Supporting Information

Pd-catalyzed C-H Arylation of Pyridazine-based Fused 1, 2, 4-Triazoles: Overriding Selectivity at the Usual Position by Undermining of Preferred Chelate Formation

Ramasamy Srinivasan,[a,b] Aniruddha Dey,[c] N. Shanmugam Nagarajan,[a]* Rajendran Senthil Kumaran,[b]* Thirumanavelan Gandhi[d]* and Debabrata Maiti[c]*

[a]Dept. of Chem., Gandhigram Rural Institute – Deemed University, Gandhigram, 624302, India.
[b]Syngene Int. Ltd, Bangalore, 560099, India
[c]Dept. of Chem., IIT Bombay, Powai, Mumbai 400076, India
[d]Dept. of Chem., VIT University, Vellore, 632014, Tamil Nadu, India

*Email: dmaiti@chem.iitb.ac.in

velan.g@vit.ac.in

senthilkr76@rediffmail.com

nsnrajan@yahoo.co.in

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1. General information:

Reagent information:

Unless otherwise stated, all the reactions were carried out in screw cap reaction tube under nitrogen atmosphere with magnetic stirring. Palladium salts were purchased from Alfa Aesar and used directly. All other reagents were purchased from Sigma Aldrich. All the dry solvents were bought from MERCK and used directly. For column chromatography silica gel (230-400 mesh) was supplied from MERCK. During elution hexane and ethyl acetate mixture was used.

Analytical information:

All the reagents were purchased commercially and used without further purification. The dry solvents were purchased directly and used as such. ^{1}H and ^{13}C NMR spectra were recorded on 300 or 400 MHz Bruker spectrometers in $CDCl_3$. The chemical shifts were reported in δ ppm relative to TMS. UPLC was recorded on Acquity ultra performance LC instrument. Melting point was measured in BÜCKI - B545 instrument. The TLC spots were visualized in UV light/$KMnO_4$ strain. For TLC, 'Silica gel-G for TLC', supplied by Merk & Co was used.

2. Experimental section:

2.1 Table 1: Optimization details

Entry	Pd catalyst (10 mol %)	Oxidant/ Base (2 eq)	Ligand/ Co-oxidant (10 mol %)	Solvent	Temp (º C)	Isolated Yield of 2a (%)
1	$Pd(OAc)_2$[(a)]	K_2CO_3	KOAc	DMF	110	-
2	$Pd(OAc)_2$	K_2CO_3	KOAc	DMF	110	5
3	$Pd(OAc)_2$	Ag_2CO_3	-	DCE	85	20
4	$Pd(OAc)_2$	$K_2S_2O_8$	-	DCE	110	-
5	$Pd(OAc)_2$	$K_2S_2O_8$	-	DMF	110	-
6	$Pd(OAc)_2$	Ag_2CO_3	1,10-phen	DMF	110	75

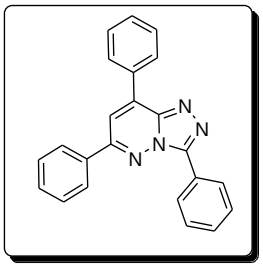
7	$Pd(OAc)_2$	Ag_2CO_3	-	DMF	100	80
8	$Pd(OAc)_2$[(b)]	Ag_2CO_3	-	DMF	100	80
9	$PdCl_2(ACN)_2$	Ag_2CO_3	-	DMF	110	35
10	$PdCl_2(PPh_3)_2$	Ag_2CO_3	-	DMF	110	26
11	$Pd(OAc)_2$	K_2CO_3	PPh_3	DMF	110	-
12	$PdCl_2$	Ag_2CO_3	-	DMF	110	10
13	CuI	Cs_2CO_3	1, 10-phen	DMF	110	-
14	$Pd(OAc)_2$	Ag_2CO_3	O_2	DMF	100	43
15	$Pd(OAc)_2$	-	O_2	DMF	100	-

2.2 General procedure for arylation:

3,6-Diphenyl-[1,2,4]triazolo pyridazine (**1a**) (0.2 g, 0.73 mmol), Iodobenzene (**2a**) (1.46 mmol), Ag_2CO_3 (1.46 mmol) were taken in dry DMF (5 mL) in a screw cap reaction tube with septum. The mixture was throughly degassed with dry nitrogen for 10 minutes. $Pd(OAc)_2$ (0.036 mmol) was added to the mixture and heated to 100 ^oC for 12 h. The mixture was filtered through the celite pad and washed with DCM (40 mL). The organic layer was washed with water (2 x 20 mL), brine (20 mL) and dried over sodium sulphate. The organic layer was concentrated under reduced pressure and the residue obtained was charged into a silica gel column using 15 to 20 % EtOAc in hexane as an eluent to afford 0.20 g (80 %) of (**3a)** as a yellow solid. The same procedure was followed for the synthesis of all the compounds.

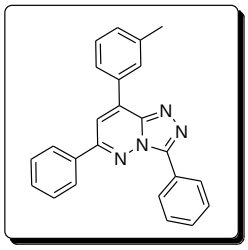
3. Characterization data

3,6,8-Triphenyl-[1,2,4]triazolo[4,3-b]pyridazine (3a)



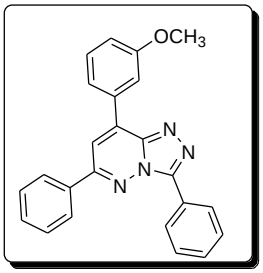
Yield: 204 mg (80 %). mp 218-220 ^{o}C. **^{1}H NMR (400 MHz, $CDCl_3$):** δ 8.63 (d, *J* = 7.80 Hz, 2H), 8.41-8.39 (m, 2H), 8.10-8.07 (m, 2H), 7.76 (s, 1H), 7.63-7.54 (m, 9H); **^{13}C NMR (100 MHz, $CDCl_3$):** δ 154.0, 148.6, 144.2, 137.5, 134.9, 132.5, 131.1, 130.8, 130.1, 129.2, 129.0, 128.7, 127.8, 127.3, 126.7, 114.7. UPLC: $(M + H)^+$ 349.5 (Purity: 100 %).

3,6-Diphenyl-8-m-tolyl-[1,2,4]triazolo[4,3-b]pyridazine (3b)



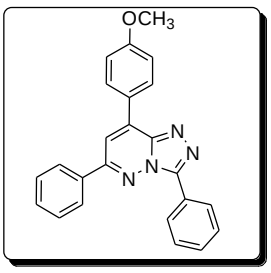
Yield: 210 mg (79 %). mp 123-125 ^{o}C. **^{1}H NMR (400 MHz, $CDCl_3$):** δ 8.65 (d, *J* = 7.80 Hz, 2H), 8.24 (s, 1H), 8.17 (d, *J* = 7.72 Hz, 1H), 8.11-8.09 (m, 2H), 7.76 (s, 1H), 7.64-7.56 (m, 6H), 7.51 (t, *J* = 7.68 Hz, 1H), 7.43-7.41 (m, 1H), 2.53 (s, 3H). **^{13}C NMR (75 MHz, $CDCl_3$):** δ 153.9, 148.4, 144.2, 138.7, 137.6, 134.9, 132.4, 131.8, 130.7, 129.9, 129.8, 129.1, 128.8, 128.6, 127.8, 127.3, 126.7, 126.2, 114.6, 21.5. UPLC: $(M + H)^+$ 363.6 (Purity: 95.7 %).

8-(3-Methoxyphenyl)-3,6-diphenyl-[1,2,4]triazolo[4,3-b]pyridazine (3c)



Yield: 208 mg (75 %). mp 179-181 ^{o}C. **^{1}H NMR (400 MHz, $CDCl_3$):** δ 8.64 (d, *J* = 7.60 Hz, 2H), 8.08-8.06 (m, 3H), 7.89 (d, *J* = 7.76 Hz, 1H), 7.76 (s, 1H), 7.62-7.55 (m, 6H), 7.50 (t, *J* = 8.0 Hz, 1H), 7.13 (d, *J* = 7.20 Hz, 1H), 3.95 (s, 3H). **^{13}C NMR (75 MHz, $CDCl_3$):** δ 159.9, 154.0, 148.6, 144.1, 137.5, 134.9, 133.7, 130.7, 130.0, 129.9, 129.2, 128.6, 127.8, 127.3, 126.6, 121.2, 117.1, 114.7, 114.6, 55.5. UPLC: $(M + H)^+$ 379.5 (Purity: 98.4 %).

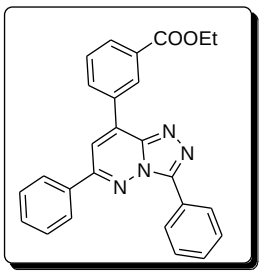
8-(4-Methoxyphenyl)-3,6-diphenyl-[1,2,4]triazolo[4,3-b]pyridazine (3d)



Yield: 191 mg (69 %). mp 205-207 ^{o}C. **^{1}H NMR (300 MHz, $CDCl_3$):** δ 8.61 (d, *J* = 7.17 Hz, 2H), 8.43 (d, *J* = 8.79 Hz, 2H), 8.06-8.04 (m, 2H), 7.68 (s, 1H), 7.61-7.52 (m, 6H), 7.07 (d, *J* = 8.79 Hz, 2H), 3.89 (s, 3H). **^{13}C NMR (75 MHz, $CDCl_3$):** δ 162.0, 154.2, 136.8, 135.1, 130.8, 130.6, 130.1, 129.1, 128.6,

127.9, 127.3, 126.4, 124.5, 114.4, 113.3, 55.4; UPLC: $(M + H)^+$ 379.5 (Purity: 98.2 %).

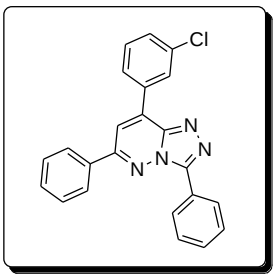
Ethyl 3-(3,6-diphenyl-[1,2,4]triazolo[4,3-b]pyridazin-8-yl)benzoate (3e)



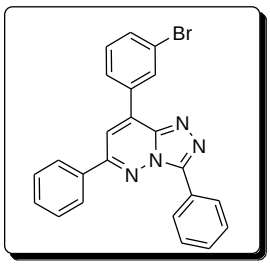
Yield: 222 mg (72 %). mp 122-124 °C. **^{1}H NMR (300 MHz, $CDCl_3$):** δ 8.82 (s, 1H**),** 8.75 (d, *J* = 7.27 Hz, 1H), 8.59 (d, *J* = 7.94 Hz, 2H), 8.21 (d, *J* = 7.27 Hz, 1H), 8.07-8.04 (m, 2H), 7.76 (s, 1H), 7.66 (t, *J* = 7.80 Hz, 1H), 7.61-7.49 (m, 6H), 4.44 (q, *J* = 7.14 Hz, 2H), 1.44 (t, *J* = 7.11 Hz, 3H). **^{13}C NMR (75 MHz, $CDCl_3$):** δ 165.9, 154.0, 148.6, 143.8, 136.5, 134.6, 134.0, 132.7, 131.7, 131.3, 130.8, 130.1, 129.4, 129.2, 129.1, 128.6, 127.8, 127.3, 126.5, 115.0, 61.4, 14.3. UPLC: $(M + H)^+$ 421.5 (Purity: 99.0 %).

8-(3-Chlorophenyl)-3,6-diphenyl-[1,2,4]triazolo[4,3-b]pyridazine (3f)

Yield: 196 mg (70 %). mp 190-192°C. **^{1}H NMR (400 MHz, $CDCl_3$):** δ 8.61 (d, *J* = 7.80 Hz, 2H), 8.34-8.31 (m, 2H), 8.06-8.04 (m, 2H), 7.70 (s, 1H), 7.61-7.49 (m, 8H). **^{13}C NMR (100 MHz, $CDCl_3$):** δ 154.1, 148.7, 143.8, 136.0, 135.1, 134.7, 134.1, 131.1, 130.9, 130.3, 130.2, 129.3, 129.0, 128.7, 127.9, 127.5, 127.4, 126.5, 115.0. UPLC: $(M + H)^+$ 383.6 & 385.6 (Cl pattern) (Purity: 94.2 %).

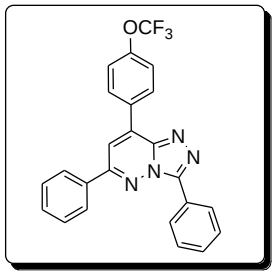


8-(3-Bromophenyl)-3,6-diphenyl-[1,2,4]triazolo[4,3-b]pyridazine (3g)



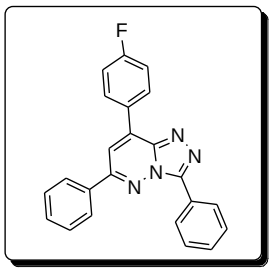
Yield: 222 mg (71 %). mp 186-188 °C. **^{1}H NMR (300 MHz, $CDCl_3$):** δ 8.62 (d, *J* = 7.57 Hz, 2H), 8.49 (s, 1H), 8.41 (d, *J* = 7.74 Hz, 1H), 8.10-8.06 (m, 2H), 7.73 (s, 1H), 7.64-7.55 (m, 7H), 7.49 (t, *J* = 7.92 Hz, 1H). **^{13}C NMR (100 MHz, $CDCl_3$):** δ 154.1, 148.7, 143.7, 136.0, 134.7, 134.4, 134.0, 131.8, 131.0, 130.6, 130.2, 129.3, 128.7, 128.1, 127.9, 127.4, 126.5, 123.1, 115.1. UPLC: $(M + H)^+$ 427.3 & 429.3 (Br pattern) (Purity: 92.9 %).

3,6-Diphenyl-8-(4-(trifluoromethoxy)phenyl)-[1,2,4]triazolo[4,3-b]pyridazine (3h)



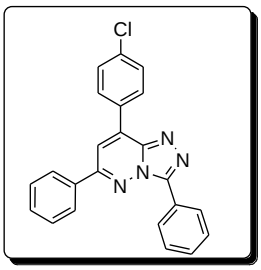
Yield: 241 mg (76 %). mp 175-177 ^{o}C. **^{1}H NMR (300 MHz, $CDCl_3$):** δ 8.62 (d, *J* = 7.59 Hz, 2H), 8.48 (d, *J* = 8.82 Hz, 2H), 8.09-8.07 (m, 2H), 7.75 (s, 1H), 7.63-7.55 (m, 6H), 7.46 (d, *J* = 8.30 Hz, 2H). **^{13}C NMR (100 MHz, $CDCl_3$):** δ 154.1, 151.2, 148.8, 143.9, 136.1, 134.8, 131.0, 130.9, 130.2, 129.3, 128.7, 127.9, 127.4, 126.5, 121.2, 119.1, 114.8. UPLC: $(M + H)^+$ 433.5 (Purity: 100 %).

8-(4-Fluorophenyl)-3,6-diphenyl-[1,2,4]triazolo[4,3-b]pyridazine (3i)



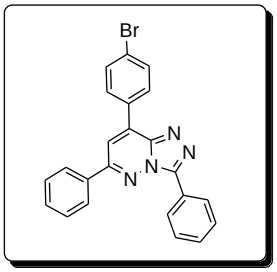
Yield: 210 mg (78 %). mp 187-189 ^{o}C. **^{1}H NMR (400 MHz, $CDCl_3$):** δ 8.62 (d, *J* = 7.80 Hz, 2H), 8.47-8.43 (m, 2H), 8.08-8.06 (m, 2H), 7.72(s, 1H), 7.62-7.55 (m, 6H), 7.32-7.27 (m, 2H). **^{13}C NMR (100 MHz, $CDCl_3$):** δ 165.8, 163.3, 154.2, 148.7, 144.1, 136.5, 134.9, 131.5, 131.4, 130.9, 130.2, 129.3, 128.7, 128.6, 128.0, 127.4, 126.5, 116.4, 116.2, 114.5. UPLC: $(M + H)^+$ 367.5 (Purity: 97.1 %).

8-(4-Chlorophenyl)-3,6-diphenyl-[1,2,4]triazolo[4,3-b]pyridazine (3j)



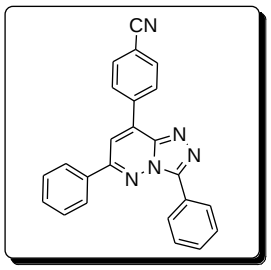
Yield: 224 mg (80 %). mp 223-225 ^{o}C. **^{1}H NMR (300 MHz, $CDCl_3$):** δ 8.59 (d, *J* = 7.47 Hz, 2H), 8.38 (d, *J* = 8.05 Hz, 2H), 8.06-8.05 (m, 2H), 7.72 (s, 1H), 7.60-7.55 (m, 8H). **^{13}C NMR (75 MHz, $CDCl_3$):** δ 154.2, 148.5, 143.5, 137.4, 136.2, 134.7, 130.9, 130.6, 130.4, 130.3, 129.3, 129.2, 128.7, 127.9, 127.3, 126.2, 114.7. UPLC: $(M + H)^+$ 383.5, 385.4 (Cl pattern) (Purity: 100 %).

8-(4-Bromophenyl)-3,6-diphenyl-[1,2,4]triazolo[4,3-b]pyridazine (3k)



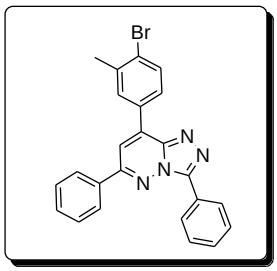
Yield: 232 mg (74 %). mp 220-222 ^{o}C. **^{1}H NMR (400 MHz, $CDCl_3$):** δ 8.60 (dd, *J* = 1.6, 7.20 Hz, 2H), 8.31 (d, *J* = 7.60 Hz, 2H), 8.08-8.05 (m, 2H), 7.74-7.71 (m, 3H), 7.62-7.52 (m, 6H); **^{13}C NMR (100 MHz, $CDCl_3$):** δ 154.2, 148.6, 143.8, 136.3, 134.8, 132.3, 131.2, 130.9, 130.7, 130.2, 129.3, 128.7, 127.9, 127.4, 126.4, 125.9, 114.6. UPLC: $(M + H)^+$ 427.5, 429.4 (Br Pattern) (Purity: 93.1 %).

4-(3,6-Diphenyl-[1,2,4]triazolo[4,3-b]pyridazin-8-yl)benzonitrile (3l)



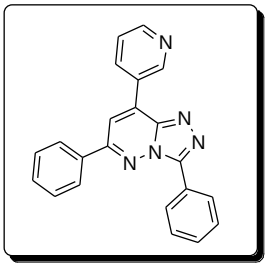
Yield: 194 mg (71 %). mp 215-217 ^{o}C. **^{1}H NMR (400 MHz, $CDCl_3$):** δ 8.62 (d, *J* = 7.20 Hz, 2H), 8.55 (d, *J* = 7.80 Hz, 2H), 8.11-8.07 (m, 2H), 7.92 (d, *J* = 7.80 Hz, 2H), 7.81 (s, 1H), 7.62-7.55 (m, 6H). **^{13}C NMR (100 MHz, $CDCl_3$):** δ 154.2, 148.9, 143.4, 136.6, 135.4, 134.4, 132.7, 131.2, 130.4, 129.8, 129.4, 128.8, 127.9, 127.4, 126.2, 118.2, 115.8, 114.5. UPLC: $(M + H)^+$ 374.6 (Purity: 97.1 %).

8-(4-Bromo-3-methylphenyl)-3,6-diphenyl-[1,2,4]triazolo[4,3-b]pyridazine (3m)



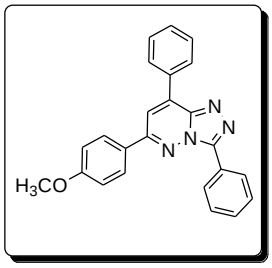
Yield: 233 mg (72 %). mp 220-222 ^{o}C. **^{1}H NMR (300 MHz, $CDCl_3$):** δ 8.62 (d, *J* = 7.29 Hz, 2H), 8.34 (s, 1H), 8.09-8.05 (m, 3H), 7.77-7.74 (m, 2H), 7.61-7.52 (m, 6H), 2.56 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$):** δ 154.0, 148.5, 143.8, 138.9, 136.4, 134.8, 133.0, 131.4, 131.3, 130.9, 130.2, 129.3, 128.7, 128.4, 127.9, 127.7, 127.4, 126.4, 114.5, 23.1. UPLC: $(M + H)^+$ 441.3 & 443.3 (Br pattern) (Purity: 97.9 %).

3,6-Diphenyl-8-(pyridin-3-yl)-[1,2,4]triazolo[4,3-b]pyridazine (3n)



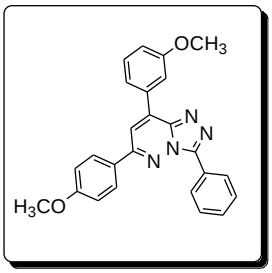
Yield: 176 mg (69 %). mp 230-232 ^{o}C. **^{1}H NMR (300 MHz, $CDCl_3$):** δ 9.42 (s, 1H), 8.93 (d, *J* = 7.80 Hz, 1H), 8.82 (d, *J* = 4.02 Hz, 1H), 8.62 (d, *J* = 7.98 Hz, 2H), 8.09-8.08 (m, 2H), 7.81 (s, 1H), 7.62-7.56 (m, 7H). **^{13}C NMR (75 MHz, $CDCl_3$):** δ 154.0, 151.5, 149.0, 148.8, 143.5, 137.3, 134.5, 131.0, 130.2, 129.3, 128.7, 127.8, 127.3, 126.3, 123.7, 114.9. UPLC: $(M + H)^+$ 350.5 (Purity: 100 %).

6-(4-Methoxyphenyl)-3,8-diphenyl-[1,2,4]triazolo[4,3-b]pyridazine (5a)



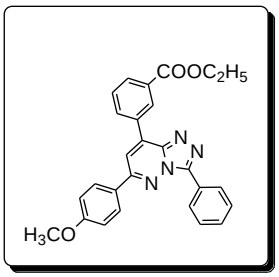
Yield: 202 mg (81 %). mp 203-205 ^{o}C. **^{1}H NMR (400 MHz, $CDCl_3$):** δ 8.62 (d, *J* = 7.2 Hz, 2H), 8.37 (dt, *J* = 6.40, 2.00 Hz, 2H), 8.03 (d, *J* = 7.80 Hz, 2H), 7.70 (s, 1H), 7.62-7.53 (m, 6H), 7.08 (d, *J* = 7.80 Hz, 2H), 3.91 (s, 3H). **^{13}C NMR (75 MHz, $CDCl_3$):** δ 161.8, 153.6, 148.5, 144.0, 137.3, 132.5, 130.9, 130.0, 129.1, 129.0, 128.7, 128.6, 127.9, 127.1, 126.6, 114.6, 55.4. UPLC: $(M + H)^+$ 379.5 (Purity: 100 %).

8-(3-Methoxyphenyl)-6-(4-methoxyphenyl)-3-phenyl-[1,2,4]triazolo[4,3-b]pyridazine (5b)



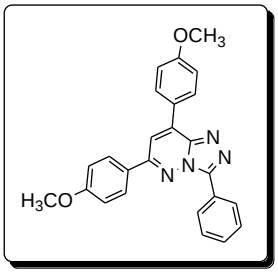
Yield: 215 mg (80 %). mp 141-143 ^{o}C. **^{1}H NMR (400 MHz, $CDCl_3$):** δ 8.63 (d, *J* = 6.80 Hz, 2H), 8.04-8.01 (m, 3H), 8.81 (d, *J* = 7.2 Hz, 1H), 7.71(s, 1H), 7.62-7.58 (m, 2H), 7.56-7.48 (m, 2H), 7.13-7.07 (m, 3H), 3.95 (s, 3H), 3.92 (s, 3H). **^{13}C NMR (75 MHz, $CDCl_3$):** δ 161.7, 159.9, 153.4, 148.3, 144.1, 137.0, 133.8, 129.9, 128.7, 128.5, 127.7, 127.1, 127.0, 126.7, 121.1, 116.9, 114.5 (2C), 55.5, 55.4. UPLC: $(M + H)^+$ 409.4 (Purity: 98.1 %).

Ethyl 3-(6-(4-methoxyphenyl)-3-phenyl-[1,2,4]triazolo[4,3-b]pyridazin-8-yl) benzoate (5c)



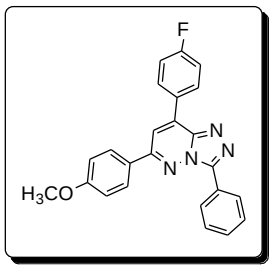
Yield: 232 mg (78 %). mp 181-183 ^{o}C. **^{1}H NMR (300 MHz, $CDCl_3$):** δ 8.83 (t, *J* = 1.60 Hz, 1H), 8.79 (dd, *J* = 7.81, 1.17 Hz, 1H), 8.62 (d, *J* = 7.62, 2H), 8.25 (dd, *J* = 7.8, 1.2 Hz, 1H), 8.06 (d, *J* = 7.86 Hz, 2H), 7.78 (s, 1H), 7.77 (t, *J* = 7.80 Hz, 1H), 7.64-7.52 (m, 3H), 7.10 (d, *J* = 8.8 Hz, 2H), 4.46 (q, *J* = 7.14, 2H), 3.92 (s, 3H), 1.45 (t, *J* = 7.11, 3H), **^{13}C NMR (75 MHz, $CDCl_3$):** δ 166.0, 161.9, 153.6, 143.8, 136.2, 134.1, 132.9, 131.7, 131.3, 130.0, 129.4, 129.1, 128.8, 128.6, 127.8, 126.9, 126.5, 114.9, 114.6, 61.4, 55.4, 14.3. UPLC: $(M + H)^+$ 451.6 (Purity: 99.5 %).

6,8-bis(4-Methoxyphenyl)-3-phenyl-[1,2,4]triazolo[4,3-b]pyridazine (5d)



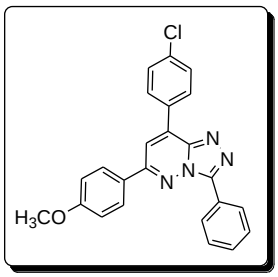
Yield: 213 mg (79 %). mp 190-192 ^{o}C. **^{1}H NMR (300 MHz, $CDCl_3$):** δ 8.62 (d, *J* = 7.77 Hz, 2H), 8.43 (d, *J* = 7.5 Hz, 2H), 8.03 (d, *J* = 7.50 Hz, 2H), 7.66 (s, 1H), 7.62-7.53 (m, 3H), 7.10-7.05 (m, 4H), 3.92 (s, 6H). **^{13}C NMR (75 MHz, $CDCl_3$):** δ 161.8, 161.6, 153.4, 148.2, 144.2, 136.4, 130.7, 129.8, 128.6, 128.5, 127.7, 127.3, 126.8, 124.7, 114.4, 114.3, 112.8, 55.4. UPLC: $(M + H)^+$ 409.4 (Purity: 95.5 %).

8-(4-Fluorophenyl)-6-(4-methoxyphenyl)-3-phenyl-[1,2,4]triazolo[4,3-b]pyridazine (5e)



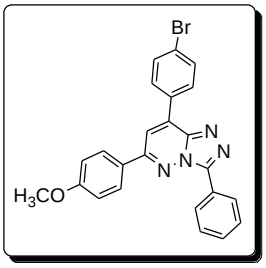
Yield: 217 mg (83 %). mp 187-189 ^{o}C. **^{1}H NMR (300 MHz, $CDCl_3$):** δ 8.60 (d, *J* = 7.5 Hz, 2H), 8.42 (t, *J* = 7.29 Hz, 2H), 8.03 (d, *J* = 8.49 Hz, 2H), 7.78 (s, 1H), 7.67-7.53 (m, 3H), 7.29 (t, *J* = 8.55 Hz, 2H), 7.09 (d, *J* = 8.34 Hz, 2H), 3.92 (s, 3H). **^{13}C NMR (75 MHz, $CDCl_3$):** δ 165.7, 163.2, 161.9, 153.5, 148.4, 143.9, 135.9, 131.4, 131.3, 130.1, 128.7, 128.6, 127.8, 127.0, 126.6, 116.2, 116.0, 114.6, 114.1, 55.5. UPLC: $(M + H)^+$ 397.5 (Purity: 90.6 %).

8-(4-Chlorophenyl)-6-(4-methoxyphenyl)-3-phenyl-[1,2,4]triazolo[4,3-b] pyridazine (5f)



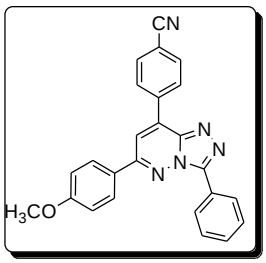
Yield: 196 mg (72 %). mp 199-201 ^{o}C. **^{1}H NMR (300 MHz, $CDCl_3$):** δ 8.60 (d, *J* = 7.20 Hz, 2H), 8.37 (d, *J* = 8.43 Hz, 2H), 8.03 (d, *J* = 8.61 Hz, 2H), 7.69 (s, 1H), 7.62-7.54 (m, 5H), 7.10 (d, *J* = 8.61 Hz, 2H), 3.92 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$):** δ 161.9, 153.4, 148.4, 143.8, 137.2, 135.7, 130.8, 130.4, 130.0, 129.2, 128.6, 127.8, 126.9, 126.6, 114.6, 114.2, 55.5. UPLC: $(M + H)^+$ 413.5 & 415.4 (Cl pattern) (Purity: 98.1 %).

8-(4-Bromophenyl)-6-(4-methoxyphenyl)-3-phenyl-[1,2,4]triazolo[4,3-b] pyridazine (5g)



Yield: 223 mg (74 %). mp 201-203 ^{o}C. **^{1}H NMR (300 MHz, $CDCl_3$):** δ 8.60 (d, *J* = 6.84 Hz, 2H), 8.30 (d, *J* = 8.55 Hz, 2H), 8.03 (d, *J* = 8.85 Hz, 2H), 7.73 (d, *J* = 8.52 Hz, 2H), 7.70 (s, 1H), 7.63-7.51 (m, 3H), 7.10 (d, *J* = 8.82 Hz, 2H), 3.92 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$):** δ 161.9, 153.6, 148.4, 143.7, 135.8, 132.2, 131.3, 130.6, 130.2, 128.8, 128.7, 127.9, 126.9, 126.4, 125.8, 114.7, 114.4, 55.5; UPLC: $(M + H)^+$ 457.5 & 459.4 (Br Pattern) (Purity: 100 %).

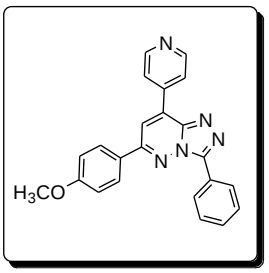
4-(6-(4-Methoxyphenyl)-3-phenyl-[1,2,4]triazolo[4,3-b]pyridazin-8-yl) benzonitrile (5h)



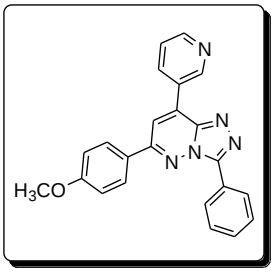
Yield: 207 mg (78 %). mp 248-250 ^{o}C. **^{1}H NMR (400 MHz, $CDCl_3$):** δ 8.62 (d, *J* = 7.20 Hz, 2H), 8.53 (d, *J* = 8.40 Hz, 2H), 8.05 (d, *J* = 8.80 Hz, 2H), 7.91 (d, *J* = 8.00 Hz, 2H), 7.77 (s, 1H), 7.64-7.57 (m, 3H), 7.12 (d, *J* = 8.40 Hz, 2H), 3.94 (s, 3H). UPLC: $(M + H)^+$ 404.7 (Purity: 99.1 %).

6-(4-Methoxyphenyl)-3-phenyl-8-(pyridin-4-yl)-[1,2,4]triazolo[4,3-b] pyridazine (5i)

Yield: 213 mg (85 %). mp 200-202 ^{o}C. **^{1}H NMR (300 MHz, CDCl$_3$):** δ 8.92-8.86 (m, 2H), 8.60 (d, *J* = 6.93 Hz, 2H), 8.28 (d, *J* = 4.74 Hz, 2H), 8.05 (d, *J* = 8.73 Hz, 2H), 7.80 (s, 1H), 7.63-7.55 (m, 3H), 7.11 (d, *J* = 8.70 Hz, 2H), 3.93 (s, 3H). **^{13}C NMR (100 MHz, CDCl$_3$):** δ 162.1, 153.6, 150.7, 148.8, 143.3, 140.0, 134.6, 130.3, 128.9, 128.7, 127.9, 126.7, 126.4, 123.0, 115.5, 114.8, 55.6. UPLC: $(M + H)^+$ 380.5 (Purity: 100 %).

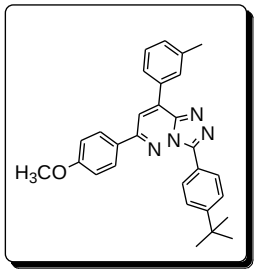


6-(4-Methoxyphenyl)-3-phenyl-8-(pyridin-3-yl)-[1,2,4]triazolo[4,3-b]pyridazine (5j)



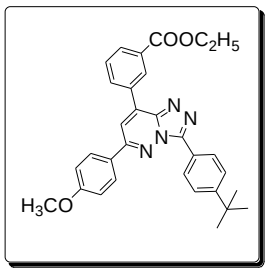
Yield: 198 mg (79 %). mp 206-208 ^{o}C. **^{1}H NMR (300 MHz, CDCl$_3$):** δ 9.40 (s, 1H), 8.92 (dt, *J* = 8.04, 2.07 Hz, 1H), 8.81 (d, *J* = 4.32 Hz, 1H), 8.61 (dd, *J* = 7.42, 1.35 Hz, 2H), 8.05 (d, *J* = 6.90 Hz, 2H), 7.77 (s, 1H), 7.64-7.53 (m, 4H), 7.10 (d, *J* = 6.90 Hz, 2H), 3.93 (s, 3H). **^{13}C NMR (75 MHz, CDCl$_3$):** δ 162.0, 153.5, 151.6, 149.1, 148.7, 143.6, 137.2, 134.3, 130.2, 128.8, 128.7, 127.9, 126.8, 126.5, 123.7, 114.7, 114.6, 55.5. UPLC: $(M + H)^+$ 380.5 (Purity: 100 %).

3-(4-tert-Butylphenyl)-6-(4-methoxyphenyl)-8-m-tolyl-[1,2,4]triazolo[4,3-b] pyridazine (7a)



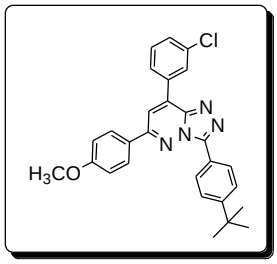
Yield: 174 mg (70 %). mp 200-202 ^{o}C. **^{1}H NMR (400 MHz, CDCl$_3$):** δ 8.57 (d, *J* = 8.40 Hz, 2H), 8.22 (s, 1H), 8.14 (d, *J* = 7.60 Hz, 1H), 8.07 (d, *J* = 7.80 Hz, 2H), 7.72 (s, 1H), 7.64 (d, *J* = 8.80 Hz, 2H), 7.49 (t, *J* = 7.60 Hz, 1H), 7.40 (d, *J* = 7.60 Hz, 1H), 7.11 (d, *J* = 7.80 Hz, 2H), 3.93 (s, 3H), 2.52 (s, 3H), 1.42 (s, 9H). **^{13}C NMR (75 MHz, CDCl$_3$):** δ 161.7, 153.4, 153.1, 148.5, 144.1, 138.7, 137.4, 132.6, 131.7, 129.8, 128.8, 128.7, 127.5, 127.3, 126.1, 125.5, 123.9, 114.5, 114.3, 55.4, 34.9, 31.2, 21.5. UPLC: $(M + H)^+$ 449.7 (Purity: 99.4 %).

Ethyl 3-(3-(4-tert-butylphenyl)-6-(4-methoxyphenyl)-[1,2,4]triazolo[4,3-b] pyridazin-8-yl)benzoate (7b)



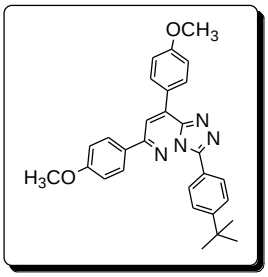
Yield: 214 mg (76 %). mp 187-191 ^{o}C. **^{1}H NMR (400 MHz, $CDCl_3$):** δ 8.84 (s, 1H), 8.81 (dd, *J* = 8.0, 1.20 Hz, 1H), 8.56 (d, *J* = 8.40 Hz, 2H), 8.26 (dd, *J* = 7.60, 1.2 Hz, 1H), 8.08 (d, *J* = 9.2 Hz, 2H), 7.78 (s, 1H), 7.72 (t, *J* = 8.00 Hz, 1H), 7.64 (d, *J* = 8.40 Hz, 2H), 7.11 (dd, *J* = 8.00, 1.6 Hz, 2H), 4.47 (q, *J* = 7.2 Hz, 2H), 3.94 (s, 3H), 1.46 (t, *J* = 7.2 Hz, 3H), 1.42 (s, 9H). **^{13}C NMR (75 MHz, $CDCl_3$):** δ 166.0, 161.9, 153.4 (2C), 148.5, 143.7, 136.1, 134.1, 132.9, 131.7, 131.3, 129.5, 129.1, 128.8, 127.6, 126.9, 125.7, 123.7, 114.7, 114.6, 61.4, 55.5, 35.0, 31.3, 14.4. UPLC: (M+ H) 507.7 (Purity: 98.4 %).

3-(4-tert-Butylphenyl)-8-(3-chlorophenyl)-6-(4-methoxyphenyl)-[1,2,4]triazolo[4,3-b]pyridazine (7c)



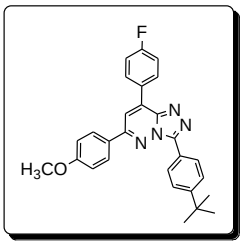
Yield: 183 mg (70 %). mp 110-112 ^{o}C. **^{1}H NMR (400 MHz, $CDCl_3$):** δ 8.54 (dd, *J* = 7.00, 2.00 Hz, 2H), 8.35-8.34 (m, 2H), 8.05 (dd, *J* = 7.20, 2.00 Hz, 2H), 7.69 (s, 1H), 7.63 (d, *J* = 7.80 Hz, 1H), 7.55-7.53 (m, 2H), 7.10 (dd, *J* = 6.80, 2.0 Hz, 2H), 3.92 (s, 3H), 1.42 (s, 9H). UPLC: $(M + H)^+$ 469.8 & 471.8 (Cl pattern) (Purity: 97.6 %).

3-(4-tert-Butylphenyl)-6,8-bis(4-methoxyphenyl)-[1,2,4]triazolo[4,3-b] pyridazine (7d)



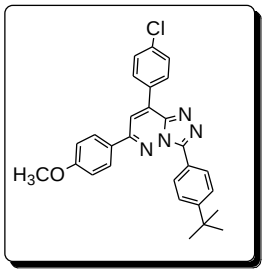
Yield: 194 mg (75 %). mp 134-136 ^{o}C. **^{1}H NMR (300 MHz, $CDCl_3$):** δ 8.58 (d, *J* = 8.40 Hz, 2H), 8.45 (d, *J* = 8.80 Hz, 2H), 8.06 (d, *J* = 8.80 Hz, 2H), 7.70 (s, 1H), 7.64 (d, *J* = 8.40 Hz, 2H), 7.13-7.09 (m, 4H), 3.93 (s, 6H), 1.42 (s, 9H). UPLC: $(M + H)^+$ 465.5 (Purity: 97.6 %).

3-(4-tert-Butylphenyl)-8-(4-fluorophenyl)-6-(4-methoxyphenyl)-[1,2,4]triazolo [4,3-b]pyridazine (7e)



Yield: 194 mg (77 %). mp 189-191 ^{o}C. **^{1}H NMR (400 MHz, CDCl$_3$):** δ 8.58 (d, *J* = 8.56 Hz, 2H), 8.45-8.41 (m, 2H), 8.06 (d, *J* = 6.92 Hz, 2H), 7.71 (s, 1H), 7.65 (d, *J* = 8.56 Hz, 2H), 7.31 (t, *J* = 8.60 Hz, 2H), 7.12 (d, *J* = 7.04 Hz, 2H), 3.94 (s, 3H), 1.43 (s, 9H). **^{13}C NMR (100 MHz, CDCl$_3$):** δ 165.7, 163.2, 161.9, 153.5, 153.4, 148.5, 143.8, 136.0, 131.4, 131.3, 128.8, 128.6 (2C), 127.6, 127.1, 125.6, 123.6, 116.2, 116.0, 114.6, 114.1, 55.5, 35.0, 31.2. UPLC: $(M + H)^+$ 453.6 (Purity: 100 %).

3-(4-tert-Butylphenyl)-8-(4-chlorophenyl)-6-(4-methoxyphenyl)-[1,2,4]triazolo [4,3-b]pyridazine (7f)



Yield: 206 mg (79 %). mp 217-219 ^{o}C. **^{1}H NMR (400 MHz, CDCl$_3$):** δ 8.52 (d, *J* = 8.00 Hz, 2H), 8.34 (d, *J* = 8.40 Hz, 2H), 8.01 (d, *J* = 8.40 Hz, 2H), 7.64 (s, 1H), 7.61 (d, *J* = 8.00 Hz, 2H), 7.53 (d, *J* = 8.00 Hz, 2H), 7.07 (d, *J* = 8.80 Hz, 2H), 3.91 (s, 3H), 1.42 (s, 9H). **^{13}C NMR (100 MHz, CDCl$_3$):** δ 161.9, 153.4 (2C), 148.6, 143.7, 137.2, 135.8, 130.9, 130.4, 129.2, 128.8, 127.6, 127.1, 125.6, 123.7, 114.6, 114.1, 55.5, 34.9, 31.2. UPLC: $(M + H)^+$ 469.8 & 471.8 (Cl pattern) (Purity: 99.1%).

6. Single crystal XRD study of (5c)

To unequivocally secure the position of C-H arylation, the single crystal X-ray study of **5c** was carried out. X-ray quality crystals of (**5c**) were developed by diffusing chloroform and toluene solution of (**5c**). The crystal data collected are presented in Table 2 and the ORTEP diagram of (**5c**) is shown in Fig. 90

Table 2 Crystal data and structure refinement for ethyl 3-(6-(4-methoxyphenyl)-3-phenyl-[1,2,4]triazolo[4,3-b]pyridazin-8-yl) benzoate **(5c)**

Identification code	shelxl
Empirical formula	$C_{27}H_{22}N_4O_3$
Formula weight	450.49
Temperature	293(2) K
Wavelength	0.71073 A
Crystal system, space group	Triclinic, P -1
Unit cell dimensions	a = 8.0109(2) Å alpha = 117.3790(10) deg. b = 12.2867(3) Å beta = 91.142(2) deg. c = 12.9925(4) Å gamma = 91.733(2) deg.
Volume	1134.23(5) $Å^3$
Z, Calculated density	2, 1.319 Mg/m^3
Absorption coefficient	0.088 mm^{-1}
F(000)	472
Crystal size	0.20 x 0.15 x 0.10 mm^3
Theta range for data collection	1.77 to 26.49 deg.
Limiting indices	-9<=h<=10, -15<=k<=15, -16<=l<=16
Reflections collected/unique	16548 / 4663 [R(int) = 0.0200]
Completeness to theta = 26.49	99.5 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9912 and 0.9826
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4663 / 0 / 310
Goodness-of-fit on F^2	1.055
Final R indices [I>2sigma(I)]	R1 = 0.0367, wR2 = 0.0881

R indices (all data)	R1 = 0.0485, wR2 = 0.0962
Extinction coefficient	0.0069(12)
Largest diff. peak and hole	0.184 and -0.144 e.Å^{-3}

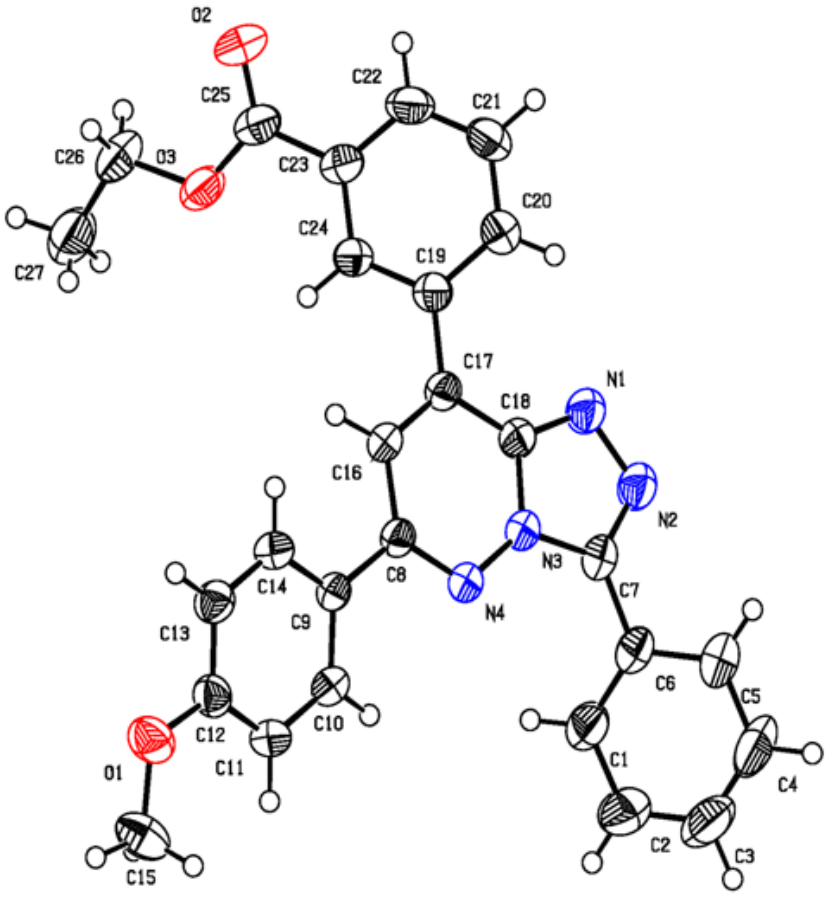


Fig. 90 ORTEP Diagram of ethyl 3-(6-(4-methoxyphenyl)-3- phenyl-[1,2,4]triazolo[4,3-b]pyridazin-8-yl)benzoate **(5c)**

CCDC number1040163 contains the supplementary crystallographic data for the compound (**5c**) given as CIF file. Crystallographic data can be obtained free of charge via http://www.ccdc.cam.ac.uk/conts/retrieving.html, or from the Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB2 1EZ, UK; fax: (+44) 1223 336 033; or e-mail: deposit@ccdc.cam.ac.uk.

4. 1H and 13C NMR spectra of compounds

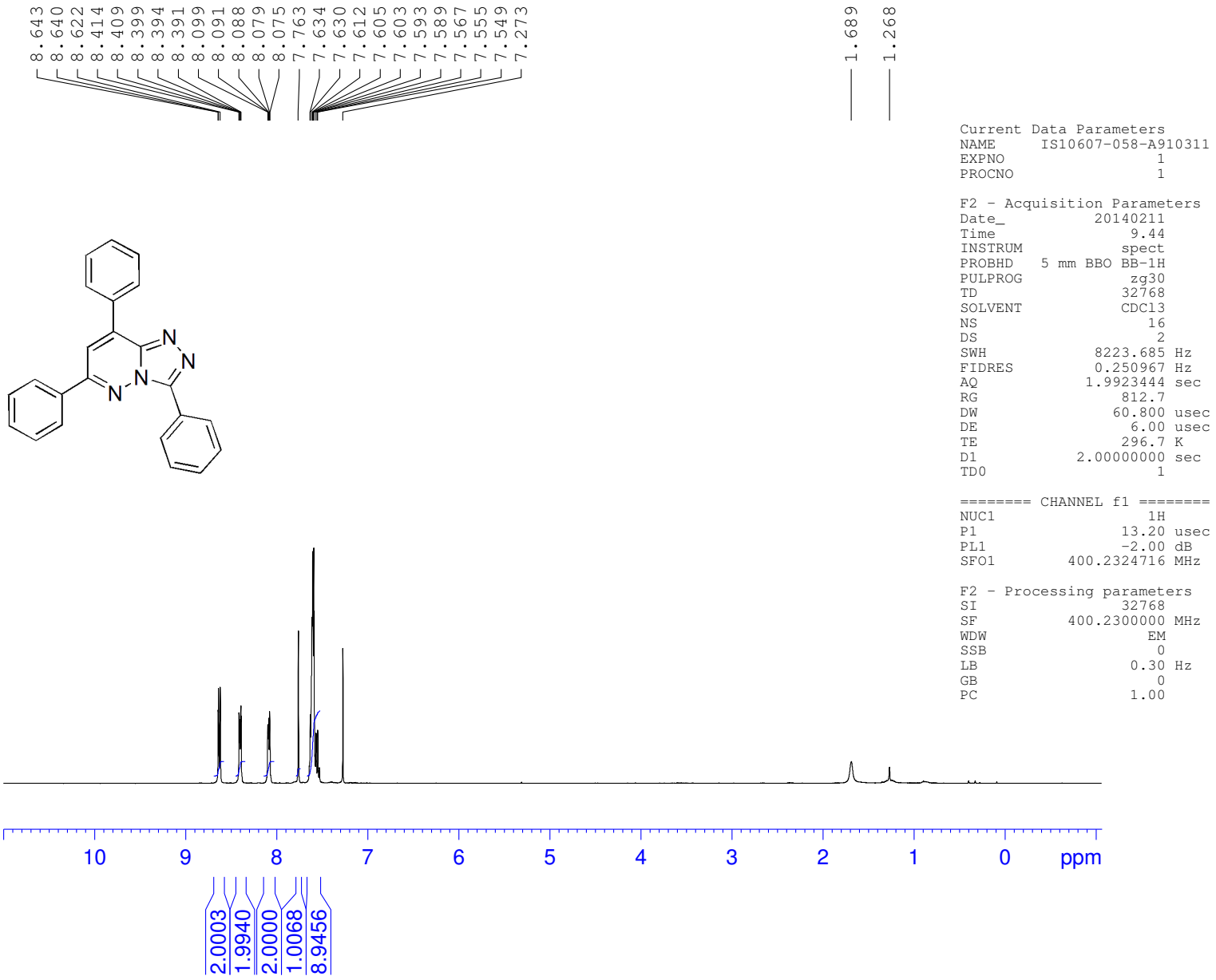
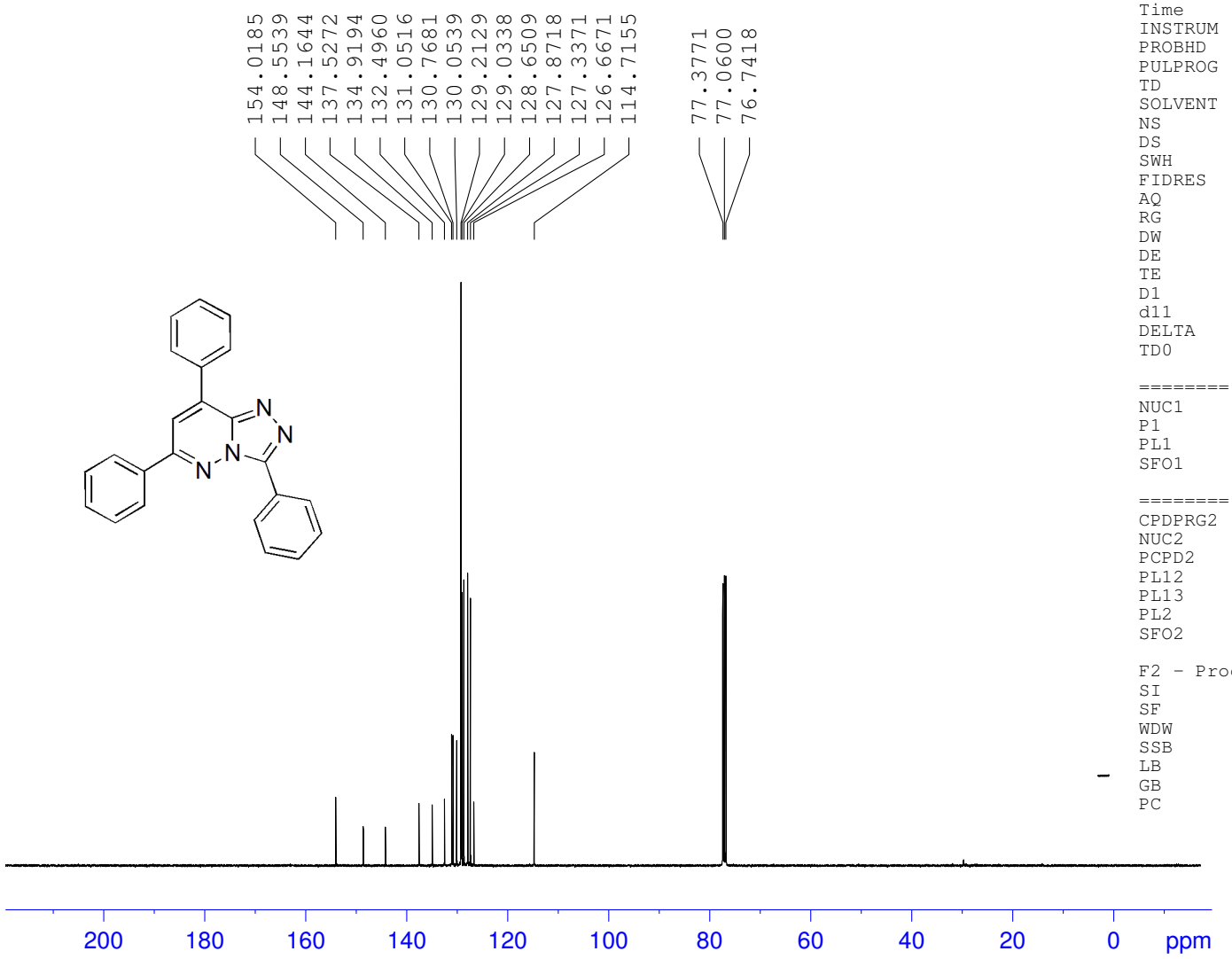


Fig 1. 1H NMR spectra of 3,6,8-triphenyl-[1,2,4]triazolo[4,3-b]pyridazine (3a)

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PL1                  -3.00 dB
SFO1          100.6278593 MHz

======== CHANNEL f2 ========
CPDPRG2            waltz16
NUC2                    1H
PCPD2                80.00 usec
PL12                 14.04 dB
PL13                 15.00 dB
PL2                  -0.50 dB
SFO2          400.1516006 MHz

F2 - Processing parameters
SI                   32768
SF            100.6177980 MHz
WDW                     EM
SSB                      0
LB                    1.00 Hz
GB                       0
PC                    1.40
```

Fig 2. 13C NMR spectra of 3,6,8-triphenyl-[1,2,4]triazolo[4,3-b]pyridazine (**3a**)

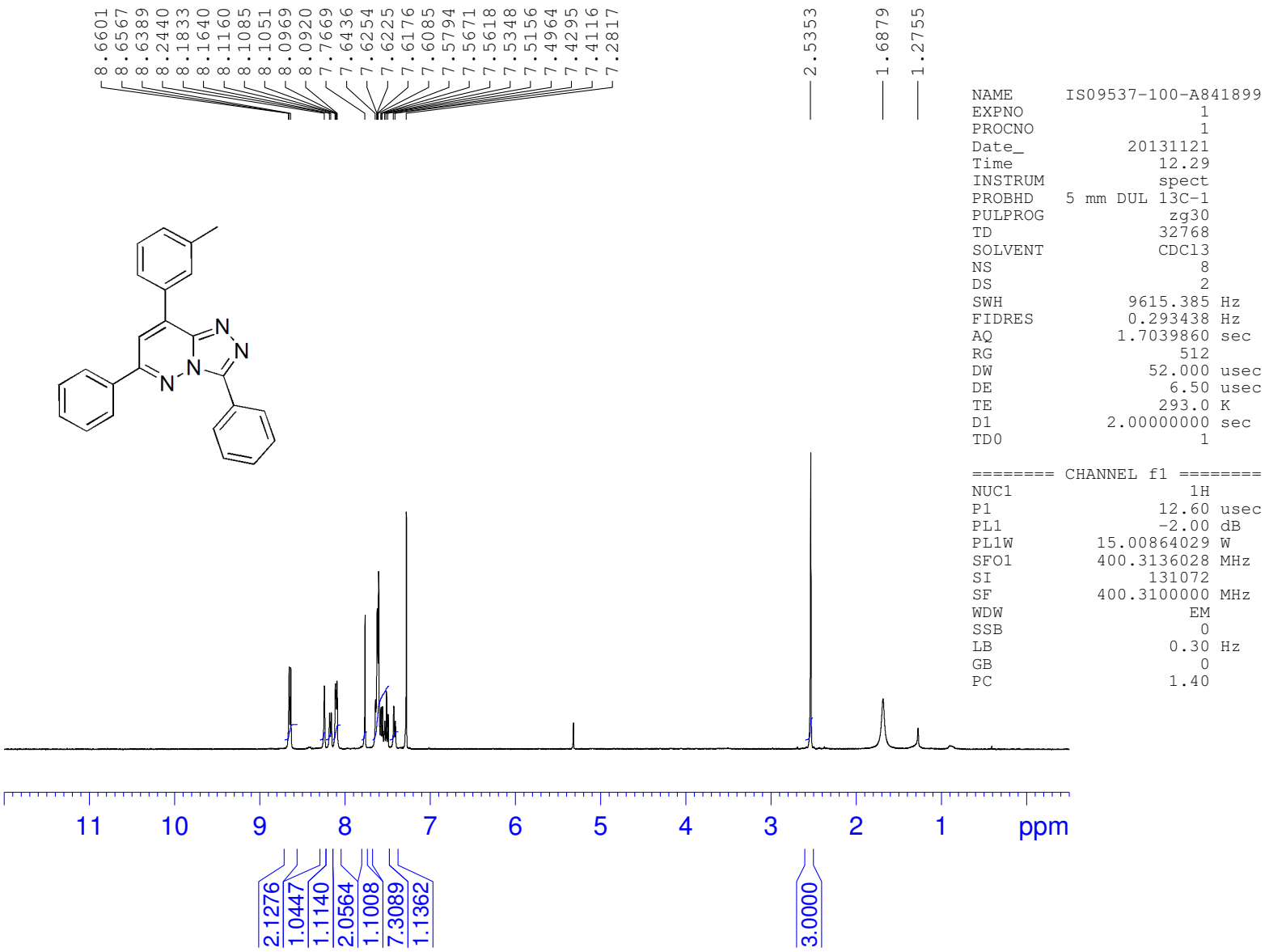
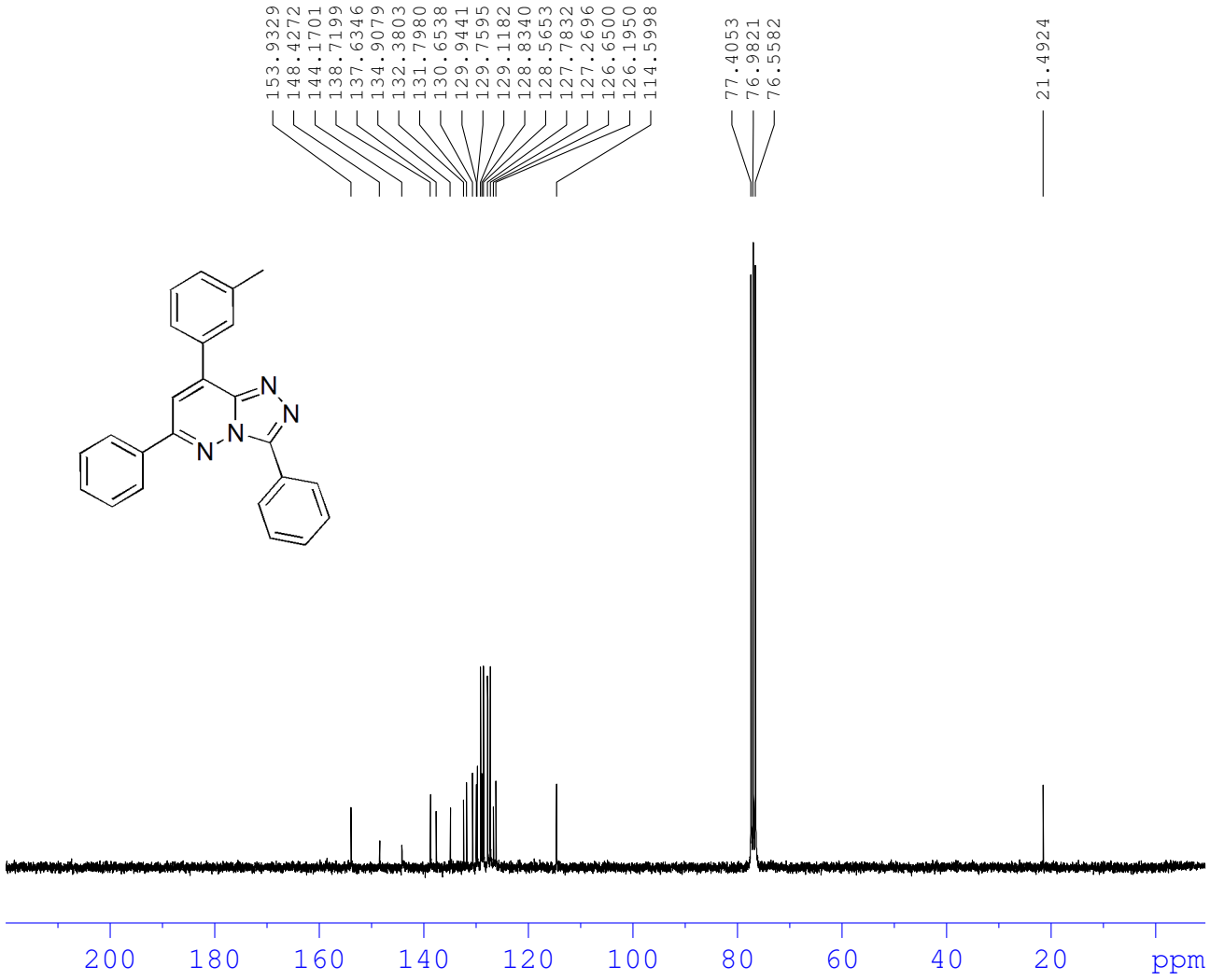


Fig 3. 1H NMR spectra of 3,6-diphenyl-8-m-tolyl-[1,2,4]triazolo[4,3-b]pyridazine (3b)

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Current Data Parameters
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EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
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Time               5.32
INSTRUM           spect
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PULPROG         zgpg30
TD              32768
SOLVENT          CDCl3
NS                2500
DS                   0
SWH          20325.203 Hz
FIDRES        0.620276 Hz
AQ           0.8061428 sec
RG               16384
DW              24.600 usec
DE               6.00 usec
TE                0.0 K
D1           2.00000000 sec
d11          0.03000000 sec
DELTA        1.89999998 sec
MCREST       0.00000000 sec
MCWRK        0.01500000 sec

======== CHANNEL f1 ========
NUC1                13C
P1                 8.50 usec
PL1                0.00 dB
SFO1         75.4771525 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                1H
PCPD2            80.00 usec
PL2                0.00 dB
PL12              14.75 dB
PL13              18.00 dB
SFO2        300.1315007 MHz

F2 - Processing parameters
SI                32768
SF          75.4677079 MHz
WDW                 EM
SSB                  0
LB                1.00 Hz
GB                   0
PC                1.70
```

Fig 4. 13C NMR spectra of 3,6-diphenyl-8-m-tolyl-[1,2,4]triazolo[4,3-b]pyridazine (**3b**)

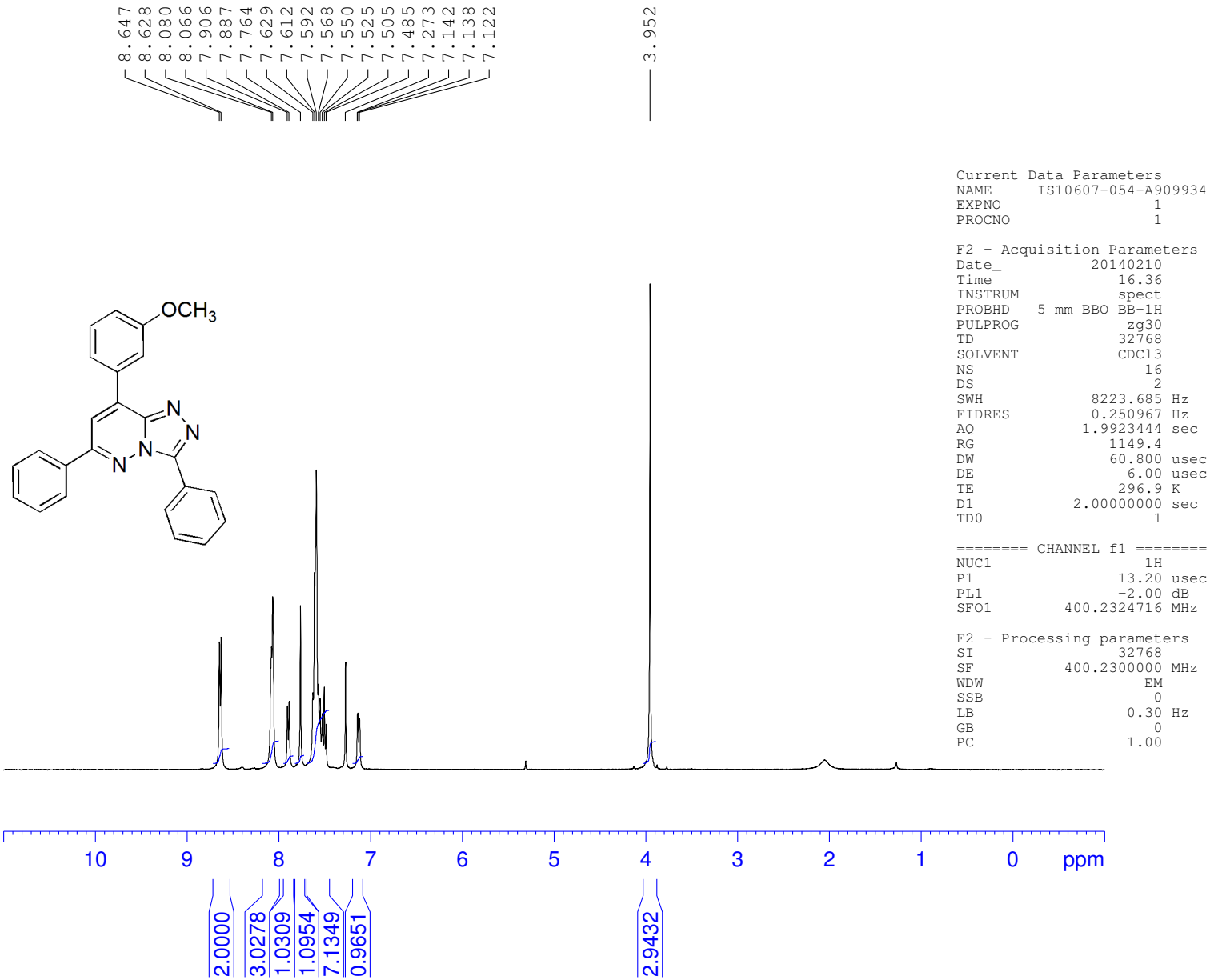
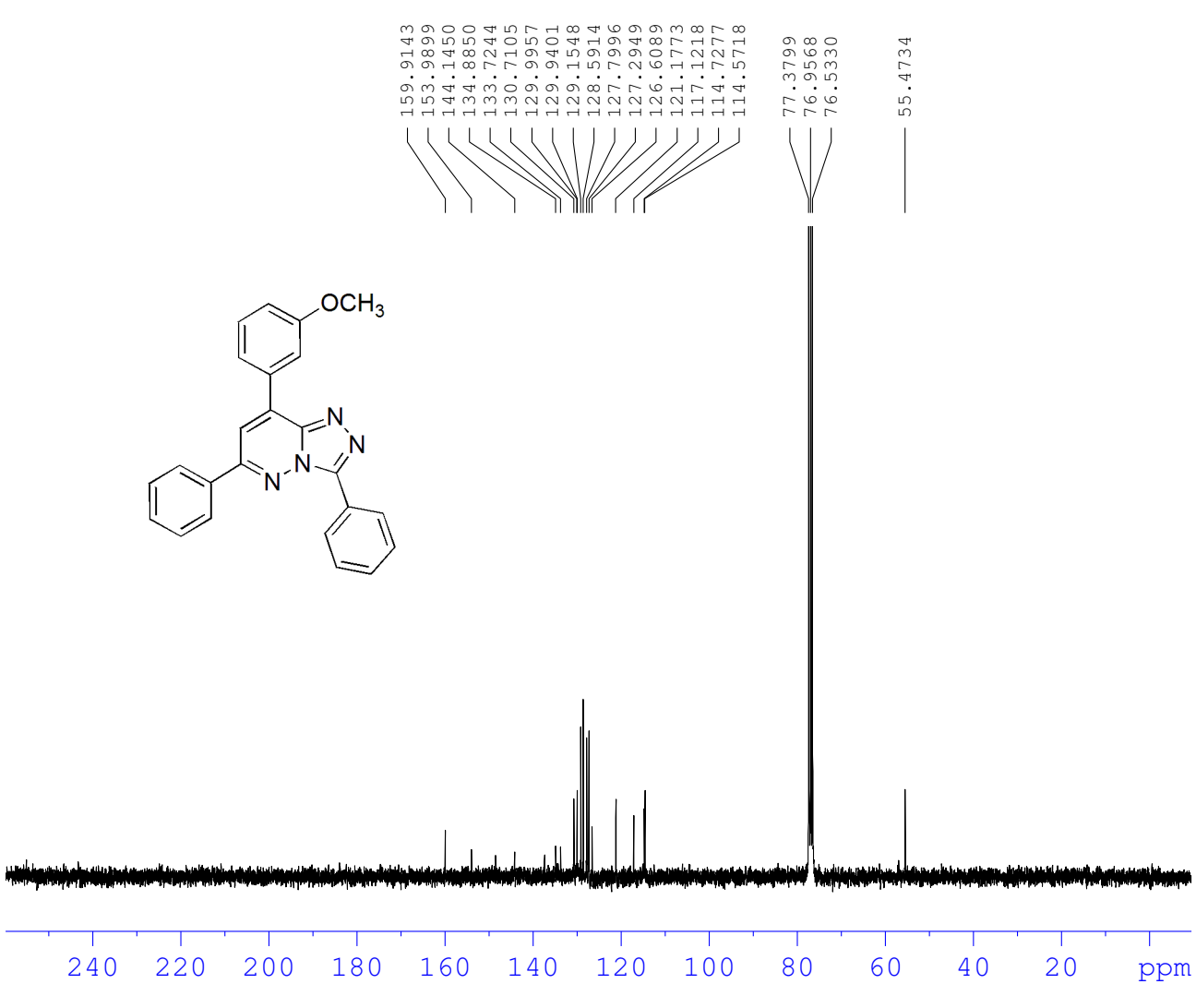


Fig 5. 1H NMR spectra of 8-(3-methoxyphenyl)-3,6-diphenyl-[1,2,4]triazolo[4,3-b]pyridazine (**3c**)

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Current Data Parameters
NAME      IS-S11042-096-A154408
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_           20141208
Time              21.03
INSTRUM           spect
PROBHD   5 mm DUL BB-1H
PULPROG          zgpg30
TD                32768
SOLVENT           CDCl3
NS                 2500
DS                    0
SWH           20325.203 Hz
FIDRES         0.620276 Hz
AQ            0.8061428 sec
RG                16384
DW               24.600 usec
DE                6.00 usec
TE                 0.0 K
D1           2.00000000 sec
d11          0.03000000 sec
DELTA        1.89999998 sec
MCREST       0.00000000 sec
MCWRK        0.01500000 sec

======== CHANNEL f1 ========
NUC1                13C
P1                 8.50 usec
PL1                0.00 dB
SFO1         75.4771525 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                1H
PCPD2             80.00 usec
PL2                0.00 dB
PL12              14.75 dB
PL13              18.00 dB
SFO2        300.1315007 MHz

F2 - Processing parameters
SI                32768
SF           75.4677079 MHz
WDW                 EM
SSB                  0
LB                1.00 Hz
GB                   0
PC                1.70
```

Fig 6. 13C NMR spectra of 8-(3-methoxyphenyl)-3,6-diphenyl-[1,2,4]triazolo[4,3-b]pyridazine (**3c**)

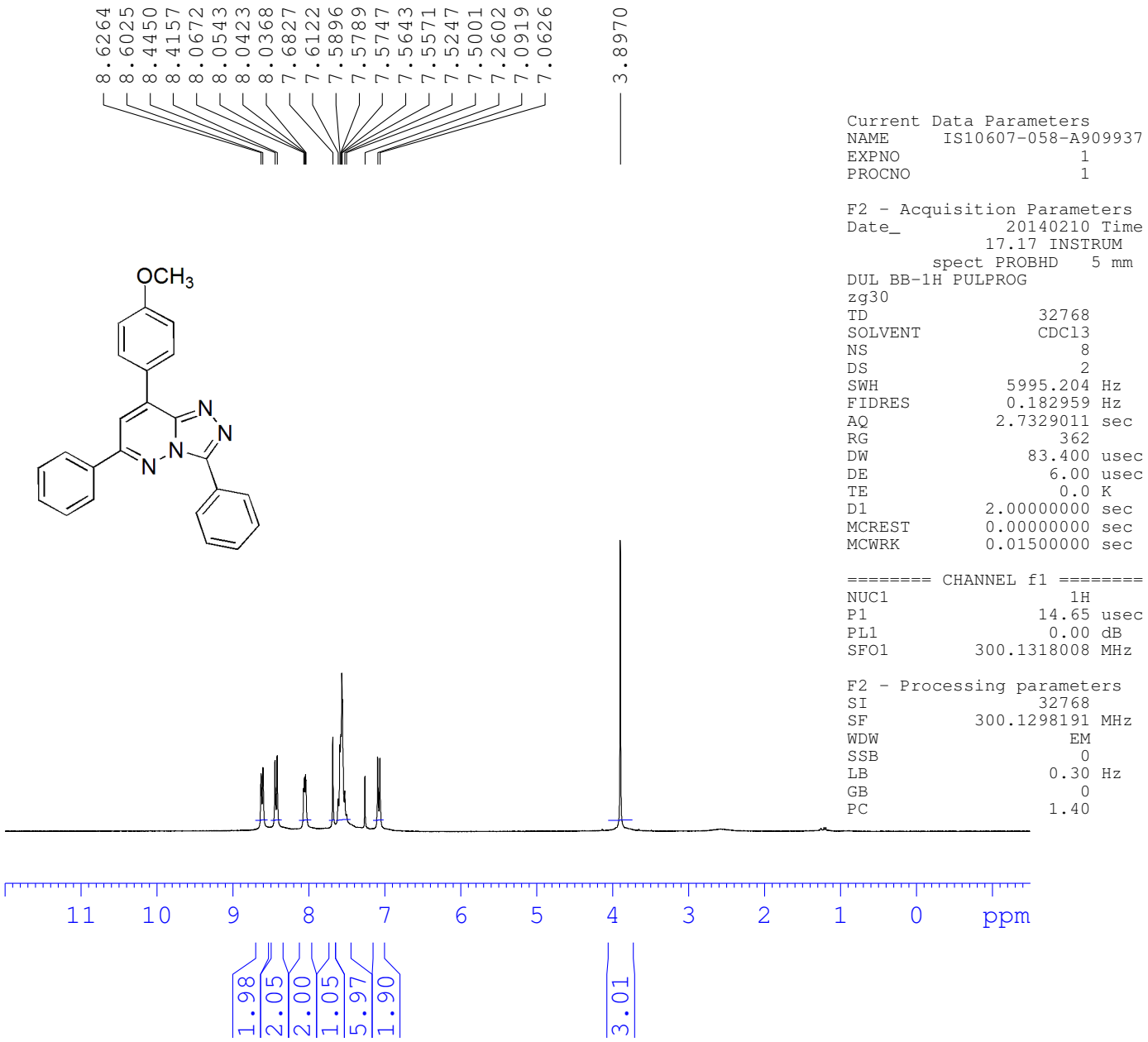
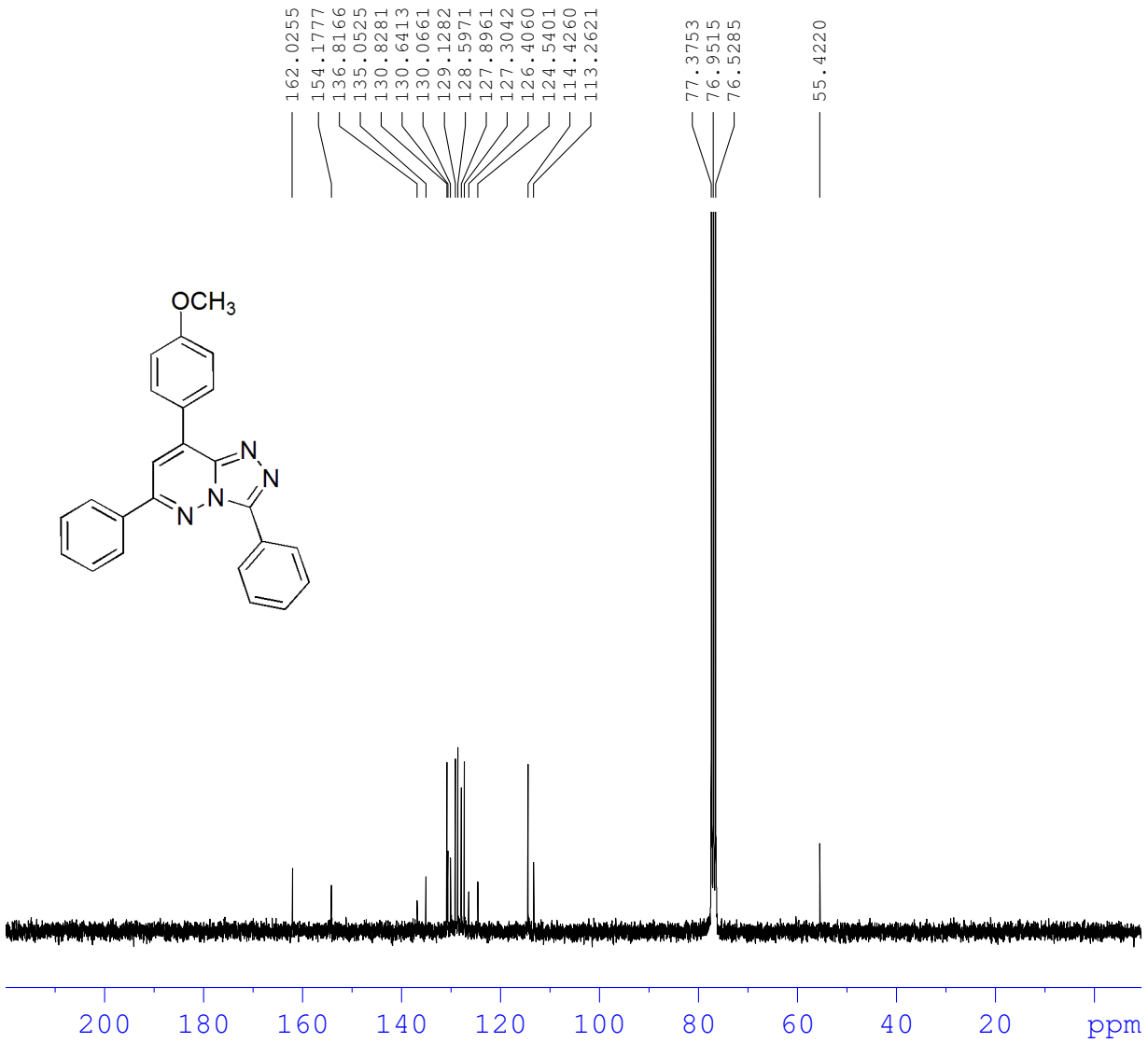


Fig 7. 1H NMR spectra of 8-(4-methoxyphenyl)-3,6-diphenyl-[1,2,4]triazolo[4,3-b]pyridazine (**3d**)

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Current Data Parameters
NAME      IS10607-058-A909937
EXPNO                       2
PROCNO                      1

F2 - Acquisition Parameters
Date_            20140212
Time                20.31
INSTRUM             spect
PROBHD   5 mm DUL BB-1H
PULPROG           zgpg30
TD                 32768
SOLVENT            CDCl3
NS                  3000
DS                     0
SWH            20325.203 Hz
FIDRES          0.620276 Hz
AQ             0.8061428 sec
RG                 16384
DW                24.600 usec
DE                 6.00 usec
TE                  0.0 K
D1           2.00000000 sec
d11          0.03000000 sec
DELTA        1.89999998 sec
MCREST       0.00000000 sec
MCWRK        0.01500000 sec

======== CHANNEL f1 ========
NUC1                  13C
P1                   8.50 usec
PL1                  0.00 dB
SFO1          75.4771525 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2              80.00 usec
PL2                 0.00 dB
PL12               14.75 dB
PL13               18.00 dB
SFO2         300.1315007 MHz

F2 - Processing parameters
SI                 32768
SF            75.4677079 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.70
```
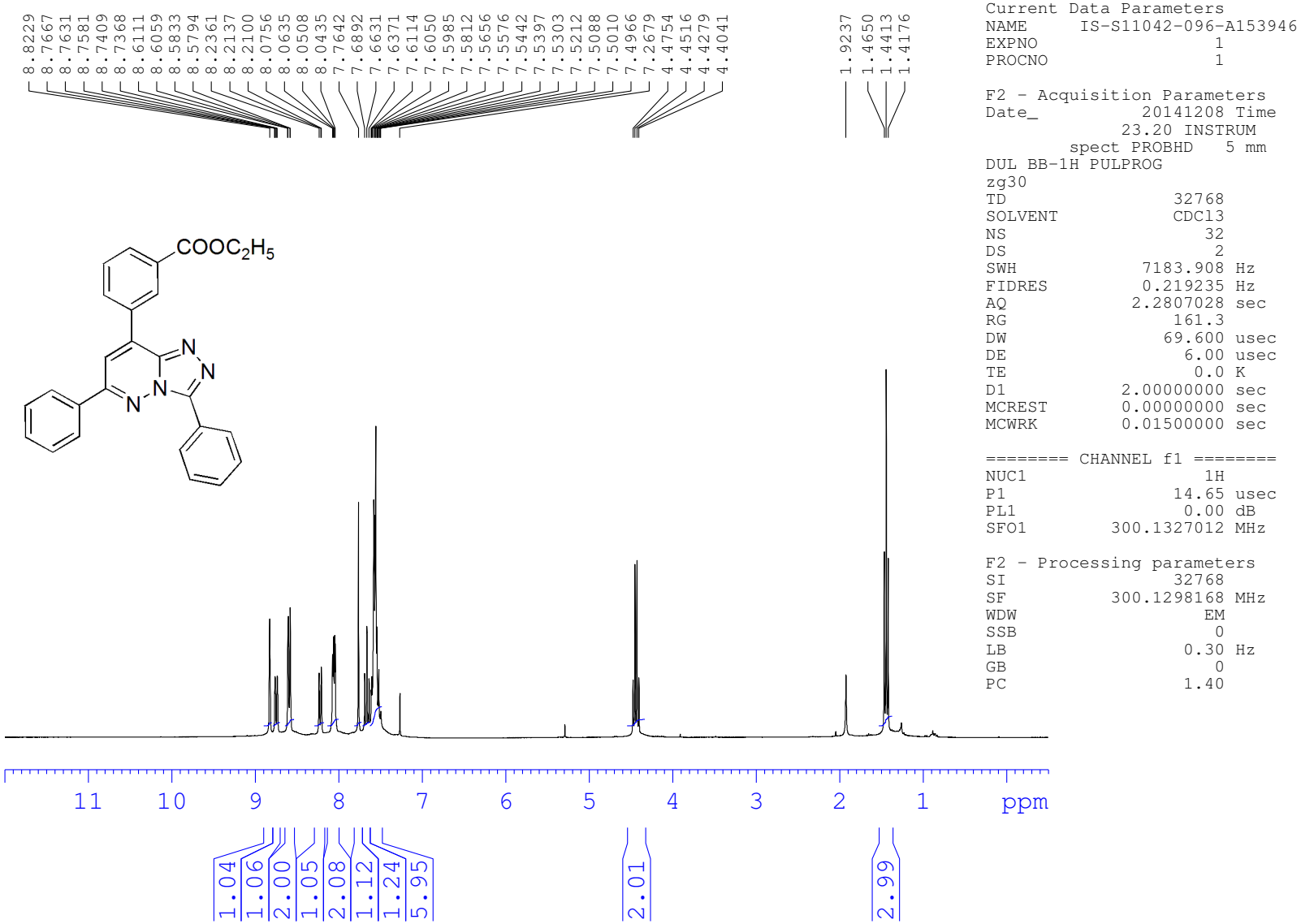

Fig 8. 13C NMR spectra of 8-(4-methoxyphenyl)-3,6-diphenyl-[1,2,4]triazolo[4,3-b]pyridazine (**3d**)

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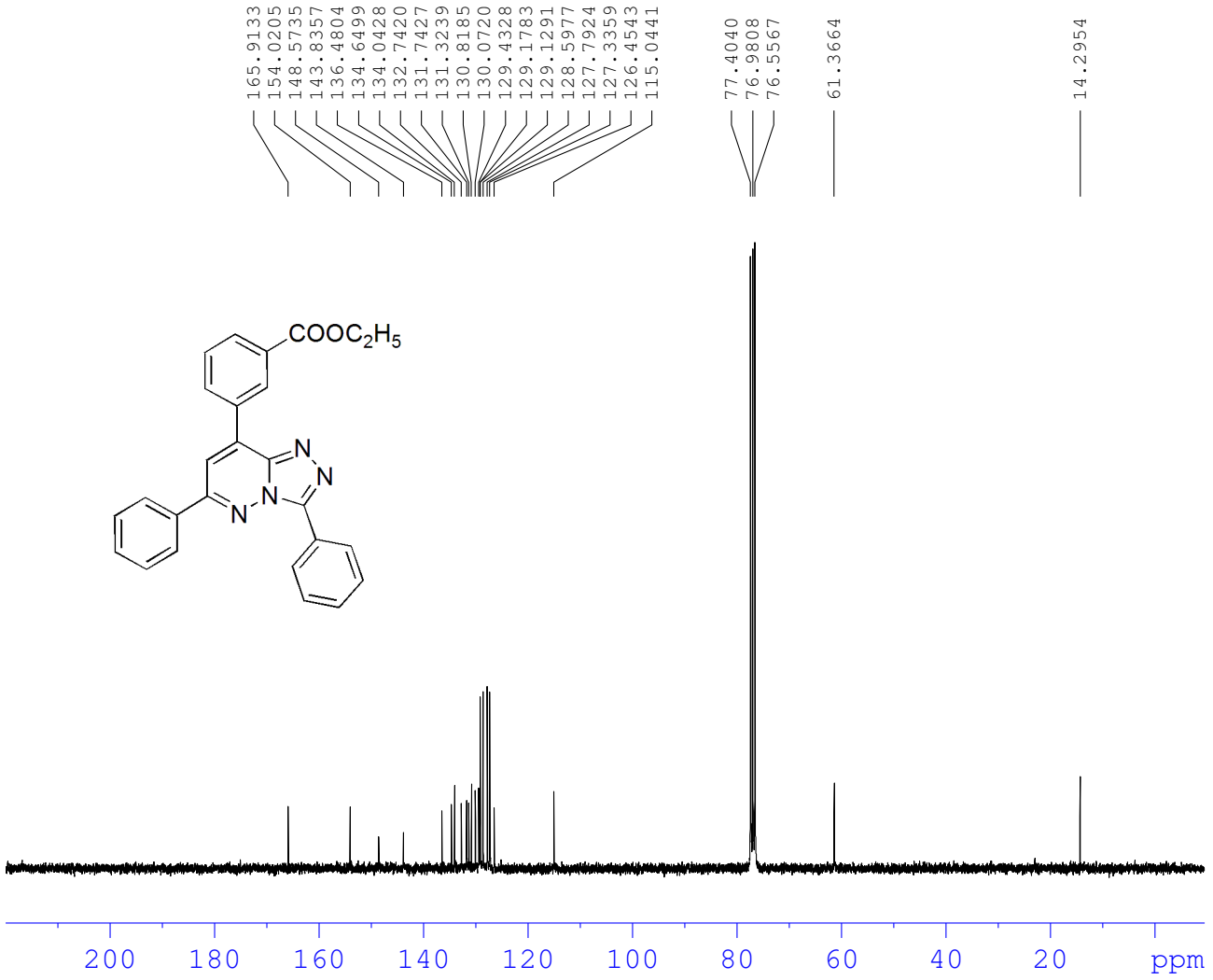
Current Data Parameters
NAME      IS-S11042-096-A153946
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_           20141208 Time
              23.20 INSTRUM
            spect PROBHD   5 mm
DUL BB-1H PULPROG
zg30
TD                32768
SOLVENT           CDCl3
NS                   32
DS                    2
SWH            7183.908 Hz
FIDRES         0.219235 Hz
AQ             2.2807028 sec
RG                161.3
DW               69.600 usec
DE                6.00 usec
TE                 0.0 K
D1            2.00000000 sec
MCREST        0.00000000 sec
MCWRK         0.01500000 sec

======== CHANNEL f1 ========
NUC1                 1H
P1                14.65 usec
PL1                0.00 dB
SFO1         300.1327012 MHz

F2 - Processing parameters
SI                32768
SF           300.1298168 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 1.40
```

Fig 9. 1H NMR spectra of ethyl 3-(3,6-diphenyl-[1,2,4]triazolo[4,3-b]pyridazin-8- yl)benzoate (**3e**)




```
Current Data Parameters
NAME      IS-S11042-096-A153946
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_          20141209
Time               1.20
INSTRUM           spect
PROBHD   5 mm DUL BB-1H
PULPROG         zgpg30
TD              32768
SOLVENT          CDCl3
NS                2500
DS                   0
SWH          20325.203 Hz
FIDRES        0.620276 Hz
AQ            0.8061428 sec
RG              14596.5
DW               24.600 usec
DE                6.00 usec
TE                 0.0 K
D1           2.00000000 sec
d11          0.03000000 sec
DELTA        1.89999998 sec
MCREST       0.00000000 sec
MCWRK        0.01500000 sec

======== CHANNEL f1 ========
NUC1                13C
P1                 8.50 usec
PL1                0.00 dB
SFO1         75.4771525 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                1H
PCPD2            80.00 usec
PL2                0.00 dB
PL12              14.75 dB
PL13              18.00 dB
SFO2        300.1315007 MHz

F2 - Processing parameters
SI                 32768
SF          75.4677079 MHz
WDW                   EM
SSB                    0
LB                1.00 Hz
GB                     0
PC                1.70
```

Fig 10. 13C NMR spectra of ethyl 3-(3,6-diphenyl-[1,2,4]triazolo[4,3-b]pyridazin-8-yl)benzoate (**3e**)

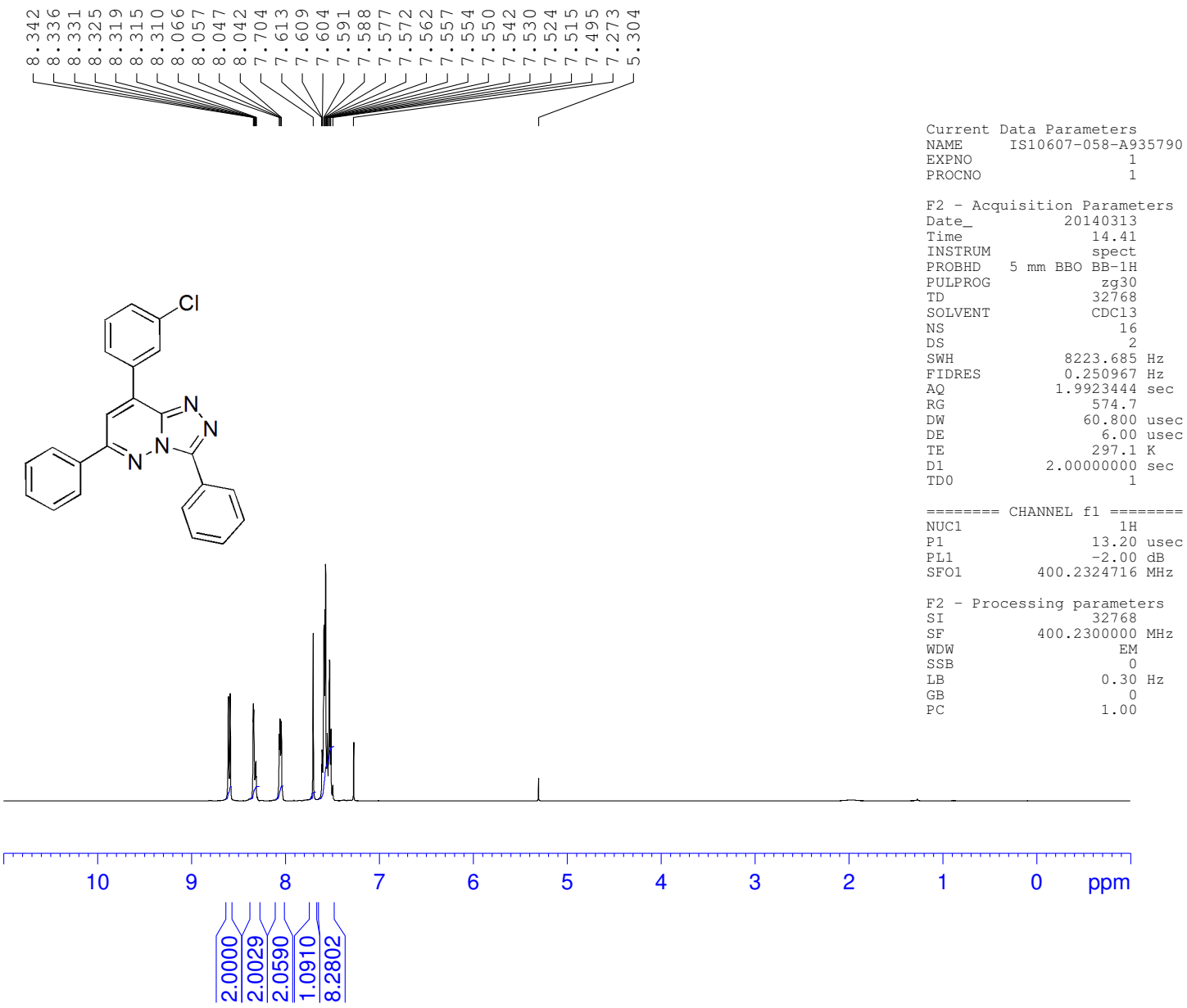
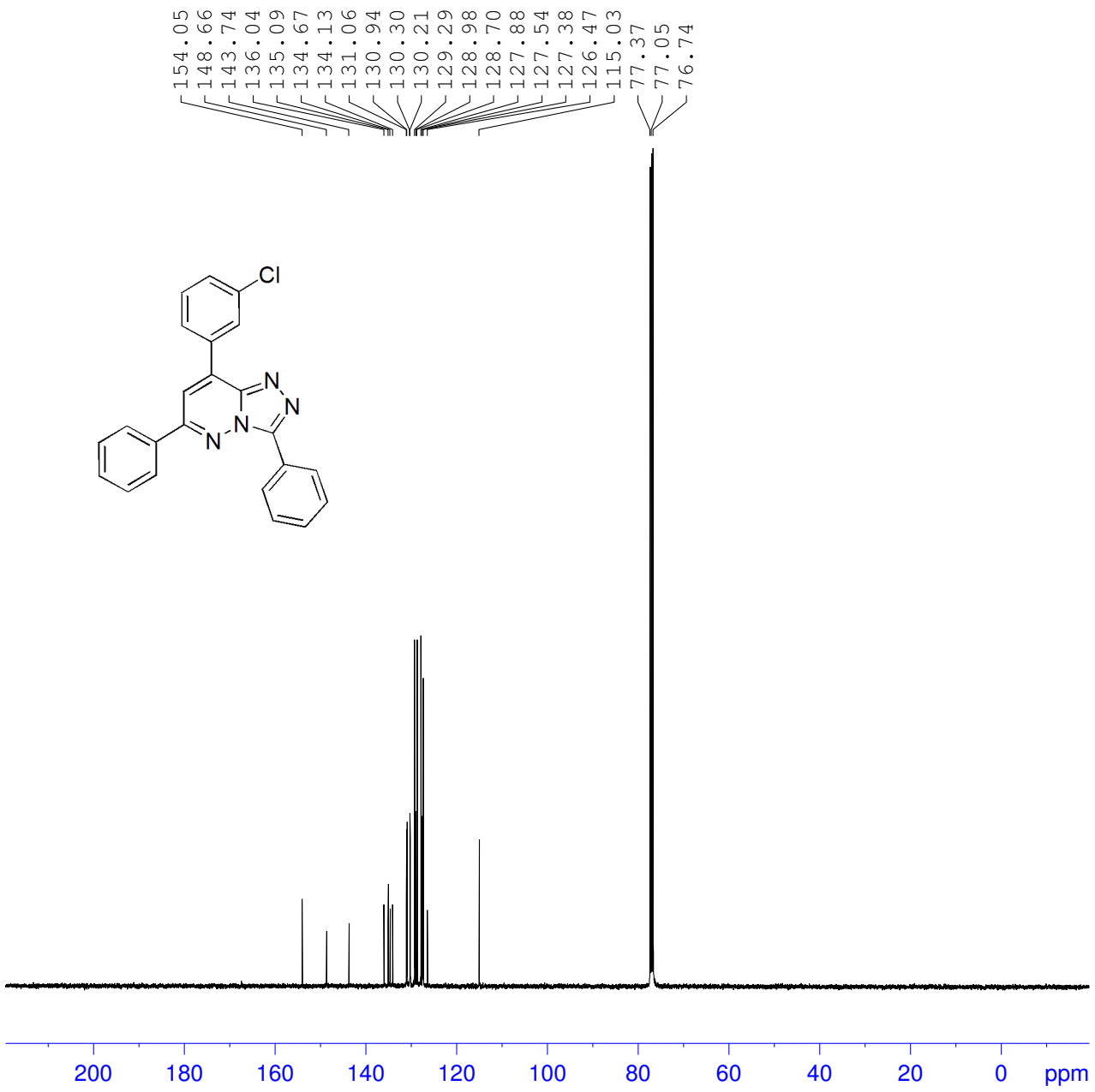


Fig 11. 1H NMR spectra of 8-(3-chlorophenyl)-3,6-diphenyl-[1,2,4]triazolo[4,3-b]pyridazine (**3f**)

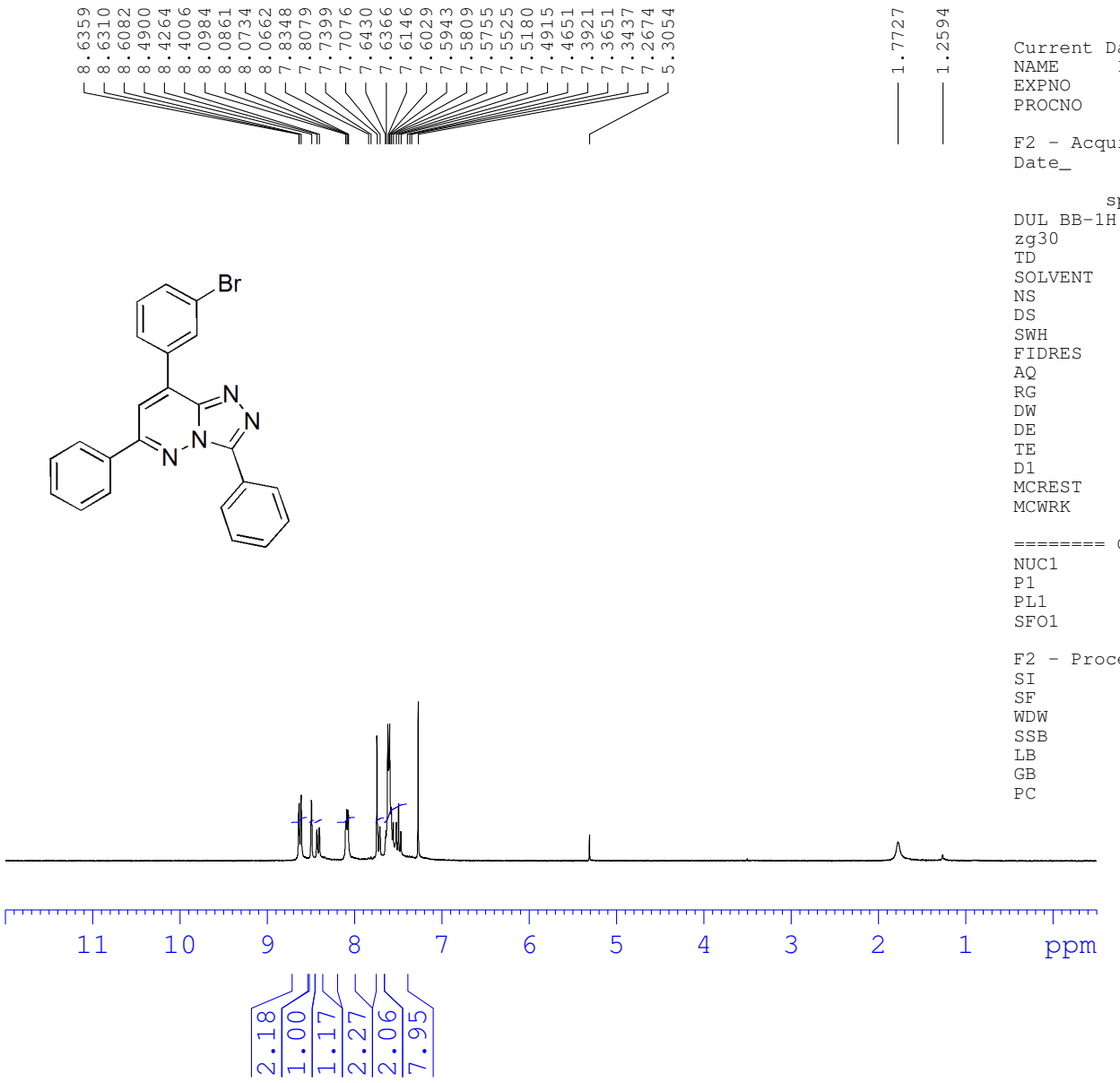



```
NAME      IS10607-058-A935790
EXPNO                       2
PROCNO                      1
Date_              20140314
Time                    8.32
INSTRUM                spect
PROBHD    5 mm DUL 13C-1
PULPROG             zgpg30
TD                      32768
SOLVENT                 CDCl3
NS                       2000
DS                          4
SWH               24038.461 Hz
FIDRES             0.733596 Hz
AQ                0.6816244 sec
RG                       2050
DW                     20.800 usec
DE                      6.50 usec
TE                     293.0 K
D1                2.00000000 sec
D11               0.03000000 sec
TD0                         1

======== CHANNEL f1 ========
NUC1                      13C
P1                       9.50 usec
PL1                     -1.50 dB
PL1W             51.09312820 W
SFO1            100.6680954 MHz

======== CHANNEL f2 ========
CPDPRG2               waltz16
NUC2                      1H
PCPD2                  100.00 usec
PL2                     -2.00 dB
PL12                    16.17 dB
PL13                    17.00 dB
PL2W             15.00864029 W
PL12W             0.22873959 W
PL13W             0.18894759 W
SFO2            400.3116012 MHz
SI                       32768
SF              100.6580300 MHz
WDW                        EM
SSB                         0
LB                       1.00 Hz
GB                          0
PC                       1.40
```

Fig 12. 13C NMR spectra of 8-(3-chlorophenyl)-3,6-diphenyl-[1,2,4]triazolo[4,3-b]pyridazine (**3f**)

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Current Data Parameters
NAME      IS10607-058-A911131
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_           20140211 Time
             17.45 INSTRUM
          spect PROBHD   5 mm
DUL BB-1H PULPROG
zg30
TD                      32768
SOLVENT                 CDCl3
NS                          8
DS                          2
SWH                  5995.204 Hz
FIDRES               0.182959 Hz
AQ                  2.7329011 sec
RG                        512
DW                     83.400 usec
DE                       6.00 usec
TE                        0.0 K
D1                 2.00000000 sec
MCREST             0.00000000 sec
MCWRK              0.01500000 sec

======== CHANNEL f1 ========
NUC1                        1H
P1                      14.65 usec
PL1                      0.00 dB
SFO1             300.1318008 MHz

F2 - Processing parameters
SI                      32768
SF               300.1298168 MHz
WDW                        EM
SSB                         0
LB                       0.30 Hz
GB                          0
PC                       1.40
```
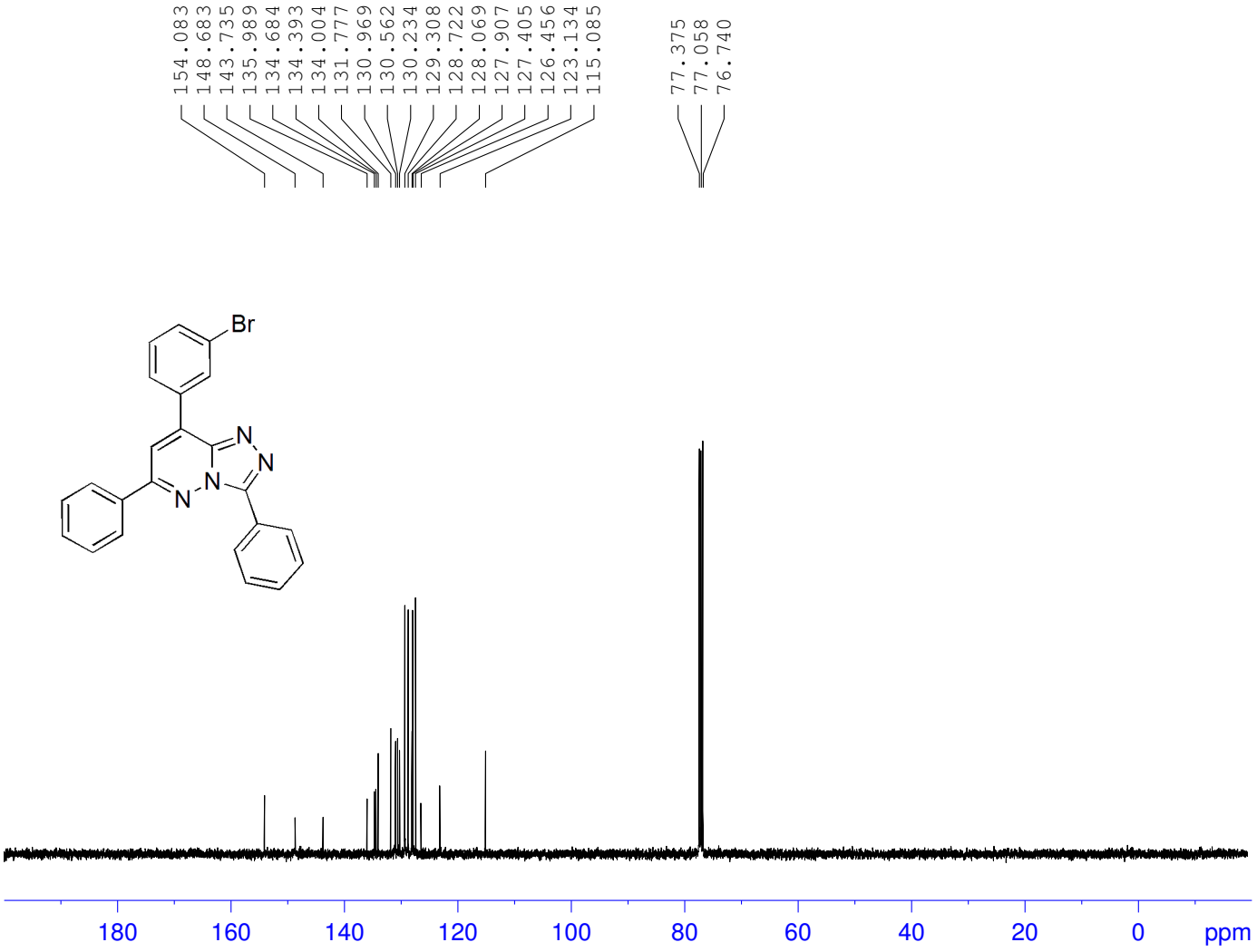

Fig 13. 1H NMR spectra of 8-(3-bromophenyl)-3,6-diphenyl-[1,2,4]triazolo[4,3-b]pyridazine (**3g**)

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Current Data Parameters
NAME      IS10607-058-A927371
EXPNO                       2
PROCNO                      1

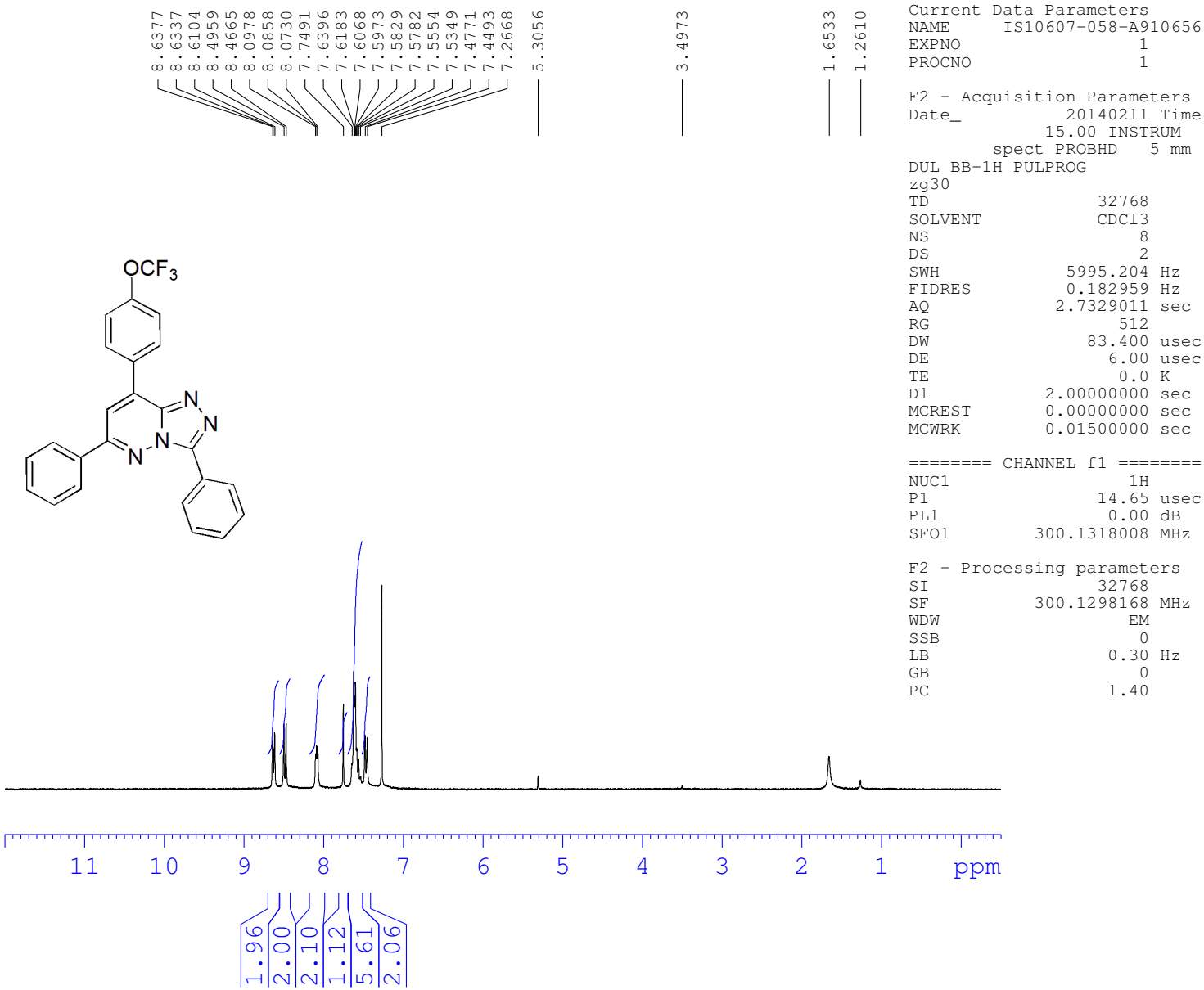
F2 - Acquisition Parameters
Date_            20140304
Time                15.32
INSTRUM             spect
PROBHD    5 mm PABBO BB-
PULPROG           zgpg30
TD                 32768
SOLVENT            CDCl3
NS                   311
DS                     2
SWH           24038.461 Hz
FIDRES         0.733596 Hz
AQ            0.6816244 sec
RG                  45.2
DW                20.800 usec
DE                 6.00 usec
TE                296.0 K
D1           2.00000000 sec
d11          0.03000000 sec
DELTA        1.89999998 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  13C
P1                   8.15 usec
PL1                 -2.00 dB
SFO1         100.6839383 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                  1H
PCPD2              80.00 usec
PL2                -2.00 dB
PL12               13.30 dB
PL13               15.50 dB
SFO2         400.3746015 MHz

F2 - Processing parameters
SI                 32768
SF          100.6738710 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

Fig 14. 13C NMR spectra of 8-(3-bromophenyl)-3,6-diphenyl-[1,2,4]triazolo[4,3-b]pyridazine (**3g**)

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Current Data Parameters
NAME      IS10607-058-A910656
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_           20140211 Time
             15.00 INSTRUM
          spect PROBHD   5 mm
DUL BB-1H PULPROG
zg30
TD                      32768
SOLVENT                 CDCl3
NS                          8
DS                          2
SWH                 5995.204 Hz
FIDRES              0.182959 Hz
AQ                  2.7329011 sec
RG                        512
DW                     83.400 usec
DE                      6.00 usec
TE                       0.0 K
D1                  2.00000000 sec
MCREST              0.00000000 sec
MCWRK               0.01500000 sec

======== CHANNEL f1 ========
NUC1                       1H
P1                      14.65 usec
PL1                      0.00 dB
SFO1             300.1318008 MHz

F2 - Processing parameters
SI                      32768
SF               300.1298168 MHz
WDW                        EM
SSB                         0
LB                       0.30 Hz
GB                          0
PC                       1.40
```
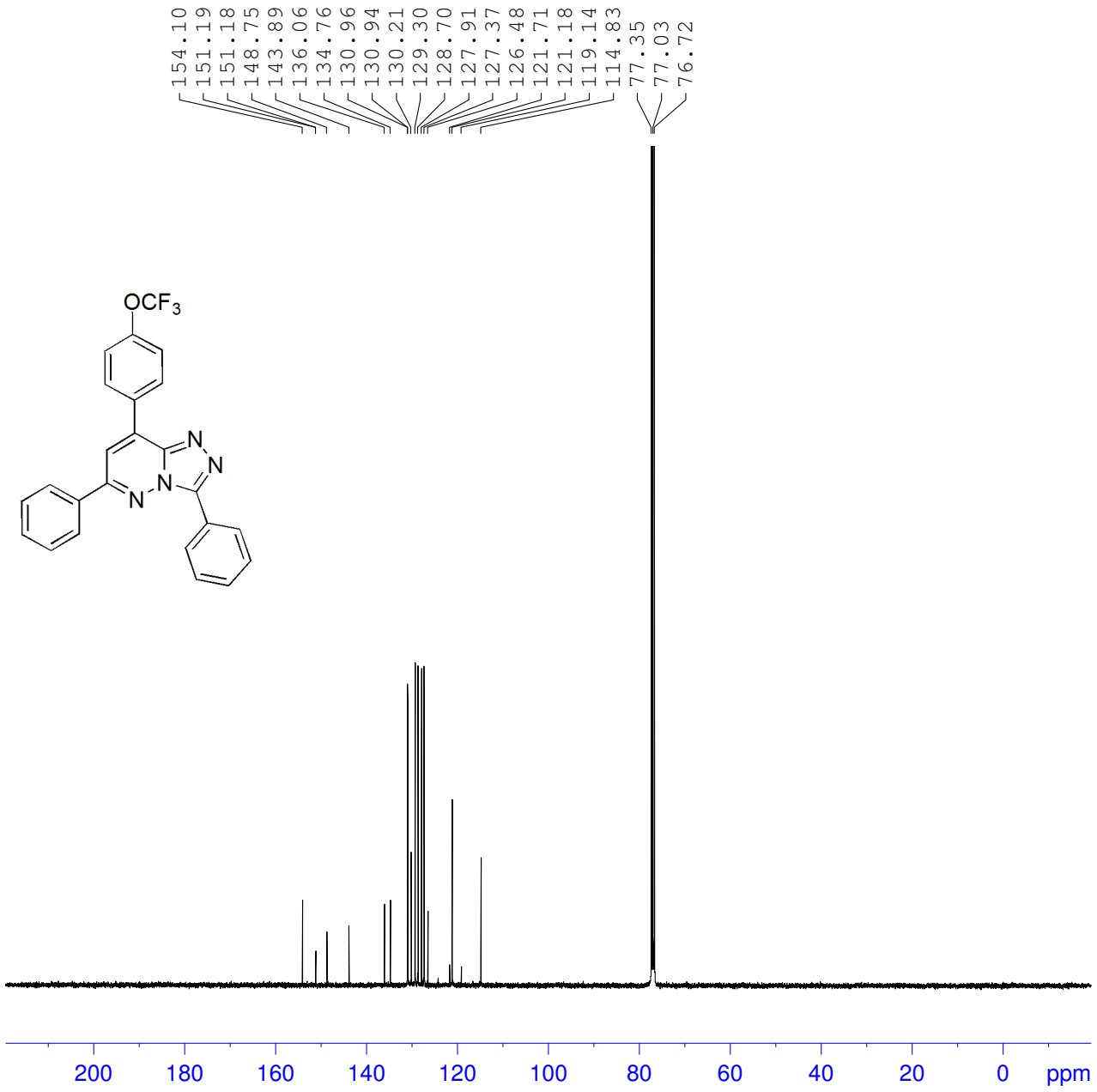

Fig 15. 1H NMR spectra of 3,6-diphenyl-8-(4-(trifluoromethoxy)phenyl)-[1,2,4]triazolo[4,3-b]pyridazine (**3h**)




```
NAME      IS10607-058-A926343
EXPNO                       2
PROCNO                      1
Date_              20140301
Time                   19.47
INSTRUM                spect
PROBHD    5 mm DUL 13C-1
PULPROG             zgpg30
TD                      32768
SOLVENT                 CDCl3
NS                       2512
DS                          4
SWH                24038.461 Hz
FIDRES              0.733596 Hz
AQ                 0.6816244 sec
RG                       2050
DW                     20.800 usec
DE                      6.50 usec
TE                     293.0 K
D1                2.00000000 sec
D11               0.03000000 sec
TD0                         1

======== CHANNEL f1 ========
NUC1                      13C
P1                       9.55 usec
PL1                     -0.50 dB
PL1W             40.58471298 W
SFO1             100.6680954 MHz

======== CHANNEL f2 ========
CPDPRG2               waltz16
NUC2                      1H
PCPD2                  100.00 usec
PL2                     -2.00 dB
PL12                    16.24 dB
PL13                    17.00 dB
PL2W             15.00864029 W
PL12W             0.22508231 W
PL13W             0.18894759 W
SFO2             400.3116012 MHz
SI                       32768
SF               100.6580300 MHz
WDW                        EM
SSB                         0
LB                       1.00 Hz
GB                          0
PC                       1.40
```

Fig 16. 13C NMR spectra of 3,6-diphenyl-8-(4-(trifluoromethoxy)phenyl)-[1,2,4]triazolo[4,3-b]pyridazine (**3h**)

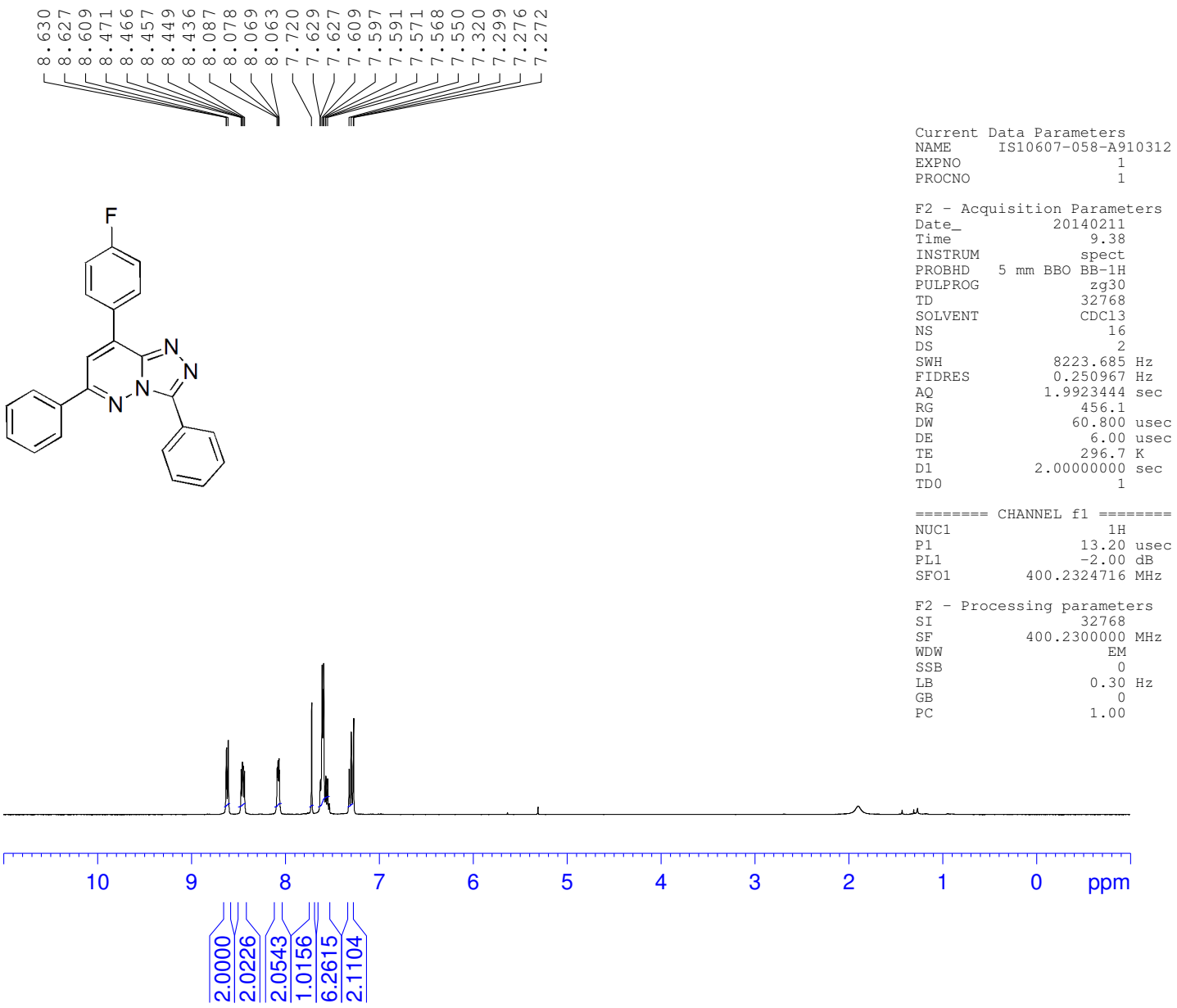
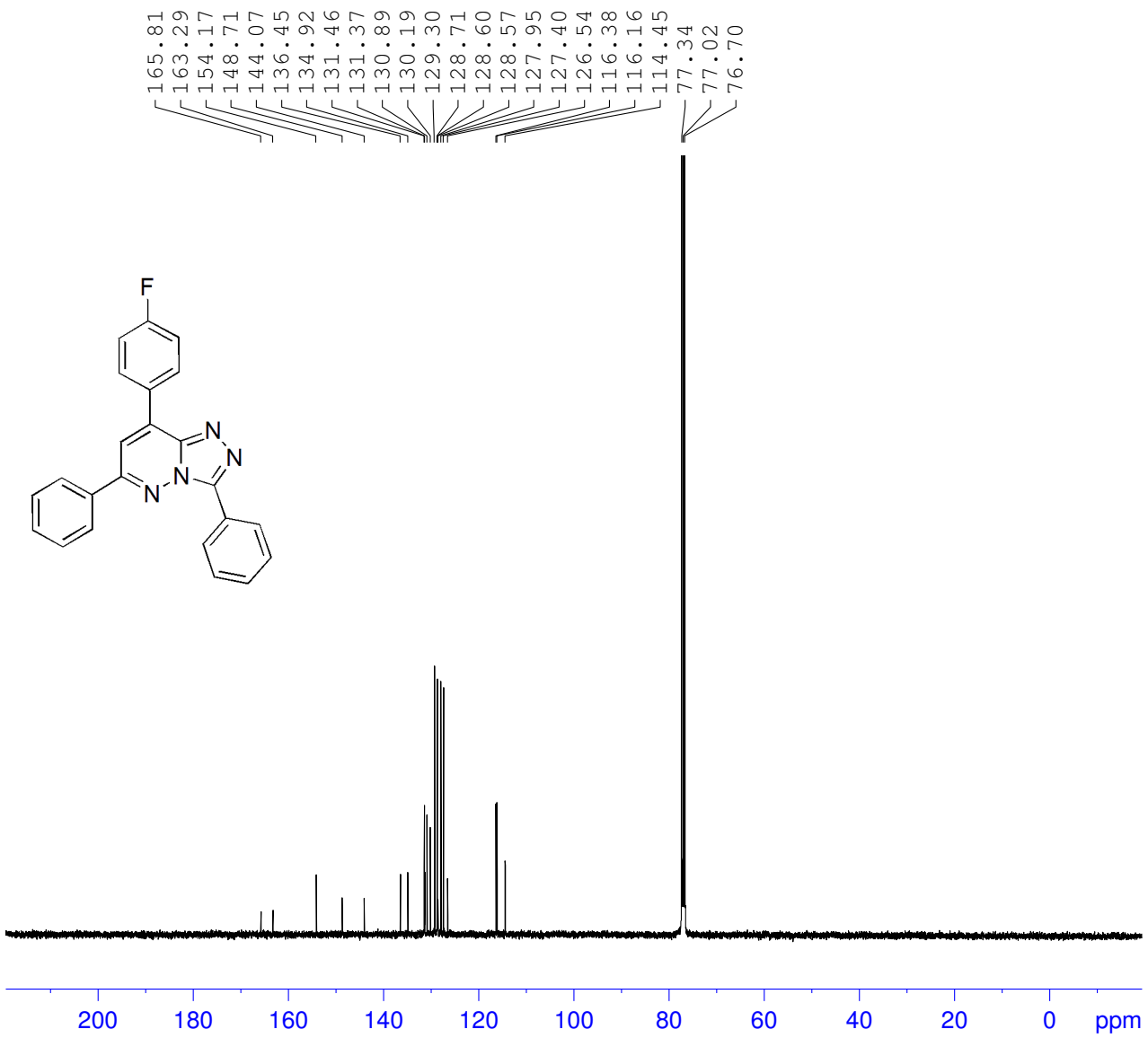


Fig 17. 1H NMR spectra of 8-(4-fluorophenyl)-3,6-diphenyl-[1,2,4]triazolo[4,3-b]pyridazine (**3i**)

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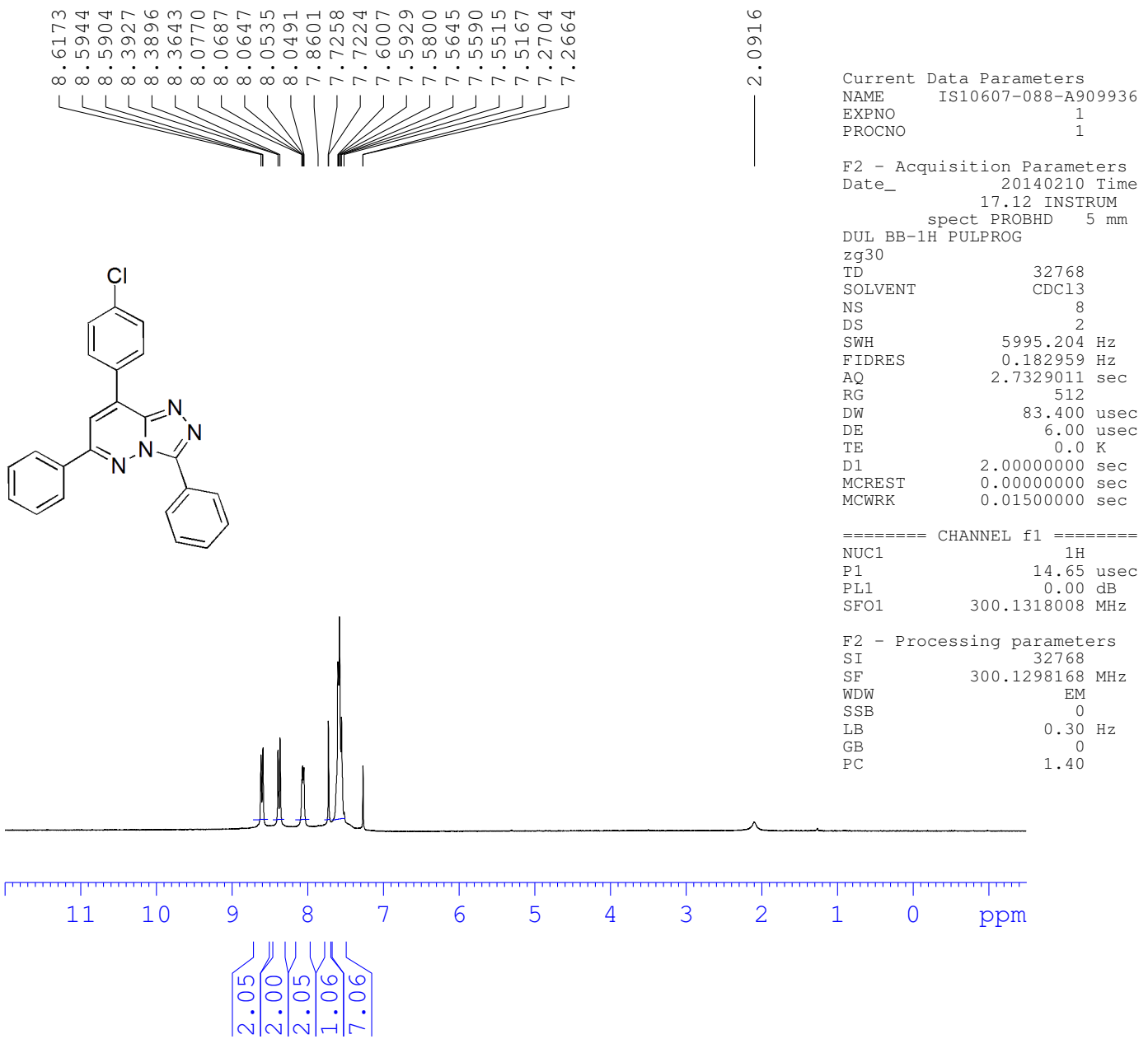
NAME      IS10607-058-A910312
EXPNO                       2
PROCNO                      1
Date_                20140216
Time                    10.24
INSTRUM                 spect
PROBHD   5 mm DUL 13C-1
PULPROG                 zgpg30
TD                       32768
SOLVENT                  CDCl3
NS                        5000
DS                           4
SWH                 24038.461 Hz
FIDRES               0.733596 Hz
AQ                  0.6816244 sec
RG                        2050
DW                      20.800 usec
DE                       6.50 usec
TE                      293.0 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                          1

======== CHANNEL f1 ========
NUC1                       13C
P1                        9.55 usec
PL1                      -0.50 dB
PL1W               40.58471298 W
SFO1              100.6680954 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                       1H
PCPD2                   100.00 usec
PL2                      -2.00 dB
PL12                     16.24 dB
PL13                     17.00 dB
PL2W               15.00864029 W
PL12W               0.22508231 W
PL13W               0.18894759 W
SFO2              400.3116012 MHz
SI                       32768
SF                100.6580300 MHz
WDW                         EM
SSB                          0
LB                        1.00 Hz
GB                           0
PC                        1.40
```

Fig 18. 13C NMR spectra of 8-(4-fluorophenyl)-3,6-diphenyl-[1,2,4]triazolo[4,3-b]pyridazine (**3i**)

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Current Data Parameters
NAME      IS10607-088-A909936
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_           20140210 Time
             17.12 INSTRUM
          spect PROBHD   5 mm
DUL BB-1H PULPROG
zg30
TD                      32768
SOLVENT                 CDCl3
NS                          8
DS                          2
SWH                  5995.204 Hz
FIDRES               0.182959 Hz
AQ                   2.7329011 sec
RG                        512
DW                     83.400 usec
DE                      6.00 usec
TE                       0.0 K
D1                 2.00000000 sec
MCREST             0.00000000 sec
MCWRK              0.01500000 sec

======== CHANNEL f1 ========
NUC1                        1H
P1                       14.65 usec
PL1                       0.00 dB
SFO1               300.1318008 MHz

F2 - Processing parameters
SI                      32768
SF                 300.1298168 MHz
WDW                        EM
SSB                         0
LB                       0.30 Hz
GB                          0
PC                       1.40
```
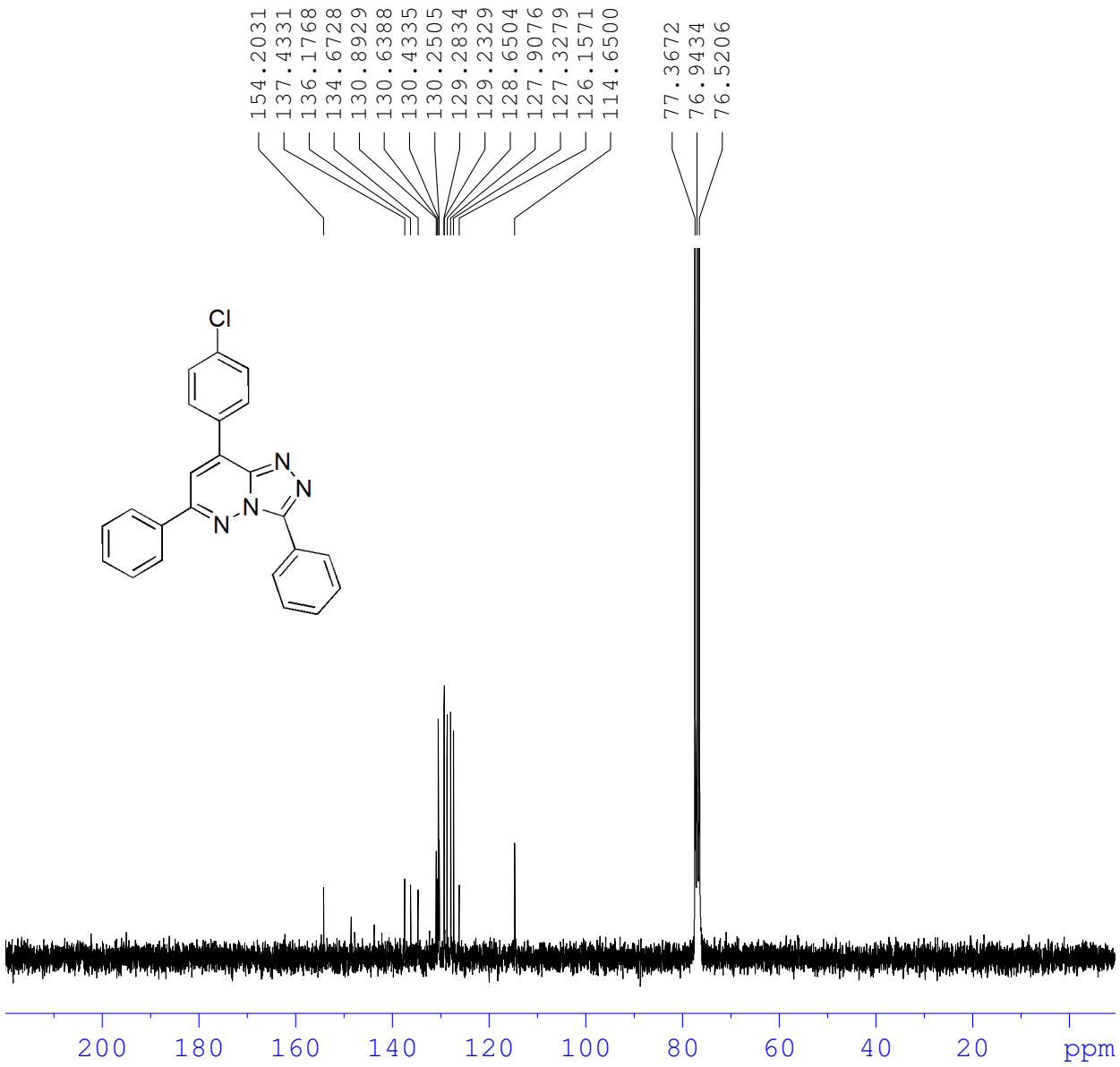

Fig 19. 1H NMR spectra of 8-(4-chlorophenyl)-3,6-diphenyl-[1,2,4]triazolo[4,3-b]pyridazine (**3j**)

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Current Data Parameters
NAME      IS10607-088-A909936
EXPNO                       2
PROCNO                      1

F2 - Acquisition Parameters
Date_            20140212
Time                 1.13
INSTRUM             spect
PROBHD    5 mm DUL BB-1H
PULPROG           zgpg30
TD                 32768
SOLVENT            CDCl3
NS                  2500
DS                     0
SWH            20325.203 Hz
FIDRES          0.620276 Hz
AQ             0.8061428 sec
RG                5792.6
DW                24.600 usec
DE                 6.00 usec
TE                  0.0 K
D1           3.00000000 sec
d11          0.03000000 sec
DELTA        2.90000010 sec
MCREST       0.00000000 sec
MCWRK        0.01500000 sec

======== CHANNEL f1 ========
NUC1                 13C
P1                  8.50 usec
PL1                 0.00 dB
SFO1          75.4771525 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2              80.00 usec
PL2                 0.00 dB
PL12               14.75 dB
PL13               18.00 dB
SFO2         300.1315007 MHz

F2 - Processing parameters
SI                 32768
SF            75.4677079 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.70
```

Fig 20. 13C NMR spectra of 8-(4-chlorophenyl)-3,6-diphenyl-[1,2,4]triazolo[4,3-b]pyridazine (**3j**)

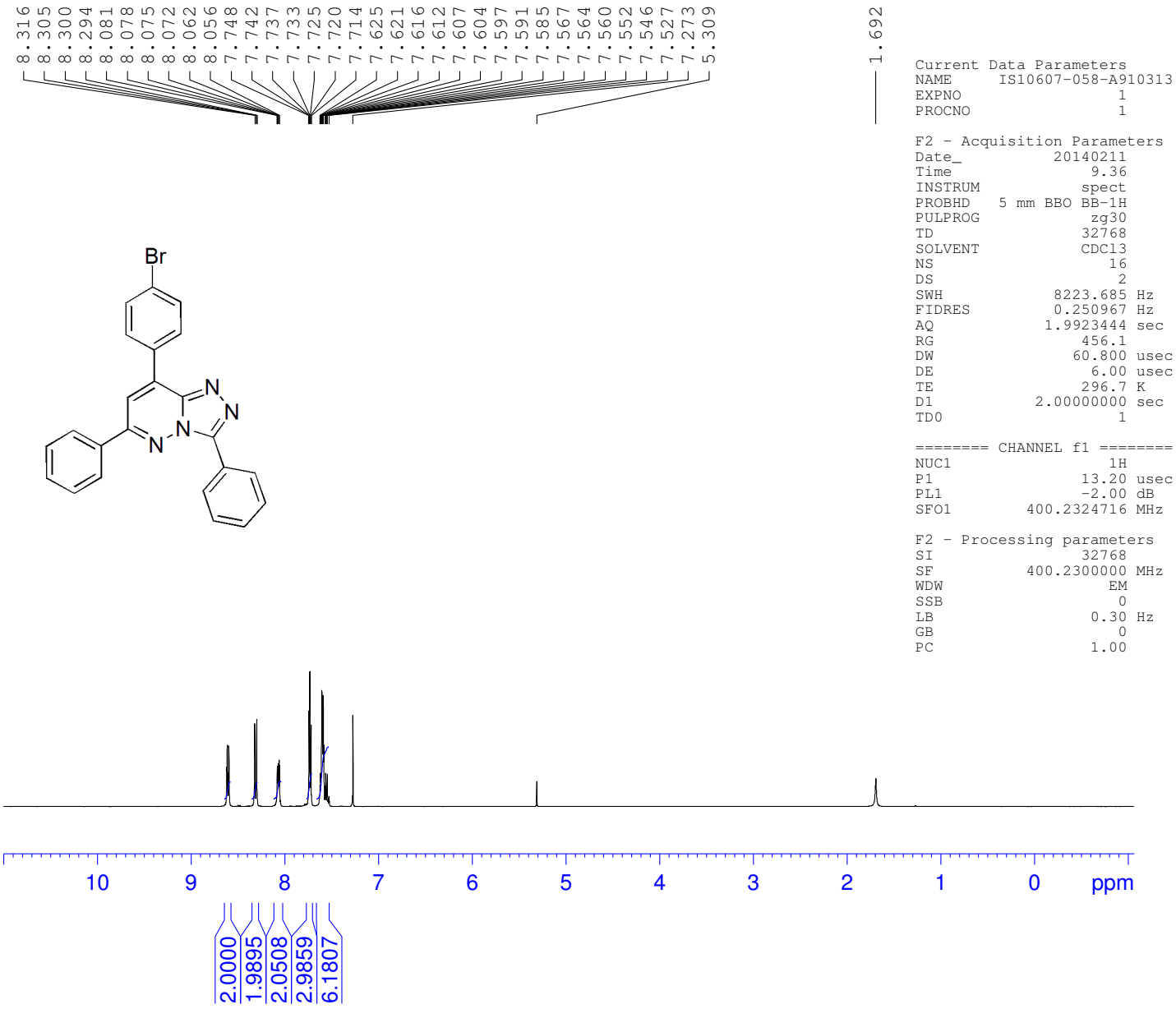
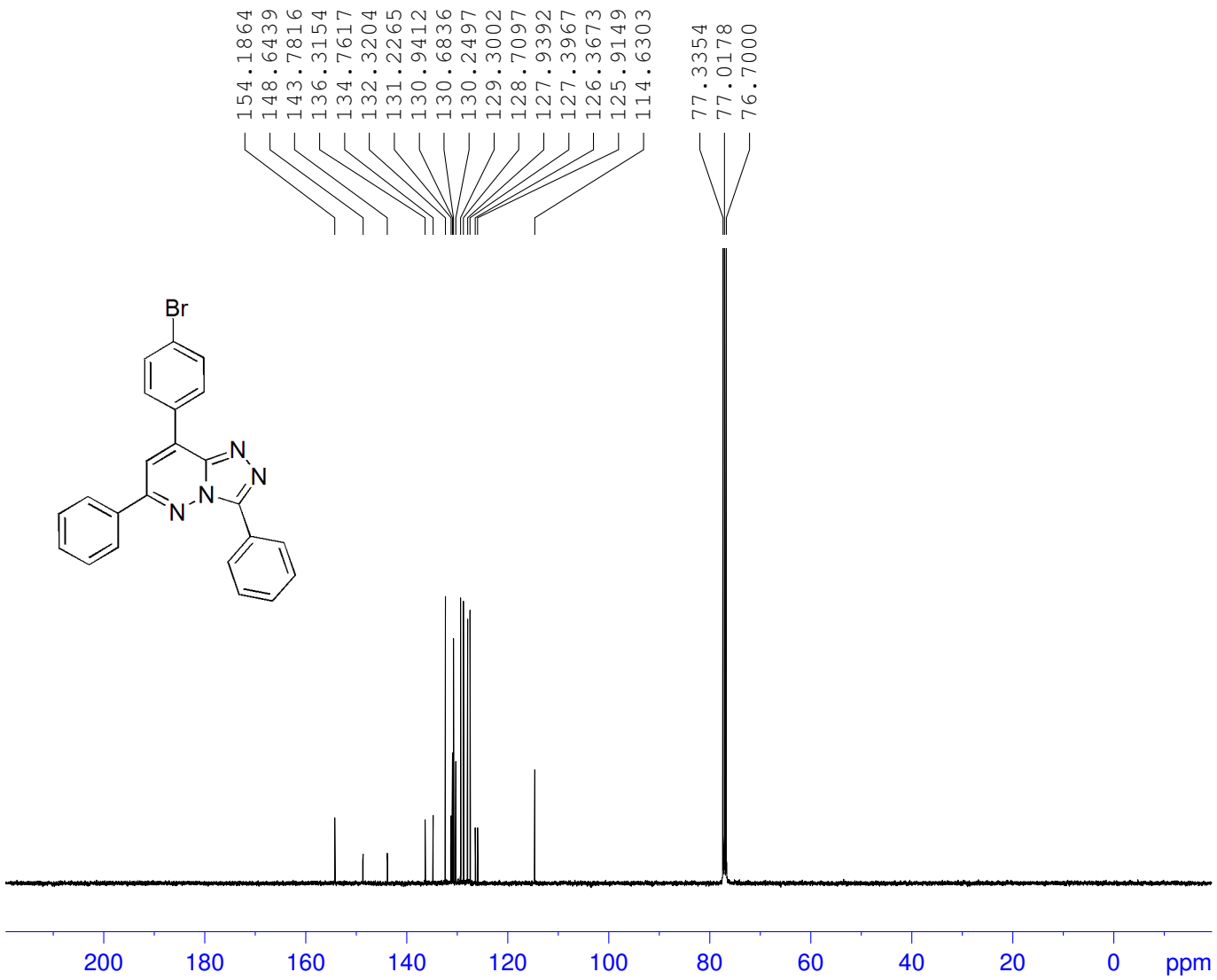


Fig 21. 1H NMR spectra of 8-(4-bromophenyl)-3,6-diphenyl-[1,2,4]triazolo[4,3-b]pyridazine (**3k**)




```
Current Data Parameters
NAME      IS10607-058-A910313
EXPNO                       2
PROCNO                      1

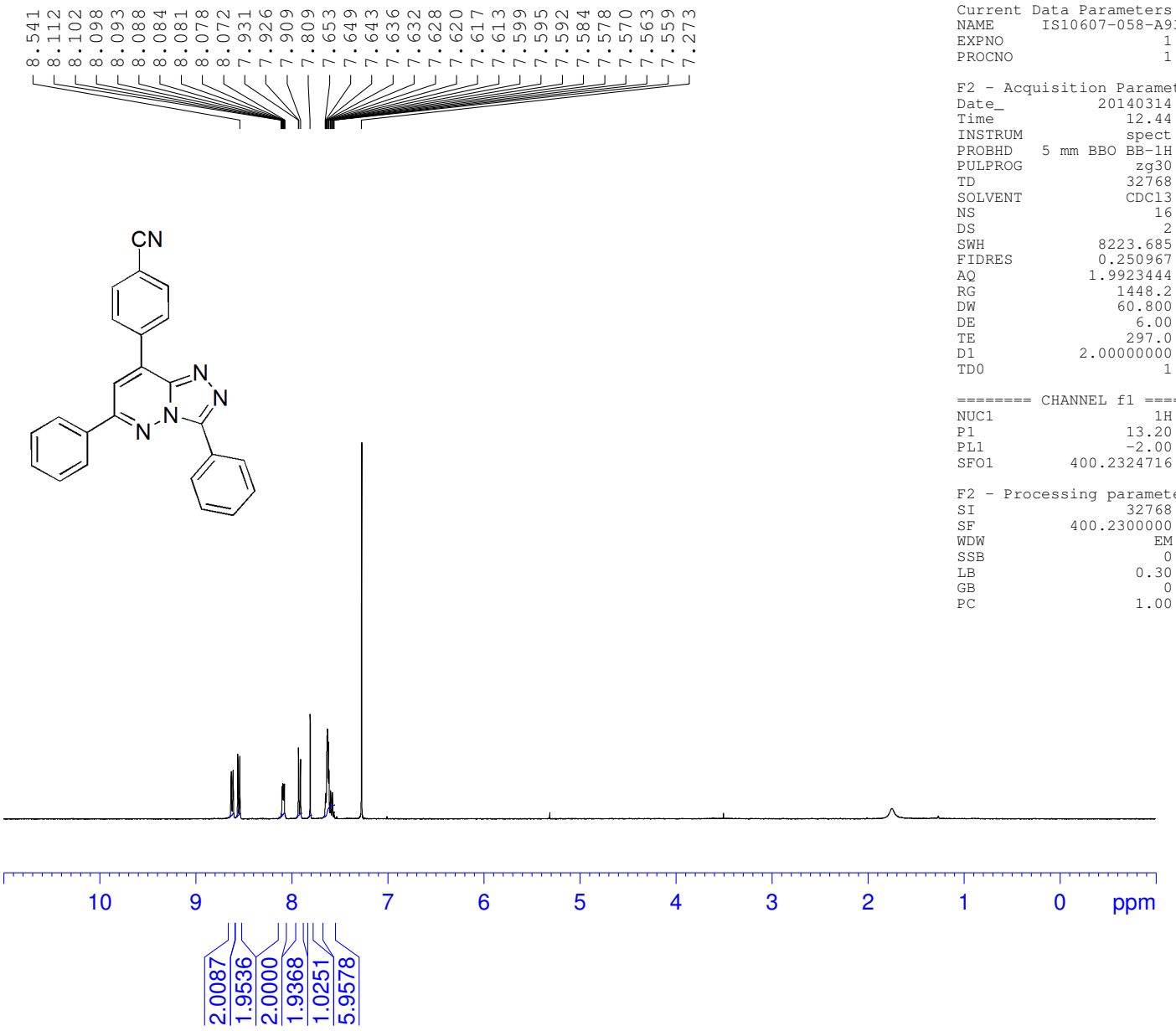
F2 - Acquisition Parameters
Date_            20140215
Time                17.37
INSTRUM             spect
PROBHD    5 mm PABBO BB-
PULPROG            zgpg30
TD                  32768
SOLVENT             CDCl3
NS                   5000
DS                      4
SWH             24038.461 Hz
FIDRES           0.733596 Hz
AQ               0.6816244 sec
RG                    203
DW                  20.800 usec
DE                   6.00 usec
TE                  297.5 K
D1              2.00000000 sec
d11             0.03000000 sec
DELTA           1.89999998 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                   13C
P1                    8.10 usec
PL1                  -3.00 dB
SFO1          100.6278593 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                   1H
PCPD2                80.00 usec
PL12                 14.04 dB
PL13                 15.00 dB
PL2                  -0.50 dB
SFO2          400.1516006 MHz

F2 - Processing parameters
SI                    32768
SF            100.6177980 MHz
WDW                     EM
SSB                      0
LB                    1.00 Hz
GB                       0
PC                    1.40
```

Fig 22. 13C NMR spectra of 8-(4-bromophenyl)-3,6-diphenyl-[1,2,4]triazolo[4,3-b]pyridazine (**3k**)



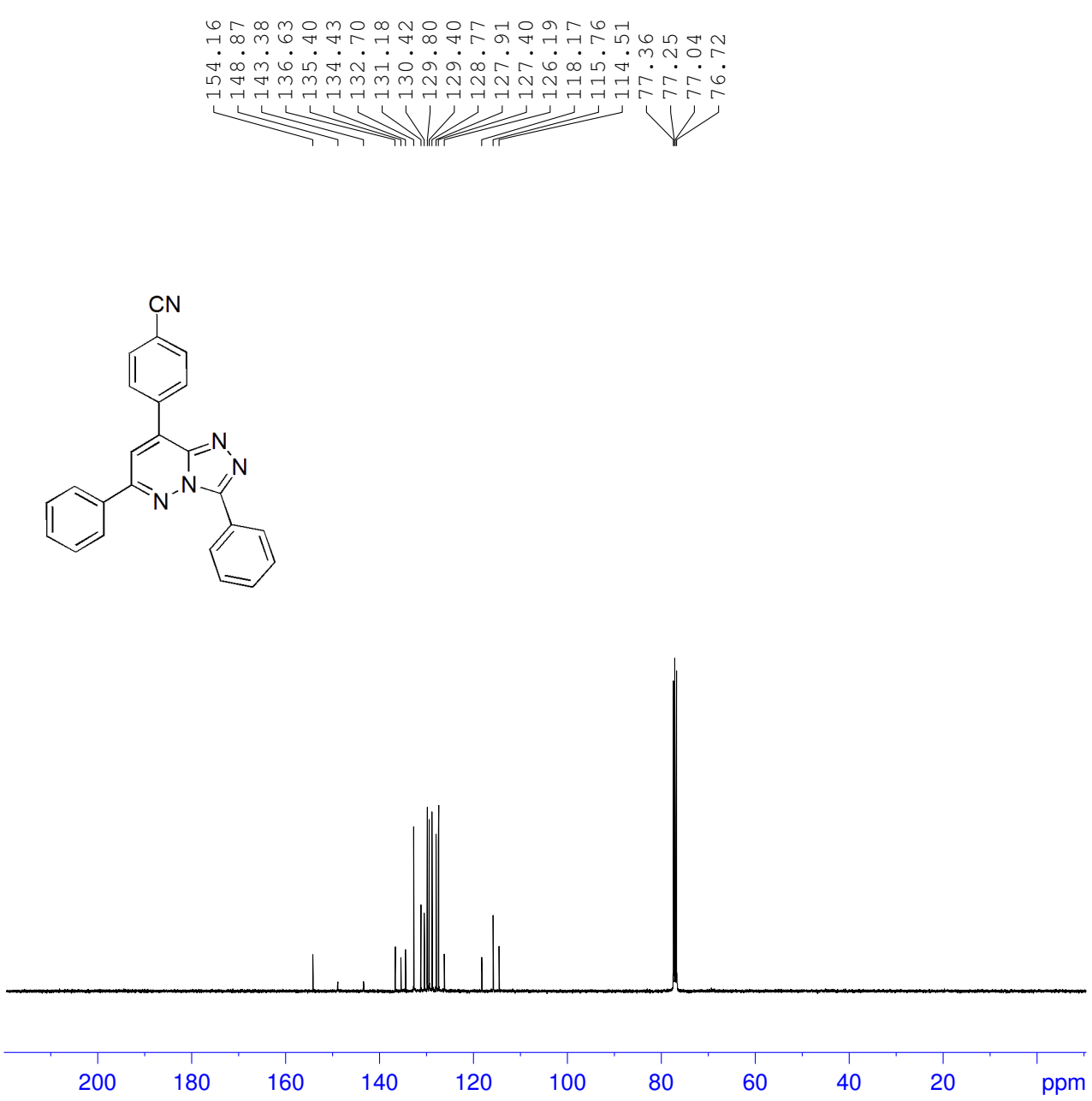

```
Current Data Parameters
NAME      IS10607-058-A936853
EXPNO                      1
PROCNO                     1

F2 - Acquisition Parameters
Date_           20140314
Time               12.44
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8223.685 Hz
FIDRES          0.250967 Hz
AQ             1.9923444 sec
RG                1448.2
DW                60.800 usec
DE                 6.00 usec
TE                297.0 K
D1           2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 13.20 usec
PL1                -2.00 dB
SFO1        400.2324716 MHz

F2 - Processing parameters
SI                 32768
SF          400.2300000 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

Fig 23. 1H NMR spectra of 4-(3,6-diphenyl-[1,2,4]triazolo[4,3-b]pyridazin-8-yl)benzonitrile (**3l**)

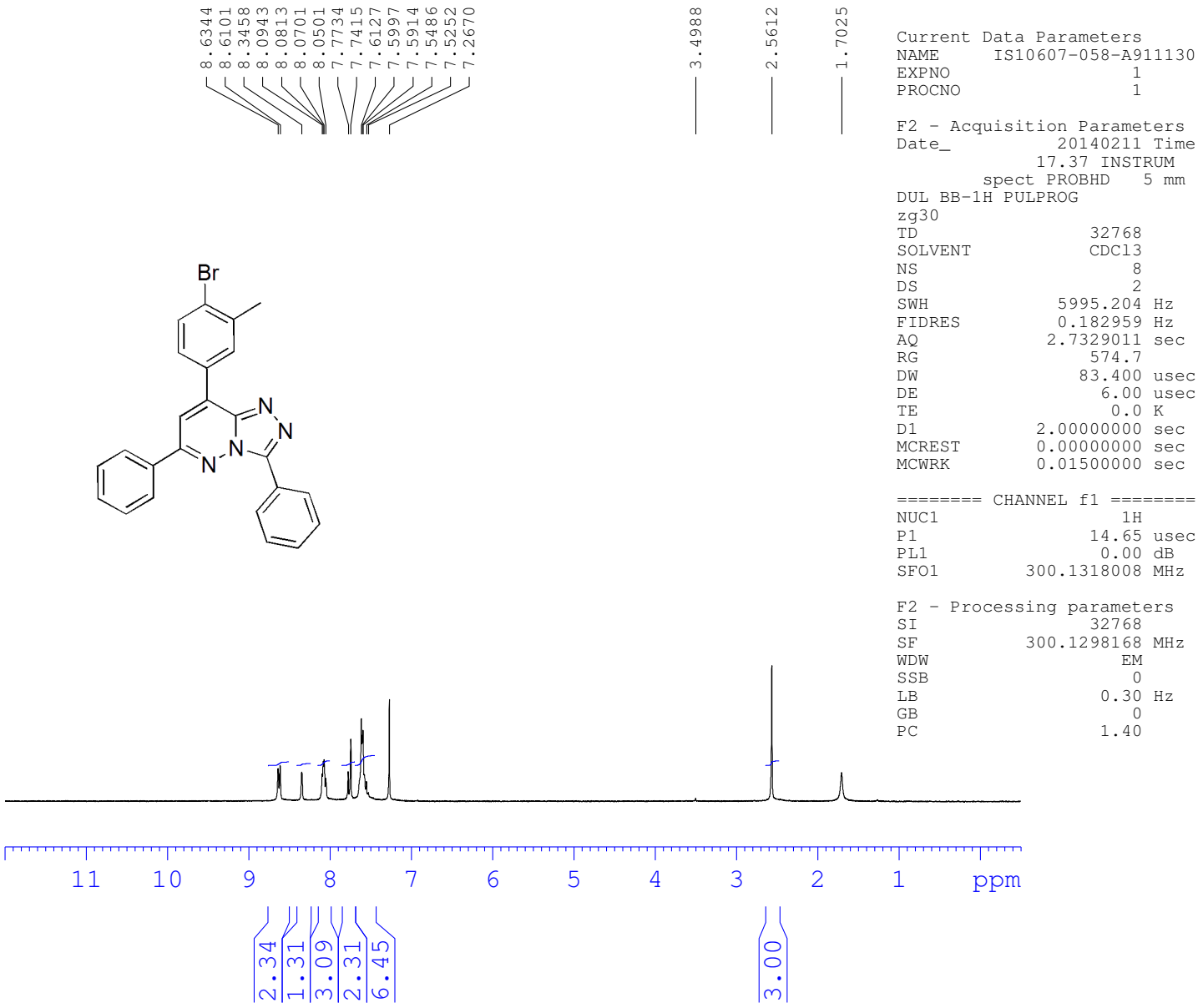



```
NAME      IS10607-058-A936853
EXPNO                   1
PROCNO                  1
Date_            20140316
Time                13.39
INSTRUM             spect
PROBHD    5 mm DUL 13C-1
PULPROG            zgpg30
TD                  32768
SOLVENT             CDCl3
NS                   3000
DS                      4
SWH            24038.461 Hz
FIDRES          0.733596 Hz
AQ             0.6816244 sec
RG                   2050
DW                 20.800 usec
DE                  6.50 usec
TE                 293.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                  13C
P1                   9.50 usec
PL1                 -1.50 dB
PL1W         51.09312820 W
SFO1        100.6680954 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                  1H
PCPD2              100.00 usec
PL2                 -2.00 dB
PL12                16.17 dB
PL13                17.00 dB
PL2W         15.00864029 W
PL12W         0.22873959 W
PL13W         0.18894759 W
SFO2        400.3116012 MHz
SI                  32768
SF          100.6580300 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

Fig 24. 13C NMR spectra of 4-(3,6-diphenyl-[1,2,4]triazolo[4,3-b]pyridazin-8-yl)benzonitrile (**3l**)



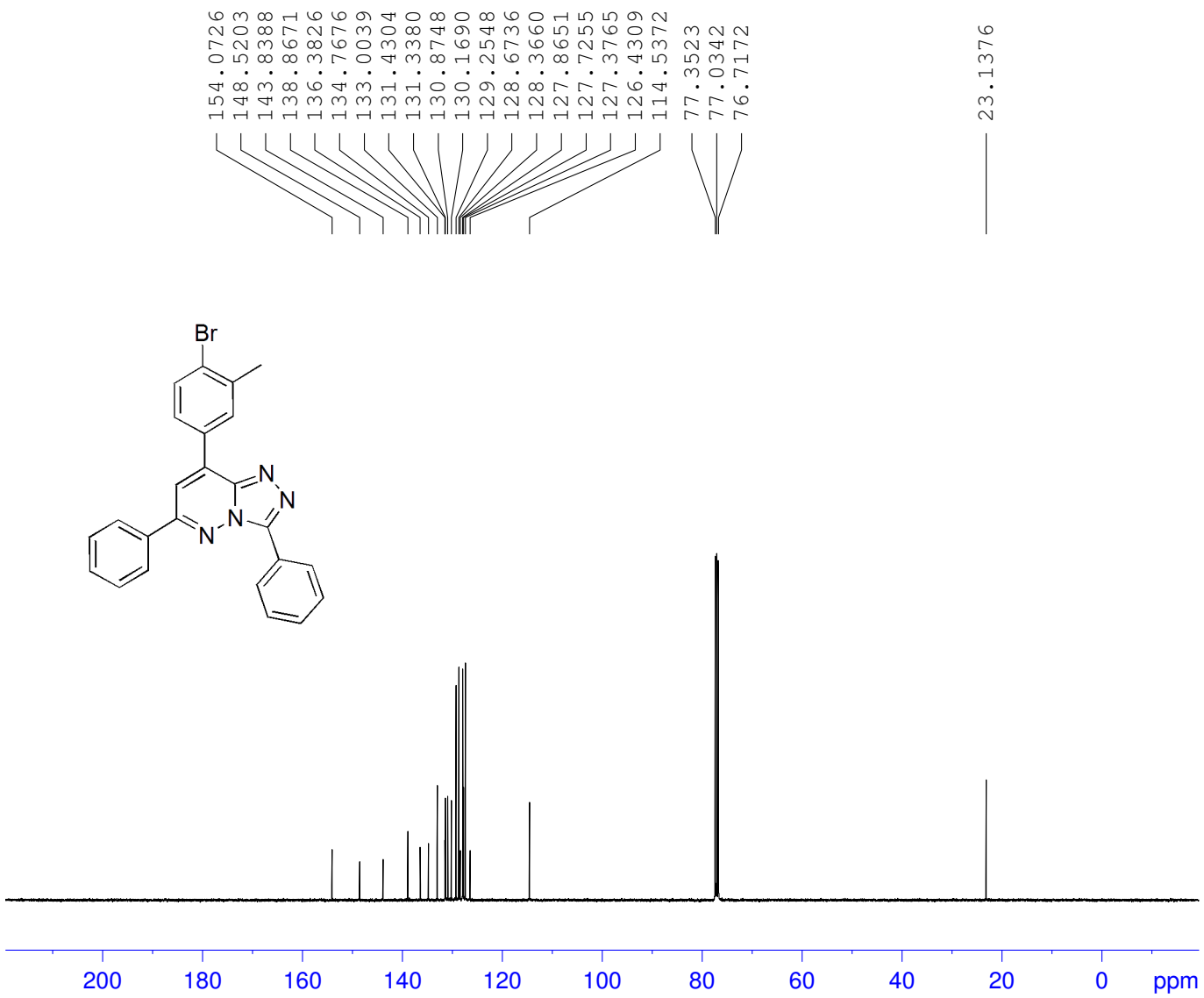

```
Current Data Parameters
NAME      IS10607-058-A911130
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_           20140211 Time
              17.37 INSTRUM
          spect PROBHD   5 mm
DUL BB-1H PULPROG
zg30
TD                      32768
SOLVENT                 CDCl3
NS                          8
DS                          2
SWH                  5995.204 Hz
FIDRES               0.182959 Hz
AQ                  2.7329011 sec
RG                      574.7
DW                     83.400 usec
DE                       6.00 usec
TE                        0.0 K
D1                 2.00000000 sec
MCREST             0.00000000 sec
MCWRK              0.01500000 sec

======== CHANNEL f1 ========
NUC1                        1H
P1                       14.65 usec
PL1                       0.00 dB
SFO1              300.1318008 MHz

F2 - Processing parameters
SI                      32768
SF                300.1298168 MHz
WDW                        EM
SSB                         0
LB                       0.30 Hz
GB                          0
PC                       1.40
```

Fig 25. 1H NMR spectra of 8-(4-bromo-3-methylphenyl)-3,6-diphenyl-[1,2,4]triazolo[4,3-b]pyridazine (**3m**)




```
Current Data Parameters
NAME      IS10607-058-A927370
EXPNO                       2
PROCNO                      1

F2 - Acquisition Parameters
Date_            20140304
Time                23.37
INSTRUM             spect
PROBHD    5 mm PABBO BB-
PULPROG            zgpg30
TD                  32768
SOLVENT             CDCl3
NS                   3000
DS                      4
SWH             24038.461 Hz
FIDRES           0.733596 Hz
AQ               0.6816244 sec
RG                    203
DW                 20.800 usec
DE                  6.00 usec
TE                 296.5 K
D1             2.00000000 sec
d11            0.03000000 sec
DELTA          1.89999998 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                   13C
P1                    8.10 usec
PL1                  -3.00 dB
SFO1          100.6278593 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                   1H
PCPD2               80.00 usec
PL12                14.04 dB
PL13                15.00 dB
PL2                 -0.50 dB
SFO2          400.1516006 MHz

F2 - Processing parameters
SI                   32768
SF            100.6177980 MHz
WDW                     EM
SSB                      0
LB                    1.00 Hz
GB                       0
PC                    1.40
```

Fig 26. 13C NMR spectra of 8-(4-bromo-3-methylphenyl)-3,6-diphenyl-[1,2,4]triazolo[4,3-b]pyridazine (**3m**)

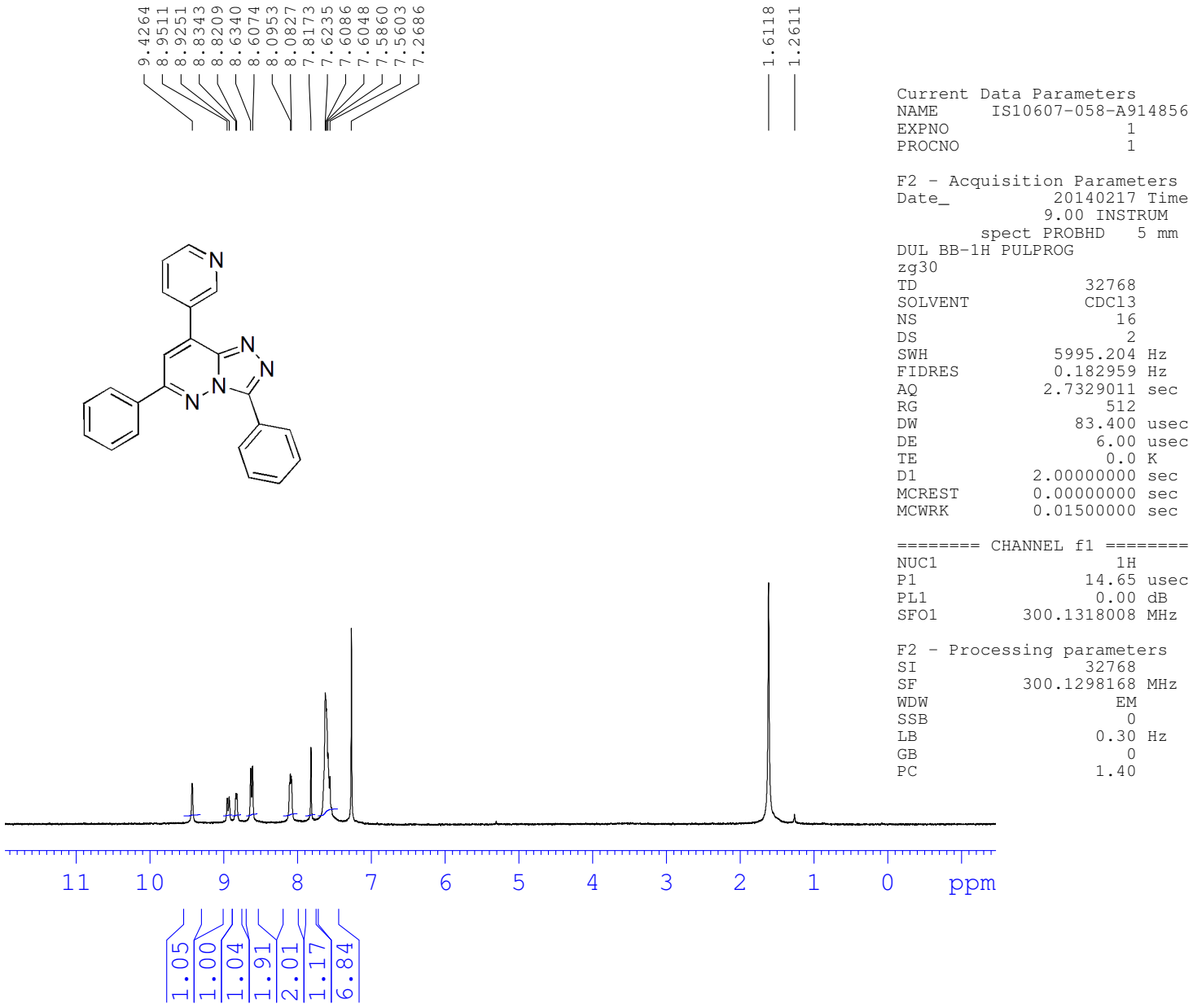
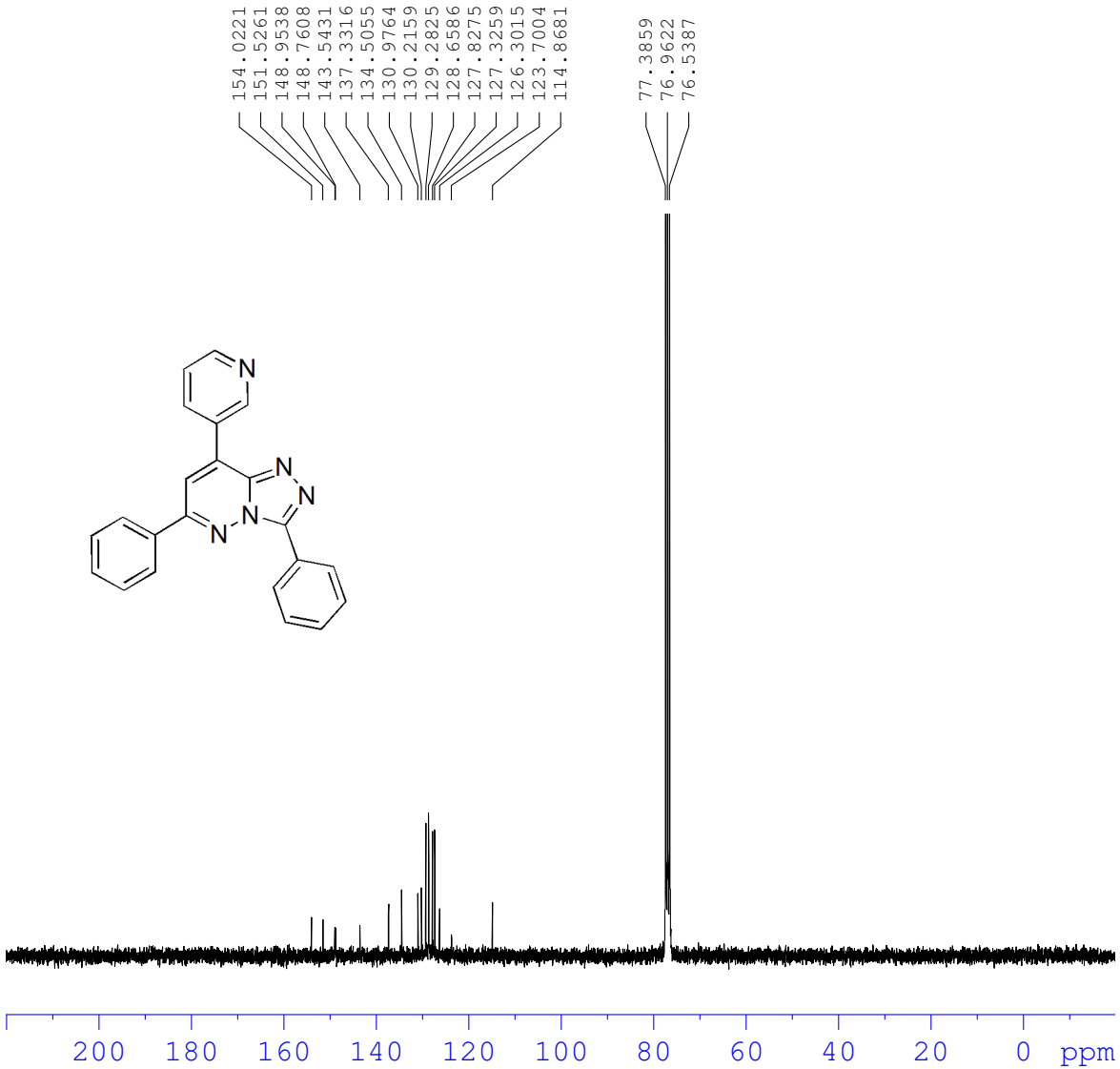


Fig 27. 1H NMR spectra of 3,6-diphenyl-8-(pyridin-3-yl)-[1,2,4]triazolo[4,3-b]pyridazine (**3n**)




```
Current Data Parameters
NAME      IS10607-058-A927372
EXPNO                       2
PROCNO                      1

F2 - Acquisition Parameters
Date_            20140304
Time                18.38
INSTRUM             spect
PROBHD    5 mm DUL BB-1H
PULPROG            zgpg30
TD                  32768
SOLVENT             CDCl3
NS                   4000
DS                      0
SWH             18115.941 Hz
FIDRES          0.552855 Hz
AQ              0.9044468 sec
RG                18390.4
DW                 27.600 usec
DE                  6.00 usec
TE                   0.0 K
D1            2.00000000 sec
d11           0.03000000 sec
DELTA         1.89999998 sec
MCREST        0.00000000 sec
MCWRK         0.01500000 sec

======== CHANNEL f1 ========
NUC1                  13C
P1                   7.75 usec
PL1                  0.00 dB
SFO1          75.4752658 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                  1H
PCPD2              80.00 usec
PL2                 0.00 dB
PL12                17.81 dB
PL13                18.00 dB
SFO2         300.1315007 MHz

F2 - Processing parameters
SI                   32768
SF            75.4677079 MHz
WDW                     EM
SSB                      0
LB                    1.00 Hz
GB                       0
PC                    1.70
```

Fig 28. 13C NMR spectra of 3,6-diphenyl-8-(pyridin-3-yl)-[1,2,4]triazolo[4,3-b]pyridazine (**3n**)

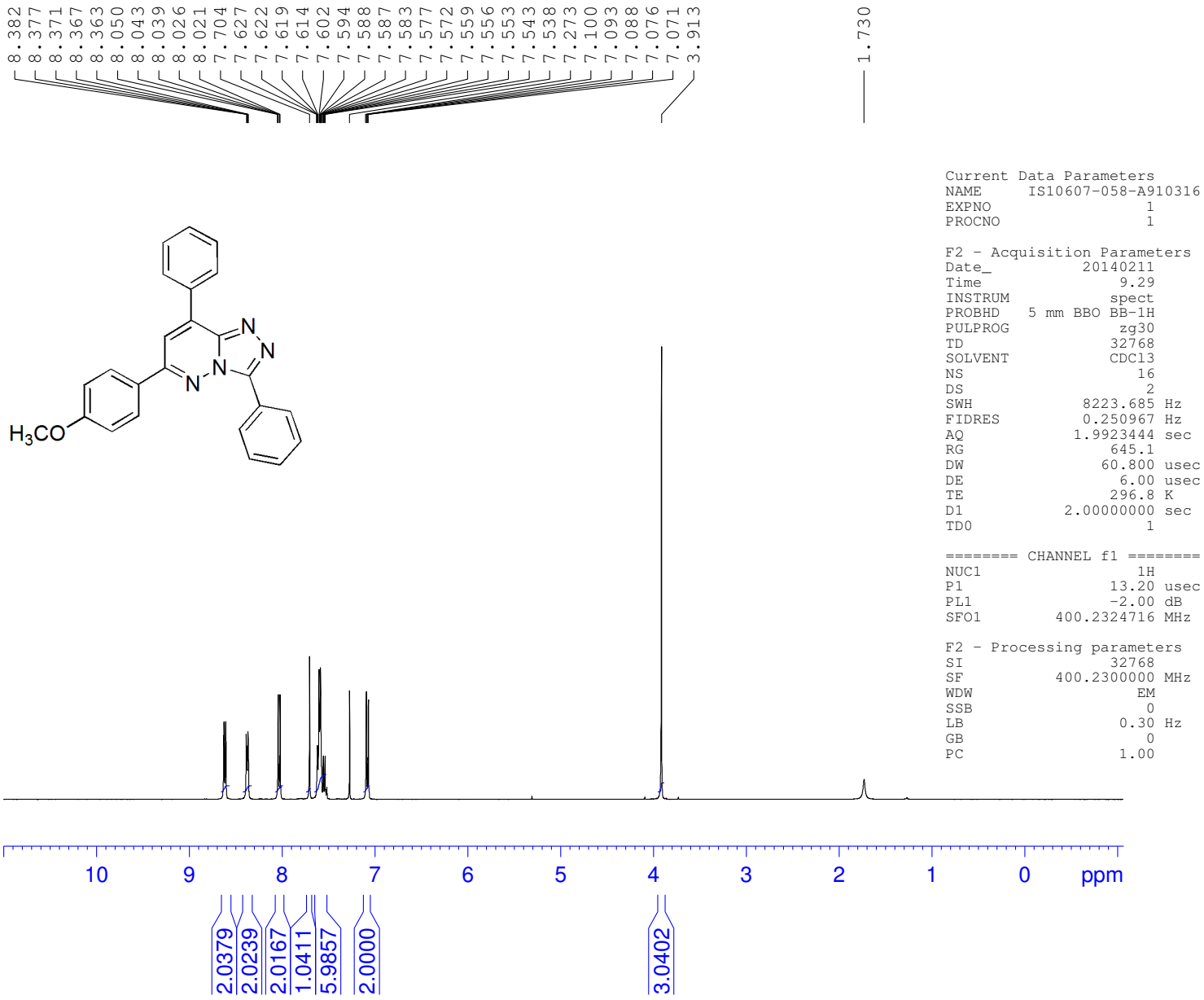
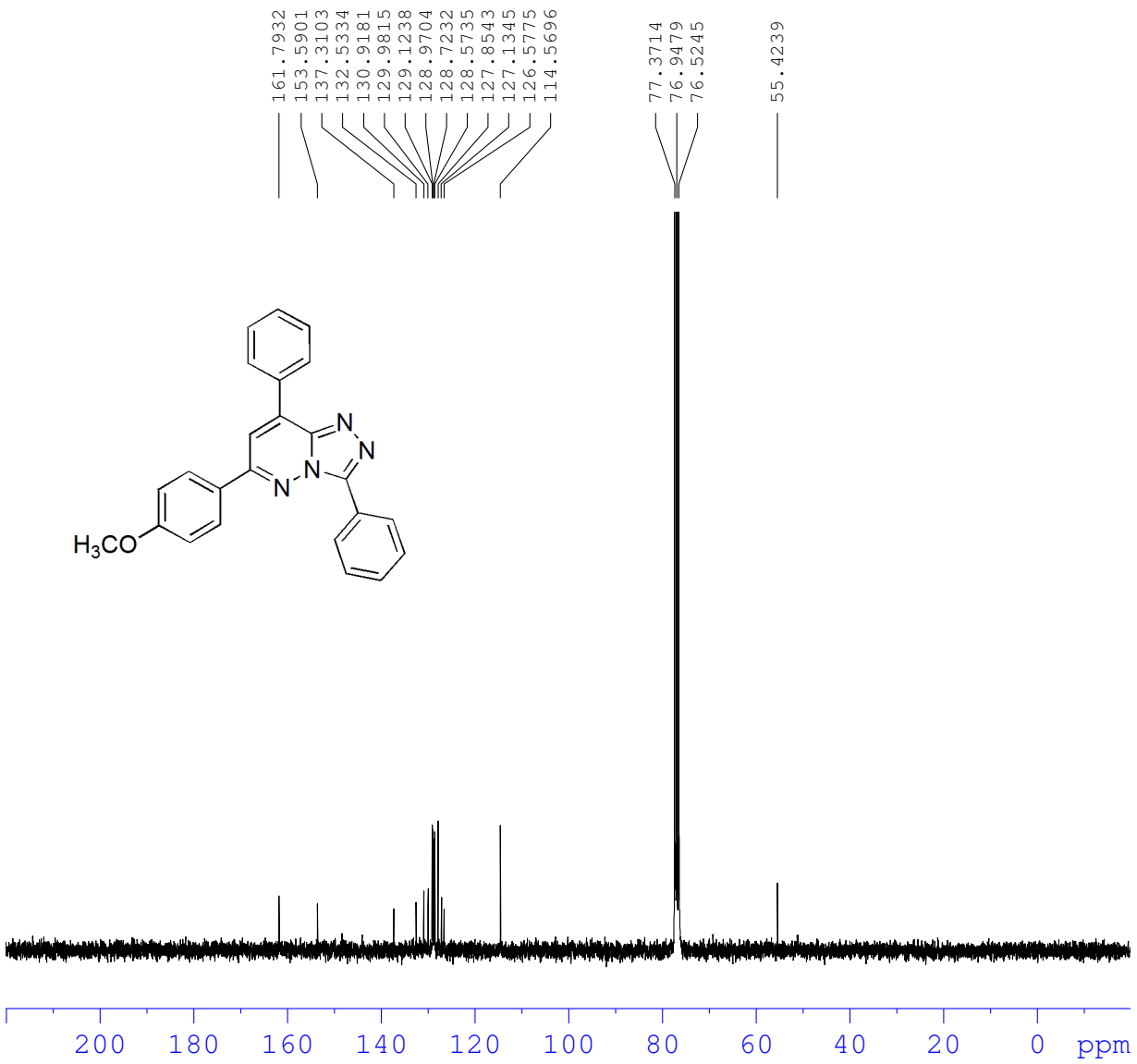


Fig 29. 1H NMR spectra of 6-(4-Methoxyphenyl)-3,8-diphenyl-[1,2,4]triazolo[4,3-b]pyridazine (**5a**)




```
Current Data Parameters
NAME      IS10607-058-A910316
EXPNO                       2
PROCNO                      1

F2 - Acquisition Parameters
Date_            20140213
Time                18.16
INSTRUM             spect
PROBHD   5 mm DUL BB-1H
PULPROG           zgpg30
TD                 32768
SOLVENT            CDCl3
NS                  4000
DS                     0
SWH            18115.941 Hz
FIDRES          0.552855 Hz
AQ             0.9044468 sec
RG               18390.4
DW                27.600 usec
DE                 6.00 usec
TE                  0.0 K
D1           2.00000000 sec
d11          0.03000000 sec
DELTA        1.89999998 sec
MCREST       0.00000000 sec
MCWRK        0.01500000 sec

======== CHANNEL f1 ========
NUC1                  13C
P1                   7.75 usec
PL1                  0.00 dB
SFO1          75.4752658 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                  1H
PCPD2              80.00 usec
PL2                 0.00 dB
PL12               17.81 dB
PL13               18.00 dB
SFO2         300.1315007 MHz

F2 - Processing parameters
SI                 32768
SF            75.4677079 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.70
```

Fig 30. 13C NMR spectra of of 6-(4-Methoxyphenyl)-3,8-diphenyl-[1,2,4]triazolo[4,3-b]pyridazine (**5a**)

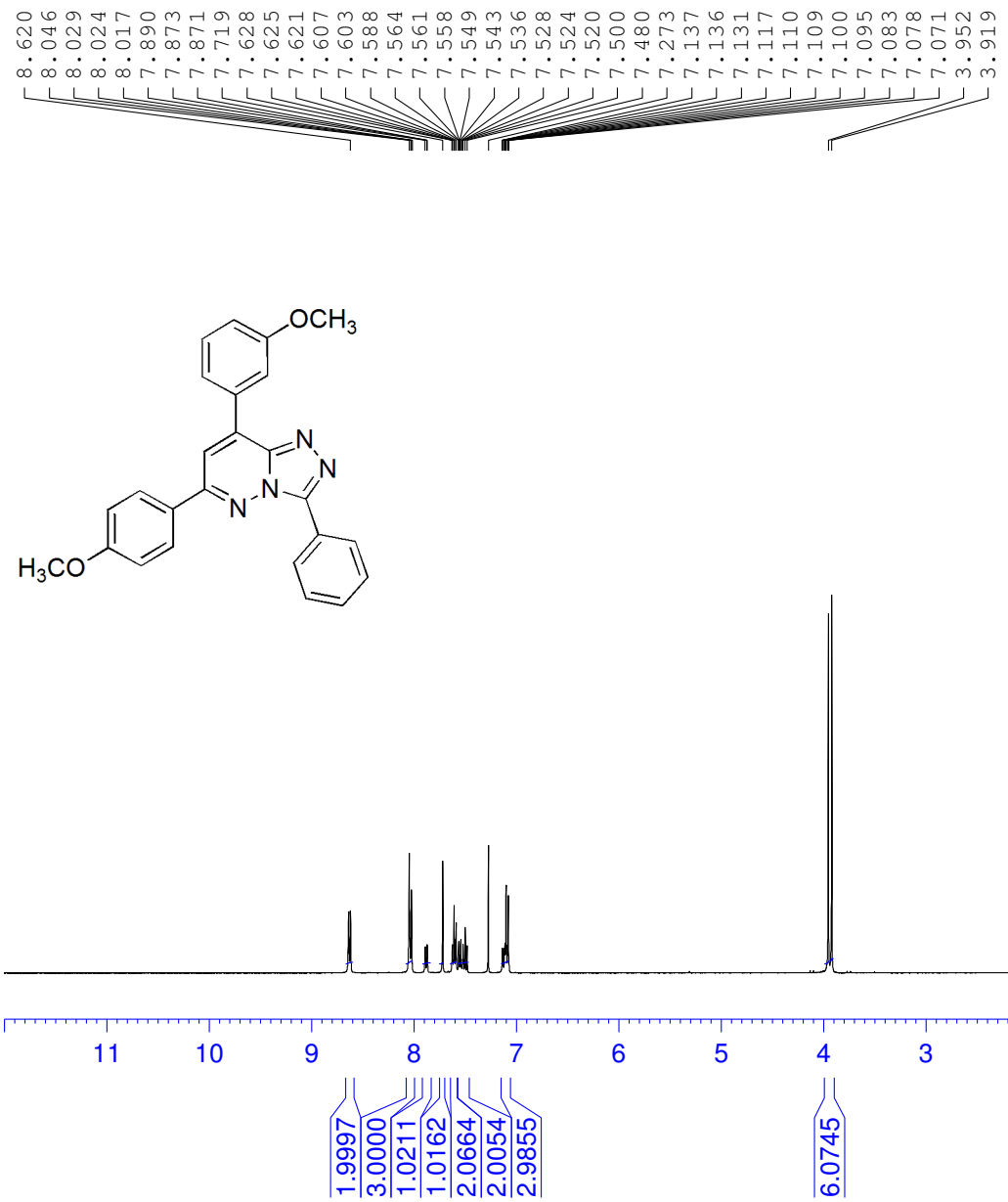
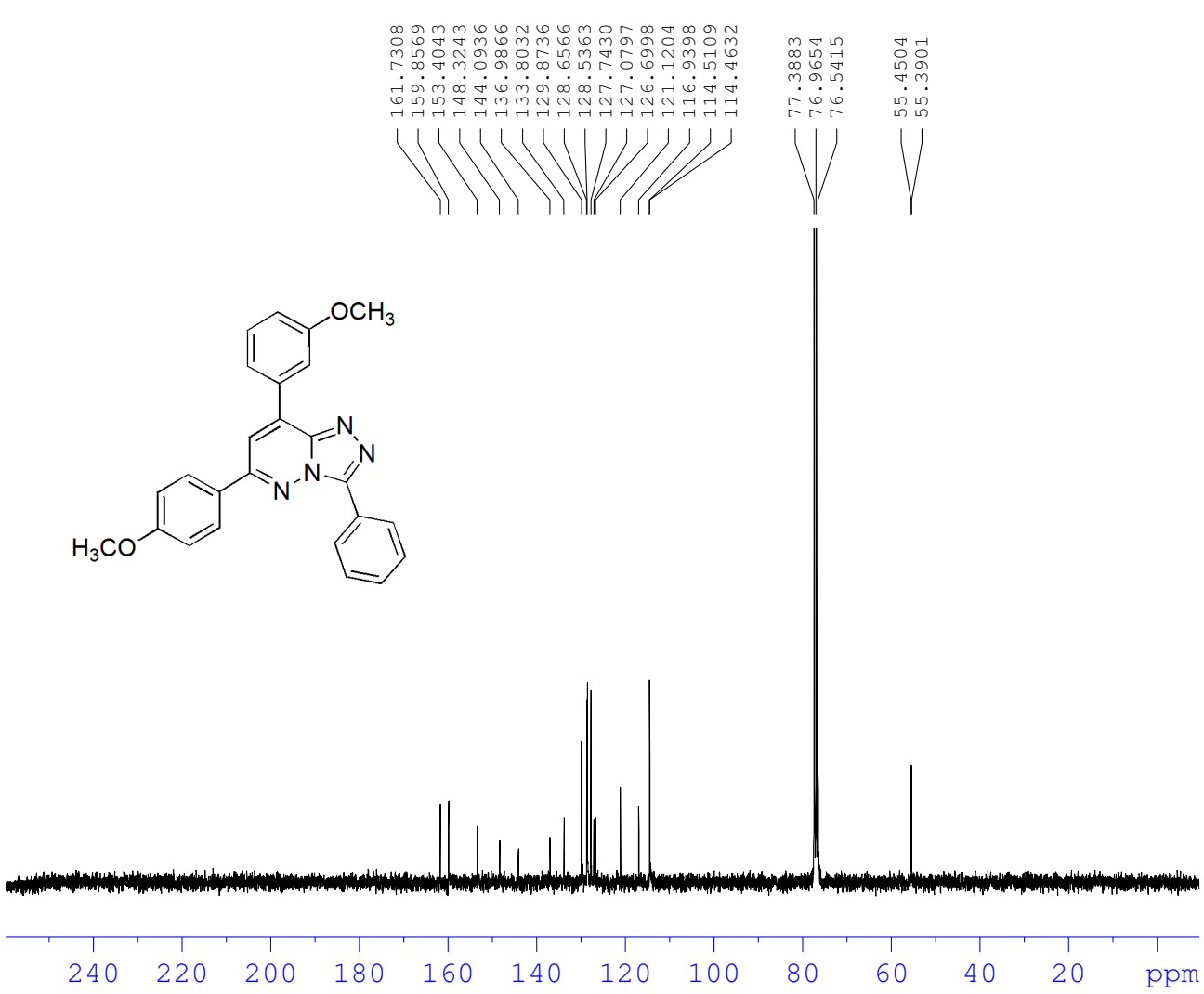


Fig 31. 1H NMR spectra of 8-(3-Methoxyphenyl)-6-(4-methoxyphenyl)-3-phenyl-[1,2,4]triazolo[4,3-b]pyridazine (**5b**)




```
Current Data Parameters
NAME      IS-S11042-096-A154411
EXPNO                 2
PROCNO                1

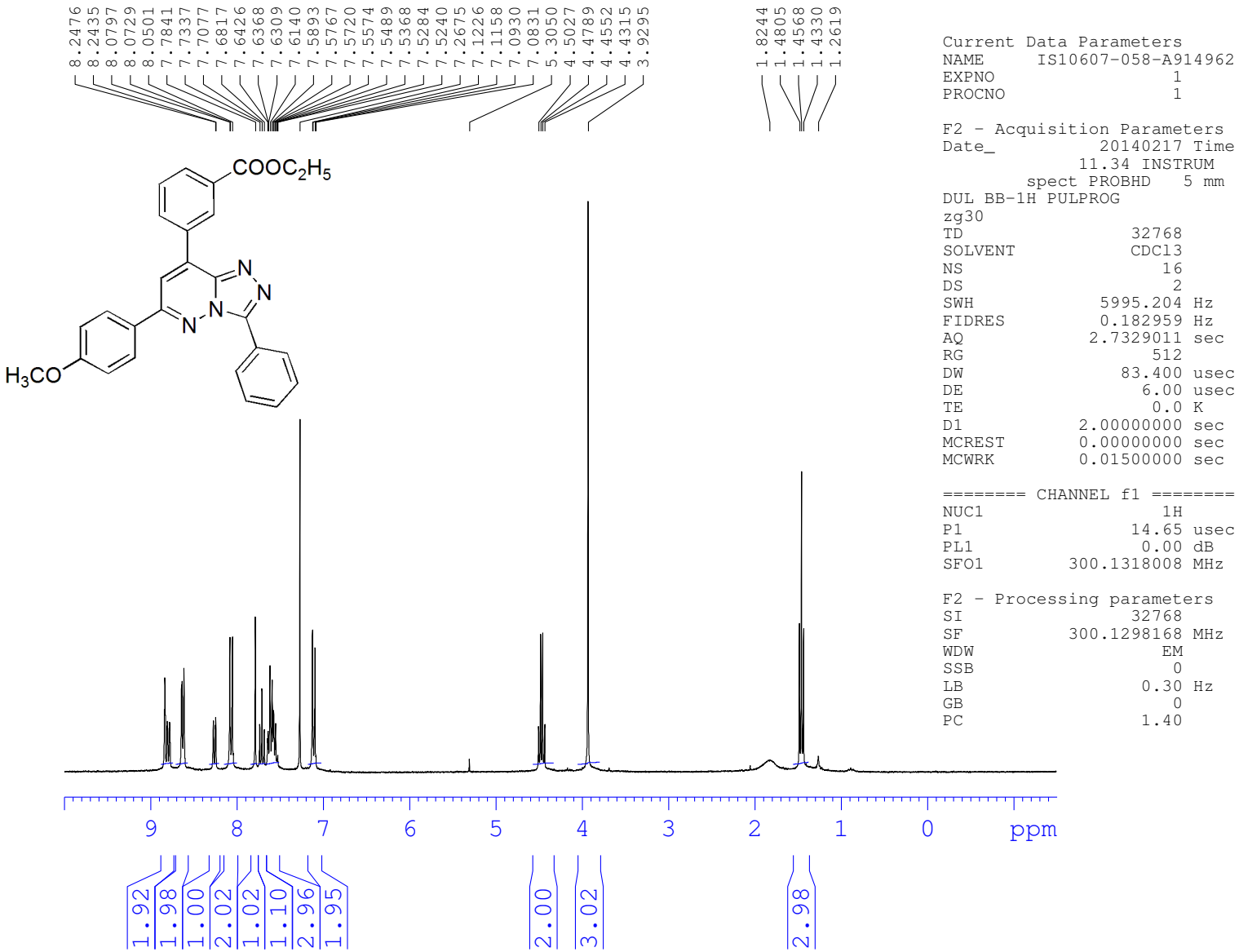
F2 - Acquisition Parameters
Date_           20141208
Time              23.12
INSTRUM           spect
PROBHD   5 mm DUL BB-1H
PULPROG          zgpg30
TD                32768
SOLVENT           CDCl3
NS                 2500
DS                    0
SWH           20325.203 Hz
FIDRES         0.620276 Hz
AQ            0.8061428 sec
RG                16384
DW               24.600 usec
DE                6.00 usec
TE                 0.0 K
D1           2.00000000 sec
d11          0.03000000 sec
DELTA        1.89999998 sec
MCREST       0.00000000 sec
MCWRK        0.01500000 sec

======== CHANNEL f1 ========
NUC1                13C
P1                 8.50 usec
PL1                0.00 dB
SFO1         75.4771525 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                1H
PCPD2             80.00 usec
PL2                0.00 dB
PL12              14.75 dB
PL13              18.00 dB
SFO2        300.1315007 MHz

F2 - Processing parameters
SI                32768
SF           75.4677079 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.70
```

Fig 32. 13C NMR spectra of 8-(3-Methoxyphenyl)-6-(4-methoxyphenyl)-3-phenyl-[1,2,4]triazolo[4,3-b] pyridazine (**5b**)



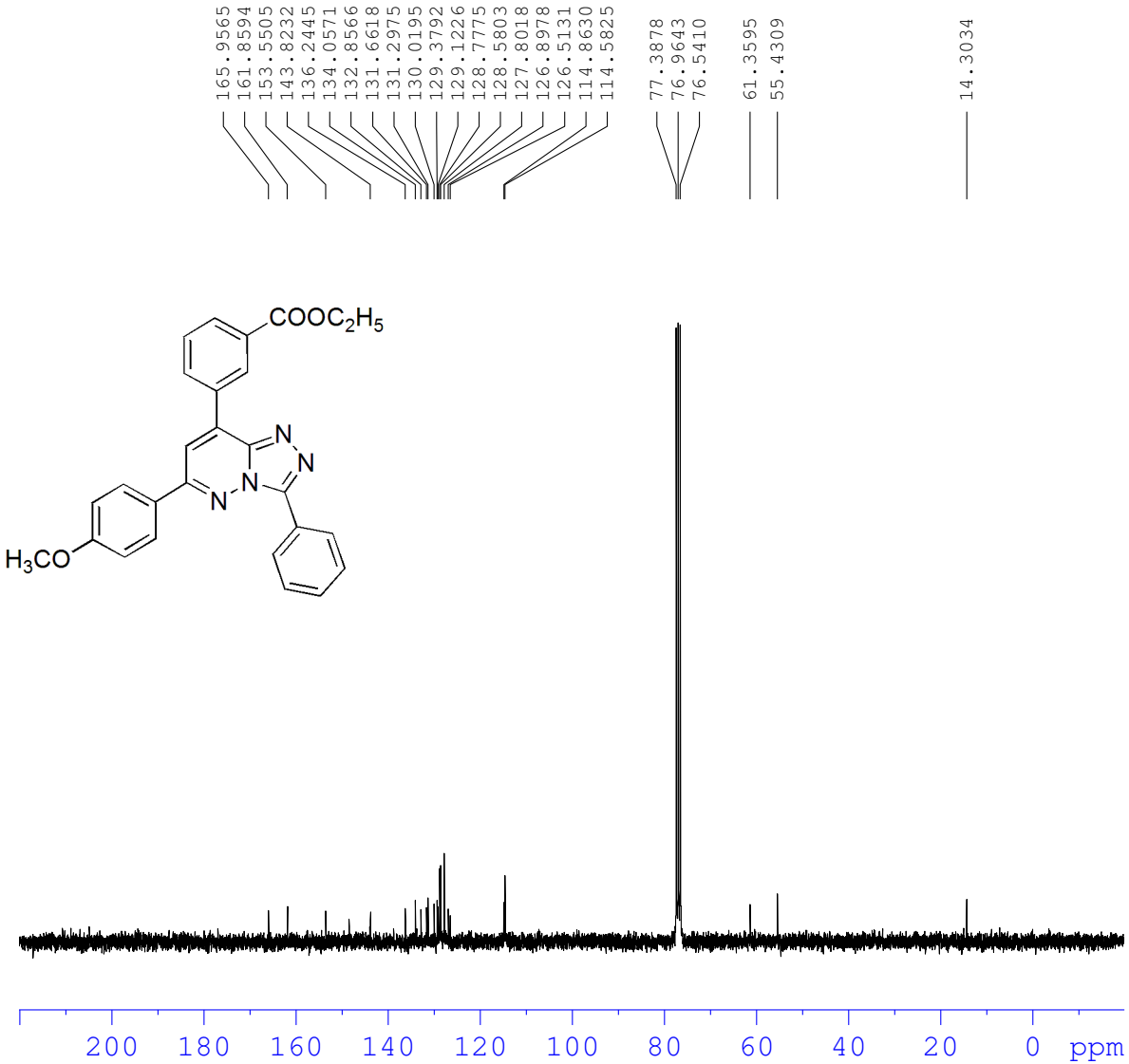

```
Current Data Parameters
NAME      IS10607-058-A914962
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_           20140217 Time
              11.34 INSTRUM
          spect PROBHD   5 mm
DUL BB-1H PULPROG
zg30
TD                  32768
SOLVENT             CDCl3
NS                     16
DS                      2
SWH              5995.204 Hz
FIDRES           0.182959 Hz
AQ               2.7329011 sec
RG                    512
DW                 83.400 usec
DE                  6.00 usec
TE                   0.0 K
D1             2.00000000 sec
MCREST         0.00000000 sec
MCWRK          0.01500000 sec

======== CHANNEL f1 ========
NUC1                   1H
P1                  14.65 usec
PL1                  0.00 dB
SFO1         300.1318008 MHz

F2 - Processing parameters
SI                  32768
SF           300.1298168 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   1.40
```

Fig 33. 1H NMR spectra of Ethyl 3-(6-(4-methoxyphenyl)-3-phenyl-[1,2,4]triazolo[4,3-b]pyridazin-8-yl) benzoate (**5c**)




```
Current Data Parameters
NAME      IS10607-058-A927373
EXPNO                       2
PROCNO                      1

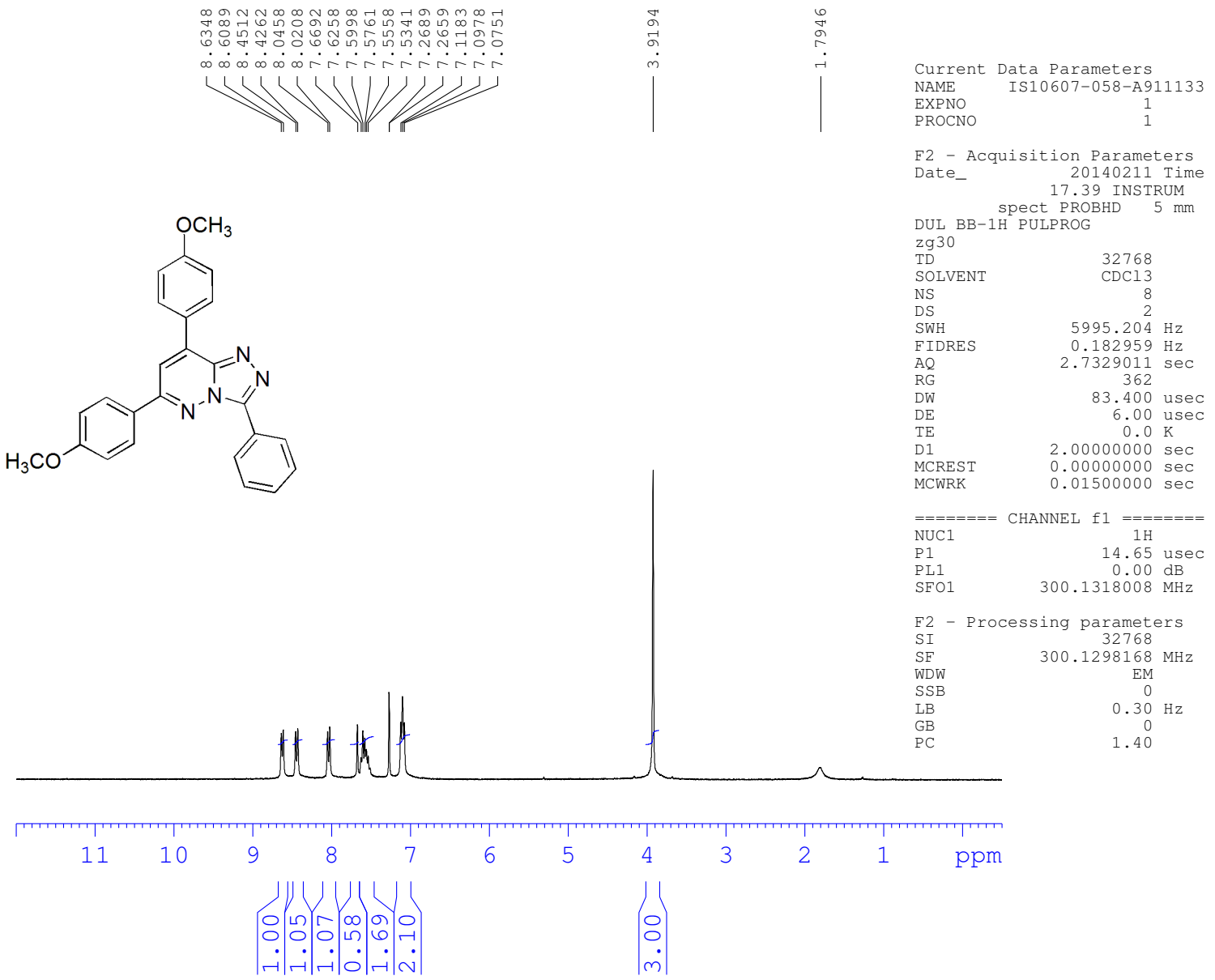
F2 - Acquisition Parameters
Date_            20140304
Time                12.42
INSTRUM             spect
PROBHD    5 mm DUL BB-1H
PULPROG           zgpg30
TD                 32768
SOLVENT            CDCl3
NS                  1084
DS                     0
SWH            18115.941 Hz
FIDRES          0.552855 Hz
AQ             0.9044468 sec
RG               18390.4
DW                27.600 usec
DE                 6.00 usec
TE                  0.0 K
D1           2.00000000 sec
d11          0.03000000 sec
DELTA        1.89999998 sec
MCREST       0.00000000 sec
MCWRK        0.01500000 sec

======== CHANNEL f1 ========
NUC1                  13C
P1                   7.75 usec
PL1                  0.00 dB
SFO1          75.4752658 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                  1H
PCPD2              80.00 usec
PL2                 0.00 dB
PL12               17.81 dB
PL13               18.00 dB
SFO2         300.1315007 MHz

F2 - Processing parameters
SI                 32768
SF            75.4677079 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.70
```

Fig 34. 13C NMR spectra of Ethyl 3-(6-(4-methoxyphenyl)-3-phenyl-[1,2,4]triazolo[4,3-b] pyridazin-8-yl) benzoate (**5c**)



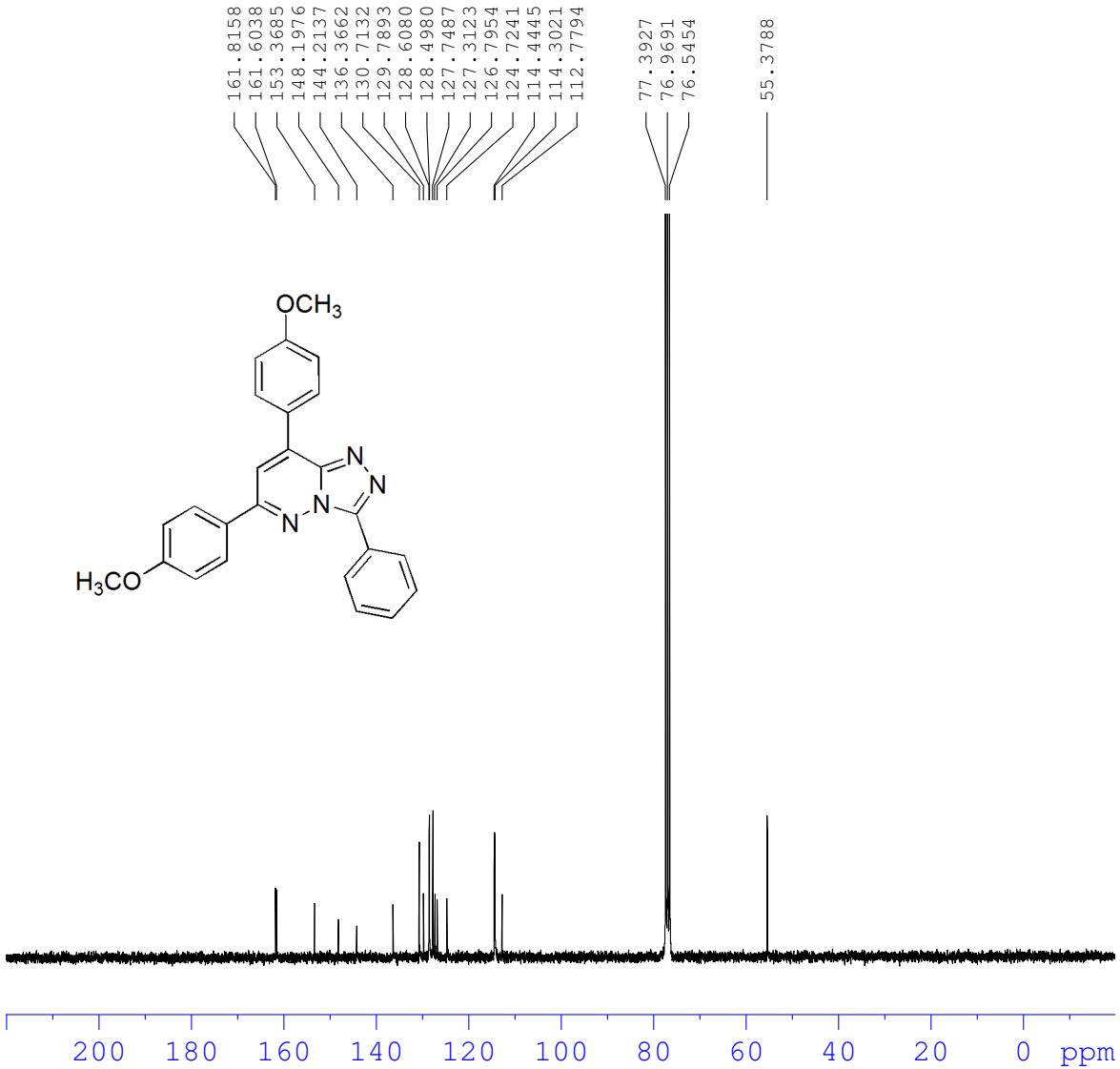

```
Current Data Parameters
NAME      IS10607-058-A911133
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_           20140211 Time
              17.39 INSTRUM
          spect PROBHD   5 mm
DUL BB-1H PULPROG
zg30
TD                      32768
SOLVENT                 CDCl3
NS                          8
DS                          2
SWH                  5995.204 Hz
FIDRES               0.182959 Hz
AQ                  2.7329011 sec
RG                        362
DW                     83.400 usec
DE                      6.00 usec
TE                       0.0 K
D1                 2.00000000 sec
MCREST             0.00000000 sec
MCWRK              0.01500000 sec

======== CHANNEL f1 ========
NUC1                        1H
P1                       14.65 usec
PL1                       0.00 dB
SFO1              300.1318008 MHz

F2 - Processing parameters
SI                      32768
SF                300.1298168 MHz
WDW                        EM
SSB                         0
LB                       0.30 Hz
GB                          0
PC                       1.40
```

Fig 35. 1H NMR spectra of 6,8-bis(4-Methoxyphenyl)-3-phenyl-[1,2,4]triazolo[4,3-b]pyridazine (**5d**)




```
Current Data Parameters
NAME      IS10607-058-A926345
EXPNO                       2
PROCNO                      1

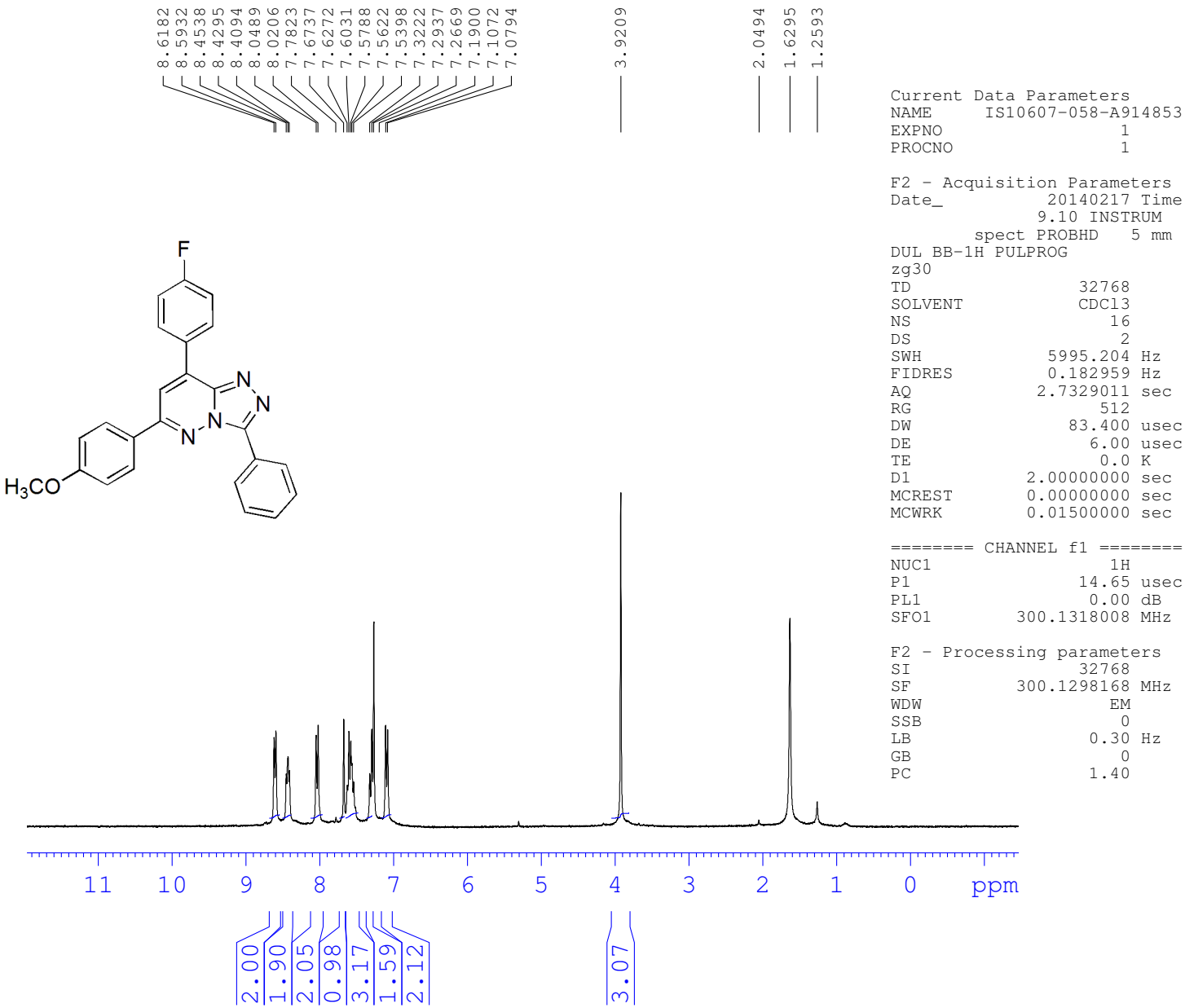
F2 - Acquisition Parameters
Date_            20140228
Time                22.04
INSTRUM             spect
PROBHD    5 mm DUL BB-1H
PULPROG           zgpg30
TD                 32768
SOLVENT            CDCl3
NS                  5000
DS                     0
SWH            18115.941 Hz
FIDRES          0.552855 Hz
AQ             0.9044468 sec
RG                  8192
DW                27.600 usec
DE                 6.00 usec
TE                  0.0 K
D1           2.00000000 sec
d11          0.03000000 sec
DELTA        1.89999998 sec
MCREST       0.00000000 sec
MCWRK        0.01500000 sec

======== CHANNEL f1 ========
NUC1                  13C
P1                   7.75 usec
PL1                  0.00 dB
SFO1          75.4752658 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                  1H
PCPD2              80.00 usec
PL2                 0.00 dB
PL12               17.81 dB
PL13               18.00 dB
SFO2         300.1315007 MHz

F2 - Processing parameters
SI                 32768
SF          75.4677079 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.70
```

Fig 36. 13C NMR spectra of 6,8-bis(4-Methoxyphenyl)-3-phenyl-[1,2,4]triazolo[4,3-b]pyridazine (**5d**)




```
Current Data Parameters
NAME      IS10607-058-A914853
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_           20140217 Time
              9.10 INSTRUM
         spect PROBHD   5 mm
DUL BB-1H PULPROG
zg30
TD                  32768
SOLVENT             CDCl3
NS                     16
DS                      2
SWH              5995.204 Hz
FIDRES           0.182959 Hz
AQ               2.7329011 sec
RG                    512
DW                 83.400 usec
DE                  6.00 usec
TE                   0.0 K
D1            2.00000000 sec
MCREST        0.00000000 sec
MCWRK         0.01500000 sec

======== CHANNEL f1 ========
NUC1                   1H
P1                 14.65 usec
PL1                 0.00 dB
SFO1         300.1318008 MHz

F2 - Processing parameters
SI                  32768
SF           300.1298168 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   1.40
```

Fig 37. 1H NMR spectra of 8-(4-Fluorophenyl)-6-(4-methoxyphenyl)-3-phenyl-[1,2,4]triazolo[4,3-b]pyridazine (**5e**)

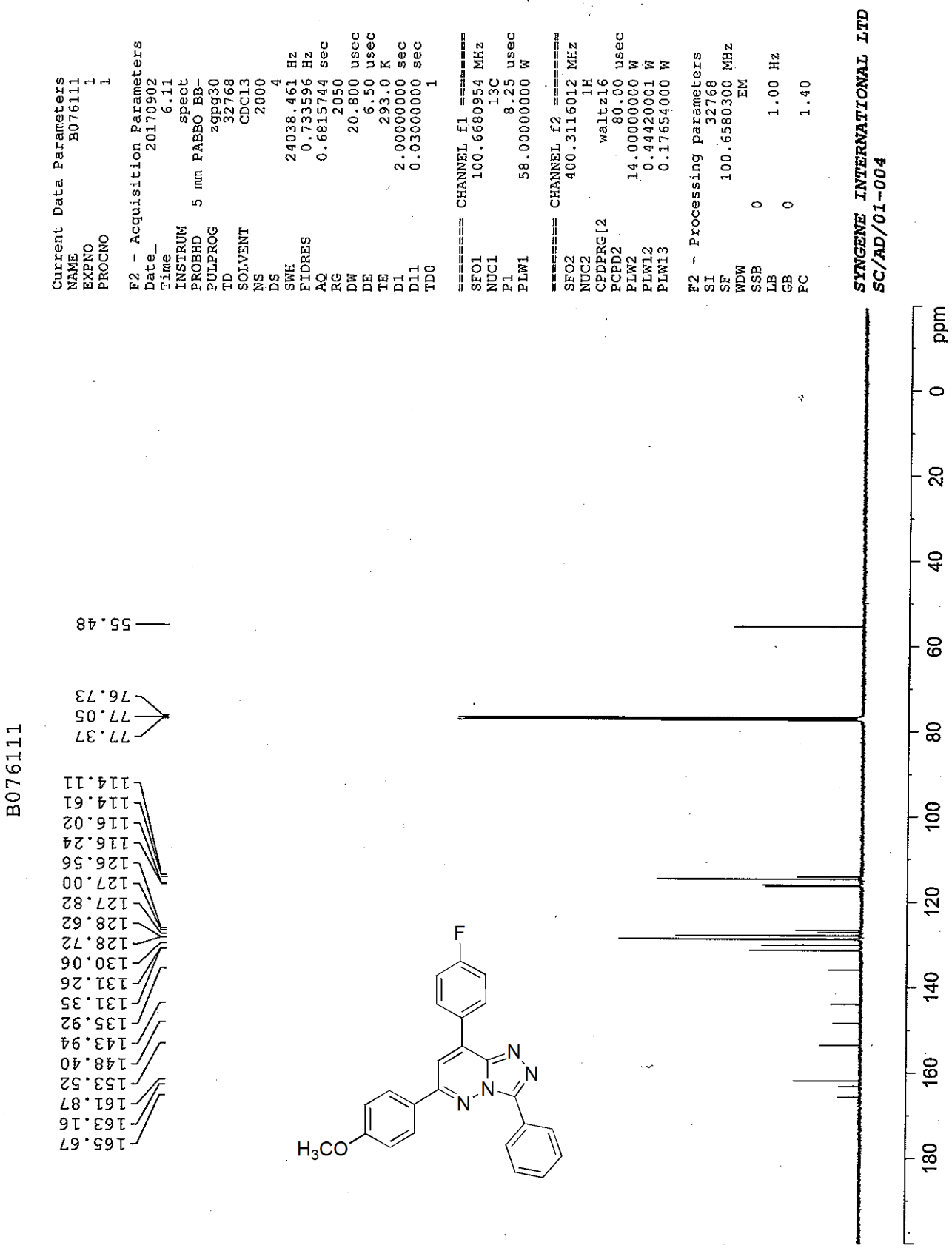


Fig 38. 13C NMR spectra of 8-(4-Fluorophenyl)-6-(4-methoxyphenyl)-3-phenyl-[1,2,4]triazolo[4,3-b] pyridazine (5e)

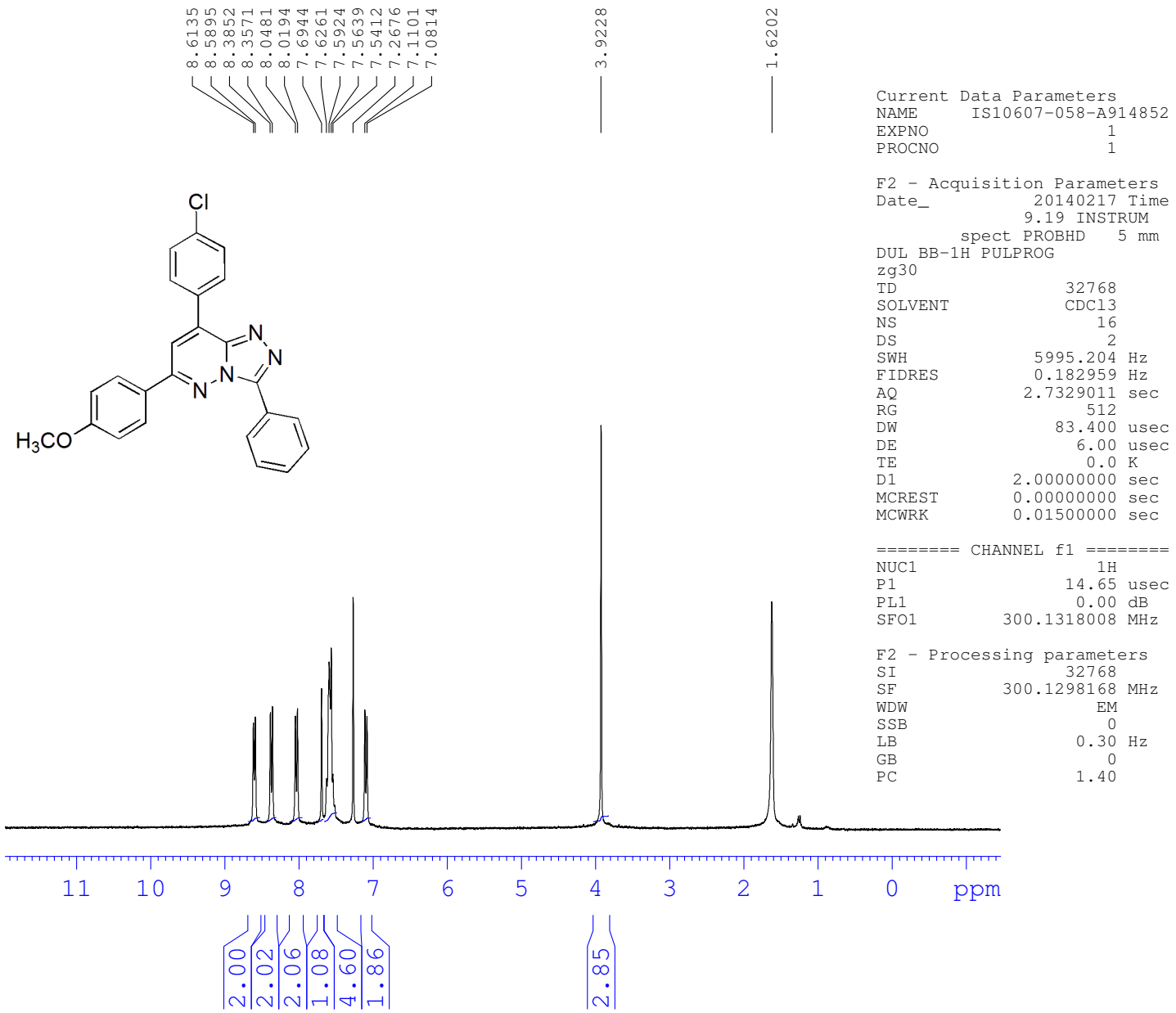
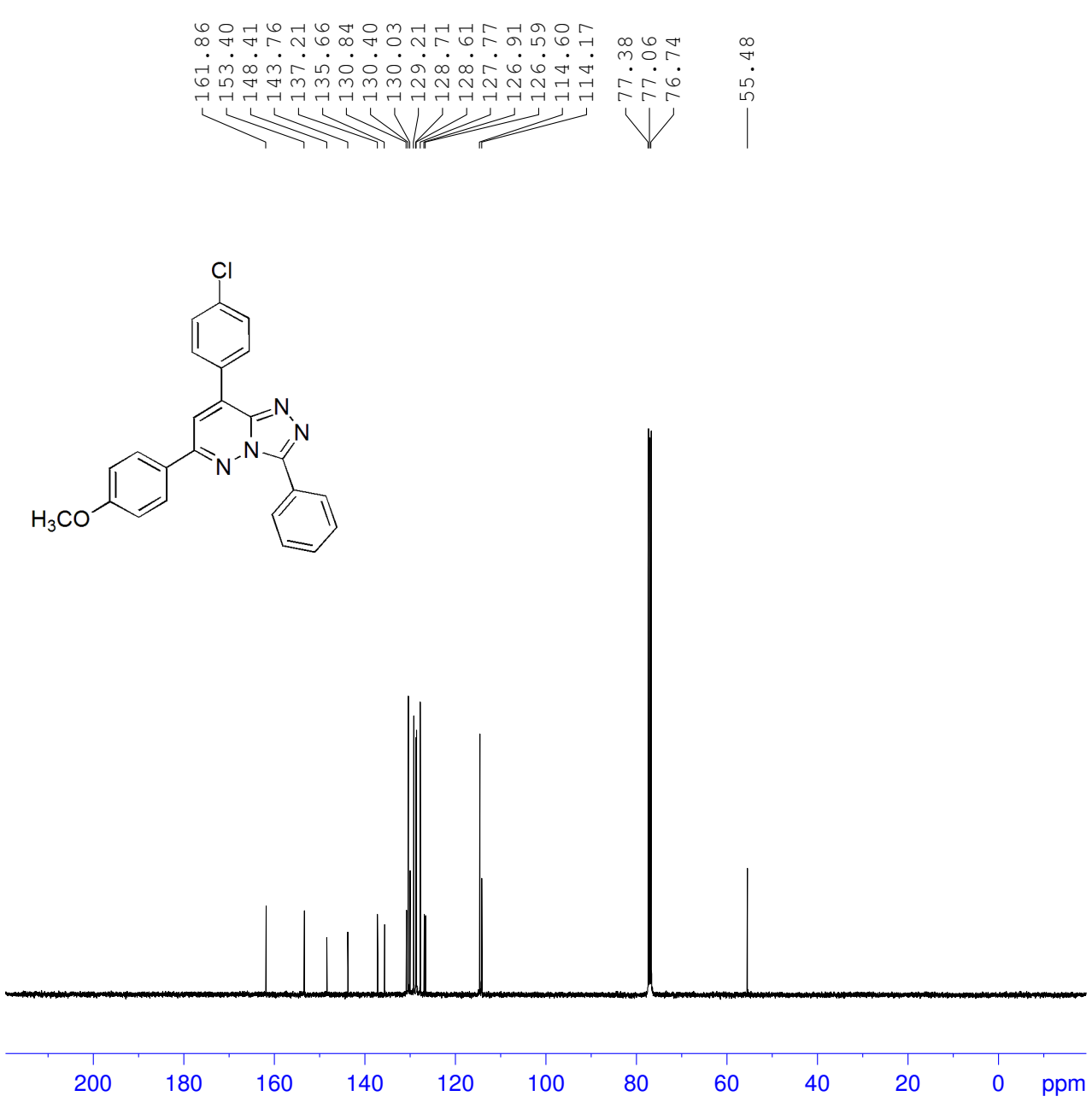


Fig 39. 1H NMR spectra of 8-(4-Chlorophenyl)-6-(4-methoxyphenyl)-3-phenyl-[1,2,4]triazolo[4,3-b] pyridazine (**5f**)

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NAME      IS10607-058-A926344
EXPNO                       2
PROCNO                      1
Date_              20140303
Time                    8.21
INSTRUM                spect
PROBHD   5 mm DUL 13C-1
PULPROG             zgpg30
TD                   32768
SOLVENT              CDCl3
NS                     965
DS                       4
SWH             24038.461 Hz
FIDRES           0.733596 Hz
AQ               0.6816244 sec
RG                    2050
DW                  20.800 usec
DE                   6.50 usec
TE                  293.0 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                   13C
P1                    9.55 usec
PL1                  -0.50 dB
PL1W          40.58471298 W
SFO1         100.6680954 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                   1H
PCPD2               100.00 usec
PL2                  -2.00 dB
PL12                 16.24 dB
PL13                 17.00 dB
PL2W          15.00864029 W
PL12W          0.22508231 W
PL13W          0.18894759 W
SFO2         400.3116012 MHz
SI                   32768
SF           100.6580300 MHz
WDW                    EM
SSB                     0
LB                   1.00 Hz
GB                      0
PC                   1.40
```

Fig 40. 13C NMR spectra of 8-(4-Chlorophenyl)-6-(4-methoxyphenyl)-3-phenyl-[1,2,4]triazolo[4,3-b] pyridazine (**5f**)

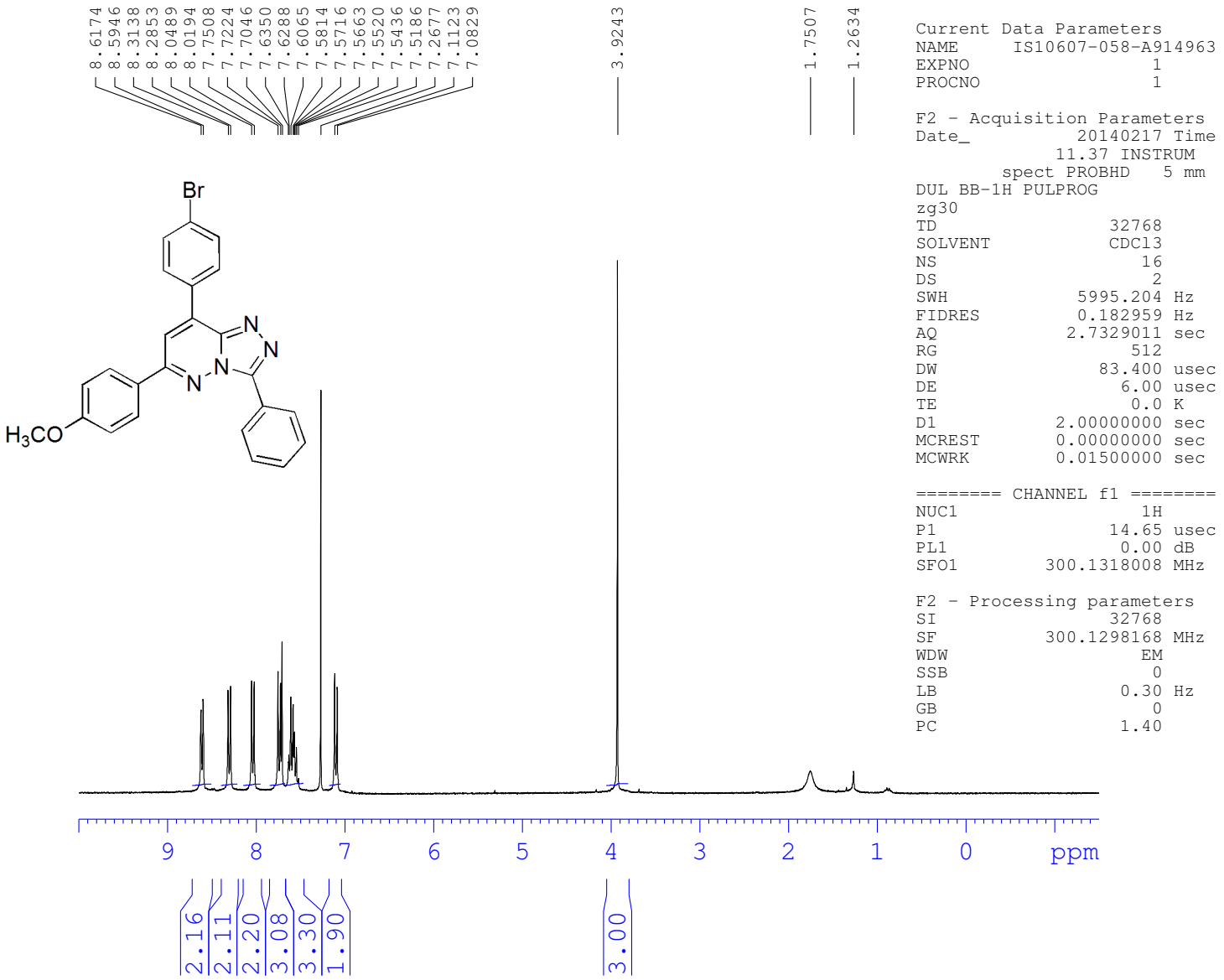


Fig 41. 1H NMR spectra of 8-(4-Bromophenyl)-6-(4-methoxyphenyl)-3-phenyl-[1,2,4]triazolo[4,3-b] pyridazine (**5g**)

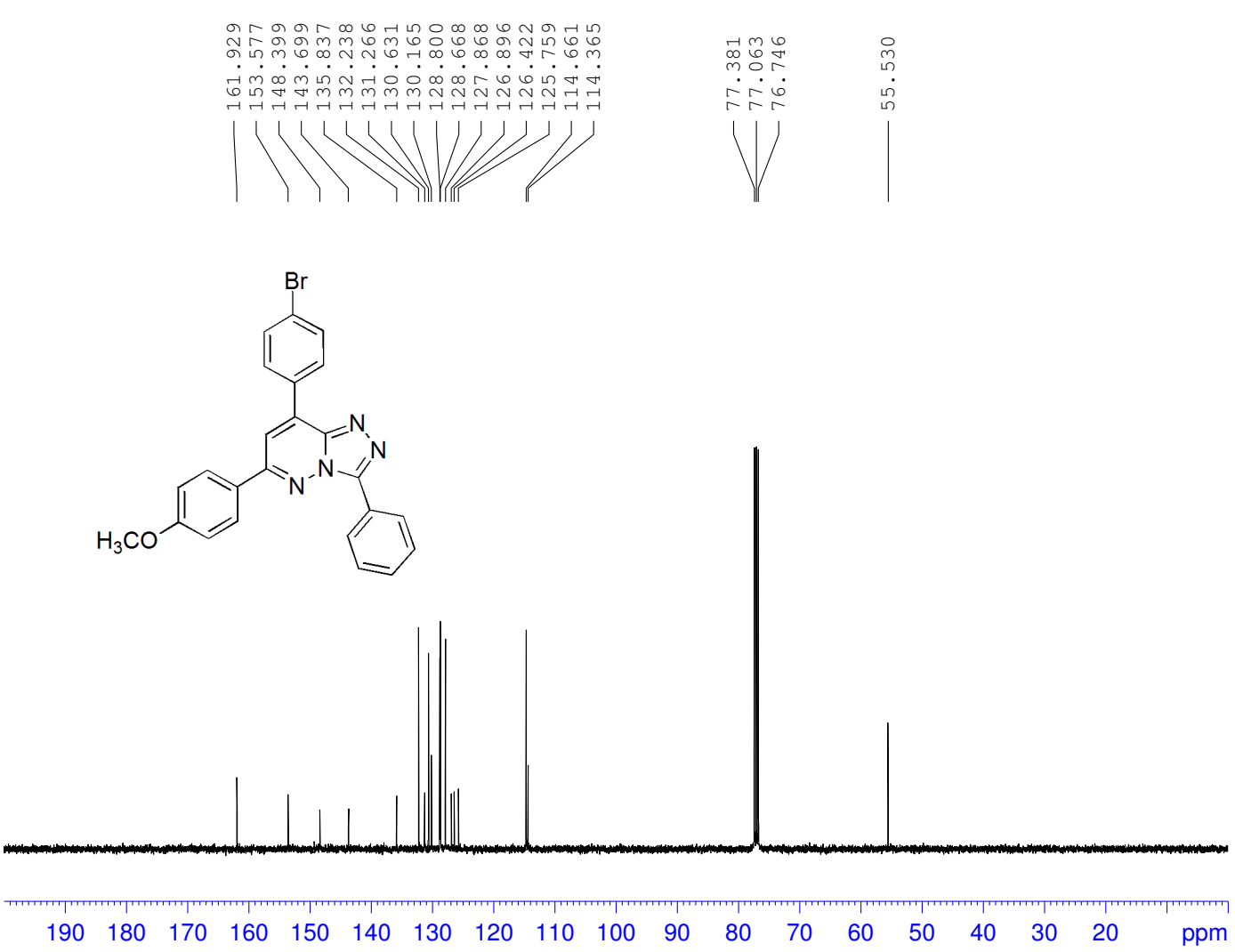


Fig 42. 13C NMR spectra of 8-(4-Bromophenyl)-6-(4-methoxyphenyl)-3-phenyl-[1,2,4]triazolo[4,3-b] pyridazine (**5g**)

```
Current Data Parameters
NAME      IS10607-058-A929348
EXPNO                       2
PROCNO                      1

F2 - Acquisition Parameters
Date_            20140306
Time                10.37
INSTRUM             spect
PROBHD    5 mm PABBO BB-
PULPROG           zgpg30
TD                 32768
SOLVENT            CDCl3
NS                   423
DS                     2
SWH            24038.461 Hz
FIDRES          0.733596 Hz
AQ             0.6816244 sec
RG                    57
DW                20.800 usec
DE                 6.00 usec
TE                295.7 K
D1            2.00000000 sec
d11           0.03000000 sec
DELTA         1.89999998 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  13C
P1                 8.15 usec
PL1               -2.00 dB
SFO1         100.6839383 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2              80.00 usec
PL2                -2.00 dB
PL12               13.30 dB
PL13               15.50 dB
SFO2         400.3746015 MHz

F2 - Processing parameters
SI                 32768
SF           100.6738710 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

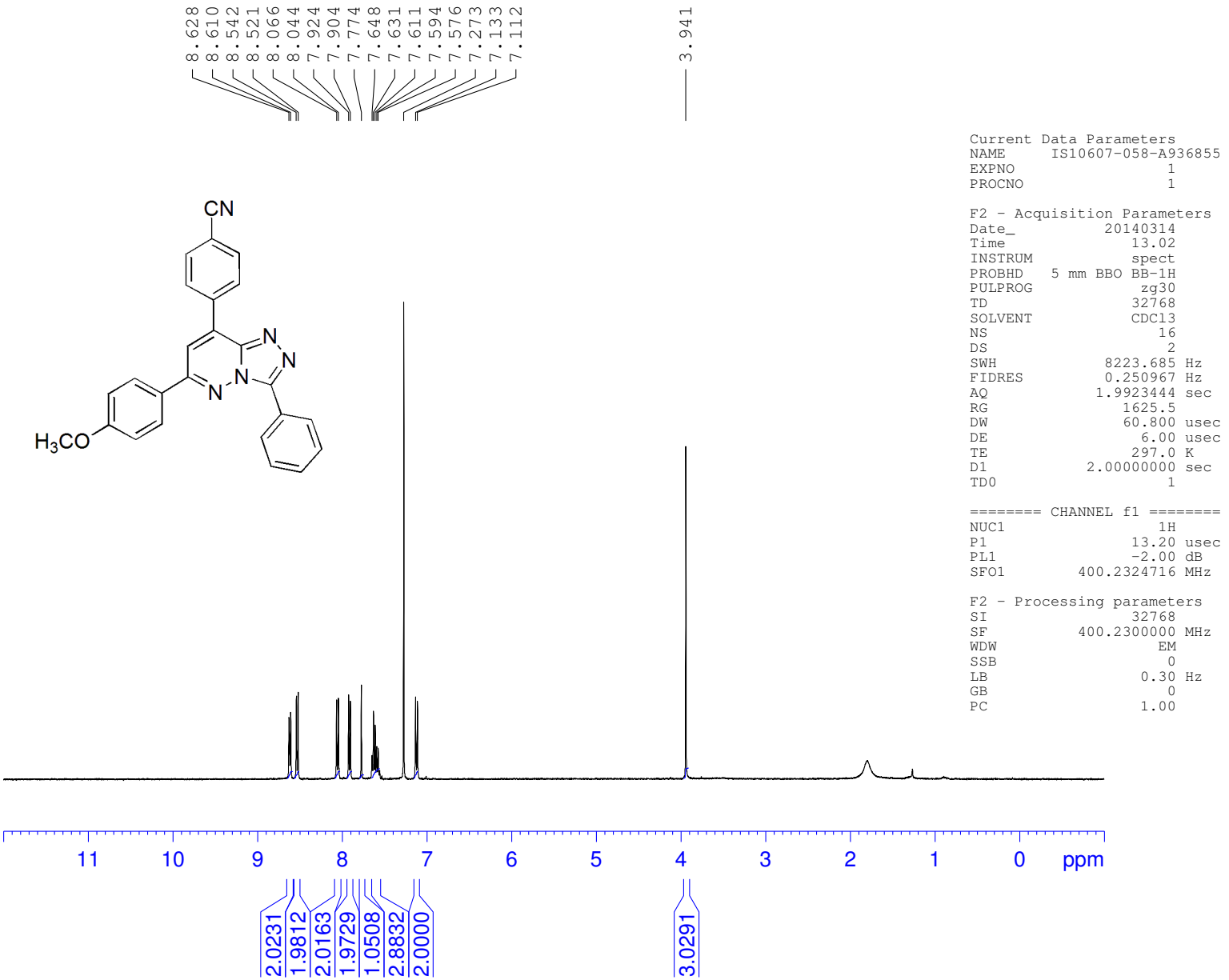


Fig 43. 1H NMR spectra of 4-(6-(4-Methoxyphenyl)-3-phenyl-[1,2,4]triazolo[4,3-b]pyridazin-8-yl) benzonitrile (**5h**)

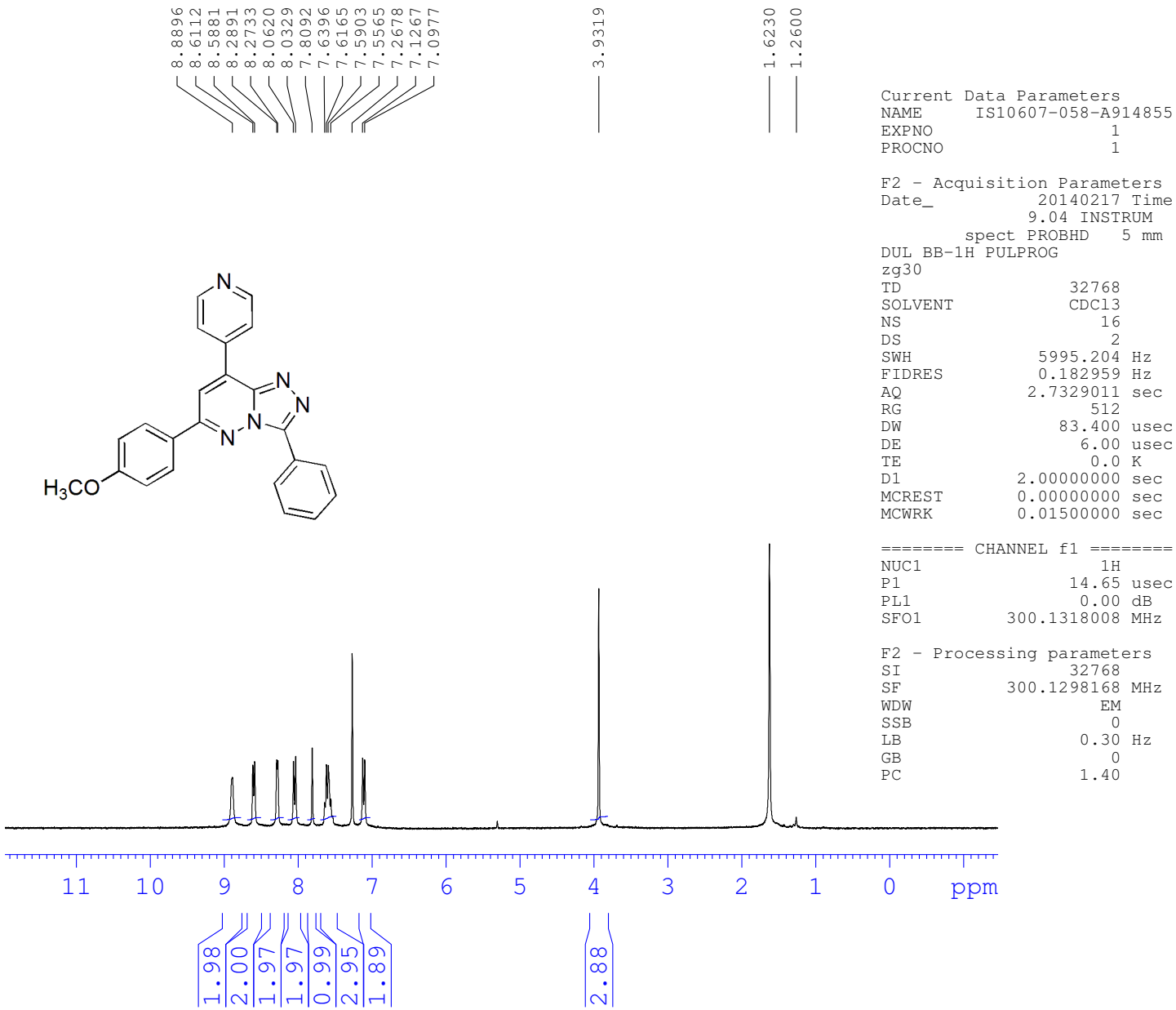
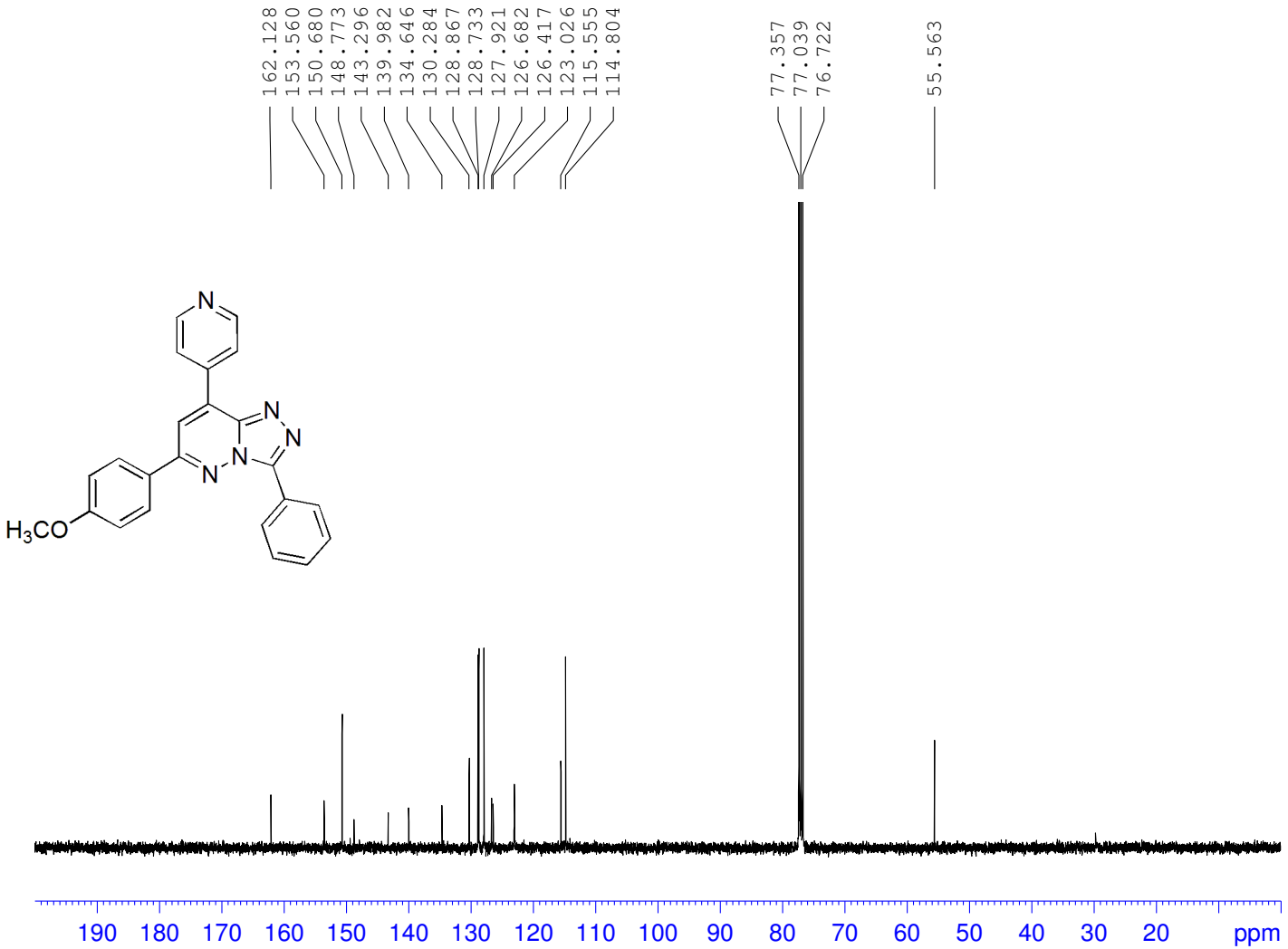


Fig 44. 1H NMR spectra of 6-(4-Methoxyphenyl)-3-phenyl-8-(pyridin-4-yl)-[1,2,4]triazolo[4,3-b]pyridazine (**5i**)

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Current Data Parameters
NAME      IS10607-058-A929350
EXPNO                       2
PROCNO                      1

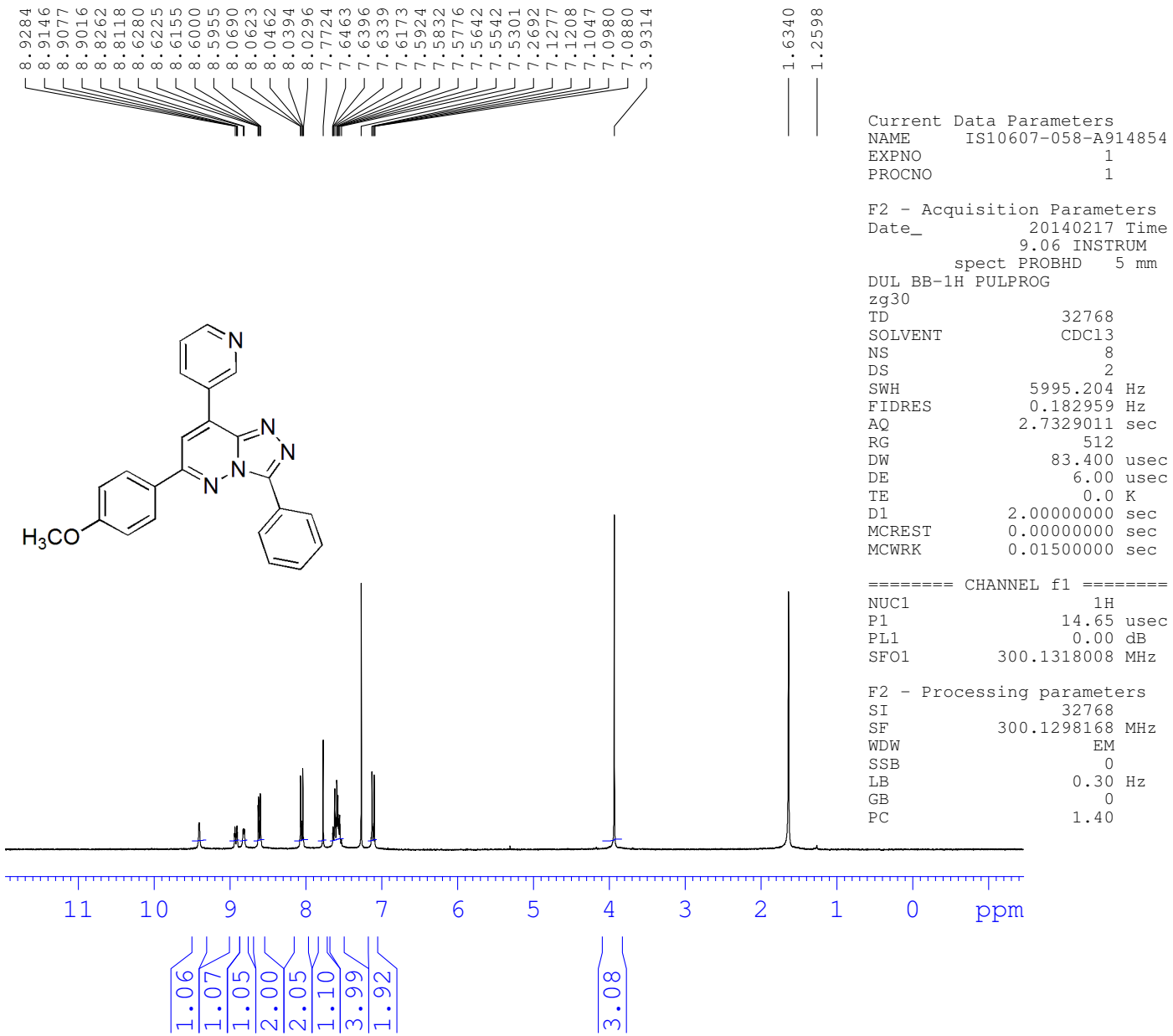
F2 - Acquisition Parameters
Date_            20140306
Time                12.34
INSTRUM             spect
PROBHD    5 mm PABBO BB-
PULPROG           zgpg30
TD                 32768
SOLVENT            CDCl3
NS                  1024
DS                     2
SWH           24038.461 Hz
FIDRES         0.733596 Hz
AQ            0.6816244 sec
RG                  45.2
DW                20.800 usec
DE                 6.00 usec
TE                296.8 K
D1           2.00000000 sec
d11          0.03000000 sec
DELTA        1.89999998 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  13C
P1                   8.15 usec
PL1                 -2.00 dB
SFO1         100.6839383 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                  1H
PCPD2              80.00 usec
PL2                -2.00 dB
PL12               13.30 dB
PL13               15.50 dB
SFO2         400.3746015 MHz

F2 - Processing parameters
SI                 32768
SF           100.6738710 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

Fig 45. 13C NMR spectra of 6-(4-Methoxyphenyl)-3-phenyl-8-(pyridin-4-yl)-[1,2,4]triazolo[4,3-b] pyridazine (**5i**)




```
Current Data Parameters
NAME      IS10607-058-A914854
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_           20140217 Time
              9.06 INSTRUM
          spect PROBHD   5 mm
DUL BB-1H PULPROG
zg30
TD                  32768
SOLVENT             CDCl3
NS                      8
DS                      2
SWH              5995.204 Hz
FIDRES           0.182959 Hz
AQ               2.7329011 sec
RG                    512
DW                 83.400 usec
DE                  6.00 usec
TE                   0.0 K
D1             2.00000000 sec
MCREST         0.00000000 sec
MCWRK          0.01500000 sec

======== CHANNEL f1 ========
NUC1                   1H
P1                  14.65 usec
PL1                  0.00 dB
SFO1         300.1318008 MHz

F2 - Processing parameters
SI                  32768
SF           300.1298168 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   1.40
```

Fig 46. 1H NMR spectra of 6-(4-Methoxyphenyl)-3-phenyl-8-(pyridin-3-yl)-[1,2,4]triazolo[4,3-b]pyridazine (**5j**)

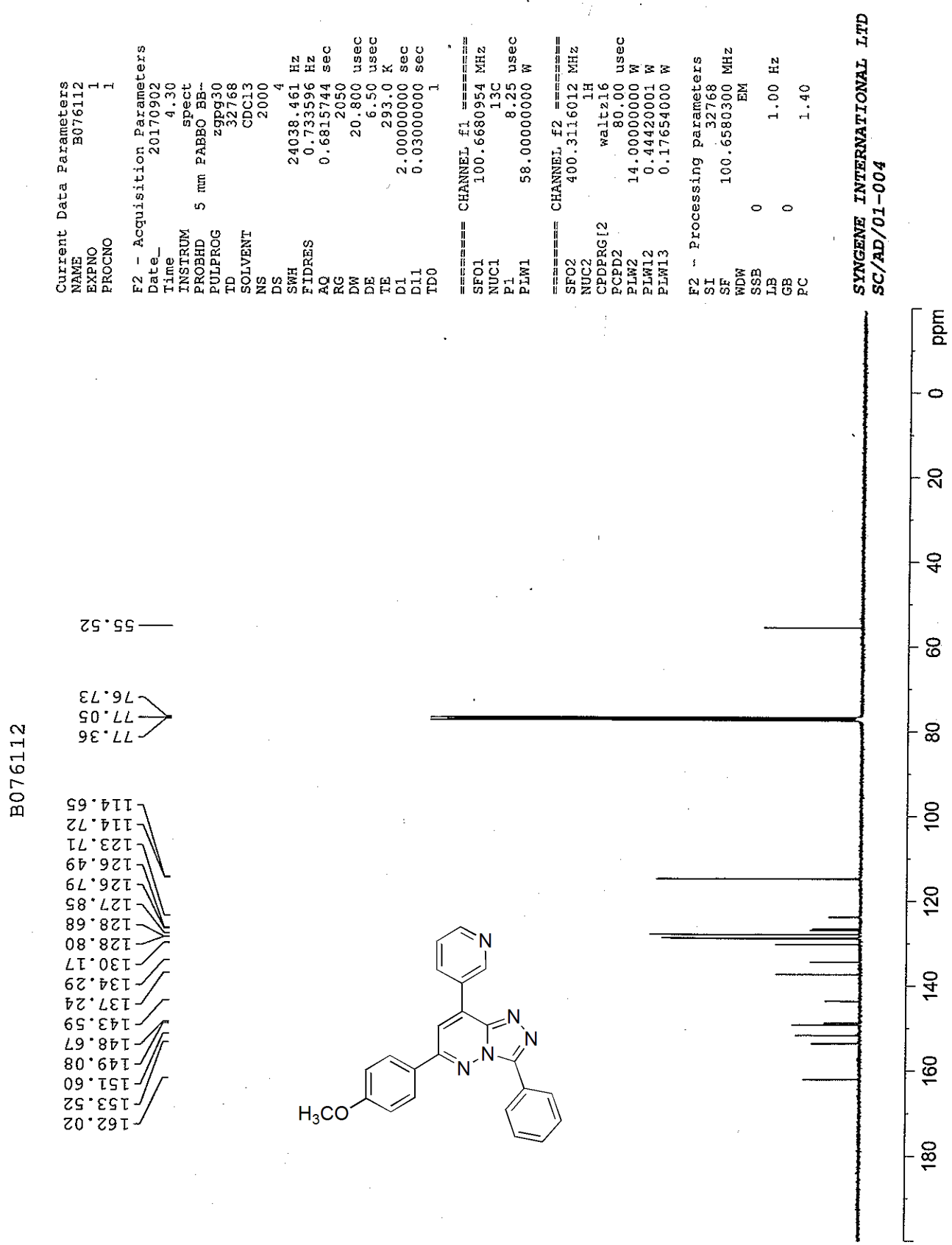


Fig 47. 13C NMR spectra of 6-(4-Methoxyphenyl)-3-phenyl-8-(pyridin-3-yl)-[1,2,4]triazolo[4,3-b] pyridazine (5j)

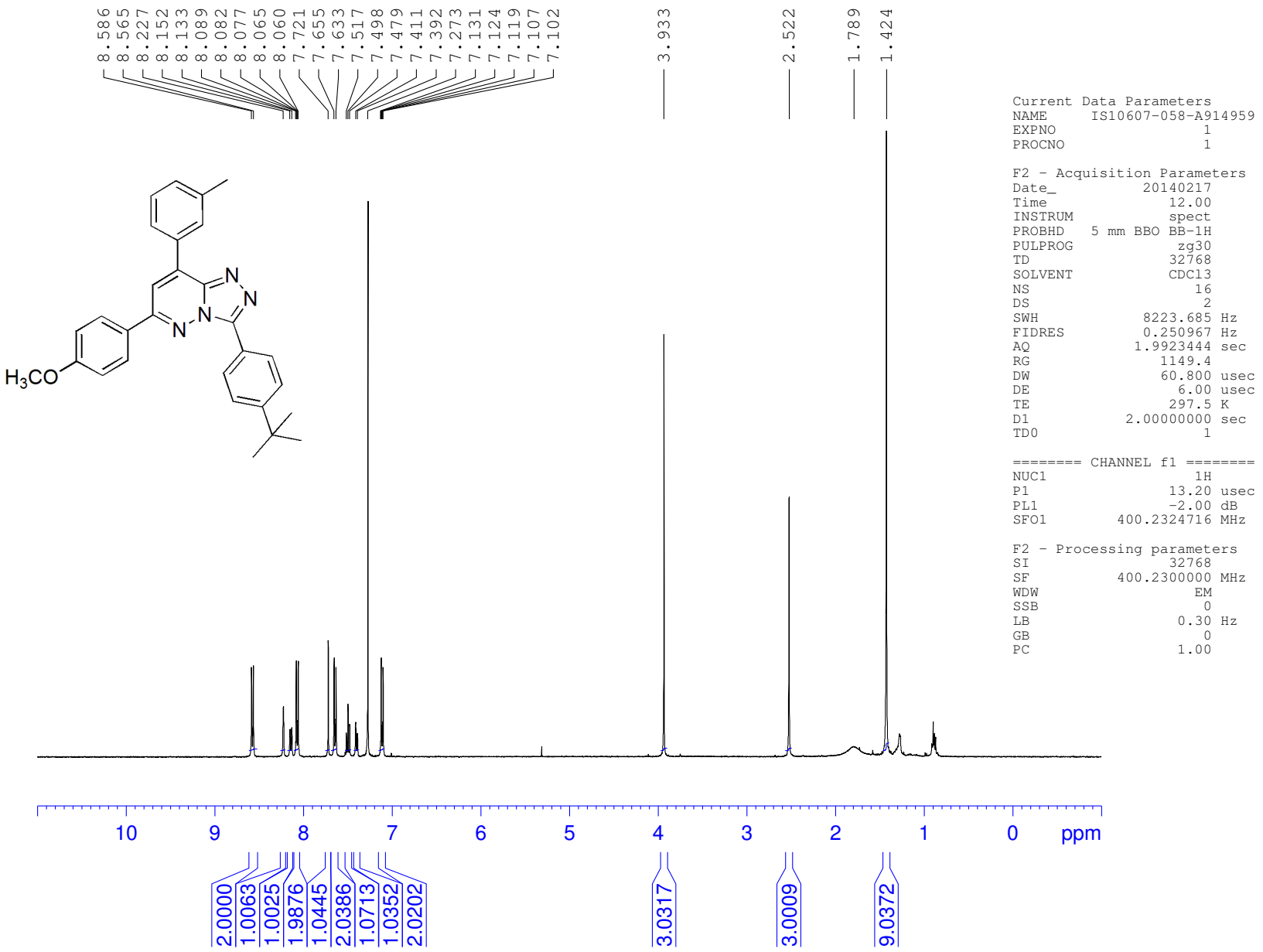
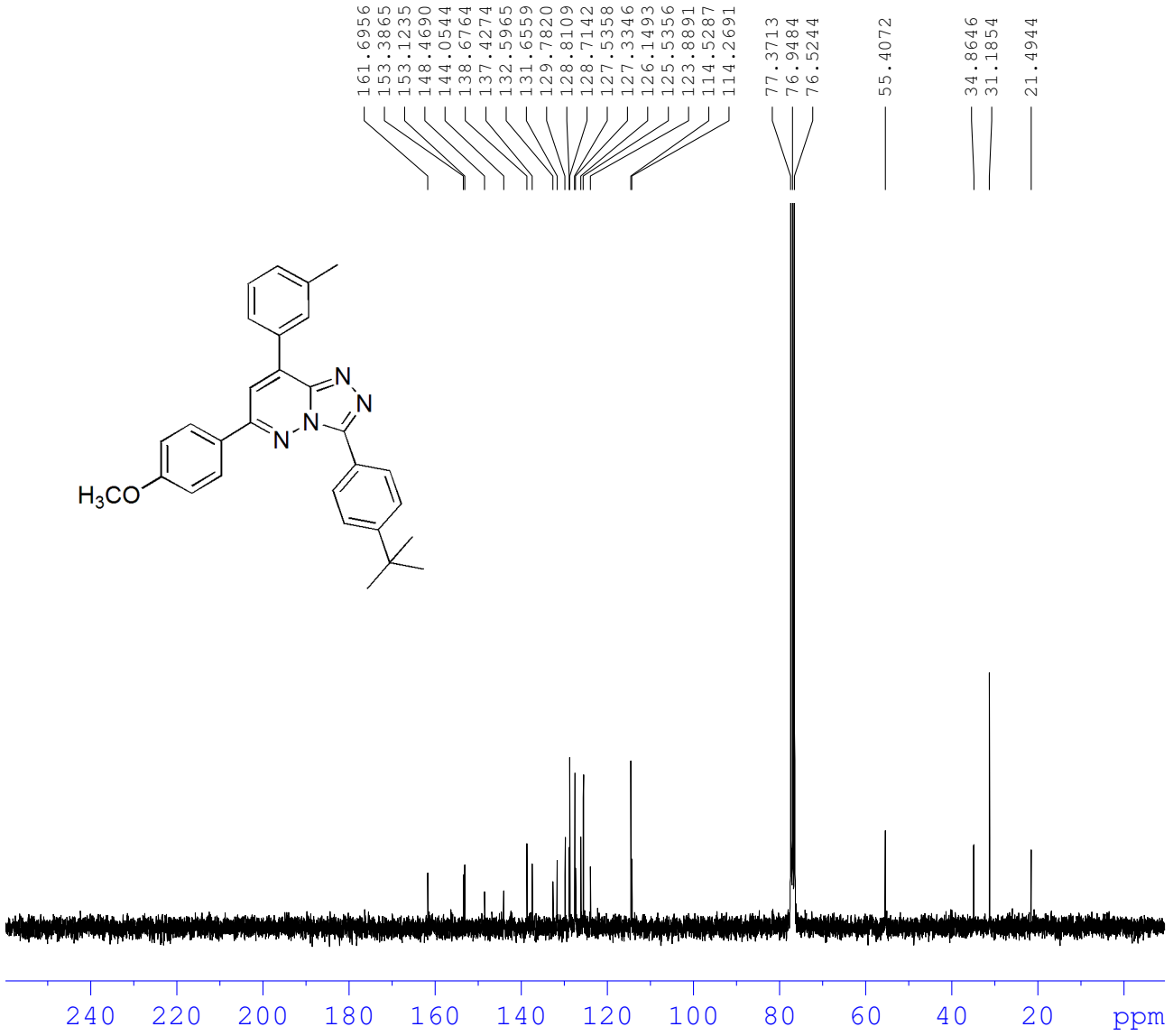


Fig 48. 1H NMR spectra of 3-(4-tert-Butylphenyl)-6-(4-methoxyphenyl)-8-m-tolyl-[1,2,4]triazolo[4,3-b] pyridazine (**7a**)

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NAME      IS_S11042_96_A155005
EXPNO                    2
PROCNO                   1

F2 - Acquisition Parameters
Date_           20141209
Time              23.52
INSTRUM           spect
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PULPROG          zgpg30
TD                32768
SOLVENT           CDCl3
NS                 2500
DS                    0
SWH           20325.203 Hz
FIDRES         0.620276 Hz
AQ            0.8061428 sec
RG                16384
DW               24.600 usec
DE                6.00 usec
TE                 0.0 K
D1           2.00000000 sec
d11          0.03000000 sec
DELTA        1.89999998 sec
MCREST       0.00000000 sec
MCWRK        0.01500000 sec

======== CHANNEL f1 ========
NUC1                13C
P1                 8.50 usec
PL1                0.00 dB
SFO1         75.4771525 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                1H
PCPD2             80.00 usec
PL2                0.00 dB
PL12              14.75 dB
PL13              18.00 dB
SFO2        300.1315007 MHz

F2 - Processing parameters
SI                 32768
SF           75.4677079 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.70
```

Fig 49. 13C NMR spectra of 3-(4-tert-Butylphenyl)-6-(4-methoxyphenyl)-8-m-tolyl-[1,2,4]triazolo[4,3-b] pyridazine (**7a**)

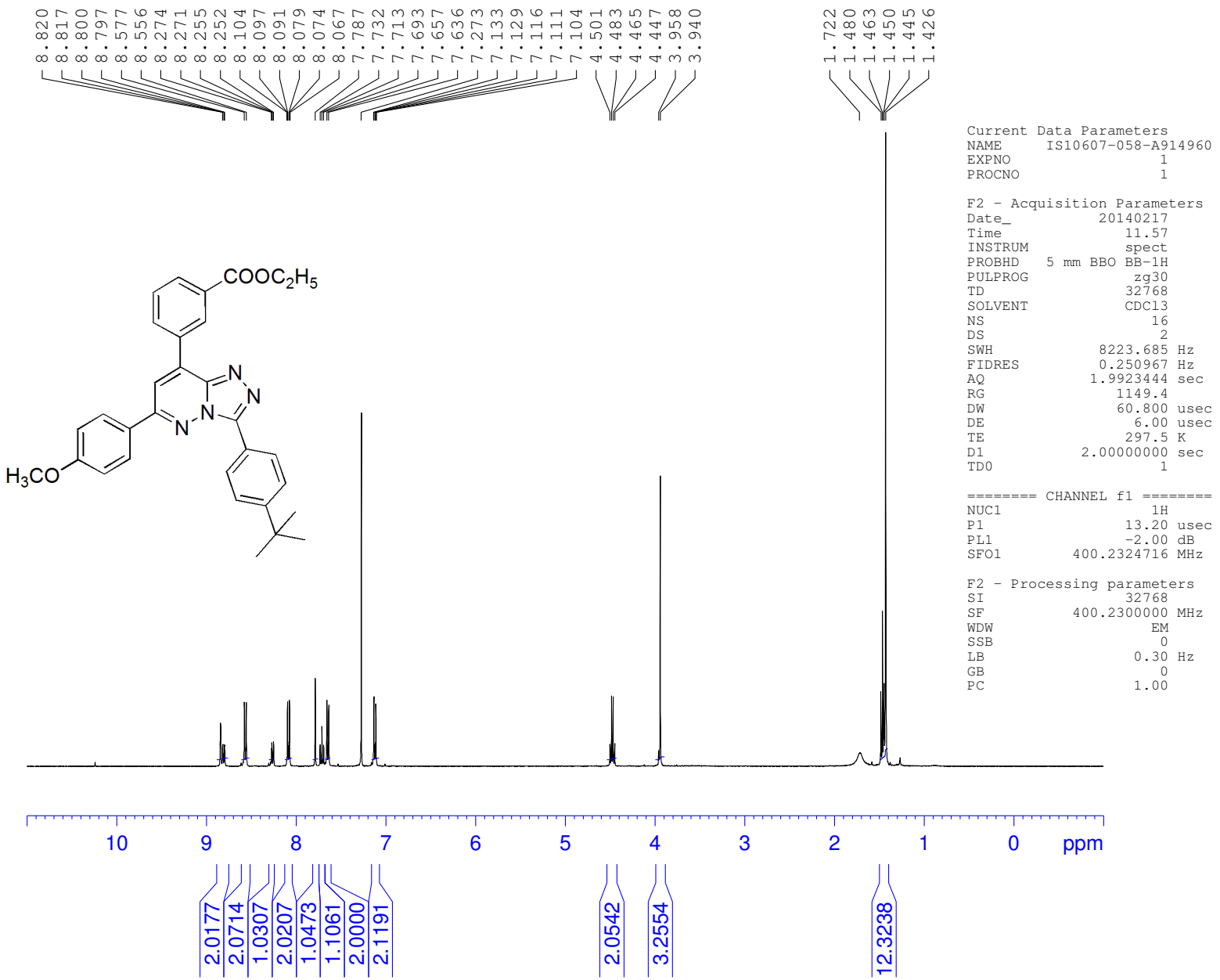


Fig 50. 1H NMR spectra of Ethyl 3-(3-(4-tert-butylphenyl)-6-(4-methoxyphenyl)-[1,2,4]triazolo[4,3-b] pyridazin-8-yl)benzoate (**7b**)

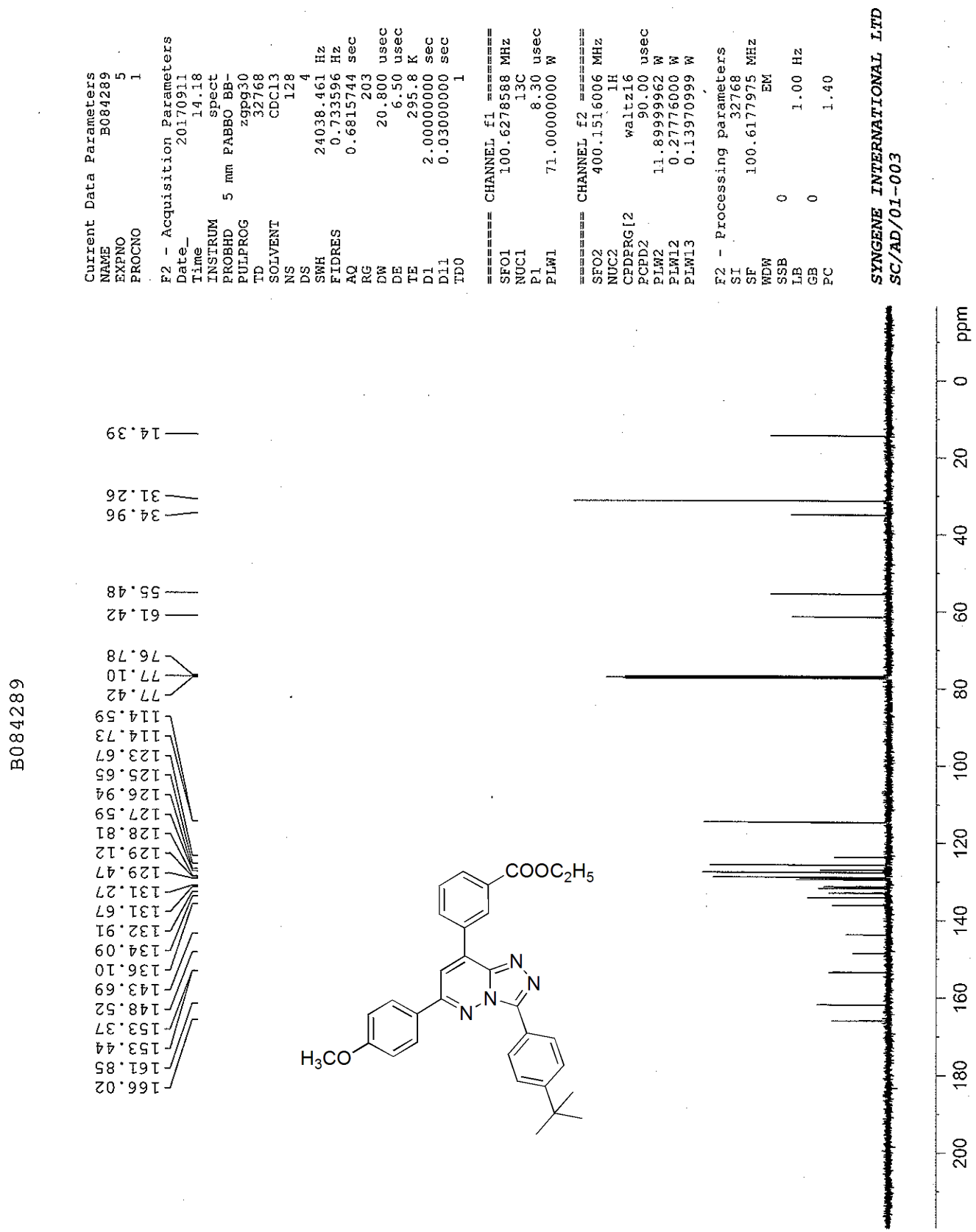
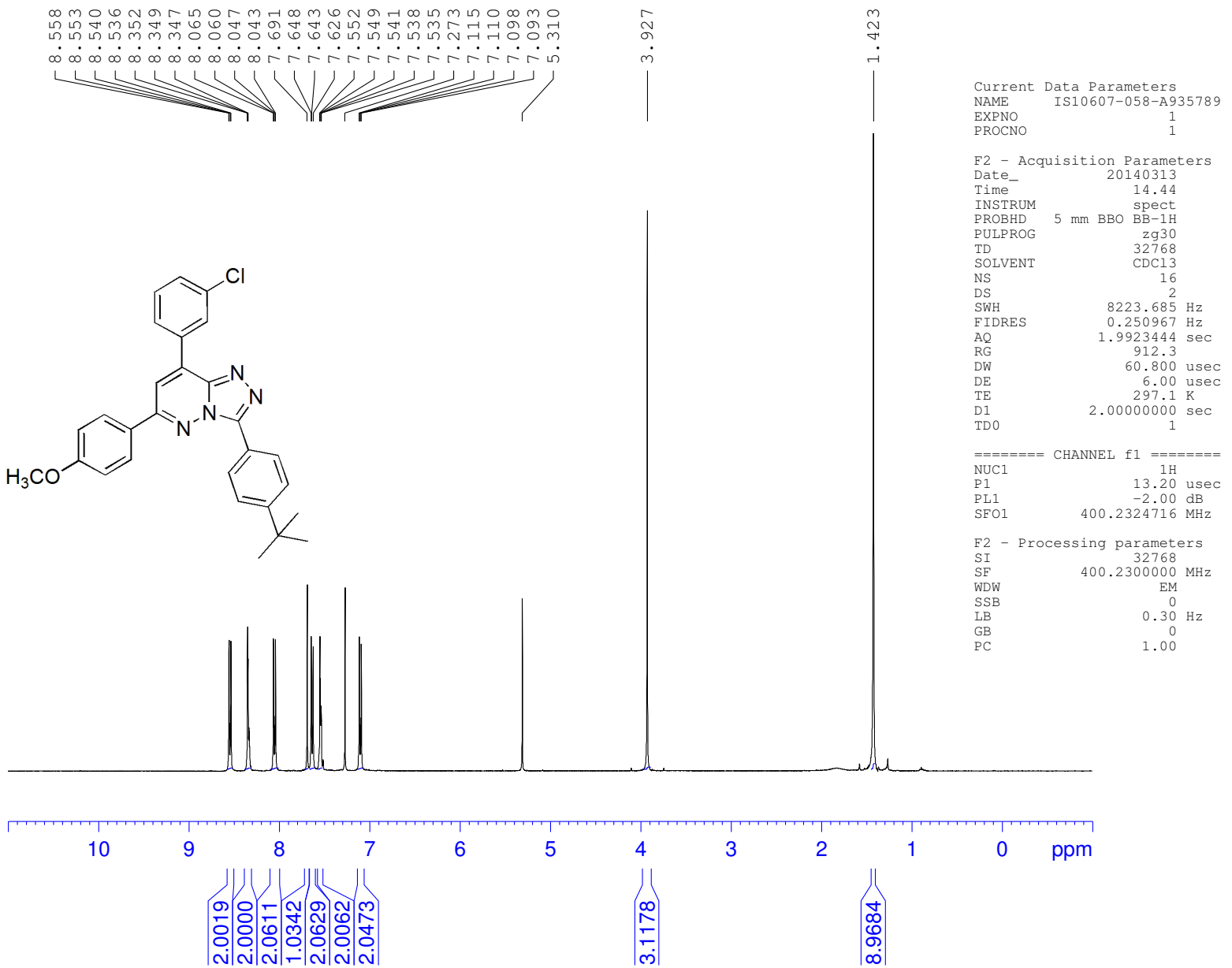


Fig 51. 13C NMR spectra of Ethyl 3-(3-(4-tert-butylphenyl)-6-(4-methoxyphenyl)-[1,2,4]triazolo[4,3-b] pyridazin-8-yl)benzoate (7b)

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Current Data Parameters
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EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
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Time               14.44
INSTRUM            spect
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PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8223.685 Hz
FIDRES          0.250967 Hz
AQ             1.9923444 sec
RG                 912.3
DW                60.800 usec
DE                 6.00 usec
TE                297.1 K
D1            2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                   1H
P1                 13.20 usec
PL1                -2.00 dB
SFO1         400.2324716 MHz

F2 - Processing parameters
SI                 32768
SF           400.2300000 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

Fig 52. 1H NMR spectra of 3-(4-tert-Butylphenyl)-8-(3-chlorophenyl)-6-(4-methoxyphenyl) [1,2,4]triazolo [4,3-b]pyridazine (**7c**)

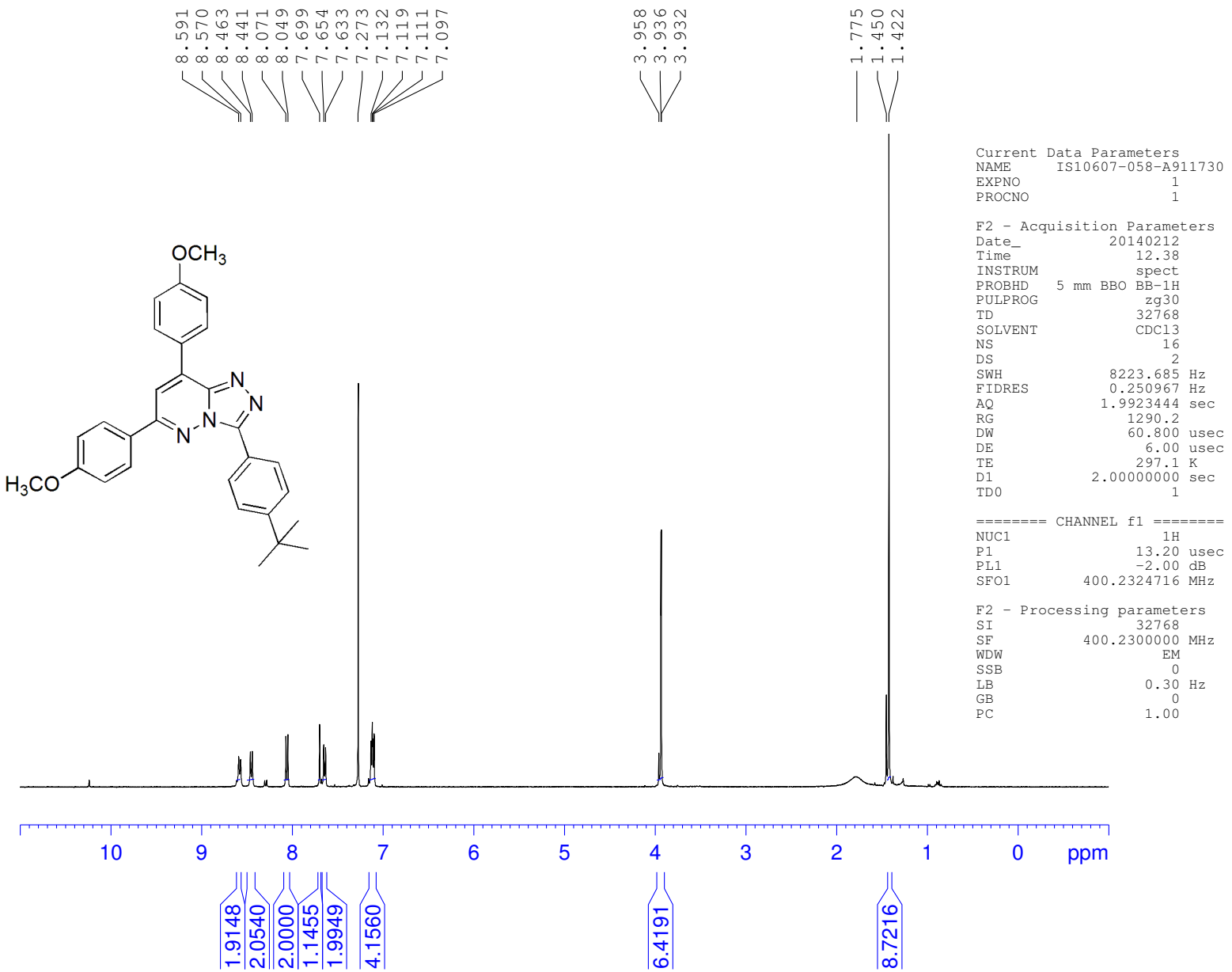


Fig 53. 1H NMR spectra of 3-(4-tert-Butylphenyl)-6,8-bis(4-methoxyphenyl)-[1,2,4]triazolo[4,3-b] pyridazine (**7d**)

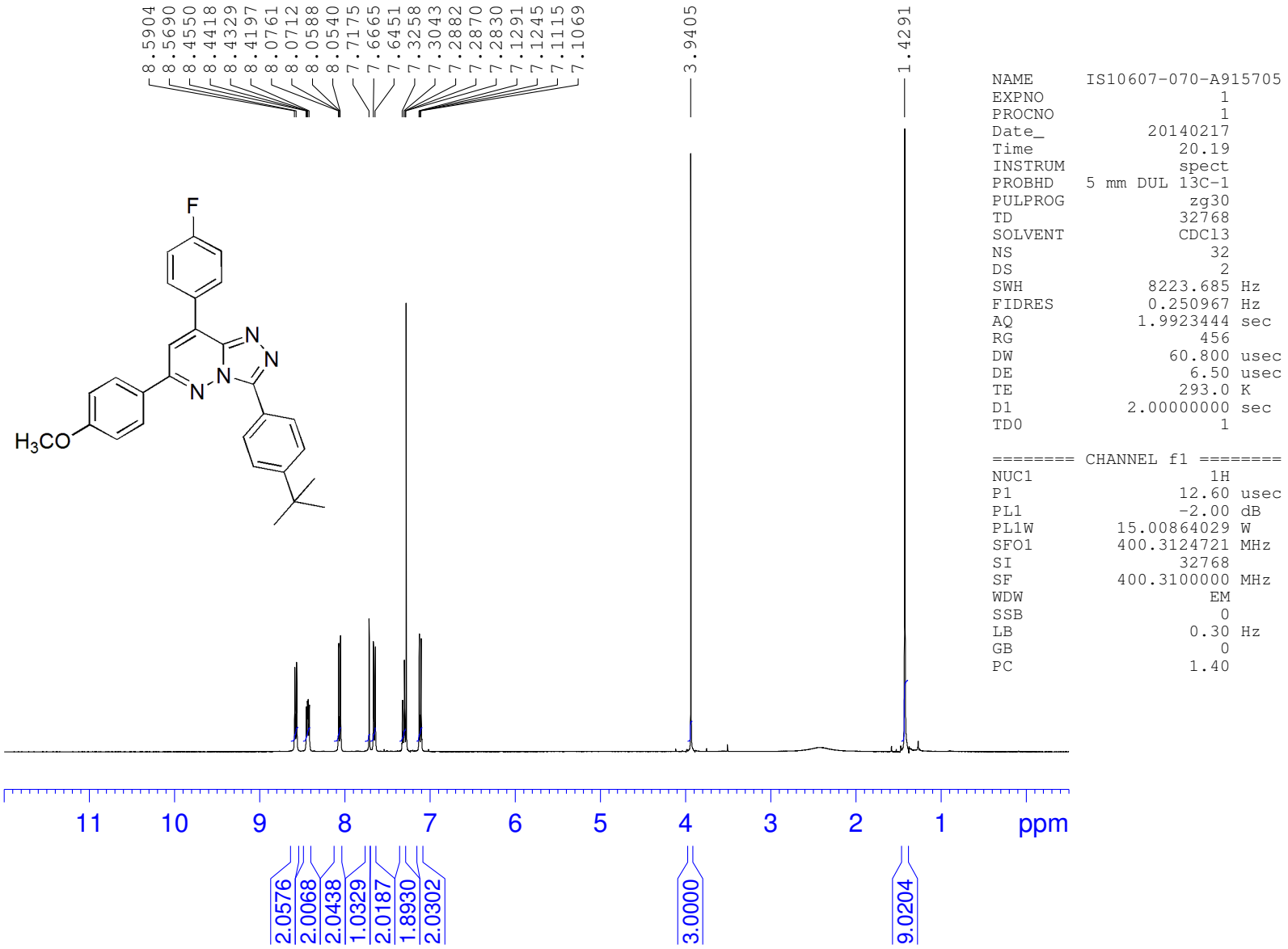
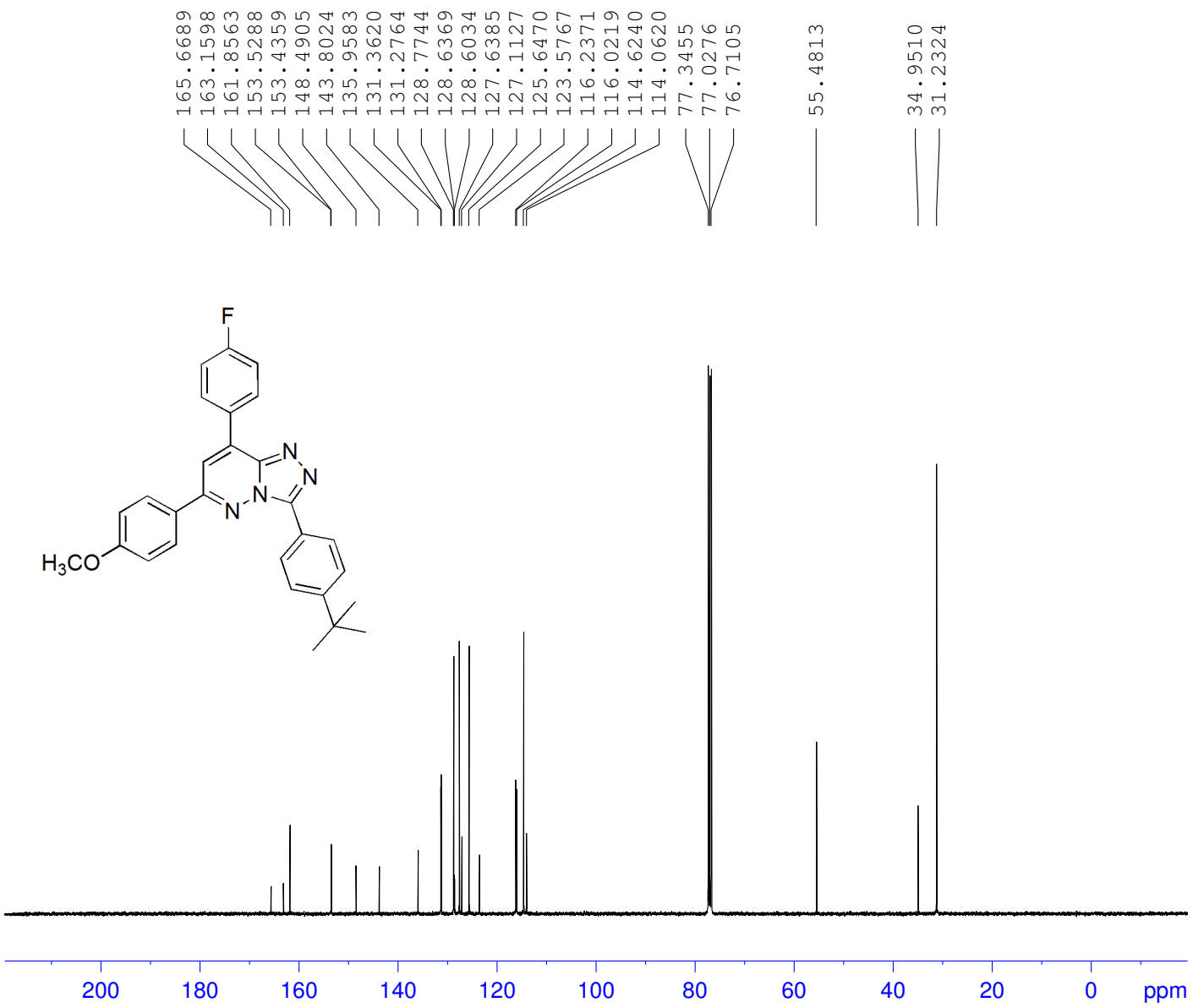


Fig 54. 1H NMR spectra of 3-(4-tert-Butylphenyl)-8-(4-fluorophenyl)-6-(4-methoxyphenyl)-[1,2,4]triazolo [4,3-b]pyridazine (**7e**)




```
Current Data Parameters
NAME      FS10607-078-A916855
EXPNO                       2
PROCNO                      1

F2 - Acquisition Parameters
Date_            20140219
Time                 6.35
INSTRUM             spect
PROBHD    5 mm PABBO BB-
PULPROG            zgpg30
TD                  65536
SOLVENT             CDCl3
NS                   3000
DS                      4
SWH             24038.461 Hz
FIDRES           0.366798 Hz
AQ               1.3631988 sec
RG                    228
DW                 20.800 usec
DE                  6.00 usec
TE                 297.6 K
D1              2.00000000 sec
d11             0.03000000 sec
DELTA           1.89999998 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                   13C
P1                    8.10 usec
PL1                  -3.00 dB
SFO1          100.6278593 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                   1H
PCPD2               80.00 usec
PL12                14.04 dB
PL13                15.00 dB
PL2                 -0.50 dB
SFO2          400.1516006 MHz

F2 - Processing parameters
SI                   32768
SF            100.6177980 MHz
WDW                     EM
SSB                      0
LB                    1.00 Hz
GB                       0
PC                    1.40
```

Fig 55. 13C NMR spectra of 3-(4-tert-Butylphenyl)-8-(4-fluorophenyl)-6-(4-methoxyphenyl)-[1,2,4]triazolo [4,3-b]pyridazine (**7e**)

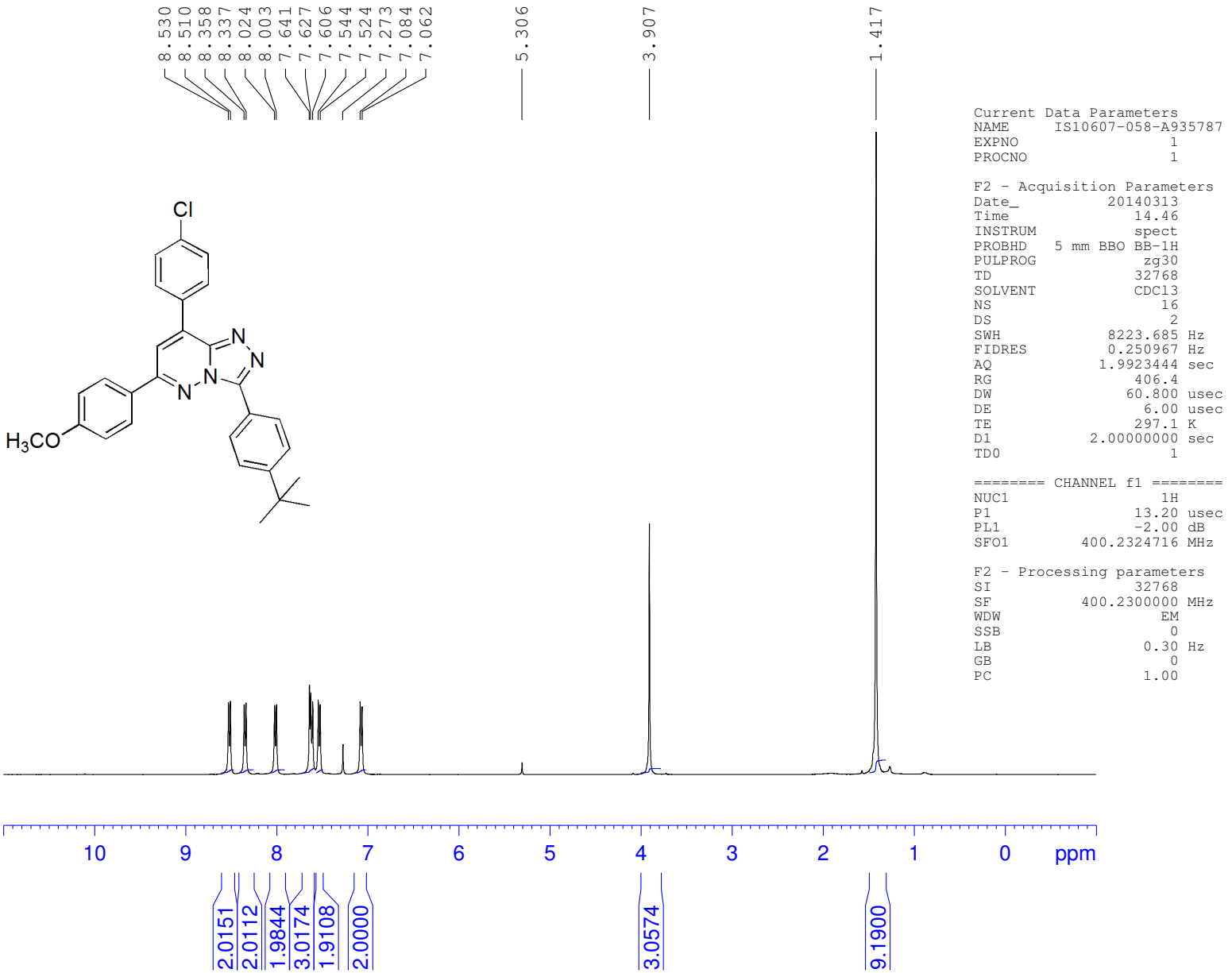
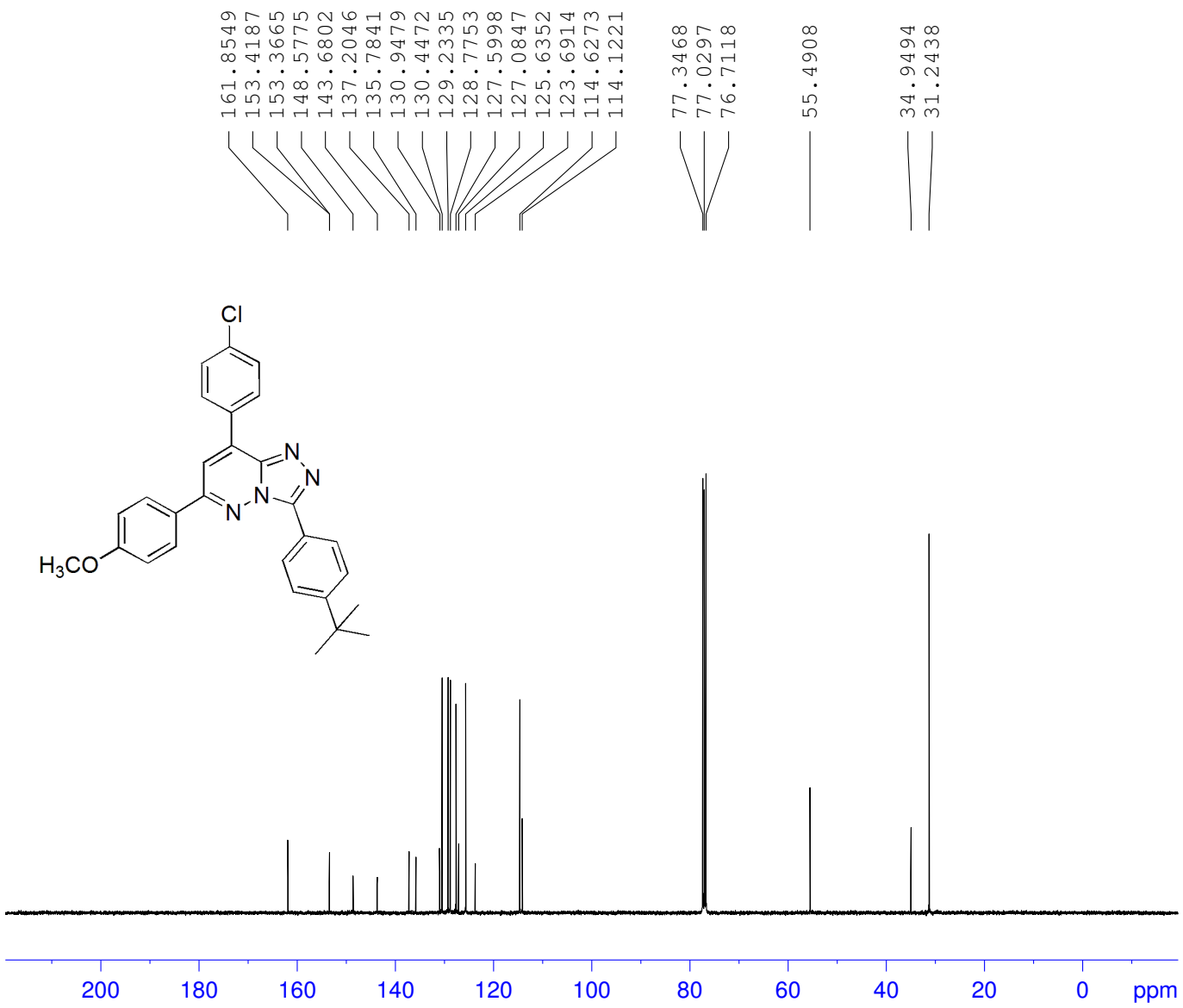


Fig 56. 1H NMR spectra of 3-(4-tert-Butylphenyl)-8-(4-chlorophenyl)-6-(4-methoxyphenyl)-[1,2,4]triazolo [4,3-b]pyridazine (**7f**)

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Current Data Parameters
NAME      IS10607-058-A935787
EXPNO                       2
PROCNO                      1

F2 - Acquisition Parameters
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Time                 5.24
INSTRUM             spect
PROBHD    5 mm PABBO BB-
PULPROG            zgpg30
TD                  32768
SOLVENT             CDCl3
NS                   3000
DS                      4
SWH             24038.461 Hz
FIDRES           0.733596 Hz
AQ               0.6816244 sec
RG                   40.3
DW                 20.800 usec
DE                  6.00 usec
TE                 296.4 K
D1             2.00000000 sec
d11            0.03000000 sec
DELTA          1.89999998 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                   13C
P1                    9.00 usec
PL1                  -3.00 dB
SFO1          100.6278593 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                   1H
PCPD2               80.00 usec
PL12                14.64 dB
PL13                15.00 dB
PL2                 -0.50 dB
SFO2          400.1516006 MHz

F2 - Processing parameters
SI                   32768
SF            100.6177980 MHz
WDW                     EM
SSB                      0
LB                    1.00 Hz
GB                       0
PC                    1.40
```

Fig 57. 13C NMR spectra of 3-(4-tert-Butylphenyl)-8-(4-chlorophenyl)-6-(4-methoxyphenyl)-[1,2,4]triazolo [4,3-b]pyridazine (**7f**)

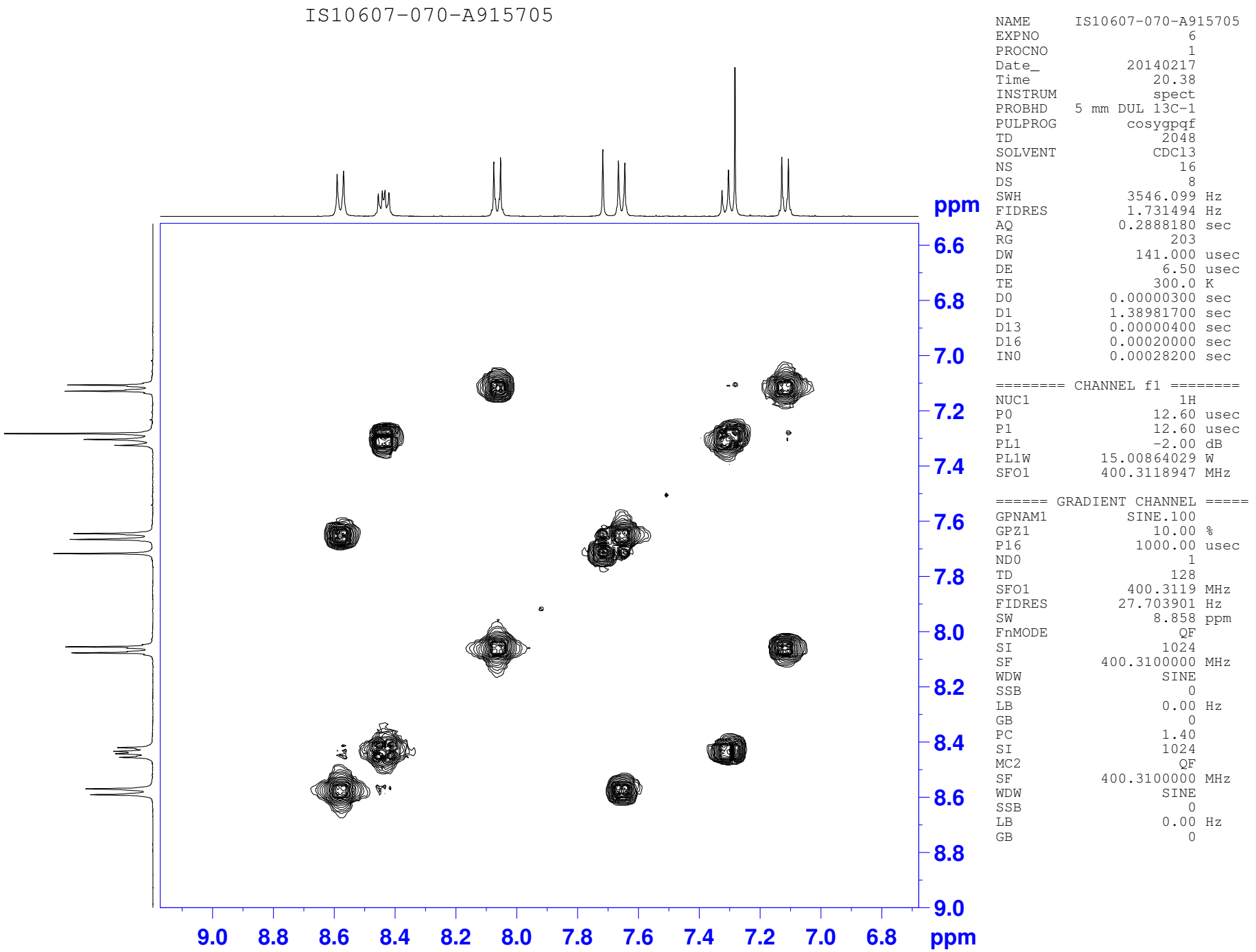


Fig 58. COSY Spectrum of 3-(4-tert-butylphenyl)-8-(4-fluorophenyl)-6-(4-methoxyphenyl)- [1,2,4]triazolo[4,3-b]pyridazine (Aromatic region) (**7e**)

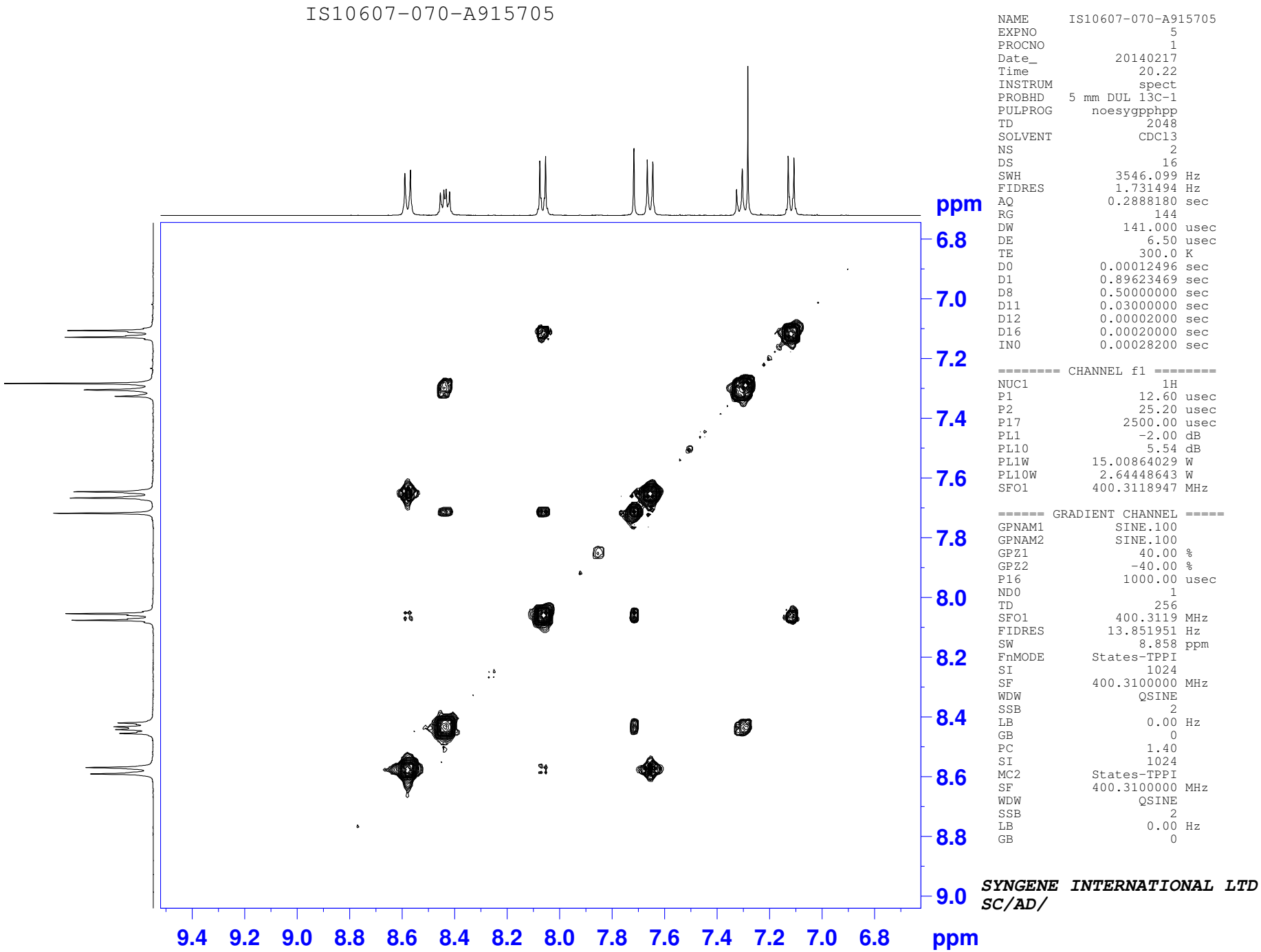


Fig 59. NOESY Spectrum of 3-(4-tert-butylphenyl)-8-(4-fluorophenyl)- 6- (4-methoxyphenyl)- [1,2,4]triazolo[4,3-b]pyridazine (Aromatic region) (**7e**)

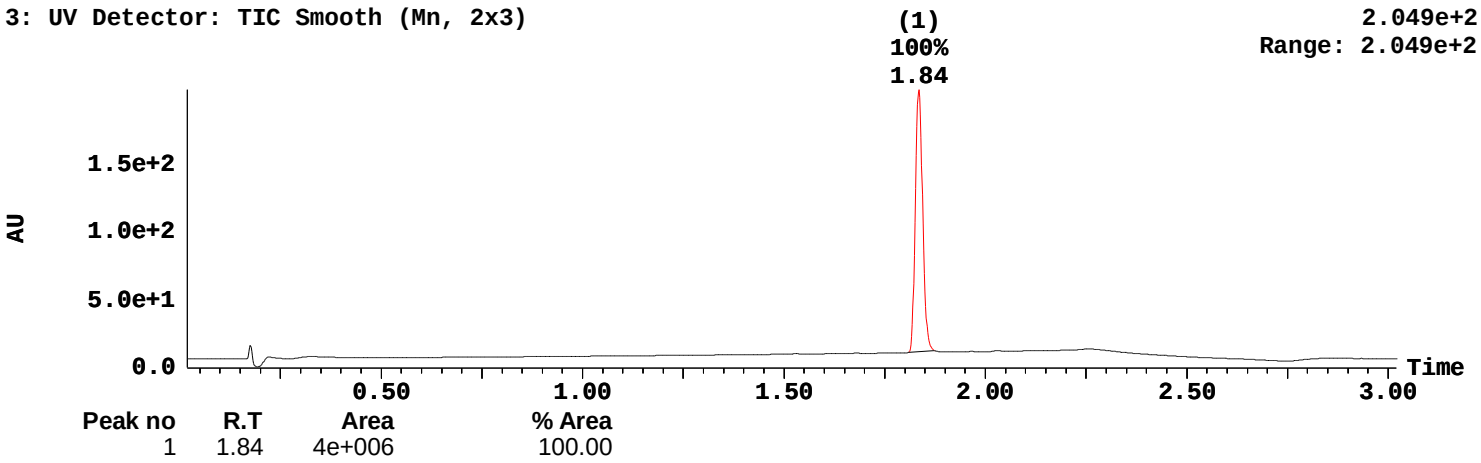
5. UPLC of compounds

Syngene International Ltd (A Biocon company) **UPLC Report** Page 1

Sample Name:IS10607-058 Mobile A:0.1%HCOOH in Water Vial:1:7
Data File:A910311 Mobile B: 0.1%HCOOH in ACN Flow Rate:1.0 ml/min
Acq.Method:595FA.olp %B: 0min=5%2min=95%2.5min=5%3min=5% Inj Date:11-Feb-2014
Instrument Code :SC\AD\17-004 Column : Acquity UPLC HSS T3 (2.1x50)mm;1.8µm:

Printed: Tue Feb 11 10:05:41 2014

Sample Report:



Peak no	R.T	Area	% Area
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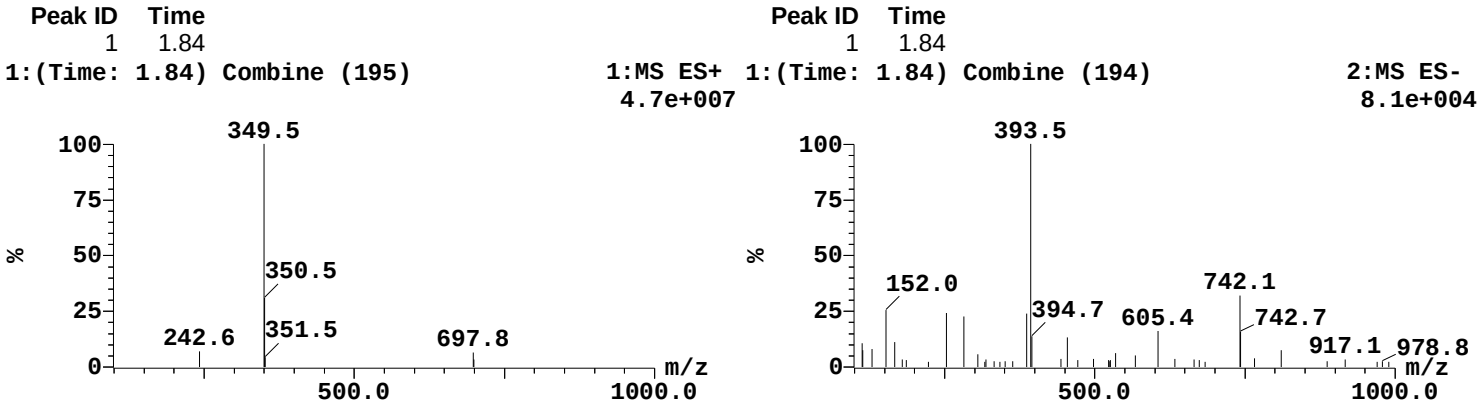


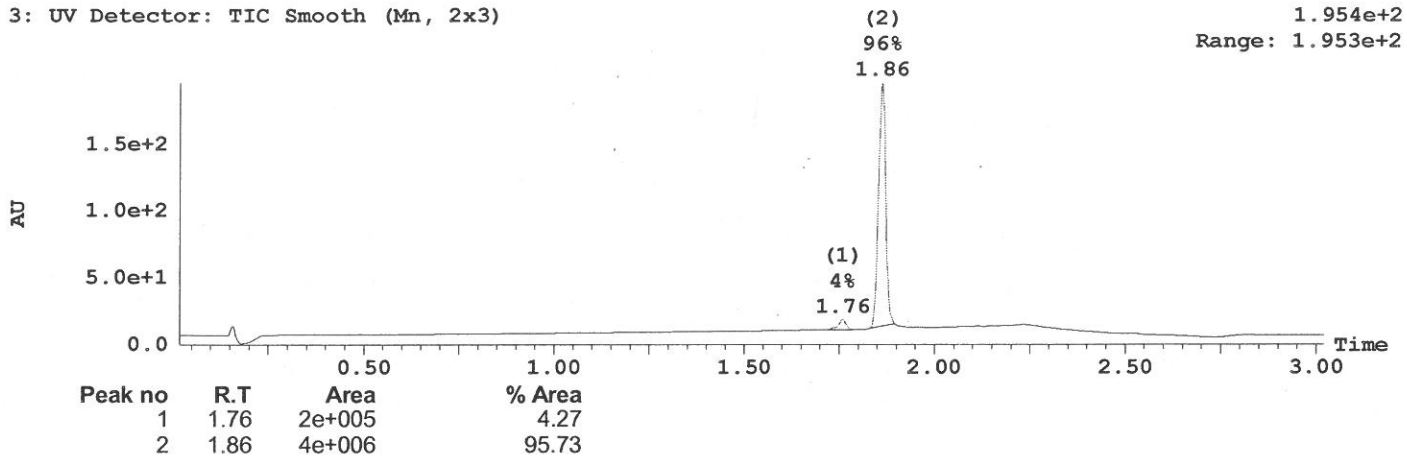
Fig 60. UPLC of 3,6,8-triphenyl-[1,2,4]triazolo[4,3-b]pyridazine **(3a)**

Syngene International Ltd (A Biocon company) — **UPLC Report**

Sample Name:IS09537-100 | Mobile A:0.1%HCOOH in Water | Vial:1:28
Data File:A841899 | Mobile B: 0.1%HCOOH in ACN | Flow Rate:1.0 ml/min
Acq.Method:595FA.olp | %B: 0min=5%2min=95%2.5min=5%3min=5% | Inj Date:21-Nov-2013
Instrument Code :SC\AD\17-004 | Column : Acquity UPLC HSS T3 (2.1x50)mm;1.8µm:

Printed: Thu Nov 21 11:25:59 2013

Sample Report:



Peak no	R.T	Area	% Area
1	1.76	2e+005	4.27
2	1.86	4e+006	95.73

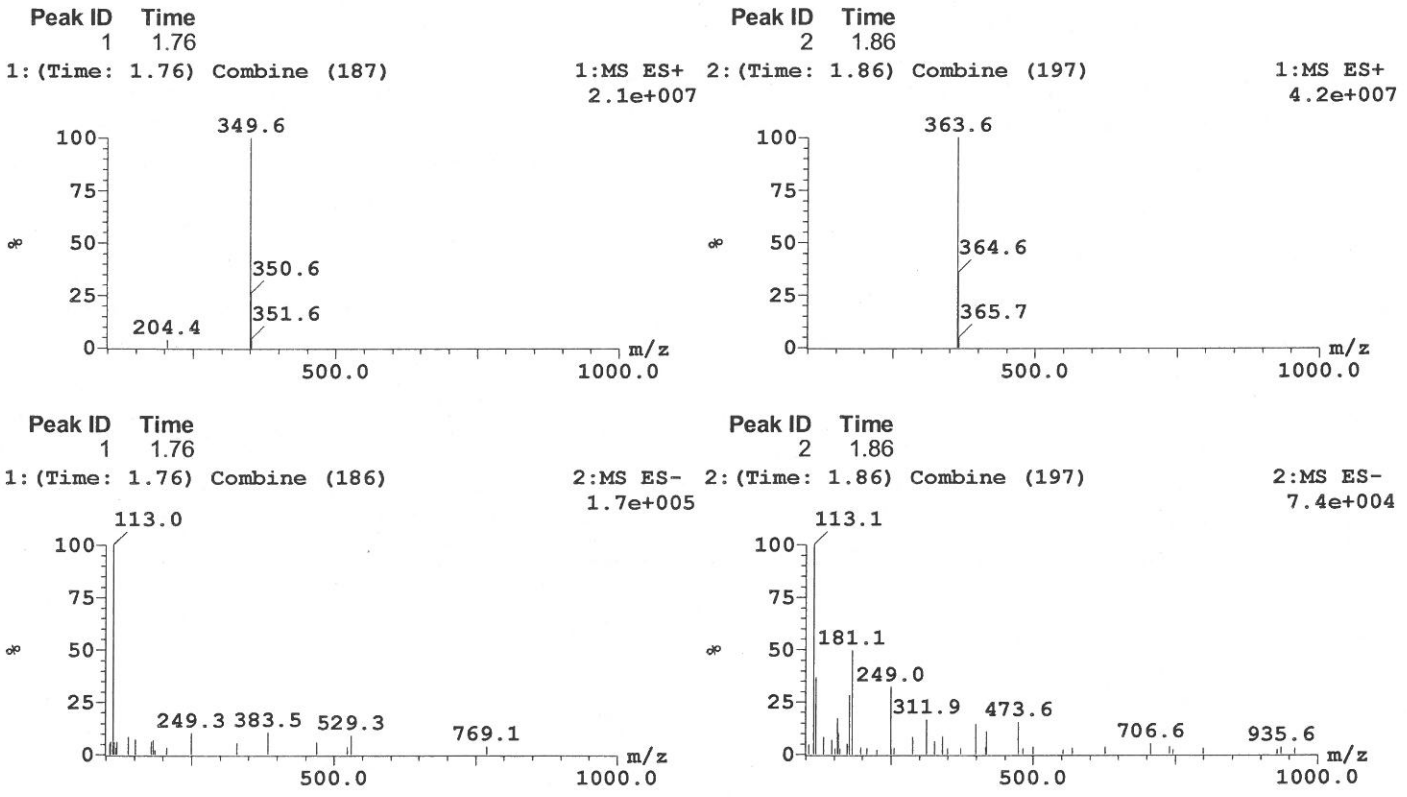
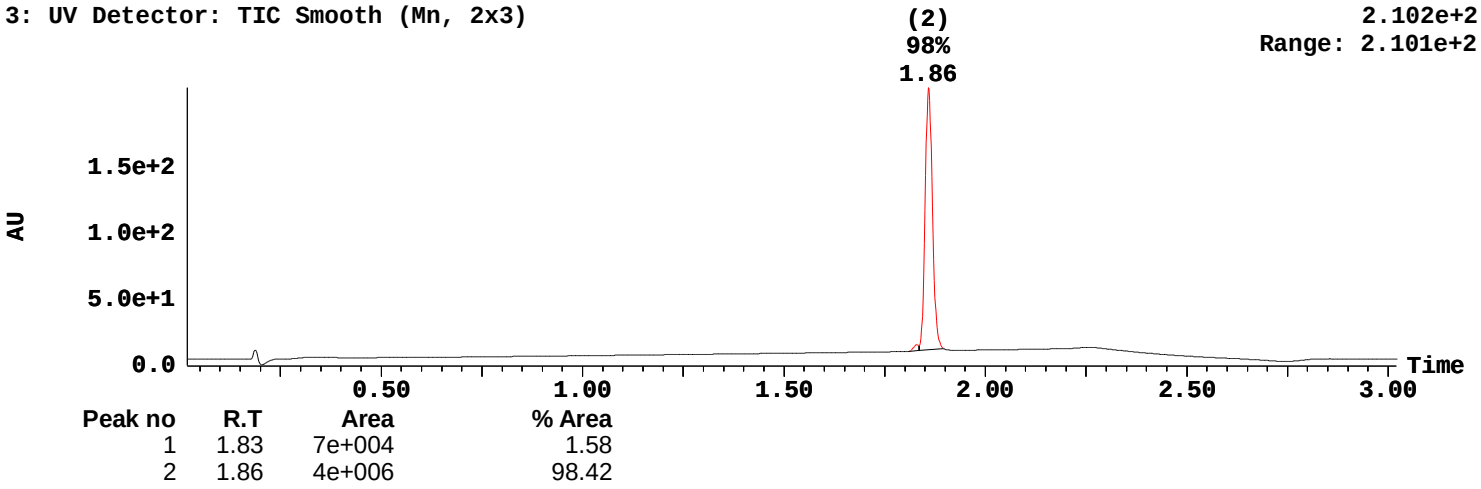


Fig 61. UPLC of 3,6-diphenyl-8-m-tolyl-[1,2,4]triazolo[4,3-b]pyridazine (**3b**)

Sample Name:IS10607-054 Mobile A:0.1%HCOOH in Water Vial:1:25
Data File:A909934 Mobile B: 0.1%HCOOH in ACN Flow Rate:1.0 ml/min
Acq.Method:595FA.olp %B: 0min=5%2min=95%2.5min=5%3min=5% Inj Date:10-Feb-2014
Instrument Code :SC\AD\17-004 Column : Acquity UPLC HSS T3 (2.1x50)mm;1.8µm:

Printed: Mon Feb 10 15:04:04 2014

Sample Report:



Peak no	R.T	Area	% Area
1	1.83	7e+004	1.58
2	1.86	4e+006	98.42

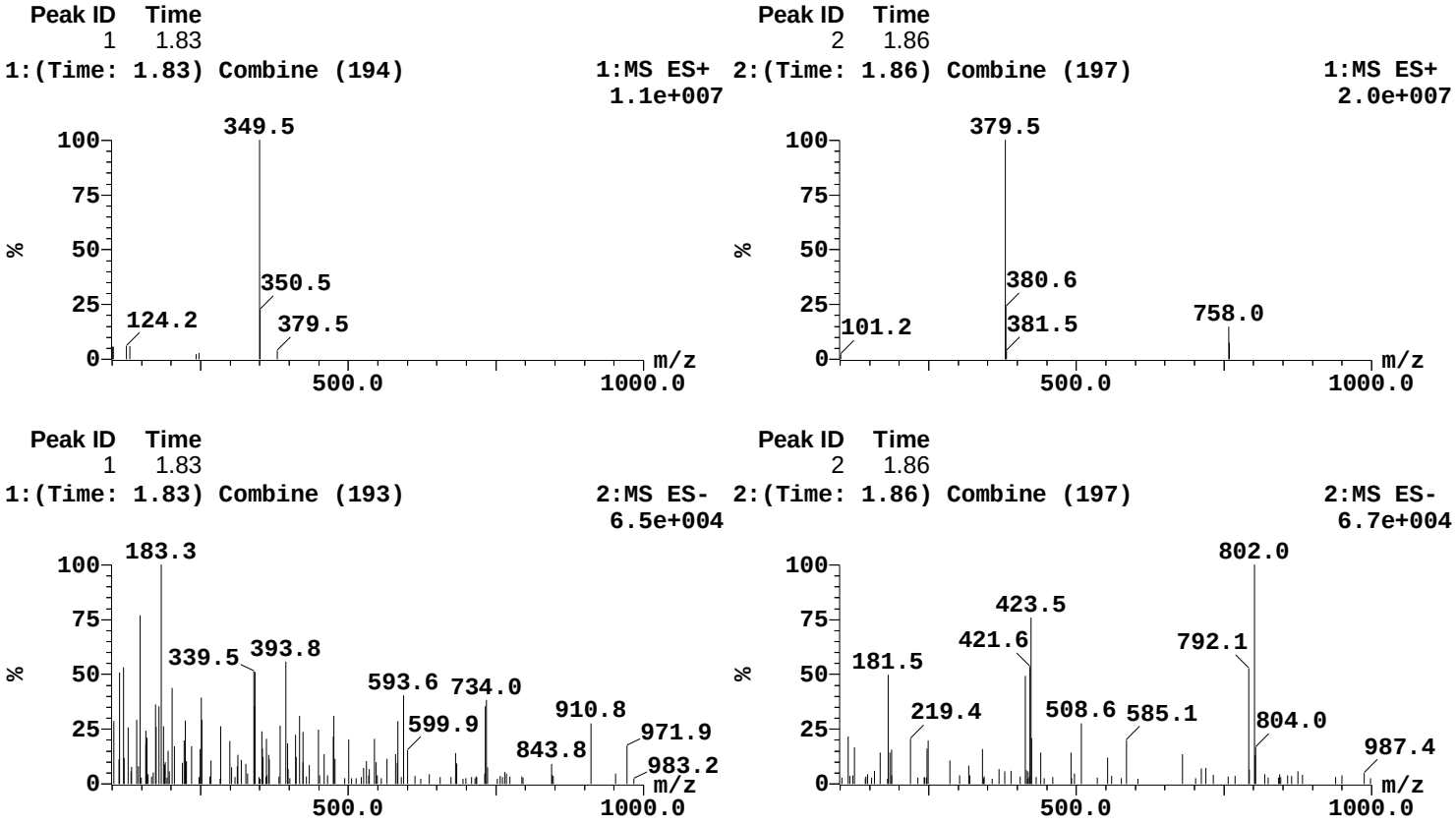
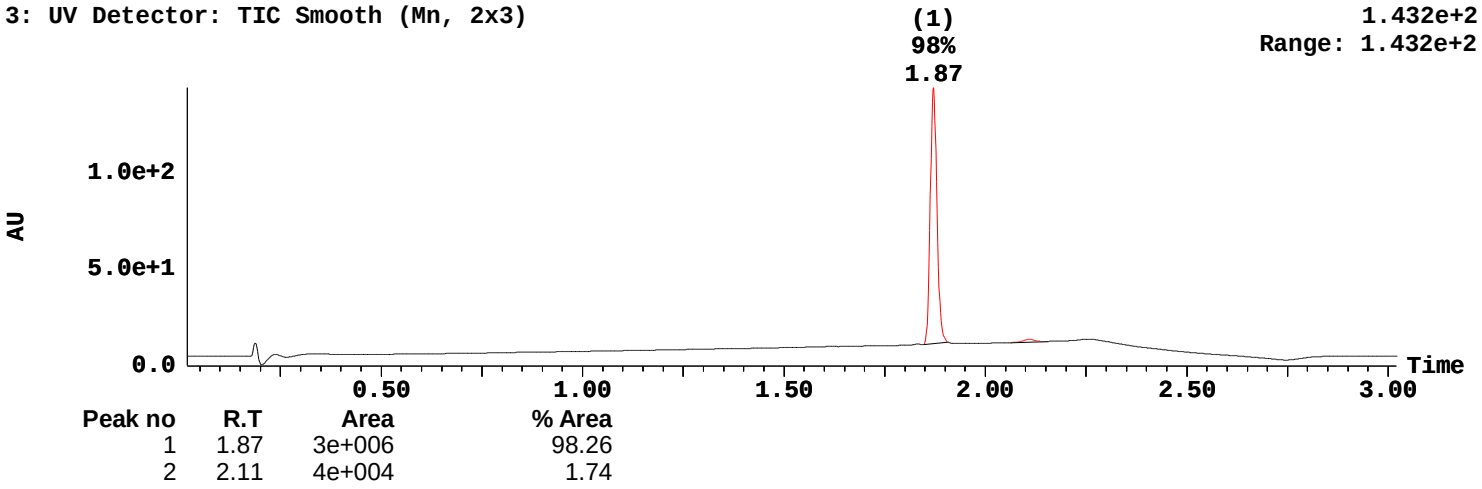


Fig 62. UPLC of 8-(3-methoxyphenyl)-3,6-diphenyl-[1,2,4]triazolo[4,3-b]pyridazine (**3c**)

Sample Name:IS10607-058 Mobile A:0.1%HCOOH in Water Vial:1:28
Data File:A909937A Mobile B: 0.1%HCOOH in ACN Flow Rate:1.0 ml/min
Acq.Method:595FA.olp %B: 0min=5%2min=95%2.5min=5%3min=5% Inj Date:10-Feb-2014
Instrument Code :SC\AD\17-004 Column : Acquity UPLC HSS T3 (2.1x50)mm;1.8µm:

Printed: Mon Feb 10 15:19:48 2014

Sample Report:



Peak no	R.T	Area	% Area
1	1.87	3e+006	98.26
2	2.11	4e+004	1.74

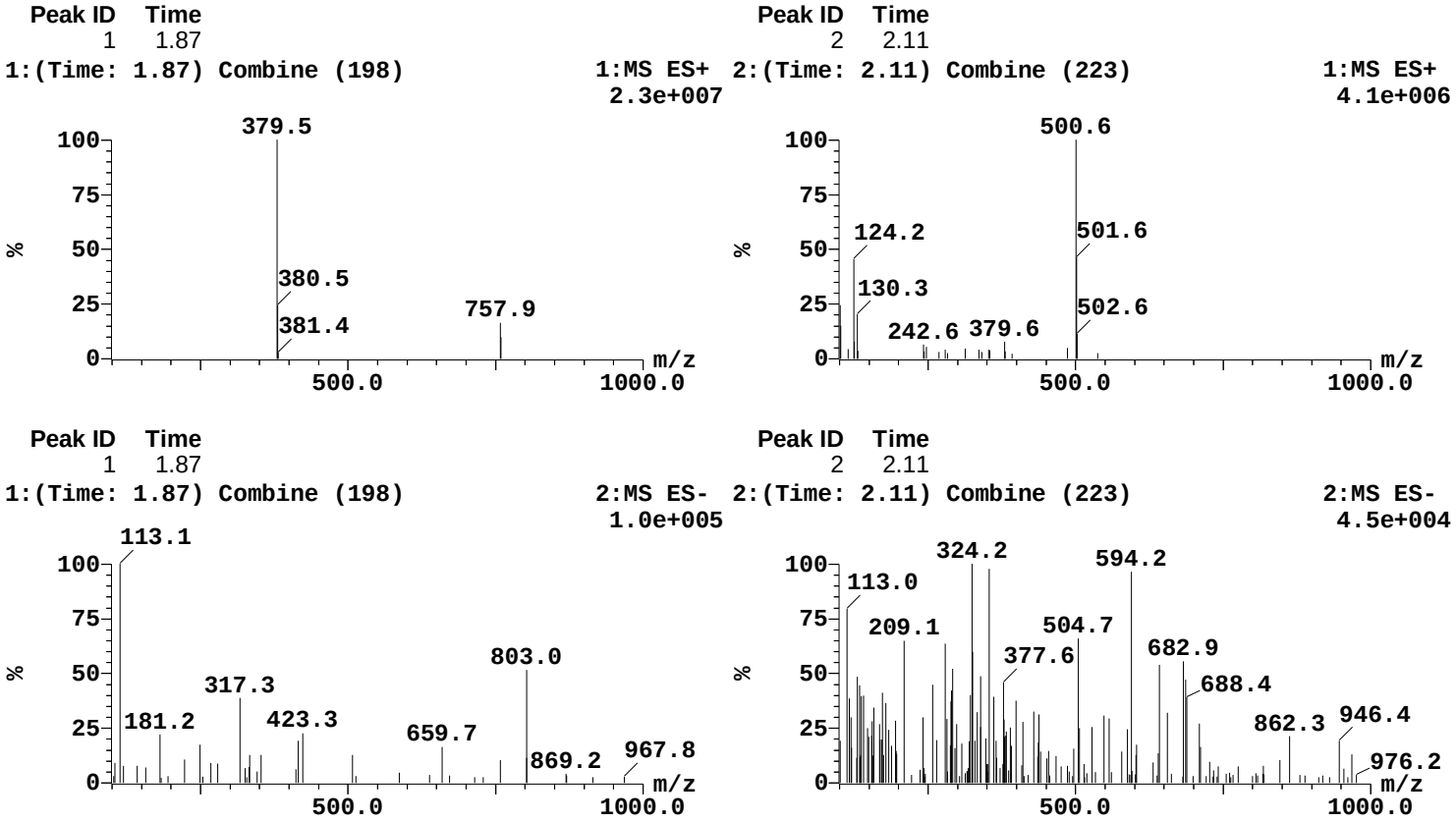
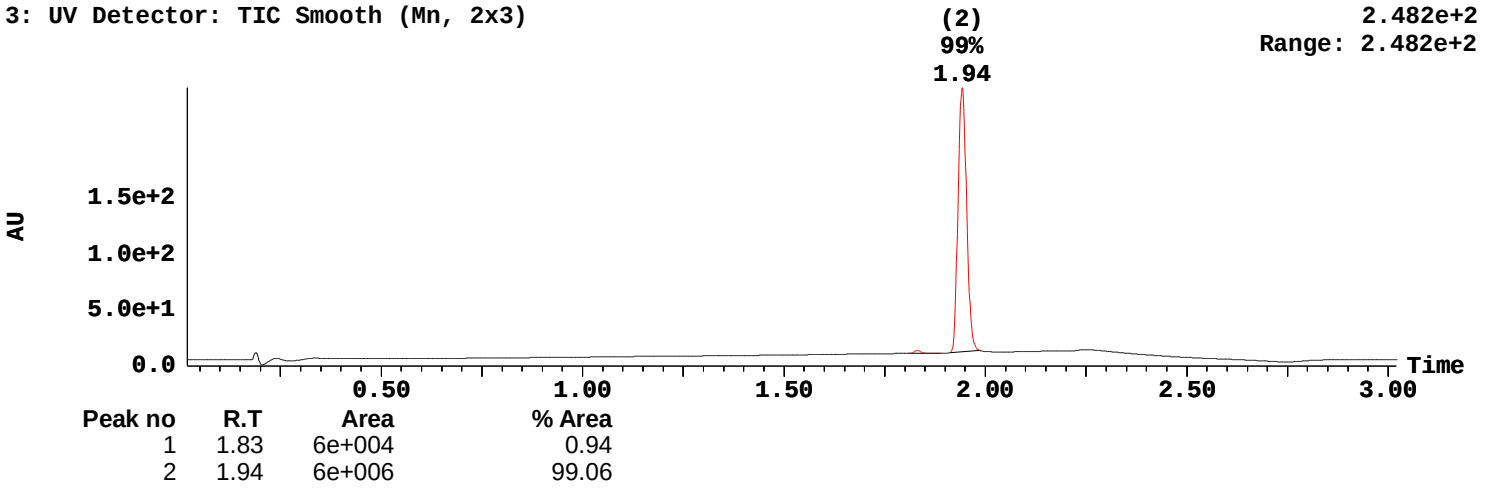


Fig 63. UPLC of 8-(4-methoxyphenyl)-3,6-diphenyl-[1,2,4]triazolo[4,3-b]pyridazine (**3d**)

Sample Name:IS10607-058 Mobile A:0.1%HCOOH in Water Vial:1:27
Data File:A909938 Mobile B: 0.1%HCOOH in ACN Flow Rate:1.0 ml/min
Acq.Method:595FA.olp %B: 0min=5%2min=95%2.5min=5%3min=5% Inj Date:10-Feb-2014
Instrument Code :SC\AD\17-004 Column : Acquity UPLC HSS T3 (2.1x50)mm;1.8µm:

Printed: Mon Feb 10 15:04:57 2014

Sample Report:



Peak no	R.T	Area	% Area
1	1.83	6e+004	0.94
2	1.94	6e+006	99.06

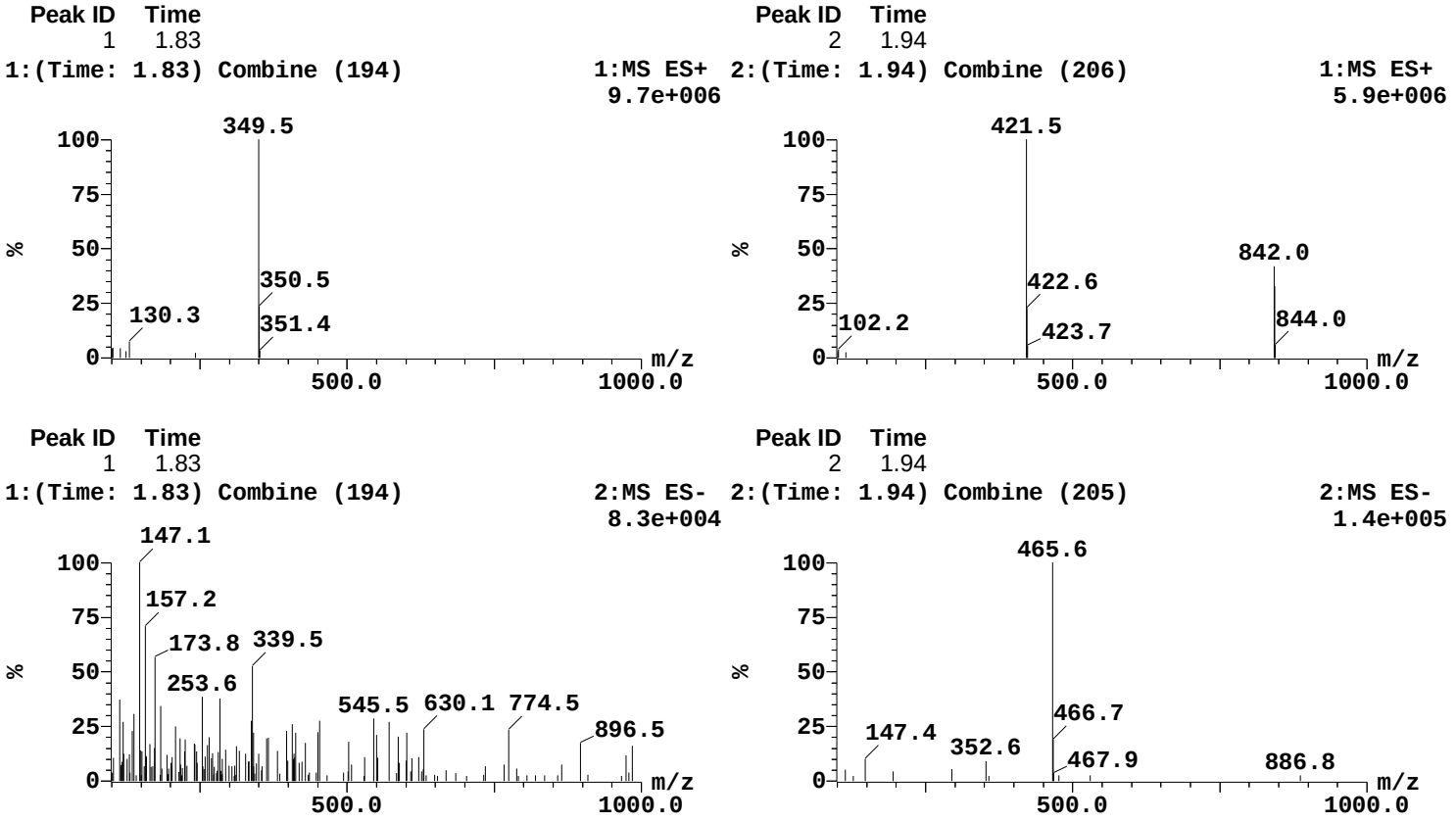
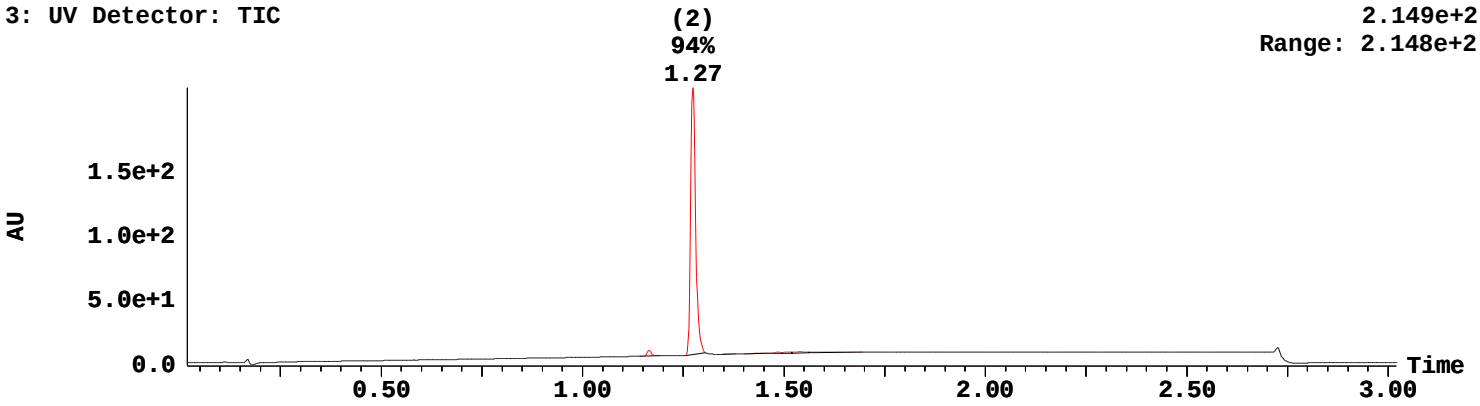


Fig 64. UPLC of ethyl 3-(3,6-diphenyl-[1,2,4]triazolo[4,3-b]pyridazin-8-yl)benzoate (**3e**)

Sample Name:IS10607-058 Mobile A:0.1%HCOOH in Water Vial:1:22
Data File:A936776 Mobile B: 0.1%HCOOH in ACN Flow Rate: 0.7 ml/min
Acq.Method:595FA.olp %B: 0min=30%1.25min=95%2min=95%3min=30% Inj Date:14-Mar-2014
Instrument Code :SC\AD\17-004 Column : Acquity UPLC HSS T3 (2.1x50)mm;1.8µm:

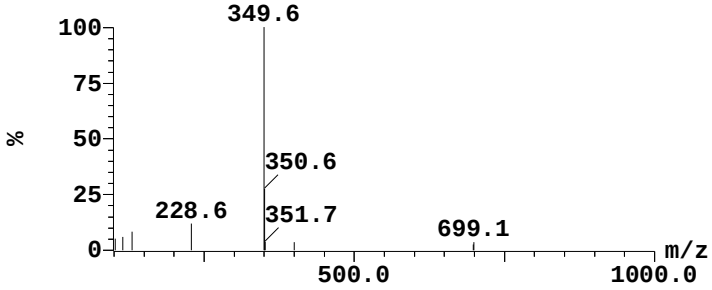
Printed: Fri Mar 14 11:02:21 2014

Sample Report:

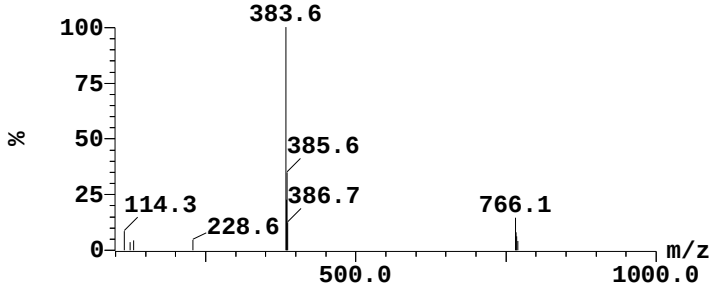


Peak no	R.T	Area	% Area
1	1.16	6e+004	1.75
2	1.27	3e+006	94.29
3	1.36	4e+003	0.14
4	1.45	7e+003	0.23
5	1.48	2e+004	0.67
6	1.51	2e+004	0.62
7	1.54	3e+004	1.04
8	1.57	4e+004	1.26

Peak ID	Time
1	1.16



Peak ID	Time
2	1.27

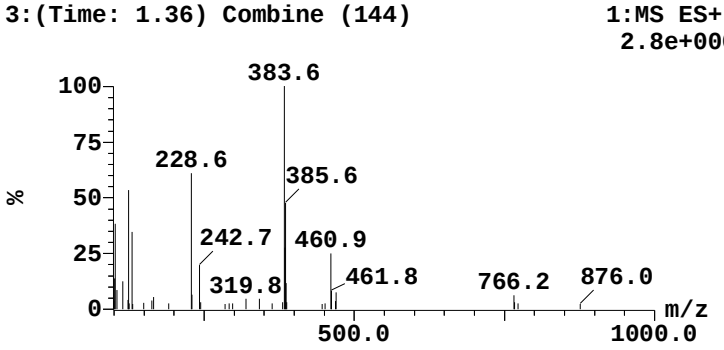


Sample Name:IS10607-058 Mobile A:0.1%HCOOH in Water Vial:1:22
Data File:A936776 Mobile B: 0.1%HCOOH in ACN Flow Rate: 0.7 ml/min
Acq.Method:595FA.olp %B: 0min=30%1.25min=95%2min=95%3min=30% Inj Date:14-Mar-2014
Instrument Code :SC\AD\17-004 Column : Acquity UPLC HSS T3 (2.1x50)mm;1.8µm:

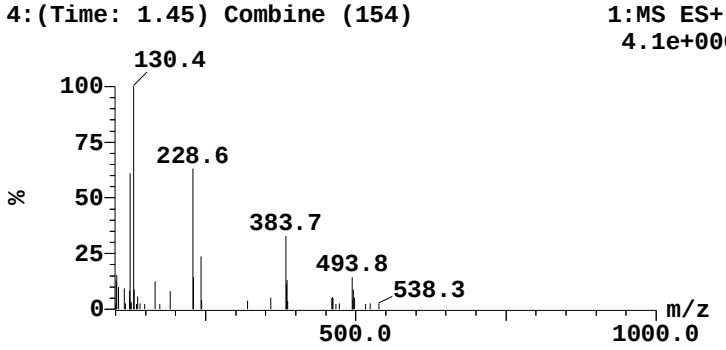
Printed: Fri Mar 14 11:02:21 2014

Sample Report (continued):

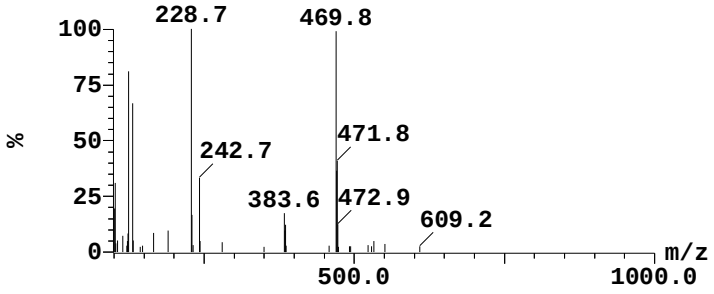
Peak ID **Time**
3 1.36



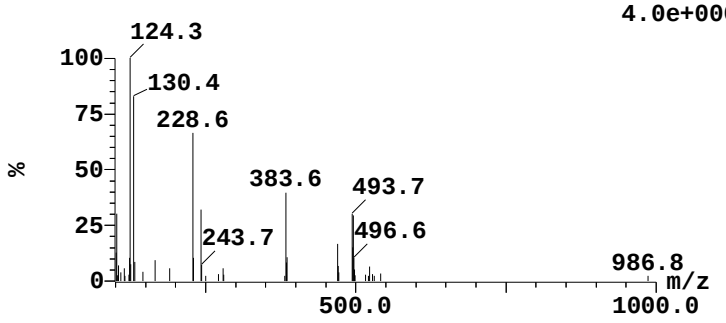
Peak ID **Time**
4 1.45



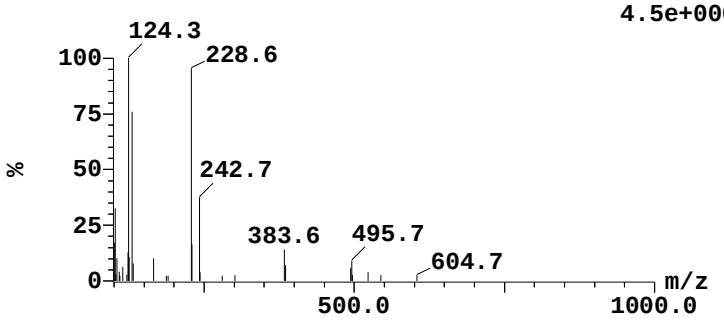
Peak ID **Time**
5 1.48



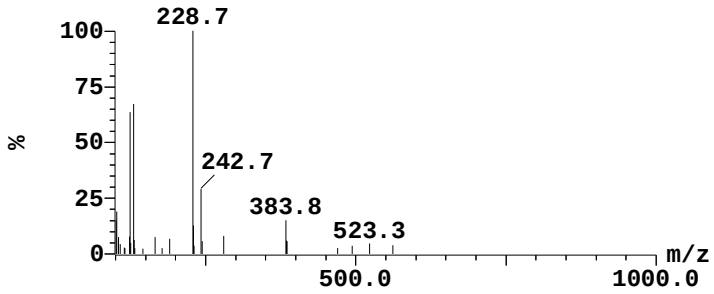
Peak ID **Time**
6 1.51



Peak ID **Time**
7 1.54



Peak ID **Time**
8 1.57



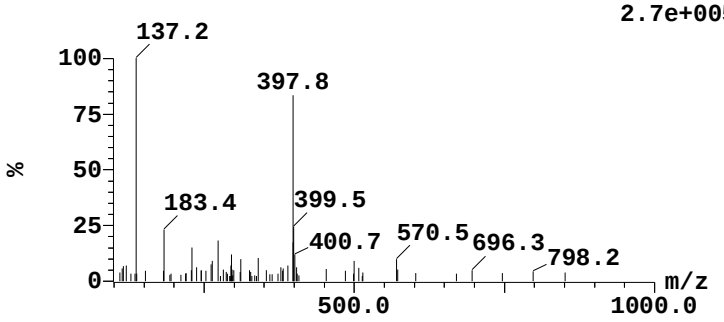
Sample Name:IS10607-058 Mobile A:0.1%HCOOH in Water Vial:1:22
Data File:A936776 Mobile B: 0.1%HCOOH in ACN Flow Rate: 0.7 ml/min
Acq.Method:595FA.olp %B: 0min=30%1.25min=95%2min=95%3min=30% Inj Date:14-Mar-2014
Instrument Code :SC\AD\17-004 Column : Acquity UPLC HSS T3 (2.1x50)mm;1.8µm:

Printed: Fri Mar 14 11:02:21 2014

Sample Report (continued):

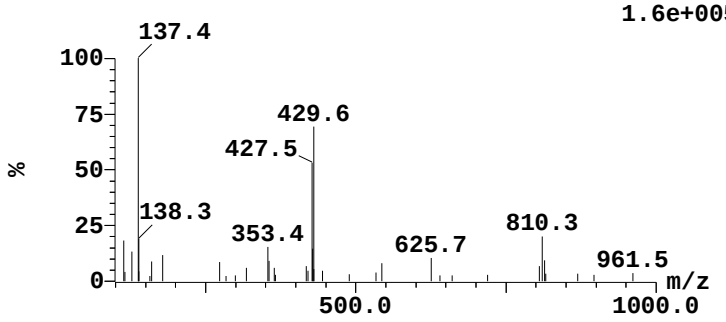
Peak ID **Time**
1 1.16

1:(Time: 1.16) Combine (123) **2:MS ES- 2.7e+005**



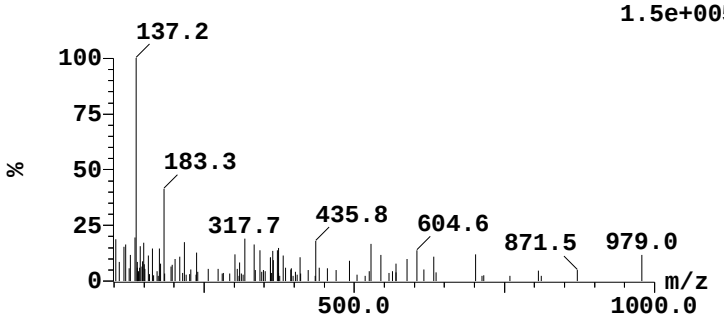
Peak ID **Time**
2 1.27

2:(Time: 1.27) Combine (135) **2:MS ES- 1.6e+005**



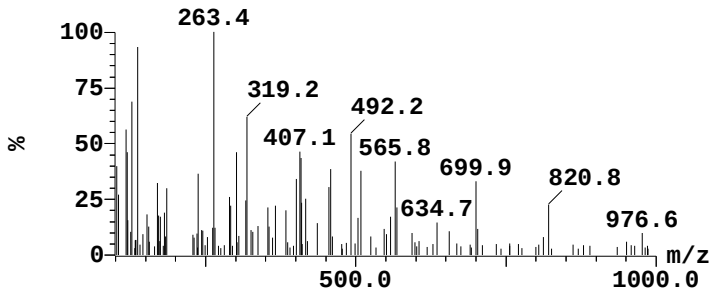
Peak ID **Time**
3 1.36

3:(Time: 1.36) Combine (144) **2:MS ES- 1.5e+005**



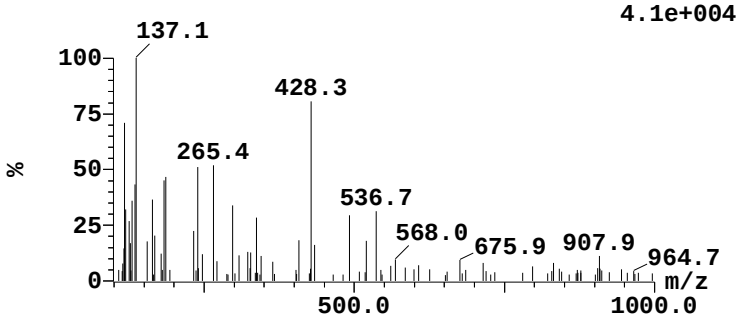
Peak ID **Time**
4 1.45

4:(Time: 1.45) Combine (153) **2:MS ES- 3.9e+004**



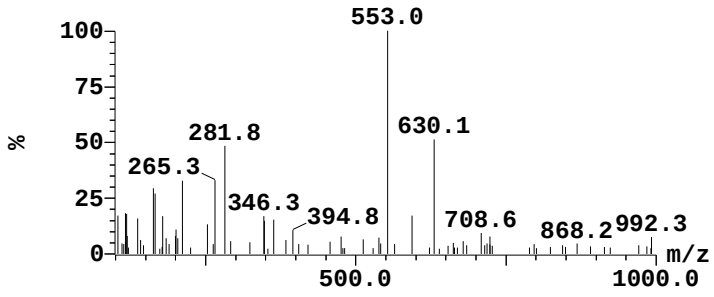
Peak ID **Time**
5 1.48

5:(Time: 1.48) Combine (157) **2:MS ES- 4.1e+004**



Peak ID **Time**
6 1.51

6:(Time: 1.51) Combine (160) **2:MS ES- 4.9e+004**



Sample Name:IS10607-058 Mobile A:0.1%HCOOH in Water Vial:1:22
Data File:A936776 Mobile B: 0.1%HCOOH in ACN Flow Rate: 0.7 ml/min
Acq.Method:595FA.olp %B: 0min=30%1.25min=95%2min=95%3min=30% Inj Date:14-Mar-2014
Instrument Code :SC\AD\17-004 Column : Acquity UPLC HSS T3 (2.1x50)mm;1.8µm:

Printed: Fri Mar 14 11:02:21 2014

Sample Report (continued):

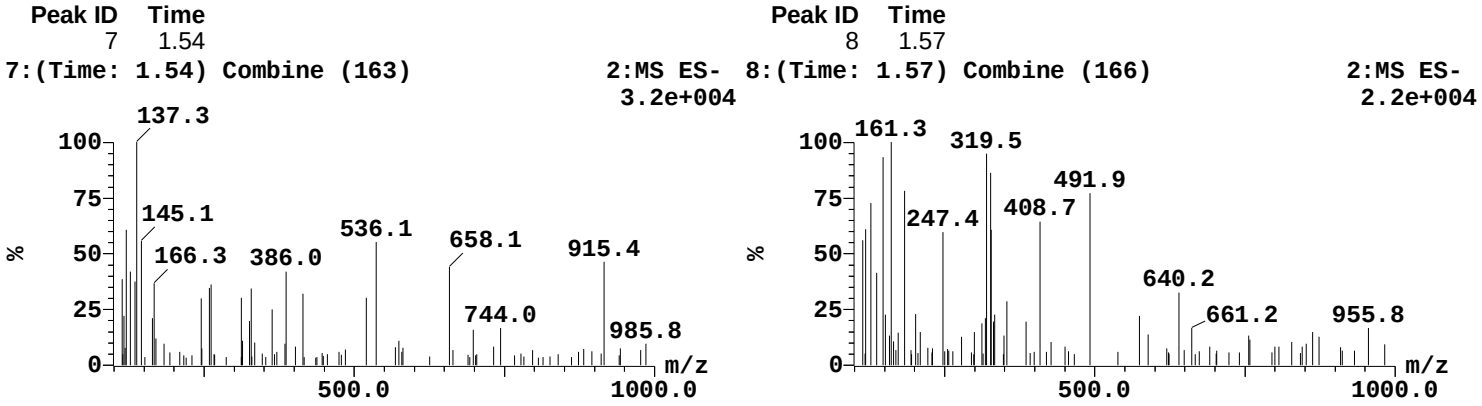


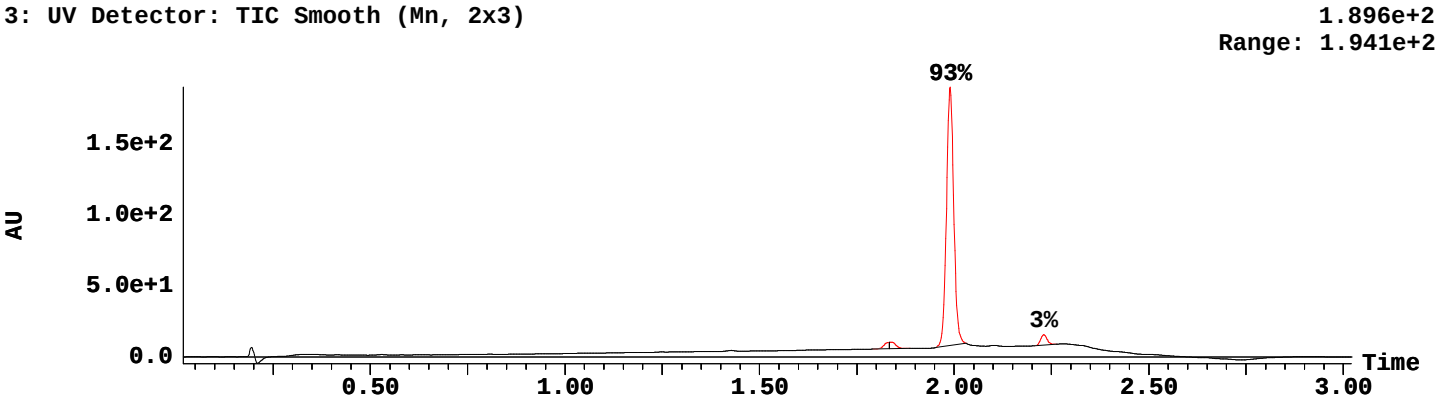
Fig 65. UPLC of 8-(3-chlorophenyl)-3,6-diphenyl-[1,2,4]triazolo[4,3-b]pyridazine (**3f**)

Sample Name:IS10607-058 Mobile A:0.1%HCOOH in Water Vial:2:D,3
Data File:A911131 Mobile B: 0.1%HCOOH in ACN Flow Rate:1.0 ml/min
Acq.Method:595FA.olp %B: 0min=5%2min=95%2.5min=5%3min=5% Inj Date:12-Feb-2014
Instrument Code :SC\AD\17-005 Column : Acquity UPLC HSS T3 (2.1x50)mm;1.8µm:

Printed: Wed Feb 12 19:06:31 2014

Sample Report:

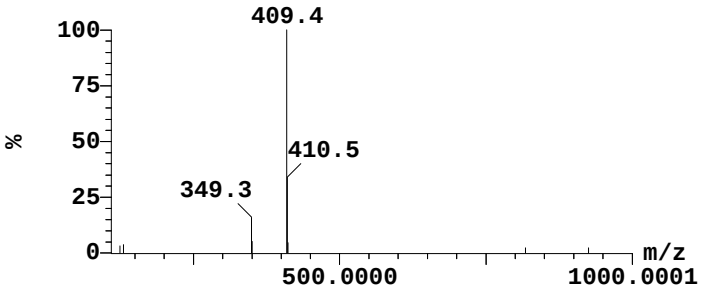
3: UV Detector: TIC Smooth (Mn, 2x3)



Peak no	R.T	Area	% Area
1	1.83	7e+004	1.63
2	1.84	9e+004	2.06
3	1.99	4e+006	92.96
4	2.23	1e+005	3.34

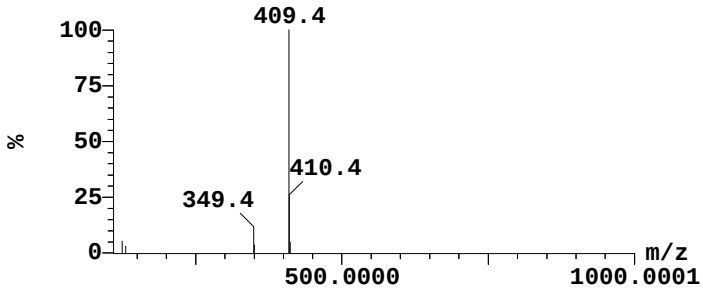
Peak ID	Time
1	1.83

1:(Time: 1.83) **1:MS ES+ 5.9e+007**



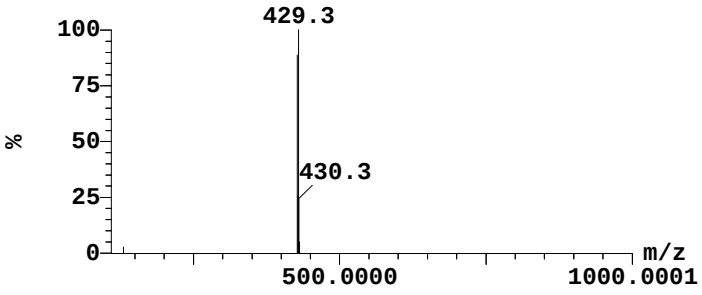
Peak ID	Time
2	1.84

2:(Time: 1.84) **1:MS ES+ 4.9e+007**



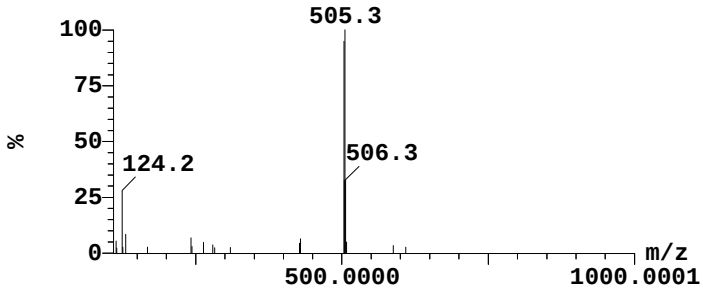
Peak ID	Time
3	1.99

3:(Time: 1.99) **1:MS ES+ 4.6e+007**



Peak ID	Time
4	2.23

4:(Time: 2.23) **1:MS ES+ 3.2e+007**



Sample Report (continued):

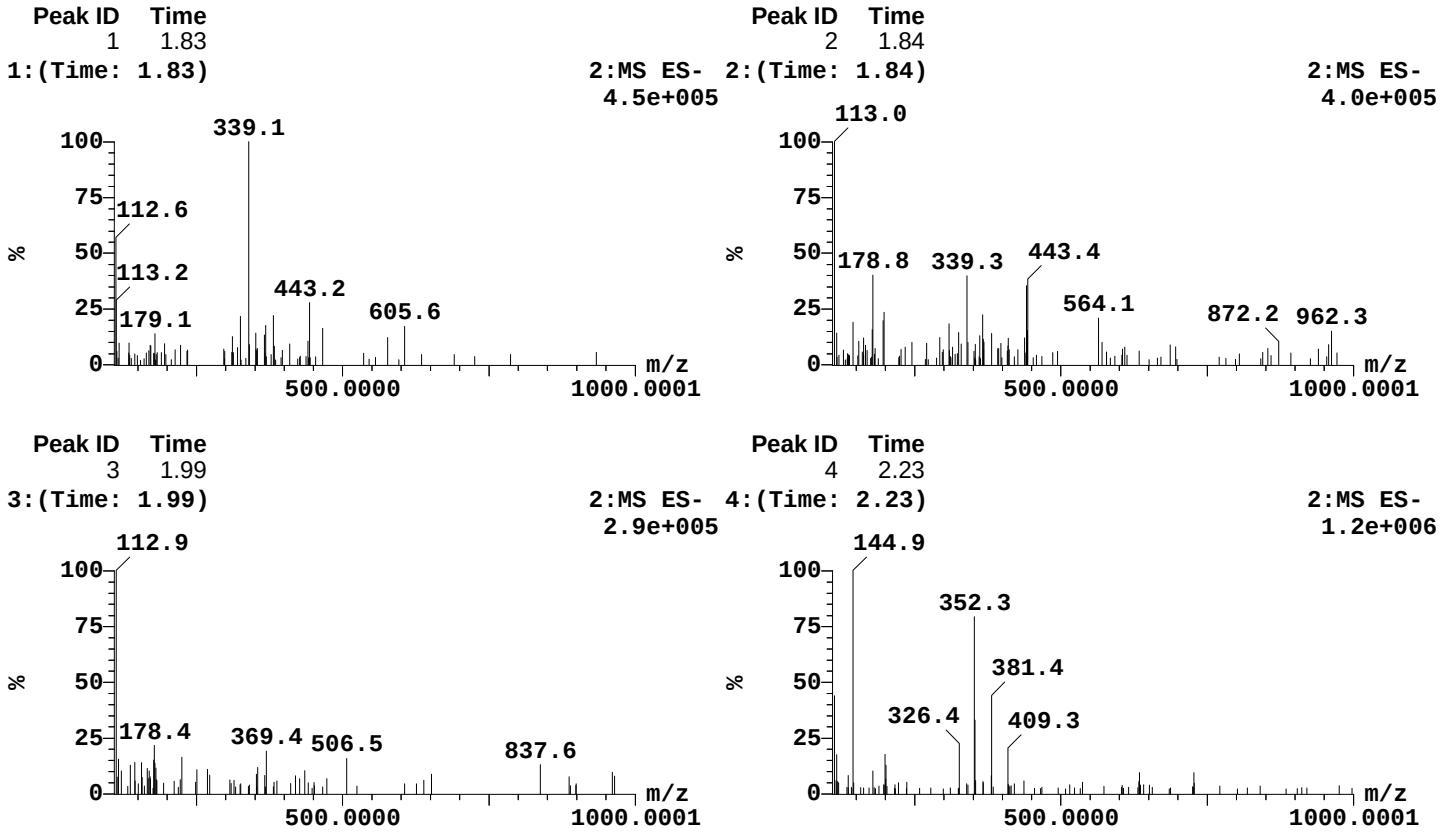
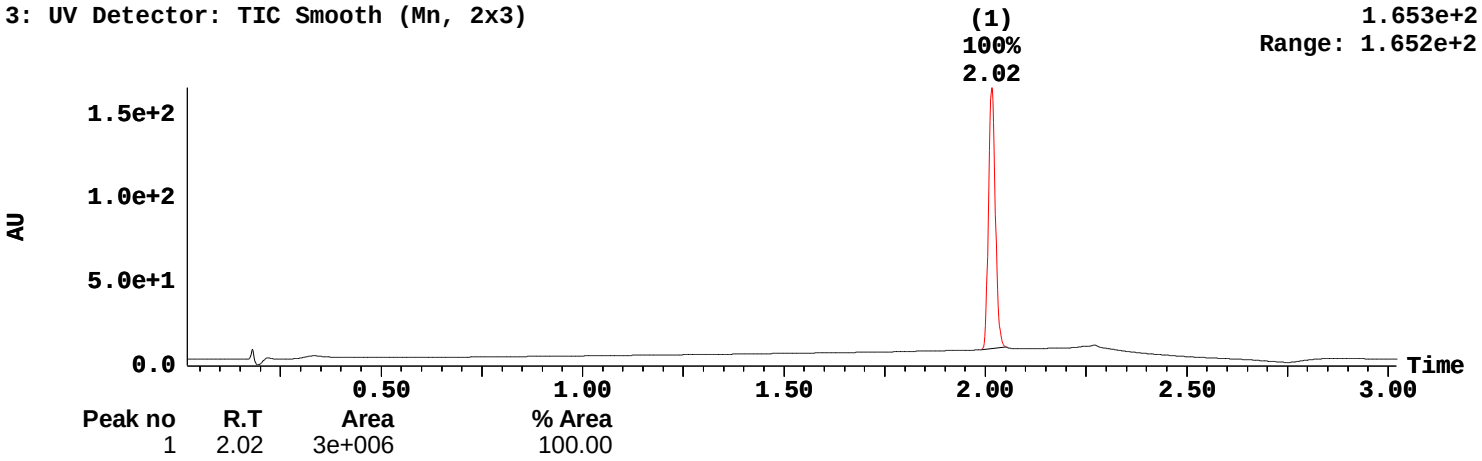


Fig 66. UPLC of 8-(3-bromophenyl)-3,6-diphenyl-[1,2,4]triazolo[4,3-b]pyridazine (**3g**)

Sample Name:IS10607-058 Mobile A:0.1%HCOOH in Water Vial:1:36
Data File:A910656A Mobile B: 0.1%HCOOH in ACN Flow Rate:1.0 ml/min
Acq.Method:595FA.olp %B: 0min=5%2min=95%2.5min=5%3min=5% Inj Date:11-Feb-2014
Instrument Code :SC\AD\17-004 Column : Acquity UPLC HSS T3 (2.1x50)mm;1.8µm:

Printed: Tue Feb 11 12:14:35 2014

Sample Report:



Peak no	R.T	Area	% Area
1	2.02	3e+006	100.00

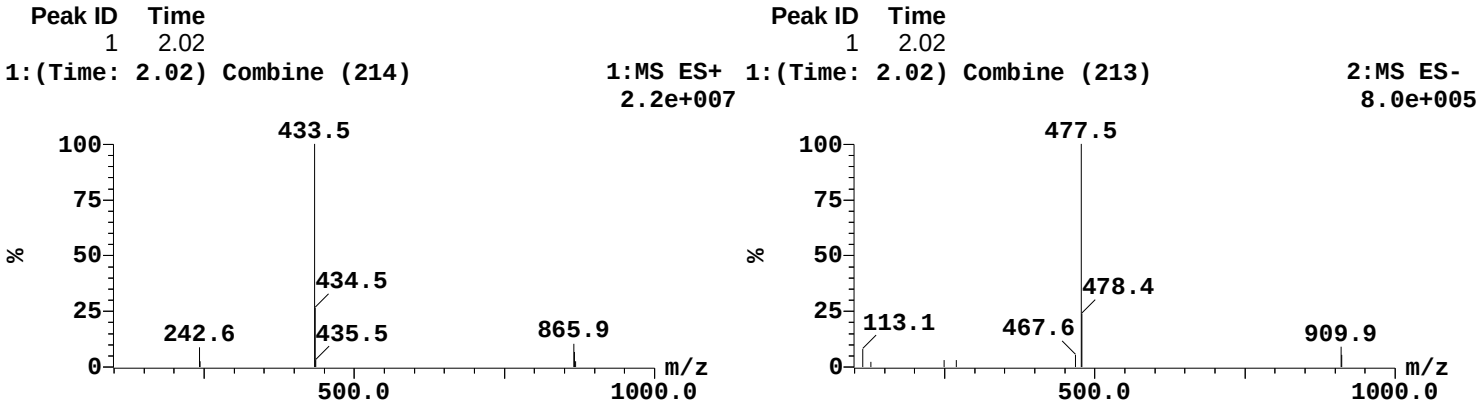
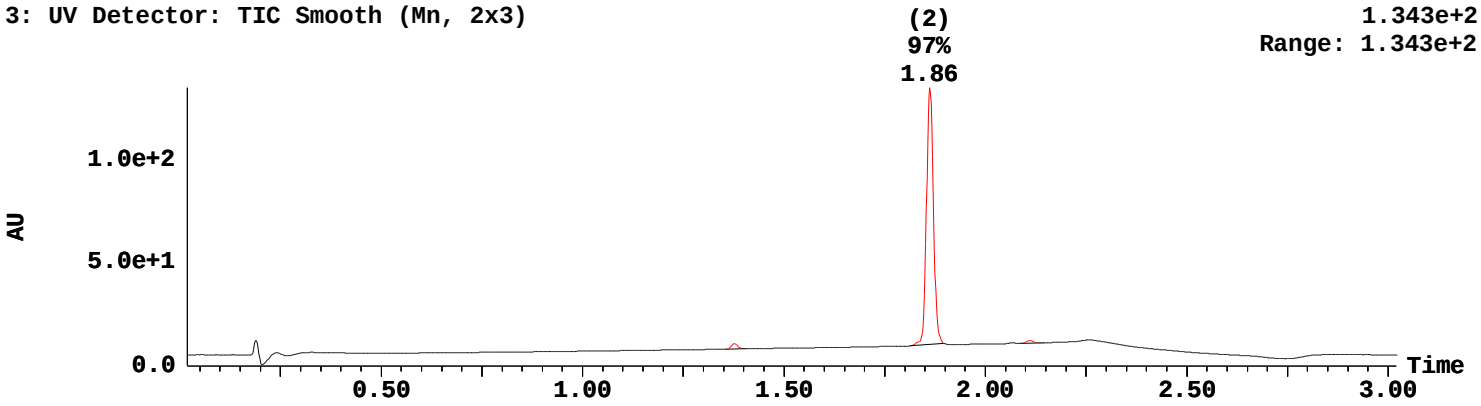


Fig 67. UPLC of 3,6-diphenyl-8-(4-(trifluoromethoxy)phenyl)-[1,2,4]triazolo[4,3-b]pyridazine (**3h**)

Sample Name:IS10607-058 Mobile A:0.1%HCOOH in Water Vial:1:6
Data File:A910312 Mobile B: 0.1%HCOOH in ACN Flow Rate:1.0 ml/min
Acq.Method:595FA.olp %B: 0min=5%2min=95%2.5min=5%3min=5% Inj Date:11-Feb-2014
Instrument Code :SC\AD\17-004 Column : Acquity UPLC HSS T3 (2.1x50)mm;1.8µm:

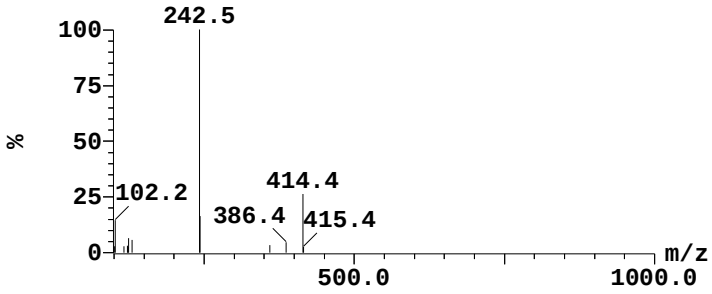
Printed: Tue Feb 11 10:05:06 2014

Sample Report:

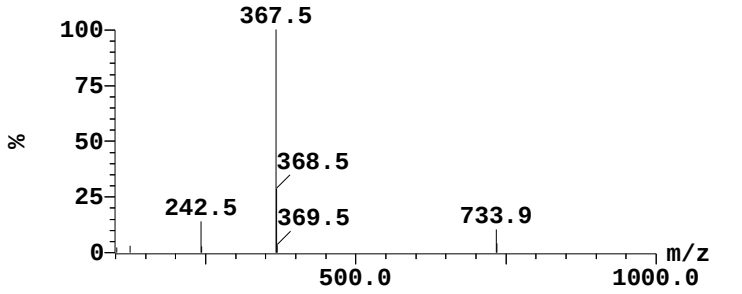


Peak no	R.T	Area	% Area
1	1.38	5e+004	1.86
2	1.86	2e+006	97.18
3	2.11	2e+004	0.96

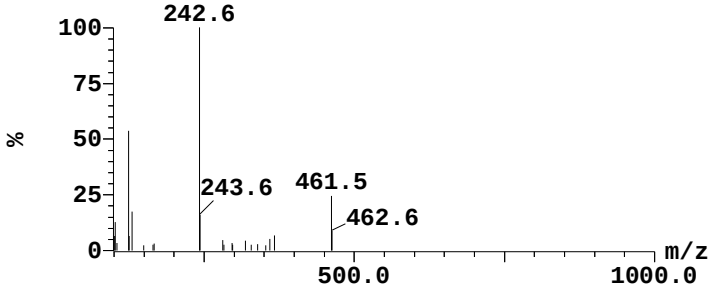
Peak ID Time
1 1.38



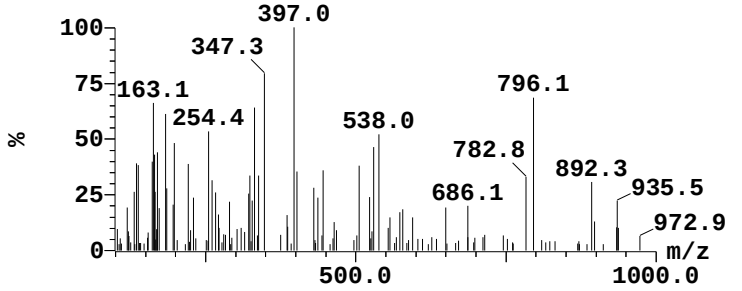
Peak ID Time
2 1.86



Peak ID Time
3 2.11



Peak ID Time
1 1.38



Sample Name:IS10607-058 Mobile A:0.1%HCOOH in Water Vial:1:6
Data File:A910312 Mobile B: 0.1%HCOOH in ACN Flow Rate:1.0 ml/min
Acq.Method:595FA.olp %B: 0min=5%2min=95%2.5min=5%3min=5% Inj Date:11-Feb-2014
Instrument Code :SC\AD\17-004 Column : Acquity UPLC HSS T3 (2.1x50)mm;1.8µm:

Printed: Tue Feb 11 10:05:06 2014

Sample Report (continued):

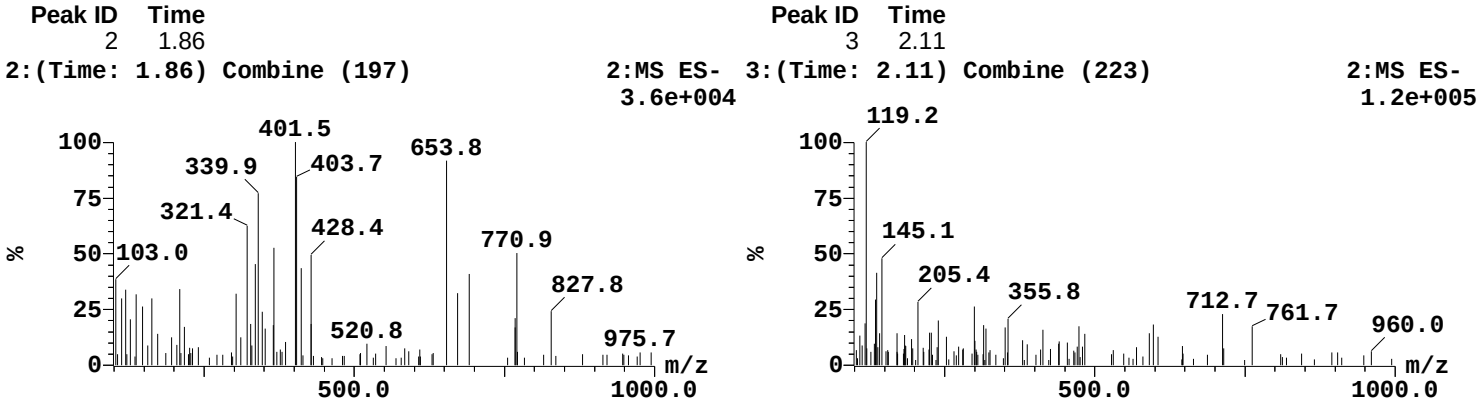
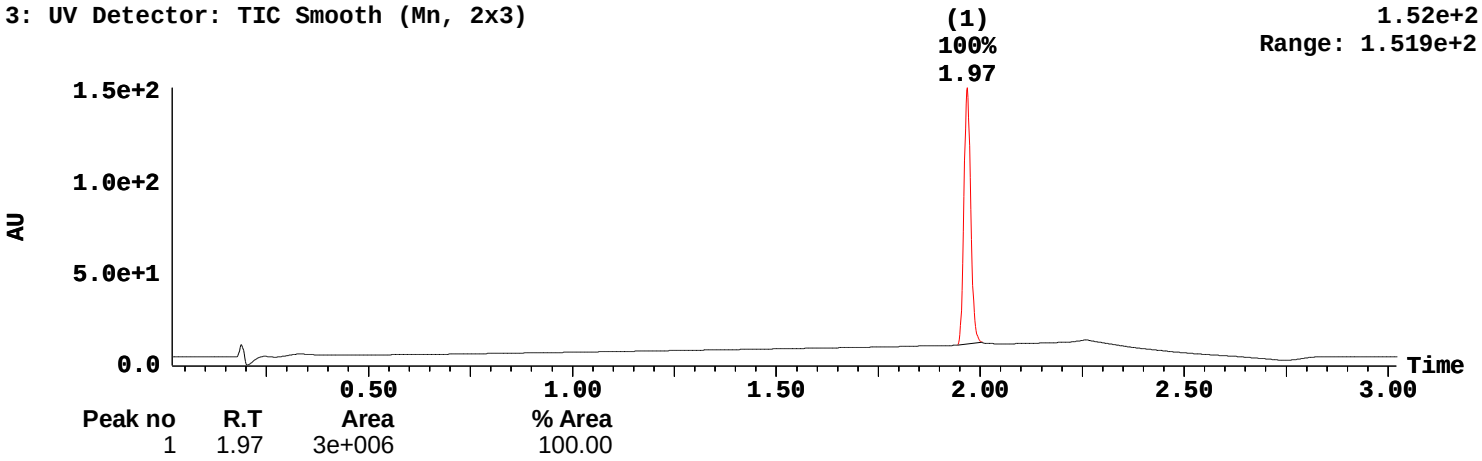


Fig 68. UPLC of 8-(4-fluorophenyl)-3,6-diphenyl-[1,2,4]triazolo[4,3-b]pyridazine (**3i**)

Sample Name:IS10607-058 Mobile A:0.1%HCOOH in Water Vial:1:26
Data File:A909936 Mobile B: 0.1%HCOOH in ACN Flow Rate:1.0 ml/min
Acq.Method:595FA.olp %B: 0min=5%2min=95%2.5min=5%3min=5% Inj Date:10-Feb-2014
Instrument Code :SC\AD\17-004 Column : Acquity UPLC HSS T3 (2.1x50)mm;1.8µm:

Printed: Mon Feb 10 15:04:34 2014

Sample Report:



Peak no	R.T	Area	% Area
1	1.97	3e+006	100.00

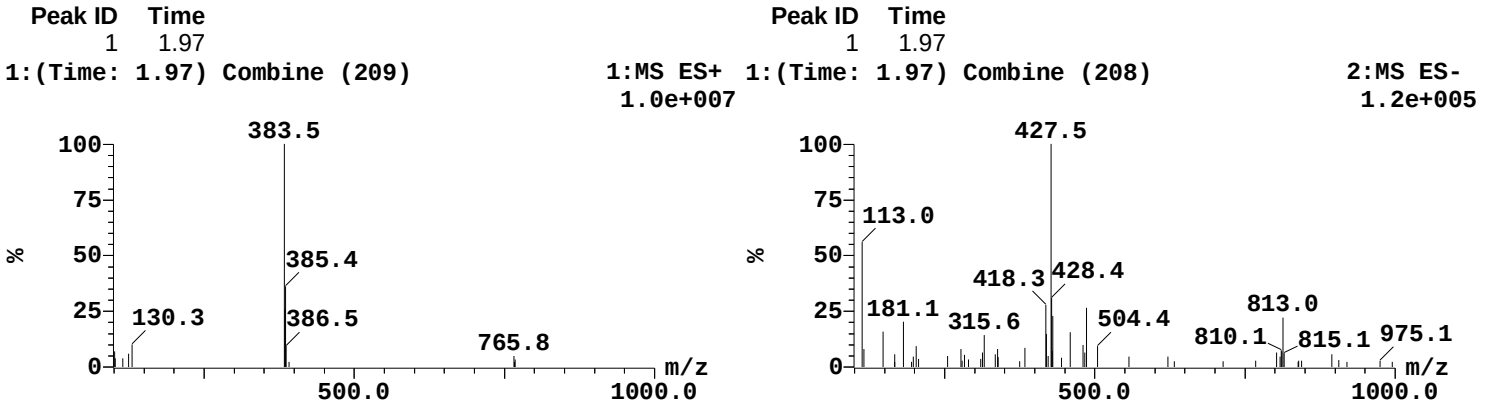
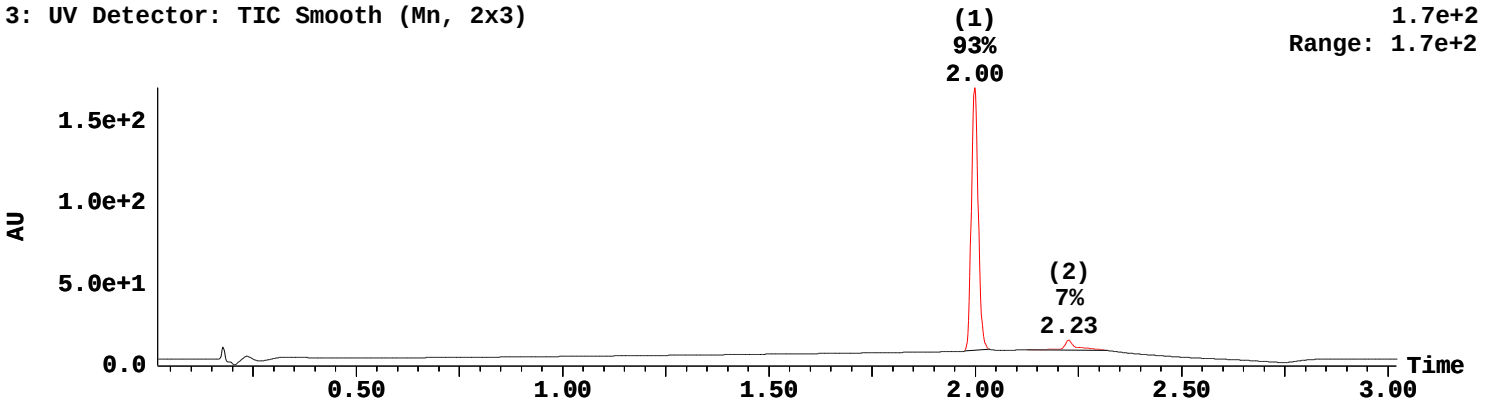


Fig 69. UPLC of 8-(4-chlorophenyl)-3,6-diphenyl-[1,2,4]triazolo[4,3-b]pyridazine (**3**j)

Sample Name:IS10607-058 Mobile A:0.1%HCOOH in Water Vial:1:2
Data File:A910313 Mobile B: 0.1%HCOOH in ACN Flow Rate:1.0 ml/min
Acq.Method:595FA.olp %B: 0min=5%2min=95%2.5min=5%3min=5% Inj Date:11-Feb-2014
Instrument Code :SC\AD\17-004 Column : Acquity UPLC HSS T3 (2.1x50)mm;1.8µm:

Printed: Tue Feb 11 09:48:13 2014

Sample Report:



Peak no	R.T	Area	% Area
1	2.00	3e+006	93.11
2	2.23	2e+005	6.89

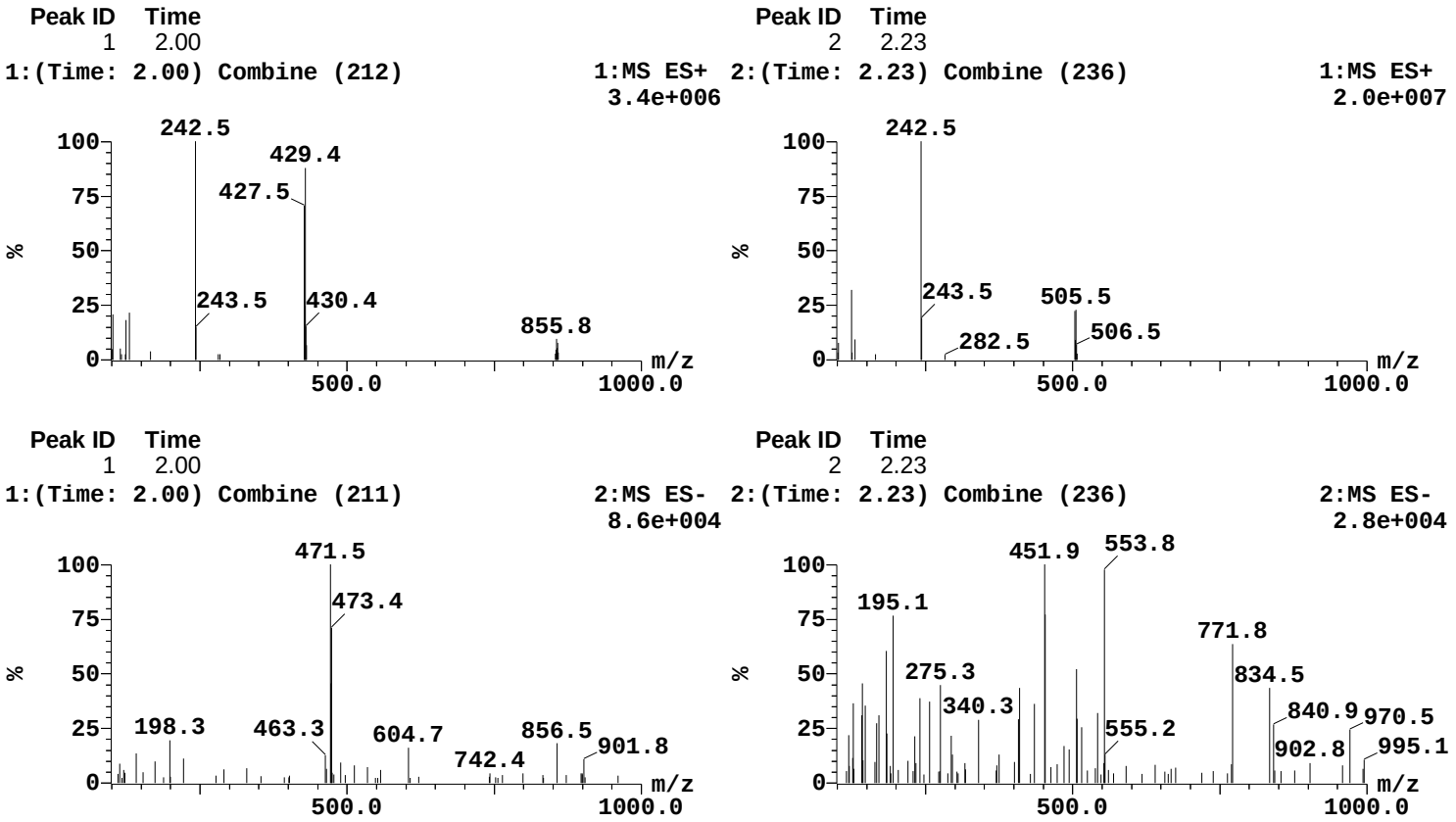
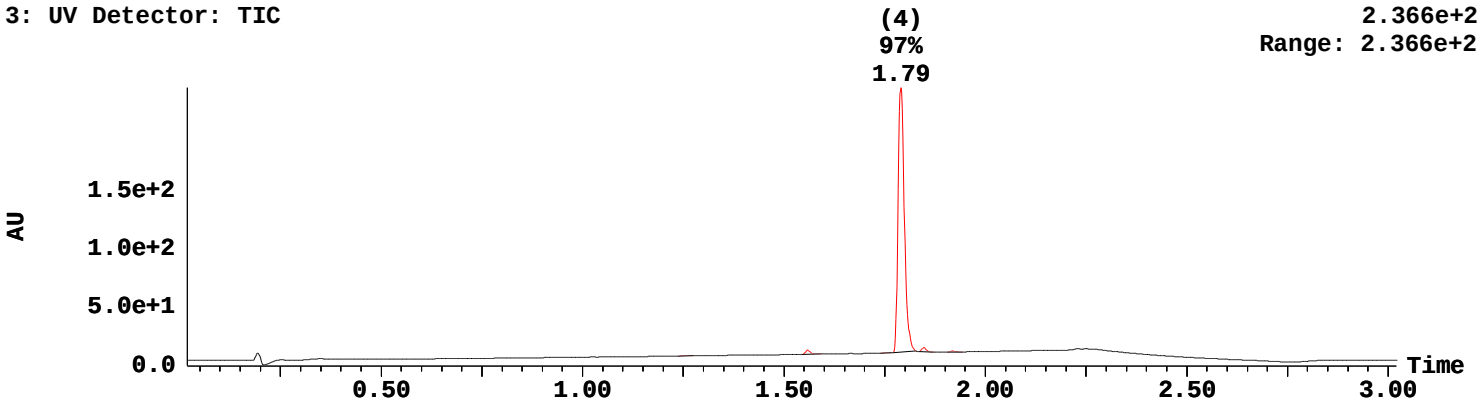


Fig 70. UPLC of 8-(4-bromophenyl)-3,6-diphenyl-[1,2,4]triazolo[4,3-b]pyridazine (**3k**)

Sample Name:IS10607-058 Mobile A:0.1%HCOOH in Water Vial:1:31
Data File:A936853 Mobile B: 0.1%HCOOH in ACN Flow Rate:1.0 ml/min
Acq.Method:595FA.olp %B: 0min=5%2min=95%2.5min=5%3min=5% Inj Date:14-Mar-2014
Instrument Code :SC\AD\17-004 Column : Acquity UPLC HSS T3 (2.1x50)mm;1.8µm:

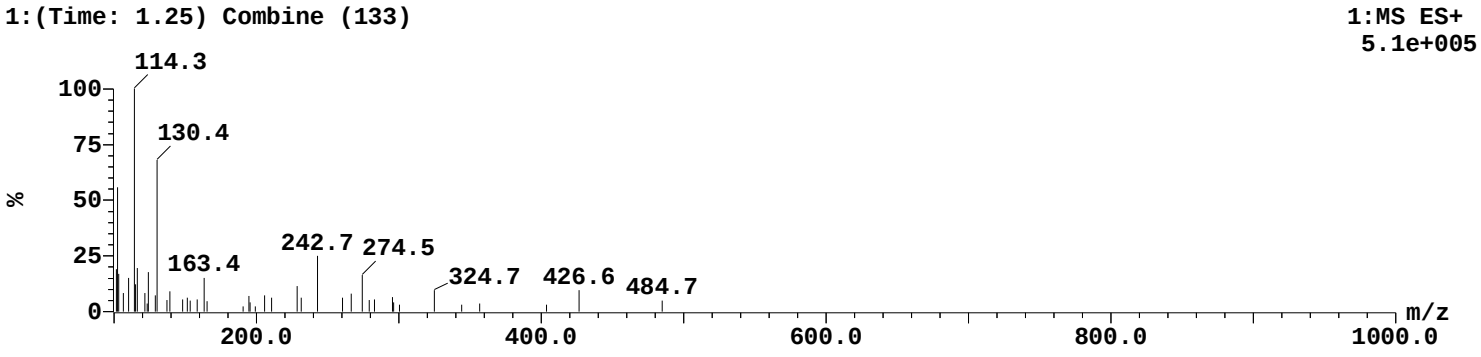
Printed: Fri Mar 14 11:53:46 2014

Sample Report:



Peak no	R.T	Area	% Area
1	1.25	6483	0.15
2	1.56	48830	1.17
3	1.75	5623	0.13
4	1.79	4068510	97.19
5	1.85	46372	1.11
6	1.92	10164	0.24

Peak ID	Time
1	1.25



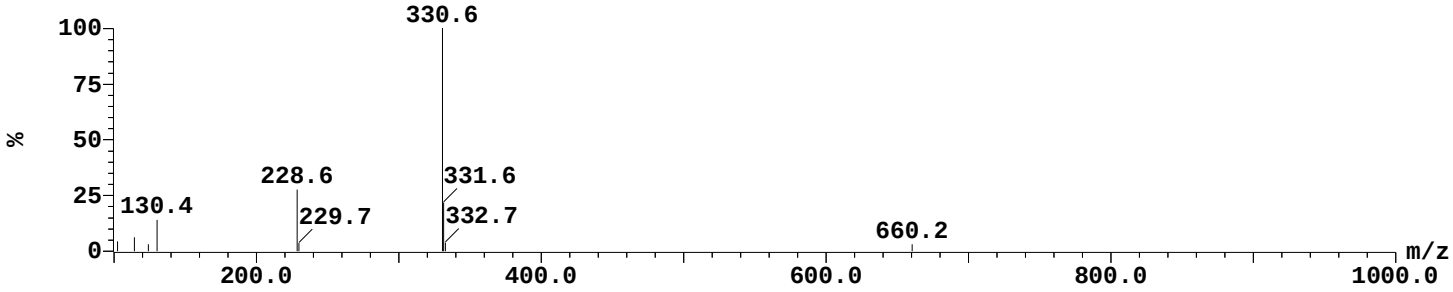
Sample Name:IS10607-058 Mobile A:0.1%HCOOH in Water Vial:1:31
Data File:A936853 Mobile B: 0.1%HCOOH in ACN Flow Rate:1.0 ml/min
Acq.Method:595FA.olp %B: 0min=5%2min=95%2.5min=5%3min=5% Inj Date:14-Mar-2014
Instrument Code :SC\AD\17-004 Column : Acquity UPLC HSS T3 (2.1x50)mm;1.8µm:

Printed: Fri Mar 14 11:53:46 2014

Sample Report (continued):

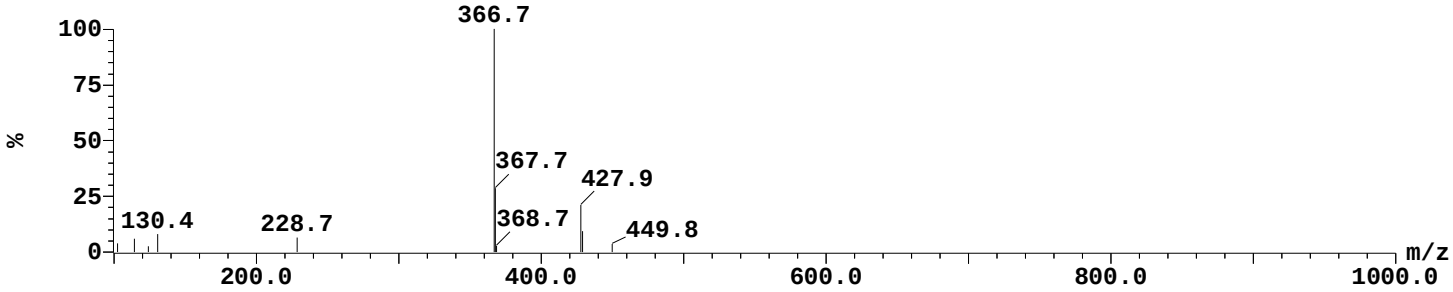
Peak ID	Time
2	1.56

2:(Time: 1.56) Combine (165) **1:MS ES+ 4.4e+006**



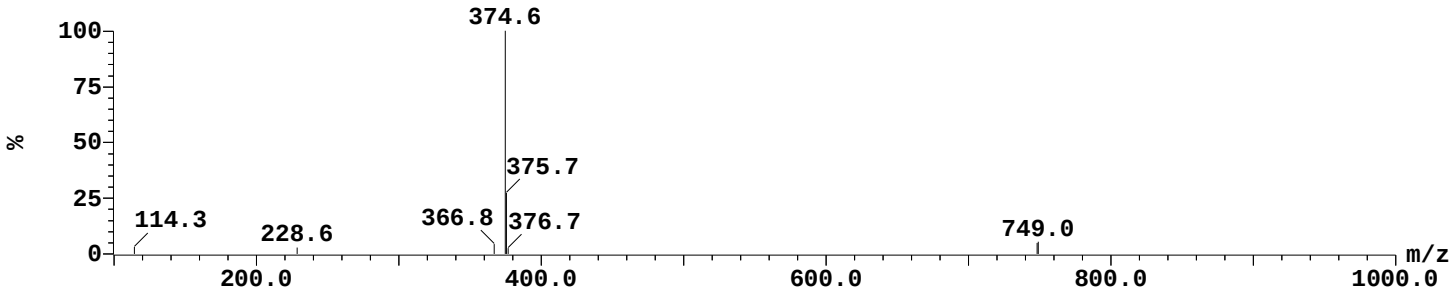
Peak ID	Time
3	1.75

3:(Time: 1.75) Combine (186) **1:MS ES+ 6.0e+006**



Peak ID	Time
4	1.79

4:(Time: 1.79) Combine (190) **1:MS ES+ 7.6e+006**



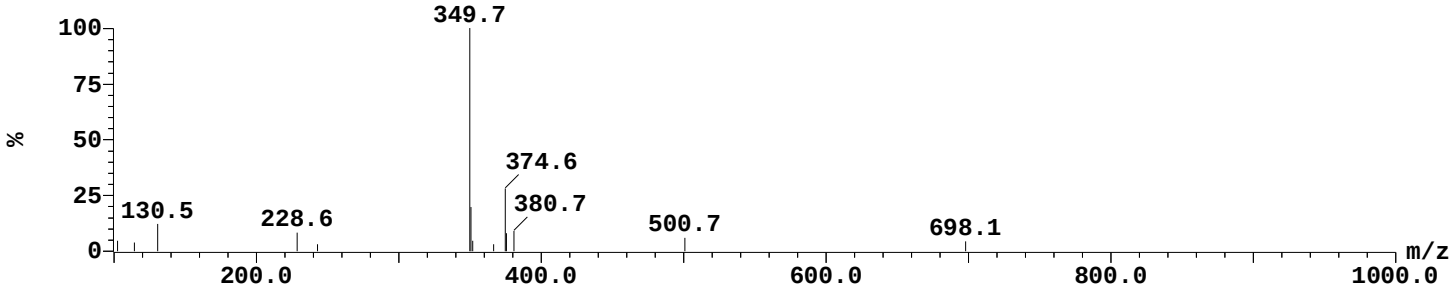
Sample Name:IS10607-058 Mobile A:0.1%HCOOH in Water Vial:1:31
Data File:A936853 Mobile B: 0.1%HCOOH in ACN Flow Rate:1.0 ml/min
Acq.Method:595FA.olp %B: 0min=5%2min=95%2.5min=5%3min=5% Inj Date:14-Mar-2014
Instrument Code :SC\AD\17-004 Column : Acquity UPLC HSS T3 (2.1x50)mm;1.8µm:

Printed: Fri Mar 14 11:53:46 2014

Sample Report (continued):

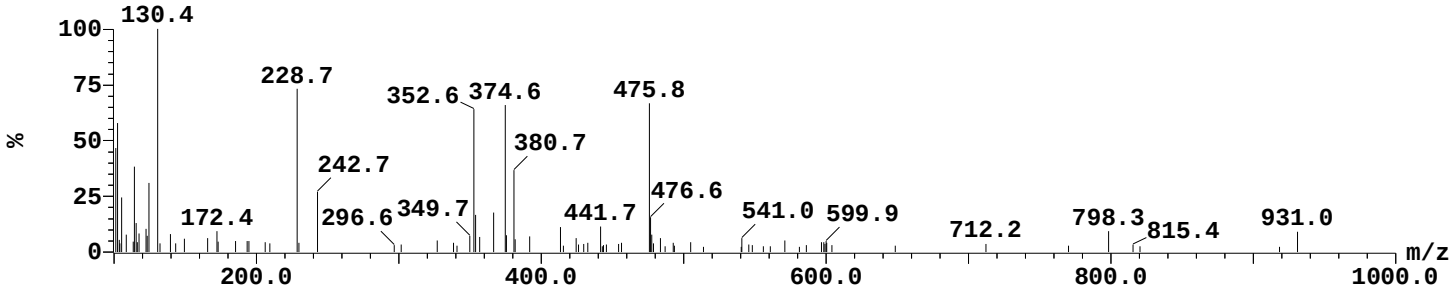
Peak ID	Time
5	1.85

5:(Time: 1.85) Combine (196) **1:MS ES+ 6.8e+006**



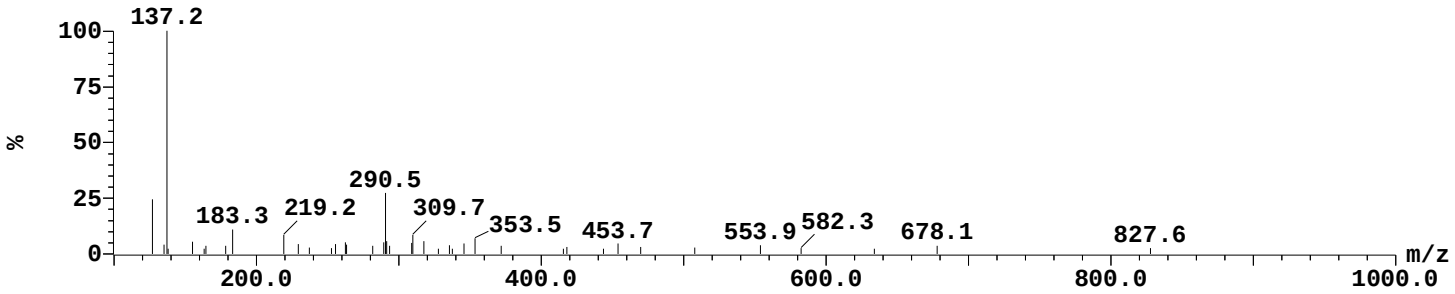
Peak ID	Time
6	1.92

6:(Time: 1.92) Combine (204) **1:MS ES+ 7.3e+005**



Peak ID	Time
1	1.25

1:(Time: 1.25) Combine (132) **2:MS ES- 8.5e+005**



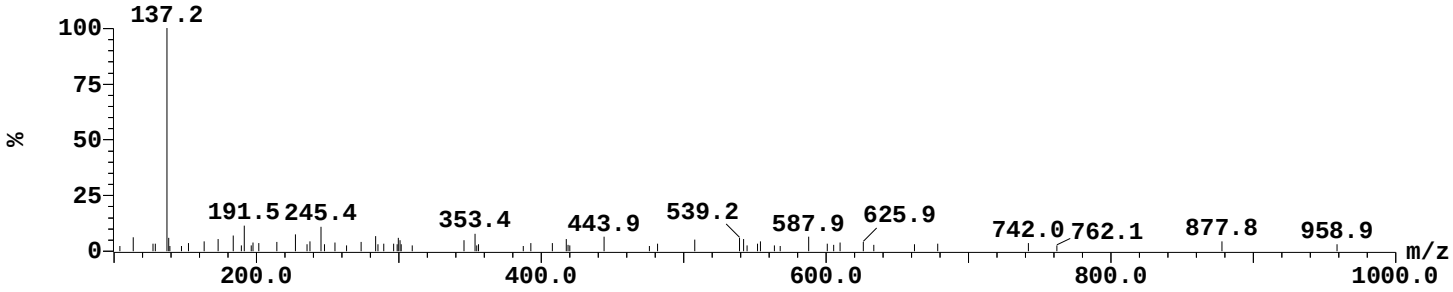
Sample Name:IS10607-058 Mobile A:0.1%HCOOH in Water Vial:1:31
Data File:A936853 Mobile B: 0.1%HCOOH in ACN Flow Rate:1.0 ml/min
Acq.Method:595FA.olp %B: 0min=5%2min=95%2.5min=5%3min=5% Inj Date:14-Mar-2014
Instrument Code :SC\AD\17-004 Column : Acquity UPLC HSS T3 (2.1x50)mm;1.8µm:

Printed: Fri Mar 14 11:53:46 2014

Sample Report (continued):

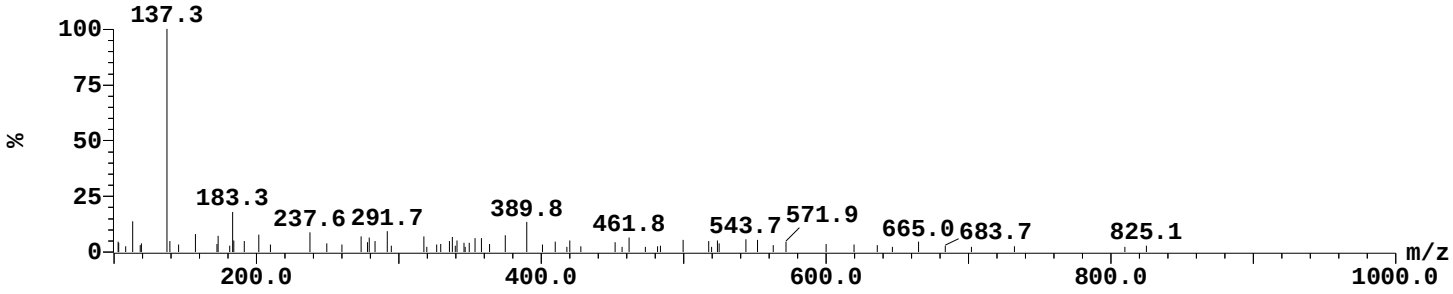
Peak ID	Time
2	1.56

2:(Time: 1.56) Combine (165) **2:MS ES- 5.5e+005**



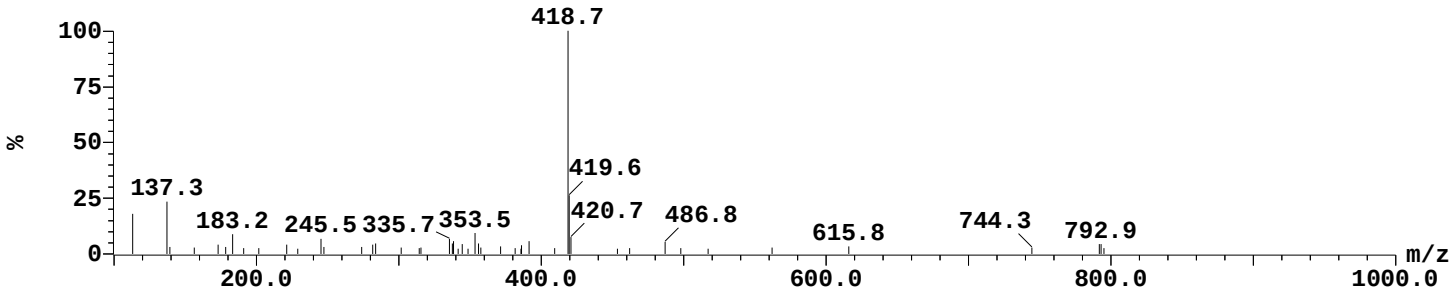
Peak ID	Time
3	1.75

3:(Time: 1.75) Combine (186) **2:MS ES- 5.2e+005**



Peak ID	Time
4	1.79

4:(Time: 1.79) Combine (189) **2:MS ES- 4.0e+005**



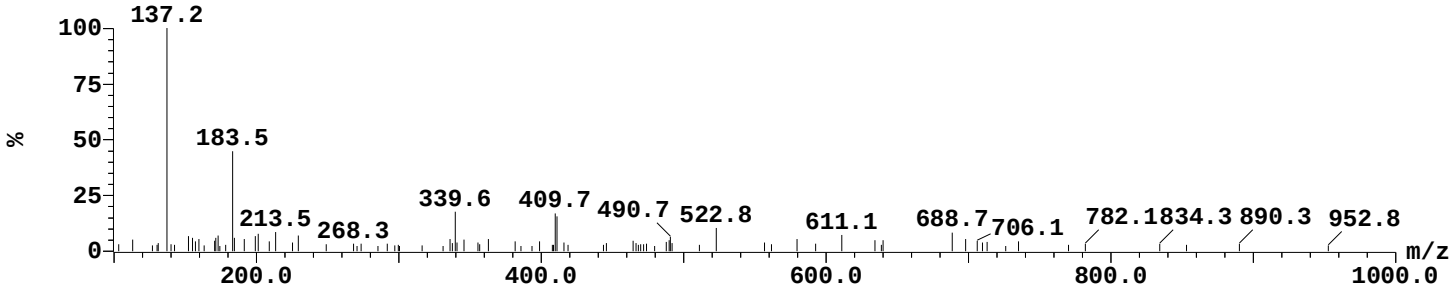
Sample Name:IS10607-058 Mobile A:0.1%HCOOH in Water Vial:1:31
Data File:A936853 Mobile B: 0.1%HCOOH in ACN Flow Rate:1.0 ml/min
Acq.Method:595FA.olp %B: 0min=5%2min=95%2.5min=5%3min=5% Inj Date:14-Mar-2014
Instrument Code :SC\AD\17-004 Column : Acquity UPLC HSS T3 (2.1x50)mm;1.8µm:

Printed: Fri Mar 14 11:53:46 2014

Sample Report (continued):

Peak ID	Time
5	1.85

5:(Time: 1.85) Combine (195) **2:MS ES- 3.6e+005**



Peak ID	Time
6	1.92

6:(Time: 1.92) Combine (203) **2:MS ES- 1.6e+005**

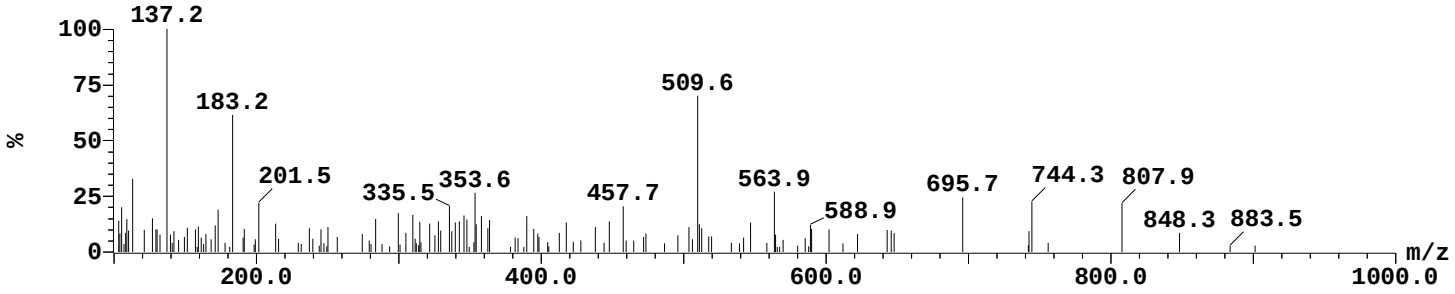
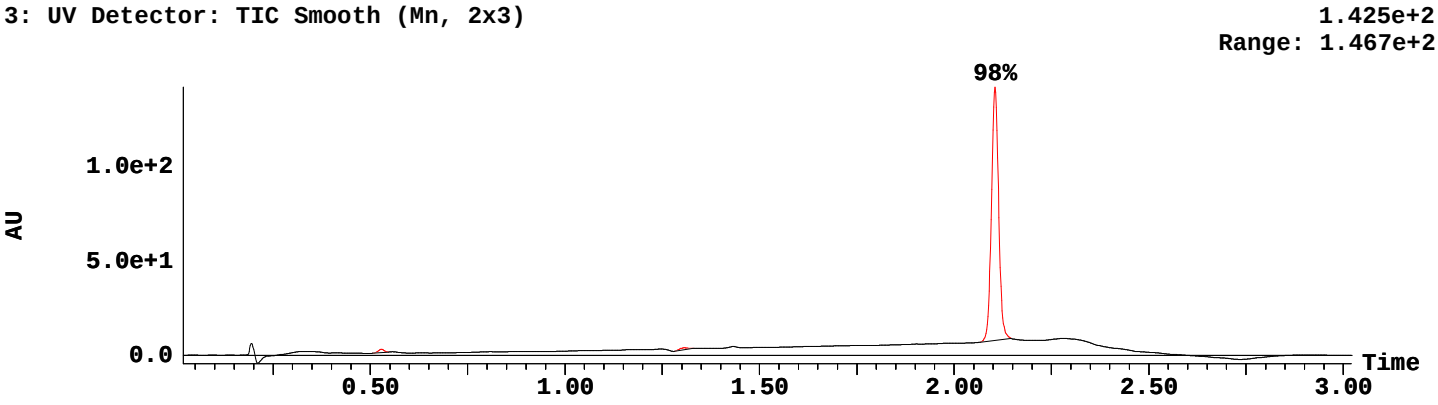


Fig 71. UPLC of 4-(3,6-diphenyl-[1,2,4]triazolo[4,3-b]pyridazin-8-yl)benzonitrile (**3l**)

Sample Name:IS10607-058 Mobile A:0.1%HCOOH in Water Vial:2:D,1
Data File:A911130 Mobile B: 0.1%HCOOH in ACN Flow Rate:1.0 ml/min
Acq.Method:595FA.olp %B: 0min=5%2min=95%2.5min=5%3min=5% Inj Date:12-Feb-2014
Instrument Code :SC\AD\17-005 Column : Acquity UPLC HSS T3 (2.1x50)mm;1.8µm:

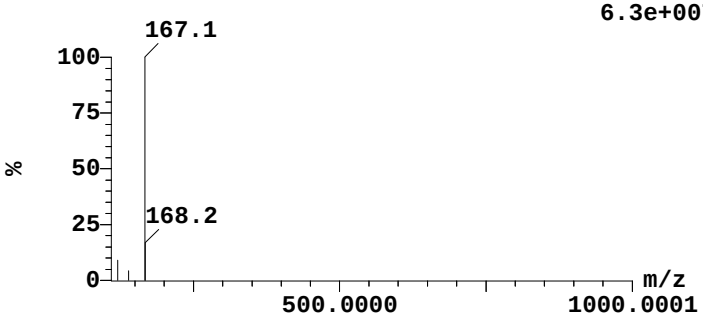
Printed: Wed Feb 12 19:05:41 2014

Sample Report:

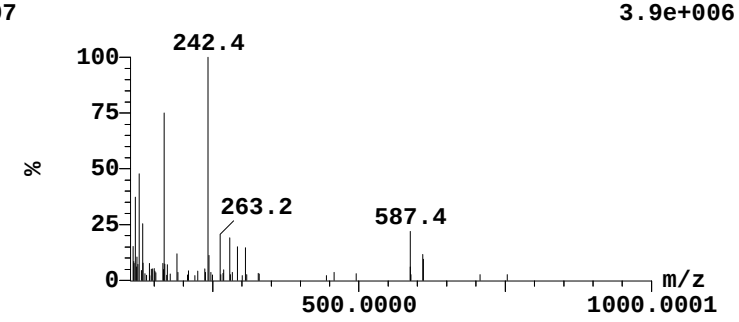


Peak no	R.T	Area	% Area
1	0.53	3e+004	1.06
2	1.31	3e+004	0.95
3	2.11	3e+006	97.98

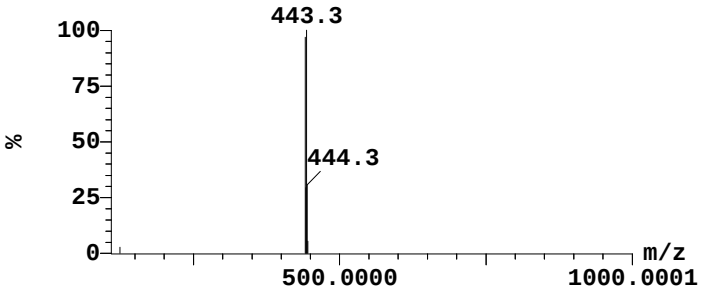
Peak ID Time
1 0.53



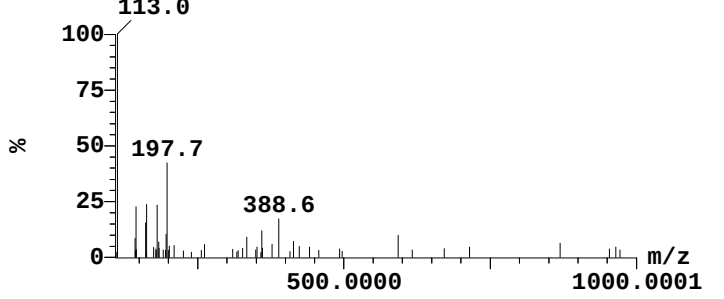
Peak ID Time
2 1.31



Peak ID Time
3 2.11



Peak ID Time
1 0.53



Sample Name:IS10607-058 Mobile A:0.1%HCOOH in Water Vial:2:D,1
Data File:A911130 Mobile B: 0.1%HCOOH in ACN Flow Rate:1.0 ml/min
Acq.Method:595FA.olp %B: 0min=5%2min=95%2.5min=5%3min=5% Inj Date:12-Feb-2014
Instrument Code :SC\AD\17-005 Column : Acquity UPLC HSS T3 (2.1x50)mm;1.8µm:

Printed: Wed Feb 12 19:05:41 2014

Sample Report (continued):

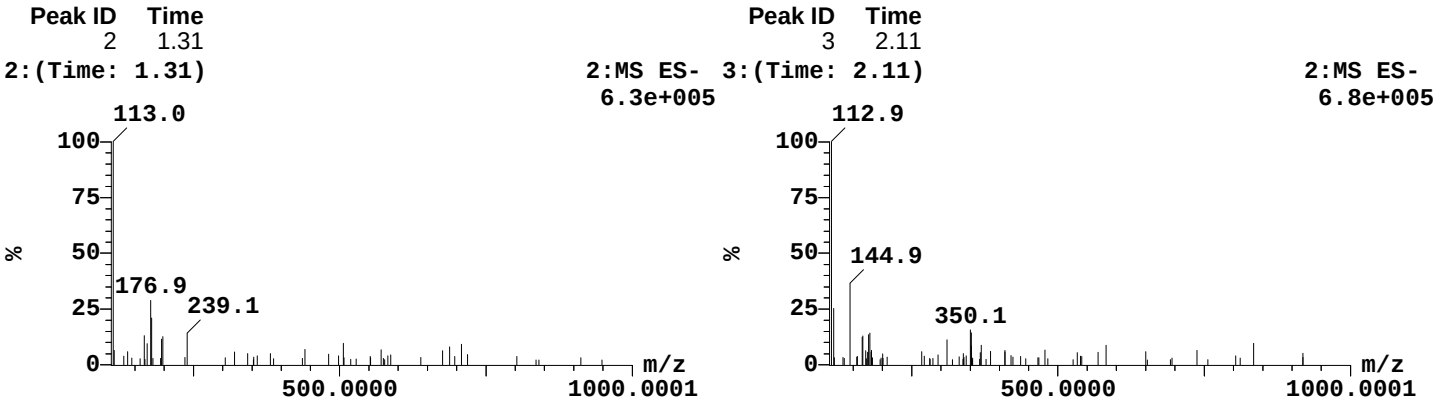
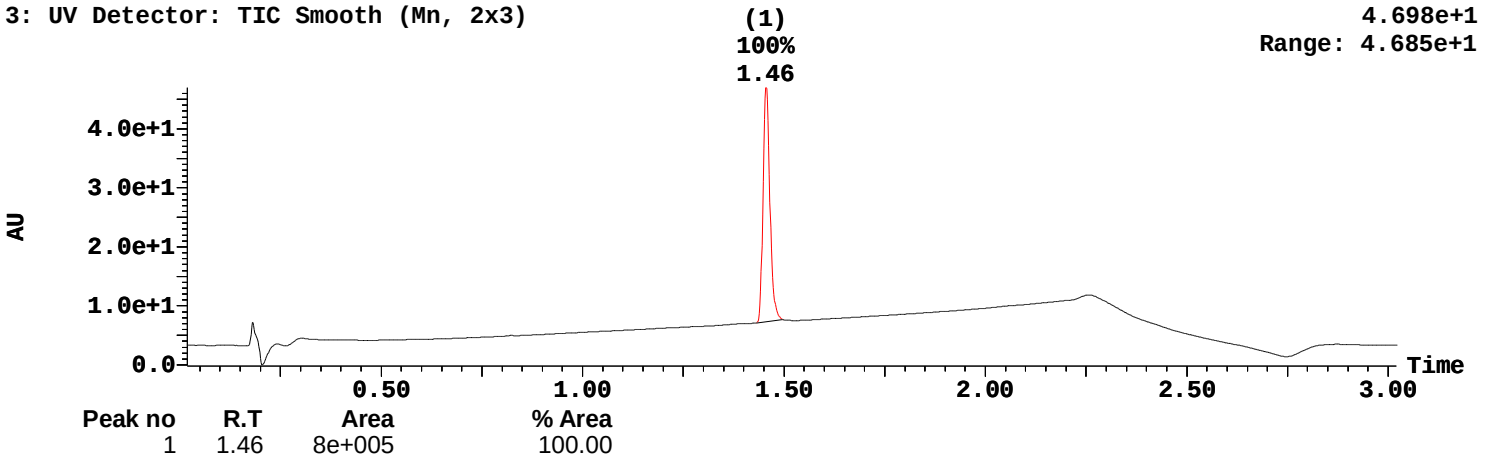


Fig 72. UPLC of 8-(4-bromo-3-methylphenyl)-3,6-diphenyl-[1,2,4]triazolo[4,3-b]pyridazine (**3m**)

Sample Name:IS10607-058 Mobile A:0.1%HCOOH in Water Vial:1:5
Data File:A914856 Mobile B: 0.1%HCOOH in ACN Flow Rate:1.0 ml/min
Acq.Method:595FA.olp %B: 0min=5%2min=95%2.5min=5%3min=5% Inj Date:17-Feb-2014
Instrument Code :SC\AD\17-004 Column : Acquity UPLC HSS T3 (2.1x50)mm;1.8µm:

Printed: Mon Feb 17 10:59:20 2014

Sample Report:



Peak no	R.T	Area	% Area
1	1.46	8e+005	100.00

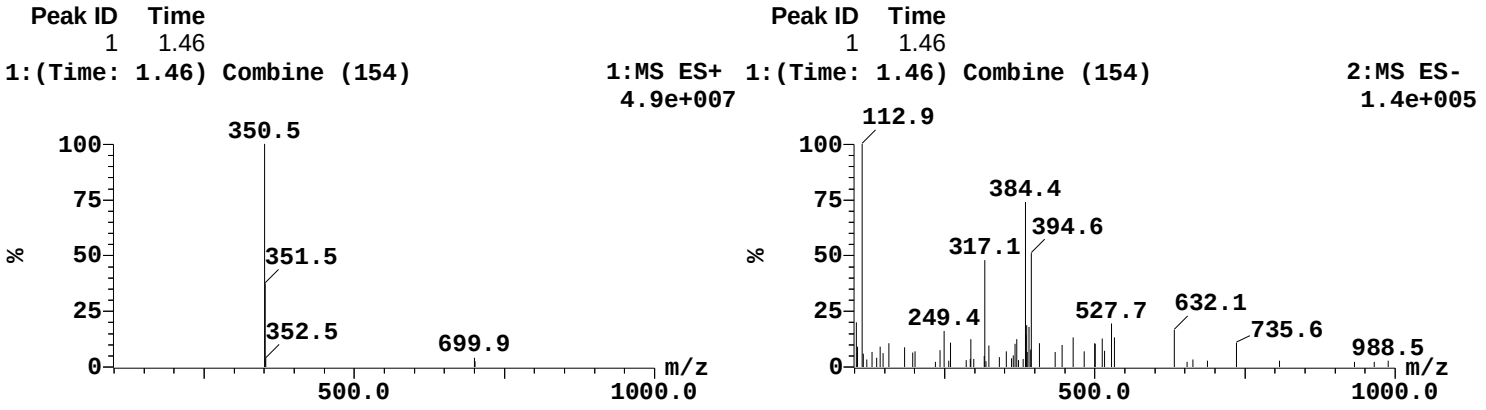
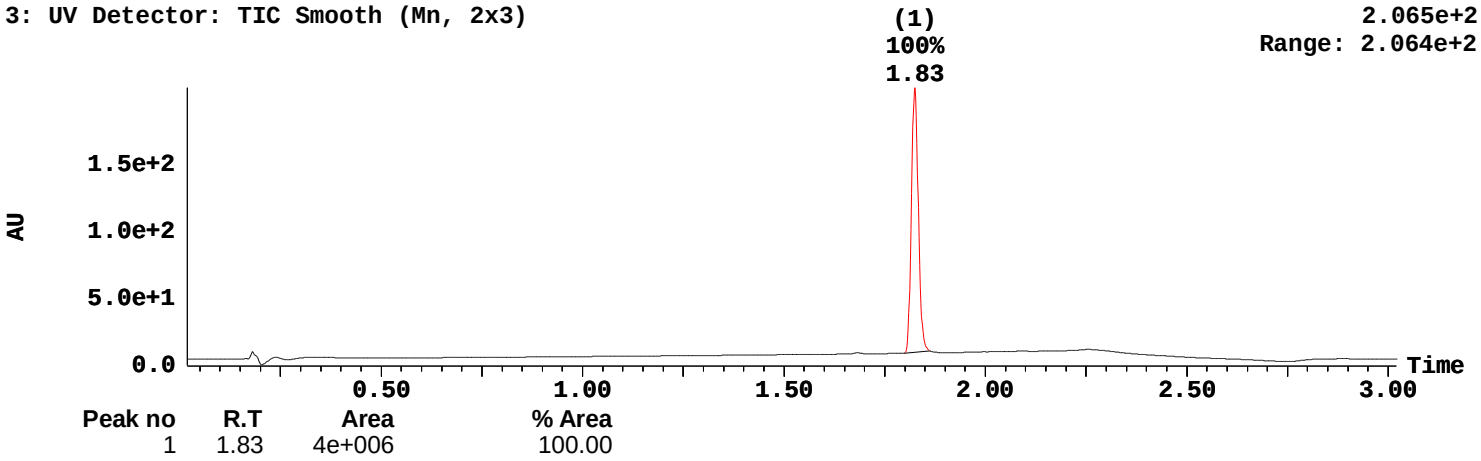


Fig 73. UPLC of 3,6-diphenyl-8-(pyridin-3-yl)-[1,2,4]triazolo[4,3-b]pyridazine (**3n**)

Sample Name:IS10607-058 Mobile A:0.1%HCOOH in Water Vial:1:3
Data File:A910316 Mobile B: 0.1%HCOOH in ACN Flow Rate:1.0 ml/min
Acq.Method:595FA.olp %B: 0min=5%2min=95%2.5min=5%3min=5% Inj Date:11-Feb-2014
Instrument Code :SC\AD\17-004 Column : Acquity UPLC HSS T3 (2.1x50)mm;1.8µm:

Printed: Tue Feb 11 09:46:58 2014

Sample Report:



Peak no	R.T	Area	% Area
1	1.83	4e+006	100.00

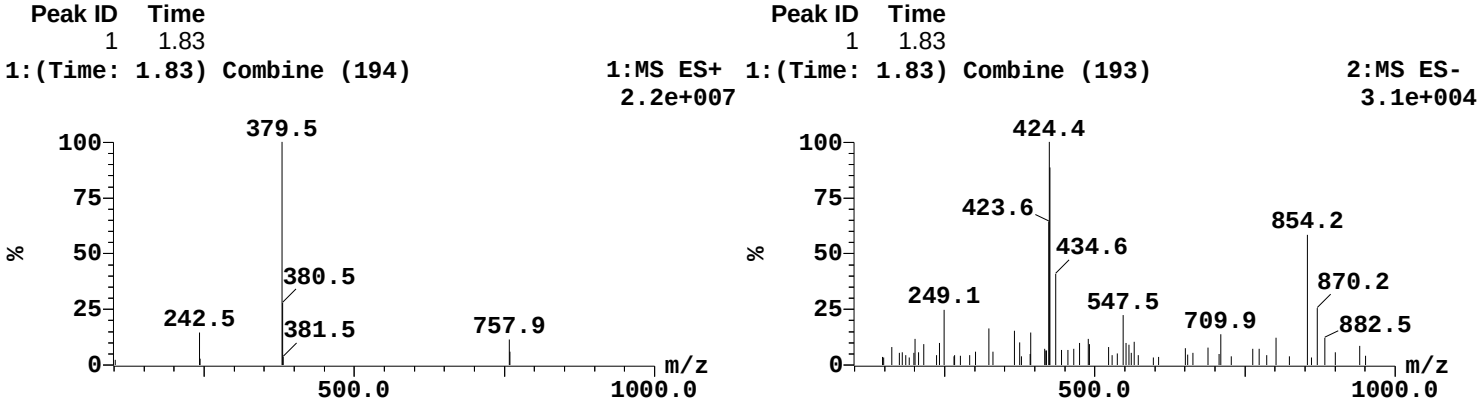
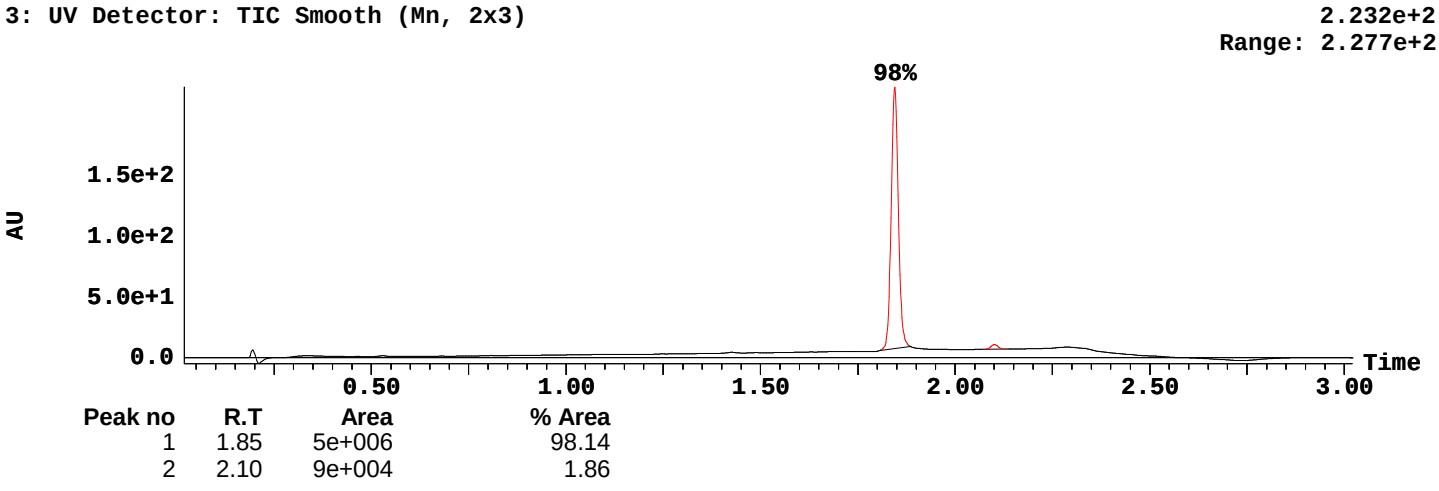


Fig 74. UPLC of 6-(4-Methoxyphenyl)-3,8-diphenyl-[1,2,4]triazolo[4,3-b]pyridazine (**5a**)

Sample Name:IS10607-058 Mobile A:0.1%HCOOH in Water Vial:2:D,2
Data File:A911132 Mobile B: 0.1%HCOOH in ACN Flow Rate:1.0 ml/min
Acq.Method:595FA.olp %B: 0min=5%2min=95%2.5min=5%3min=5% Inj Date:12-Feb-2014
Instrument Code :SC\AD\17-005 Column : Acquity UPLC HSS T3 (2.1x50)mm;1.8µm:

Printed: Wed Feb 12 19:06:04 2014

Sample Report:



Peak no	R.T	Area	% Area
1	1.85	5e+006	98.14
2	2.10	9e+004	1.86

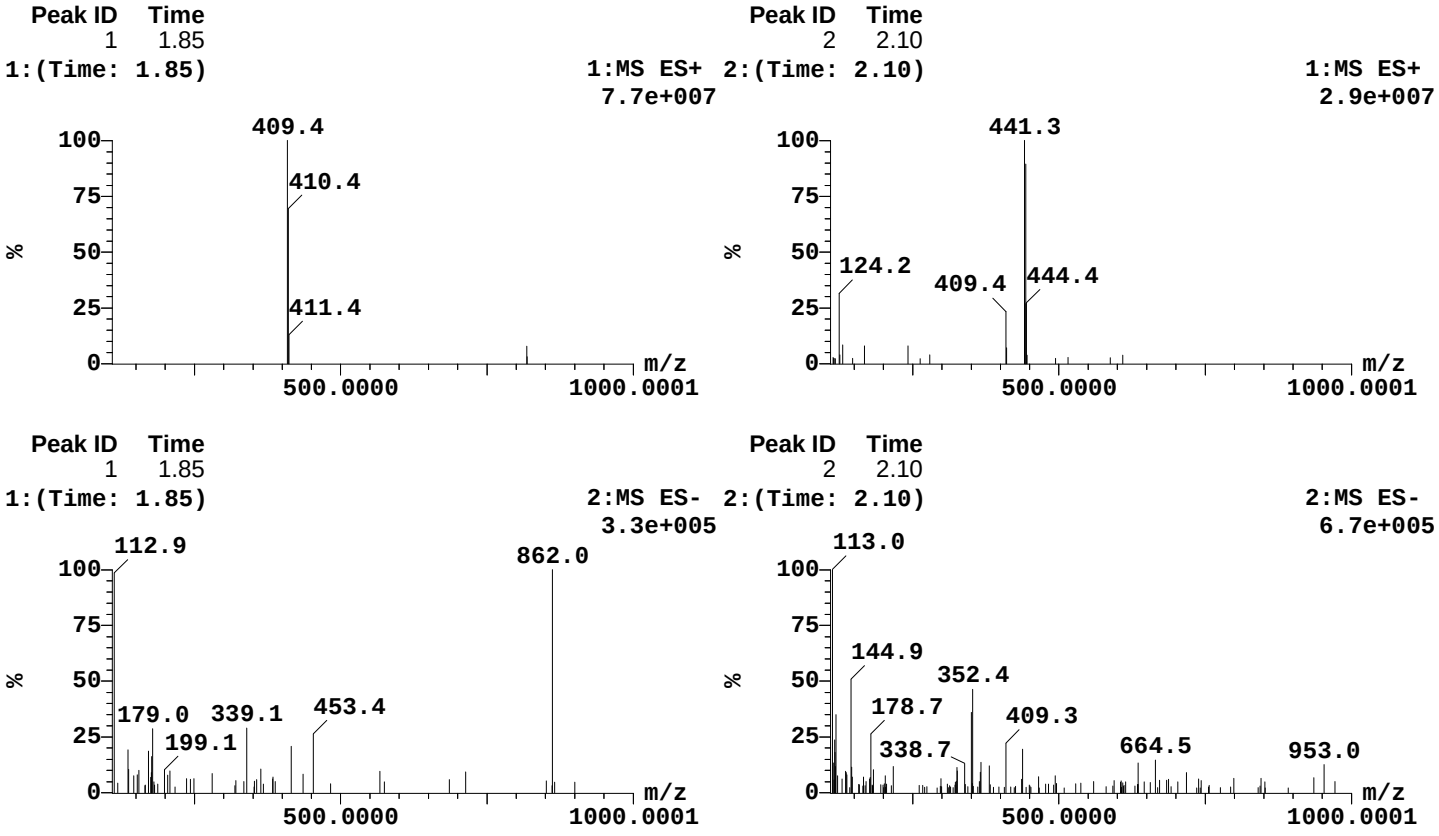
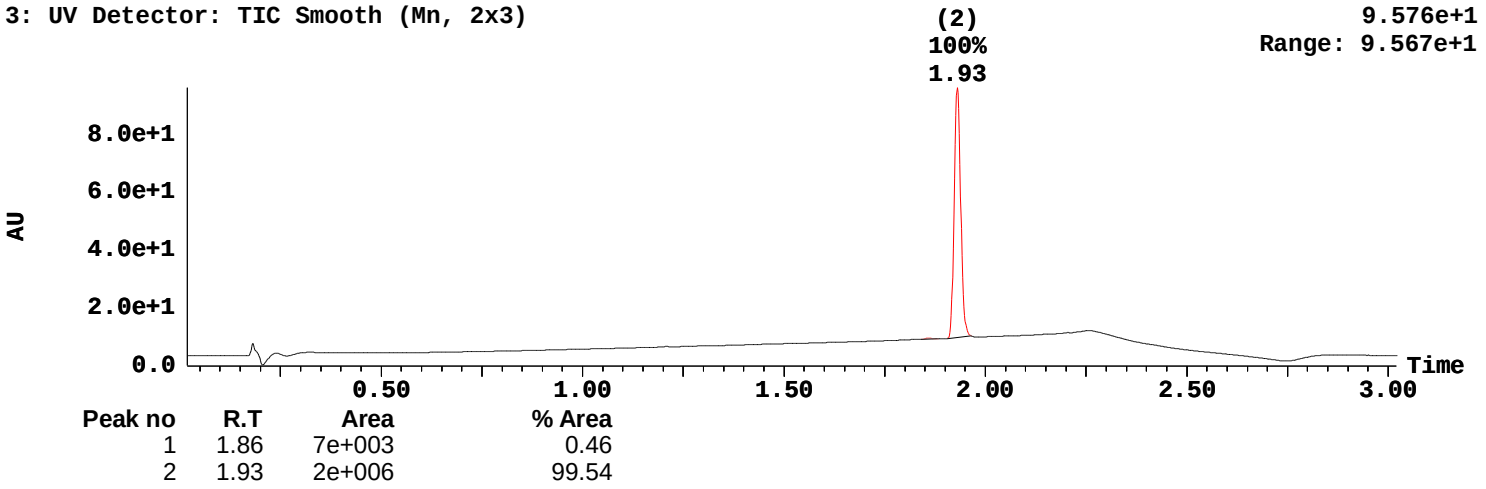


Fig 75. UPLC of 8-(3-Methoxyphenyl)-6-(4-methoxyphenyl)-3-phenyl-[1,2,4]triazolo[4,3-b] pyridazine (**5b**)

Sample Name:IS10607-058 Mobile A:0.1%HCOOH in Water Vial:1:8
Data File:A914962 Mobile B: 0.1%HCOOH in ACN Flow Rate:1.0 ml/min
Acq.Method:595FA.olp %B: 0min=5%2min=95%2.5min=5%3min=5% Inj Date:17-Feb-2014
Instrument Code :SC\AD\17-004 Column : Acquity UPLC HSS T3 (2.1x50)mm;1.8µm:

Printed: Mon Feb 17 12:18:21 2014

Sample Report:



Peak no	R.T	Area	% Area
1	1.86	7e+003	0.46
2	1.93	2e+006	99.54

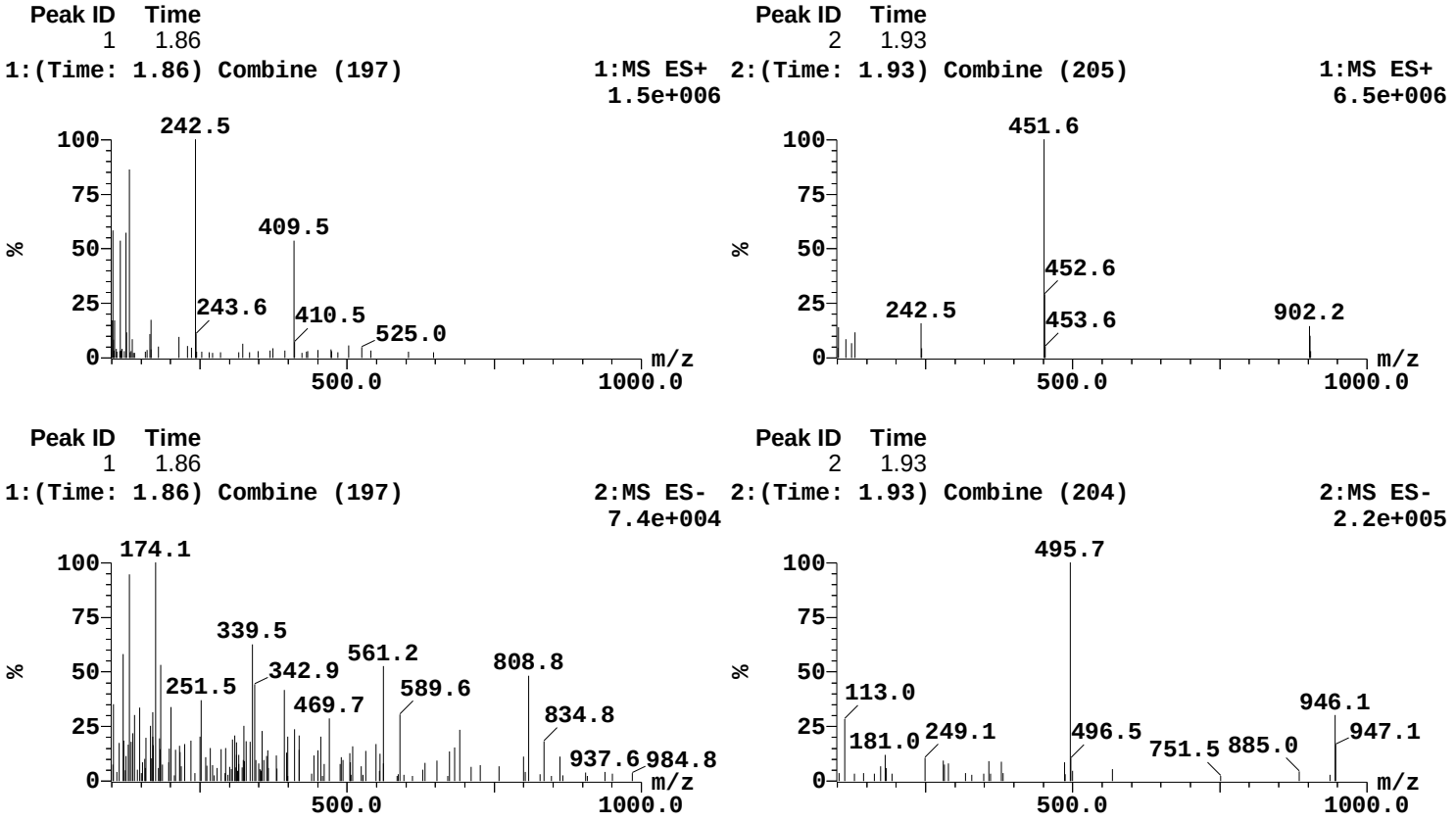
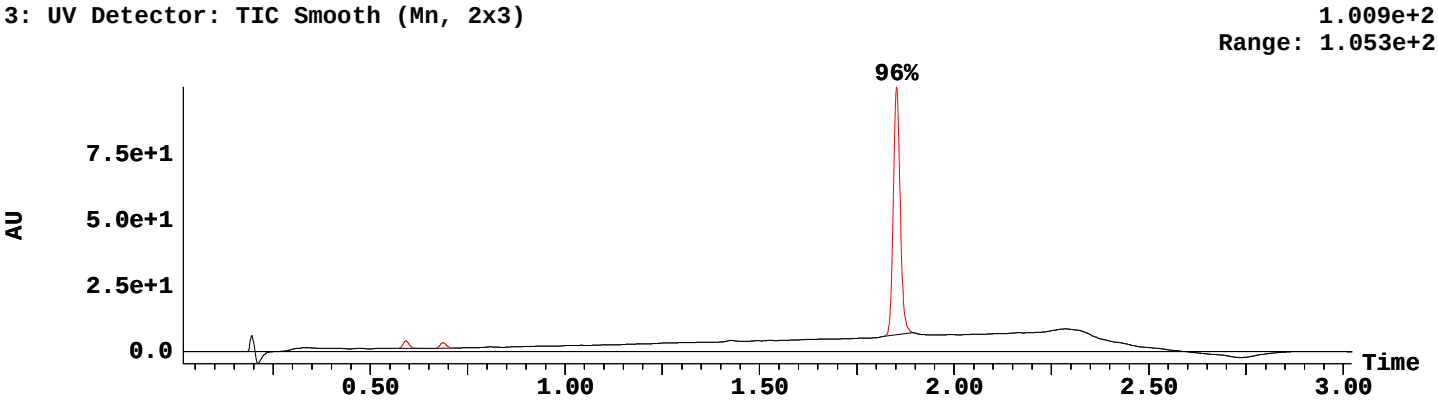


Fig 76. UPLC of Ethyl 3-(6-(4-methoxyphenyl)-3-phenyl-[1,2,4]triazolo[4,3-b]pyridazin-8-yl) benzoate (**5c**)

Sample Name:IS10607-058 Mobile A:0.1%HCOOH in Water Vial:2:D,4
Data File:A911133A Mobile B: 0.1%HCOOH in ACN Flow Rate:1.0 ml/min
Acq.Method:595FA.olp %B: 0min=5%2min=95%2.5min=5%3min=5% Inj Date:12-Feb-2014
Instrument Code :SC\AD\17-005 Column : Acquity UPLC HSS T3 (2.1x50)mm;1.8µm:

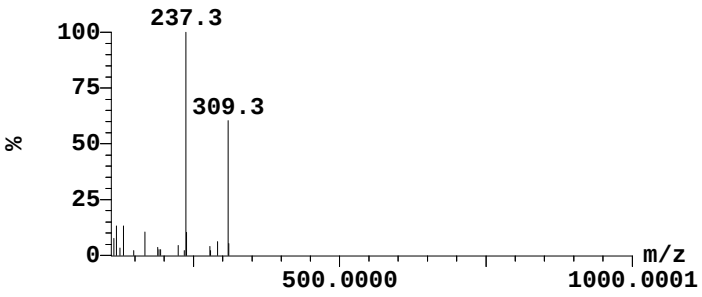
Printed: Wed Feb 12 19:32:47 2014

Sample Report:

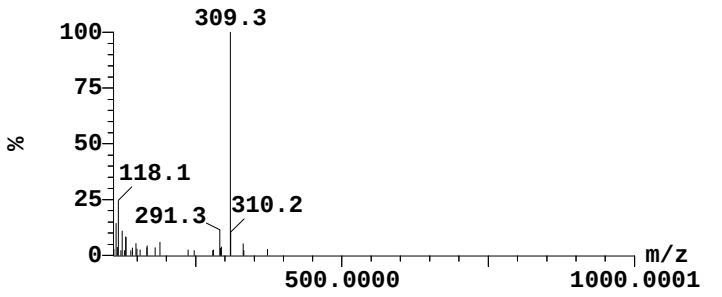


Peak no	R.T	Area	% Area
1	0.59	5e+004	2.49
2	0.69	4e+004	1.93
3	1.85	2e+006	95.58

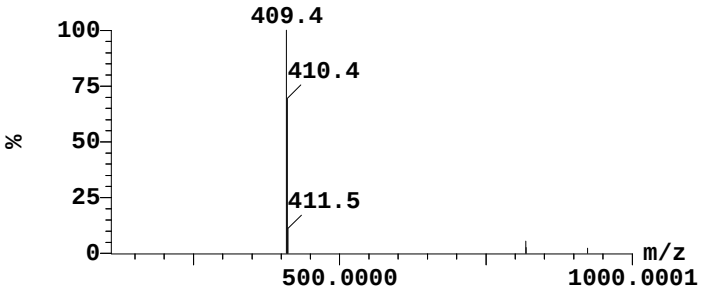
Peak ID Time
1 0.59



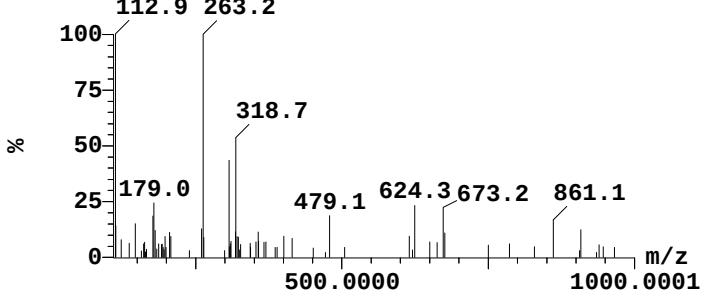
Peak ID Time
2 0.69



Peak ID Time
3 1.85



Peak ID Time
1 0.59



Sample Name:IS10607-058 Mobile A:0.1%HCOOH in Water Vial:2:D,4
Data File:A911133A Mobile B: 0.1%HCOOH in ACN Flow Rate:1.0 ml/min
Acq.Method:595FA.olp %B: 0min=5%2min=95%2.5min=5%3min=5% Inj Date:12-Feb-2014
Instrument Code :SC\AD\17-005 Column : Acquity UPLC HSS T3 (2.1x50)mm;1.8µm:

Printed: Wed Feb 12 19:32:47 2014

Sample Report (continued):

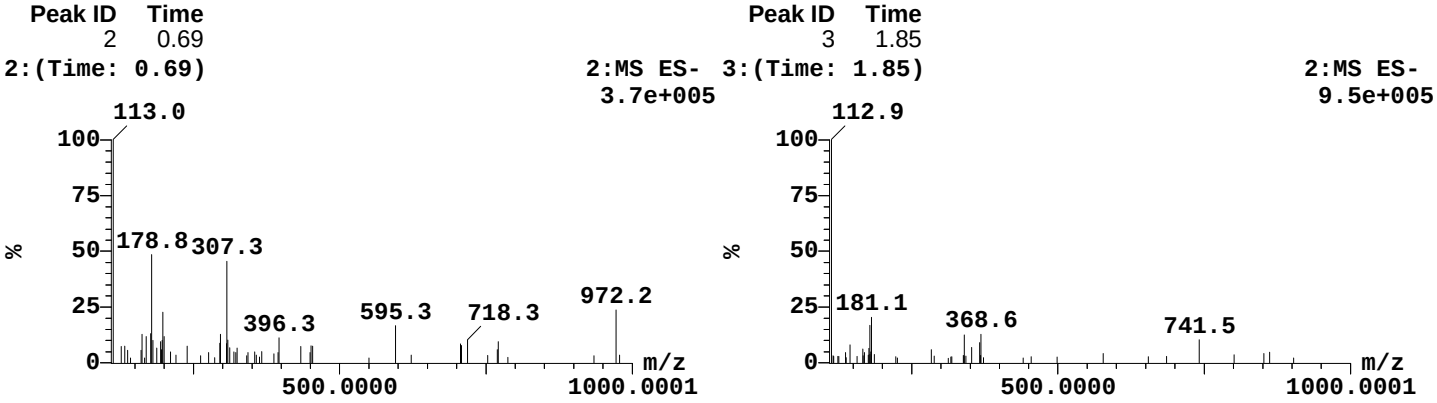
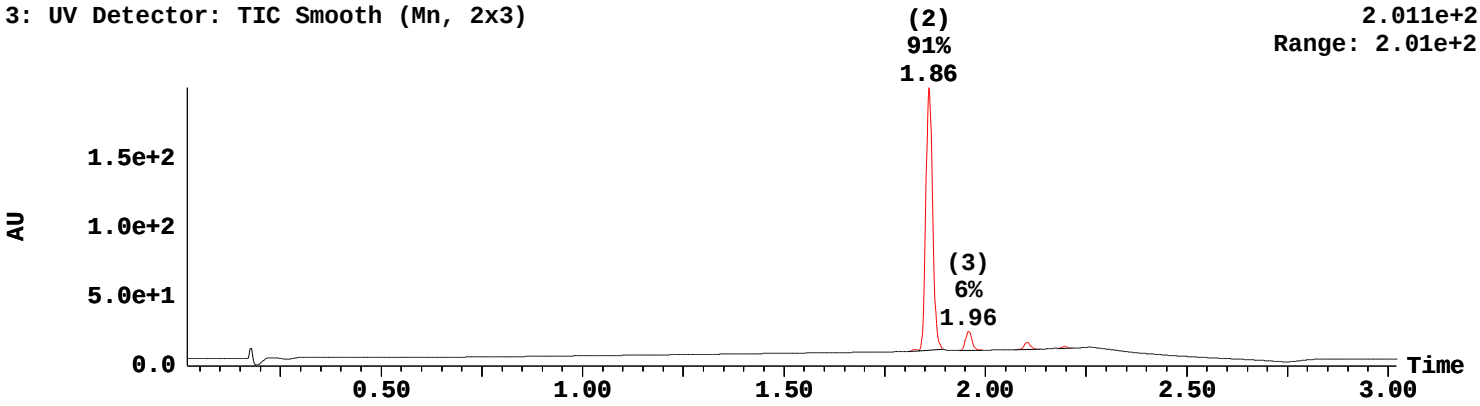


Fig 77. UPLC of 6,8-bis(4-Methoxyphenyl)-3-phenyl-[1,2,4]triazolo[4,3-b]pyridazine (**5d**)

Sample Name:IS10607-058 Mobile A:0.1%HCOOH in Water Vial:1:1
Data File:A914853 Mobile B: 0.1%HCOOH in ACN Flow Rate:1.0 ml/min
Acq.Method:595FA.olp %B: 0min=5%2min=95%2.5min=5%3min=5% Inj Date:17-Feb-2014
Instrument Code :SC\AD\17-004 Column : Acquity UPLC HSS T3 (2.1x50)mm;1.8µm:

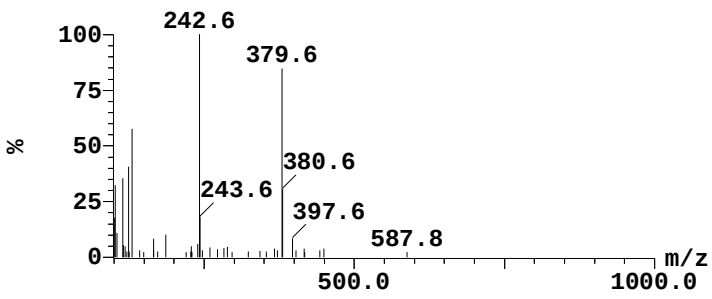
Printed: Mon Feb 17 10:28:14 2014

Sample Report:

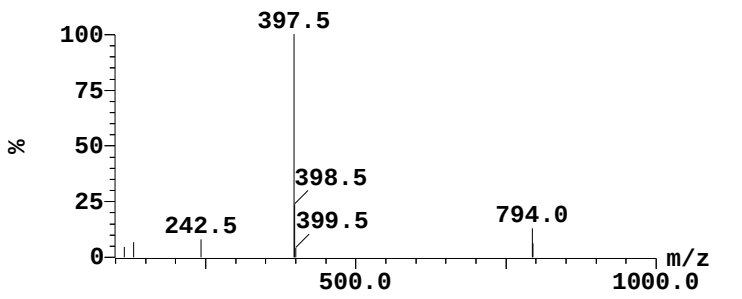


Peak no	R.T	Area	% Area
1	1.83	2e+004	0.43
2	1.86	4e+006	90.67
3	1.96	3e+005	6.17
4	2.10	9e+004	2.22
5	2.20	2e+004	0.51

Peak ID	Time
1	1.83



Peak ID	Time
2	1.86



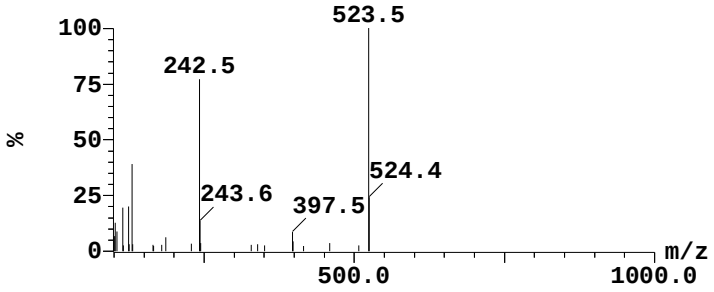
Sample Name:IS10607-058 Mobile A:0.1%HCOOH in Water Vial:1:1
Data File:A914853 Mobile B: 0.1%HCOOH in ACN Flow Rate:1.0 ml/min
Acq.Method:595FA.olp %B: 0min=5%2min=95%2.5min=5%3min=5% Inj Date:17-Feb-2014
Instrument Code :SC\AD\17-004 Column : Acquity UPLC HSS T3 (2.1x50)mm;1.8µm:

Printed: Mon Feb 17 10:28:14 2014

Sample Report (continued):

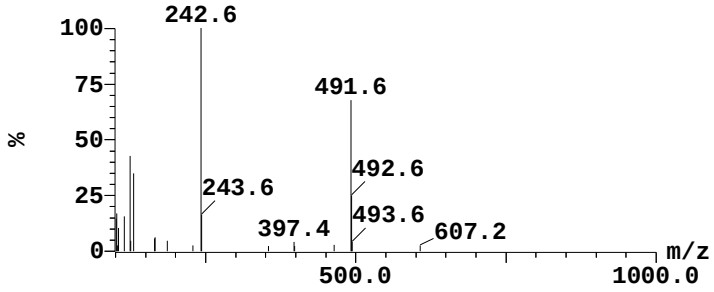
Peak ID Time
3 1.96

3:(Time: 1.96) Combine (208) **1:MS ES+** **4.4e+006**



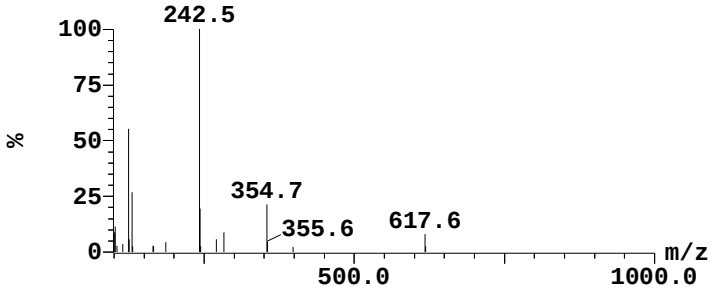
Peak ID Time
4 2.10

4:(Time: 2.10) Combine (223) **1:MS ES+** **5.6e+006**



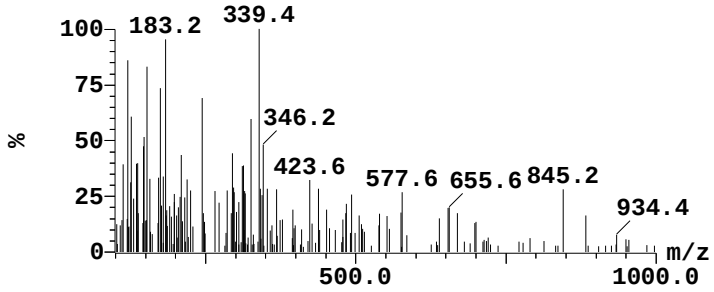
Peak ID Time
5 2.20

5:(Time: 2.20) Combine (233) **1:MS ES+** **1.2e+007**



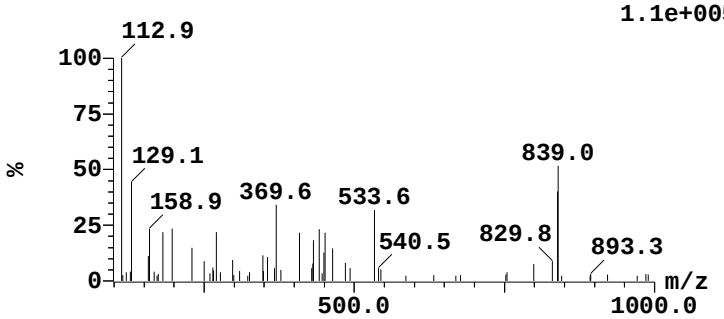
Peak ID Time
1 1.83

1:(Time: 1.83) Combine (193) **2:MS ES-** **6.2e+004**



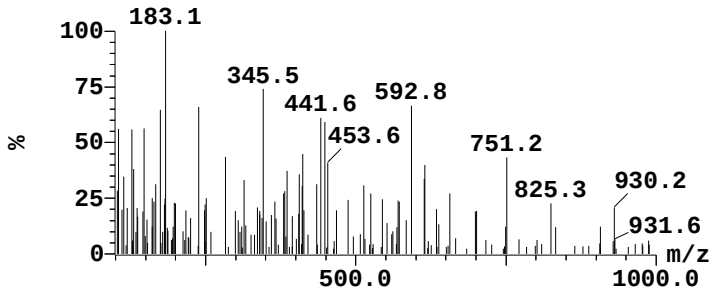
Peak ID Time
2 1.86

2:(Time: 1.86) Combine (197) **2:MS ES-** **1.1e+005**



Peak ID Time
3 1.96

3:(Time: 1.96) Combine (207) **2:MS ES-** **5.1e+004**



Sample Name:IS10607-058 Mobile A:0.1%HCOOH in Water Vial:1:1
Data File:A914853 Mobile B: 0.1%HCOOH in ACN Flow Rate:1.0 ml/min
Acq.Method:595FA.olp %B: 0min=5%2min=95%2.5min=5%3min=5% Inj Date:17-Feb-2014
Instrument Code :SC\AD\17-004 Column : Acquity UPLC HSS T3 (2.1x50)mm;1.8µm:

Printed: Mon Feb 17 10:28:14 2014

Sample Report (continued):

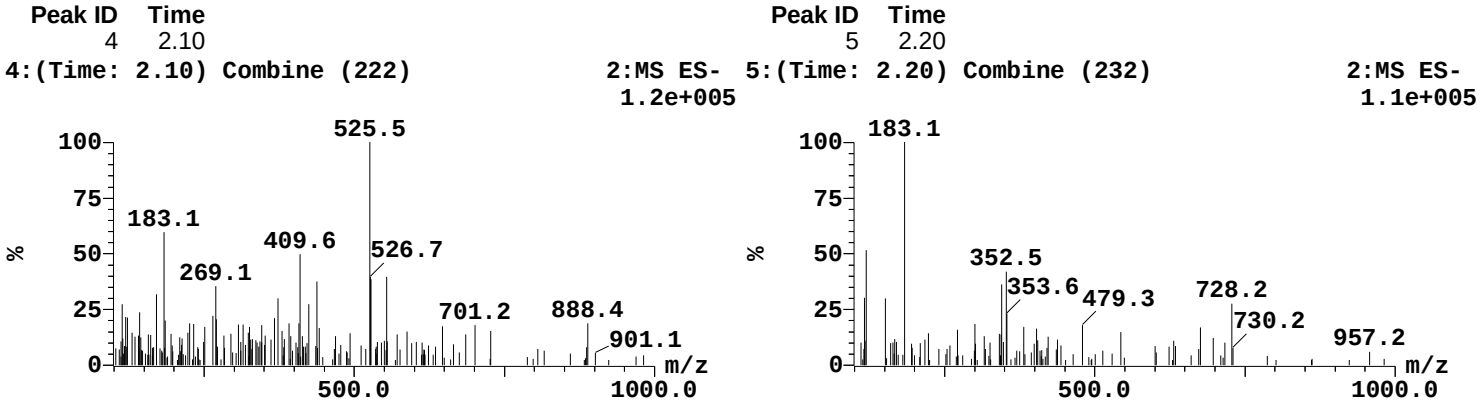


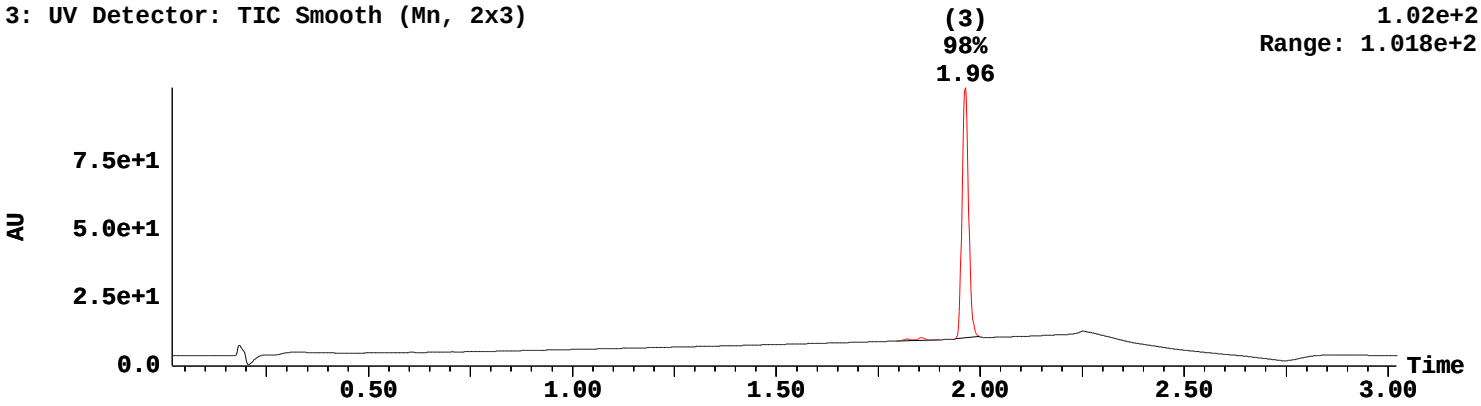
Fig 78. UPLC of 8-(4-Fluorophenyl)-6-(4-methoxyphenyl)-3-phenyl-[1,2,4]triazolo[4,3-b]pyridazine (**5e**)

Sample Name:IS10607-058 Mobile A:0.1%HCOOH in Water Vial:1:2
Data File:A914852 Mobile B: 0.1%HCOOH in ACN Flow Rate:1.0 ml/min
Acq.Method:595FA.olp %B: 0min=5%2min=95%2.5min=5%3min=5% Inj Date:17-Feb-2014
Instrument Code :SC\AD\17-004 Column : Acquity UPLC HSS T3 (2.1x50)mm;1.8µm:

Printed: Mon Feb 17 10:28:45 2014

Sample Report:

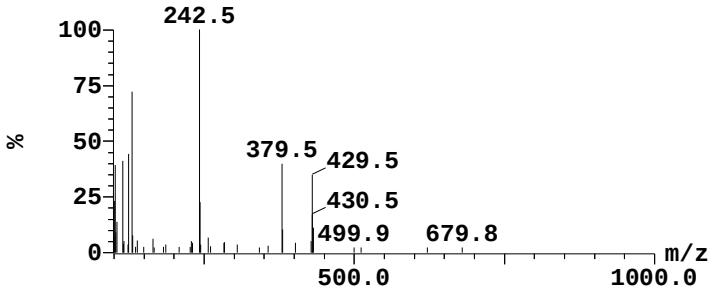
3: UV Detector: TIC Smooth (Mn, 2x3)



Peak no	R.T	Area	% Area
1	1.82	1e+004	0.78
2	1.86	2e+004	1.07
3	1.96	2e+006	98.16

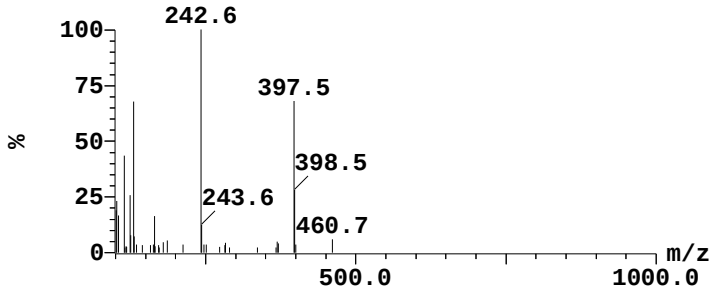
Peak ID Time
1 1.82

1:(Time: 1.82) Combine (193) **1:MS ES+ 1.8e+006**



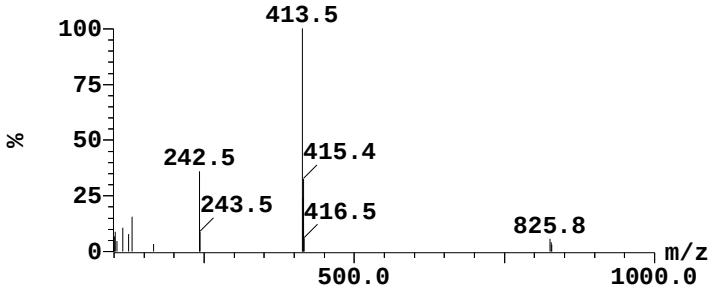
Peak ID Time
2 1.86

2:(Time: 1.86) Combine (197) **1:MS ES+ 2.0e+006**



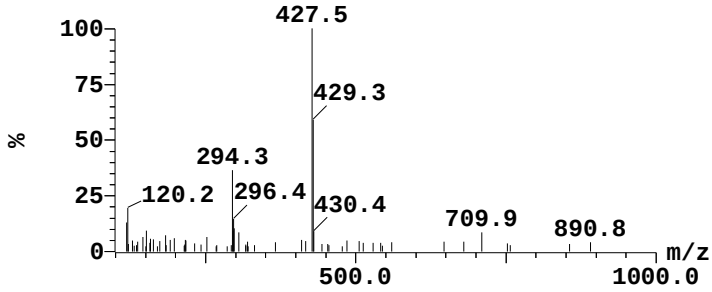
Peak ID Time
3 1.96

3:(Time: 1.96) Combine (208) **1:MS ES+ 5.0e+006**



Peak ID Time
1 1.82

1:(Time: 1.82) Combine (192) **2:MS ES- 3.8e+005**



Sample Name:IS10607-058 Mobile A:0.1%HCOOH in Water Vial:1:2
Data File:A914852 Mobile B: 0.1%HCOOH in ACN Flow Rate:1.0 ml/min
Acq.Method:595FA.olp %B: 0min=5%2min=95%2.5min=5%3min=5% Inj Date:17-Feb-2014
Instrument Code :SC\AD\17-004 Column : Acquity UPLC HSS T3 (2.1x50)mm;1.8µm:

Printed: Mon Feb 17 10:28:45 2014

Sample Report (continued):

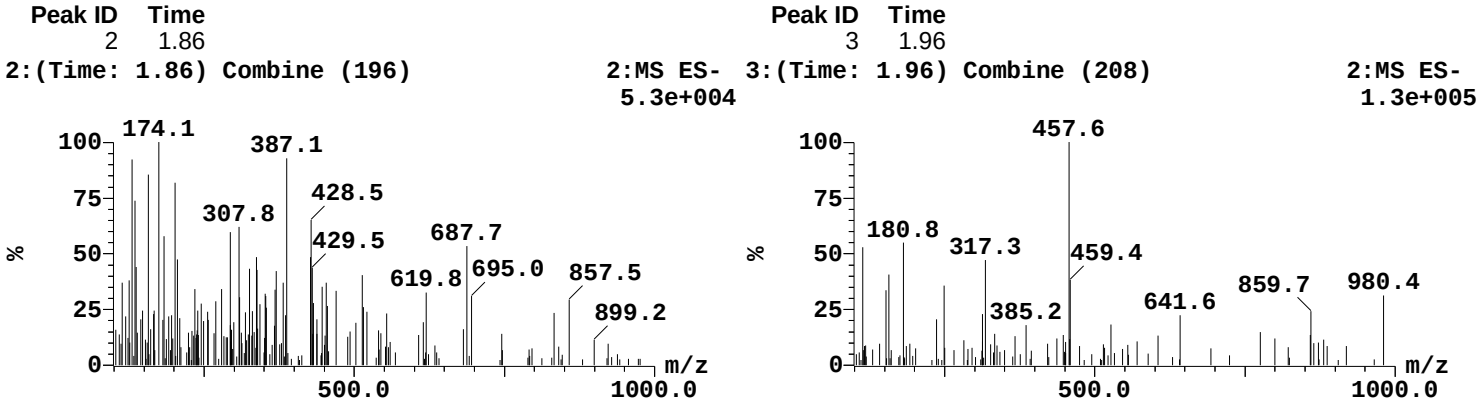
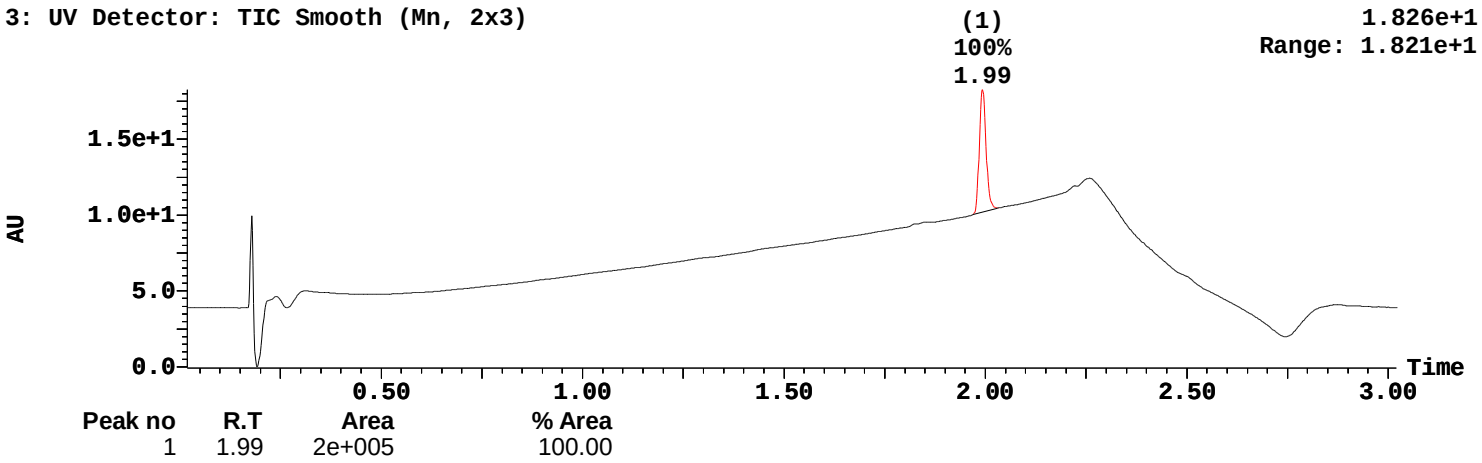


Fig 79. UPLC of 8-(4-Chlorophenyl)-6-(4-methoxyphenyl)-3-phenyl-[1,2,4]triazolo[4,3-b] pyridazine (**5f**)

Sample Name:IS10607-058 Mobile A:0.1%HCOOH in Water Vial:1:10
Data File:A914963 Mobile B: 0.1%HCOOH in ACN Flow Rate:1.0 ml/min
Acq.Method:595FA.olp %B: 0min=5%2min=95%2.5min=5%3min=5% Inj Date:17-Feb-2014
Instrument Code :SC\AD\17-004 Column : Acquity UPLC HSS T3 (2.1x50)mm;1.8µm:

Printed: Mon Feb 17 12:19:13 2014

Sample Report:



Peak no	R.T	Area	% Area
1	1.99	2e+005	100.00

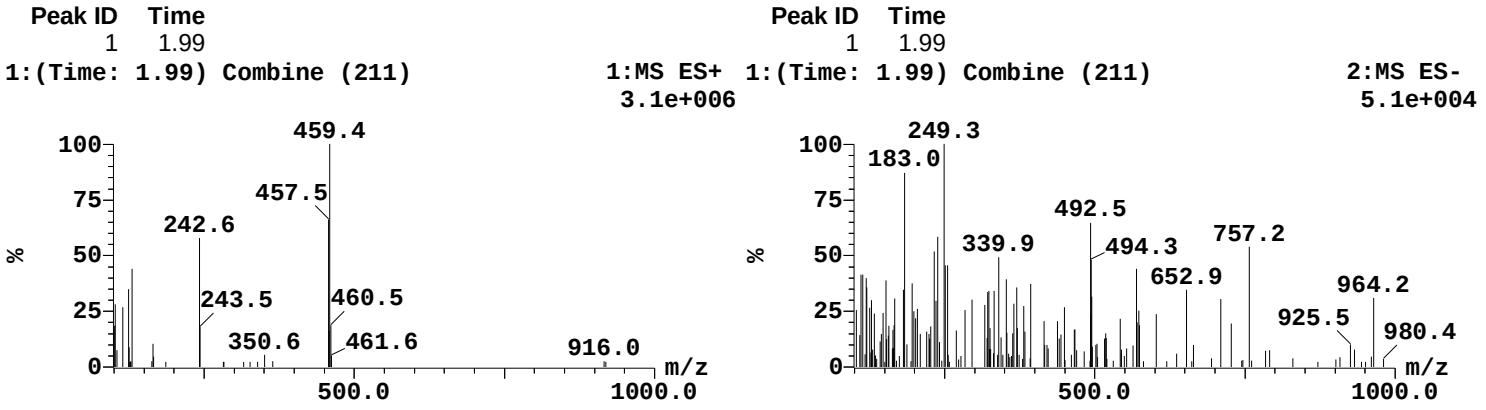
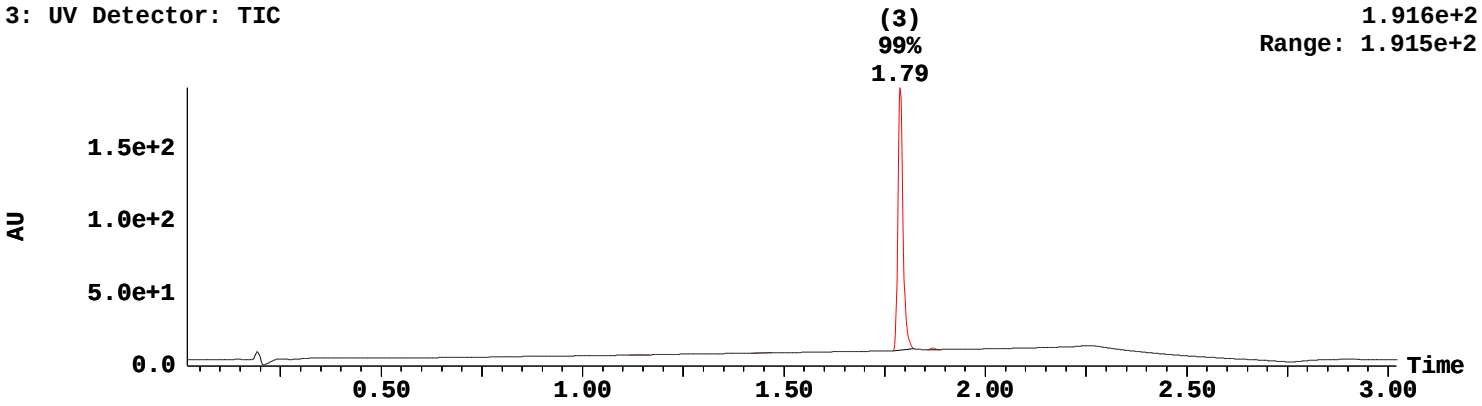


Fig 80. UPLC of 8-(4-Bromophenyl)-6-(4-methoxyphenyl)-3-phenyl-[1,2,4]triazolo[4,3-b] pyridazine (**5g**)

Sample Name:IS10607-058 Mobile A:0.1%HCOOH in Water Vial:1:30
Data File:A936855 Mobile B: 0.1%HCOOH in ACN Flow Rate:1.0 ml/min
Acq.Method:595FA.olp %B: 0min=5%2min=95%2.5min=5%3min=5% Inj Date:14-Mar-2014
Instrument Code :SC\AD\17-004 Column : Acquity UPLC HSS T3 (2.1x50)mm;1.8µm:

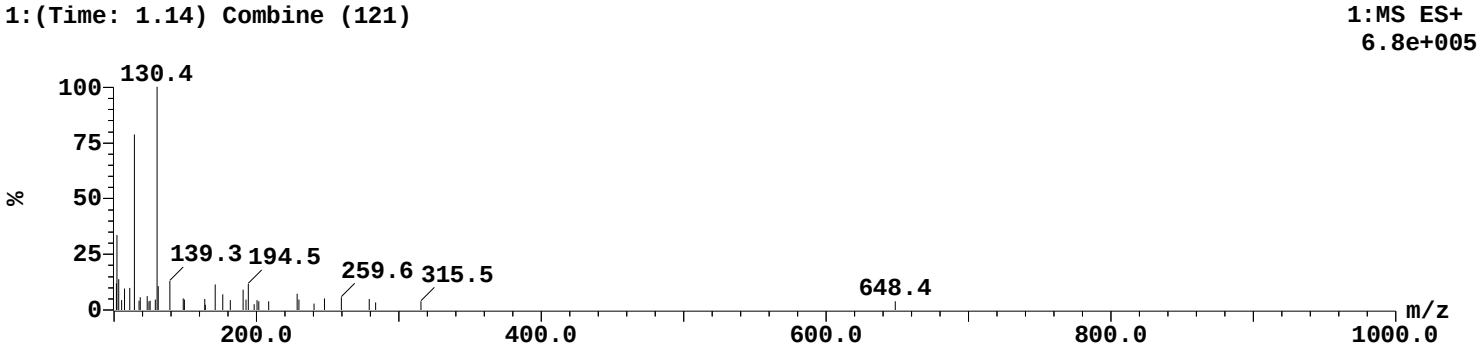
Printed: Fri Mar 14 11:53:08 2014

Sample Report:

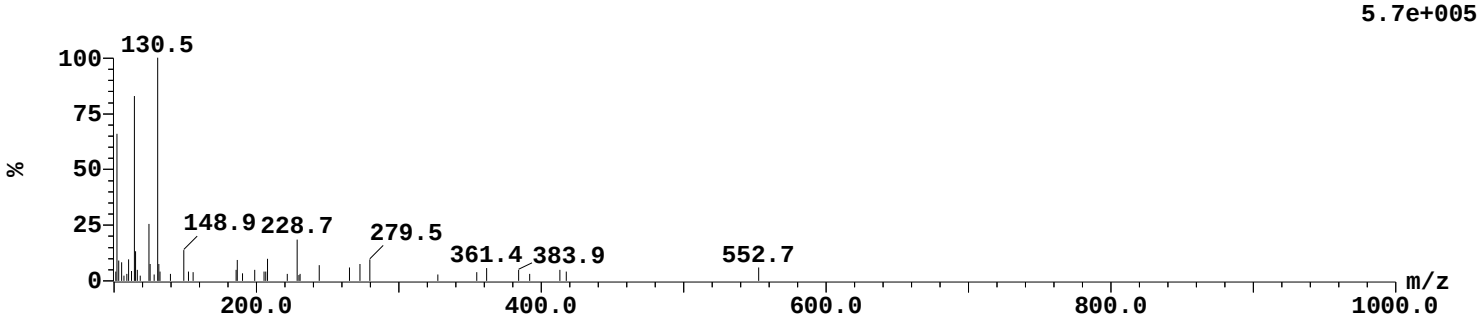


Peak no	R.T	Area	% Area
1	1.14	4617	0.17
2	1.44	3922	0.15
3	1.79	2619277	99.10
4	1.87	15185	0.57

Peak ID	Time
1	1.14



Peak ID	Time
2	1.44



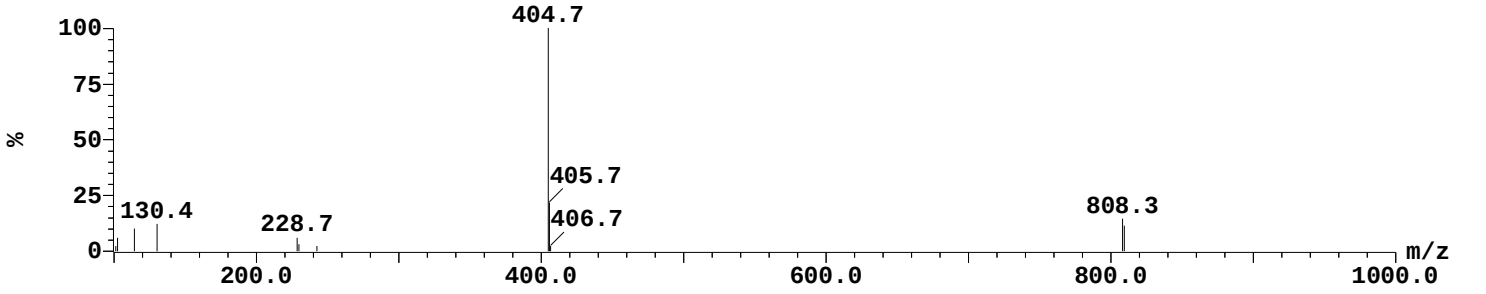
Sample Name:IS10607-058 Mobile A:0.1%HCOOH in Water Vial:1:30
Data File:A936855 Mobile B: 0.1%HCOOH in ACN Flow Rate:1.0 ml/min
Acq.Method:595FA.olp %B: 0min=5%2min=95%2.5min=5%3min=5% Inj Date:14-Mar-2014
Instrument Code :SC\AD\17-004 Column : Acquity UPLC HSS T3 (2.1x50)mm;1.8µm:

Printed: Fri Mar 14 11:53:08 2014

Sample Report (continued):

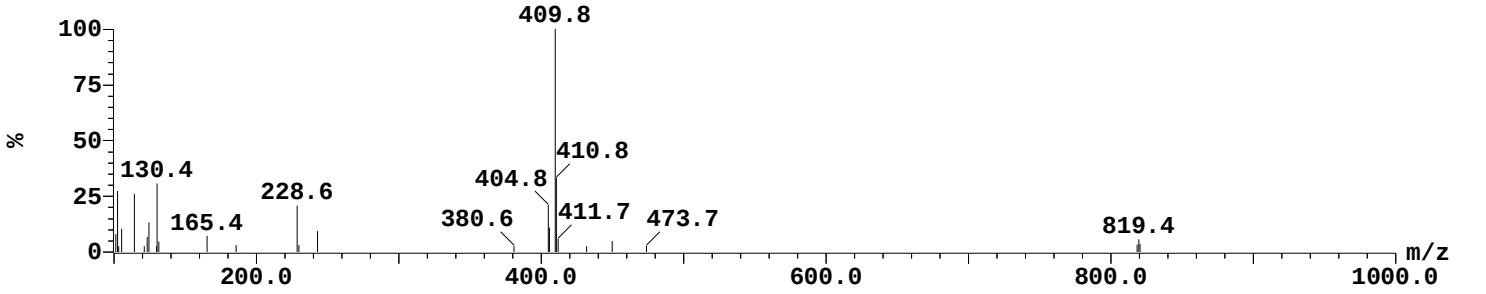
Peak ID	Time
3	1.79

3:(Time: 1.79) Combine (190) **1:MS ES+ 3.5e+006**



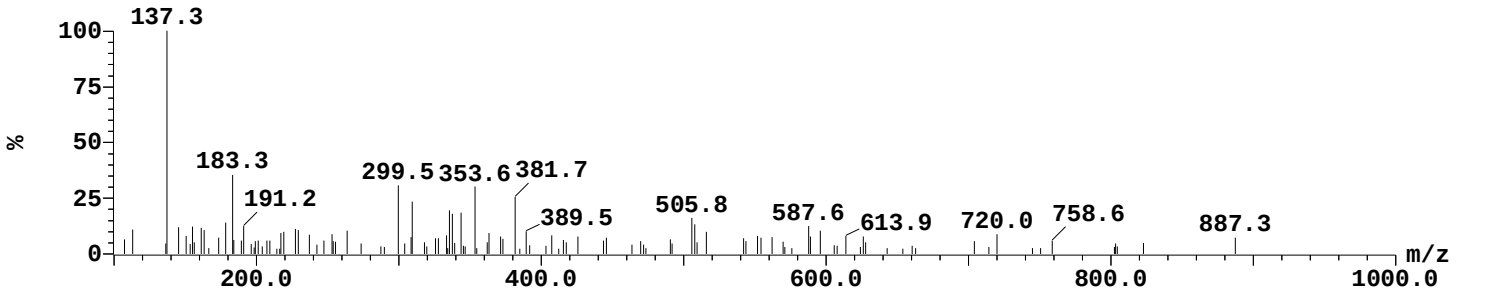
Peak ID	Time
4	1.87

4:(Time: 1.87) Combine (198) **1:MS ES+ 2.3e+006**



Peak ID	Time
1	1.14

1:(Time: 1.14) Combine (121) **2:MS ES- 2.6e+005**



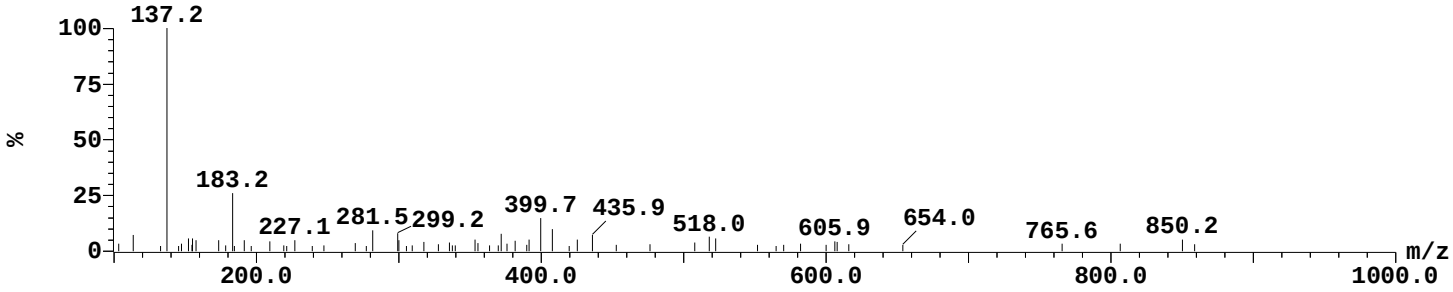
Sample Name:IS10607-058 Mobile A:0.1%HCOOH in Water Vial:1:30
Data File:A936855 Mobile B: 0.1%HCOOH in ACN Flow Rate:1.0 ml/min
Acq.Method:595FA.olp %B: 0min=5%2min=95%2.5min=5%3min=5% Inj Date:14-Mar-2014
Instrument Code :SC\AD\17-004 Column : Acquity UPLC HSS T3 (2.1x50)mm;1.8µm:

Printed: Fri Mar 14 11:53:08 2014

Sample Report (continued):

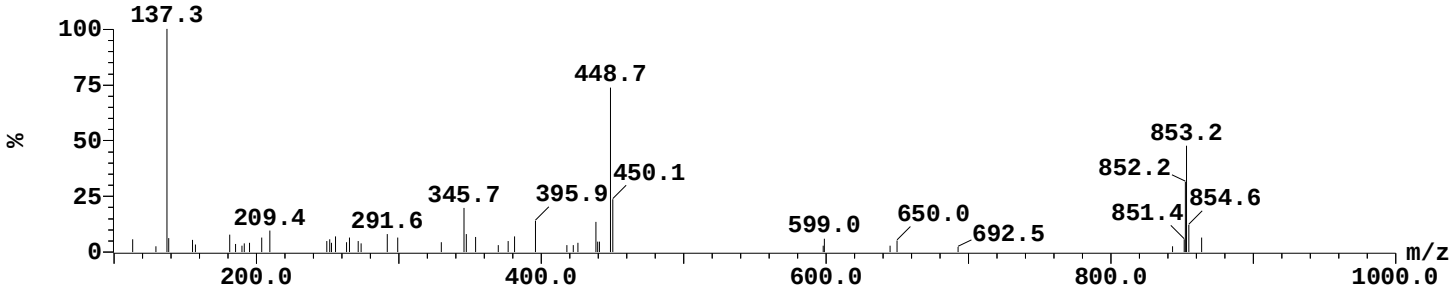
Peak ID	Time
2	1.44

2:(Time: 1.44) Combine (152) **2:MS ES- 5.2e+005**



Peak ID	Time
3	1.79

3:(Time: 1.79) Combine (189) **2:MS ES- 2.0e+005**



Peak ID	Time
4	1.87

4:(Time: 1.87) Combine (198) **2:MS ES- 2.1e+005**

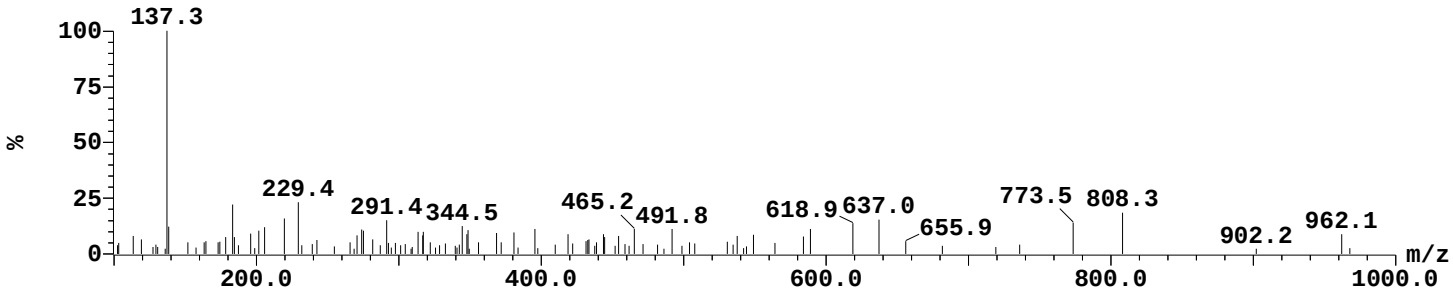


Fig 81. UPLC of 4-(6-(4-Methoxyphenyl)-3-phenyl-[1,2,4]triazolo[4,3-b]pyridazin-8-yl) benzonitrile (**5h**)

Sample Name:IS10607-058 Mobile A:0.1%HCOOH in Water Vial:1:4
Data File:A914855 Mobile B: 0.1%HCOOH in ACN Flow Rate:1.0 ml/min
Acq.Method:595FA.olp %B: 0min=5%2min=95%2.5min=5%3min=5% Inj Date:17-Feb-2014
Instrument Code :SC\AD\17-004 Column : Acquity UPLC HSS T3 (2.1x50)mm;1.8µm:

Printed: Mon Feb 17 10:58:53 2014

Sample Report:

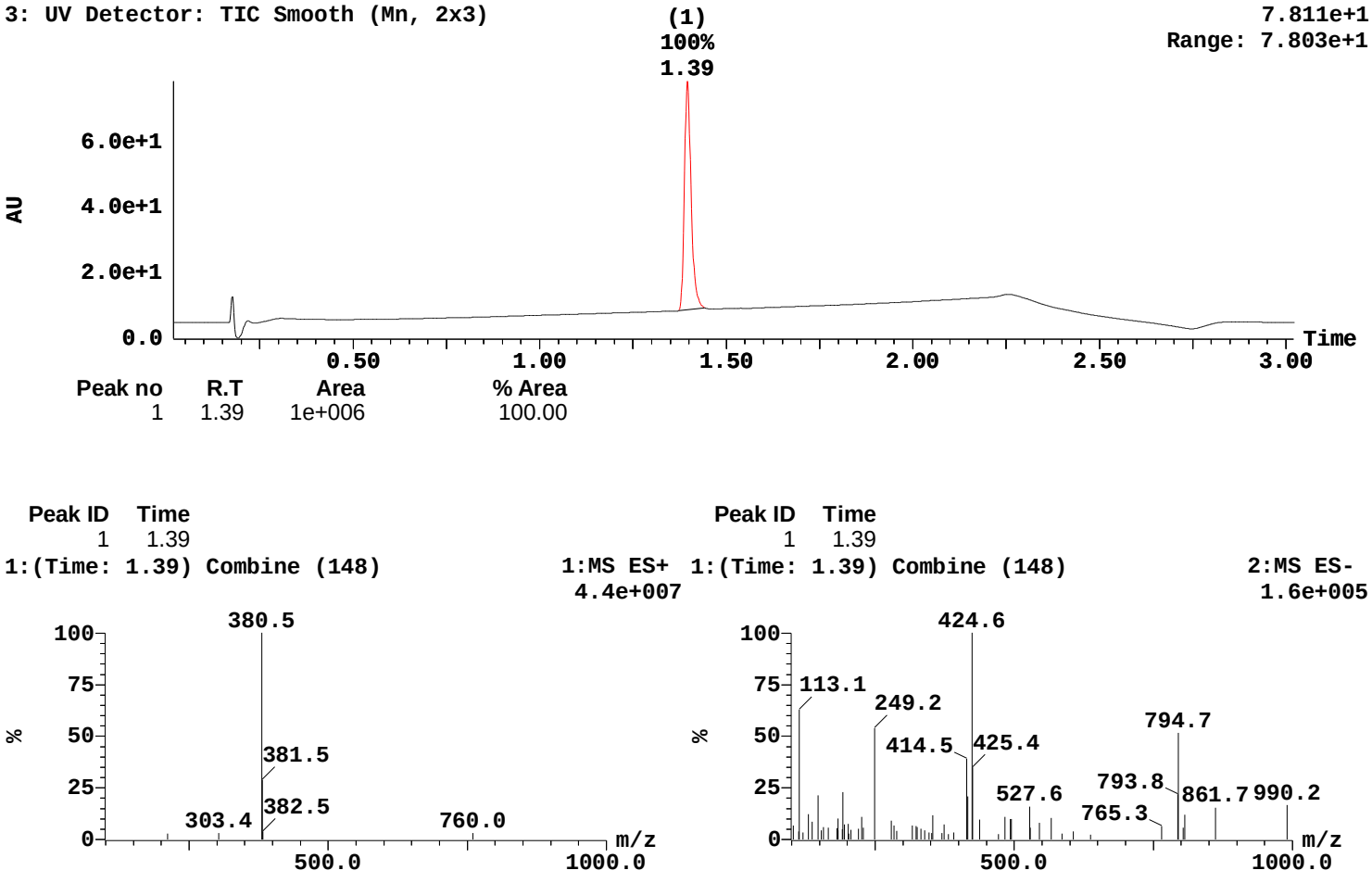
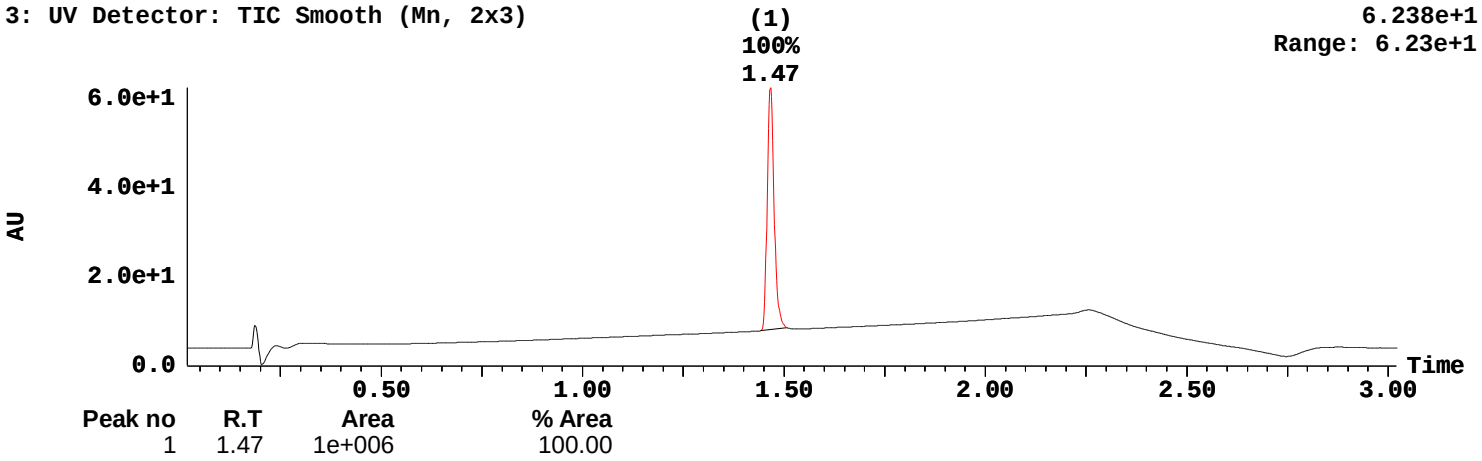


Fig 82. UPLC of 6-(4-Methoxyphenyl)-3-phenyl-8-(pyridin-4-yl)-[1,2,4]triazolo[4,3-b]pyridazine (**5i**)

Sample Name:IS10607-058 Mobile A:0.1%HCOOH in Water Vial:1:6
Data File:A914854 Mobile B: 0.1%HCOOH in ACN Flow Rate:1.0 ml/min
Acq.Method:595FA.olp %B: 0min=5%2min=95%2.5min=5%3min=5% Inj Date:17-Feb-2014
Instrument Code :SC\AD\17-004 Column : Acquity UPLC HSS T3 (2.1x50)mm;1.8µm:

Printed: Mon Feb 17 10:59:40 2014

Sample Report:



Peak no	R.T	Area	% Area
1	1.47	1e+006	100.00

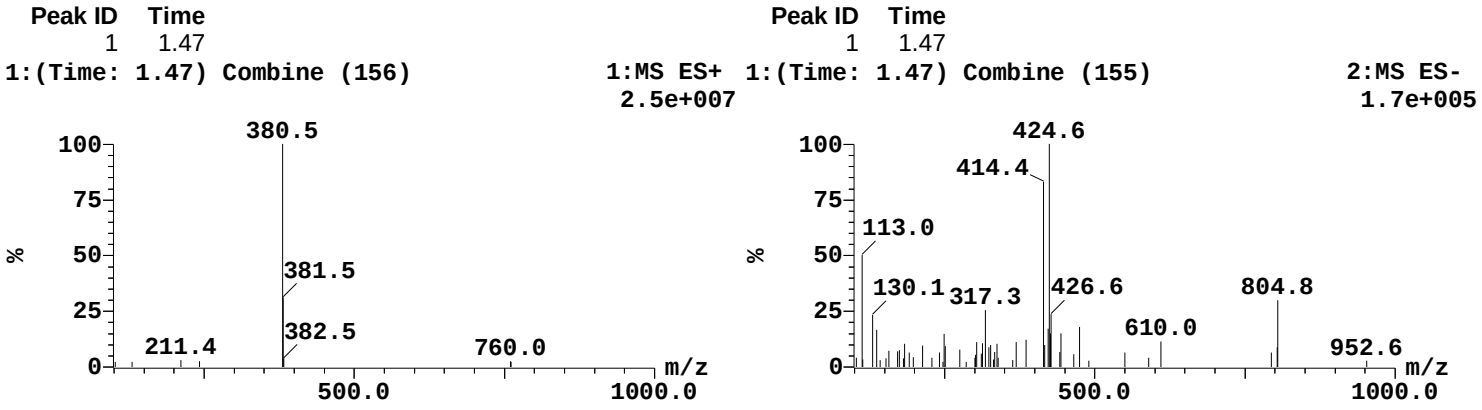
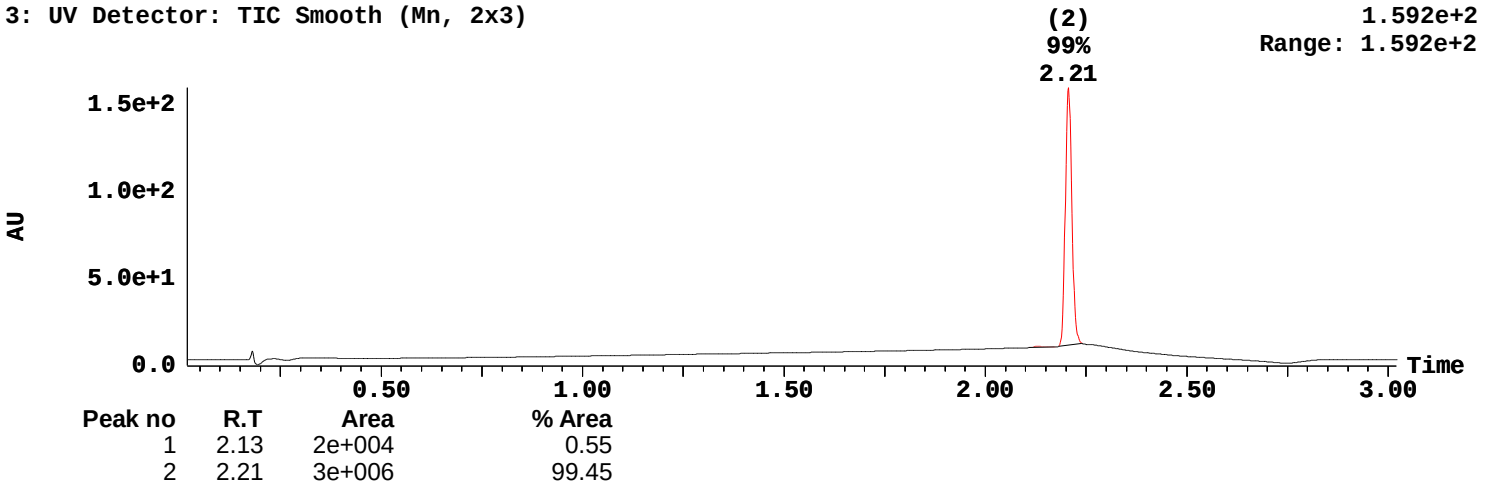


Fig 83. UPLC of 6-(4-Methoxyphenyl)-3-phenyl-8-(pyridin-3-yl)-[1,2,4]triazolo[4,3-b]pyridazine (**5j**)

Sample Name:IS10607-058 Mobile A:0.1%HCOOH in Water Vial:1:7
Data File:A914959 Mobile B: 0.1%HCOOH in ACN Flow Rate:1.0 ml/min
Acq.Method:595FA.olp %B: 0min=5%2min=95%2.5min=5%3min=5% Inj Date:17-Feb-2014
Instrument Code :SC\AD\17-004 Column : Acquity UPLC HSS T3 (2.1x50)mm;1.8µm:

Printed: Mon Feb 17 12:20:02 2014

Sample Report:



Peak no	R.T	Area	% Area
1	2.13	2e+004	0.55
2	2.21	3e+006	99.45

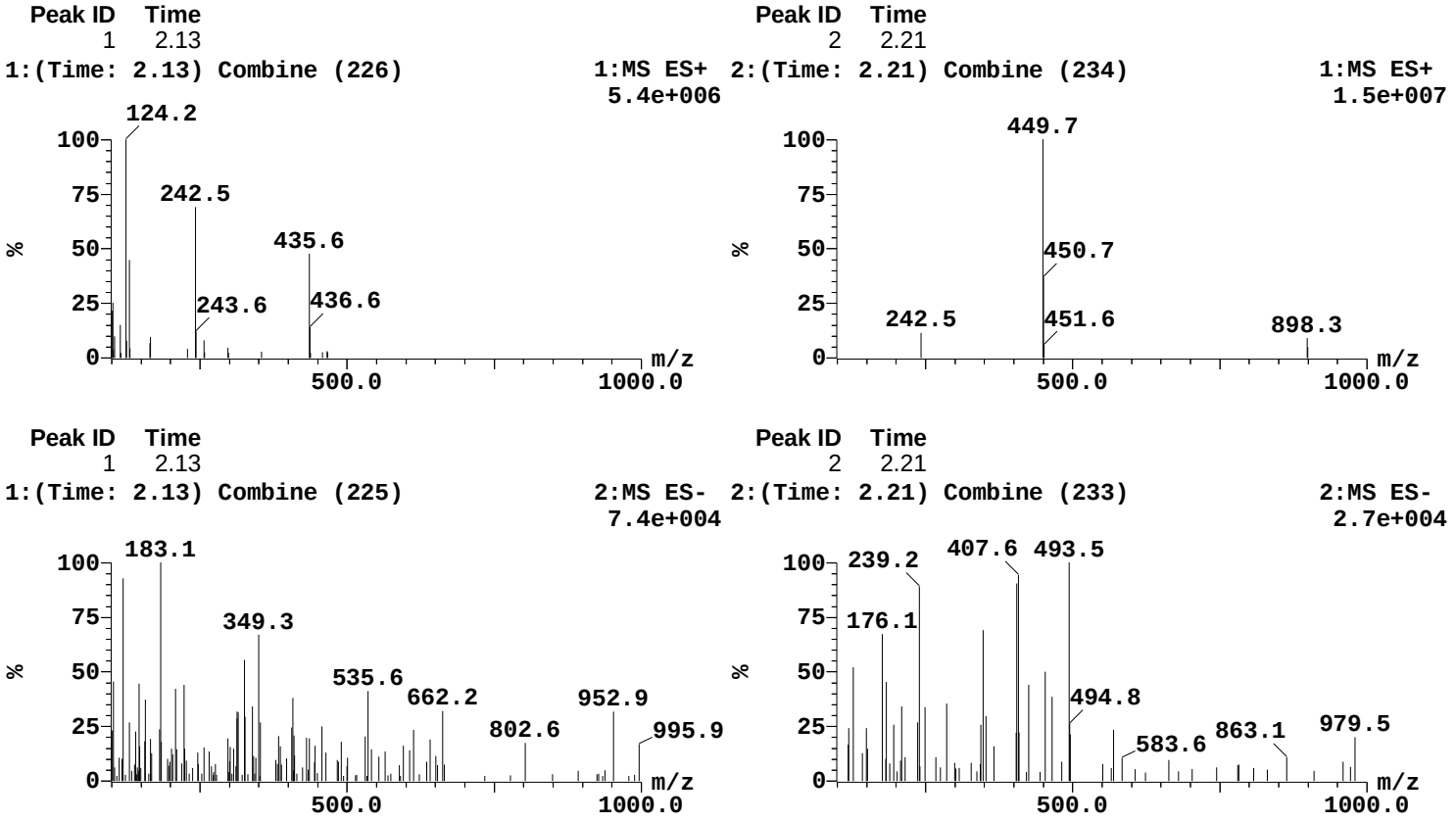
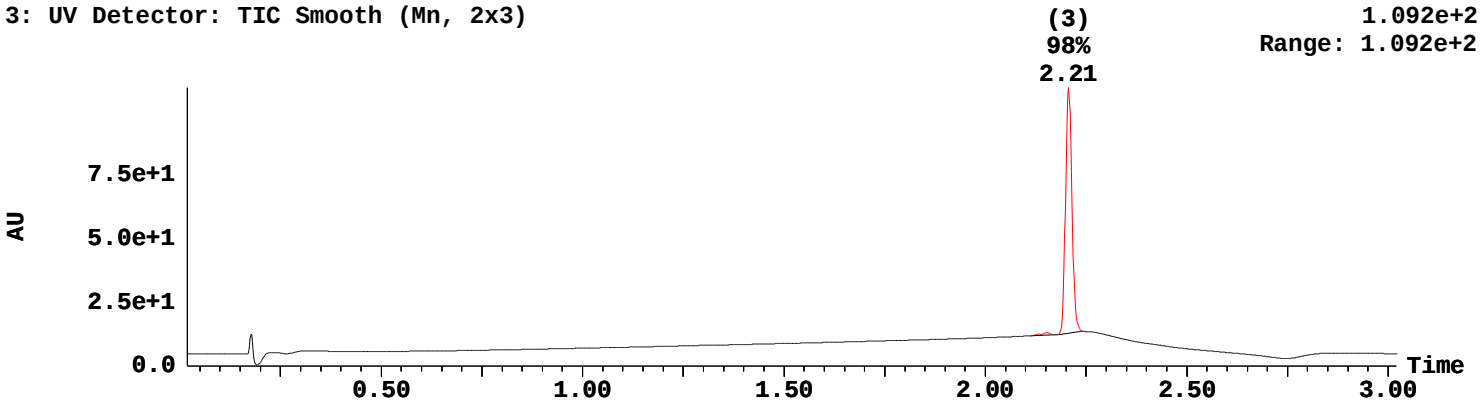


Fig 84. UPLC of 3-(4-tert-Butylphenyl)-6-(4-methoxyphenyl)-8-m-tolyl-[1,2,4]triazolo[4,3-b] pyridazine (**7a**)

Sample Name:IS10607-058 Mobile A:0.1%HCOOH in Water Vial:1:9
Data File:A914960 Mobile B: 0.1%HCOOH in ACN Flow Rate:1.0 ml/min
Acq.Method:595FA.olp %B: 0min=5%2min=95%2.5min=5%3min=5% Inj Date:17-Feb-2014
Instrument Code :SC\AD\17-004 Column : Acquity UPLC HSS T3 (2.1x50)mm;1.8µm:

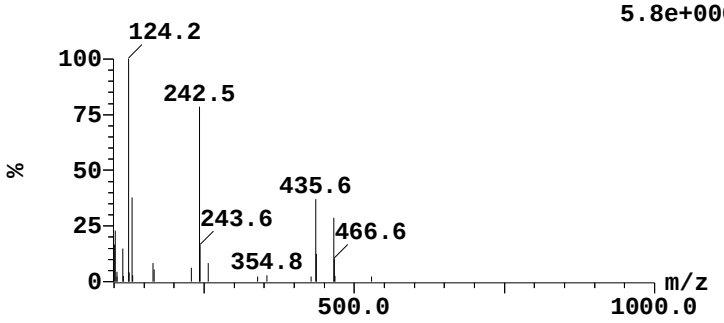
Printed: Mon Feb 17 12:20:26 2014

Sample Report:

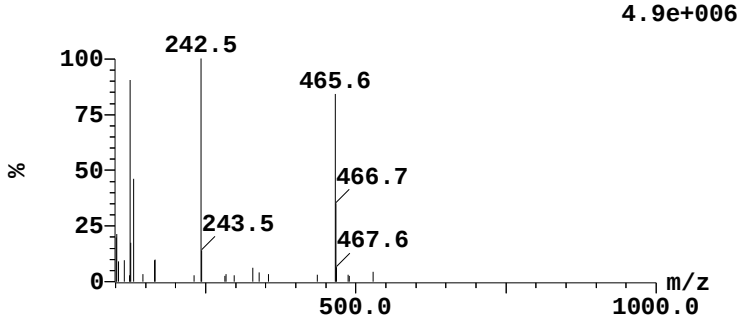


Peak no	R.T	Area	% Area
1	2.13	9e+003	0.49
2	2.15	2e+004	1.05
3	2.21	2e+006	98.46

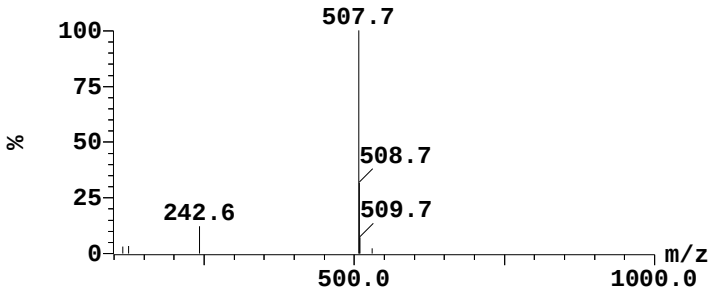
Peak ID Time
1 2.13



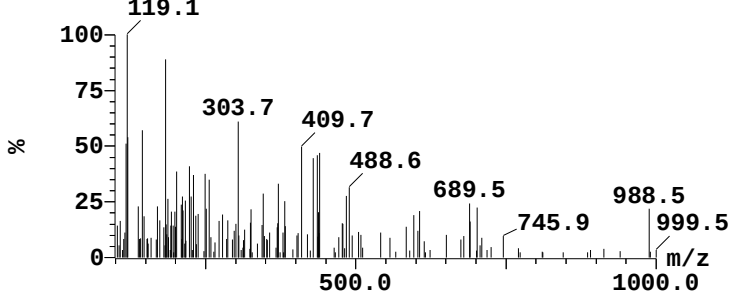
Peak ID Time
2 2.15



Peak ID Time
3 2.21



Peak ID Time
1 2.13



Sample Name:IS10607-058 Mobile A:0.1%HCOOH in Water Vial:1:9
Data File:A914960 Mobile B: 0.1%HCOOH in ACN Flow Rate:1.0 ml/min
Acq.Method:595FA.olp %B: 0min=5%2min=95%2.5min=5%3min=5% Inj Date:17-Feb-2014
Instrument Code :SC\AD\17-004 Column : Acquity UPLC HSS T3 (2.1x50)mm;1.8µm:

Printed: Mon Feb 17 12:20:26 2014

Sample Report (continued):

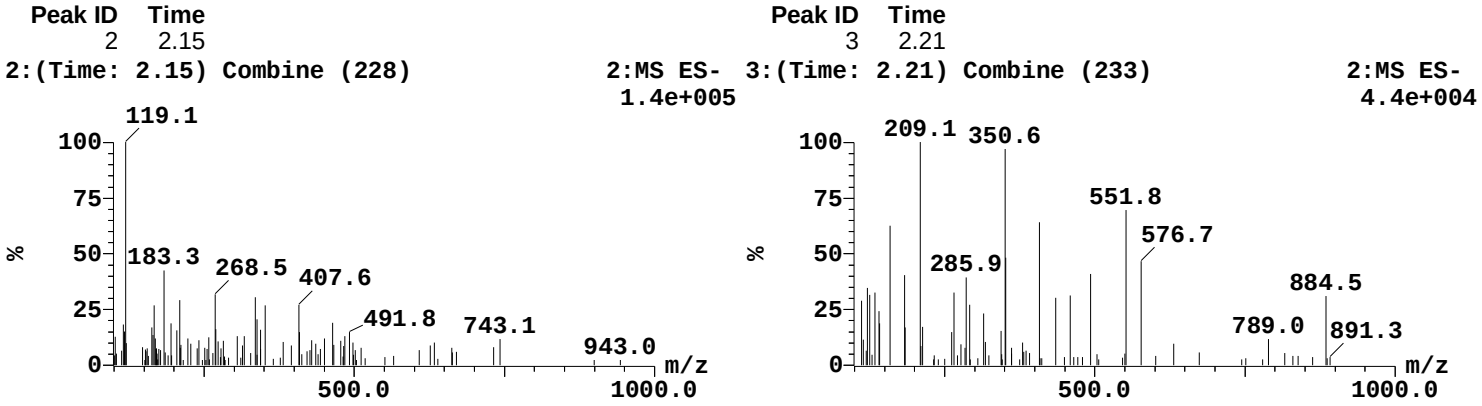
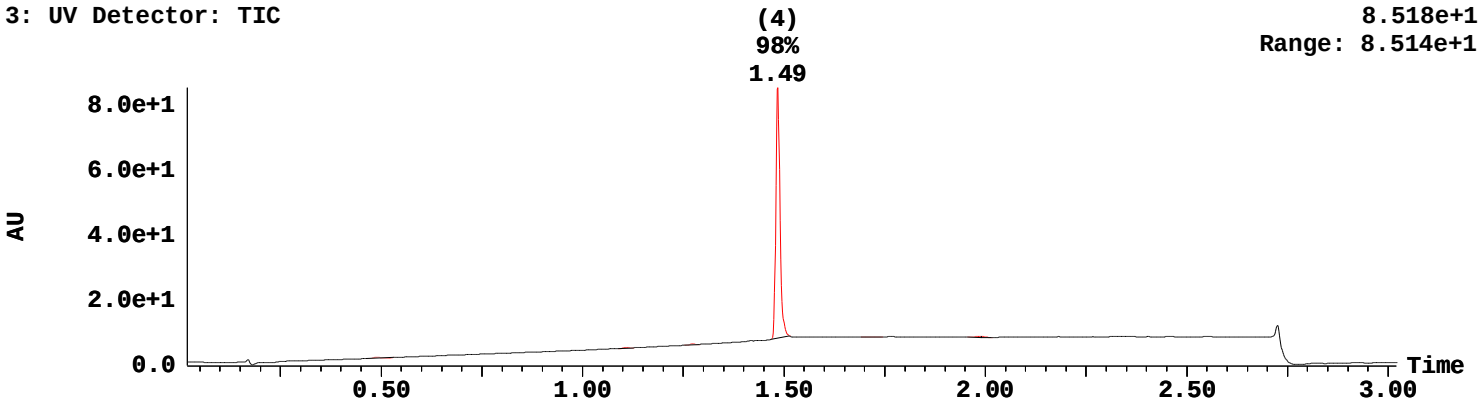


Fig 85. UPLC of Ethyl 3-(3-(4-tert-butylphenyl)-6-(4-methoxyphenyl)-[1,2,4]triazolo[4,3-b] pyridazin-8-yl)benzoate (**7b**)

Sample Name:IS10607-058 Mobile A:0.1%HCOOH in Water Vial:1:20
Data File:A936775A Mobile B: 0.1%HCOOH in ACN Flow Rate: 0.7 ml/min
Acq.Method:595FA.olp %B: 0min=30%1.25min=95%2min=95%3min=30% Inj Date:14-Mar-2014
Instrument Code :SC\AD\17-004 Column : Acquity UPLC HSS T3 (2.1x50)mm;1.8µm:

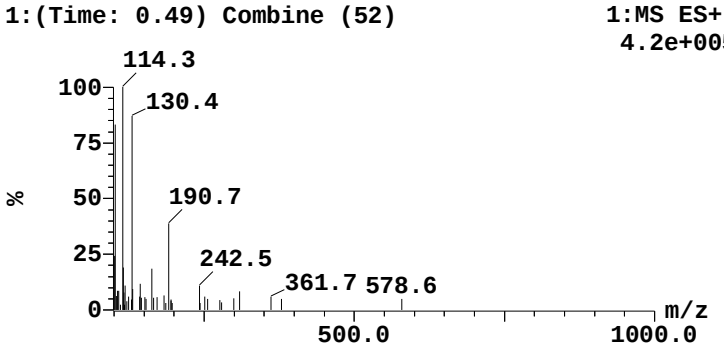
Printed: Fri Mar 14 11:17:09 2014

Sample Report:

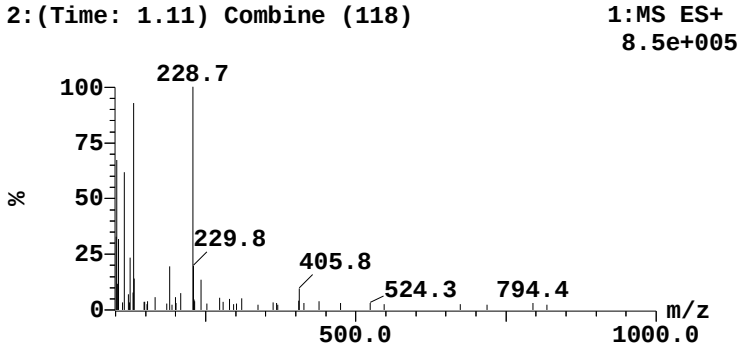


Peak no	R.T	Area	% Area
1	0.49	6e+003	0.65
2	1.11	3e+003	0.35
3	1.27	4e+003	0.39
4	1.49	9e+005	97.65
5	1.71	2e+003	0.24
6	1.99	4e+003	0.44
7	1.99	3e+003	0.27

Peak ID	Time
1	0.49



Peak ID	Time
2	1.11



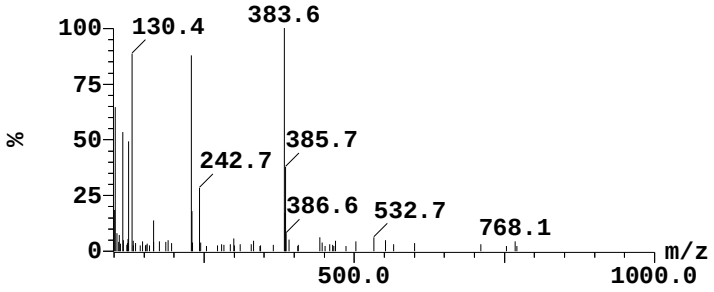
Sample Name:IS10607-058 Mobile A:0.1%HCOOH in Water Vial:1:20
Data File:A936775A Mobile B: 0.1%HCOOH in ACN Flow Rate: 0.7 ml/min
Acq.Method:595FA.olp %B: 0min=30%1.25min=95%2min=95%3min=30% Inj Date:14-Mar-2014
Instrument Code :SC\AD\17-004 Column : Acquity UPLC HSS T3 (2.1x50)mm;1.8µm:

Printed: Fri Mar 14 11:17:09 2014

Sample Report (continued):

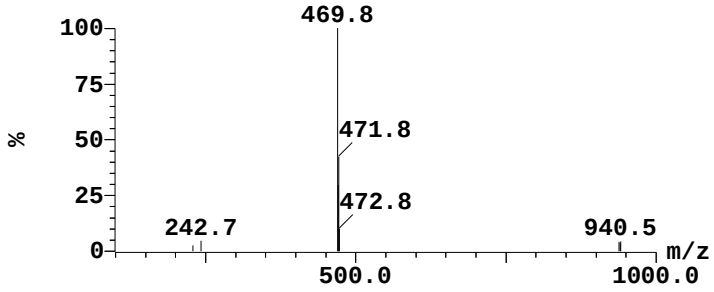
Peak ID 3 **Time** 1.27

3:(Time: 1.27) Combine (135) **1:MS ES+** **1.2e+006**



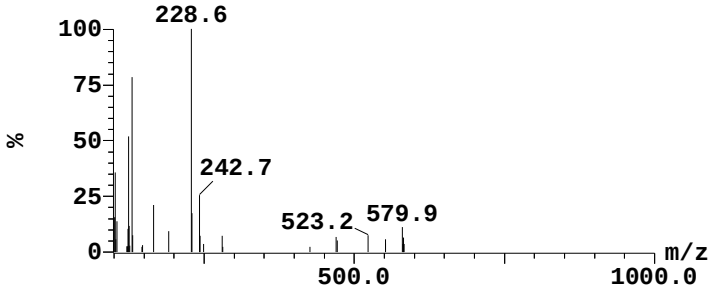
Peak ID 4 **Time** 1.49

4:(Time: 1.49) Combine (158) **1:MS ES+** **1.1e+007**



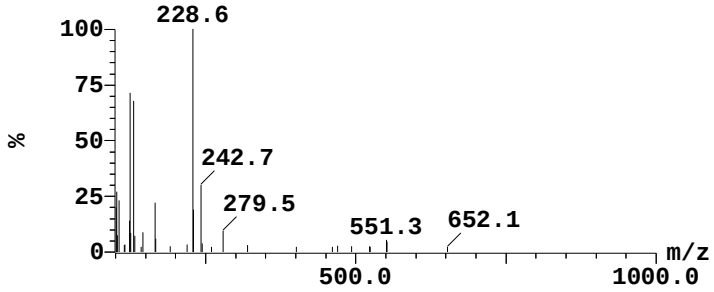
Peak ID 5 **Time** 1.71

5:(Time: 1.71) Combine (181) **1:MS ES+** **3.8e+006**



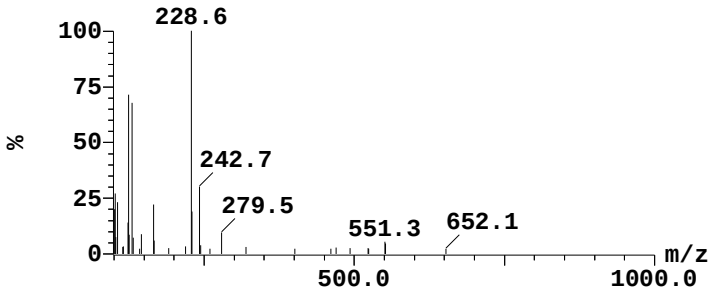
Peak ID 6 **Time** 1.99

6:(Time: 1.99) Combine (211) **1:MS ES+** **3.5e+006**



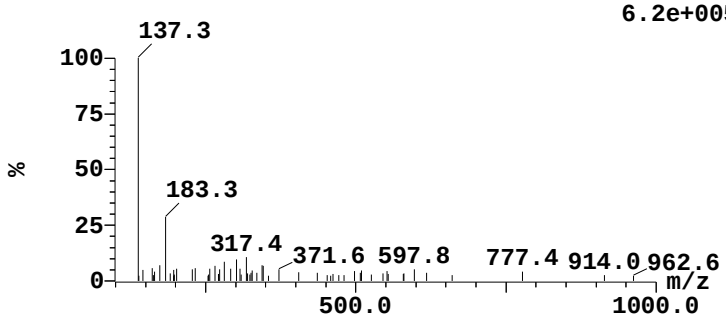
Peak ID 7 **Time** 1.99

7:(Time: 1.99) Combine (211) **1:MS ES+** **3.5e+006**



Peak ID 1 **Time** 0.49

1:(Time: 0.49) Combine (52) **2:MS ES-** **6.2e+005**



Sample Name:IS10607-058 Mobile A:0.1%HCOOH in Water Vial:1:20
Data File:A936775A Mobile B: 0.1%HCOOH in ACN Flow Rate: 0.7 ml/min
Acq.Method:595FA.olp %B: 0min=30%1.25min=95%2min=95%3min=30% Inj Date:14-Mar-2014
Instrument Code :SC\AD\17-004 Column : Acquity UPLC HSS T3 (2.1x50)mm;1.8µm:

Printed: Fri Mar 14 11:17:09 2014

Sample Report (continued):

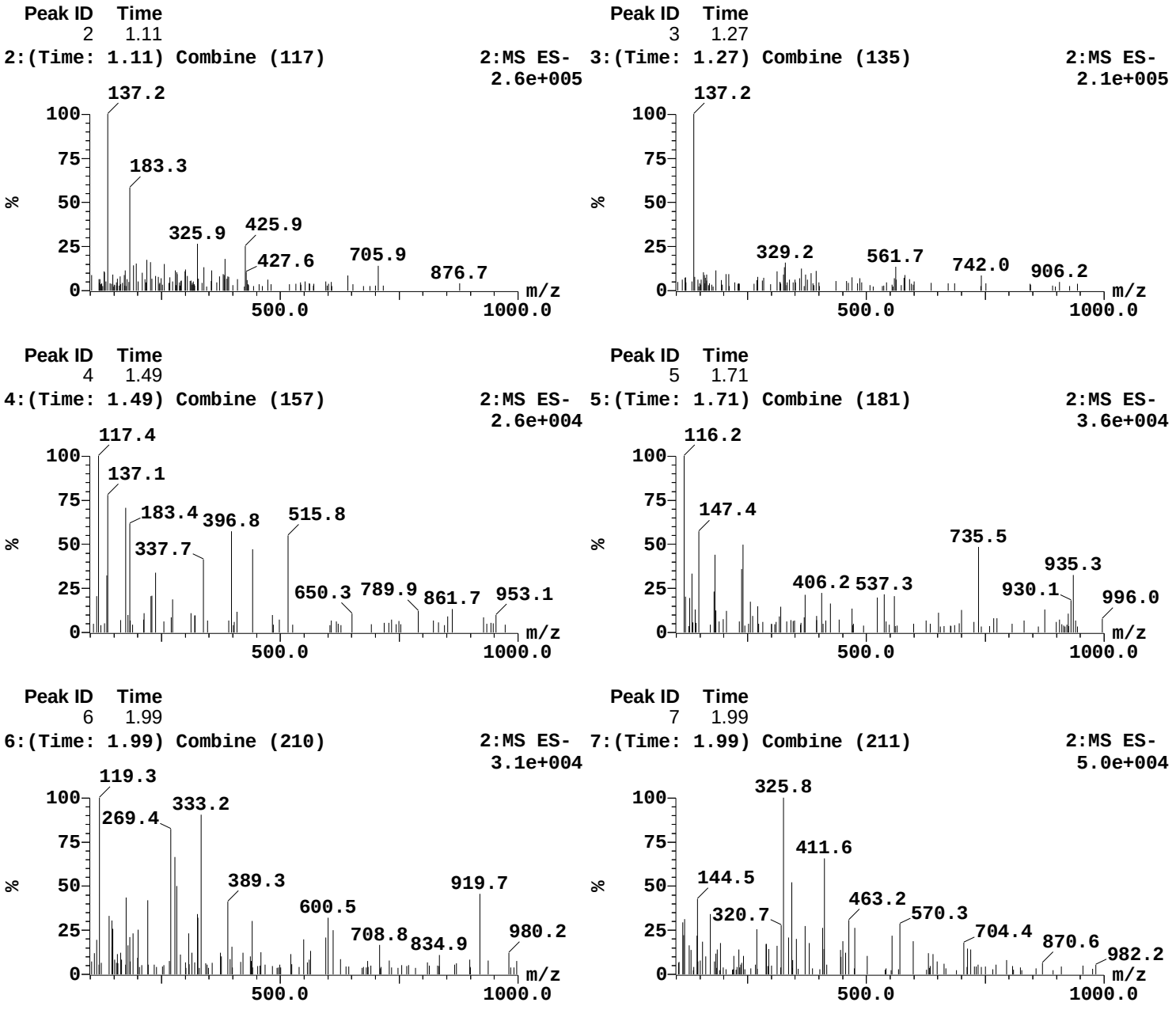
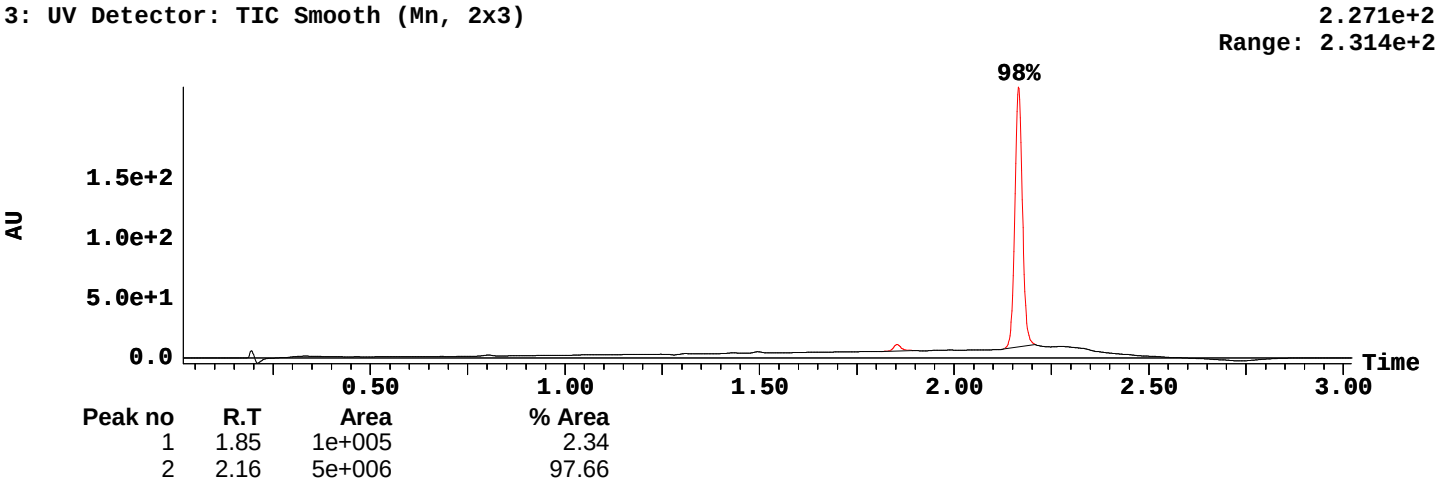


Fig 86. UPLC of 3-(4-tert-Butylphenyl)-8-(3-chlorophenyl)-6-(4-methoxyphenyl) [1,2,4]triazolo[4,3-b] pyridazine (**7c**)

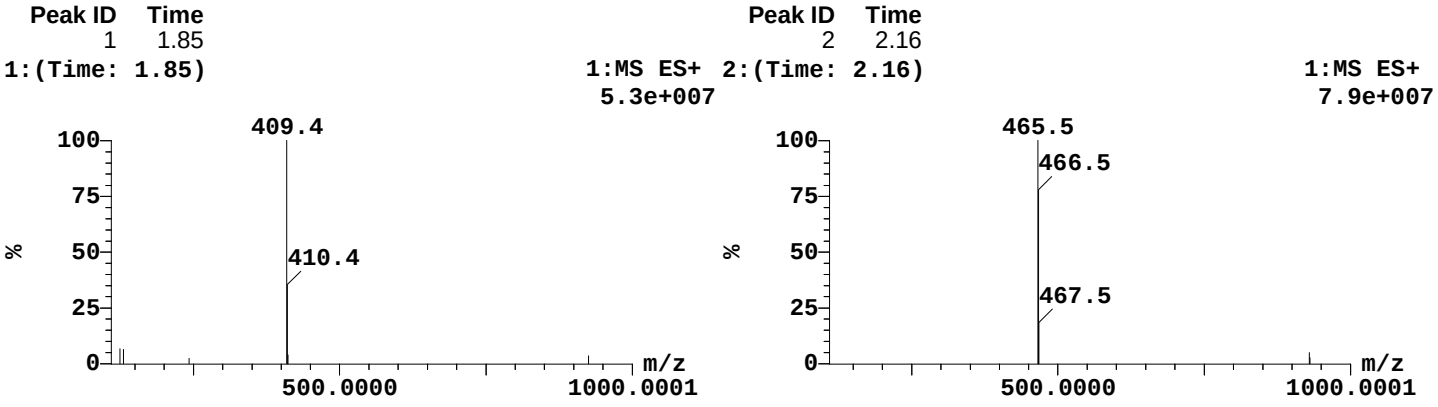
Sample Name:IS10607-058 Mobile A:0.1%HCOOH in Water Vial:2:D,5
Data File:A911730 Mobile B: 0.1%HCOOH in ACN Flow Rate:1.0 ml/min
Acq.Method:595FA.olp %B: 0min=5%2min=95%2.5min=5%3min=5% Inj Date:12-Feb-2014
Instrument Code :SC\AD\17-005 Column : Acquity UPLC HSS T3 (2.1x50)mm;1.8µm:

Printed: Wed Feb 12 19:09:18 2014

Sample Report:



Peak no	R.T	Area	% Area
1	1.85	1e+005	2.34
2	2.16	5e+006	97.66



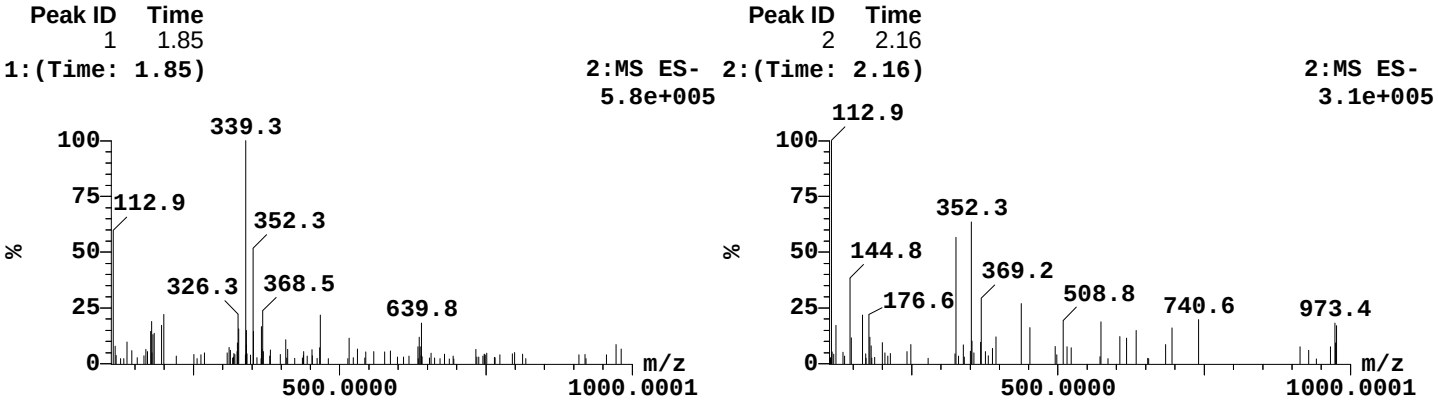
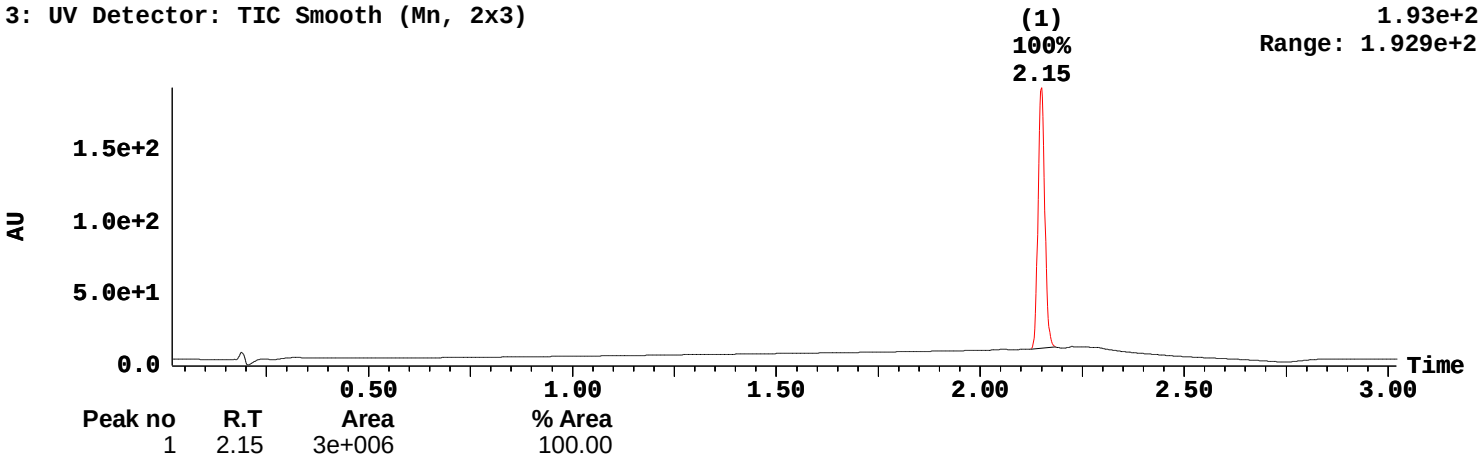


Fig 87. UPLC of 3-(4-tert-Butylphenyl)-6,8-bis(4-methoxyphenyl)-[1,2,4]triazolo[4,3-b]pyridazine (**7d**)

Sample Name:IS10607-058 Mobile A:0.1%HCOOH in Water Vial:1:11
Data File:A914961 Mobile B: 0.1%HCOOH in ACN Flow Rate:1.0 ml/min
Acq.Method:595FA.olp %B: 0min=5%2min=95%2.5min=5%3min=5% Inj Date:17-Feb-2014
Instrument Code :SC\AD\17-004 Column : Acquity UPLC HSS T3 (2.1x50)mm;1.8µm:

Printed: Mon Feb 17 12:19:33 2014

Sample Report:



Peak no	R.T	Area	% Area
1	2.15	3e+006	100.00

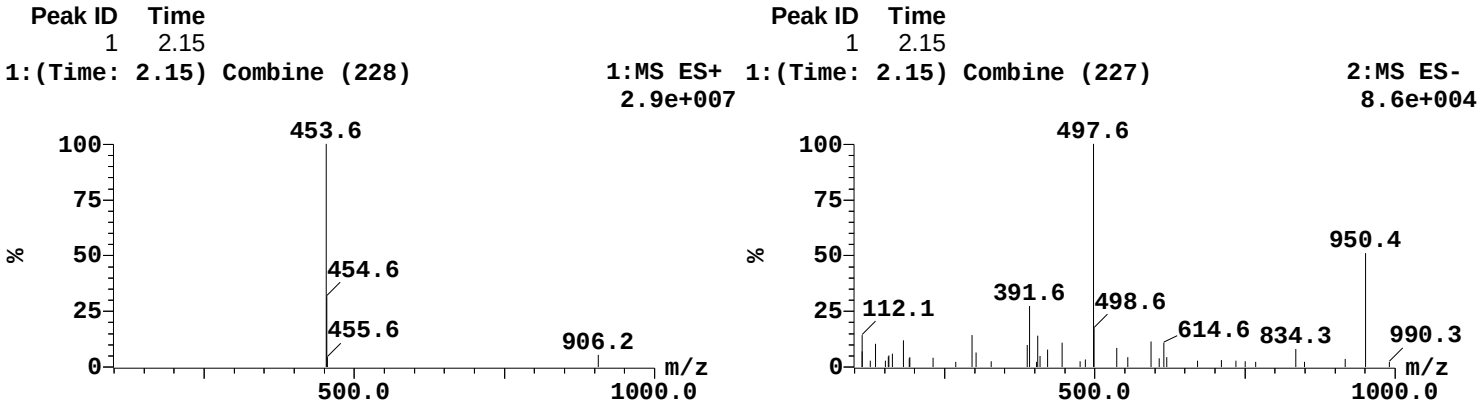
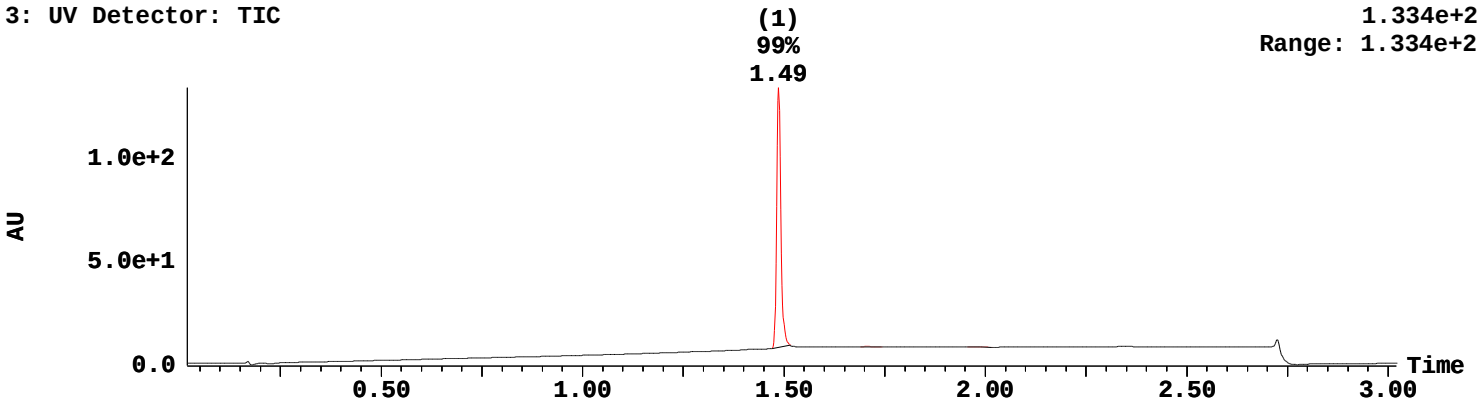


Fig 88. UPLC spectra of 3-(4-tert-Butylphenyl)-8-(4-fluorophenyl)-6-(4-methoxyphenyl)-[1,2,4]triazolo [4,3-b]pyridazine (**7e**)

Sample Name:IS10607-058 Mobile A:0.1%HCOOH in Water Vial:1:23
Data File:A936770A Mobile B: 0.1%HCOOH in ACN Flow Rate: 0.7 ml/min
Acq.Method:595FA.olp %B: 0min=30%1.25min=95%2min=95%3min=30% Inj Date:14-Mar-2014
Instrument Code :SC\AD\17-004 Column : Acquity UPLC HSS T3 (2.1x50)mm;1.8µm:

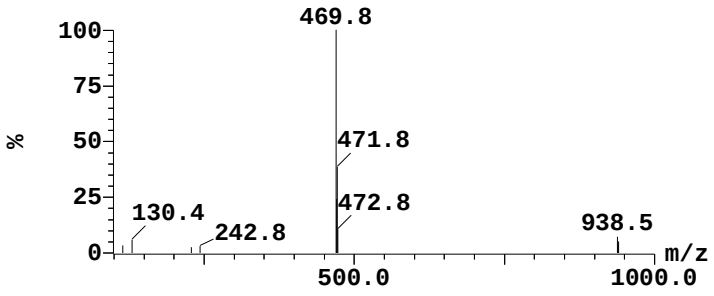
Printed: Fri Mar 14 11:17:39 2014

Sample Report:

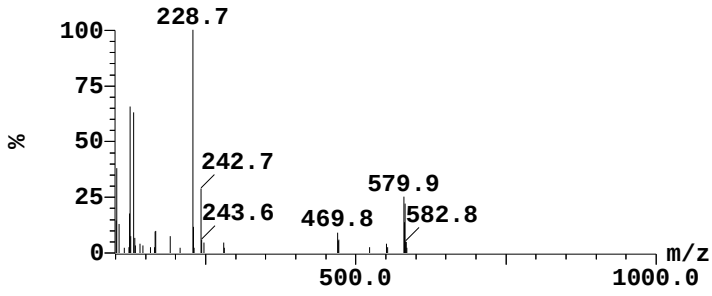


Peak no	R.T	Area	% Area
1	1.49	1e+006	99.13
2	1.71	7e+003	0.48
3	1.99	3e+003	0.21
4	1.99	3e+003	0.19

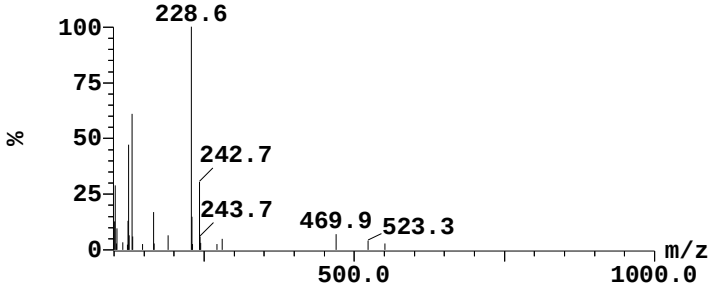
Peak ID Time
1 1.49



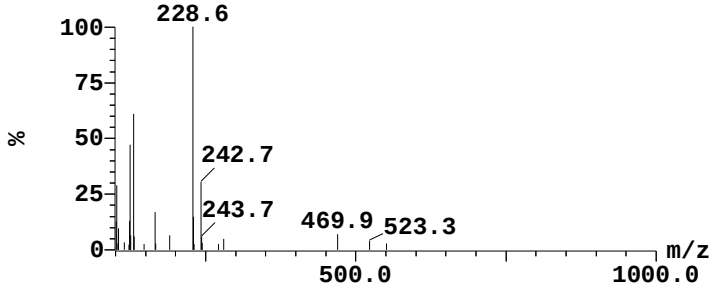
Peak ID Time
2 1.71



Peak ID Time
3 1.99



Peak ID Time
4 1.99



Sample Name:IS10607-058 Mobile A:0.1%HCOOH in Water Vial:1:23
Data File:A936770A Mobile B: 0.1%HCOOH in ACN Flow Rate: 0.7 ml/min
Acq.Method:595FA.olp %B: 0min=30%1.25min=95%2min=95%3min=30% Inj Date:14-Mar-2014
Instrument Code :SC\AD\17-004 Column : Acquity UPLC HSS T3 (2.1x50)mm;1.8µm:

Printed: Fri Mar 14 11:17:39 2014

Sample Report (continued):

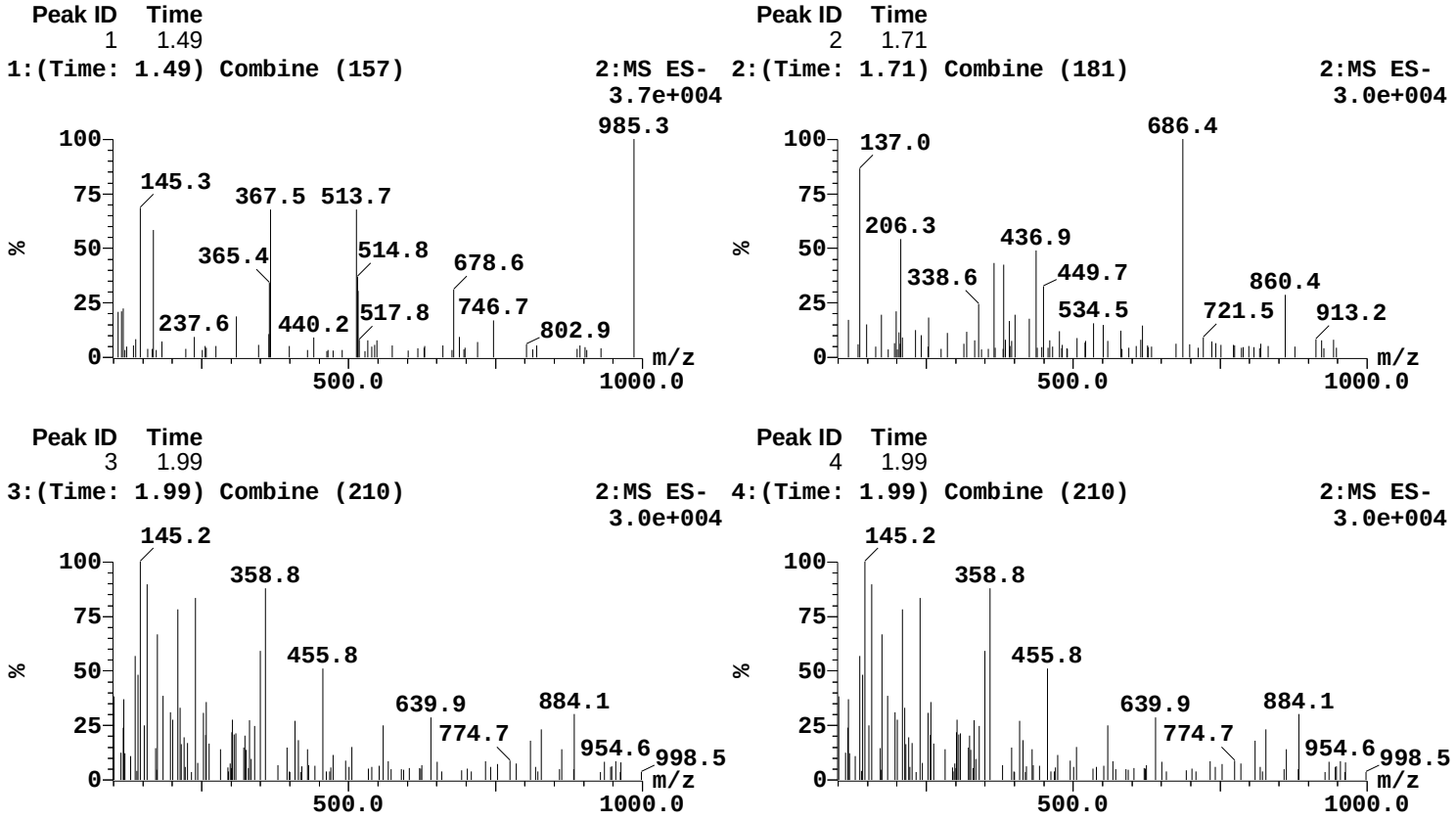


Fig 89. UPLC of 3-(4-tert-Butylphenyl)-8-(4-chlorophenyl)-6-(4-methoxyphenyl)-[1,2,4]triazolo [4,3-b]pyridazine (**7f**)