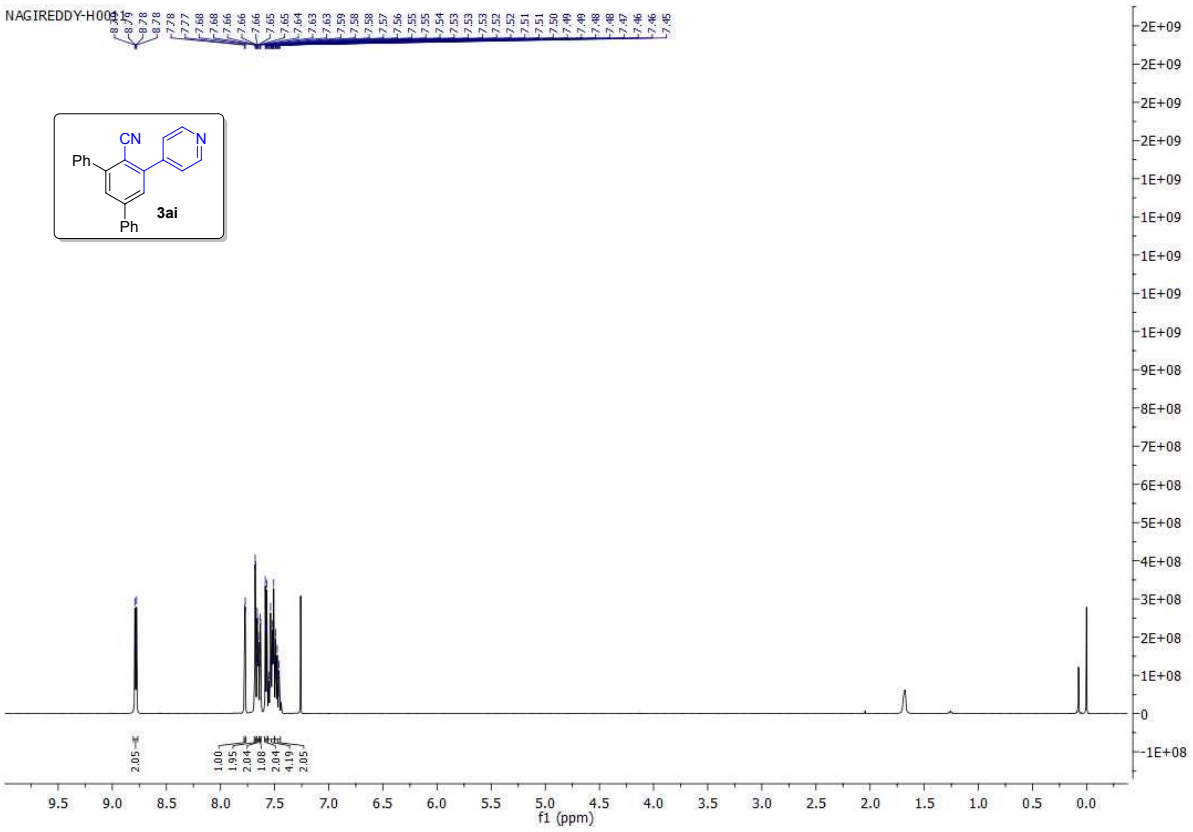

NAGIREDDY-H001a
CN
OMe
OMe
Ph
Ph
3ag
56.08
55.96
f1 (ppm)

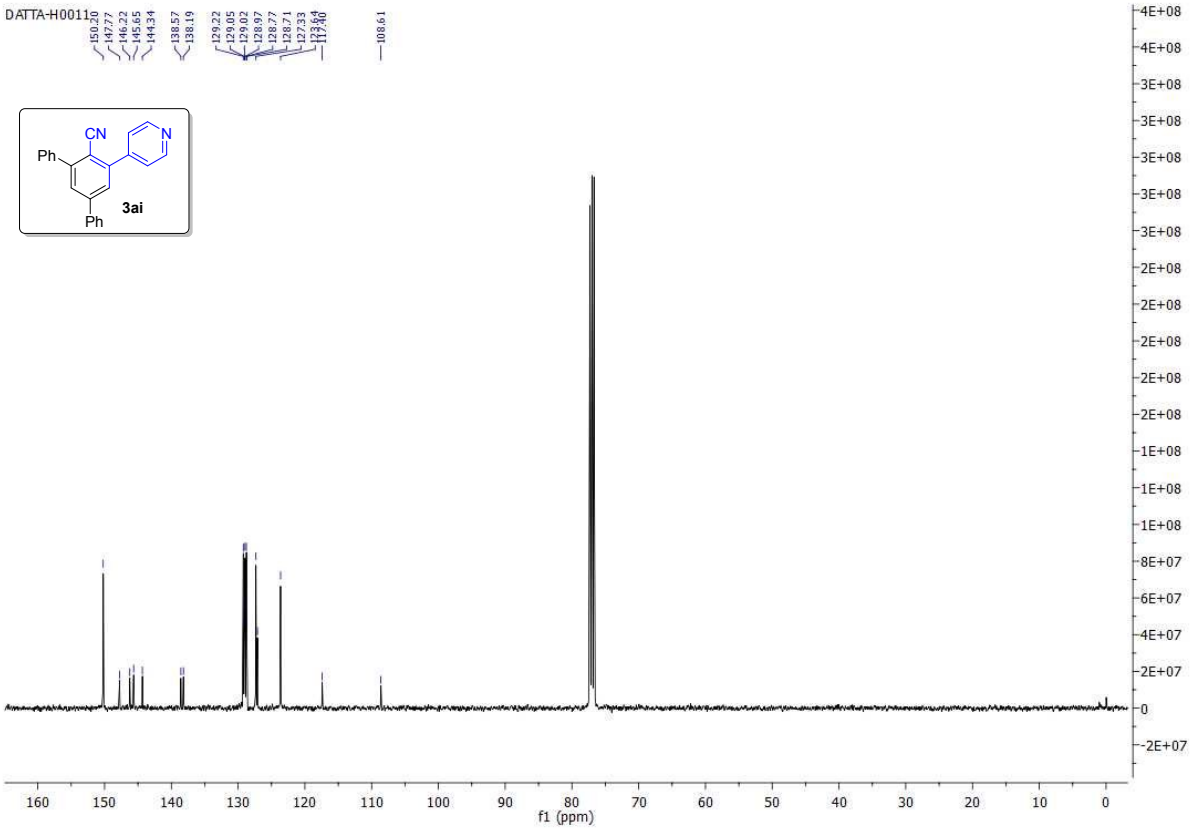

MSR_95_C_392
CSIR-Indian Inistiute of Chemical Technology
XEVO-G2-XS-QToF
17DEC_2019_8 26 (0.502) AM2 (Ar,22000.0,0.00,0.00); ABS
1: TOF MS ES+
1.48e5
392.1649
409.1914
414.1463
430.1207
437.2228
226.9517
438.2251
441.1895
242.9249
279.0940
253.9092
288.9226
301.1424
352.8943
362.9280
482.1330
498.9057
546.8340
556.8457
586.3671
593.2259
629.3870
647.4250
m/z
%
3ag

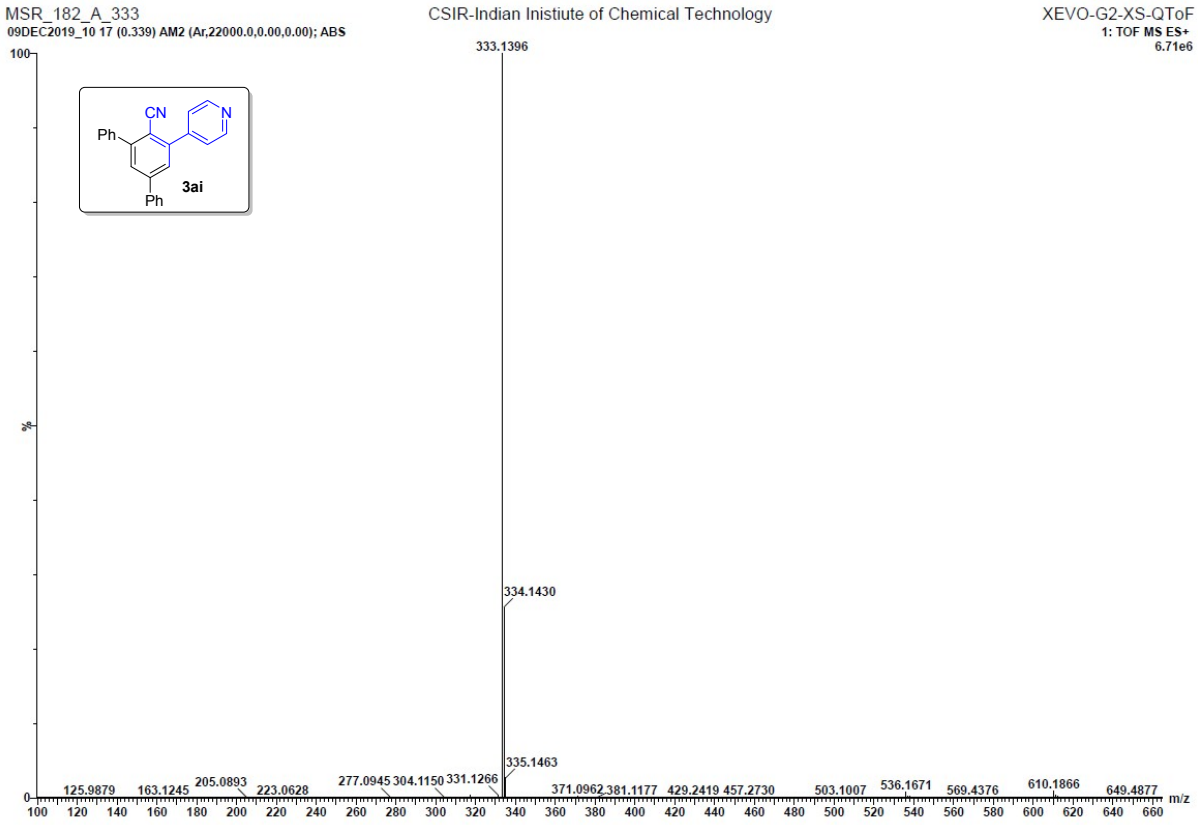

3ah
f1 (ppm)

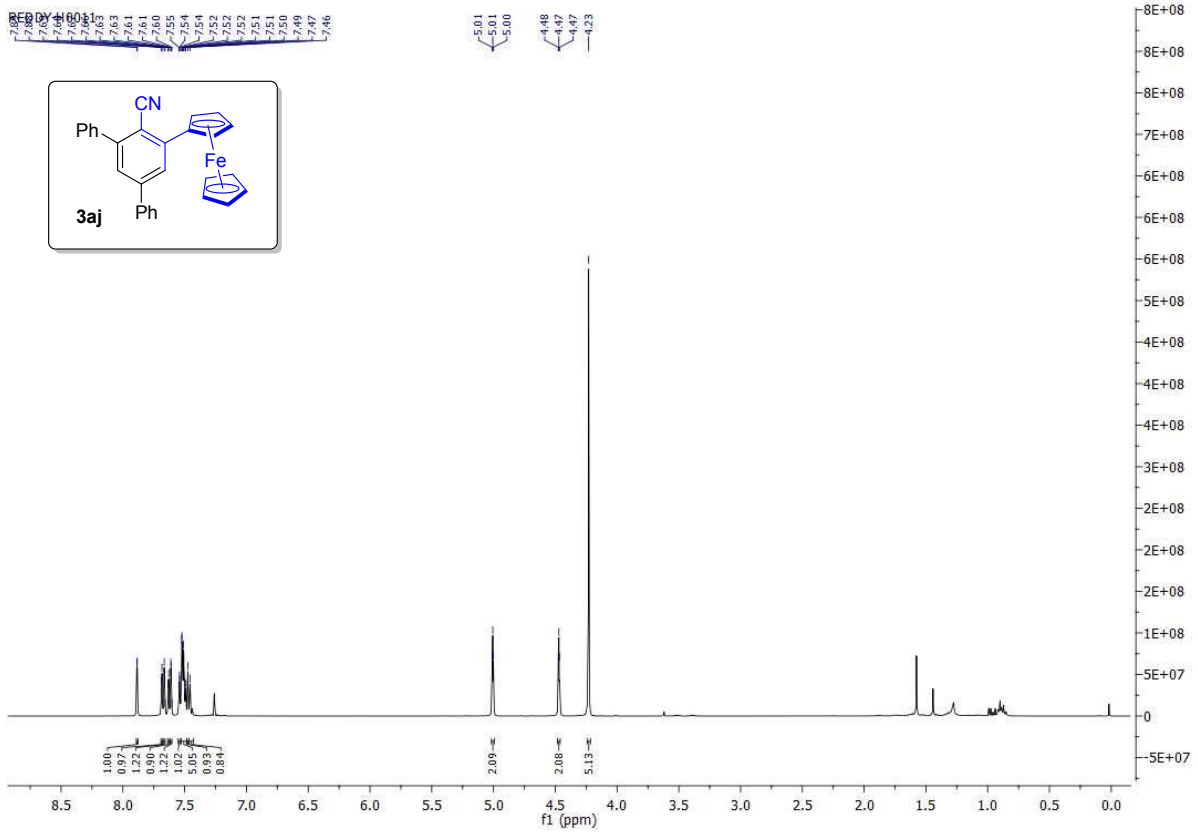

MANEESH-H0011
148.18
147.37
147.02
145.08
139.04
138.69
129.10
129.02
128.74
128.64
127.41
123.33
123.04
118.12
109.52
108.97
108.52
101.43
CN
Ph
Ph
3ah
f1 (ppm)

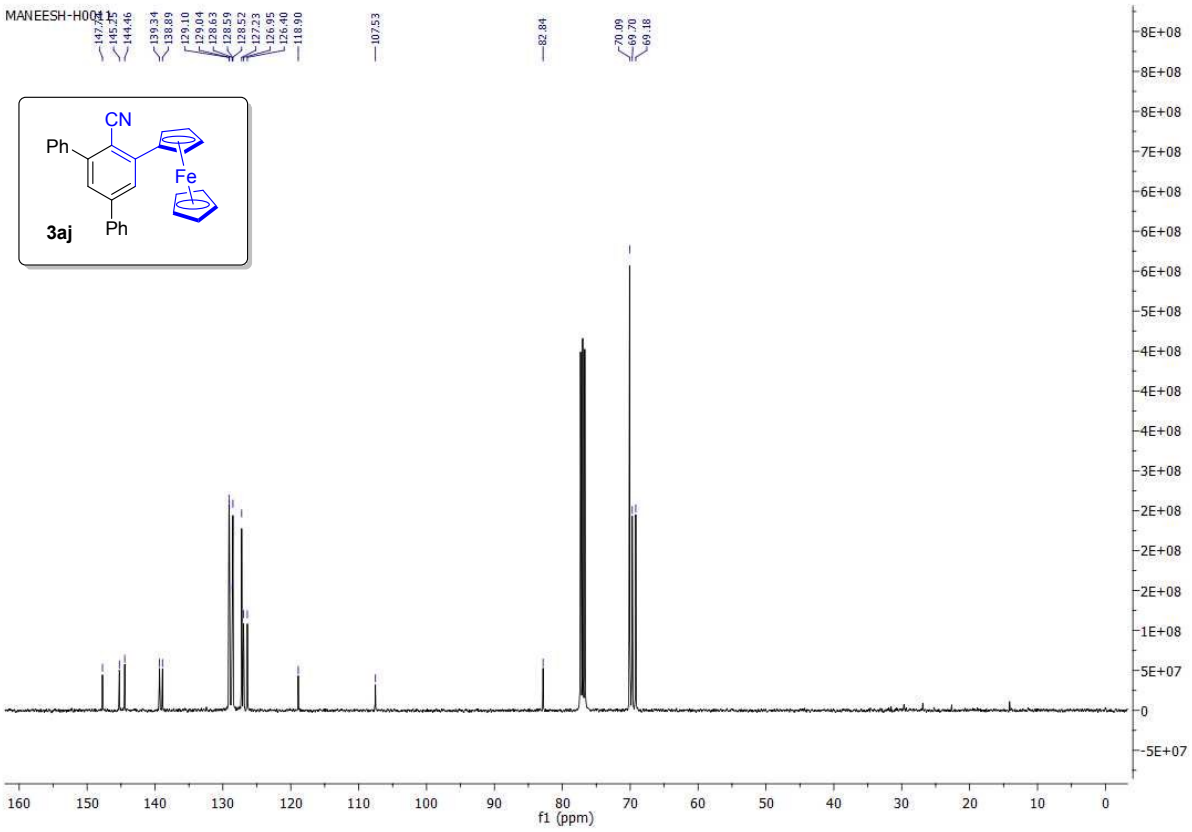

MSR_95_B_376
CSIR-Indian Inistiute of Chemical Technology
XEVO-G2-XS-QToF
17DEC_2019_9 37 (0.700) AM2 (Ar,22000.0,0.00,0.00); ABS
1: TOF MS ES+
1.21e4
CN
Ph
Ph
3ah
376.1336
392.1649
414.0888
393.1665
288.9218
301.1423
279.0948
430.9132
420.8883
250.1439
362.9245
377.1384
437.2260
441.1896
317.1176
315.1542
352.8951
278.8910
329.1694
342.8694
378.8999
478.8483
253.9120
272.9443
294.9418
368.8668
446.8862
460.2909
254.8208
%
m/z

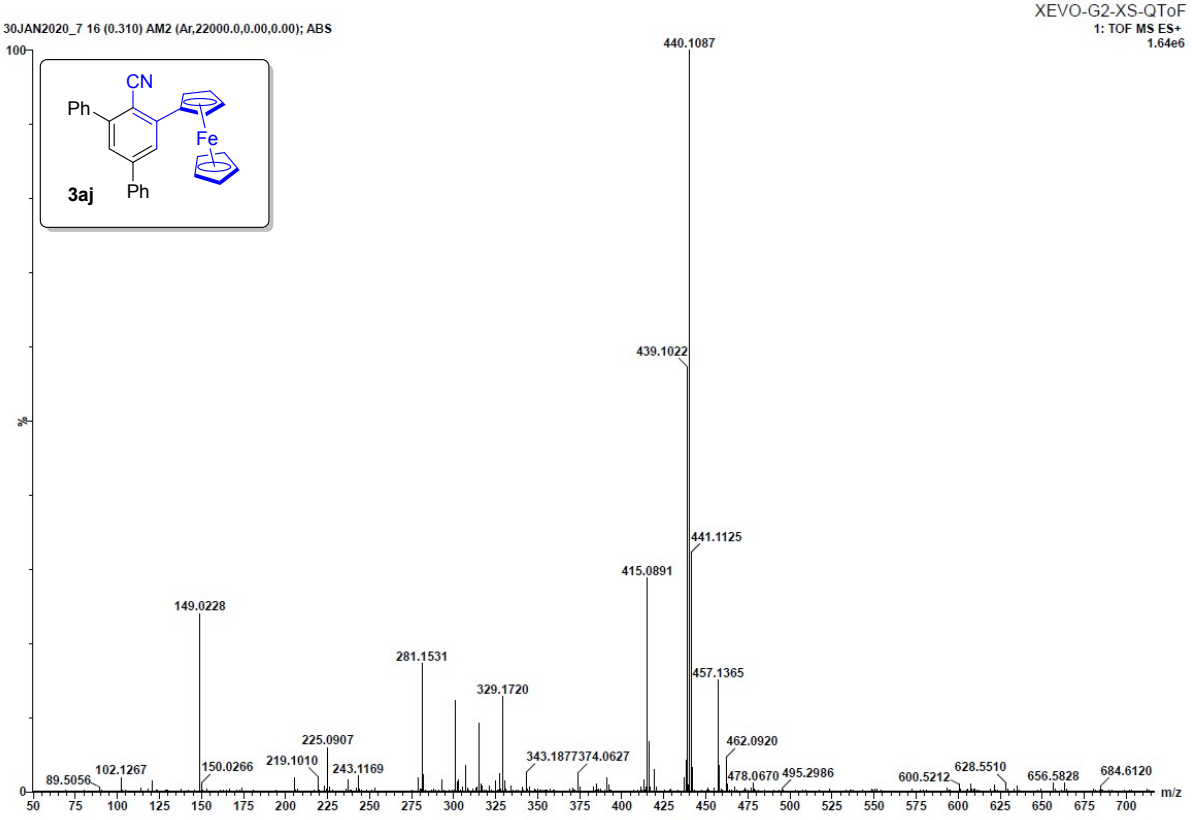

NAGIREDDY-H0011
CN
N
Ph
Ph
3ai
f1 (ppm)

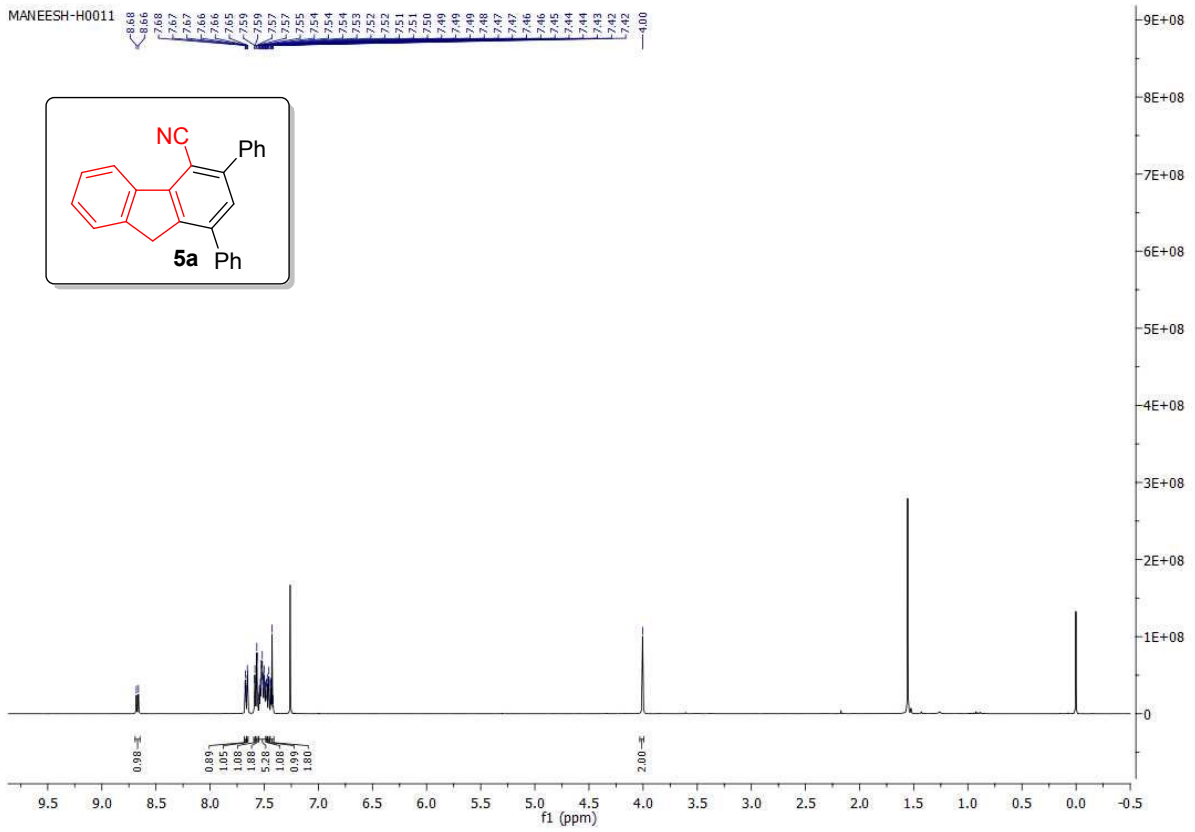

DATTA-H0011
CN
N
Ph
Ph
3ai
f1 (ppm)

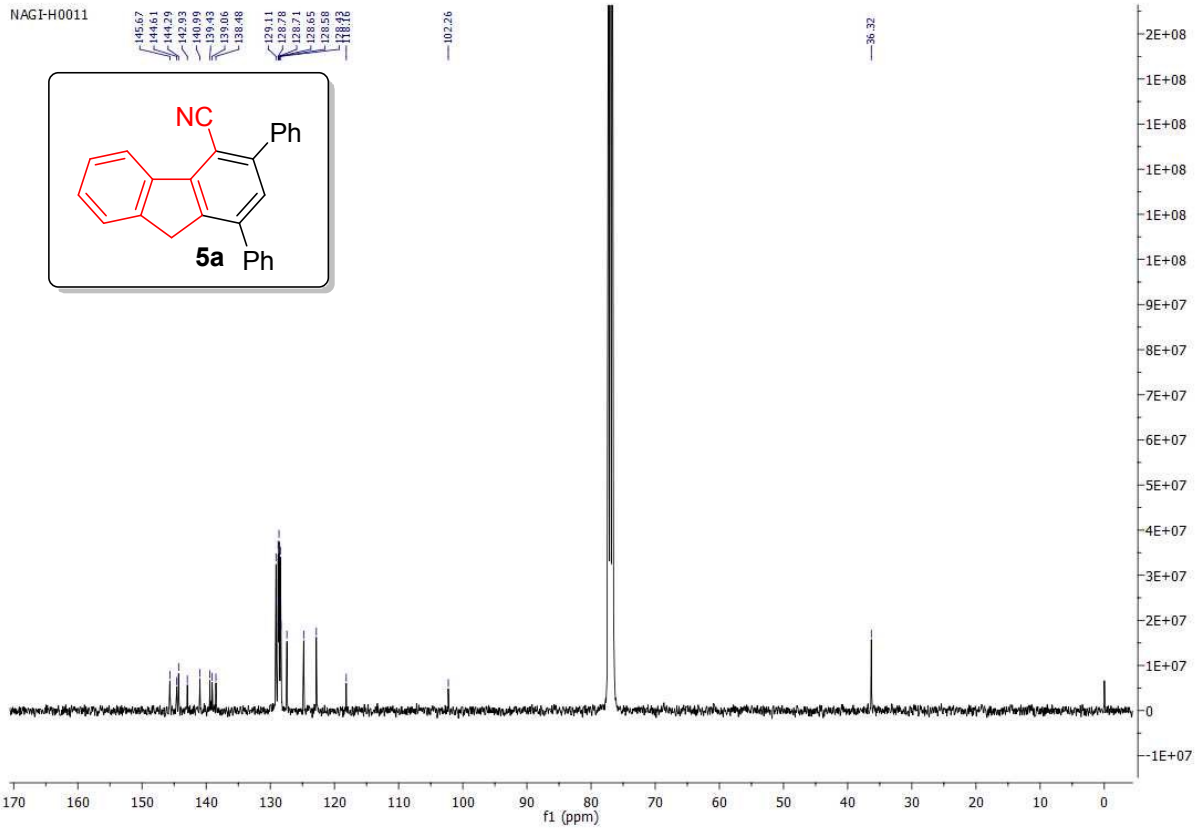

MSR_182_A_333
CSIR-Indian Institute of Chemical Technology
XEVO-G2-XS-QToF
09DEC2019_10 17 (0.339) AM2 (Ar,22000.0,0.00,0.00); ABS
1: TOF MS ES+
6.71e6
333.1396
334.1430
335.1463
CN
N
Ph
Ph
3ai
%
m/z

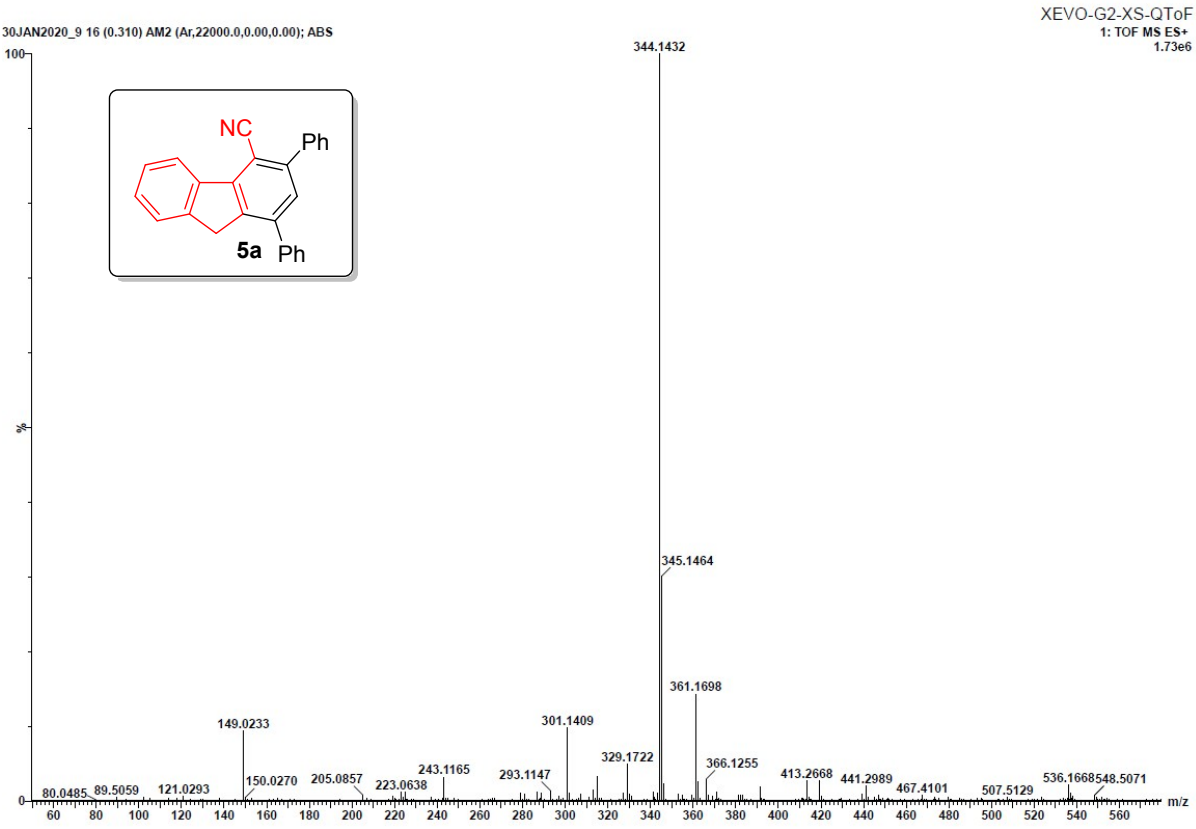

CN
Ph
Fe
Ph
3aj
f1 (ppm)

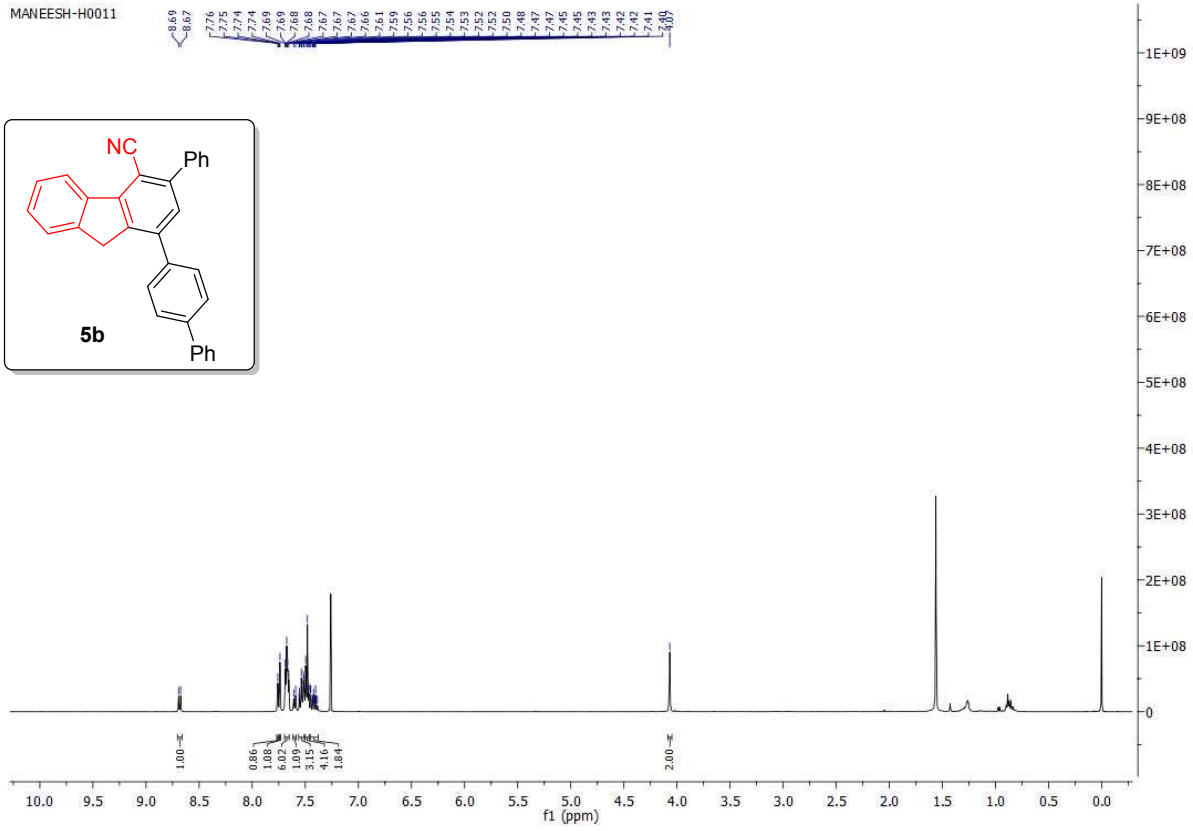

MANEESH-H0001
147.74
145.25
144.46
139.34
138.89
129.10
129.04
128.63
128.59
128.52
127.23
126.95
126.40
118.90
107.53
82.84
70.09
69.70
69.18
CN
Ph
Fe
Ph
3aj
f1 (ppm)

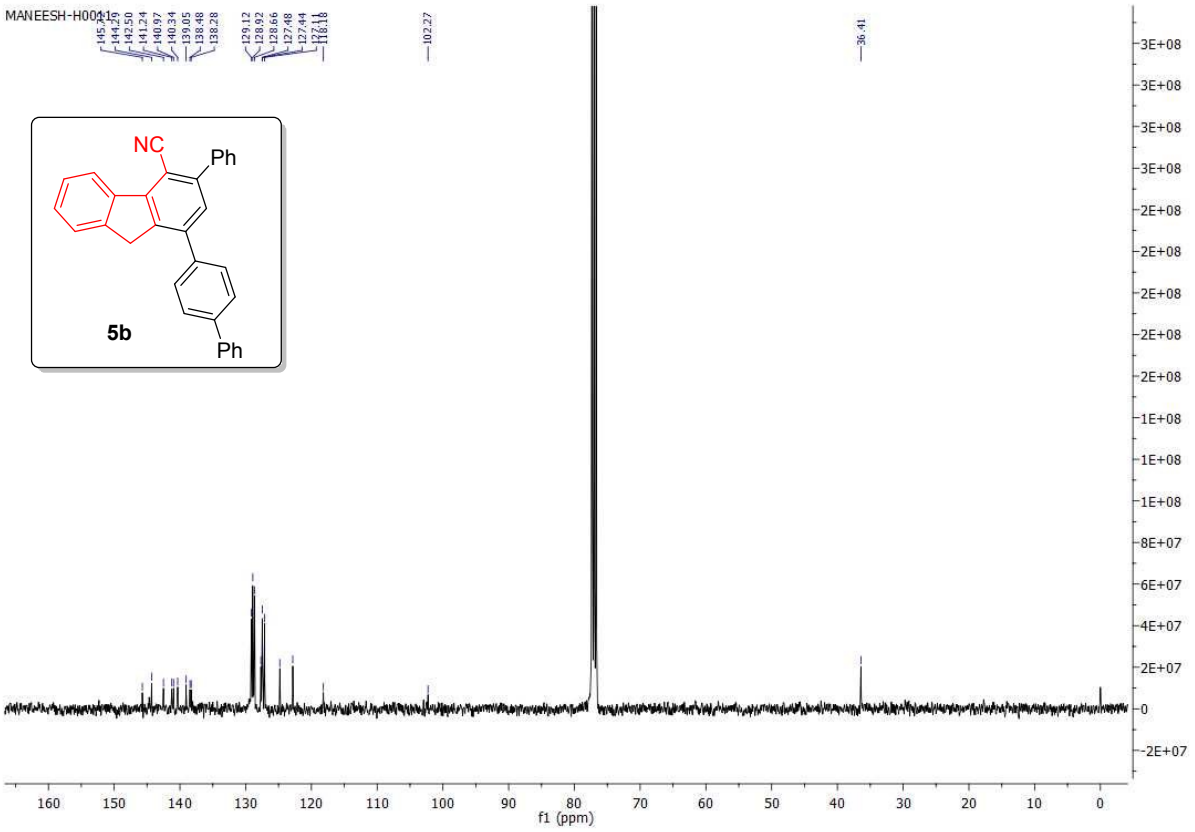

30JAN2020_7 16 (0.310) AM2 (Ar,22000.0,0.00,0.00); ABS
XEVO-G2-XS-QToF
1: TOF MS ES+
1.64e6
CN
Ph
Fe
Ph
3aj
%
m/z
440.1087
439.1022
441.1125
415.0891
149.0228
281.1531
457.1365
329.1720
462.0920
225.0907
219.1010
243.1169
150.0266
102.1267
89.5056
343.1877374.0627
478.0670
495.2986
600.5212
628.5510
656.5828
684.6120

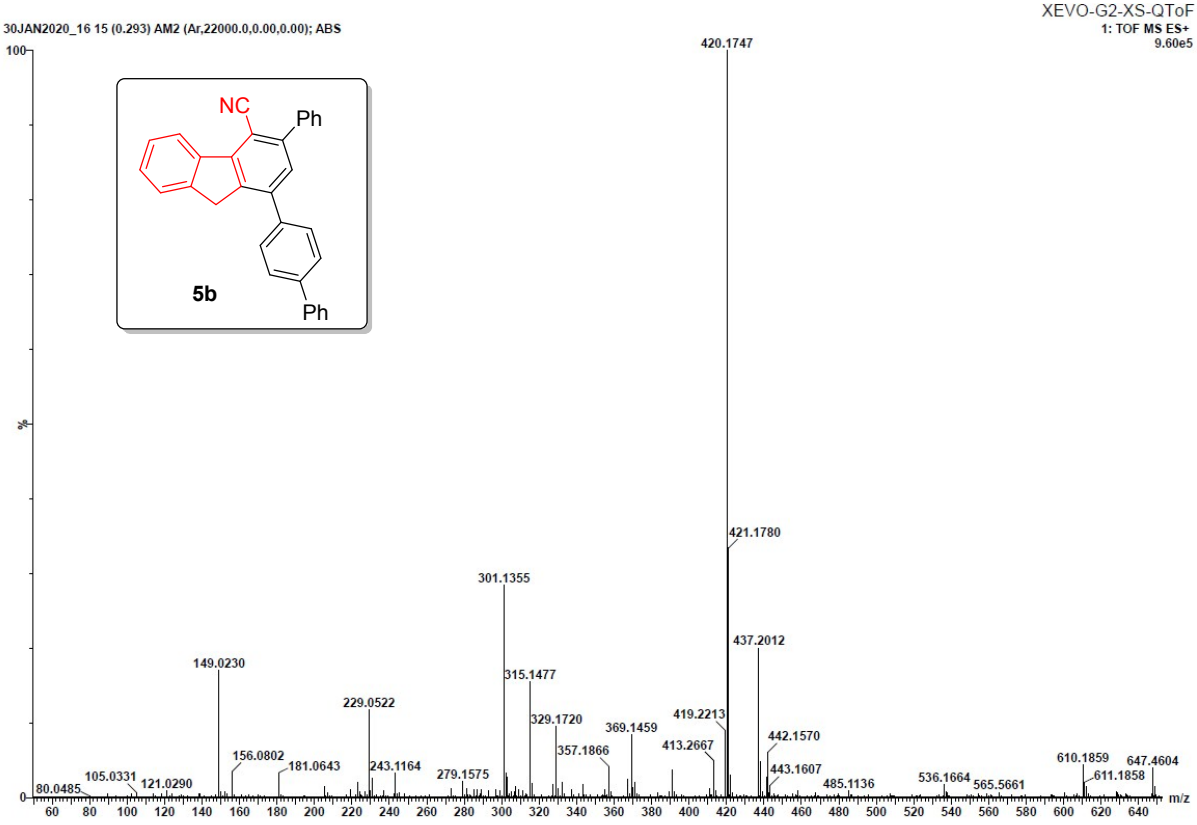

MANEESH-H0011
NC
Ph
5a
Ph
f1 (ppm)

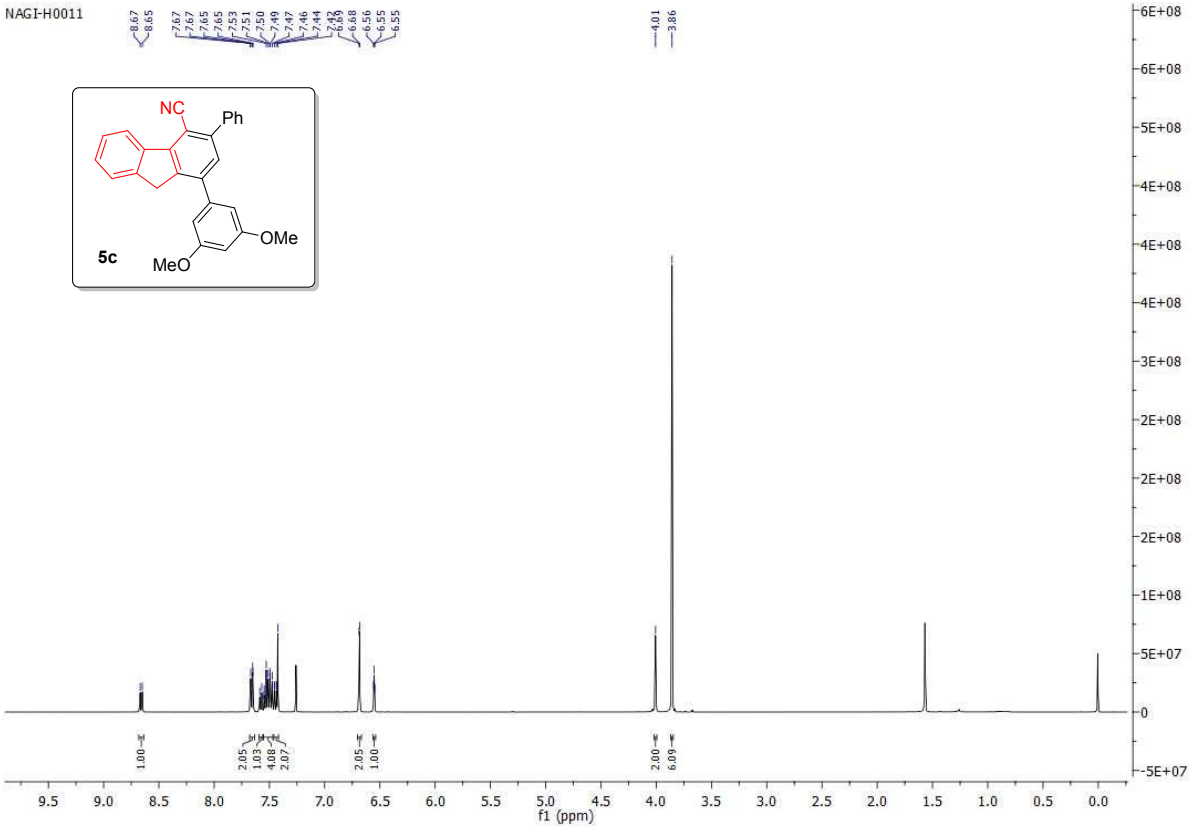

NAGI-H0011
NC
Ph
5a
Ph
f1 (ppm)

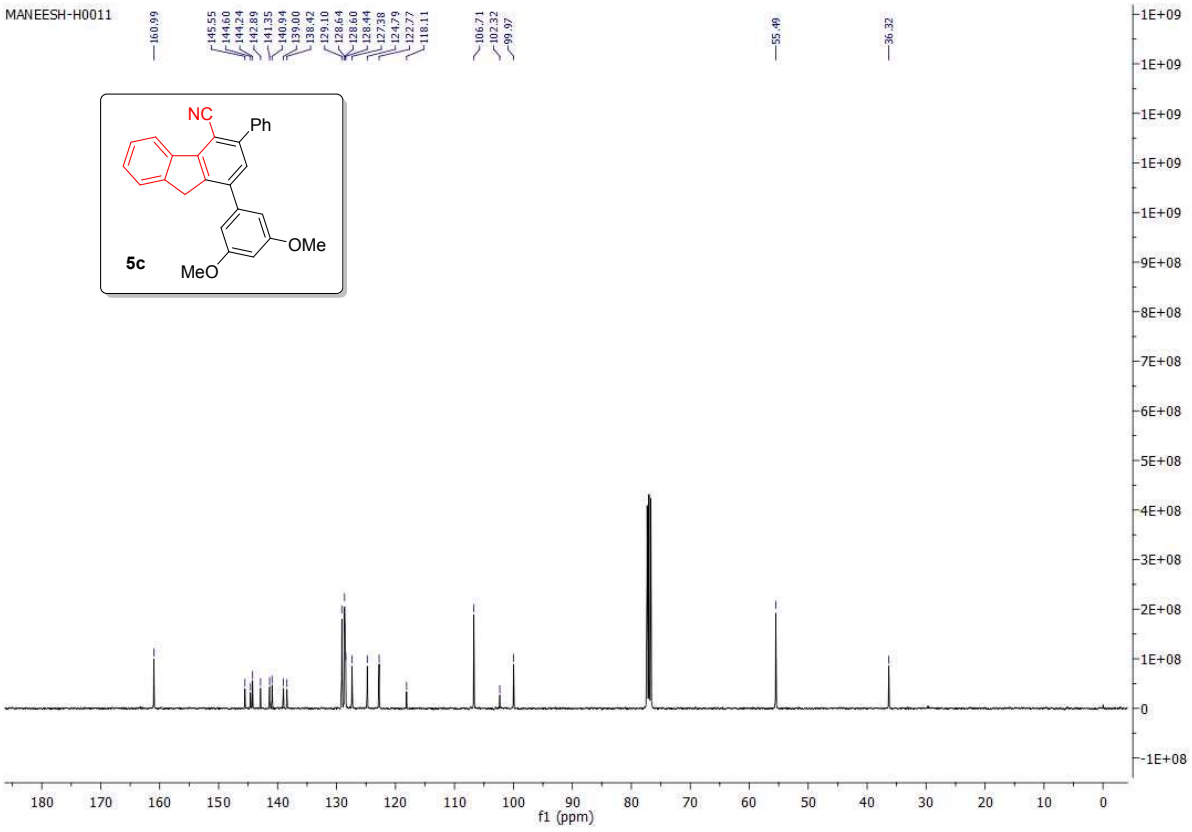

30JAN2020_9 16 (0.310) AM2 (Ar,22000.0,0.00,0.00); ABS
XEVO-G2-XS-QToF
1: TOF MS ES+
1.73e6
NC
Ph
5a
Ph
344.1432
345.1464
361.1698
149.0233
301.1409
329.1722
366.1255
243.1165
293.1147
150.0270
205.0857
223.0638
413.2668
441.2989
467.4101
507.5129
536.1668548.5071
80.0485
89.5059
121.0293
%
m/z

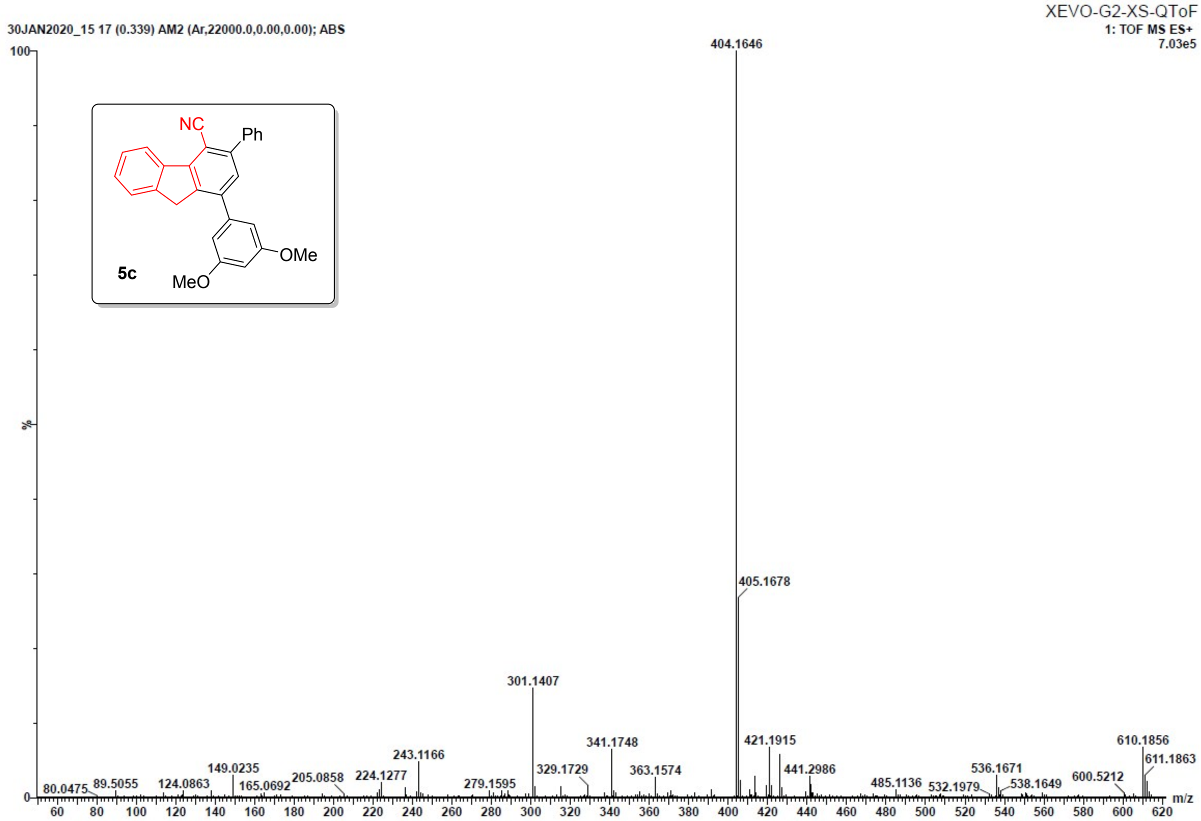

MANEESH-H0011
NC
Ph
5b
Ph
f1 (ppm)

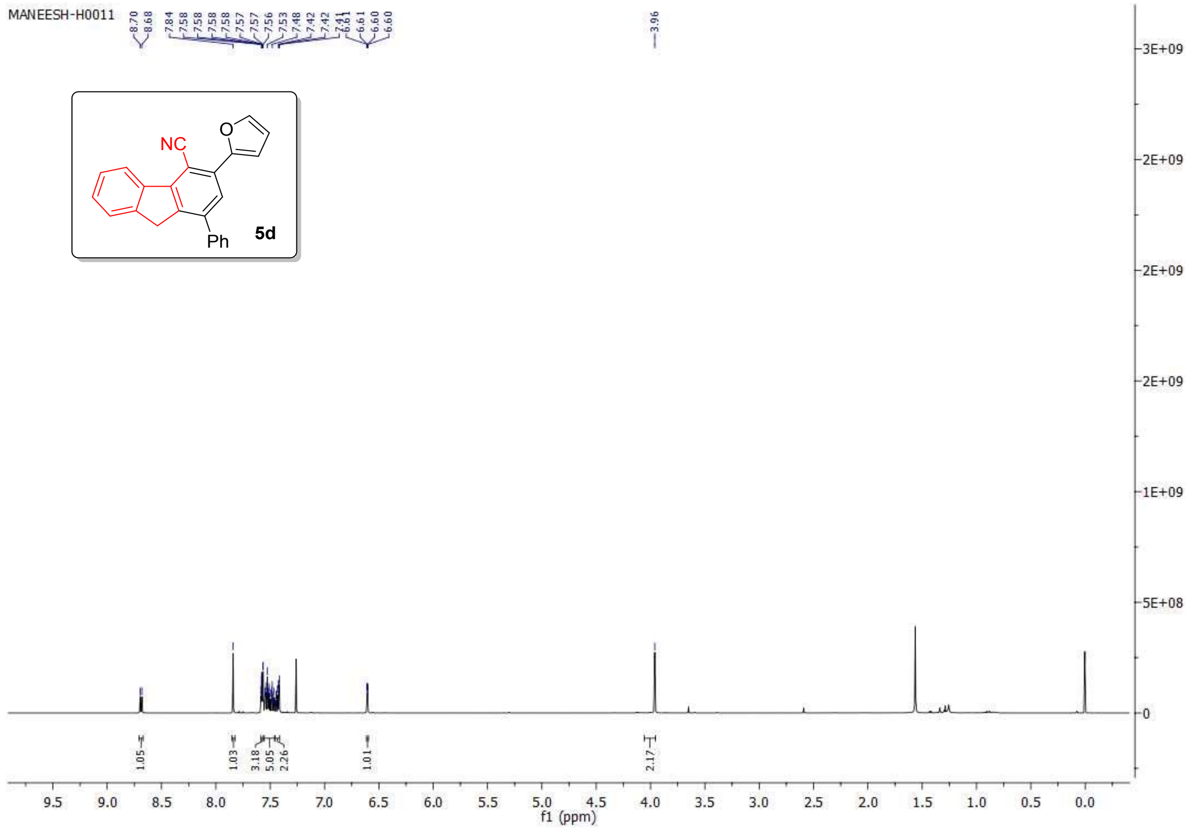

MANEESH-H0041
NC
Ph
5b
Ph
f1 (ppm)

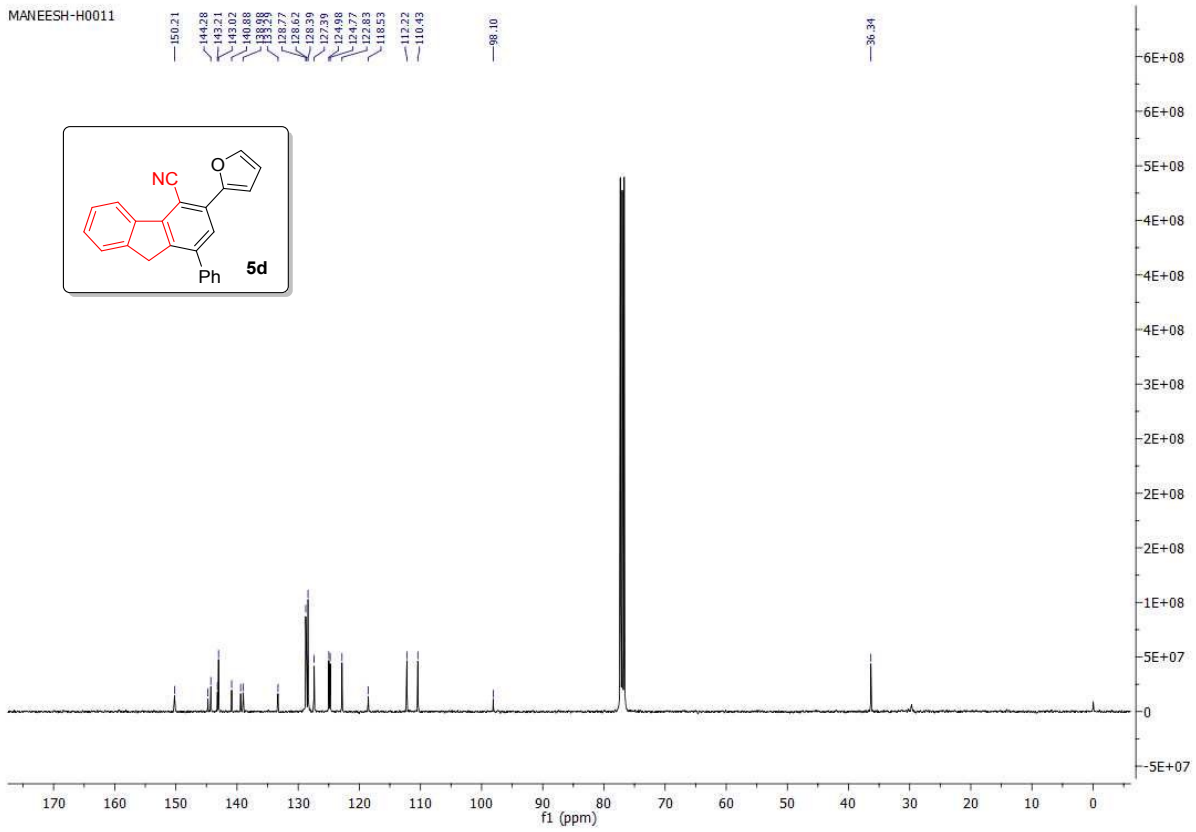

30JAN2020_16 15 (0.293) AM2 (Ar,22000.0,0.00,0.00); ABS
XEVO-G2-XS-QToF
1: TOF MS ES+
9.60e5
NC
Ph
5b
Ph
%
m/z
420.1747
421.1780
301.1355
437.2012
149.0230
315.1477
229.0522
329.1720
369.1459
419.2213
442.1570
357.1866
413.2667
443.1607
156.0802
181.0643
243.1164
279.1575
105.0331
121.0290
80.0485
485.1136
536.1664
565.5661
610.1859
647.4604
611.1858

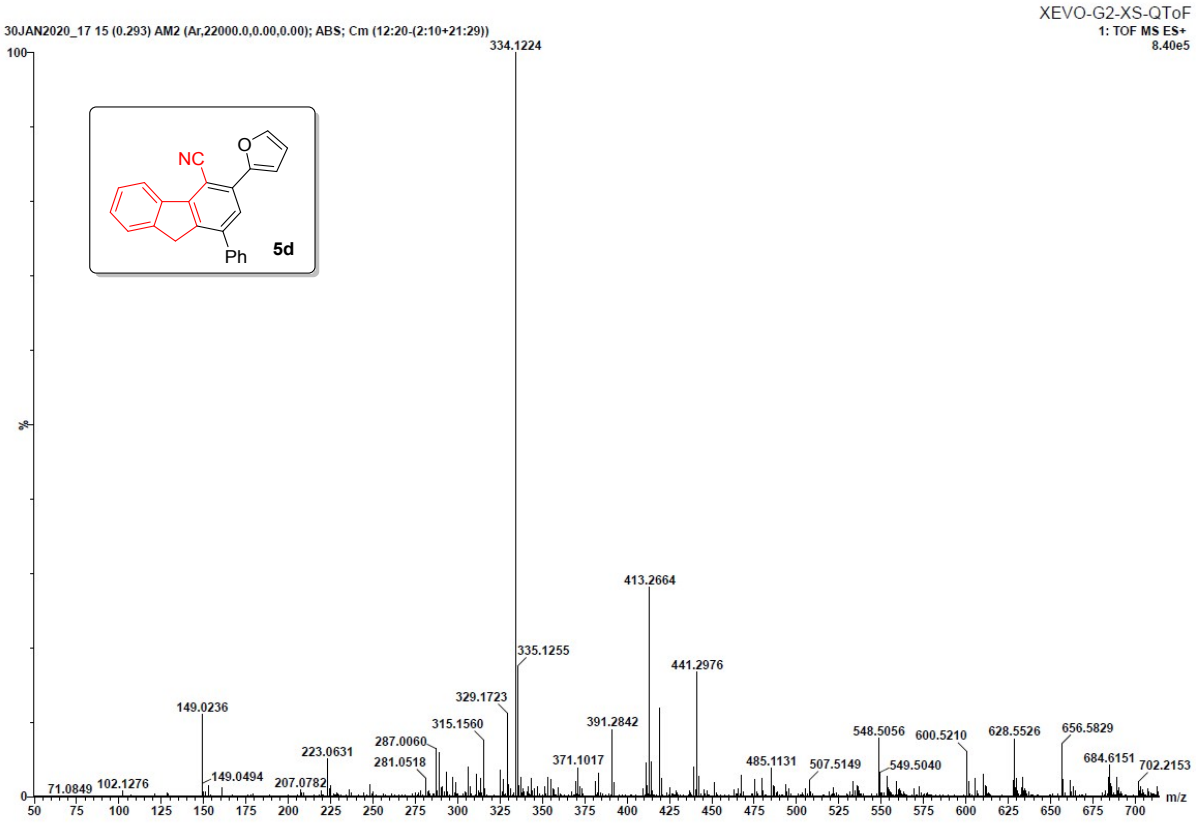

NAGI-H0011
NC
Ph
OMe
MeO
5c
f1 (ppm)

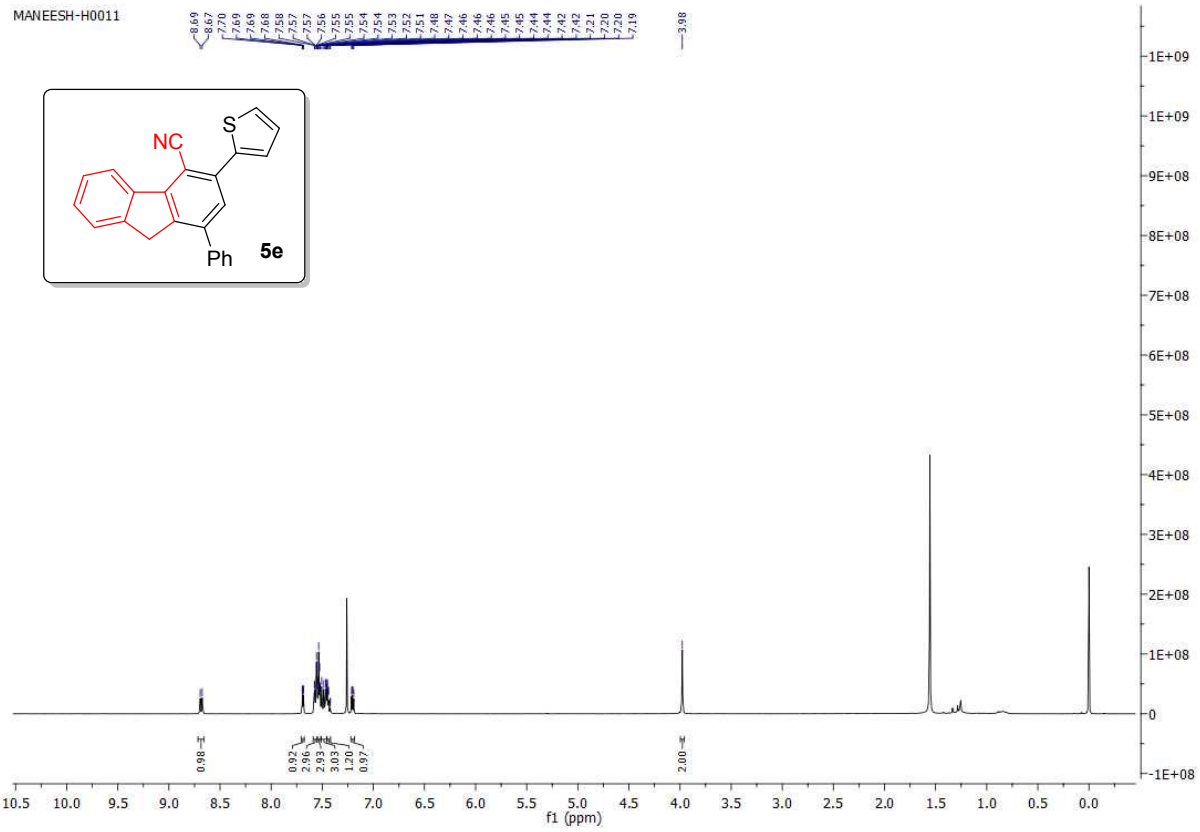

MANEESH-H0011
NC
Ph
OMe
MeO
5c
f1 (ppm)

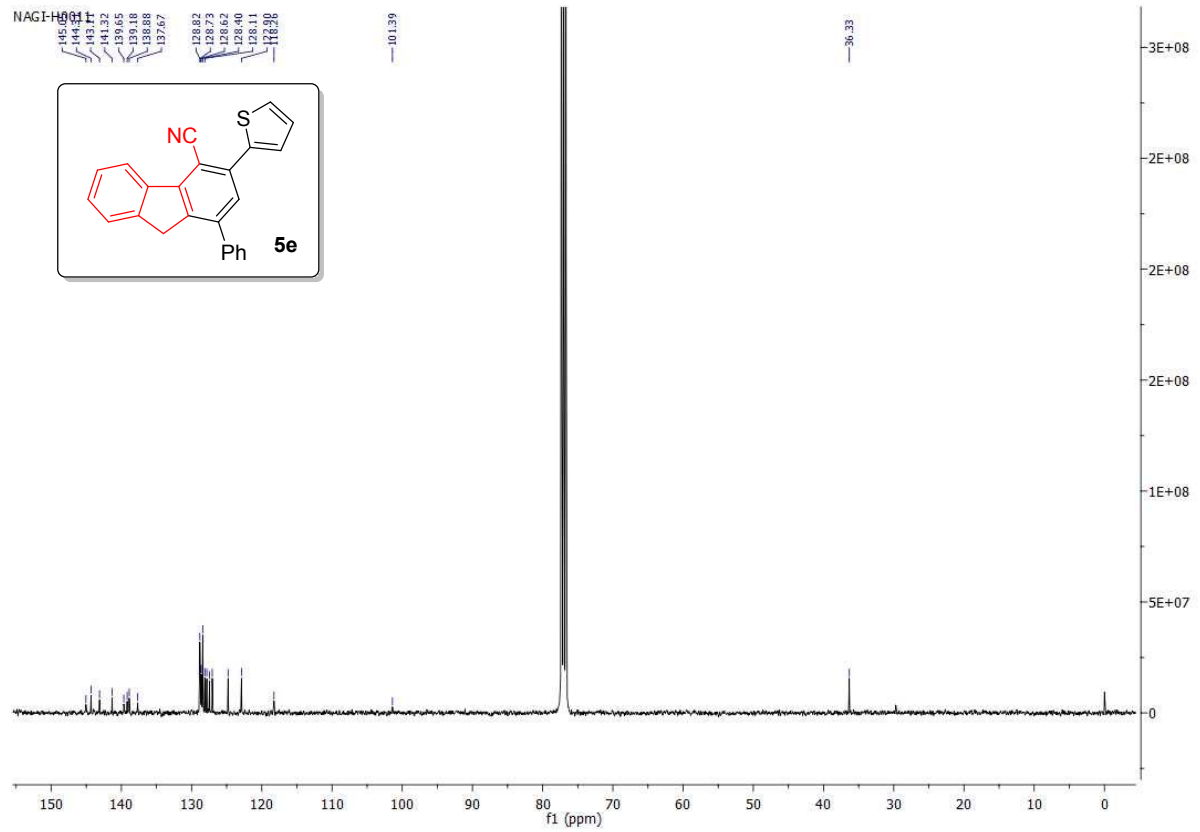

30JAN2020_15 17 (0.339) AM2 (Ar,22000.0,0.00,0.00); ABS
XEVO-G2-XS-QToF
1: TOF MS ES+
7.03e5
404.1646
405.1678
301.1407
341.1748
421.1915
610.1856
611.1863
243.1166
149.0235
441.2986
536.1671
329.1729
363.1574
80.0475
89.5055
124.0863
165.0692
205.0858
224.1277
279.1595
485.1136
532.1979
538.1649
600.5212
m/z
%
NC
Ph
OMe
MeO
5c

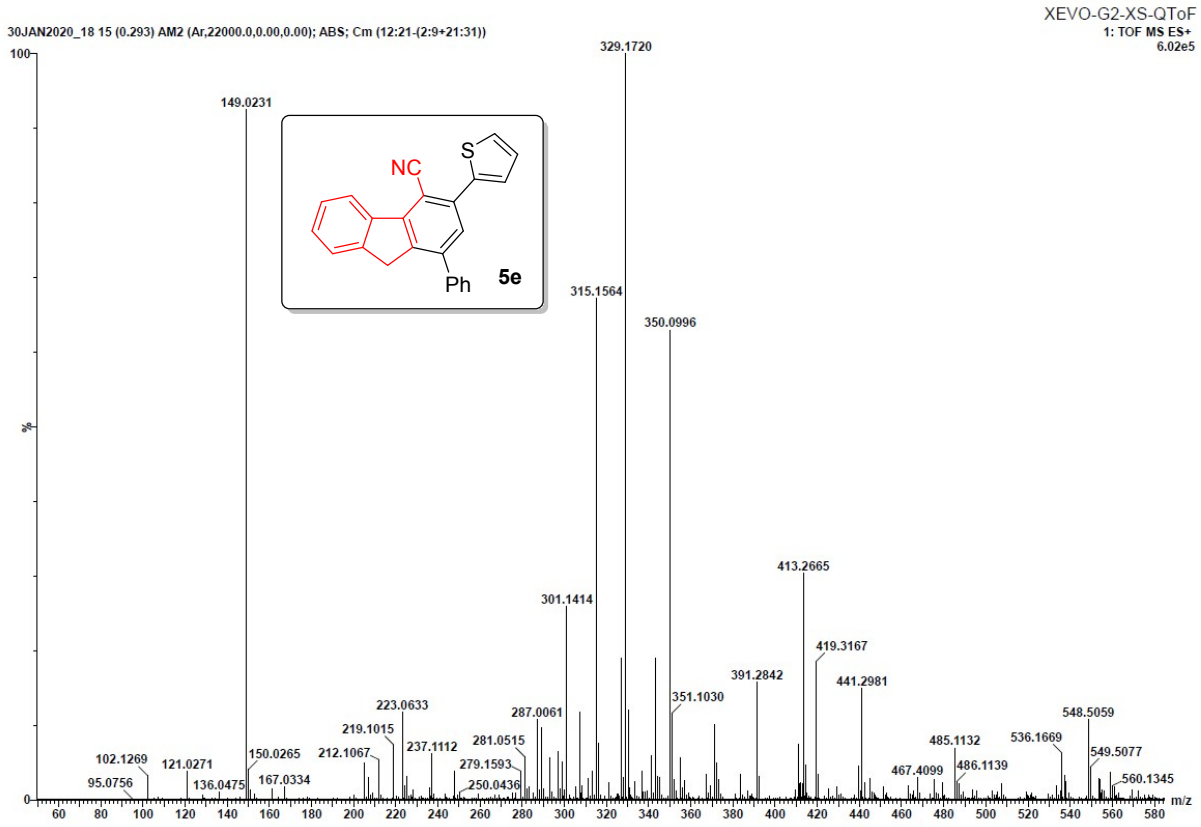

MANEESH-H0011
NC
O
Ph
5d
f1 (ppm)

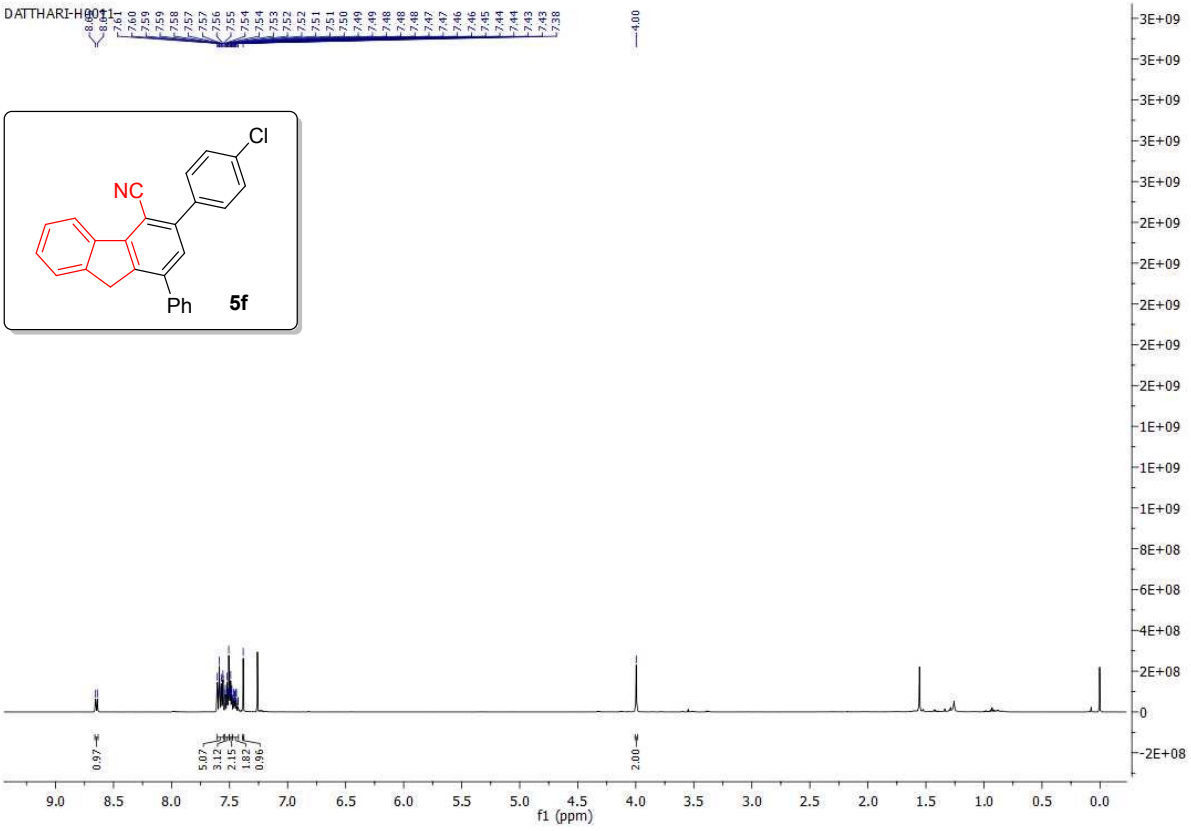

MANEESH-H0011
150.21
144.28
143.21
143.02
140.88
133.29
128.77
128.62
128.39
127.39
124.98
124.77
122.83
118.53
112.22
110.43
98.10
36.34
NC
O
Ph
5d
f1 (ppm)

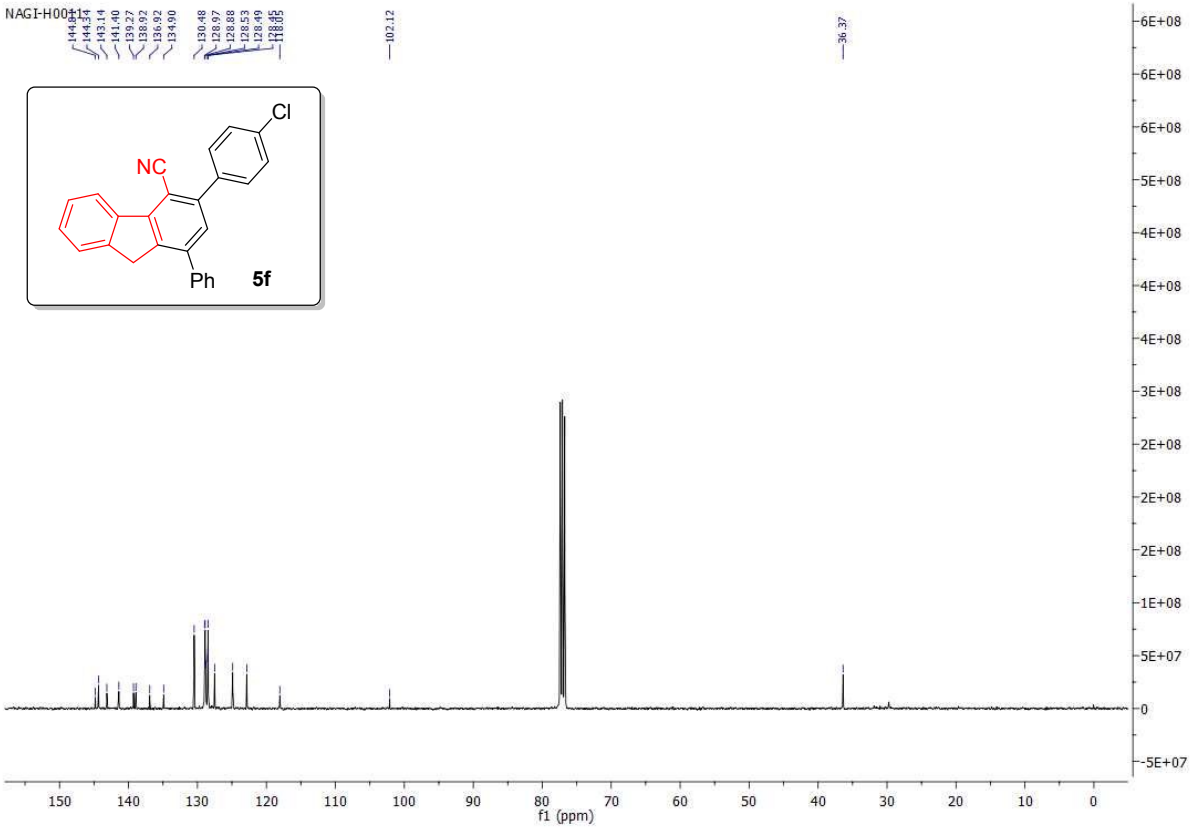

30JAN2020_17 15 (0.293) AM2 (Ar,22000.0,0.00,0.00); ABS; Cm (12:20-(2:10+21:29))
XEVO-G2-XS-QToF
1: TOF MS ES+
8.40e5
NC
O
Ph
5d
334.1224
413.2664
335.1255
441.2976
329.1723
149.0236
315.1560
391.2842
287.0060
223.0631
281.0518
371.1017
548.5056
600.5210
628.5526
656.5829
485.1131
507.5149
549.5040
684.6151
702.2153
71.0849
102.1276
149.0494
207.0782
%
m/z

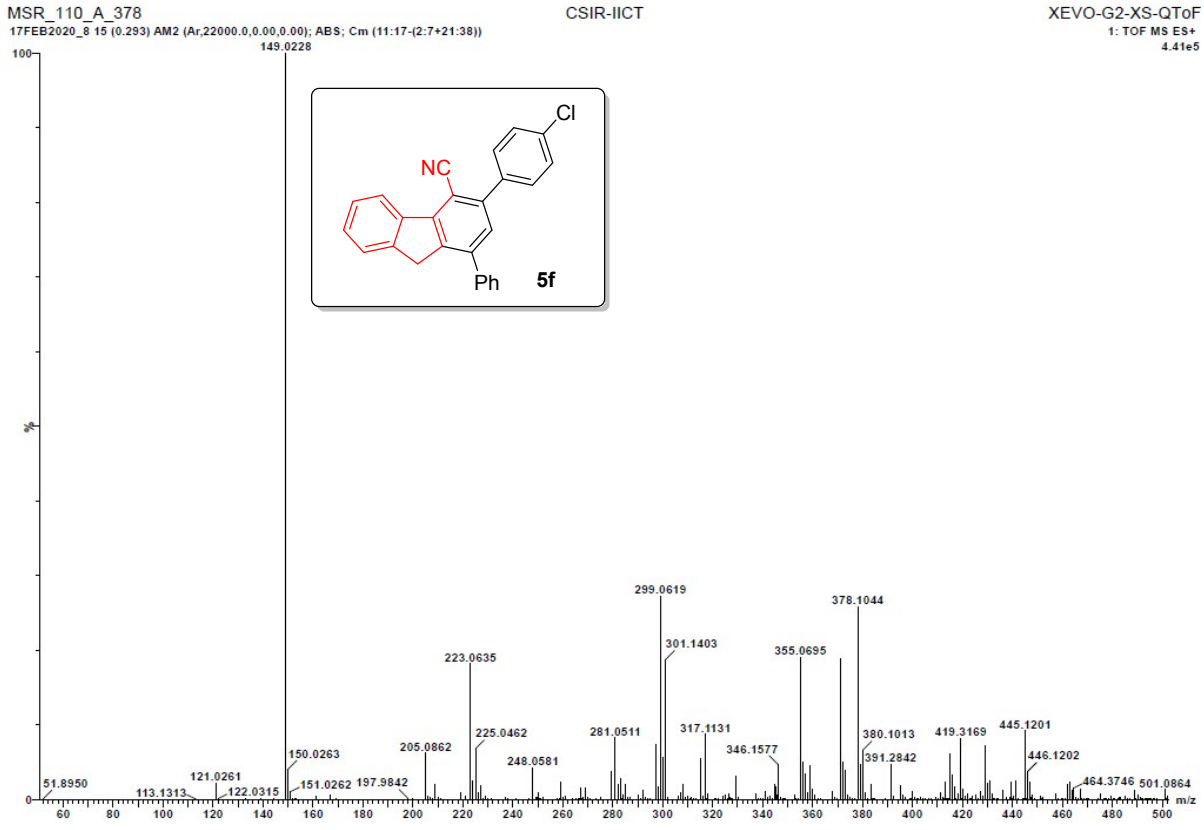

MANEESH-H0011
NC
S
Ph
5e
f1 (ppm)

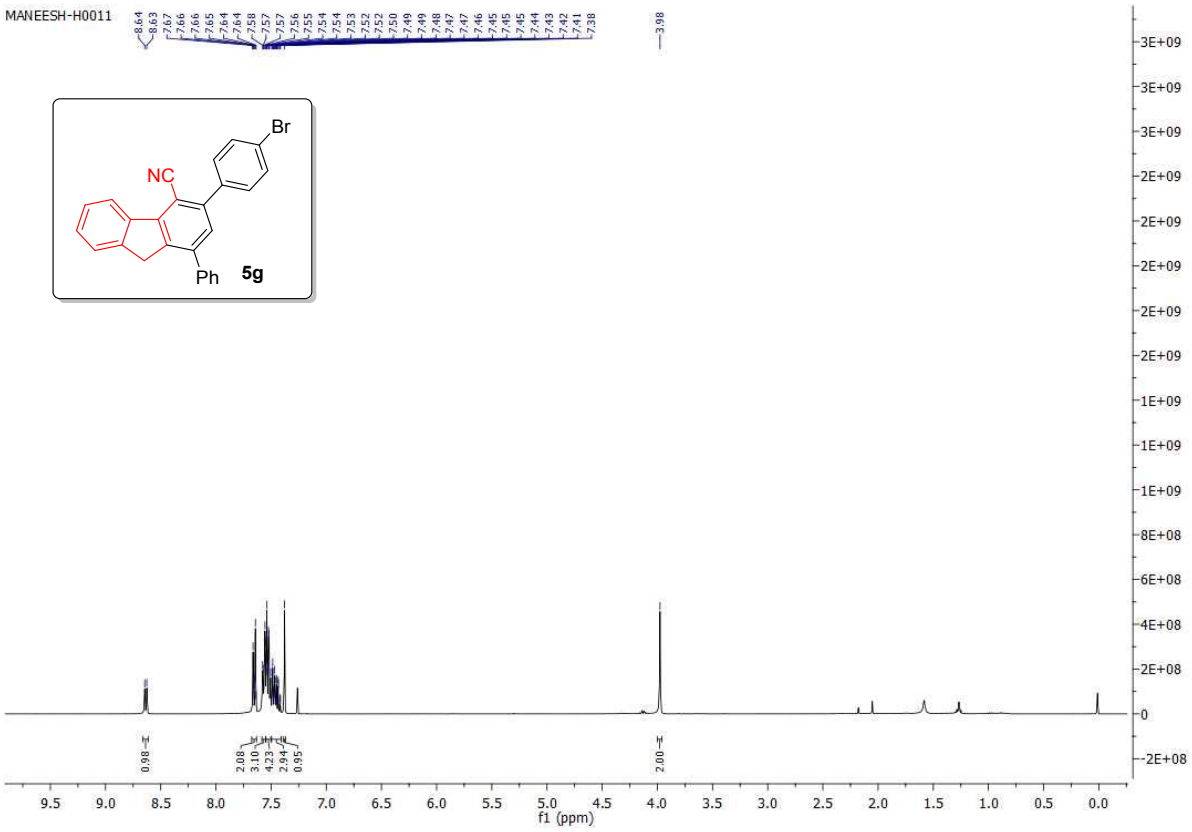

NAGI-H0011
NC
S
Ph
5e
f1 (ppm)

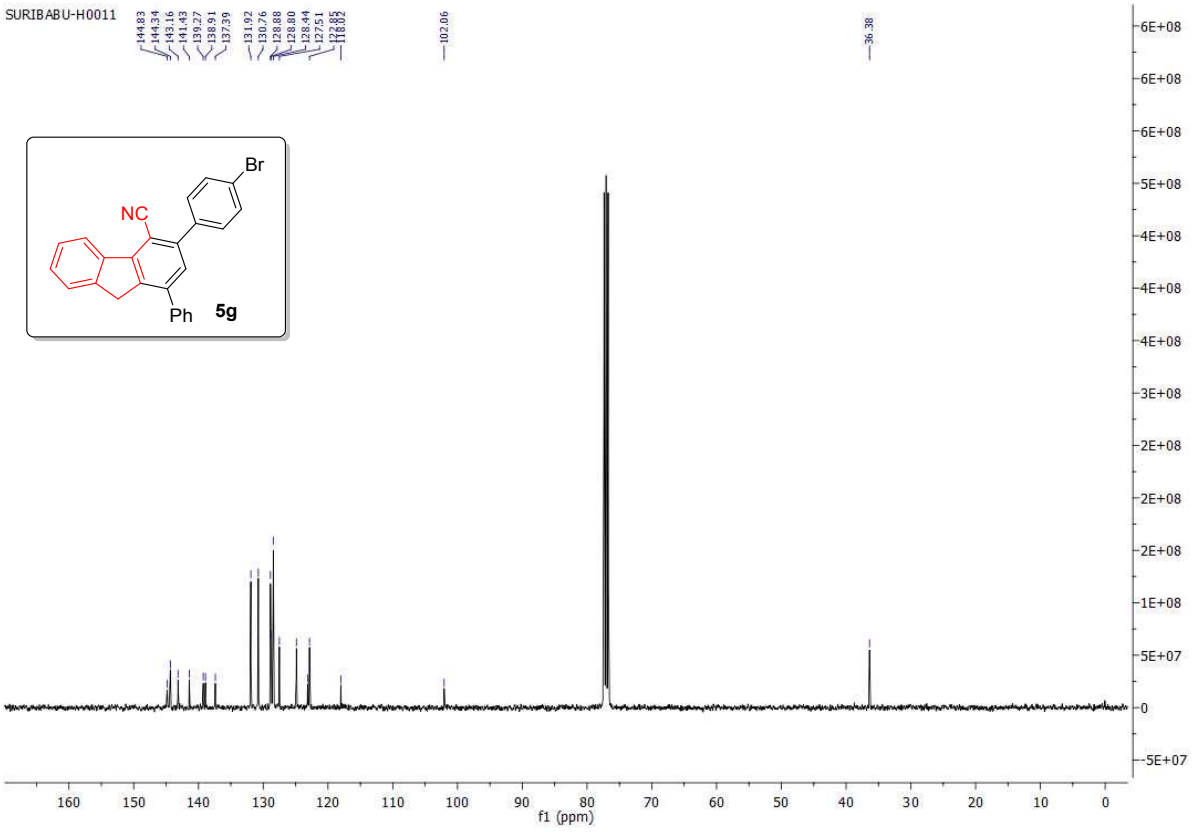

XEVO-G2-XS-QToF
1: TOF MS ES+
6.02e5
30JAN2020_18 15 (0.293) AM2 (Ar,22000.0,0.00,0.00); ABS; Cm (12:21-(2:9+21:31))
NC
S
Ph
5e
329.1720
149.0231
315.1564
350.0996
413.2665
301.1414
419.3167
391.2842
441.2981
351.1030
223.0633
287.0061
548.5059
219.1015
281.0515
485.1132
536.1669
237.1112
549.5077
102.1269
121.0271
150.0265
212.1067
279.1593
467.4099
486.1139
95.0756
136.0475
167.0334
250.0436
560.1345
%
m/z

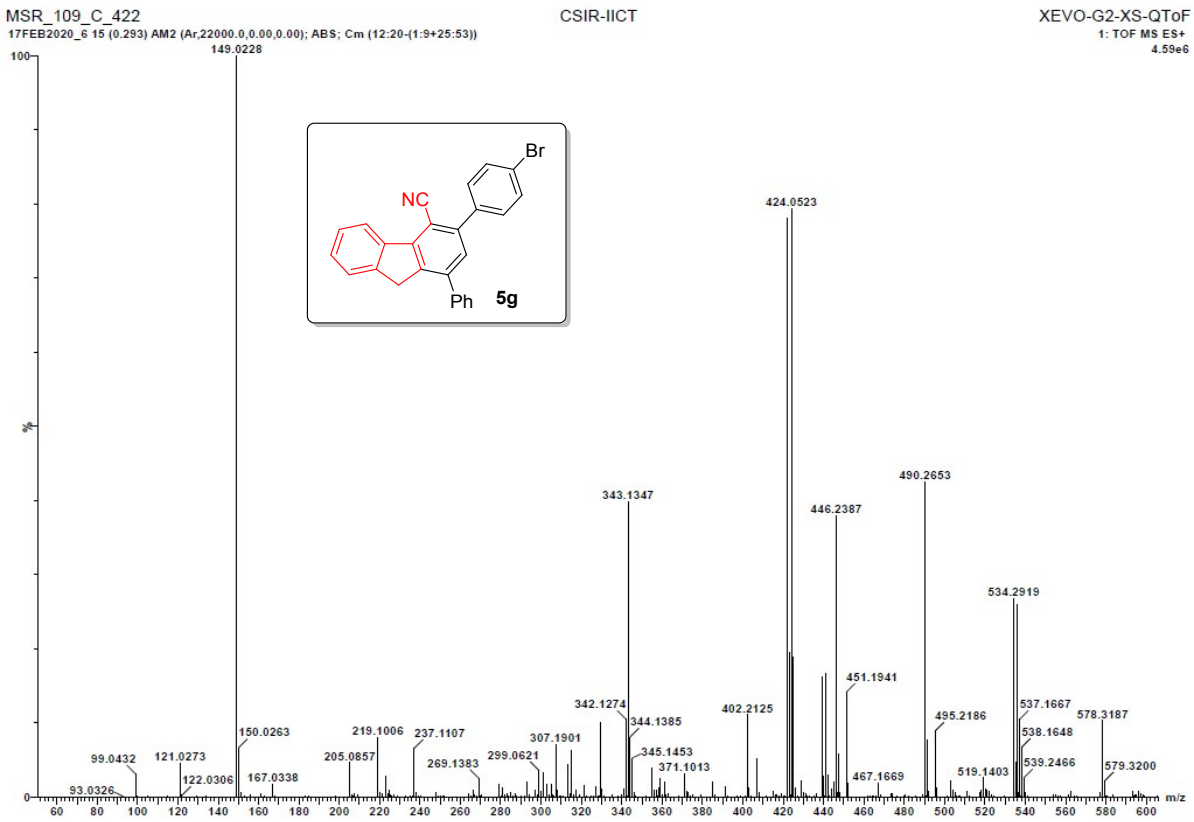

DATTHARI-H9011
NC
Cl
Ph
5f
f1 (ppm)

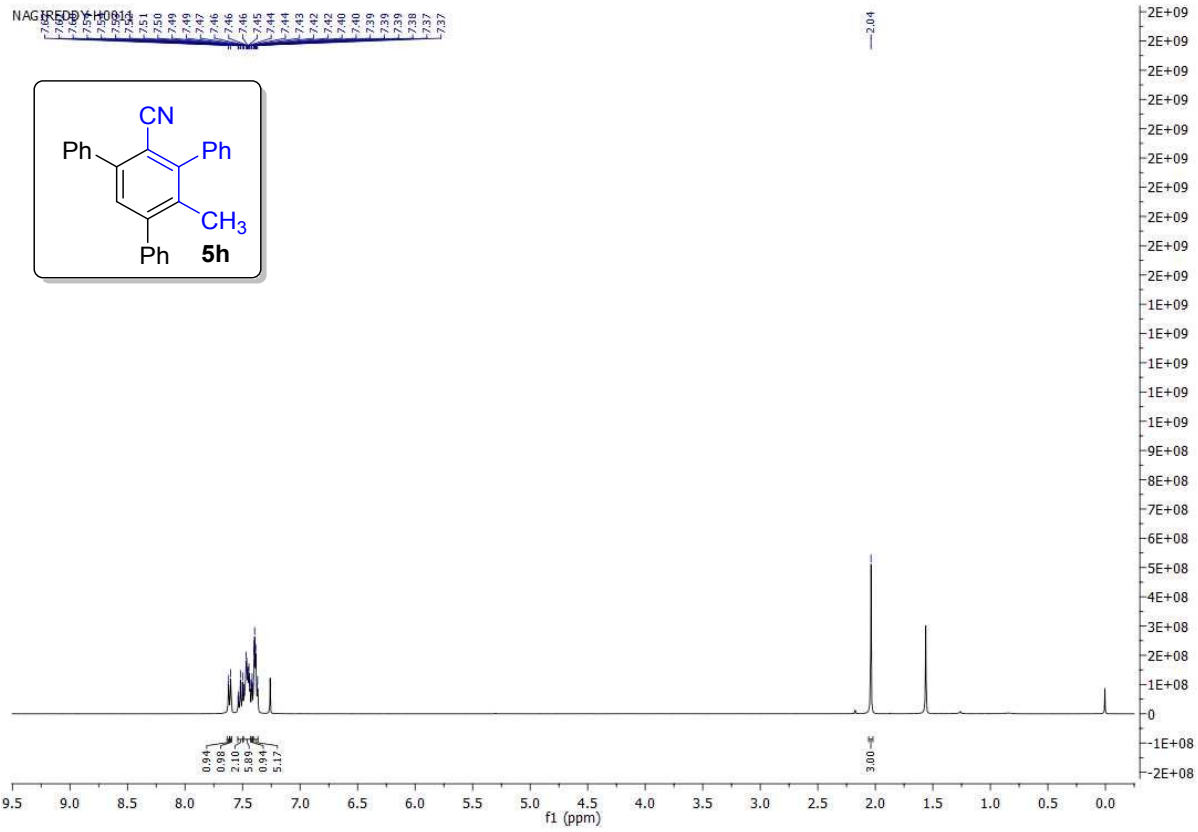

NAGI-H0041
144.81
144.34
143.14
141.40
139.27
138.92
136.92
134.90
130.48
128.97
128.88
128.53
128.49
128.45
118.85
102.12
36.37
Cl
NC
Ph
5f
6E+08
6E+08
6E+08
5E+08
4E+08
4E+08
4E+08
4E+08
3E+08
2E+08
2E+08
2E+08
1E+08
5E+07
0
-5E+07
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

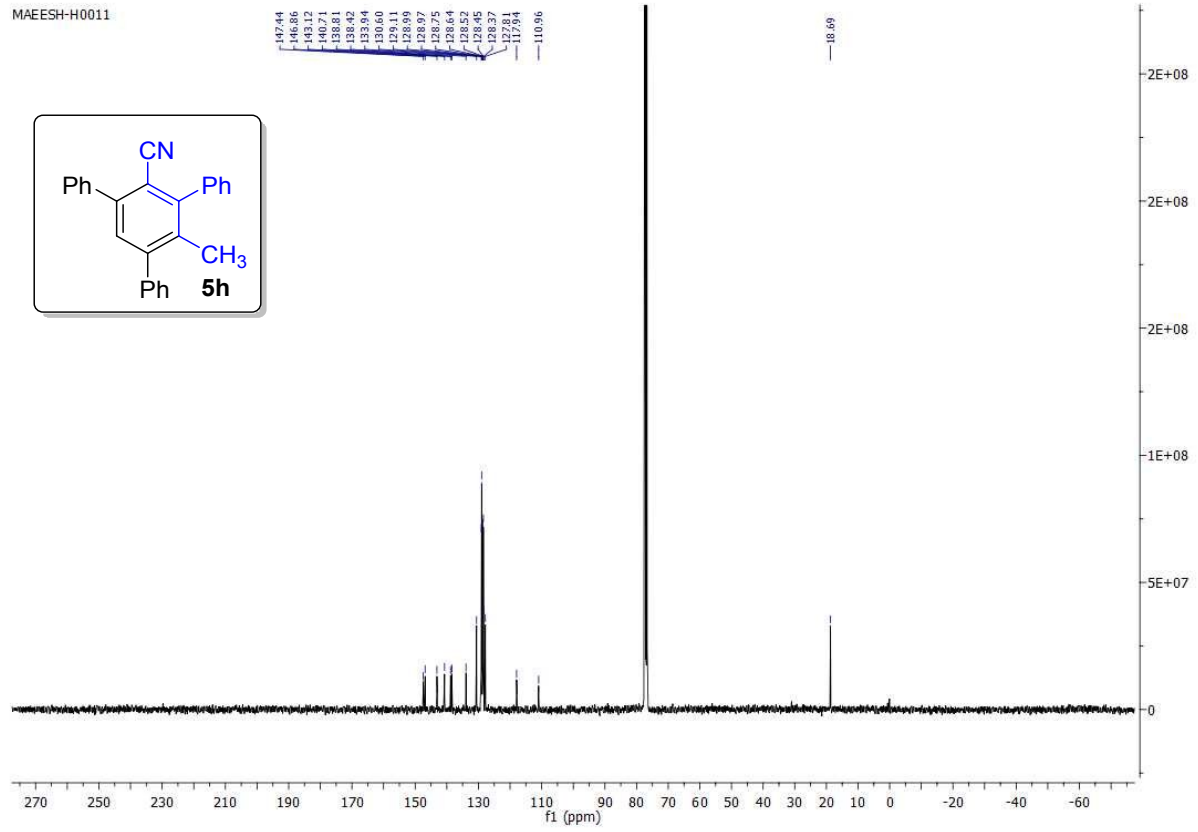

MSR_110_A_378
CSIR-IICT
XEVO-G2-XS-QToF
17FEB2020_8 15 (0.293) AM2 (Ar,22000.0,0.00,0.00); ABS; Cm (11:17-(2:7+21:38))
1: TOF MS ES+
4.41e5
100
%
0
149.0228
Cl
NC
Ph
5f
299.0619
378.1044
301.1403
355.0695
223.0635
225.0462
281.0511
317.1131
346.1577
380.1013
419.3169
445.1201
446.1202
391.2842
205.0862
248.0581
150.0263
121.0261
51.8950
113.1313
122.0315
151.0262
197.9842
464.3746
501.0864
60
80
100
120
140
160
180
200
220
240
260
280
300
320
340
360
380
400
420
440
460
480
500
m/z

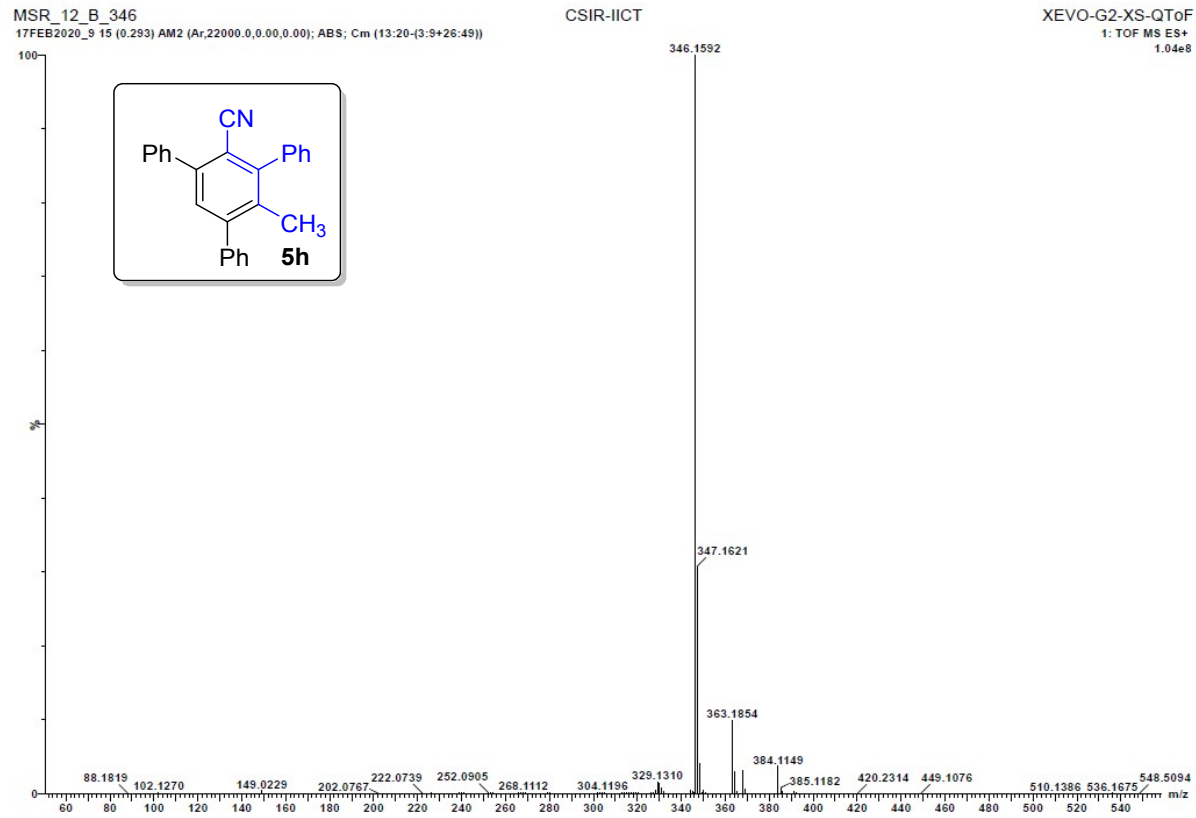

MANEESH-H0011
Br
NC
Ph
5g
f1 (ppm)

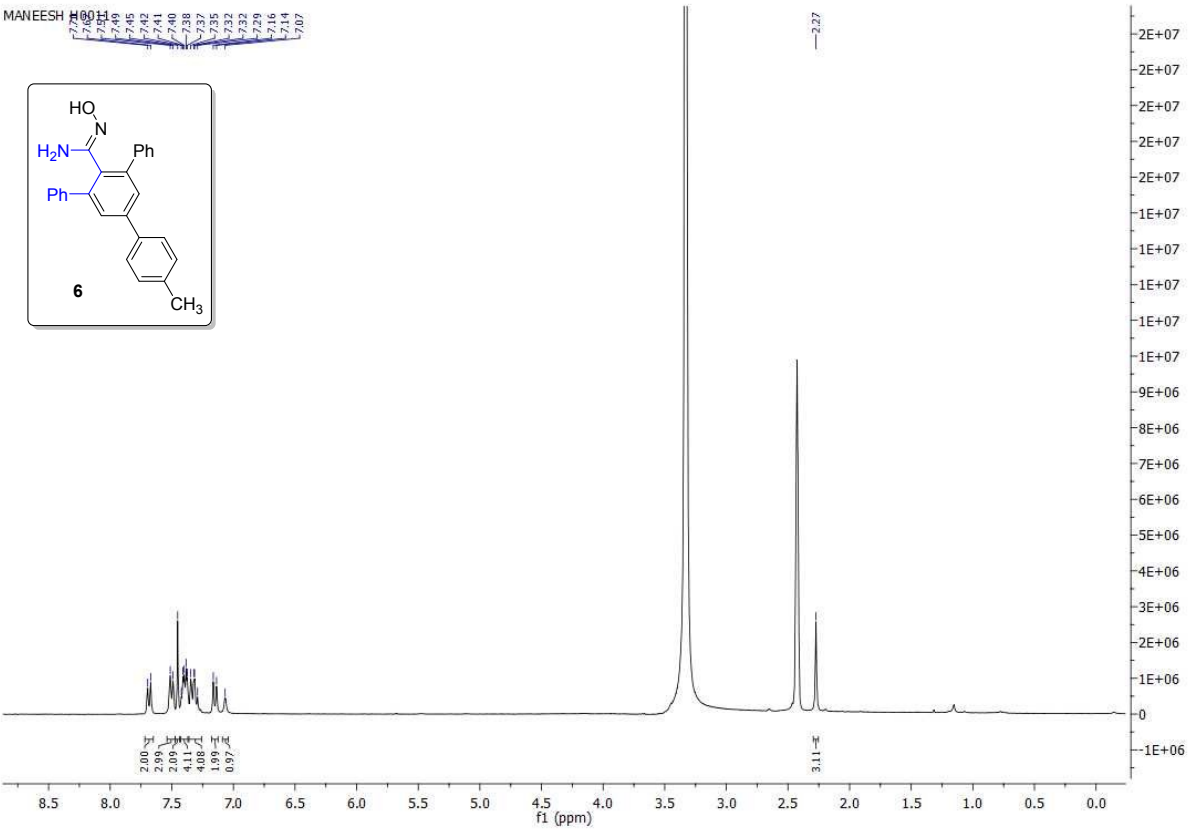

SURIBABU-H0011
Br
NC
Ph
5g
f1 (ppm)

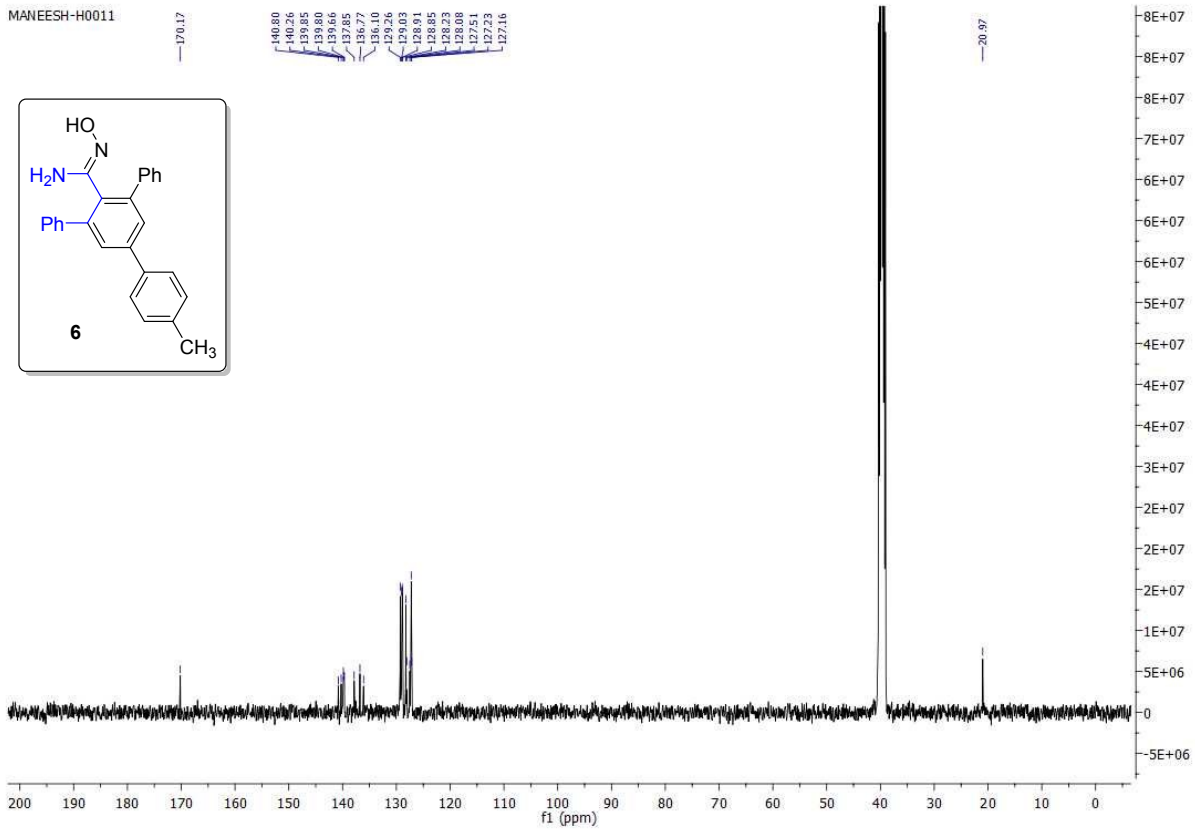

MSR_109_C_422
CSIR-IICT
XEVO-G2-XS-QToF
17FEB2020_6 15 (0.293) AM2 (Ar,22000.0,0.00,0.00); ABS; Cm (12:20-(1:9+25:53))
1: TOF MS ES+
4.59e6
Br
NC
Ph
5g
%
m/z
149.0228
424.0523
490.2653
343.1347
446.2387
534.2919
451.1941
342.1274
344.1385
537.1667
578.3187
402.2125
495.2186
538.1648
150.0263
219.1006
237.1107
307.1901
345.1453
539.2466
579.3200
99.0432
121.0273
205.0857
269.1383
299.0621
371.1013
519.1403
122.0306
167.0338
467.1669
93.0326

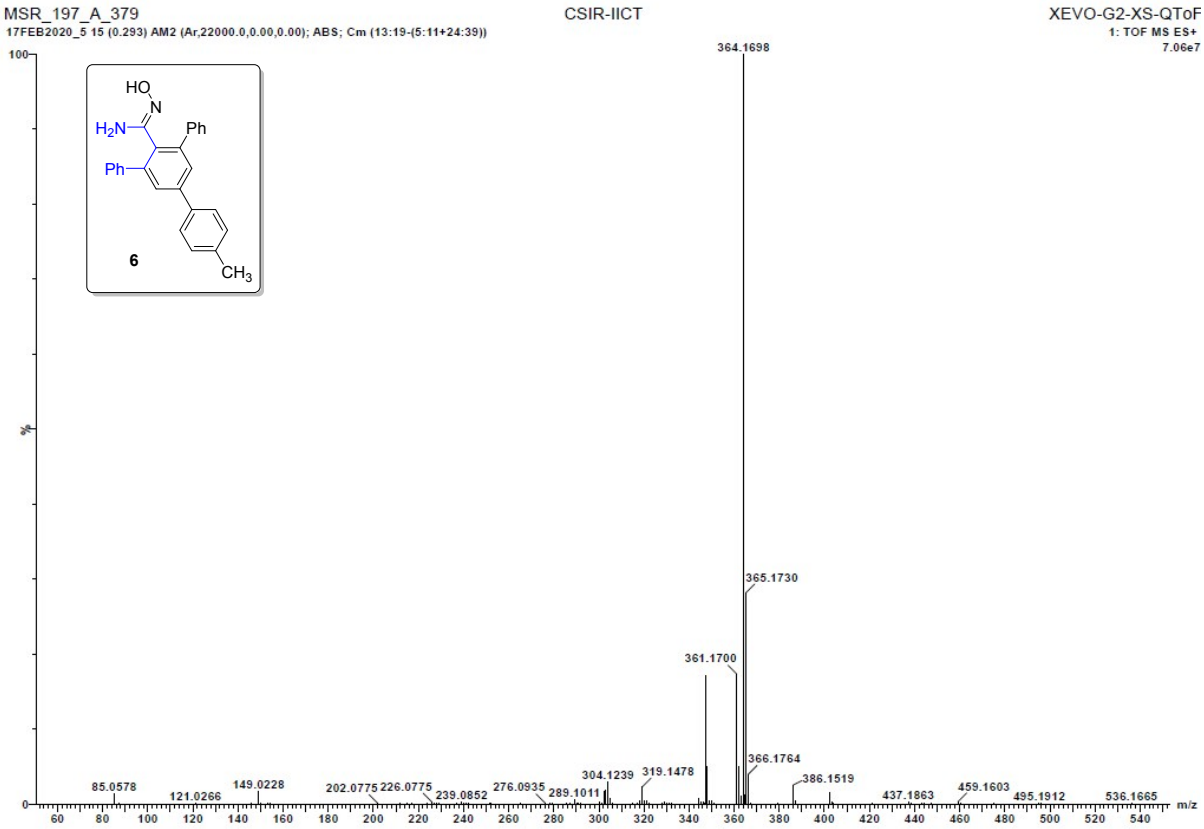

NAGIREDDY-H0014
CN
Ph
Ph
CH3
Ph
5h
f1 (ppm)

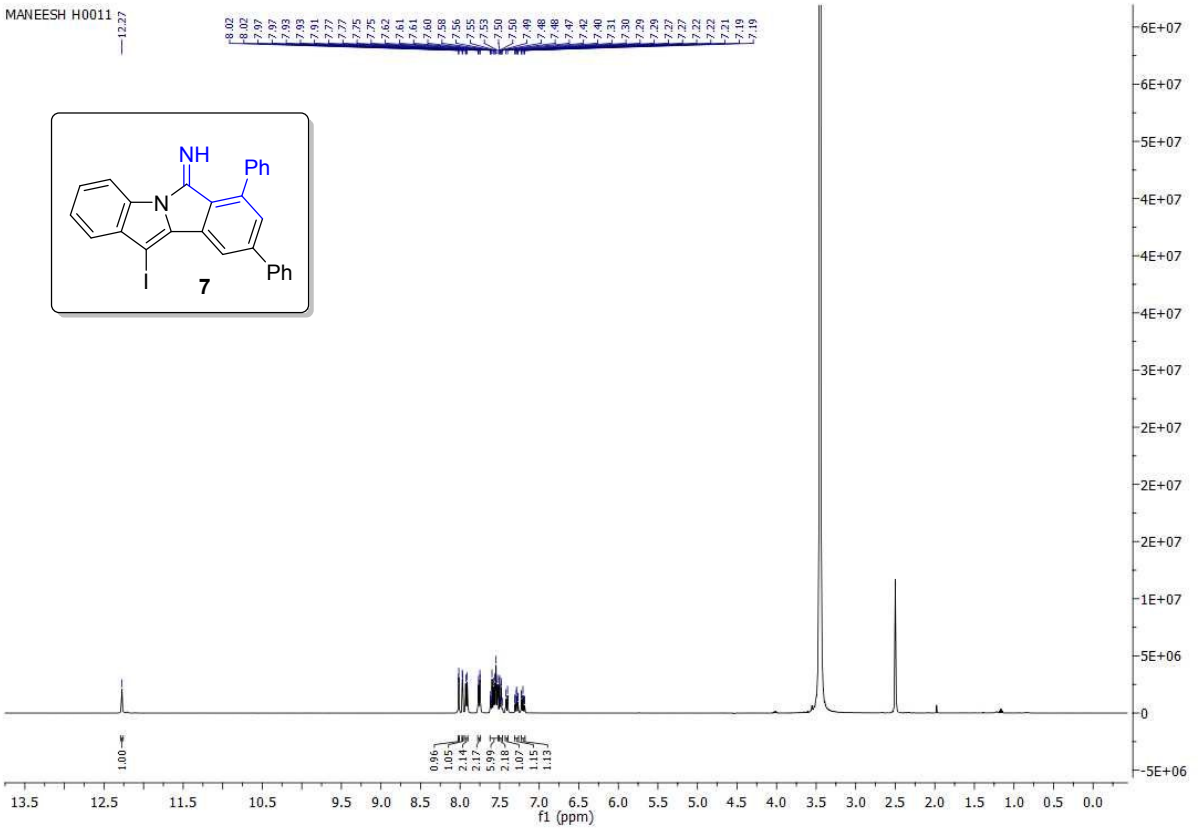

MAEESH-H0011
CN
Ph
Ph
CH3
Ph
5h
f1 (ppm)

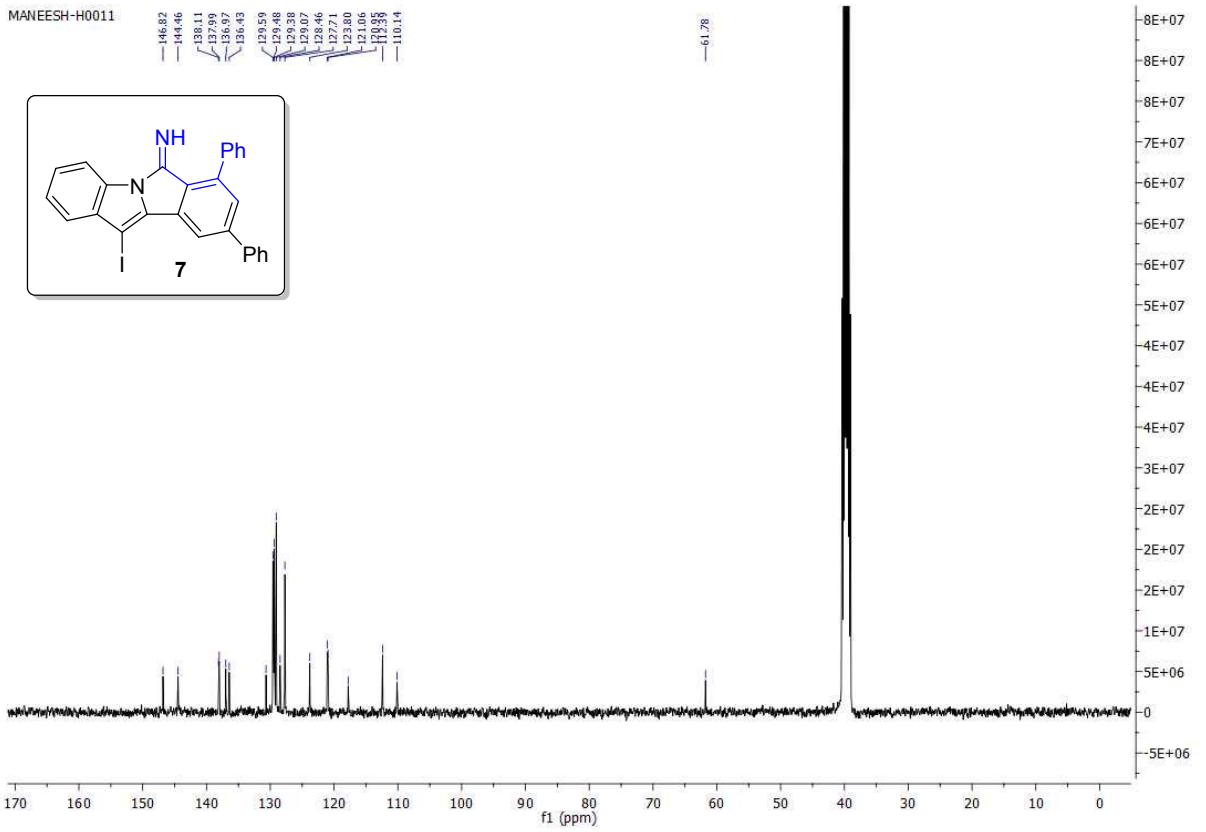

MSR_12_B_346
17FEB2020_9 15 (0.293) AM2 (Ar,22000.0,0.00,0.00); ABS; Cm (13:20-(3:9+26:49))
CSIR-IICT
XEVO-G2-XS-QToF
1: TOF MS ES+
1.04e8
CN
Ph
Ph
CH3
Ph
5h
346.1592
347.1621
363.1854
384.1149
385.1182
420.2314
449.1076
548.5094
m/z

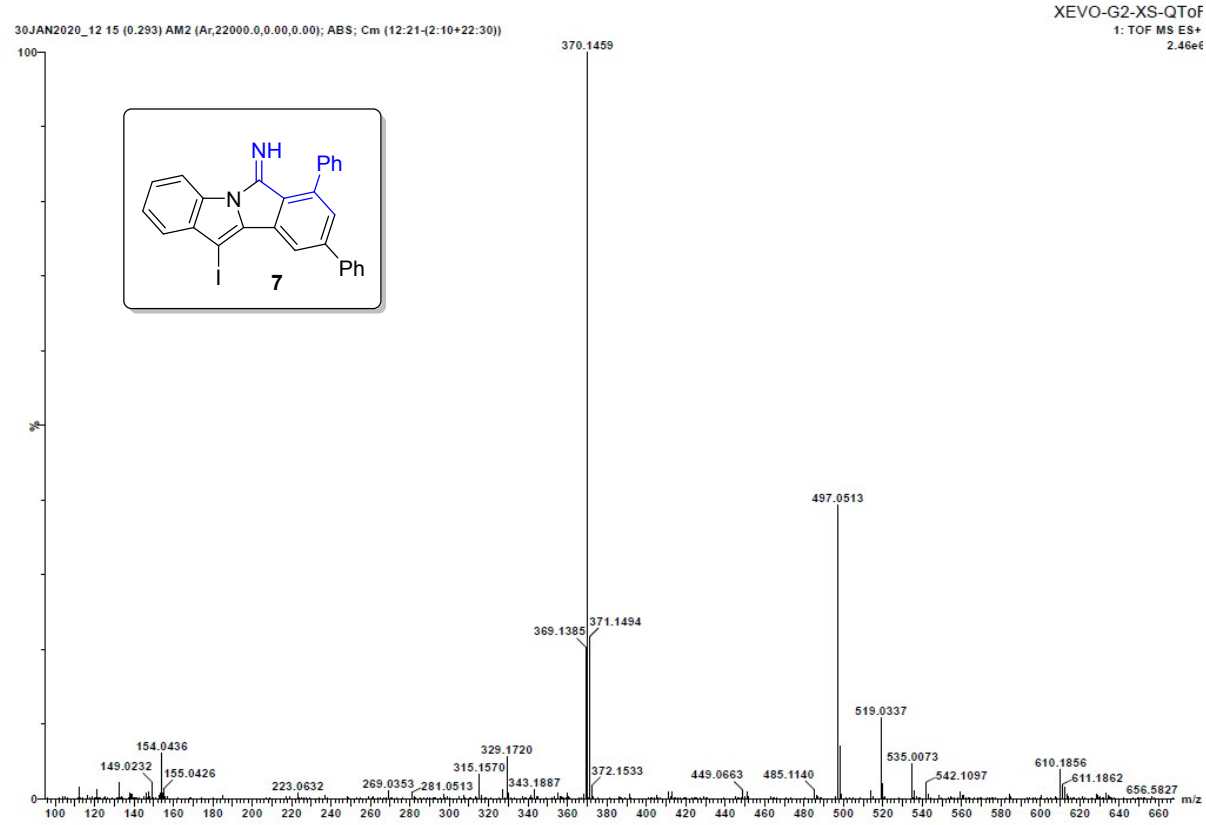

MANEESH 1001
HO
N
H2N
Ph
Ph
6
CH3
2.27
f1 (ppm)

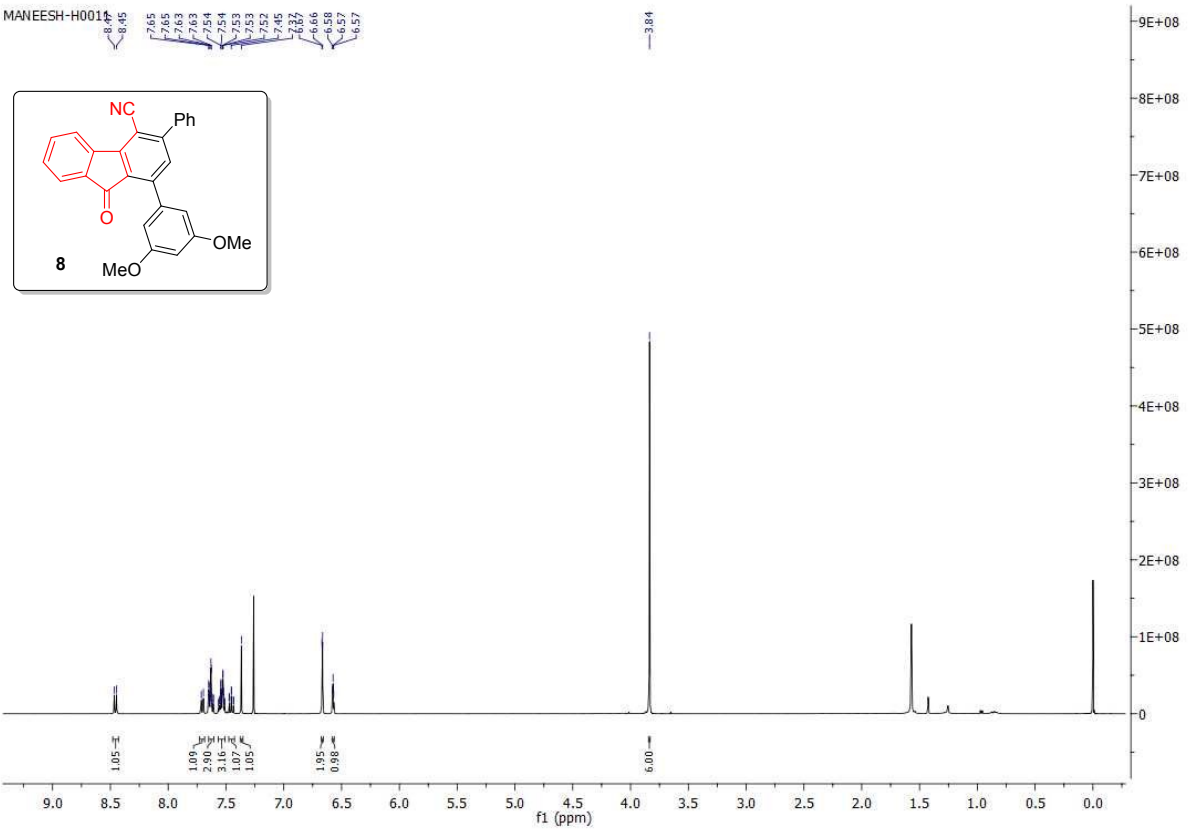

MANEESH-H0011
170.17
140.80
140.26
139.85
139.80
139.66
137.85
136.77
136.10
129.26
129.03
128.91
128.85
128.23
128.08
127.51
127.23
127.16
20.97
HO
N
H2N
Ph
Ph
6
CH3
8E+07
8E+07
8E+07
7E+07
6E+07
6E+07
6E+07
5E+07
4E+07
4E+07
4E+07
3E+07
2E+07
2E+07
2E+07
1E+07
5E+06
0
-5E+06
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

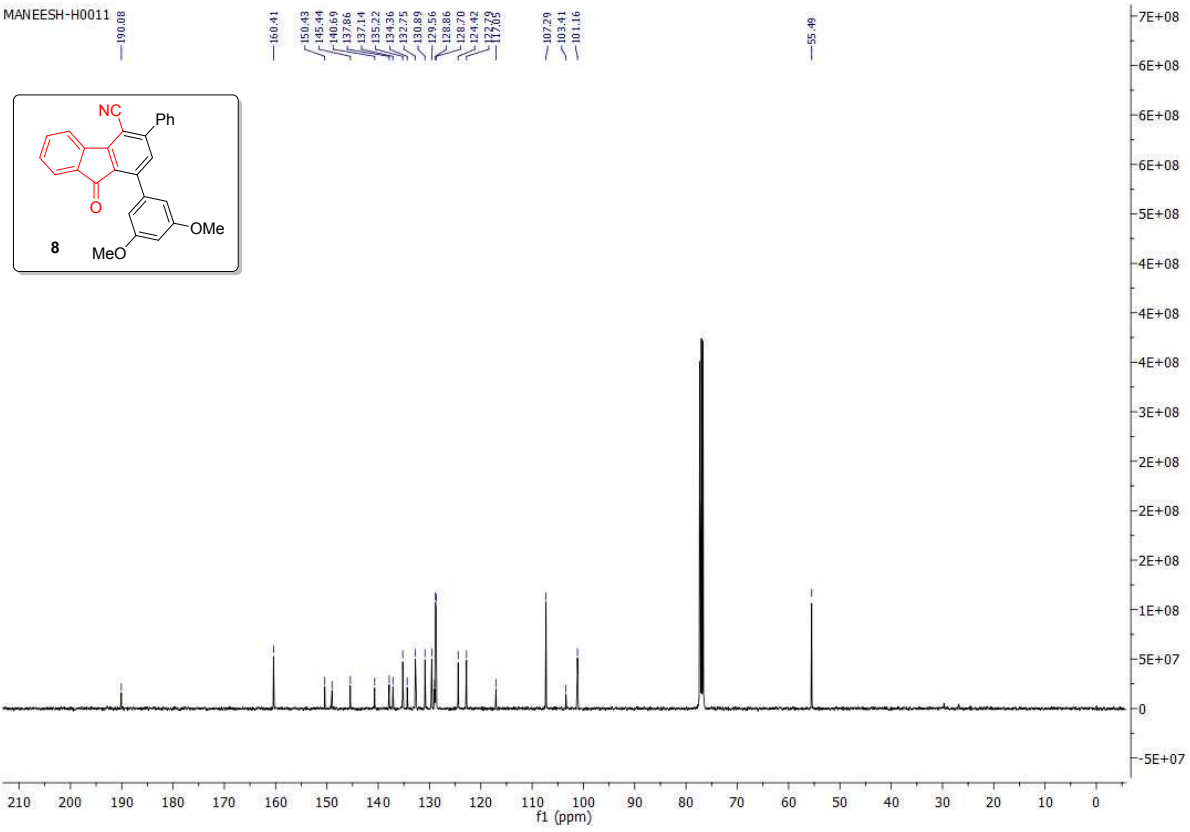

MSR_197_A_379
CSIR-IICT
XEVO-G2-XS-QToF
17FEB2020_5 15 (0.293) AM2 (Ar,22000.0,0.00,0.00); ABS; Cm (13:19-(5:11+24:39))
1: TOF MS ES+
7.06e7
HO
N
H2N
Ph
Ph
6
CH3
364.1698
365.1730
361.1700
366.1764
386.1519
304.1239
319.1478
85.0578
121.0266
149.0228
202.0775
226.0775
239.0852
276.0935
289.1011
437.1863
459.1603
495.1912
536.1665
m/z

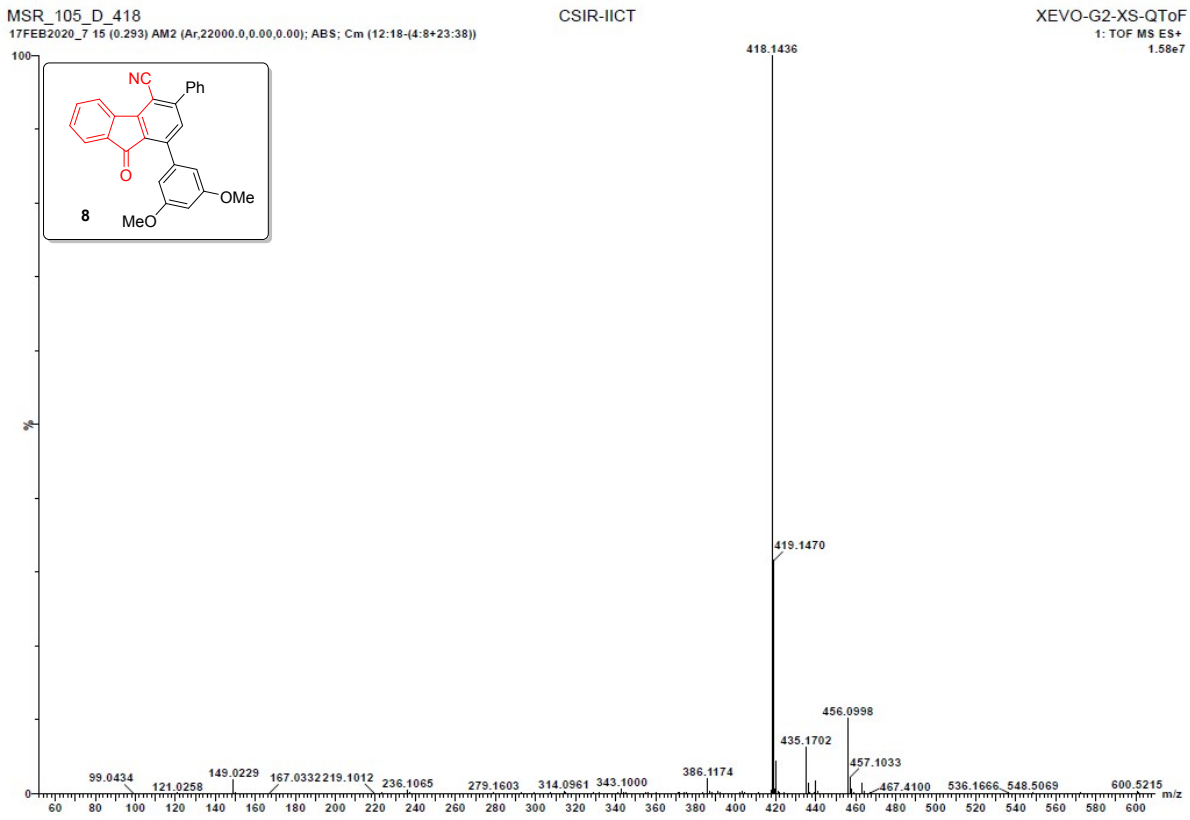

MANEESH H0011
NH
Ph
N
I
Ph
7
f1 (ppm)


MANEESH-H0011
146.82
144.46
138.11
137.99
136.97
136.43
129.59
129.48
129.38
129.07
128.46
127.71
123.80
121.06
112.39
110.14
61.78
NH
Ph
N
I
Ph
7
f1 (ppm)


30JAN2020_12 15 (0.293) AM2 (Ar,22000.0,0.00,0.00); ABS; Cm (12:21-(2:10+22:30))
XEVO-G2-XS-QToF
1: TOF MS ES+
370.1459
497.0513
369.1385
371.1494
519.0337
154.0436
149.0232
155.0426
329.1720
315.1570
343.1887
372.1533
223.0632
269.0353
281.0513
449.0663
485.1140
535.0073
542.1097
610.1856
611.1862
656.5827
NH
Ph
N
I
Ph
7
m/z


MANEESH-H0011
NC
Ph
O
OMe
MeO
8
f1 (ppm)


MANEESH-H0011
NC
Ph
O
OMe
MeO
8
f1 (ppm)


MSR_105_D_418
17FEB2020_7 15 (0.293) AM2 (Ar,22000.0,0.00,0.00); ABS; Cm (12:18-(4:8+23:38))
CSIR-IICT
XEVO-G2-XS-QToF
1: TOF MS ES+
1.58e7
NC
Ph
O
OMe
MeO
8
418.1436
419.1470
456.0998
435.1702
457.1033
99.0434
121.0258
149.0229
167.0332
219.1012
236.1065
279.1603
314.0961
343.1000
386.1174
467.4100
536.1666
548.5069
600.5215
%
m/z