Supporting Information

On Water: Iodine-Mediated Direct Construction of 1, 3-Benzothiazines from ortho-Alkynylanilines by Regioselective *6-Exo-dig* Cyclization

*Kapil Mohan Saini, Rakesh K. Saunthwal, Shiv Kumar and Akhilesh K. Verma**

Synthetic Organic Chemistry Research Laboratory, Department of Chemistry, University of Delhi, Delhi-110007, India

X-Ray Crystallographic Studies

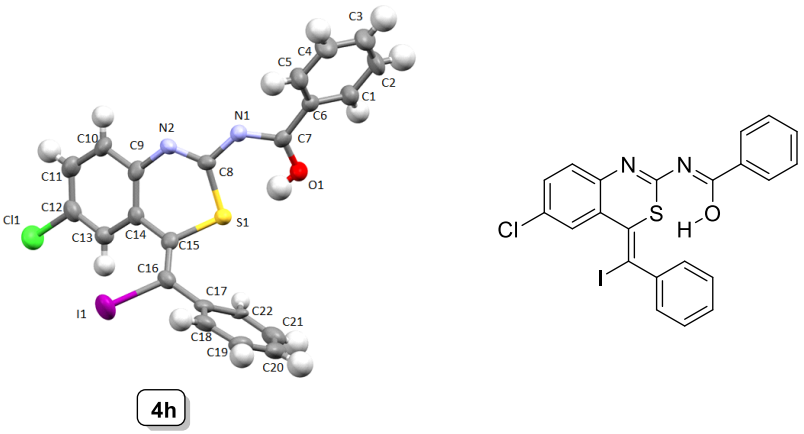


Figure I. ORTEP structure of compound **4h.**

The crystal of **4h** of suitable quality was obtained from MeOH/$CHCl_3$. The compound **4h** crystallized in Orthorhombic crystal system with space group *P c c n*. The single-crystal X-ray data were collected on an Oxford X Calibur CCD diffractometer using graphite monochromated Mo Kα radiation (λ = 0.71073 Å). The structures was solved using SIR-92 and refined by full matrix least square technique on F^2 using the SHELXL-97[1-4] program within the WinGX v 1.80.05 software package. In **4h** hydrogens are mixed and all non-hydrogen atoms were refined anisotropically. Atomic coordinates, bond lengths, bond angles, and thermal parameters for compound **4h** have been deposited at the Cambridge Crystallographic Data Centre. CCDC deposit number for **4h** is 1872209.

Table I. Crystallographic data and structure refinement for compounds **4h**

Formula weight	516.76
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system	Orthorhombic
Space group	P c c n
A	9.8708(4) Å
B	40.1183(17) Å
C	9.9473(5) Å
α	90°
β	90°
γ	90°
Volume	3939.1(3) $Å^3$
Z	8
Density (calculated)	1.743 Mg/m^3
Absorption coefficient	1.883 mm^{-1}
F(000)	2032
Crystal size	0.20 x 0.18 x 0.16 mm^3
Theta range for data collection	3.272 to 29.542°
Index ranges	-13<=h<=13, -54<=k<=55, -13<=l<=13
Reflections collected	56114
Independent reflections	5137 [R(int) = 0.1507]
Completeness to theta = 25.00°	99.8 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5137 / 0 / 253
Goodness-of-fit on F^2	1.026
Final *R* indices [I>2sigma(I)][a, b]	R1 = 0.0766, wR2 = 0.1418
R indices (all data)	R1 = 0.1807, wR2 = 0.1766
Largest diff. peak and hole	0.995 and -1.048 $e.Å^{-3}$

[a]$R = \sum(\| Fo | - | Fc \|) / \sum | Fo |$; [b]$wR = \{\sum[w(F_o^2 - F_c^2)^2] / \sum[w(F_o^2)^2]\}^{1/2}$

References:

1. CrysAlisPro, Agilent Technologies, Version 1.171.34.49, **2011**.

2. Sheldrick, G. M., *ActaCryst*. **2008**, *A64*, 112.

3. Farrugia, L. J. WinGX Version 1.80.05, An integrated system of Windows Programs for the Solution, Refinement and Analysis of Single Crystal X-Ray Diffraction Data*;* Department of Chemistry, University of Glasgow,**1997-2009**.

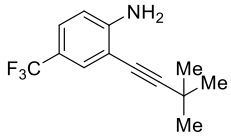
4. (a) Foresman, J. B.; Frisch, A. E. *Exploring Chemistry with Electronic Structure Methods*; Gaussian, Inc.: Pittsburgh, PA. **1995**. (b) Hehre, W. J., Radom, L., Schleyer, P. V. R.; Pople, J. A. *Ab Initio Molecular Orbital Theory*; Wiley: New York, **1985**.

General Experimental

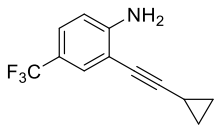
General Information and Method. All the reactions were performed in an oven-dried Schlenk flask under an argon atmosphere. Column chromatography was performed using silica gel (mesh 100-200). TLC analysis was performed on commercially prepared 60 F_{254} silica gel plates. Visualization of spots on TLC plate was accomplished with UV light (254 nm) and staining over I_2 chamber. ^{1}H NMR (400 MHz) and ^{13}C NMR (100 MHz) spectra were recorded in $CDCl_3$ and $(CD_3)_2SO$. Chemical shifts for carbons are reported in ppm from tetramethylsilane and are referenced to the carbon resonance of the solvent. Data are reported as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, dd = doublet of doublet, br s = broad singlet), coupling constants in Hertz, and integration. High-resolution mass spectra were recorded with q−TOF electrospray mass spectrometer. All purchased chemicals were used as received. All melting points are uncorrected.

General Procedure for the Synthesis of Starting Substrate 1a-o: To a solution of substituted 2-iodoaniline (0.5 mmol) in MeCN (2 mL), 3 mol% of $Pd(PPh_3)_2Cl_2$ was added. The reaction vial was then sealed and flushed with nitrogen. Then, 1.5 equiv of Et_3N and 0.51 mmol of alkyne were added to the reaction mixture. The reaction was then stirred at 70 °C until TLC revealed complete conversion of the starting material. The reaction mixture was then allowed to cool, was diluted with H_2O, and was extracted with EtOAc (3 × 10 mL). The combined organic layers were dried over Na_2SO_4, concentrated under vacuum, and purified by column chromatography using 100−200 mesh size silica gels (hexane: ethyl acetate) to afford the corresponding product. The structure and purity of known starting materials **1a-o** were confirmed by comparison of their physical and NMR-spectral data (^{1}H NMR and ^{13}C NMR) with those reported in the literature.[17-20]

General Procedure for the Synthesis of Starting Substrate 1p-u: To a solution of substituted 2-iodoaniline (0.5 mmol) in Et_3N (3 mL), 3 mol% of $Pd(PPh_3)_2Cl_2$ and 1 mol% of CuI were added. The reaction vial was then sealed and flushed with nitrogen. Then 0.51 mmol of alkyne was added to the reaction mixture. The reaction was then stirred at 25 °C until TLC revealed complete conversion of the starting material. The reaction mixture was then allowed to cool, was diluted with H_2O, and was extracted with EtOAc (3 × 10 mL). The combined organic layers were dried over Na_2SO_4, concentrated under vacuum, and purified by column chromatography using 100−200 mesh size silica gels (hexane: ethyl acetate) to afford the corresponding product. The structure and purity of known starting materials **1p, 1q, 1t, 1u** were confirmed by comparison of their physical and NMR-spectral data (^{1}H NMR and ^{13}C NMR) with those reported in the literature.[17-20]



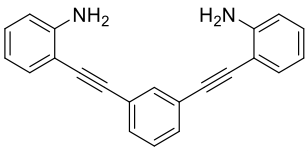
2-(3,3-Dimethylbut-1-yn-1-yl)-4-(trifluoromethyl)aniline (**1r**). The product was obtained as a colourless oil, (110.9 mg, 92%); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.49 (s, 1H), 7.28 (d, J = 8.8 Hz, 1H), 6.67 (d, J = 8.8 Hz, 1H), 4.44 (s, 2H), 1.35 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 150.1, 129.3 (q, $J_{C\text{-}F}$ = 3.9 Hz), 125.7 (q, $J_{C\text{-}F}$ = 3.9 Hz), 124.4 (q, $J_{C\text{-}F}$ = 270.3 Hz), 119.7 (q, $J_{C\text{-}F}$ = 32.8 Hz), 113.4, 108.5, 105.4, 74.3, 31.2, 28.4. HRMS (ESI) $[M+H]^+$ Calcd for $[C_{13}H_{14}F_3N]$ 242.1157, found 242.1159.



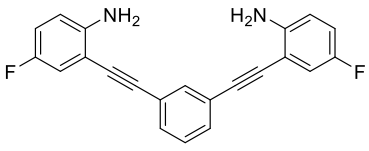
2-(Cyclopropylethynyl)-4-(trifluoromethyl)aniline (**1s**). The product was obtained as a colourless oil, (101.2 mg, 90%); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.47 (s, 1H), 7.26 (dd, J = 8.5 and 1.9 Hz, 1H), 6.65 (d, J = 8.5 Hz, 1H), 4.46 (br s, 2H), 1.52–1.46 (m, 1H), 0.93–0.88 (m, 2H), 0.83–0.79 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 150.5, 129.6 (q,

$J_{C\text{-}F}$ = 3.9 Hz), 125.8 (q, $J_{C\text{-}F}$ = 3.9 Hz), 124.6 (q, $J_{C\text{-}F}$ = 270.3 Hz), 119.6 (q, $J_{C\text{-}F}$ = 32.7 Hz), 113.5, 108.4, 100.2, 70.9, 9.0, 0.3. HRMS (ESI) $[M+H]^+$ Calcd for $[C_{12}H_{10}F_3N]$ 226.0844, found 226.0837.

General Procedure for the Synthesis of Starting Substrate 6a-b: To a solution of substituted 2-iodoaniline (0.5 mmol) in MeCN (2 mL), 5 mol% of $Pd(PPh_3)_2Cl_2$ was added. The reaction vial was then sealed and flushed with nitrogen. Then, 3 equiv of Et_3N and 0.26 mmol of terminal alkyne were added to the reaction mixture. The reaction was then stirred at 70 °C until TLC revealed complete conversion of the starting material. The reaction mixture was then allowed to cool, was diluted with H_2O, and was extracted with EtOAc (3 × 10 mL). The combined organic layers were dried over Na_2SO_4, concentrated under vacuum, and purified by column chromatography using 100−200 mesh size silica gels (hexane:ethyl acetate) to afford the corresponding product.



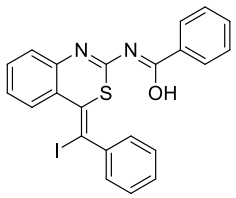
2,2'-(1,3-Phenylenebis(ethyne-2,1-diyl))dianiline (**6a**). The product was obtained as a yellow needles, mp: 127–129 ^oC (135.5 mg, 88%); ^1H NMR (400 MHz, $CDCl_3$) δ 7.68 (s, 1H), 7.47–7.45 (m, 2H), 7.37–7.29 (m, 3H), 7.16–7.12 (m, 2H), 6.73– 6.70 (m, 4H), 4.19 (br s, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 148.0, 134.3, 132.3, 131.1, 130.1, 128.7, 123.8, 118.1, 114.5, 107.7, 94.0, 86.8. HRMS (ESI) $[M+H]^+$ Calcd for $[C_{22}H_{16}N_2]$ 309.1392, found 309.1389.



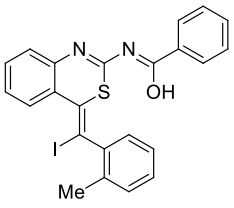
2,2'-(1,3-Phenylenebis(ethyne-2,1-diyl))bis(4-fluoroaniline) (**6b**). The product was obtained as a yellow needles, mp: 121–123 ^oC (146.2mg, 85%); ^1H NMR (400 MHz, $CDCl_3$) δ 7.67 (s, 1H), 7.48–7.46 (m, 2H), 7.36–7.31 (m, 1H), 7.07 (d, J =

2.9 Hz, 1H), 7.05 (d, *J* = 3.0 Hz, 1H), 6.88 (td, *J* = 8.6 and 2.9 Hz, 2H), 6.65 (dd, *J* = 8.9 and 4.7 Hz, 2H), 4.15 (br s, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 155.3 (d, J_{C-F} = 237.0 Hz), 144.4, 135.3, 134.4, 132.4 (d, J_{C-F} = 16.4 Hz), 131.5, 130.3, 128.8, 127.8, 123.4, 117.9 (d, J_{C-F} = 23.1 Hz), 117.3 (d, J_{C-F} = 23.1 Hz), 115.5 (d, J_{C-F} = 8.7 Hz), 108.3 (d, J_{C-F} = 9.6 Hz), 94.4, 85.9. HRMS (ESI) $[M+H]^+$ Calcd for $[C_{22}H_{14}F_2N_2]$ 345.1203, found 345.1198.

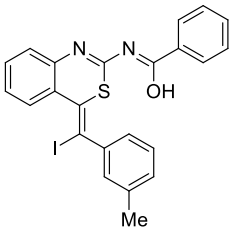
General experimental procedure for green one-pot synthesis of benzo[1,3]thiazin-2-yl)benzimidic acid 3-5: To a solution of *ortho*-alkynlanilines **1** (0.5 mmol), aroyl isothiocyanates **2** (0.52 mmol) and 2.0 equiv of I_2 was added in water (2.0 mL). The reaction was then stirred at room temperature until TLC revealed a complete conversion of the starting material. After the completion of the reaction, the reaction mixture was quenched with saturated aq sodium thiosulfate solution and extracted with EtOAc (3X10 mL). The combined organic layers were dried over Na_2SO_4, concentrated under vacuum, and purified by column chromatography using 100−200 mesh size silica gels (EtOAc: hexane) to afford the corresponding product.



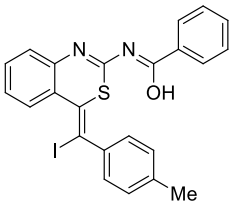
(Z)-N-((E)-4-(Iodo(phenyl)methylene)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (**3a**). The product was obtained as a pale yellow needles, mp: 155–157 ^{o}C (216.9 mg, 90%); FTIR (Zn−Se ATR, cm^{-1}) 3429, 2922, 1597, 1554, 1411, 1310, 1285, 1079, 762, 748, 708; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.55 (s, 1H), 8.12 (d, *J* = 7.8 Hz, 1H), 7.96 (d, *J* = 7.8 Hz, 2H), 7.48–7.27 (m, 10H), 7.09 (d, *J* = 7.8 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 143.1, 138.6, 134.3, 132.8, 130.6, 129.9, 129.5, 129.3, 129.0, 128.9, 128.7, 128.6, 128.5, 126.3, 125.4, 124.4, 121.3, 114.2, 98.1. HRMS (ESI) $[M+H]^+$ Calcd for $[C_{22}H_{15}IN_2OS]$ 483.0028, found 483.0022.



(Z)-N-((E)-4-(Iodo(o-tolyl)methylene)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (**3b**). The product was obtained as a yellow needles, mp: 154–156 ^{o}C (207.9 mg, 84%); FTIR (Zn–Se ATR, cm^{-1}) 3495, 2988, 1611, 1584, 1501, 1399, 1310, 1089, 712, 698, 658; ^{1}H NMR (400 MHz, $CDCl_3$) δ 11.64 (br s, 1H), 8.22 (d, J = 7.8 Hz, 1H), 7.99 (d, J = 6.8 Hz, 2H), 7.50–7.46 (m, 1H), 7.42–7.36(m, 3H), 7.32–7.28 (m, 1H), 7.26–7.17 (m, 4H), 7.07 (d, J = 7.8 Hz, 1H), 2.28 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 146.7, 143.2, 139.0, 137.0, 135.3, 134.9, 133.6, 133.3, 132.7, 131.2, 131.1, 129.5, 127.5, 125.5, 100.0, 23.7. HRMS (ESI) $[M+H]^+$ Calcd for $[C_{23}H_{17}IN_2OS]$ 497.0185, found 497.0172.

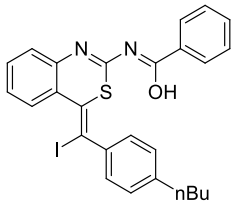


(Z)-N-((E)-4-(Iodo(m-tolyl)methylene)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (**3c**). The product was obtained as a yellow needles, mp: 86–88 ^{o}C (215.7 mg, 87%); FTIR (Zn–Se ATR, cm^{-1}) 3299, 2838, 1610, 1588, 1420, 1338, 1198, 1038, 1001, 848, 708, 690; ^{1}H NMR (400 MHz, $CDCl_3$) δ 11.79 (br s, 1H), 8.10 (d, J = 7.8 Hz, 1H), 8.00 (d, J = 7.8 Hz, 2H), 7.49–7.46 (m, 1H), 7.42–7.35 (m, 3H), 7.30–7.25 (m, 2H), 7.16–7.14 (m, 3H), 7.07 (d, J = 8.8 Hz, 1H), 2.37 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) 142.1, 137.6, 133.9, 131.6, 129.5, 129.4, 128.7, 128.1, 127.7, 127.4, 125.3, 124.2, 123.4, 119.8, 97.0, 20.5. HRMS (ESI) $[M+H]^+$ Calcd for $[C_{23}H_{17}IN_2OS]$ 497.0185, found 497.0186.

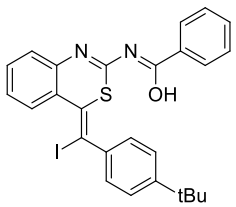


(Z)-N-((E)-4-(Iodo(p-tolyl)methylene)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (**3d**). The product was obtained as a yellow needles, mp: 146–148 ^{o}C

(230.6 mg, 93%); FTIR (Zn–Se ATR, cm^{-1}) 3313, 1691, 1546, 1446, 1388, 1232, 1074, 817, 748, 702, 617; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.24 (br s, 1H), 8.09 (dd, J = 7.8 and 1.4 Hz, 1H), 7.97 (d, J = 7.3 Hz, 2H), 7.47–7.43 (m, 1H), 7.39–7.32 (m, 3H), 7.29–7.24 (m, 3H), 7.18 (d, J = 8.2 Hz, 2H), 7.09 (dd, J = 7.8 and 0.9 Hz, 1H), 2.35 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 140.2, 139.7, 138.5, 134.3, 132.8, 130.5, 129.8, 129.5, 129.3, 129.1, 129.0, 128.7, 128.5, 125.7, 125.4, 124.5, 121.2, 98.7, 21.6. HRMS (ESI) $[M+H]^+$ Calcd for $[C_{23}H_{17}IN_2OS]$ 497.0185, found 497.0196.

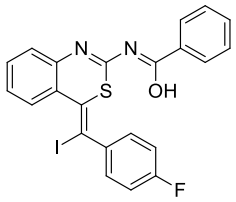


(Z)-N-((E)-4-((4-Butylphenyl)iodomethylene)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (**3e**). The product was obtained as a yellow needles, mp: 161–163 ^{o}C (236.7 mg, 88%); FTIR (Zn–Se ATR, cm^{-1}) 3310, 2968, 1605, 1585, 1433, 1355, 1275, 1040, 862, 748, 690; ^{1}H NMR (400 MHz, $CDCl_3$) δ 11.83 (s, 1H), 8.08 (d, J = 7.8 Hz, 1H), 7.95 (d, J = 6.8 Hz, 2H), 7.46–7.42 (m, 1H), 7.38–7.24 (m, 6H), 7.19 (d, J = 8.8 Hz, 2H), 7.03 (d, J = 7.8 Hz, 1H), 2.61 (t, J = 7.8 Hz, 2H), 1.66–1.58 (m, 2H), 1.43–1.36 (m, 2H), 0.94 (t, J = 7.3 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 144.6, 140.4, 134.9, 132.6, 130.5, 129.4, 129.1, 129.06, 128.8, 128.4, 125.8, 125.2, 124.7, 121.0, 98.6, 35.6, 33.4, 22.6, 14.1. HRMS (ESI) $[M+H]^+$ Calcd for $[C_{26}H_{23}IN_2OS]$ 539.0654, found 539.0667.

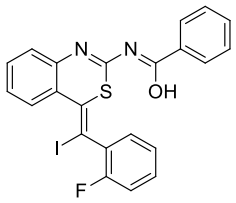


(Z)-N-((E)-4-((4-(tert-Butyl)phenyl)iodomethylene)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (**3f**). The product was obtained as a pale yellow needles, mp: 184–186 ^{o}C (231.3 mg, 86%); FTIR (Zn–Se ATR, cm^{-1}) 3267, 2958, 1653, 1577, 1562, 1465, 1257, 1186, 914, 754, 661; ^{1}H NMR (400 MHz, $CDCl_3$) δ 11.78 (br s, 1H), 8.01

(d, *J* = 8.8 Hz, 1H), 7.88 (d, *J* = 6.8 Hz, 2H), 7.38–7.31 (m, 3H), 7.29–7.24 (m, 5H), 7.20–7.16 (m, 1H), 6.96 (d, *J* = 8.8 Hz, 1H), 1.26 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 151.6, 138.9, 137.4, 133.8, 131.5, 129.4, 128.6, 128.2, 128.1, 128.0, 127.8, 127.5, 127.3, 124.7, 124.4, 124.1, 123.6, 119.9, 97.7, 33.9, 30.3. HRMS (ESI) $[M+H]^+$ Calcd for $[C_{26}H_{23}IN_2OS]$ 539.0654, found 539.0646.

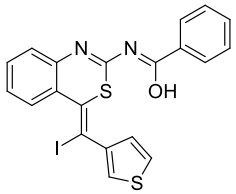


(Z)-N-((E)-4-((4-Fluorophenyl)iodomethylene)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (**3g**). The product was obtained as a brown needles, mp: 135–137 ^{o}C (212.4 mg, 85%); FTIR (Zn–Se ATR, cm^{-1}) 3237, 2920, 1893, 1696, 1502, 1466, 1259, 1232, 1156, 1026, 836, 750, 702; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.46 (br s, 1H), 8.07 (d, *J* = 7.8 Hz, 1H), 7.97 (d, *J* = 7.8 Hz, 1H), 7.56–7.24 (m, 7H), 7.20–7.04 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.9 (d, *J* = 250.5 Hz, 1C), 139.1 (d, *J* = 2.9 Hz, 1C), 138.5, 133.8, 133.0, 131.3 (d, *J* = 8.7 Hz, 1C), 130.7, 129.0, 128.8, 128.6, 126.7, 125.7, 124.2, 121.5, 116.0 (d, *J* = 22.2 Hz, 1C), 96.7. HRMS (ESI) $[M+H]^+$ Calcd for $[C_{22}H_{14}FIN_2OS]$ 500.9934, found 500.9932.

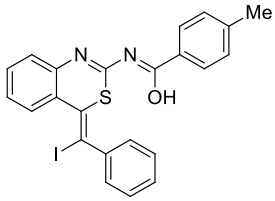


(Z)-N-((E)-4-((2-Fluorophenyl)iodomethylene)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (**3h**). The product was obtained as a pale yellow needles, mp: 226–228 ^{o}C (199.8 mg, 80%); FTIR (Zn–Se ATR, cm^{-1}) 3228, 3068, 1693, 1581, 1543, 1446, 1269, 1217, 744, 698, 677; ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.97 (br s, 1H), 8.07 (d, *J* = 7.8 Hz, 1H), 7.96 (d, *J* = 5.9 Hz, 2H), 7.55–7.33 (m, 8H), 7.26–7.19 (m, 2H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 157.9 (d, *J* = 246.6 Hz, 1C), 133.1, 131.8 (d, *J* = 8.7 Hz, 1C),

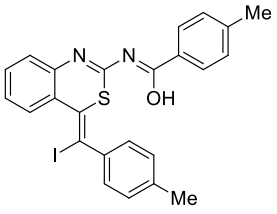
131.5, 131.4, 131.2, 131.0, 130.3, 129.4, 128.9, 128.1, 125.5, 123.7, 116.6 (d, J = 21.2 Hz, 1C), 89.6. HRMS (ESI) $[M+H]^+$ Calcd for $[C_{22}H_{14}FIN_2OS]$ 500.9934, found 500.9936.



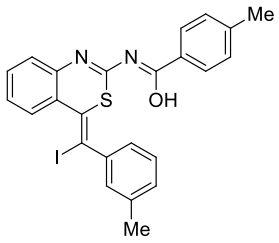
(Z)-N-((E)-4-(Iodo(thiophen-3-yl)methylene)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (**3i**). The product was obtained as a yellow needles, mp: 126–128 ^oC (200.1 mg, 82%); FTIR (Zn–Se ATR, cm^{-1}) 3210, 3020, 1697, 1534, 1424, 1316, 1280, 1235, 979, 752, 728, 688; ^1H NMR (400 MHz, $CDCl_3$) δ 11.14 (br s, 1H), 8.04 (d, J = 7.8 Hz, 1H), 7.94 (d, J = 7.8 Hz, 2H), 7.47–7.42 (m, 2H), 7.40–7.33 (m, 4H), 7.27–7.24 (m, 1H), 7.18 (d, J = 3.9 Hz, 1H), 7.05 (d, J = 7.8, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 141.7, 137.8, 133.3, 131.6, 129.4, 128.1, 127.8, 127.6, 127.4, 126.6, 126.3, 125.4, 124.9, 124.1, 123.4, 120.4, 90.0. HRMS (ESI) $[M+H]^+$ Calcd for $[C_{20}H_{13}IN_2OS_2]$ 488.9592, found 488.9592.



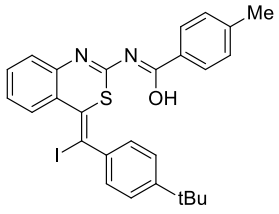
(Z)-N-((E)-4-(Iodo(phenyl)methylene)-4H-benzo[d][1,3]thiazin-2-yl)-4-methylbenzimidic acid (**3j**). The product was obtained as a yellow needles, mp: 146–148 ^oC (213.2 mg, 86%); FTIR (Zn–Se ATR, cm^{-1}) 3320, 2822, 1589, 1554, 1429, 1318, 1293, 1179, 832, 762, 718, 688; ^1H NMR (400 MHz, $CDCl_3$) δ 9.70 (s, 1H), 8.09 (d, J = 7.8 Hz, 1H), 7.83 (d, J = 7.8 Hz, 2H), 7.39–7.21 (m, 7H), 7.13 (d, J = 8.8 Hz, 2H), 7.07 (d, J = 7.8 Hz, 1H), 2.32 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 143.6, 143.1, 139.0, 131.3, 130.5, 129.9, 129.7, 129.5, 129.3, 129.26, 129.0, 128.8, 128.79, 128.6, 126.5, 125.4, 124.4, 121.6, 97.9, 21.8. HRMS (ESI) $[M+H]^+$ Calcd for $[C_{23}H_{17}IN_2OS]$ 497.0185, found 497.0169.



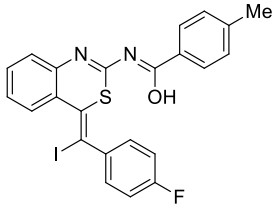
(Z)-N-((E)-4-(Iodo(p-tolyl)methylene)-4H-benzo[d][1,3]thiazin-2-yl)-4-methylbenzimidic acid (**3k**). The product was obtained as a pale yellow needles, mp: 144–146 ^{o}C (224.4 mg, 88%); FTIR (Zn–Se ATR, cm^{-1}) 3626, 3280, 2917, 1721, 1592, 1555, 1406, 1303, 1286, 1186, 1018, 954, 817, 793, 749; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.97 (br s, 1H), 8.06 (d, J = 7.8 Hz, 1H), 7.83 (d, J = 7.8 Hz, 2H), 7.36–7.32 (m, 1H), 7.25–7.24 (m, 3H), 7.17–7.12 (m, 4H), 7.05 (d, J = 7.8 Hz, 1H), 2.33 (s, 3H), 2.32 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 143.6, 140.2, 139.7, 138.9, 131.5, 130.4, 129.9, 129.5, 129.3, 129.27, 129.0, 128.9, 125.9, 125.4, 124.5, 121.5, 98.5, 21.8, 21.6. HRMS (ESI) $[M+H]^+$ Calcd for $[C_{24}H_{19}IN_2OS]$ 511.0341, found 511.0319.



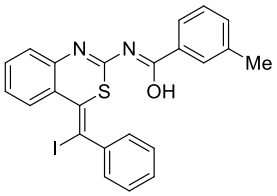
(Z)-N-((E)-4-(Iodo(m-tolyl)methylene)-4H-benzo[d][1,3]thiazin-2-yl)-4-methylbenzimidic acid (**3l**). The product was obtained as a yellow needles, mp: 161–163 ^{o}C (221.8 mg, 87%); FTIR (Zn–Se ATR, cm^{-1}) 3301, 2920, 2852, 1683, 1604, 1546, 1467, 1442, 1259, 1211, 1111, 1039, 920, 790, 738, 719; ^{1}H NMR (400 MHz, $CDCl_3$) δ 11.39 (br s, 1H), 8.08 (d, J = 7.8 Hz, 1H), 7.86 (d, J = 7.8 Hz, 2H), 7.39–7.35 (m, 1H), 7.28–7.24 (m, 2H), 7.16–7.12 (m, 5H), 7.07 (d, J = 7.8 Hz, 1H), 2.35 (s, 3H), 2.33 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 142.30, 141.9, 137.4, 129.3, 129.2, 128.6, 128.2, 128.0, 127.9, 127.7, 127.5, 125.2, 125.0, 124.1, 123.2, 120.2, 96.8, 20.5, 20.4. HRMS (ESI) $[M+H]^+$ Calcd for $[C_{24}H_{19}IN_2OS]$ 511.0341, found 511.0328.



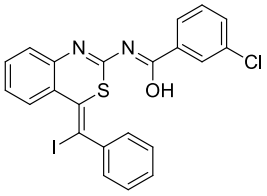
(Z)-N-((E)-4-((4-(tert-butyl)phenyl)iodomethylene)-4H-benzo[d][1,3]thiazin-2-yl)-4-methylbenzimidic acid (**3m**). The product was obtained as a yellow needles, mp: 147–149 ^{o}C (248.4 mg, 90%); FTIR (Zn–Se ATR, cm^{-1}) 3216, 2812, 1610, 1552, 1472, 1343, 1285, 1179, 1099, 755, 688; ^{1}H NMR (400 MHz, $CDCl_3$) δ 11.86 (br s, 1H), 8.06 (d, J = 7.8 Hz, 1H), 7.85 (d, J = 7.8 Hz, 2H), 7.38–7.33 (m, 3H), 7.30–7.22 (m, 3H), 7.14 (d, J = 8.8 Hz, 2H), 7.02 (d, J = 7.8 Hz, 1H), 2.32 (s, 3H), 1.31 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 151.5, 142.2, 138.9, 129.3, 128.2, 128.1, 124.6, 124.0, 123.6, 119.9, 97.4, 33.8, 30.2, 20.6. HRMS (ESI) $[M+H]^+$ Calcd for $[C_{27}H_{25}IN_2OS]$ 553.0811, found 553.0808.



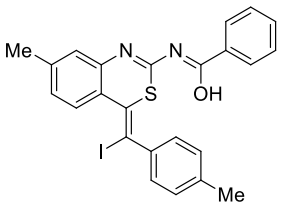
(Z)-N-((E)-4-((4-Fluorophenyl)iodomethylene)-4H-benzo[d][1,3]thiazin-2-yl)-4-methylbenzimidic acid (**3n**). The product was obtained as a pale yellow needles, mp: 193–195 ^{o}C (210.7 mg, 82%); FTIR (Zn–Se ATR, cm^{-1}) 3360, 3062, 2922, 1664, 1604, 1558, 1462, 1436, 1259, 1226, 1151, 1085, 1041, 958, 827, 738, 650, 586; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.29 (br s, 1H), 8.07 (dd, J = 7.8 and 1.4 Hz, 1H), 7.83 (d, J = 7.8 Hz, 2H), 7.38–7.32 (m, 3H), 7.28–7.24 (m, 1H), 7.15 (d, J = 8.2 Hz, 2H), 7.08–7.04 (m, 3H), 2.33 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.9 (d, J = 250.5 Hz, 1C), 143.7, 139.2 (d, J = 2.9 Hz, 1C), 131.3 (d, J = 8.7 Hz, 1C), 130.6, 129.5, 129.3, 129.0, 128.7, 127.2, 125.4, 124.2, 121.8, 115.9 (d, J = 22.2 Hz, 1C), 114.2, 96.0, 21.7. HRMS (ESI) $[M+H]^+$ Calcd for $[C_{23}H_{16}FIN_2OS]$ 515.0090, found 515.0085.



(Z)-N-((E)-4-(Iodo(phenyl)methylene)-4H-benzo[d][1,3]thiazin-2-yl)-3-methylbenzimidic acid (**3o**). The product was obtained as a pale yellow needles, mp: 140–142 ^{o}C (213.2 mg, 86%); FTIR (Zn–Se ATR, cm^{-1}) 3220, 2918, 1681, 1595, 1537, 1446, 1352, 1282, 1192, 1072, 999, 866, 760, 738, 698, 677; ^{1}H NMR (400 MHz, $CDCl_3$) δ 11.14 (br s, 1H), 8.11 (d, J = 7.8Hz, 1H), 7.74–7.72 (m, 2H), 7.41–7.22 (m, 9H), 7.07 (d, J = 7.83, 1H), 2.32 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 143.2, 139.3, 138.3, 134.4, 133.5, 130.5, 129.5, 129.3, 128.8, 128.4, 126.7, 126.0, 125.3, 124.4, 121.7, 115.6, 97.5. HRMS (ESI) $[M+H]^+$ Calcd for $[C_{23}H_{17}IN_2OS]$ 497.0185, found 497.0201.

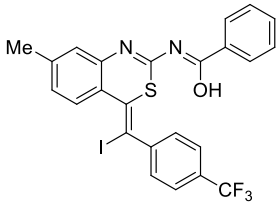


(Z)-3-Chloro-N-((E)-4-(iodo(phenyl)methylene)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (**3p**). The product was obtained as a yellow needles, mp: 129–131 ^{o}C (216.6 mg, 84%); FTIR (Zn–Se ATR, cm^{-1}) 3066, 2922, 1687, 1546, 1357, 1284, 1251, 1072, 788, 713, 678; ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.05 (br s, 1H), 8.13 (d, J = 7.8 Hz, 1H), 8.03 (s, 1H), 7.91 (d, J = 7.8 Hz, 1H), 7.43–7.34 (m, 7H), 7.32–7.24 (m, 2H), 7.05 (d, J = 7.8 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 143.1, 137.3, 134.5, 132.5, 130.7, 129.6, 129.55, 129.2, 129.1, 128.9, 127.4, 125.9, 125.3, 124.3, 120.1, 98.5. HRMS (ESI) $[M+H]^+$ Calcd for $[C_{22}H_{14}ClIN_2OS]$ 516.9638, found 516.9627.

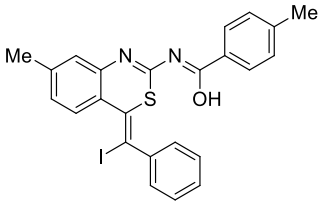


(Z)-N-((E)-4-(Iodo(p-tolyl)methylene)-7-methyl-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (**4a**). The product was obtained as a yellow needles,

mp: 167–169 ^{o}C (232.1 mg, 91%); FTIR (Zn–Se ATR, cm^{-1}) 3230, 2918, 1693, 1570, 1541, 1467, 1267, 1024, 997, 817, 704, 655; ^{1}H NMR (400 MHz, DMSO-d$_6$) δ 7.93 (d, J = 8.3 Hz, 2H), 7.86 (d, J = 8.3 Hz, 1H), 7.50 (d, J = 7.3Hz, 1H), 7.42–7.38 (m, 2H), 7.19–7.09 (m, 4H), 7.06–7.03 (m, 2H), 2.32 (s, 3H), 2.25 (s, 3H); ^{13}C NMR (100 MHz, DMSO-d$_6$) δ 140.8, 140.6, 139.1, 134.3, 133.0, 130.0, 129.7, 129.6, 129.4, 129.0, 128.9, 128.6, 127.2, 126.2, 122.2, 98.7, 21.5, 21.4. HRMS (ESI) [M+H]$^{+}$ Calcd for [$C_{24}H_{19}IN_2OS$] 511.0341, found 511.0343.

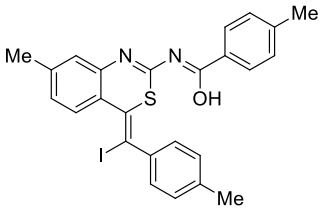


(Z)-N-((E)-4-(Iodo(4-(trifluoromethyl)phenyl)methylene)-7-methyl-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (**4b**). The product was obtained as a yellow needles, mp: 170–172 ^{o}C (234.05 mg, 83%); FTIR (Zn–Se ATR, cm^{-1}) 3275, 2924, 1699, 1546, 1489, 1319, 1284, 1114, 1064, 1016, 786, 711; ^{1}H NMR (400 MHz, $CDCl_3$) δ 11.31 (br s, 1H), 8.01 (d, J = 7.8 Hz, 3H), 7.66 (d, J = 7.8 Hz, 2H), 7.50–7.45 (m, 3H), 7.40–7.36 (m, 2H), 7.13 (d, J = 7.8 Hz, 1H), 6.94 (s, 1H), 2.39 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 146.6, 141.6, 133.0, 130.8 (q, J_{C-F} = 32.7 Hz), 129.6, 129.0, 128.6, 128.3, 126.6 126.2 (q, J_{C-F} = 272.3 Hz), 125.9 (q, J_{C-F} = 3.5 Hz), 121.6, 120.9, 94.1, 21.4. HRMS (ESI) [M+H]$^{+}$ Calcd for [$C_{24}H_{16}F_3IN_2OS$] 565.0058, found 565.0041.

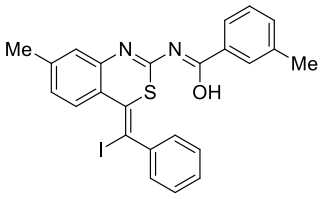


(Z)-N-((E)-4-(Iodo(phenyl)methylene)-7-methyl-4H-benzo[d][1,3]thiazin-2-yl)-4-methylbenzimidic acid (**4c**). The product was obtained as a yellow needles, mp: 152–154 ^{o}C (221.8 mg, 87%); FTIR (Zn–Se ATR, cm^{-1}) 3226, 2918, 1691, 1544, 1467, 1265, 1213, 1024, 977, 815, 754, 694; ^{1}H NMR (400 MHz, DMSO-d$_6$) δ 10.52 (br s, 1H), 7.91 (d, J = 7.8 Hz, 1H), 7.85 (d, J = 8.8 Hz, 2H), 7.41–7.37 (m, 2H),

7.32–7.28 (m, 3H), 7.24 (d, *J* = 7.8 Hz, 2H), 7.14 (d, *J* = 8.8 Hz, 1H), 7.09 (s, 1H), 2.36 (s, 3H), 2.32 (s, 3H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 143.8, 143.3, 140.7, 130.0, 129.5, 129.46, 129.4, 129.2, 129.1, 128.4, 127.8, 126.2, 122.0, 98.1, 21.6, 21.5. HRMS (ESI) $[M+H]^+$ Calcd for $[C_{24}H_{19}IN_2OS]$ 511.0341, found 511.0346.

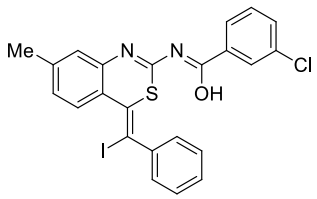


(Z)-N-((E)-4-(Iodo(p-tolyl)methylene)-7-methyl-4H-benzo[d][1,3]thiazin-2-yl)-4-methylbenzimidic acid (**4d**). The product was obtained as a dark yellow needles, mp: 135–137 ^{o}C (235.8 mg, 90%); FTIR (Zn–Se ATR, cm^{-1}) 3288, 2890, 1695, 1580, 1482, 1301, 1225, 1201, 1024, 997, 801, 754, 680; ^{1}H NMR (400 MHz, $CDCl_3$) δ 11.53 (br s, 1H), 7.99 (d, *J* = 8.8 Hz, 1H), 7.93 (d, *J* = 8.8 Hz, 2H), 7.26 (d, *J* = 7.8 Hz, 2H), 7.20–7.17 (m, 4H), 7.11 (d, *J* = 8.8 Hz, 1H), 6.97 (s, 1H), 2.39 (s, 3H), 2.37 (s, 3H), 2.36 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 143.8, 141.2, 140.2, 139.7, 137.6, 131.8, 129.9, 129.6, 129.3, 129.2, 128.8, 127.7, 126.6, 125.1, 121.6, 121.2, 114.2, 98.0, 21.8, 21.5, 21.4. HRMS (ESI) $[M+H]^+$ Calcd for $[C_{25}H_{21}IN_2OS]$ 525.0498, found 525.0495.

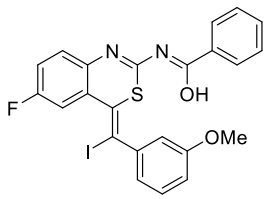


(Z)-N-((E)-4-(Iodo(phenyl)methylene)-7-methyl-4H-benzo[d][1,3]thiazin-2-yl)-3-methylbenzimidic acid (**4e**). The product was obtained as a yellow needles, mp: 151–153 ^{o}C (221.8 mg, 87%); FTIR (Zn–Se ATR, cm^{-1}) 3494, 3024, 1587, 1535, 1419, 1344, 1282, 1190, 858, 808, 777, 736, 653; ^{1}H NMR (400 MHz, $CDCl_3$) δ 11.17 (br s, 1H), 8.01 (d, *J* = 8.2 Hz, 1H), 7.78–7.76 (m, 2H), 7.41–7.31 (m, 5H), 7.28–7.22 (m, 2H), 7.11–7.08 (m, 1H), 6.88 (s, 1H), 2.37 (s, 3H), 2.32 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 143.3, 141.1, 138.2, 134.7, 133.5, 129.6, 129.4, 129.3, 128.8, 128.6, 128.4, 126.6,

126.2, 121.6, 96.4, 21.5, 21.4. HRMS (ESI) $[M+H]^+$ Calcd for $[C_{24}H_{19}IN_2OS]$ 511.0341, found 511.0329.

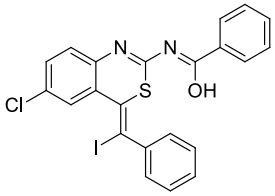


(Z)-3-Chloro-N-((E)-4-(iodo(phenyl)methylene)-7-methyl-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (**4f**). The product was obtained as a yellow needles, mp: 175–177 ^oC (227.8 mg, 86%); FTIR (Zn–Se ATR, cm^{-1}) 3515, 2918, 1585, 1533, 1429, 1419, 1344, 1284, 1155, 1068, 777, 690; ^1H NMR (400 MHz, $CDCl_3$) δ 12.65 (br s, 1H), 8.06 (s, 1H), 8.02 (d, J = 7.8 Hz, 1H), 7.94 (d, J = 7.8 Hz, 1H), 7.43–7.34 (m, 6H), 7.31–7.27 (m, 1H), 7.24 (d, J = 6.8 Hz, 1H), 7.11 (d, J = 7.8 Hz, 1H), 6.86 (s, 1H), 2.40 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 143.2, 141.4, 137.7, 136.8, 134.4, 132.4, 129.8, 129.6, 129.55, 129.2, 128.9, 128.9, 128.6, 127.5, 126.2, 125.9, 121.5, 120.1, 97.1, 21.5. HRMS (ESI) $[M+H]^+$ Calcd for $[C_{23}H_{16}ClIN_2OS]$ 530.9795, found 530.9783.

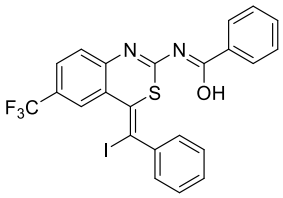


(Z)-N-((E)-6-Fluoro-4-(iodo(3-methoxyphenyl)methylene)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (**4g**). The product was obtained as a yellow needles, mp: 165–167 ^oC (222.5 mg, 84%); FTIR (Zn–Se ATR, cm^{-1}) 3311, 2910, 1688, 1539, 1467, 1400, 1218, 1155, 1085, 1024, 977, 815, 710; ^1H NMR (400 MHz, $CDCl_3$) δ 10.32 (br s, 1H), 7.85–7.83 (m, 2H), 7.82 (d, J = 2.7 Hz, 1H), 7.47–7.43 (m, 1H), 7.36–7.32 (m, 2H), 7.29–7.25 (m, 1H), 7.07–6.98 (m, 2H), 6.92–6.90 (m, 1H), 6.86–6.84 (m, 2H), 3.78 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.1 (d, J = 245.6 Hz, 1C), 159.6, 144.1, 133.5, 132.9, 129.9, 128.6, 128.5, 126.2, 125.7 (d, J = 7.7 Hz, 1C), 124.4, 121.6, 117.4 (d, J = 2.3 Hz, 1C), 115.3, 115.1,

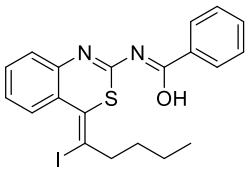
114.6, 93.0, 55.5. HRMS (ESI) $[M+H]^+$ Calcd for $[C_{23}H_{16}FIN_2O_2S]$ 531.0039, found 531.0028.



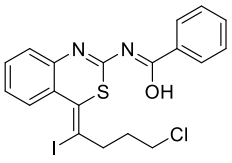
(Z)-N-((E)-6-Chloro-4-(iodo(phenyl)methylene)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (**4h**). The product was obtained as a pale yellow needles, mp: 154–156 ^oC (211.5 mg, 82%); FTIR (Zn–Se ATR, cm^{-1}) 3257, 2851, 1654, 1571, 1548, 1506, 1458, 1396, 1263, 1199, 1178, 1080, 1026, 966, 817, 709, 684; ^1H NMR (400 MHz, DMSO-d_6) δ 11.81 (br s, 1H), 8.02 (d, J = 1.8 Hz, 1H), 7.91 (d, J = 7.3 Hz, 2H), 7.53–7.48 (m, 2H), 7.42–7.34 (m, 4H), 7.31–7.25 (m, 4H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 143.4, 133. 2, 130.4, 129.6, 129.5, 129.3, 129.2, 128.9, 128.3, 126.4, 126.2, 101.2. HRMS (ESI) $[M+H]^+$ Calcd for $[C_{22}H_{14}ClIN_2OS]$ 516.9638, found 516.9636.



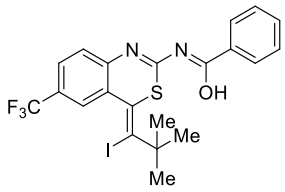
(Z)-N-((E)-4-(Iodo(phenyl)methylene)-6-(trifluoromethyl)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (**4i**). The product was obtained as a pale yellow needles, mp: 139–141 ^oC (219.9 mg, 80%); FTIR (Zn–Se ATR, cm^{-1}) 3429, 2855, 1720, 1627, 1555, 1441, 1328, 1277, 1157, 1122, 1073, 1025, 968, 832, 710; ^1H NMR (400 MHz, DMSO-d_6) δ 12.46 (br s, 1H), 8.35 (s, 1H), 7.96 (d, J = 7.8 Hz, 2H), 7.81 (d, J = 7.8 Hz, 1H), 7.58–7.51 (m, 1H), 7.48–7.28 (m, 8H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 143.3, 133.3, 129.7, 129.5, 129.4, 129.2, 129.0, 127.3, 127.26, 126.4, 126.35, 126.0, 125.95, 125.0, 123.3, 102.3. HRMS (ESI) $[M+H]^+$ Calcd for $[C_{23}H_{14}F_3IN_2OS]$ 550.9902, found 550.9897.



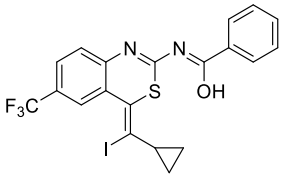
(Z)-N-((E)-4-(1-Iodopentylidene)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (**5a**). The product was obtained as a yellow needles, mp: 129–131 ^{o}C (182.4 mg, 79%); FTIR (Zn–Se ATR, cm^{-1}) 3365, 2980, 2855, 1685, 1556, 1504, 1437, 1305, 1210, 1039, 955, 815, 754, 684; ^{1}H NMR (400 MHz, $CDCl_3$) δ 11.47 (br s, 1H), 7.99 (d, J = 7.8 Hz, 2H), 7.84 (d, J = 7.8 Hz, 1H), 7.48–7.45 (m, 1H), 7.38–7.34 (m, 2H), 7.30–7.25 (m, 1H), 7.21–7.17 (m, 1H), 6.97 (d, J = 7.8 Hz, 1H), 3.07 (t, J = 7.3 Hz, 2H), 1.65–1.58 (m, 2H), 1.44–1.35 (m, 2H), 0.95 (t, J = 7.3 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 138.8, 134.5, 132.7, 129.8, 129.0, 128.9, 128.6, 125.4, 125.0, 123.1, 121.1, 107.8, 44.0, 31.6, 21.7, 14.1. HRMS (ESI) $[M+H]^+$ Calcd for $[C_{20}H_{19}IN_2OS]$ 463.0341, found 463.0340.



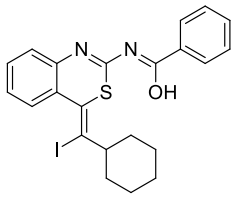
(Z)-N-((E)-4-(4-Chloro-1-iodobutylidene)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (**5b**). The product was obtained as a yellow needles, mp: 135–137 ^{o}C (192.7 mg, 80%); FTIR (Zn–Se ATR, cm^{-1}) 3231, 2985, 1665, 1574, 1477, 1385, 1301, 1287, 1153, 1101, 1029, 932, 732, 704; ^{1}H NMR (400 MHz, $CDCl_3$) δ 11.23 (br s, 1H), 8.03 (d, J = 6.8 Hz, 2H), 7.85 (d, J = 7.8 Hz, 1H), 7.54–7.50 (m, 1H), 7.44–7.40 (m, 2H), 7.36–7.32 (m, 1H), 7.25–7.21 (m, 1H), 7.03 (d, J = 7.8 Hz, 1H), 3.61 (t, J = 6.4 Hz, 2H), 3.25 (t, J = 7.3 Hz, 2H), 2.17–2.10 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 139.1, 134.3, 132.9, 130.0, 129.0, 128.8, 128.6, 125.2, 125.1, 124.8, 121.4, 104.8, 43.3, 41.3, 32.0. HRMS (ESI) $[M+H]^+$ Calcd for $[C_{19}H_{16}ClIN_2OS]$ 482.9795, found 482.9800.



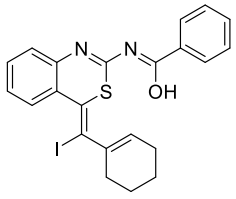
(Z)-N-((E)-4-(1-Iodo-2,2-dimethylpropylidene)-6-(trifluoromethyl)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (**5c**). The product was obtained as a pale yellow needles, mp: 121–123 ^{o}C (204.1 mg, 77%); FTIR (Zn–Se ATR, cm^{-1}) 3205, 2972, 1660, 1554, 1469, 1327, 1257, 1153, 1114, 1070, 904, 732, 704, 671; ^{1}H NMR (400 MHz, $CDCl_3$) δ 11.02 (br s, 1H), 7.96–7.94 (m, 3H), 7.51–7.43 (m, 2H), 7.40–7.34 (m, 2H), 7.04–7.01 (m, 1H), 1.56 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 142.8, 133.5, 133.1, 129.5, 128.8, 128.2, 127.4 (q, $J_{C\text{-}F}$ = 32.7 Hz), 125.9, 125.4, 122.7, 122.2, 121.8, 42.4, 33.2. HRMS (ESI) $[M+H]^+$ Calcd for $[C_{21}H_{18}F_3IN_2OS]$ 531.0215, found 531.0222.



(Z)-N-((E)-4-(Cyclopropyliodomethylene)-6-(trifluoromethyl)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (**5d**). The product was obtained as a pale yellow needles, mp: 117–119 ^{o}C (200.4 mg, 78%); FTIR (Zn–Se ATR, cm^{-1}) 3272, 2933, 1640, 1562, 1473, 1390, 1272, 1151, 1112, 1070, 1032, 955, 732, 701; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.82 (br s, 1H), 7.98 (s, 1H), 7.81 (d, J = 7.8 Hz, 2H), 7.38–7.31 (m, 2H), 7.27–7.24 (m, 2H), 6.91 (d, J = 7.8 Hz, 1H), 2.04–1.96 (m, 1H), 0.85–0.83 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 143.1, 133.2, 133.1, 128.7, 128.6, 126.9, 126.6 (br s, *C-F*), 126.1, 125.9 (br s, C-F), 125.6 (q, $J_{C\text{-}F}$ = 270.3 Hz), 122.7 (br s, *C-F*), 121.8, 115.2, 82.0, 20.9, 11.4. HRMS (ESI) $[M+H]^+$ Calcd for $[C_{20}H_{14}F_3IN_2OS]$ 514.9902, found 514.9892.



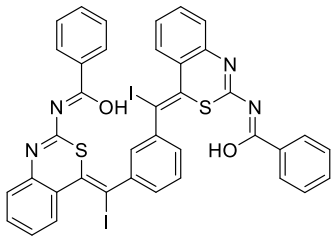
(Z)-N-((E)-4-(Cyclohexyliodomethylene)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (**5e**). The product was obtained as a yellow needles, mp: 125–127 ^{o}C (190.3 mg, 78%); FTIR (Zn–Se ATR, cm^{-1}) 3255, 2853, 1601, 1554, 1459, 1337, 1257, 1114, 1070, 904, 855, 732, 702, 688; ^{1}H NMR (400 MHz, $CDCl_3$) δ 11.39 (br s, 1H), 8.11 (d, J = 7.8 Hz, 2H), 7.87 (d, J = 7.8 Hz, 1H), 7.55–7.51 (m, 1H), 7.46–7.40 (m, 2H), 7.36–7.30 (m, 1H), 7.28–7.20 (m, 1H), 7.08–7.02 (m, 1H), 2.79–2.73 (m, 1H), 1.91–1.70 (m, 4H), 1.60–1.49 (m, 4H), 1.37–1.20 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) 138.5, 135.0, 132.7, 132.65, 129.9, 129.8, 129.2, 129.1, 128.5, 125.6, 125.4, 124.8, 120.6, 120.2, 113.6, 45.9, 33.5, 25.6, 25.4. HRMS (ESI) $[M+H]^+$ Calcd for $[C_{22}H_{21}IN_2OS]$ 489.0498, found 489.0519.



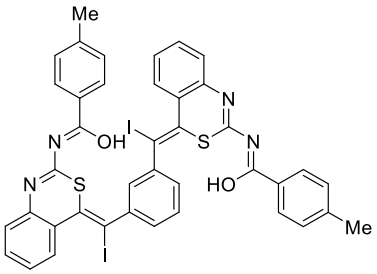
(Z)-N-((E)-4-(Cyclohex-1-en-1-yliodomethylene)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (**5f**). The product was obtained as a yellow needles, mp: 125–127 ^{o}C (157.9 mg, 65%); FTIR (Zn–Se ATR, cm^{-1}) 3198, 2972, 1654, 1567, 1439, 1257, 1201, 1153, 1114, 1070, 910, 832, 732, 671; ^{1}H NMR (400 MHz, $CDCl_3$) δ 11.89 (br s, 1H), 8.09–7.99 (m, 2H), 7.55–7.47 (m, 2H), 7.43–7.39 (m, 2H), 7.37–7.31 (m, 1H), 7.27–7.20 (m, 1H), 7.02 (d, J = 7.8 Hz, 1H), 5.91 (t, J = 3.9 Hz, 1H), 2.70–2.56 (m, 2H), 2.15–2.12 (m, 2H), 1.79–1.63 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 140.9, 132.7, 132.6, 130.3, 129.7, 129.2, 128.6, 128.5, 128.2, 124.9, 123.2, 120.7, 103.6, 26.5, 25.9, 22.3, 21.7. HRMS (ESI) $[M+H]^+$ Calcd for $[C_{22}H_{19}IN_2OS]$ 487.0341, found 487.0349.

General experimental procedure for green one-pot synthesis of Bisbenzo[1,3]thiazin-2-yl)di benzimidic acid 7: To a solution of *ortho*-haloanilines **1** (0.5 mmol), aroyl

isothiocyanates **2** (1.04 mmol) and 3.5 equiv of I_2 were added in water (2.0 mL). The reaction was then stirred at room temperature until TLC revealed complete conversion of the starting material. After the completion of the reaction, the reaction mixture was quenched with saturated aq sodium thiosulfate solution and extracted with EtOAc (3X10 mL). The combined organic layers were dried over Na_2SO_4, concentrated under vacuum, and purified by column chromatography using 100−200 mesh size silica gels (EtOAc:hexane) to afford the corresponding product.

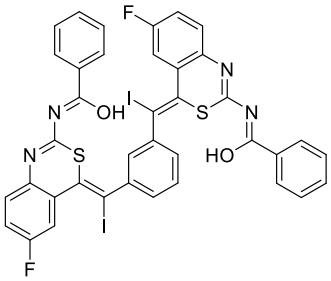


(1Z,1'Z)-N,N'-((4Z,4'E)-(1,3-Phenylenebis(iodomethanylylidene))bis(4H-benzo[d][1,3]thiazine-2-yl-4-ylidene))dibenzimidic acid (**7a**). The product was obtained as a yellow needles, mp: 136–138 ^oC (314.1 mg, 71%); FTIR (Zn–Se ATR, cm^{-1}) 3310, 2990, 2868, 1616, 1578, 1503, 1210, 926, 743; ^1H NMR (400 MHz, $CDCl_3$) δ 11.06 (br s, 2H), 8.11–8.06 (m, 4H), 7.95 (d, J = 7.8 Hz, 3H), 7.60–7.56 (m, 1H), 7.47–7.39 (m, 6H), 7.33–7.27 (m, 6H), 7.17 (d, J = 7.8 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 143.2, 139.6, 134.0, 133.5, 132.7, 130.6, 130.5, 130.2, 130.0, 129.3, 129.0, 128.6, 128.5, 128.4, 127.4, 125.6, 124.5, 122.0, 96.3. HRMS (ESI) $[M+H]^+$ Calcd for $[C_{38}H_{24}I_2N_4O_2S_2]$ 886.9508, found 886.9505.

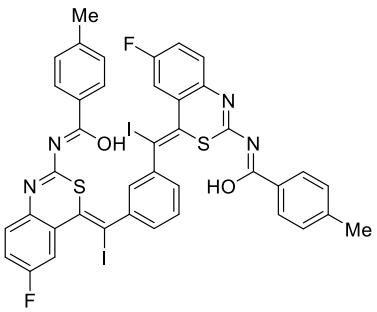


(1Z,1'Z)-N,N'-((4Z,4'E)-(1,3-Phenylenebis(iodomethanylylidene))bis(4H-benzo[d][1,3]thiazine-2-yl-4-ylidene))bis(4-methylbenzimidic acid) (**7b**). The product was obtained as a yellow needles, mp: 156–158 ^oC

(342.2 mg, 75%); FTIR (Zn–Se ATR, cm^{-1}) 3290, 2916, 2848, 1676, 1602, 1541, 1255, 906, 721; ^{1}H NMR (400 MHz, $CDCl_3$) δ 11.80 (br s, 2H), 8.06 (d, J = 7.8 Hz, 2H), 7.82 (m, 3H), 7.43–7.37 (m, 4H), 7.33 (d, J = 7.8 Hz, 2H), 7.29–7.24 (m, 3H), 7.11–7.07 (m, 6H), 2.31 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 143.3, 130.6, 130.2, 130.15, 129.3, 129.2, 129.0, 128.7, 127.6, 125.3, 124.3, 95.9, 21.7. HRMS (ESI) $[M+H]^+$ Calcd for $[C_{40}H_{28}I_2N_4O_2S_2]$ 914.9798, found 914.9791.

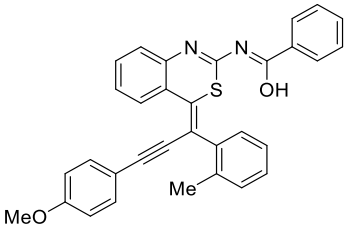


(1Z,1'Z)-N,N'-((4Z,4'E)-(1,3-Phenylenebis(iodomethanylylidene))bis(6-fluoro-4H-benzo[d][1,3]thiazine-2-yl-4-ylidene))dibenzimidic acid (**7c**). The product was obtained as a pale yellow needles, mp: 134–136 ^{o}C (322.3 mg, 70%); FTIR (Zn–Se ATR, cm^{-1}) 3197, 2922, 2852, 1674, 1550, 1462, 1259, 1195, 999, 817, 702; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.55 (br s, 2H), 7.85–7.80 (m, 5H), 7.50–7.42 (m, 3H), 7.35–7.26 (m, 8H), 7.13 (d, J = 6.4 Hz, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.2 (d, $J_{C\text{-}F}$ = 244.7 Hz), 143.4, 143.2, 133.6, 132.9, 132.8, 130.5 (d, $J_{C\text{-}F}$ = 8.7 Hz), 130.1, 129.7, 129.5, 129.3, 128.9, 128.6, 128.4, 125.5 (d, $J_{C\text{-}F}$ = 7.7 Hz), 117.6 (d, $J_{C\text{-}F}$ = 22.1 Hz), 115.1 (d, $J_{C\text{-}F}$ = 26.0 Hz), 96.5. HRMS (ESI) $[M+H]^+$ Calcd for $[C_{38}H_{22}F_2I_2N_4O_2S_2]$ 922.9320, found 922.9295.

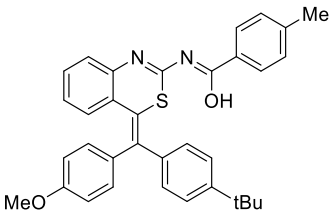


(*1Z,1'Z)-N,N'-((4Z,4'E)-(1,3-Phenylenebis(iodomethanylylidene))bis(6-fluoro-4H-benzo[d][1,3]thiazine-2-yl-4-*

ylidene))bis(4-methylbenzimidic acid) (**7d**). The product was obtained as a pale yellow needles, mp: 148–150 ^{o}C (341.6 mg, 72%); FTIR (Zn–Se ATR, cm^{-1}) 3238, 2965, 2823, 1624, 1543, 1476, 1320, 1211, 1156, 923, 817, 710; ^{1}H NMR (400 MHz, $CDCl_3$) δ 11.12 (br s, 2H), 7.98 (d, J = 7.8 Hz, 1H), 7.79 (d, J = 8.8 Hz, 2H), 7.73–7.68 (m, 3H), 7.43–7.40 (m, 1H), 7.35–7.24 (m, 3H), 7.13–7.06 (m, 8H), 2.30 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.3 (d, $J_{C\text{-}F}$ = 245.6 Hz), 144.3, 143.6, 143.1, 130.2, 130.17, 130.0, 129.4, 129.3, 128.5, 127.6, 127.2, 125.7 (d, $J_{C\text{-}F}$ = 8.7 Hz), 117.5 (d, $J_{C\text{-}F}$ = 23.1 Hz), 114.9 (d, $J_{C\text{-}F}$ = 25.1 Hz), 96.5, 21.7. HRMS (ESI) $[M+H]^+$ Calcd for $[C_{40}H_{26}F_2I_2N_4O_2S_2]$ 950.9633, found 950.9638.

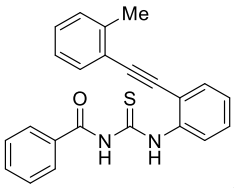


(Z)-N-((Z)-4-(3-(4-Methoxyphenyl)-1-(o-tolyl)prop-2-yn-1-ylidene)-4H-benzo[d][1,3] thiazin-2-yl)benzimidic acid (**9**). The product was obtained as a yellow needles, mp: 205–207 ^{o}C (197.5 mg, 79%); FTIR (Zn–Se ATR, cm^{-1}) 3297, 2852, 2176, 1682, 1592, 1552, 1503, 1363, 1249, 1023, 825, 719; ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.17 (br s, 1H), 8.72 (d, J = 7.8 Hz, 1H), 8.04 (d, J = 6.8 Hz, 2H), 7.49–7.45 (m, 1H), 7.41–7.35 (m, 3H), 7.32–7.24 (m, 7H), 7.07 (d, J = 7.8 Hz, 1H), 6.81 (d, J = 8.8 Hz, 2H), 3.78 (s, 3H), 2.39 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.7, 137.0, 135.9, 135.0, 133.0, 132.7, 132.2, 130.7, 130.5, 130.4, 129.1, 128.8, 128.6, 128.2, 128.1, 127.6, 126.4, 124.9, 121.1, 120.6, 114.9, 113.9, 96.2, 88.0, 55.1, 19.2. HRMS (ESI) $[M+H]^+$ Calcd for $[C_{32}H_{24}N_2O_2S]$ 501.1637, found 501.1625.

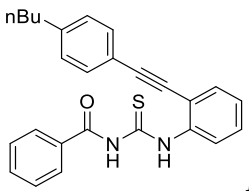


(Z)-N-((E)-4-((4-(tert-Butyl)phenyl)(4-methoxyphenyl)methylene)-4H-benzo[d][1,3] thiazin-2-yl)-4-methylbenzimidic acid (**11**). The

product was obtained as a yellow needles, mp: 96–98 ^{o}C (199.5 mg, 75%); FTIR (Zn–Se ATR, cm^{-1}) 3215, 2838, 1644, 1592, 1544, 1501, 1415, 1240, 1123, 1033, 825, 710; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.42 (br s, 1H), 7.97 (d, J = 7.8 Hz, 2H), 7.36 (d, J = 7.8 Hz, 2H), 7.17 (d, J = 7.8 Hz, 3H), 7.08 (d, J = 7.8 Hz, 2H), 6.98 (d, J = 7.8 Hz, 1H), 6.92–6.81 (m, 4H), 6.69 (d, J = 8.8 Hz, 2H), 3.73 (s, 3H), 2.35 (s, 3H), 1.33 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.3, 151.9, 145.4, 143.2, 138.0, 133.7, 132.4, 130.3, 130.2, 129.4, 129.1, 129.0, 125.3, 124.9, 124.0, 120.1, 116.1, 114.9, 113.7, 55.3, 34.9, 31.4, 21.7. HRMS (ESI) $[M+H]^+$ Calcd for $[C_{34}H_{32}N_2O_2S]$ 533.2263, found 533.2254.

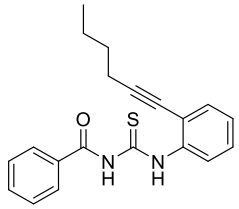


N-((2-(o-Tolylethynyl)phenyl)carbamothioyl)benzamide (**12a**). The product was obtained as a white needles, mp: 130–132 ^{o}C (175.8 mg, 95%); FTIR (Zn–Se ATR, cm^{-1}) 3323, 2923, 2197, 1682, 1602, 1526, 1340, 1147, 1078, 832, 708, 656; ^{1}H NMR (400 MHz, $CDCl_3$) δ 13.03 (s, 1H), 9.19 (br s, 1H), 8.53 (d, J = 7.8 Hz, 1H), 7.88 (d, J = 7.8 Hz, 2H), 7.68 (d, J = 7.8 Hz, 1H), 7.65–7.60 (m, 2H), 7.54–7.50 (m, 2H), 7.42–7.38 (m, 1H), 7.27–7.14 (m, 4H), 2.50 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 182.6, 170.7, 144.7, 143.2, 138.1, 136.9, 136.8, 136.0, 133.8, 133.6, 133.1, 132.8, 132.0, 130.8, 130.0, 128.6, 127.0, 122.5, 99.9, 92.9, 25.11. HRMS (ESI) $[M+H]^+$ Calcd for $[C_{23}H_{18}N_2OS]$ 371.1218, found 371.1210.



N-((2-((4-Butylphenyl)ethynyl)phenyl)carbamothioyl)benzamide (**12b**). The product was obtained as a white needles, mp: 113–115 ^{o}C (191.6 mg, 93%); FTIR (Zn–Se ATR, cm^{-1}) 3315, 2897, 2210, 1680, 1612, 1565, 1410, 1147, 1078, 813, 707; ^{1}H

NMR (400 MHz, $CDCl_3$) δ 13.17 (s, 1H), 9.17 (s, 1H), 8.74 (d, J = 8.8 Hz, 1H), 7.91 (d, J = 7.8 Hz, 2H), 7.67–7.59 (m, 4H), 7.57–7.53 (m, 2H), 7.42–7.38 (m, 1H), 7.26–7.22 (m, 1H), 7.18 (d, J = 8.8 Hz, 2H), 2.63 (t, J = 7.8 Hz, 2H), 1.64–1.57 (m, 2H), 1.39–1.33 (m, 2H), 0.94 (t, J = 7.3 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 177.7, 166.3, 143.9, 139.1, 133.7, 132.4, 131.9, 131.8, 129.3, 128.5, 128.3, 127.6, 126.1, 123.4, 120.0, 117.5, 97.3, 84.1, 35.7, 33.5, 22.4, 14.0. HRMS (ESI) $[M+H]^+$ Calcd for $[C_{26}H_{24}N_2OS]$ 413.1688, found 413.1699.



N-((2-(Hex-1-yn-1-yl)phenyl)carbamothioyl)benzamide (**12c**). The product was obtained as a white needles, mp: 140–142 ^{o}C (159.6 mg, 95%); FTIR (Zn–Se ATR, cm^{-1}) 3110, 2995, 2190, 1622, 1570, 1323, 1147, 1078, 1000, 921, 832, 701; ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.96 (s, 1H), 9.10 (s, 1H), 8.70 (d, J = 8.2 Hz, 1H), 7.90–7.88 (m, 2H), 7.65–7.61 (m, 1H), 7.54–7.51 (m, 2H), 7.45 (dd, J = 7.7, 1.4 Hz, 1H), 7.34–7.30 (m, 1H), 7.16 (td, J = 7.6, 1.0 Hz, 1H), 2.54 (t, J = 7.1 Hz, 2H), 1.68–1.60 (m, 2H), 1.51–1.44 (m, 2H), 0.91 (t, J = 7.4 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 177.5, 166.1, 139.5, 133.7, 132.1, 131.9, 129.3, 127.7, 127.9, 126.0, 123.0, 117.9, 99.1, 75.8, 30.6, 22.2, 19.6, 13.8. HRMS (ESI) $[M+H]^+$ Calcd for $[C_{20}H_{20}N_2OS]$ 337.1375, found 337.1375.

References

(1) (a) X. Wang, J. Li, Y. Huang, J. Zhu, R. Hu, W. Wu, H. Jiang, *J. Org. Chem.* **2018**, *83*, 10453−10464. (b) C. M. Le, T. Sperger, R. Fu, X. Hou, Y. H. Lim, F. Schoenebeck, M. Lautens, *J. Am. Chem. Soc.* **2016**, *138*, 14441−14448. (c) L. Z. Yu, Y. Wei, M. Shi, *Chem. Commun*. **2017**, *53*, 8980−8983.

(2) F. Gao, J. T. Wang, L. L. Liu, N. Ma, C. Yang, Y. Gao, W. Xia, *Chem. Commun*., **2017**, *53*, 8533−8536. (b) Y. Zhao, Y. Hu, H. Wang, X. Li, B. Wan, *J. Org. Chem.* **2016**, *81*,

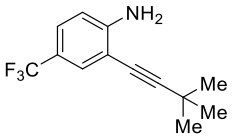
4412−4420. (c) P. Li, Y. Weng, X. Xu, X. Cui, *J. Org. Chem.* **2016**, *81*, 3994−4001. (d) R. J. Liu, P. F. Wang, W. K. Yuan, L. R. Wen, M. Li, *Adv. Synth. Catal*. **2017**, *359*, 1373–1378.

(3) (a) L. Tang, C. Wu, Q. Hu, Q. Li, Zhang, *Appl Organometal Chem.* **2018**, *32*, 3980. (b) X. F. Xia, G. W. Zhang, D. Wang, S. L. Zhu, *J. Org. Chem.* **2017**, *82*, 8455−8463. (c) F. D. Zhuang, J. M. Han, S. Tang, J. H. Yang, Q. R. Chen, J. Y. Wang, J. Pei, *Organometallics* **2017**, *36*, 2479−2482. (d) C. Koradin, W. Dohle, A. L. Rodriguez, B. Schmid, P. Knochel, *Tetrahedron* **2003**, *59*, 1571–1587.

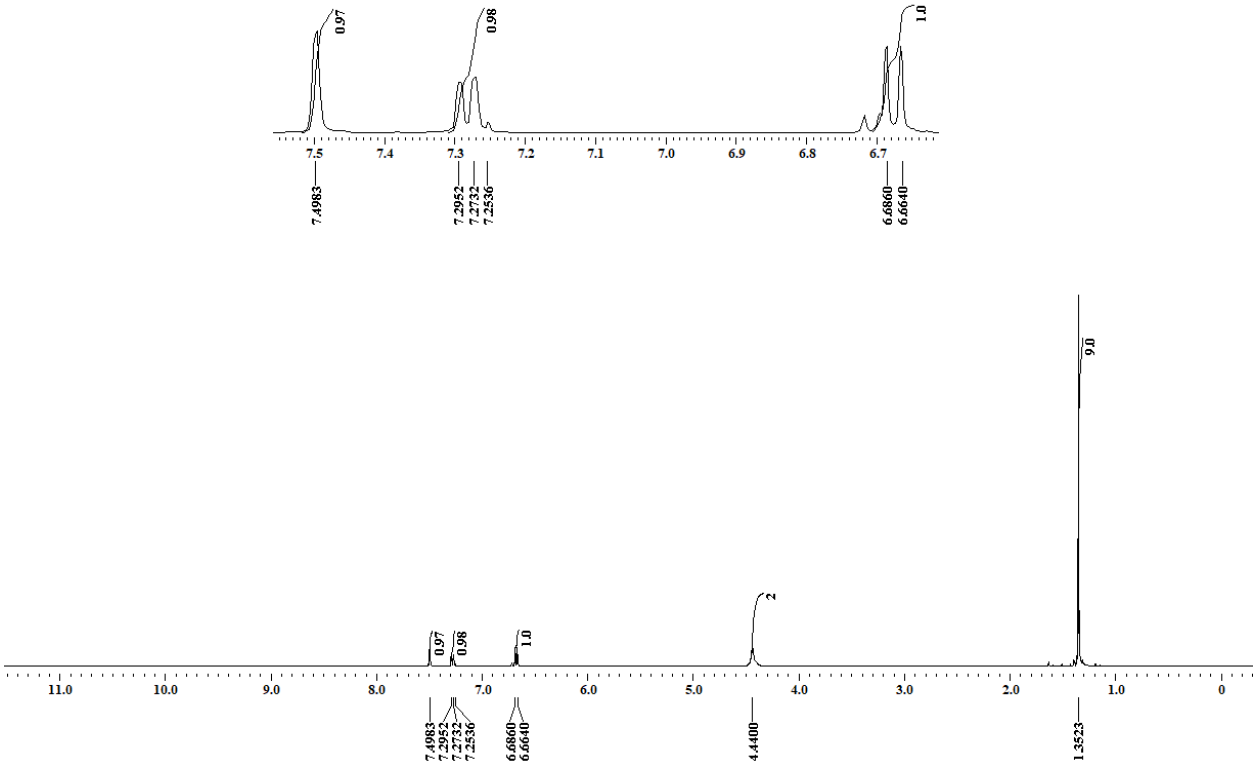
(4) (a) C. Peng, Y. Wang, L. Liu, H. Wang, J. Zhao, Q. Zhu, *Eur. J. Org. Chem.* **2010**, 818–822. (b) X. F. Xia, L. L. Zhang, X. R. Song, X. Y. Liu, Y. M. Liang, *Org. Lett*. **2012**, *14*, 2480–2483. (c) A. Carpita, A. Ribecai, *Tetrahedron Lett.* **2009**, *50*, 204–207. (d) J. S. Kim, J. H. Han, J. J. Lee, Y. M. Jun, B. M. Lee, B. H. Kim, *Tetrahedron Lett.* **2008**, *49*, 3733–3738.

Copies of ^{1}H and ^{13}C NMR

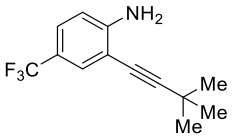
^{1}H NMR



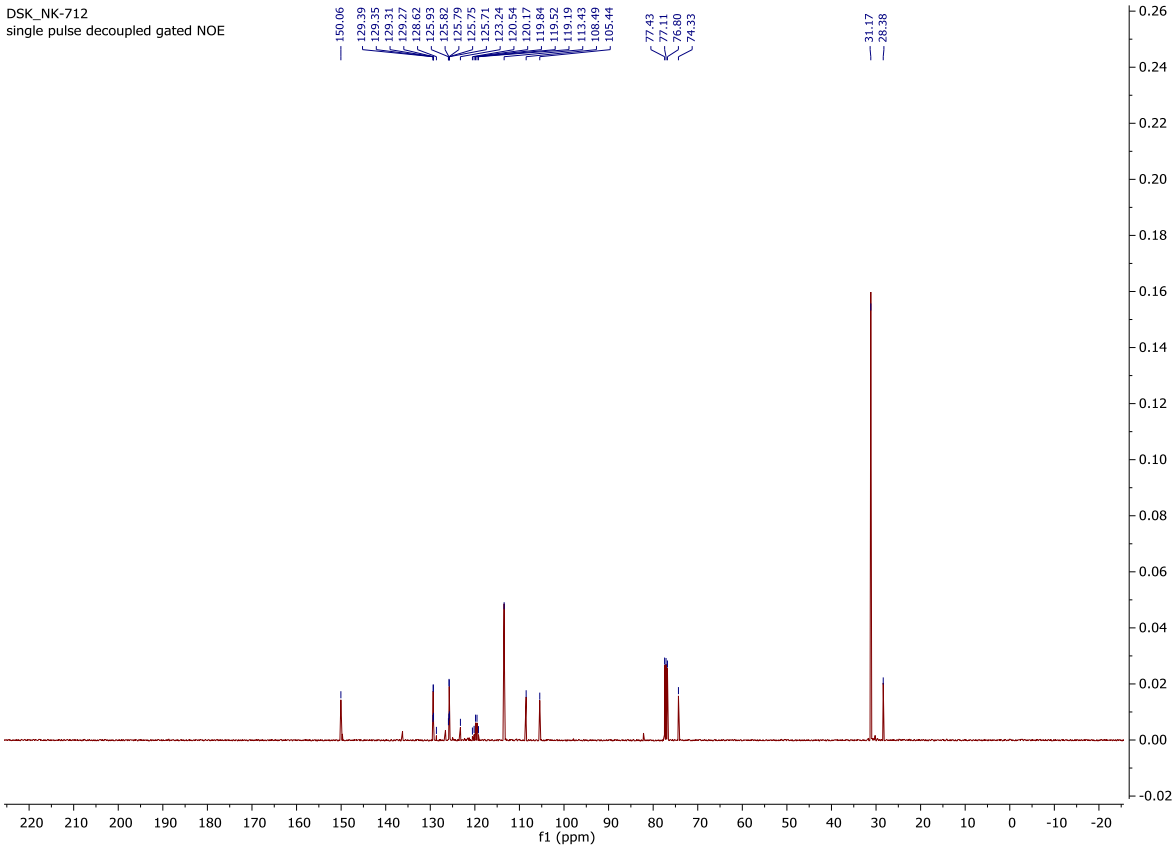
2-(3,3-Dimethylbut-1-yn-1-yl)-4-(trifluoromethyl)aniline (1r)



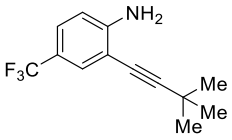
^{13}C NMR



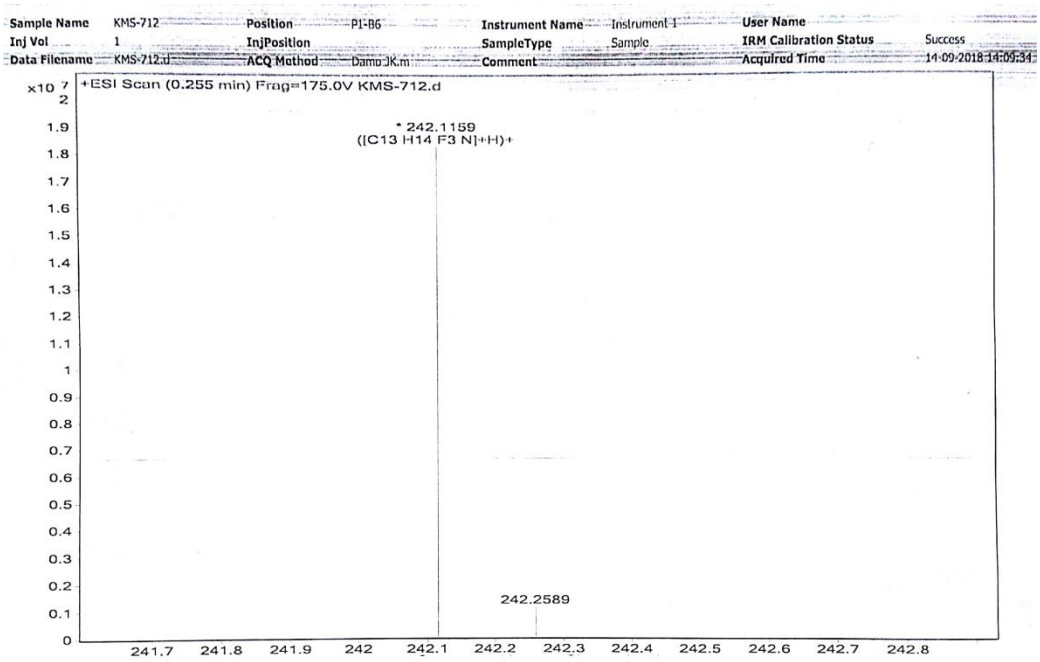
2-(3,3-Dimethylbut-1-yn-1-yl)-4-(trifluoromethyl)aniline (1r)



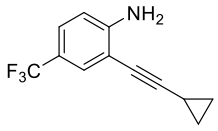
HRMS



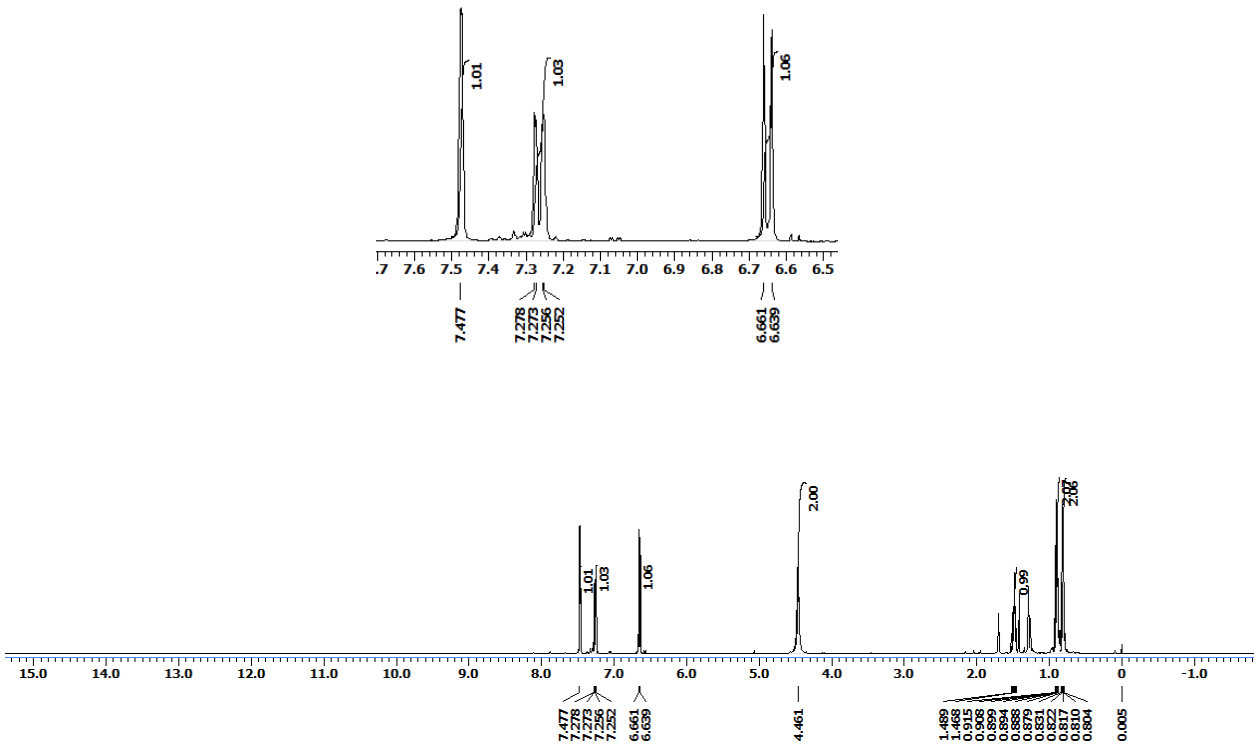
2-(3,3-Dimethylbut-1-yn-1-yl)-4-(trifluoromethyl)aniline (1r)



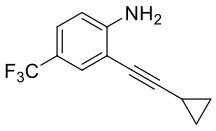
^{1}H NMR



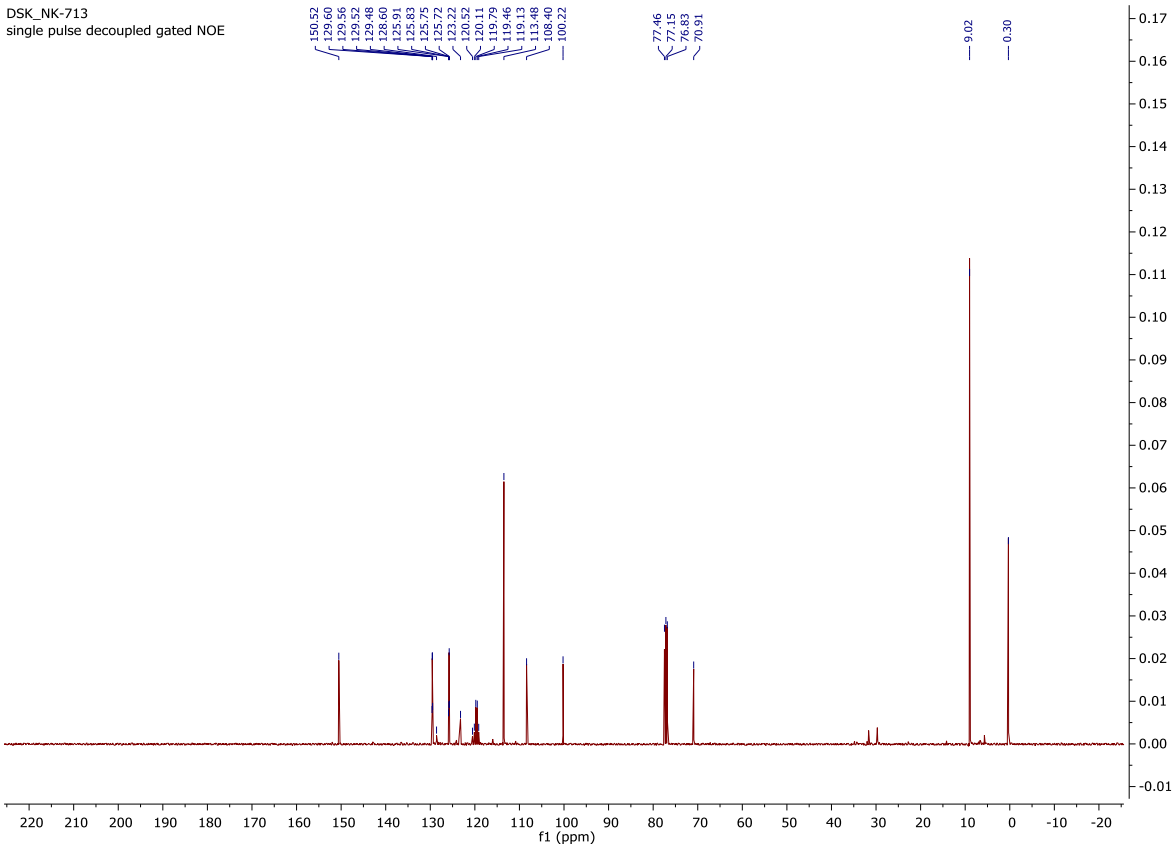
2-(cyclopropylethynyl)-4-(trifluoromethyl)aniline (1s)



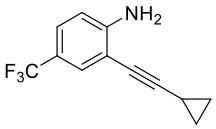
^{13}C NMR



2-(cyclopropylethynyl)-4-(trifluoromethyl)aniline (1s)



HRMS



2-(cyclopropylethynyl)-4-(trifluoromethyl)aniline (1s)

Qualitative Compound Report

Data File	KMS-713.d	Sample Name	KMS-713
Sample Type	Sample	Position	P1-D3
Instrument Name	Instrument 1	User Name	
Acq Method	Damo JK.m	Acquired Time	18-09-2018 12:05:23
IRM Calibration Status	Success	DA Method	Default.m
Comment			

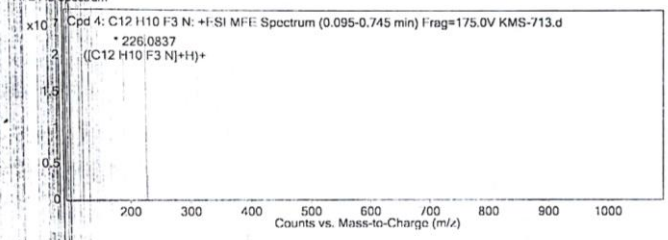
Sample Group — Info.
Acquisition SW Version: 6200 series TOF/6500 series Q-TOF B.05.01 (B5175.1)

Compound Table

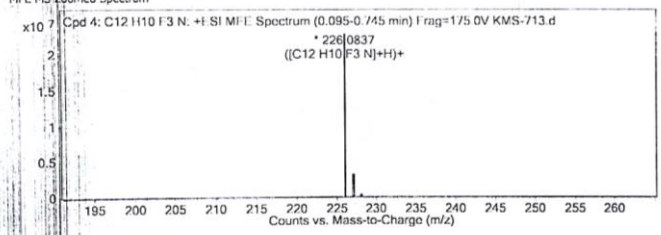
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 4: C12 H10 F3 N	0.184	225.0765	C12 H10 F3 N	C12 H10 F3 N	0.2	C12 H10 F3 N

Compound Label	m/z	RT	Algorithm	Mass
Cpd 4: C12 H10 F3 N	226.0837	0.184	Find by Molecular Feature	225.0765

MFE MS Spectrum



MFE MS Zoomed Spectrum

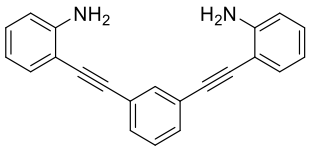


MS Spectrum Peak List

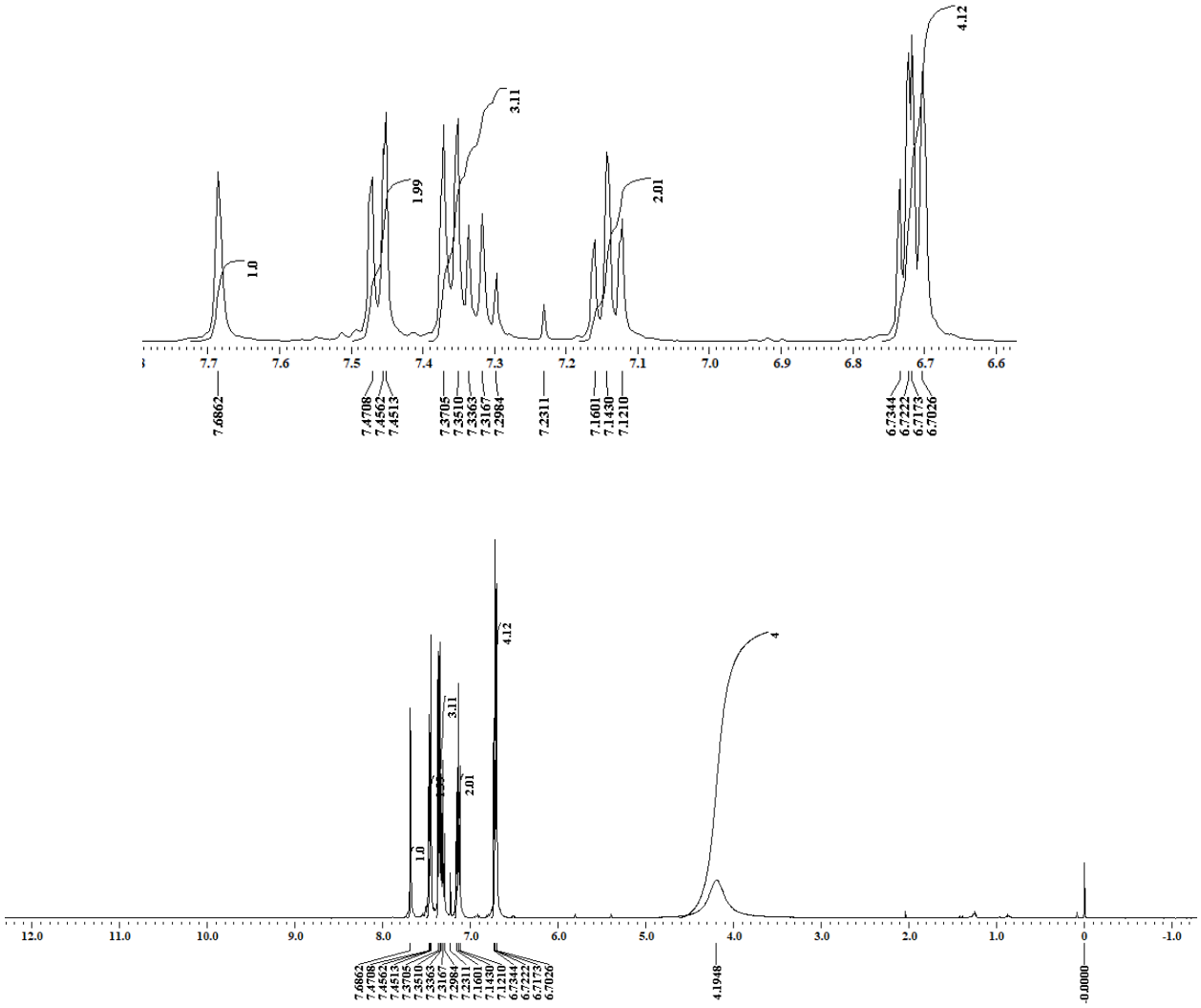
m/z	z	Abund	Formula	Ion
226.0837	1	23027524	C12 H10 F3 N	(M+H)+
227.087	1	3384047.14	C12 H10 F3 N	(M+H)+
228.0934	1	249224.99	C12 H10 F3 N	(M+H)+
229.1002	1	17439.6	C12 H10 F3 N	(M+H)+
230.0961	1	5156.09	C12 H10 F3 N	(M+H)+

--- End Of Report ---

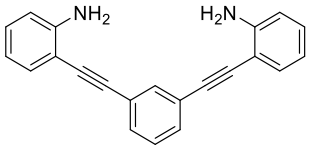
^{1}H NMR



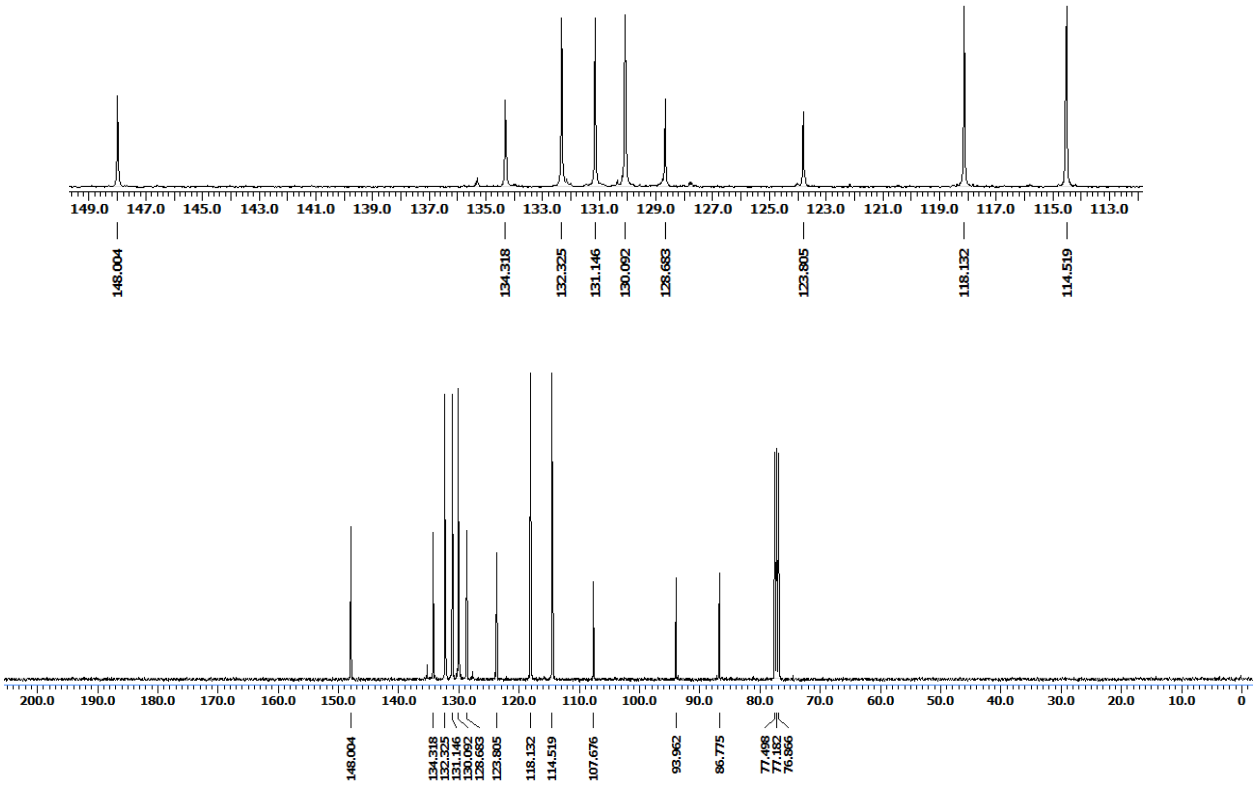
2,2'-(1,3-phenylenebis(ethyne-2,1-diyl))dianiline (6a)



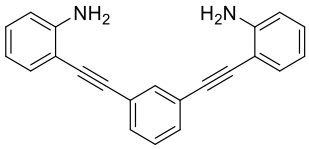
^{13}C NMR



2,2'-(1,3-phenylenebis(ethyne-2,1-diyl))dianiline (6a)



HRMS



2,2'-(1,3-phenylenebis(ethyne-2,1-diyl))dianiline (6a)

Qualitative Compound Report

Data File	KMS-721.d	Sample Name	KMS-721
Sample Type	Sample	Position	P1-B7
Instrument Name	Instrument 1	User Name	
Acq Method	Damo JK.m	Acquired Time	25-09-2018 12:09:37
IRM Calibration Status	Success	DA Method	Default.m
Comment			

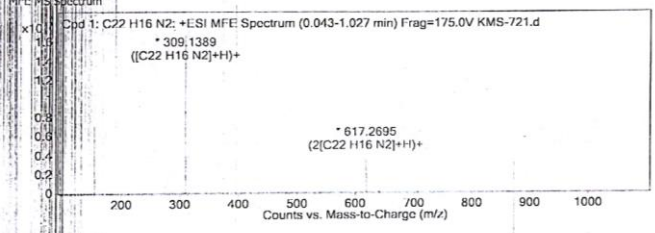
Sample Group Info.
Acquisition SW 6200 series TOF/6500 series
Version Q-TOF B.05.01 (B5125.1)

Compound Table

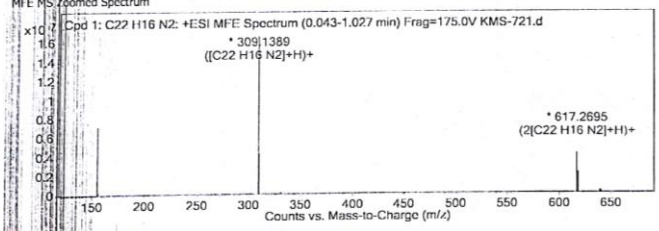
	Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
1	Cpd 1: C22 H16 N2	0.145	308.1321	C22 H16 N2	C22 H16 N2	-2.46	C22 H16 N2

Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: C22 H16 N2	309.1389	0.145	Find by Molecular Feature	308.1321

MFE MS Spectrum



MFE MS Zoomed Spectrum

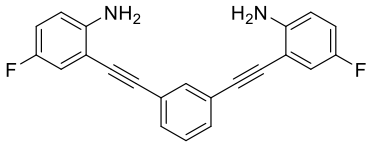


MS Spectrum Peak List

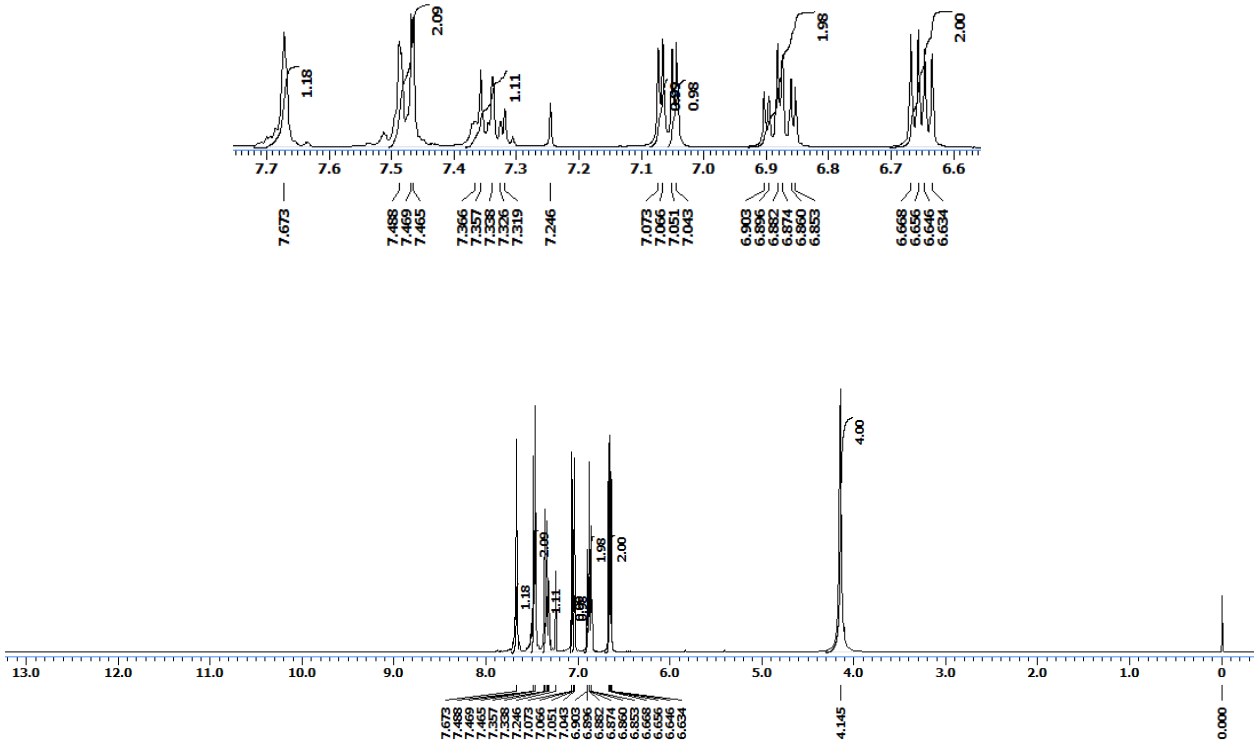
m/z	z	Abund	Formula	Ion
155.0733	2	7070489.5	C22 H16 N2	(M+2H)+2
155.5751	2	1745167.84	C22 H16 N2	(M+2H)+2
156.0778	2	234020.54	C22 H16 N2	(M+2H)+2
309.1389	1	16776508	C22 H16 N2	(M+H)+
310.1422	1	3980917.77	C22 H16 N2	(M+H)+
331.1205	1	1077772.73	C22 H16 N2	(M+Na)+
617.2695	1	4161893.75	C22 H16 N2	(2M+H)+
618.273	1	2080140.31	C22 H16 N2	(2M+H)+
639.2511	1	149815.66	C22 H16 N2	(2M+Na)+
640.2541	1	77217.66	C22 H16 N2	(2M+Na)+

--- End Of Report ---

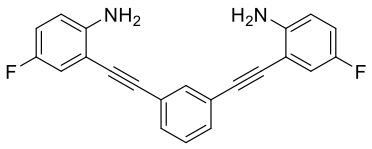
^{1}H NMR



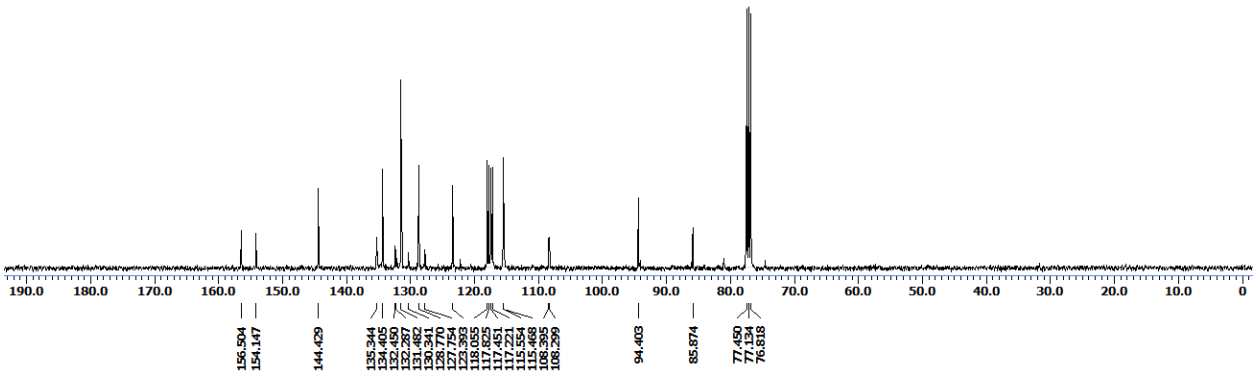
2,2'-(1,3-phenylenebis(ethyne-2,1-diyl))bis(4-fluoroaniline) (6b)



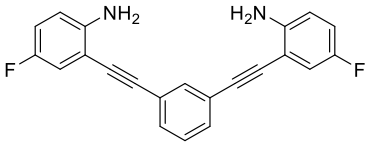
^{13}C NMR



2,2'-(1,3-phenylenebis(ethyne-2,1-diyl))bis(4-fluoroaniline) (6b)



HRMS



2,2'-(1,3-phenylenebis(ethyne-2,1-diyl))bis(4-fluoroaniline) (6b)

Qualitative Compound Report

Data File	KMS-724.d	Sample Name	KMS-724
Sample Type	Sample	Position	P1-A7
Instrument Name	Instrument 1	User Name	
Acq Method	Damo JK.m	Acquired Time	25-09-2018 11:54:33
IRM Calibration Status	Success	DA Method	Default.m
Comment			

Sample Group — Info.

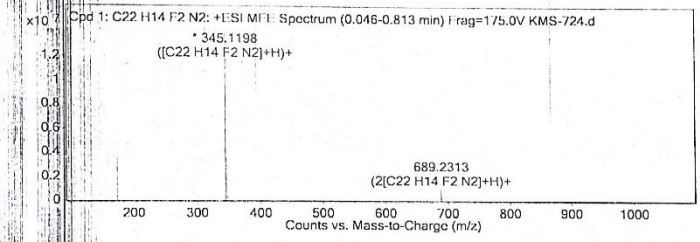
Acquisition SW Version: 6200 series TOF/6500 series Q-TOF B.05.01 (B5125.1)

Compound Table

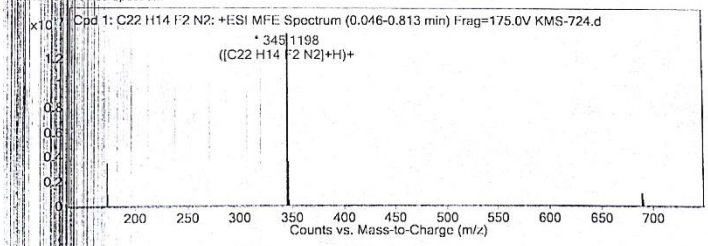
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 1: C22 H14 F2 N2	0.154	344.1125	C22 H14 F2 N2	C22 H14 F2 N2	0.02	C22 H14 F2 N2

Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: C22 H14 F2 N2	345.1198	0.154	Find by Molecular Feature	344.1125

MFE MS Spectrum



MFE MS Zoomed Spectrum

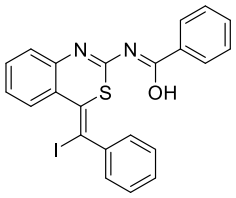


MS Spectrum Peak List

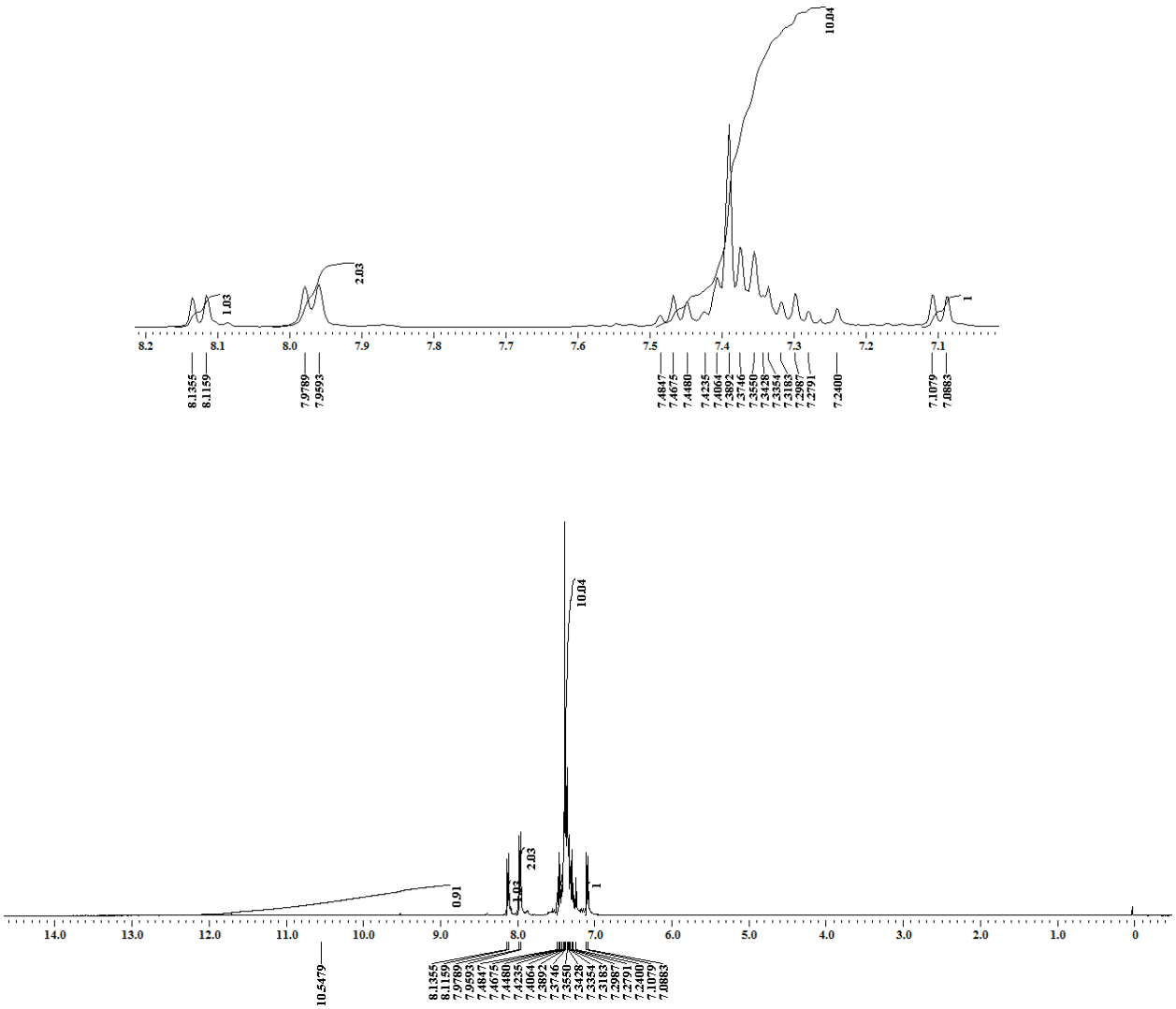
m/z	z	Abund	Formula	Ion
173.0639	2	3493346.75	C22 H14 F2 N2	(M+2H)+2
173.5655	2	842409.31	C22 H14 F2 N2	(M+2H)+2
174.0678	2	1060709	C22 H14 F2 N2	(M+2H)+2
174.5704	2	8119.58	C22 H14 F2 N2	(M+2H)+2
345.1198	1	14140078	C22 H14 F2 N2	(M+H)+
346.1229	1	3561240.08	C22 H14 F2 N2	(M+H)+
347.1267	1	419789.99	C22 H14 F2 N2	(M+H)+
348.1308	1	32479.57	C22 H14 F2 N2	(M+H)+
689.2313	1	953115	C22 H14 F2 N2	(2M+H)+
690.2343	1	467887.88	C22 H14 F2 N2	(2M+H)+

--- End Of Report ---

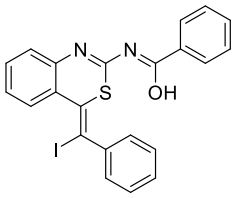
^{1}H NMR



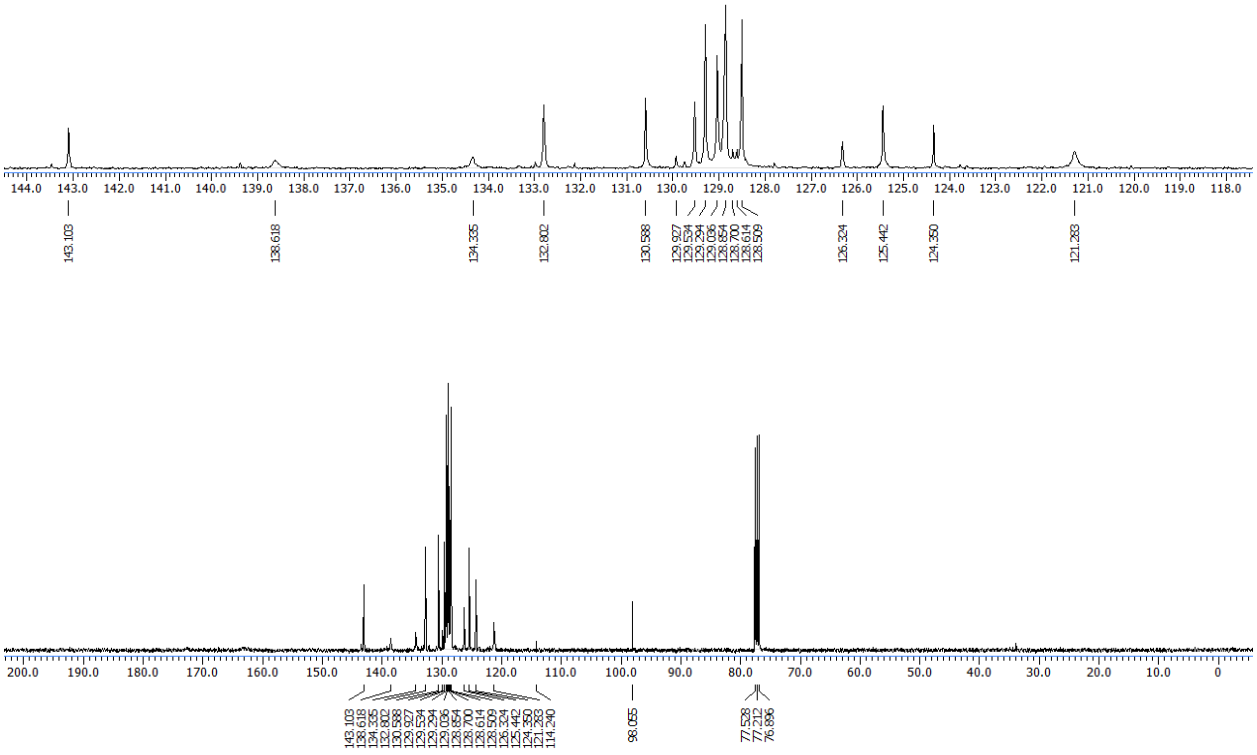
(Z)-N-((E)-4-(iodo(phenyl)methylene)-4*H*-benzo[*d*][1,3]thiazin-2-yl)benzimidic acid (3a)



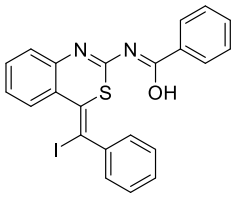
^{13}C NMR



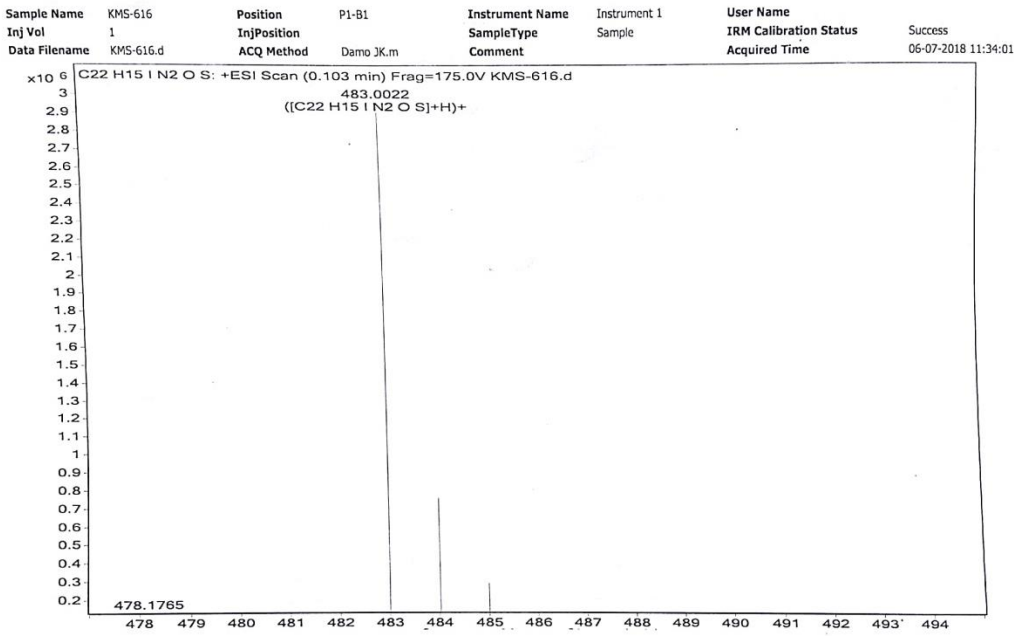
(Z)-N-((E)-4-(iodo(phenyl)methylene)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (3a)



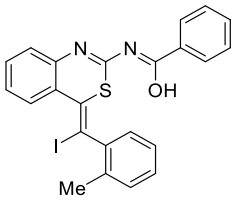
HRMS



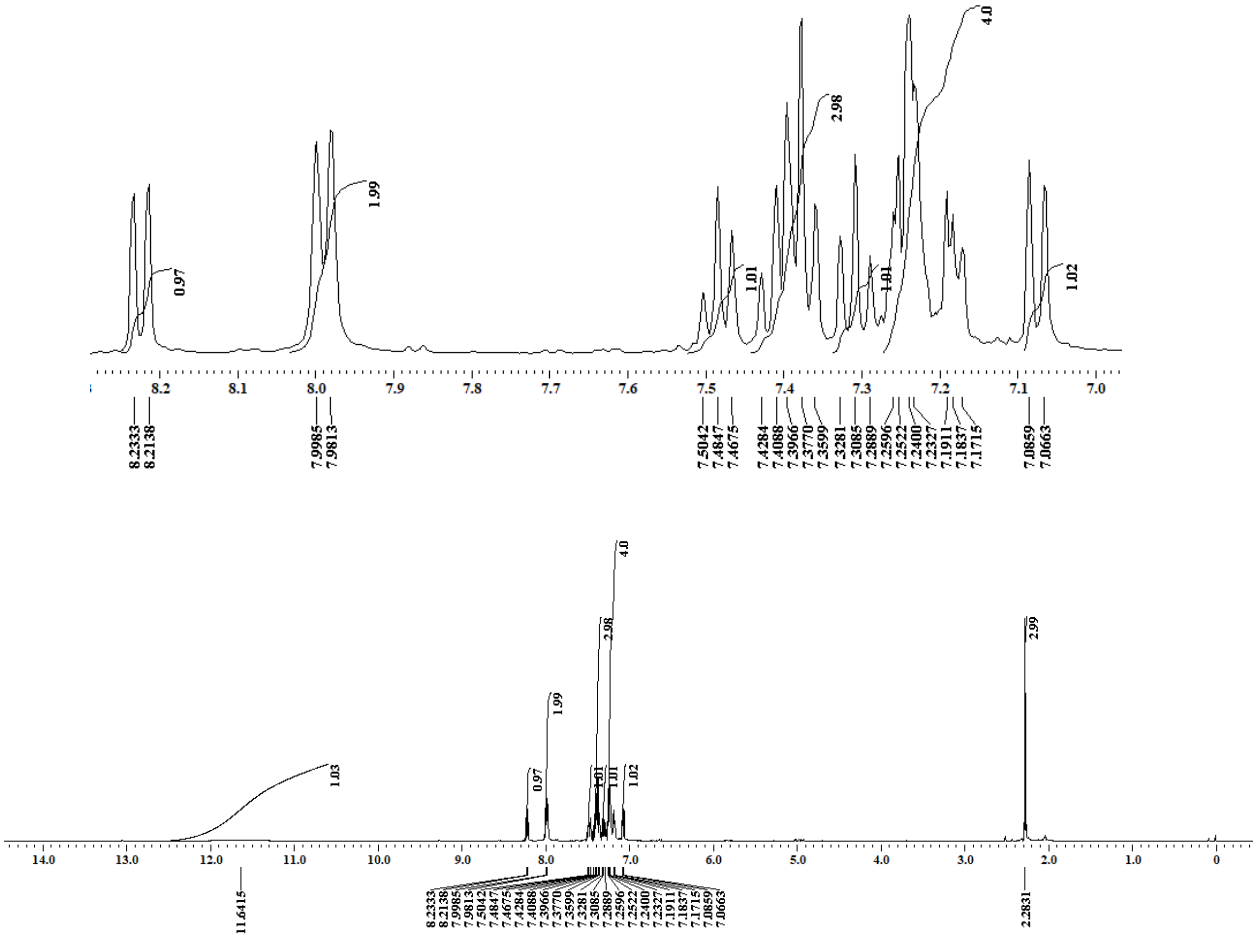
(Z)-N-((E)-4-(iodo(phenyl)methylene)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (3a)



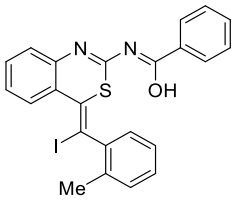
^{1}H NMR



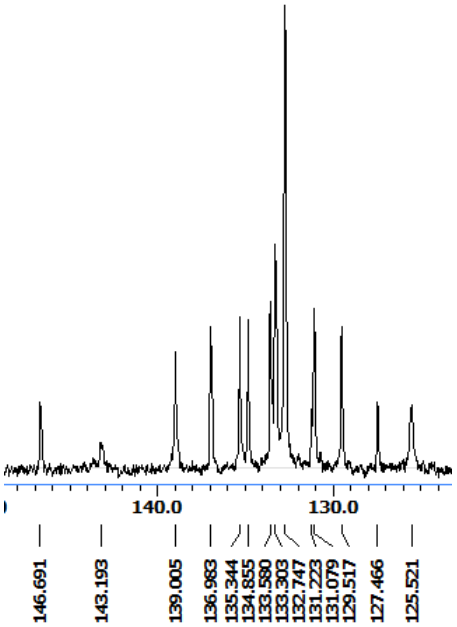
(Z)-N-((E)-4-(iodo(*o*-tolyl)methylene)-4*H*-benzo[*d*][1,3]thiazin-2-yl)benzimidic acid (3b)

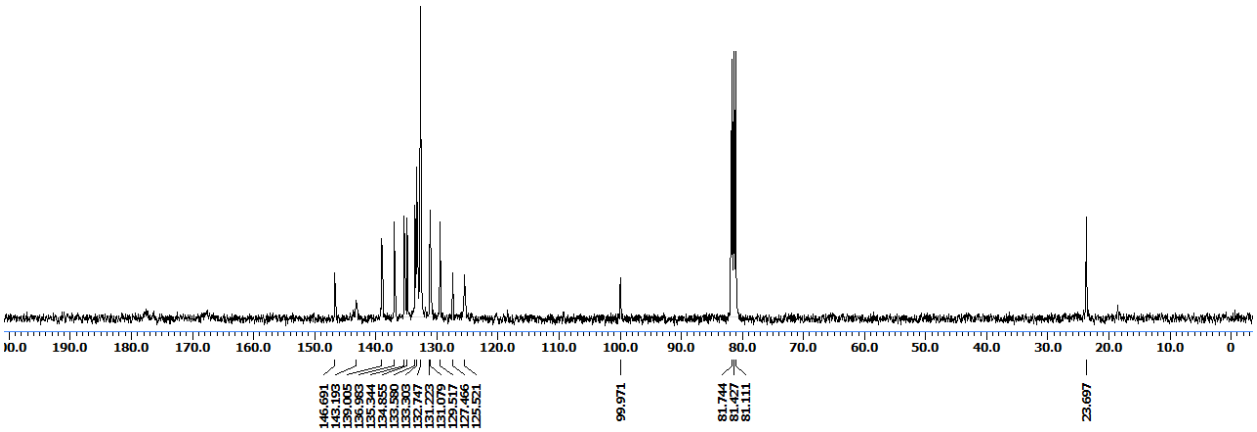


^{13}C NMR

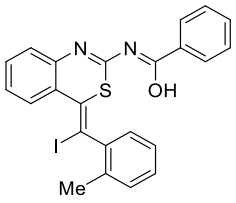


(Z)-N-((E)-4-(iodo(o-tolyl)methylene)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (3b)

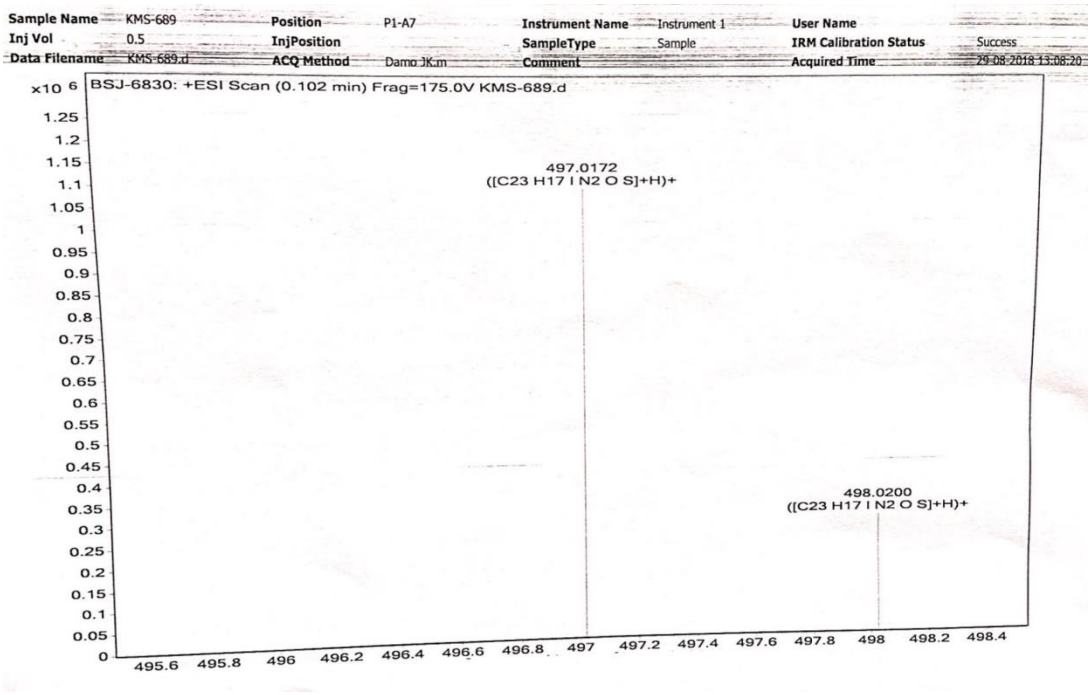




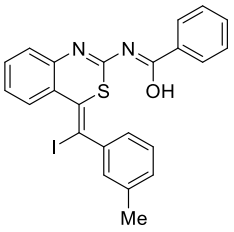
HRMS



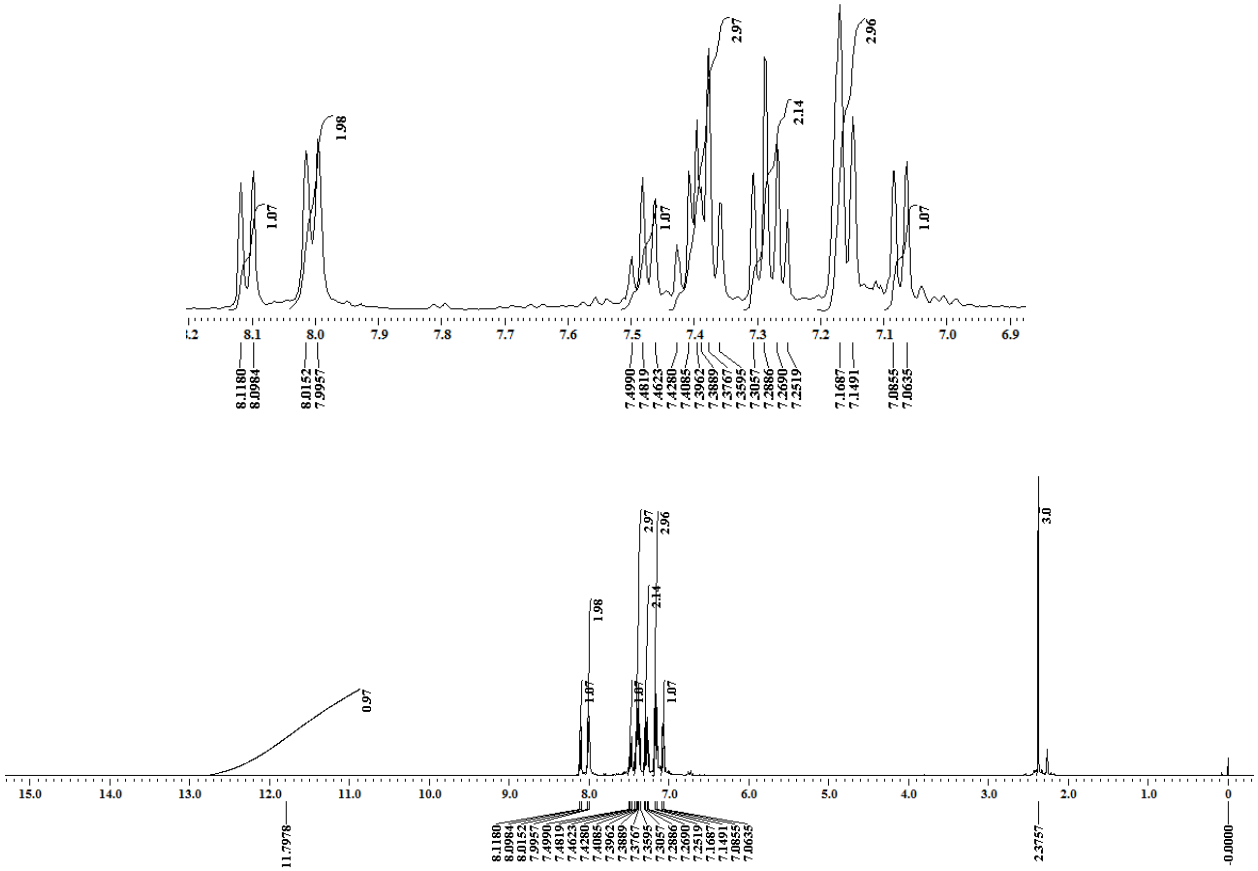
(Z)-N-((E)-4-(iodo(o-tolyl)methylene)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (3b)



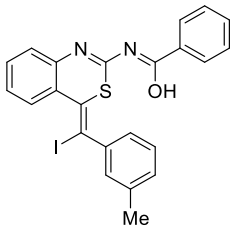
^{1}H NMR



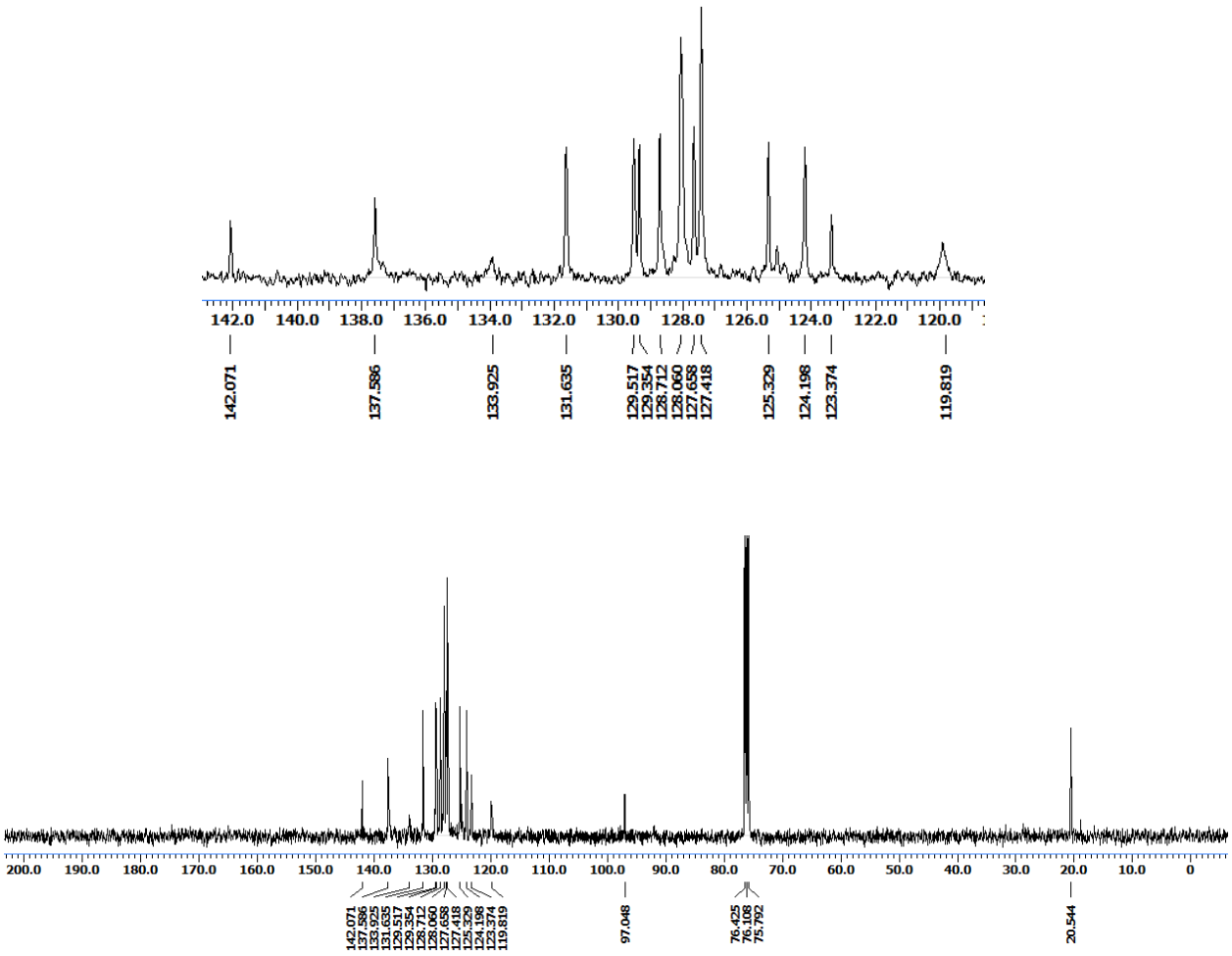
(Z)-N-((E)-4-(Iodo(m-tolyl)methylene)-4*H*-benzo[d][1,3]thiazin-2-yl)benzimidic acid (3c)



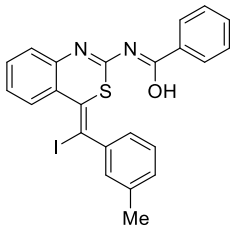
^{13}C NMR



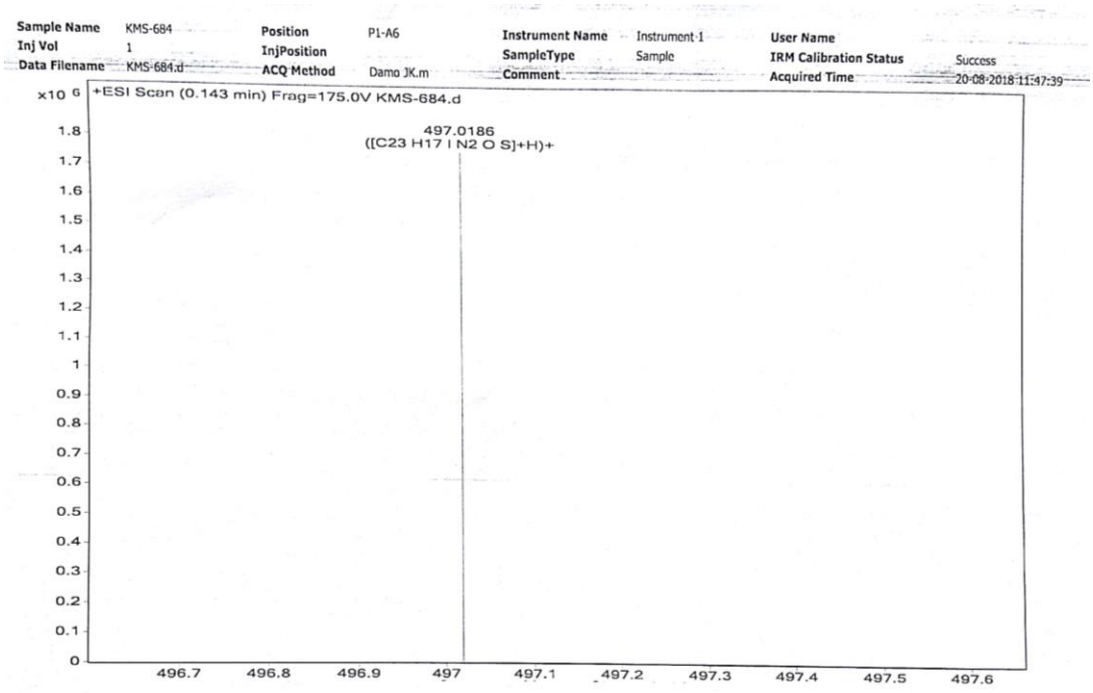
(Z)-N-((E)-4-(Iodo(m-tolyl)methylene)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (3c)



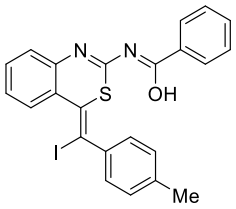
HRMS



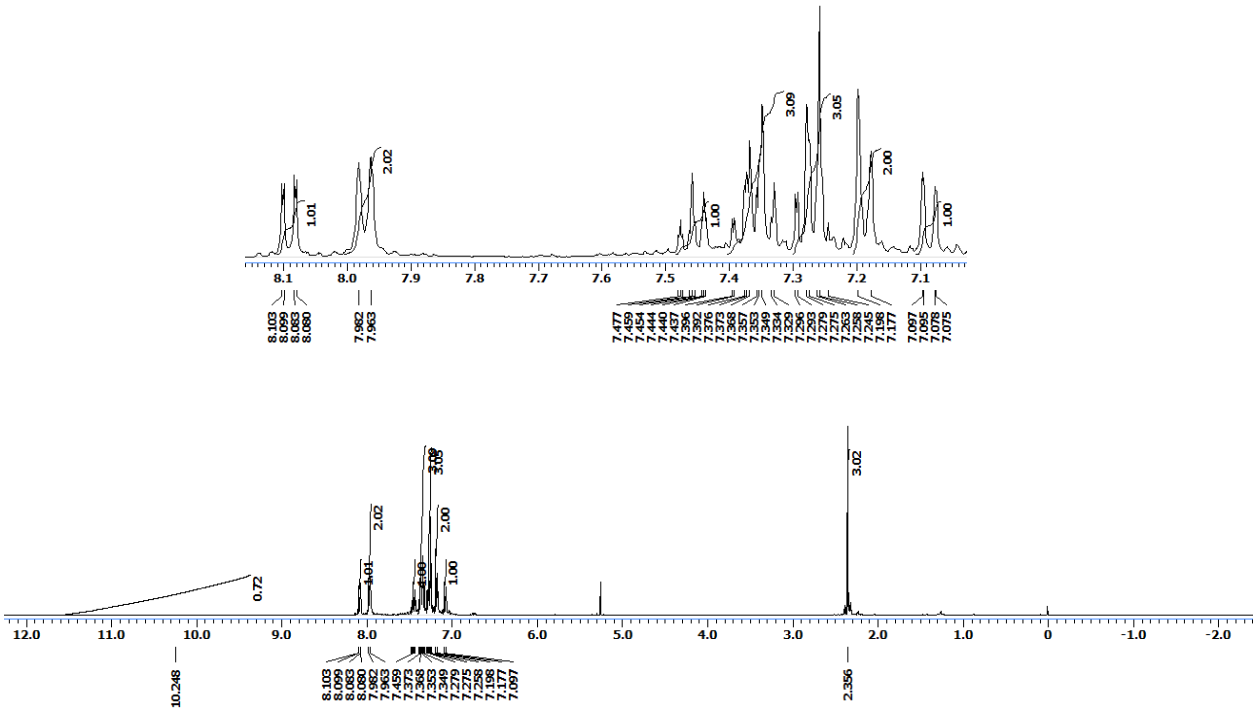
(Z)-N-((E)-4-(Iodo(m-tolyl)methylene)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (3c)



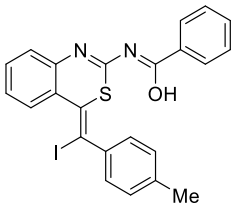
^{1}H NMR



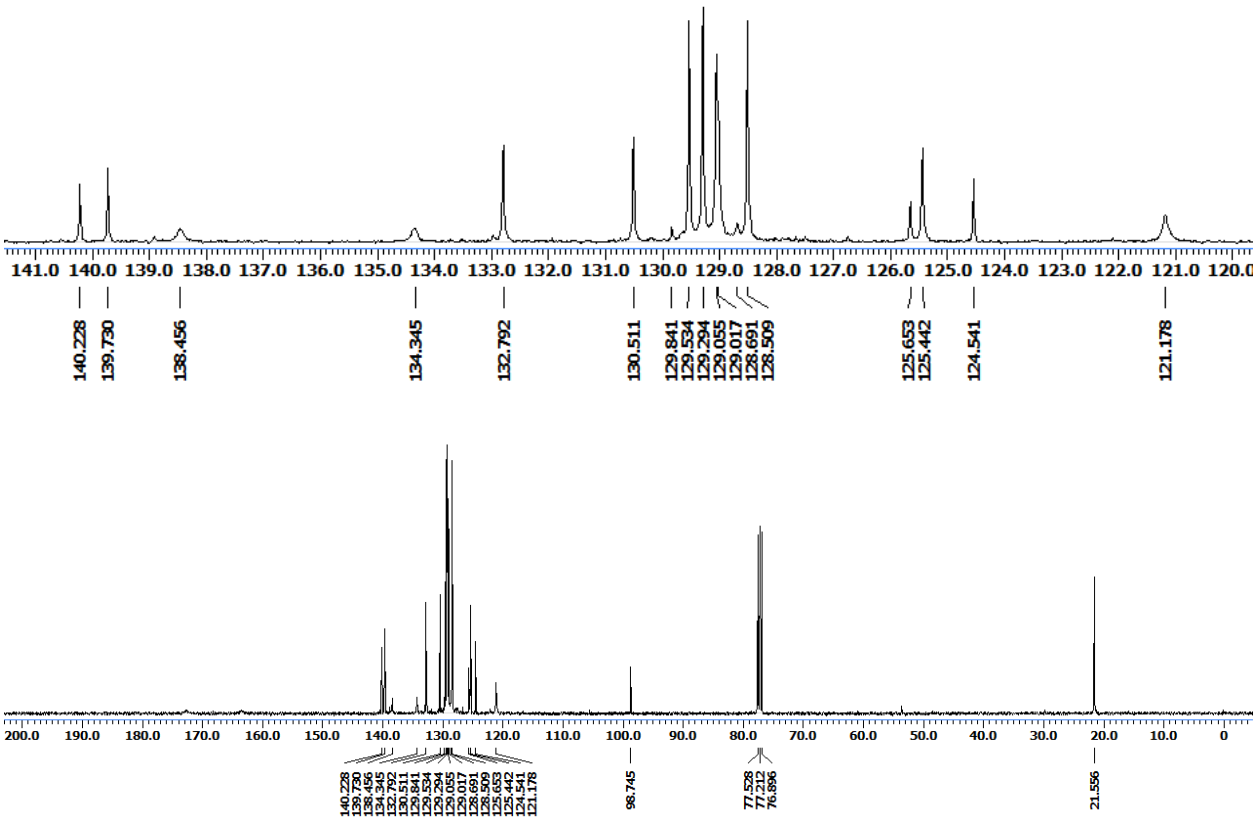
(Z)-N-((E)-4-(Iodo (*p*-tolyl)methylene)-4*H*-benzo[*d*][1,3]thiazin-2-yl)benzimidic acid (3d)



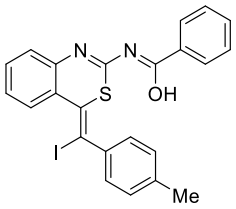
^{13}C NMR



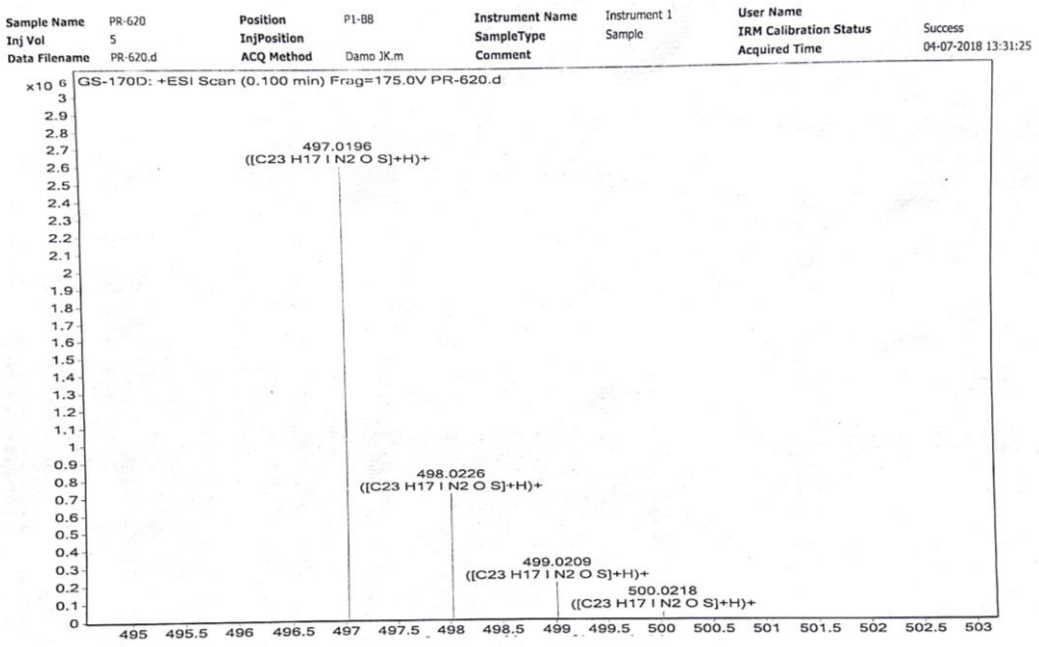
(Z)-N-((E)-4-(Iodo(p-tolyl)methylene)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (3d)



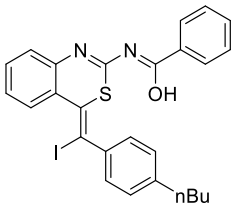
HRMS



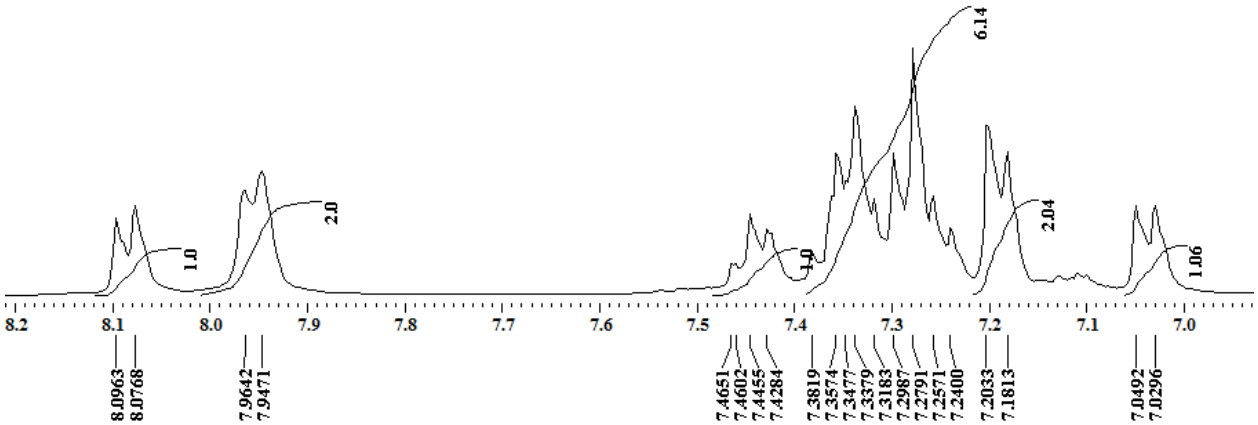
(Z)-N-((E)-4-(Iodo(p-tolyl)methylene)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (3d)

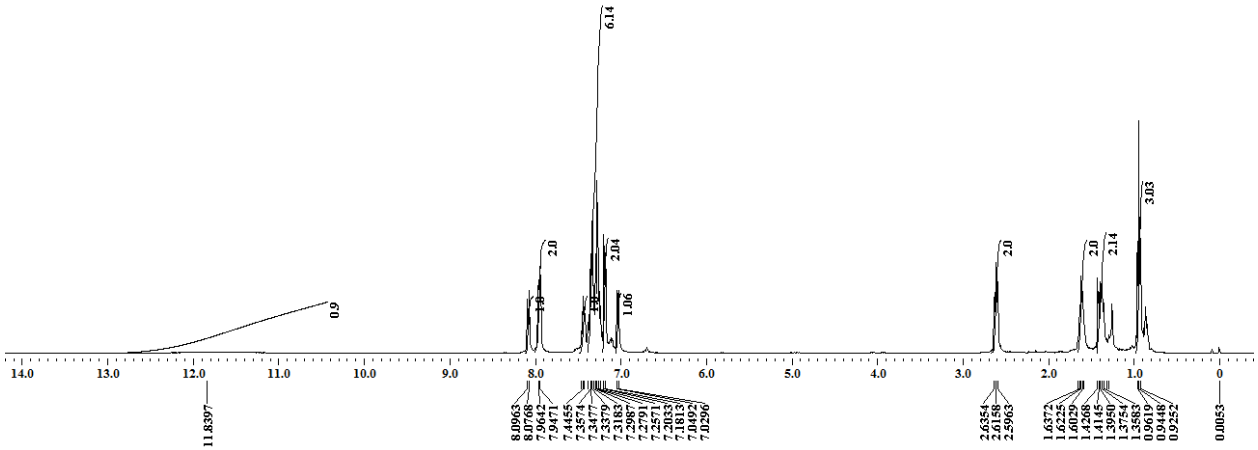


^{1}H NMR

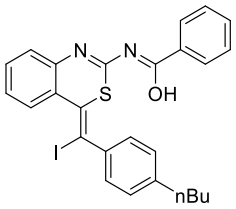


(Z)-N-((E)-4-((4-butylphenyl)iodomethylene)-4*H*-benzo[*d*][1,3]thiazin-2-yl)benzimidic acid (3e)

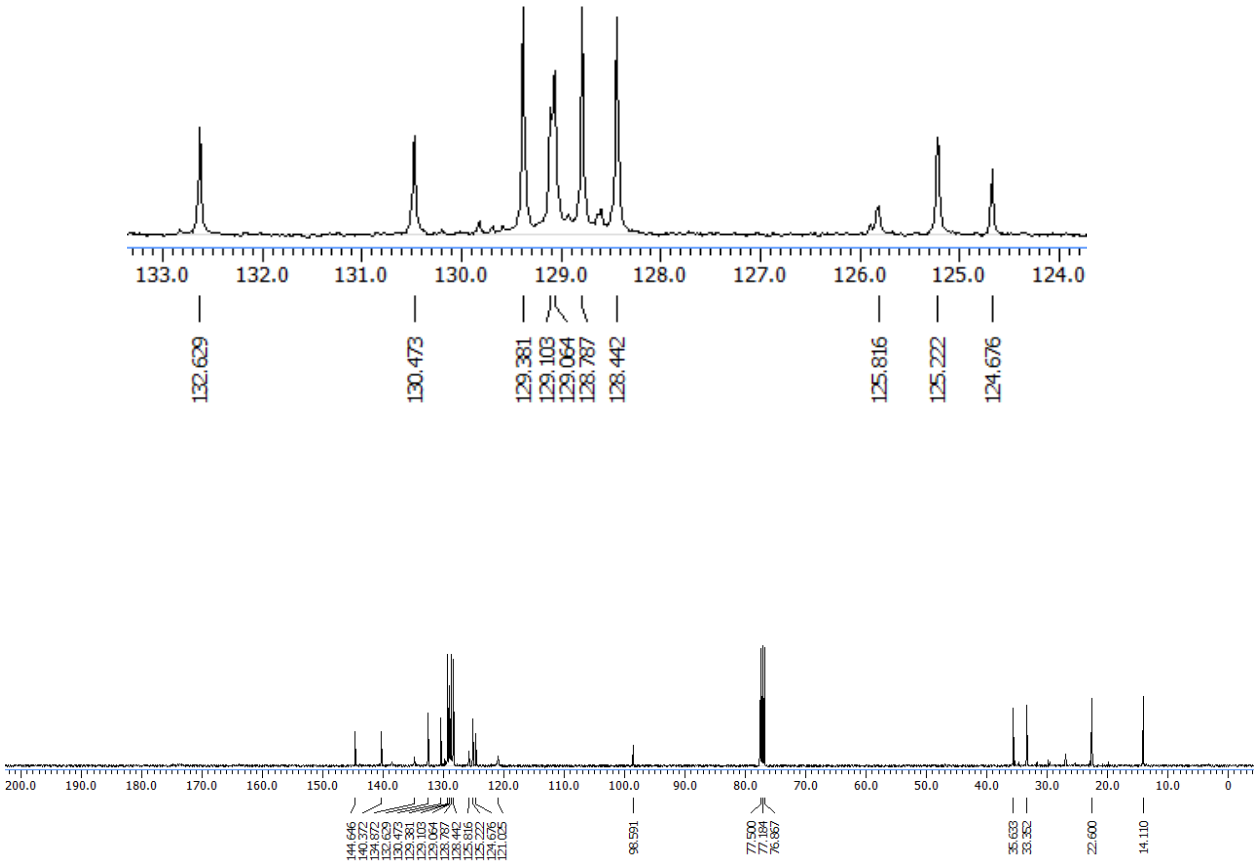




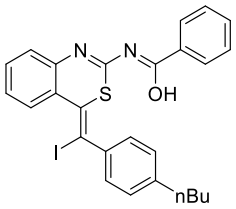
^{13}C NMR



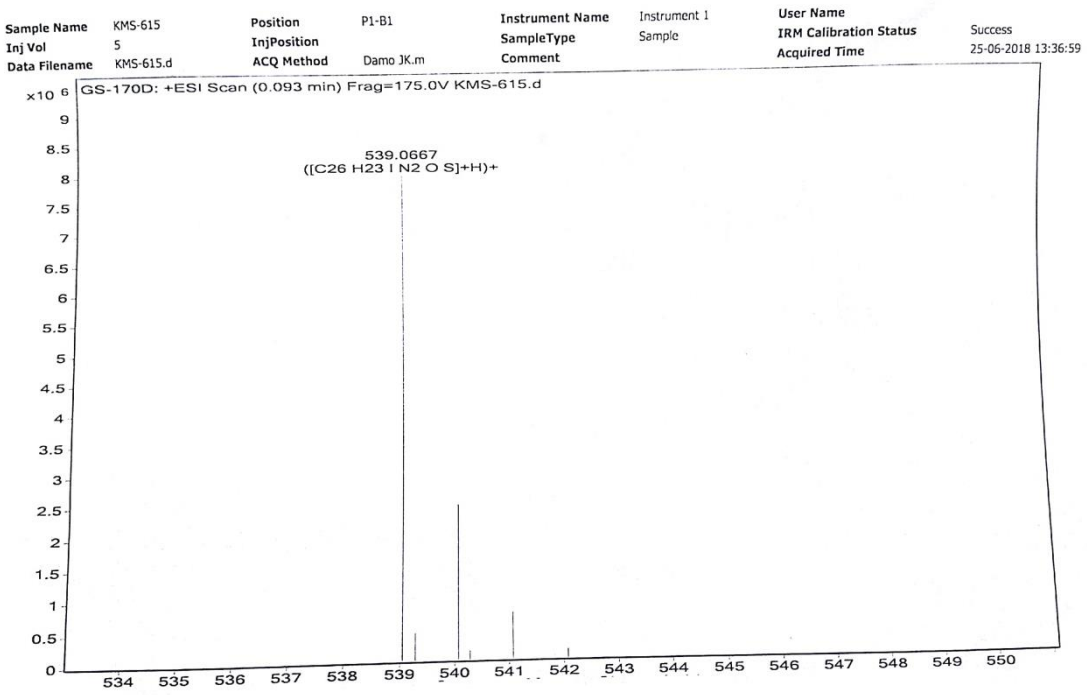
(Z)-N-((E)-4-((4-butylphenyl)iodomethylene)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (3e)



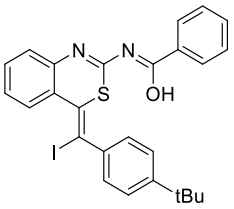
HRMS



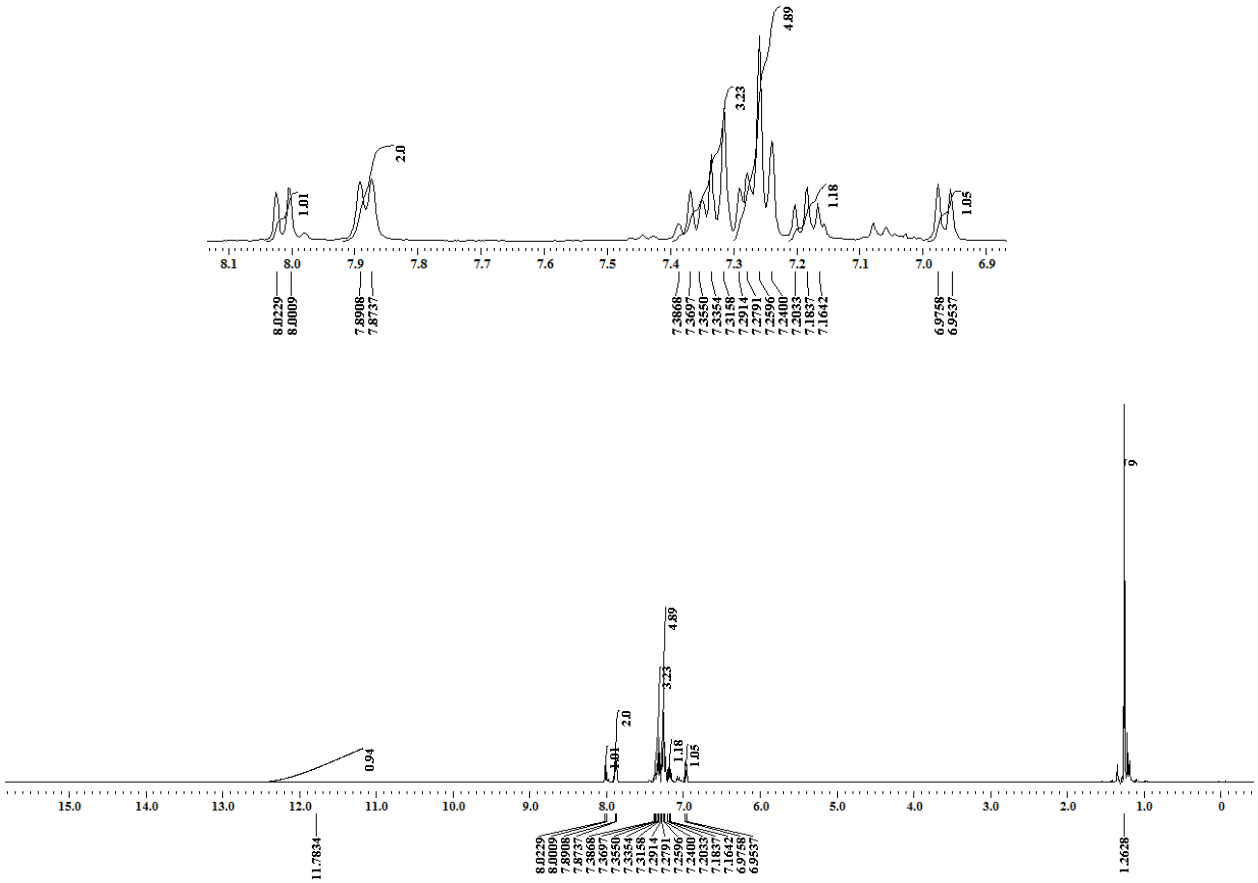
(Z)-N-((E)-4-((4-butylphenyl)iodomethylene)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (3e)



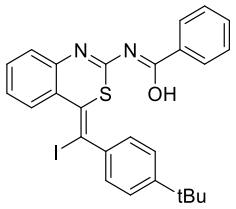
^{1}H NMR



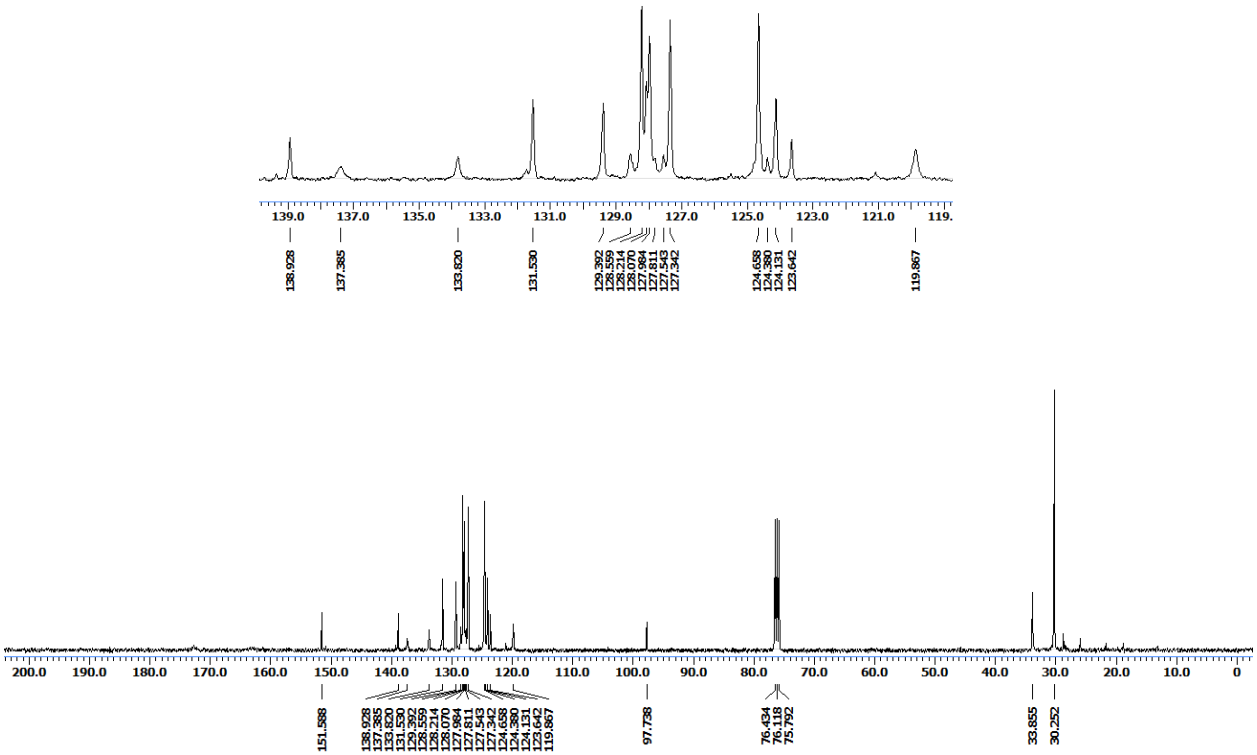
(Z)-N-((E)-4-((4-(*tert*-butyl)phenyl)iodomethylene)-4*H*-benzo[*d*][1,3]thiazin-2-yl)benzimidic acid (3f)



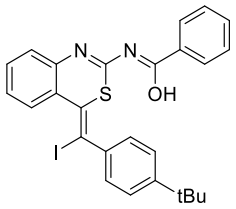
^{13}C NMR



(Z)-N-((E)-4-((4-(tert-butyl)phenyl)iodomethylene)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (3f)



HRMS



(Z)-N-((E)-4-((4-(tert-butyl)phenyl)iodomethylene)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (3f)

Qualitative Compound Report

Data File	KMS-683.d	**Sample Name**	KMS-683
Sample Type	Sample	**Position**	P1-C2
Instrument Name	Instrument 1	**User Name**	
Acq Method	Damo JK.m	**Acquired Time**	30-08-2018 14:07:37
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

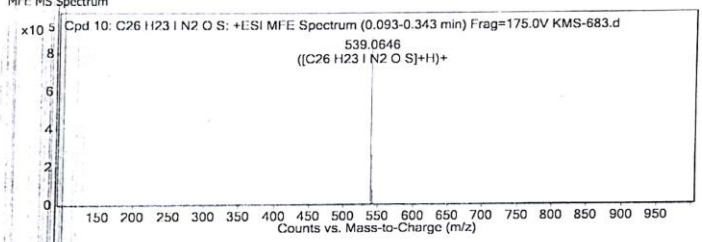
Sample Group **Info.**
Acquisition SW Version 6200 series TOF/6500 series Q-TOF B.05.01 (B5125.1)

Compound Table

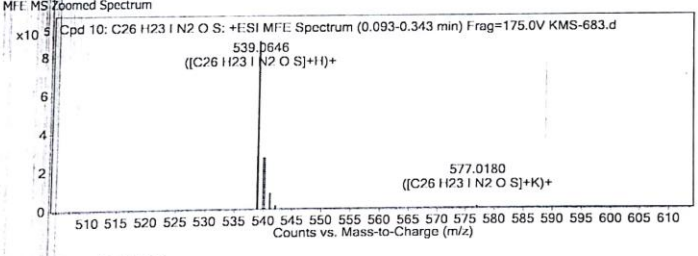
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 10: C26 H23 I N2 O S	0.146	538.0573	C26 H23 I N2 O S	C26 H23 I N2 O S	0.56	C26 H23 I N2 O S

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 10: C26 H23 I N2 O S	539.0646	0.146	Find by Molecular Feature	538.0573

MFE MS Spectrum



MFE MS Zoomed Spectrum

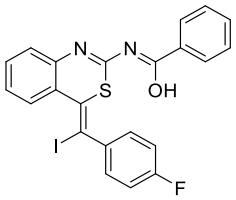


MS Spectrum Peak List

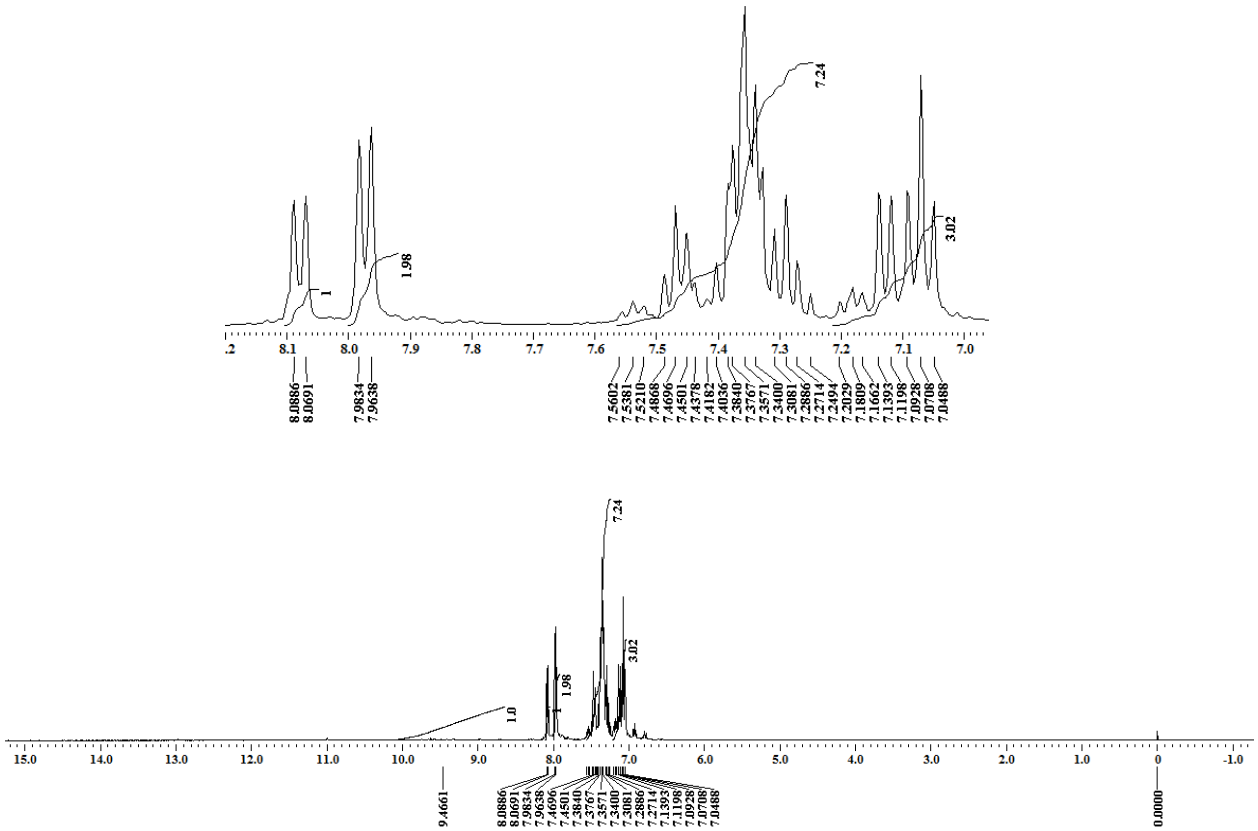
m/z	z	Abund	Formula	Ion
539.0646	1	884134.06	C26 H23 I N2 O S	(M+H)+
540.0672	1	261978.43	C26 H23 I N2 O S	(M+H)+
541.0664	1	74011.3	C26 H23 I N2 O S	(M+H)+
542.0675	1	14650.73	C26 H23 I N2 O S	(M+H)+
543.071	1	2394.14	C26 H23 I N2 O S	(M+H)+
577.018	1	3166.65	C26 H23 I N2 O S	(M+K)+
578.0202	1	1103.57	C26 H23 I N2 O S	(M+K)+
579.0251	1	651.26	C26 H23 I N2 O S	(M+K)+

--- End Of Report ---

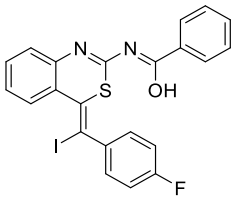
^{1}H NMR



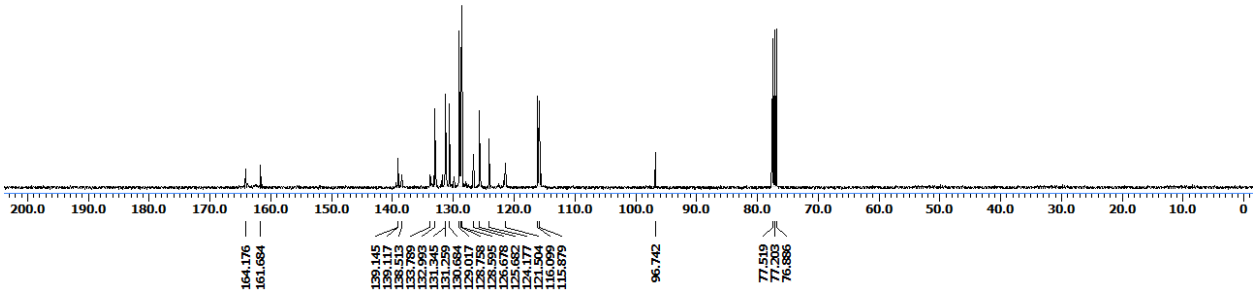
(Z)-N-((E)-4-((4-Fluorophenyl)iodomethylene)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (3g)



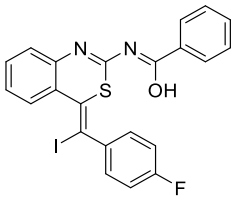
^{13}C NMR



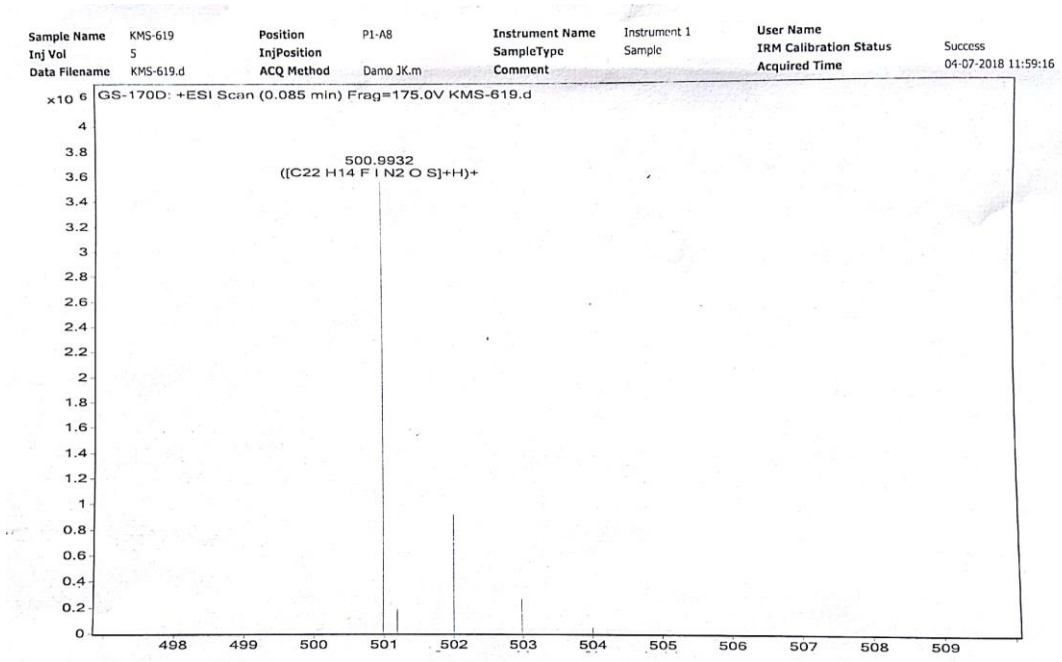
(Z)-N-((E)-4-((4-Fluorophenyl)iodomethylene)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (3g)



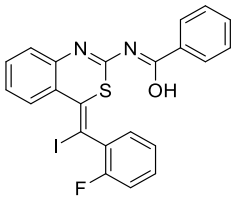
HRMS



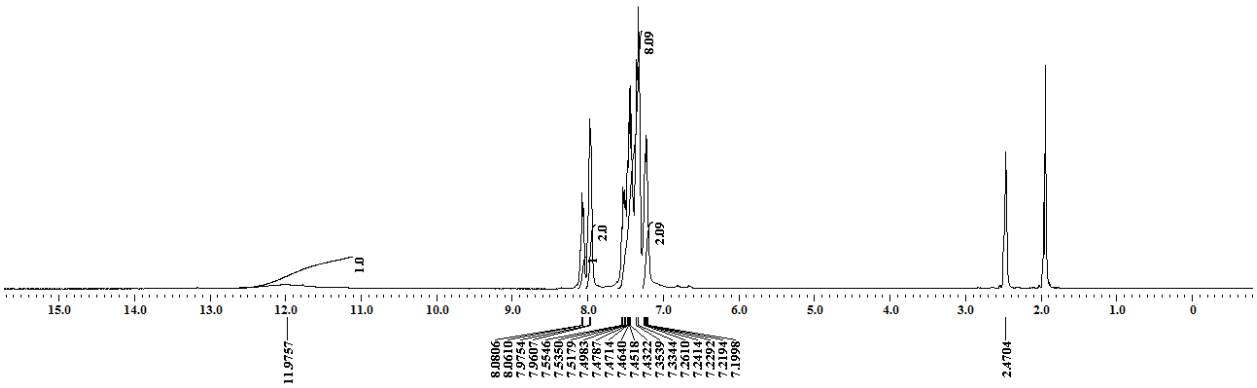
(Z)-N-((E)-4-((4-Fluorophenyl)iodomethylene)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (3g)



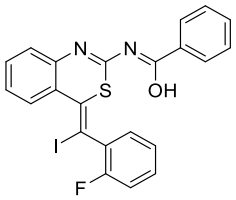
^{1}H NMR



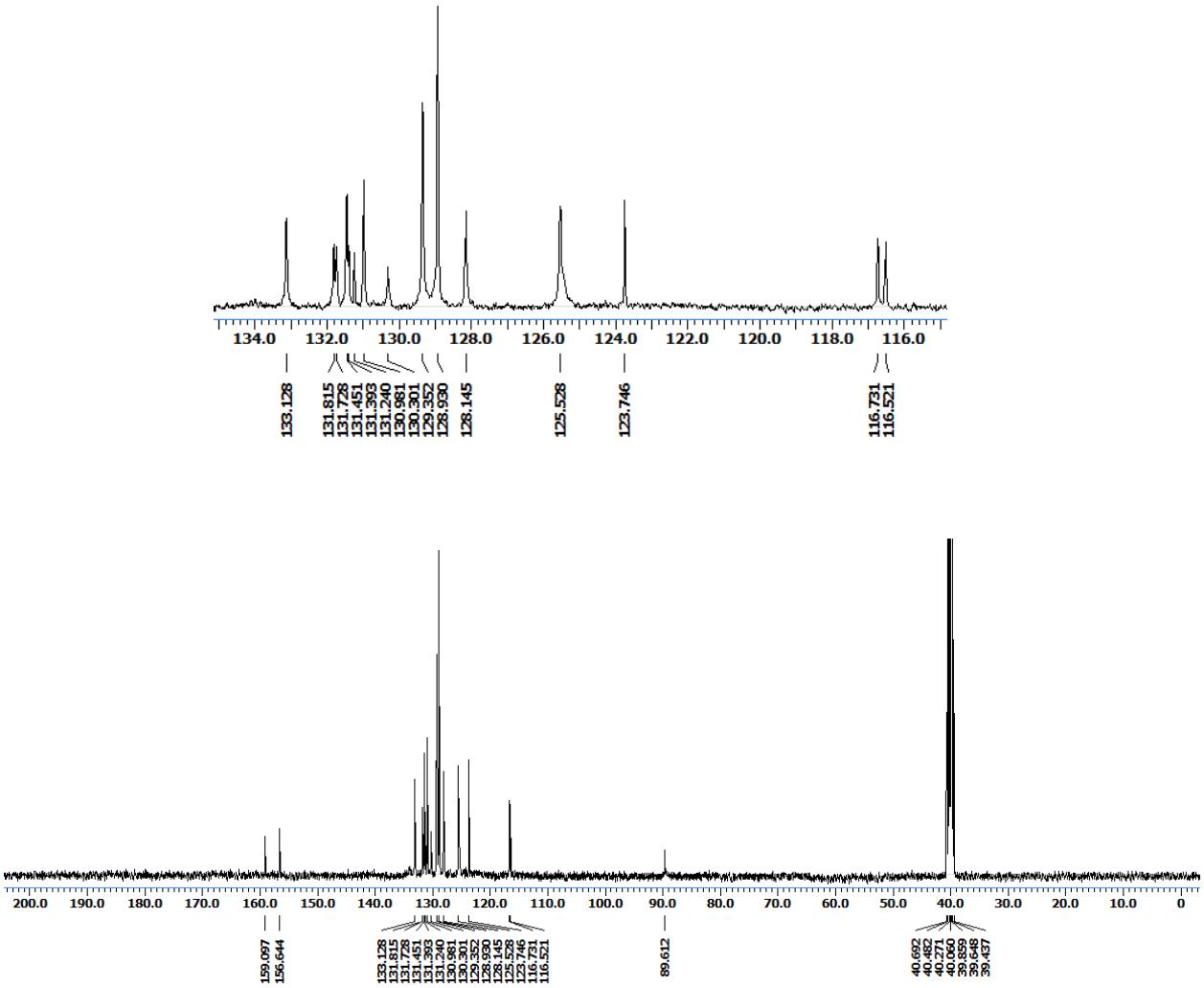
(Z)-N-((E)-4-((2-Fluorophenyl)iodomethylene)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (3h)



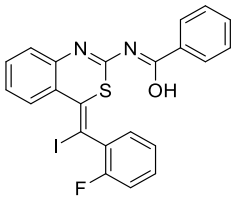
^{13}C NMR



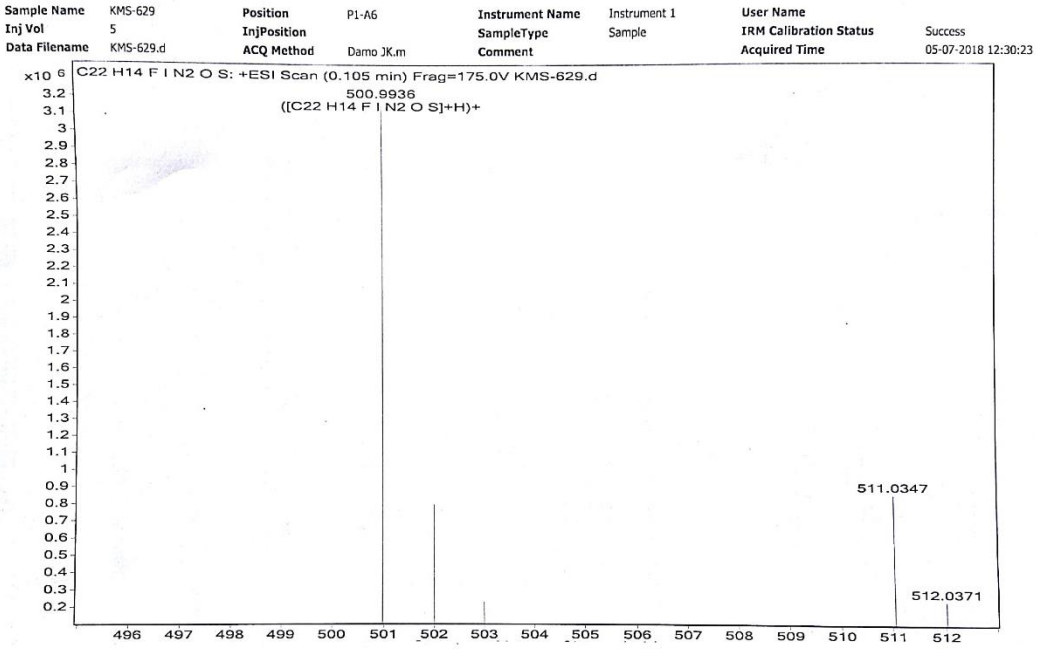
(Z)-N-((E)-4-((2-Fluorophenyl)iodomethylene)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (3h)



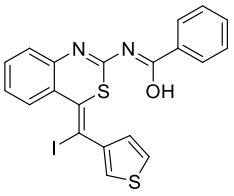
HRMS



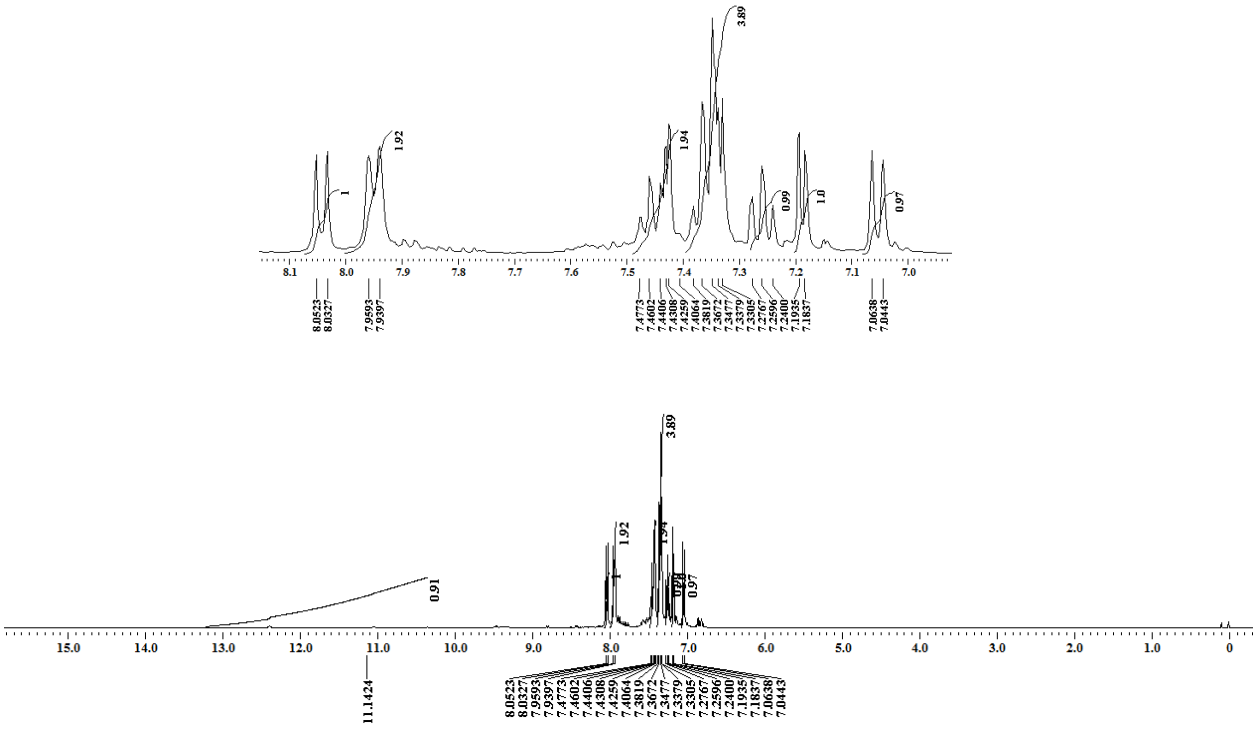
(Z)-N-((E)-4-((2-Fluorophenyl)iodomethylene)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (3h)



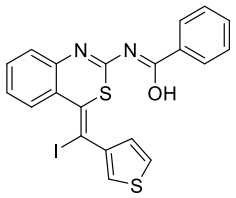
^{1}H NMR



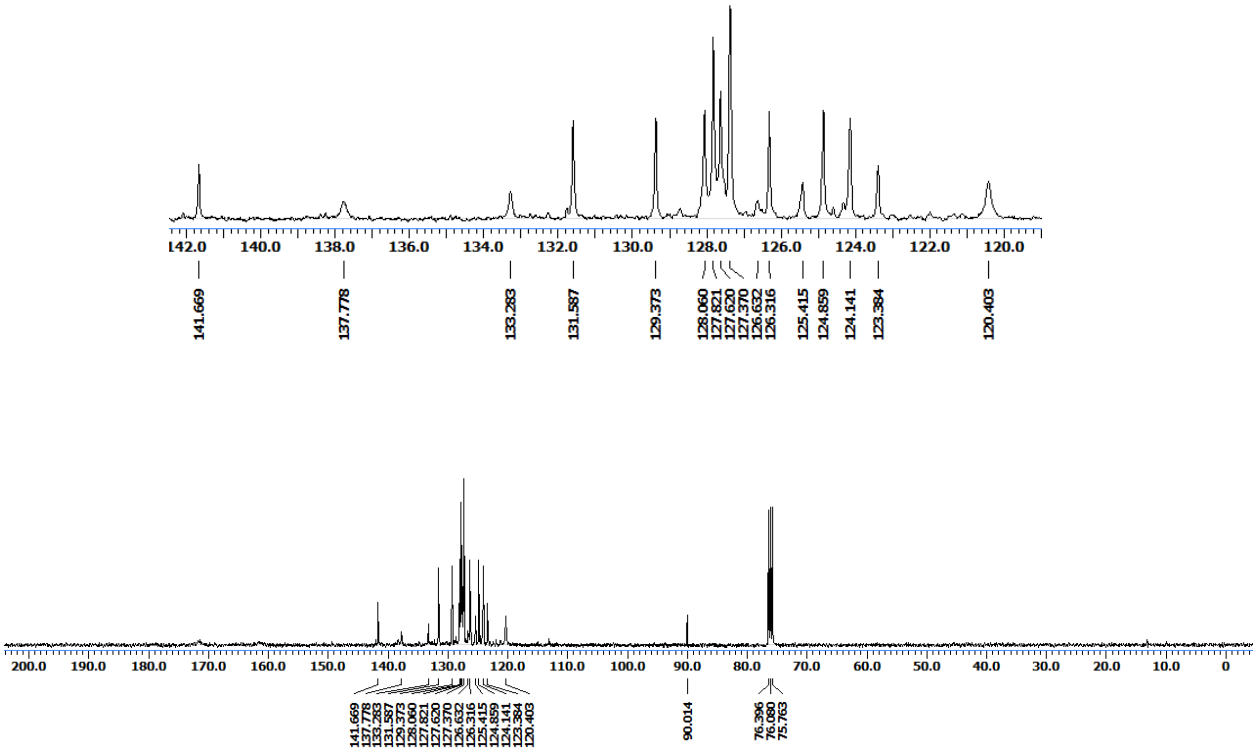
(Z)-N-((E)-4-(Iodo(thiophen-3-yl)methylene)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (3i)



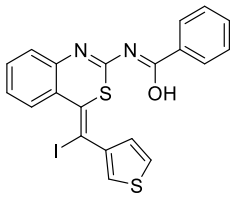
^{13}C NMR



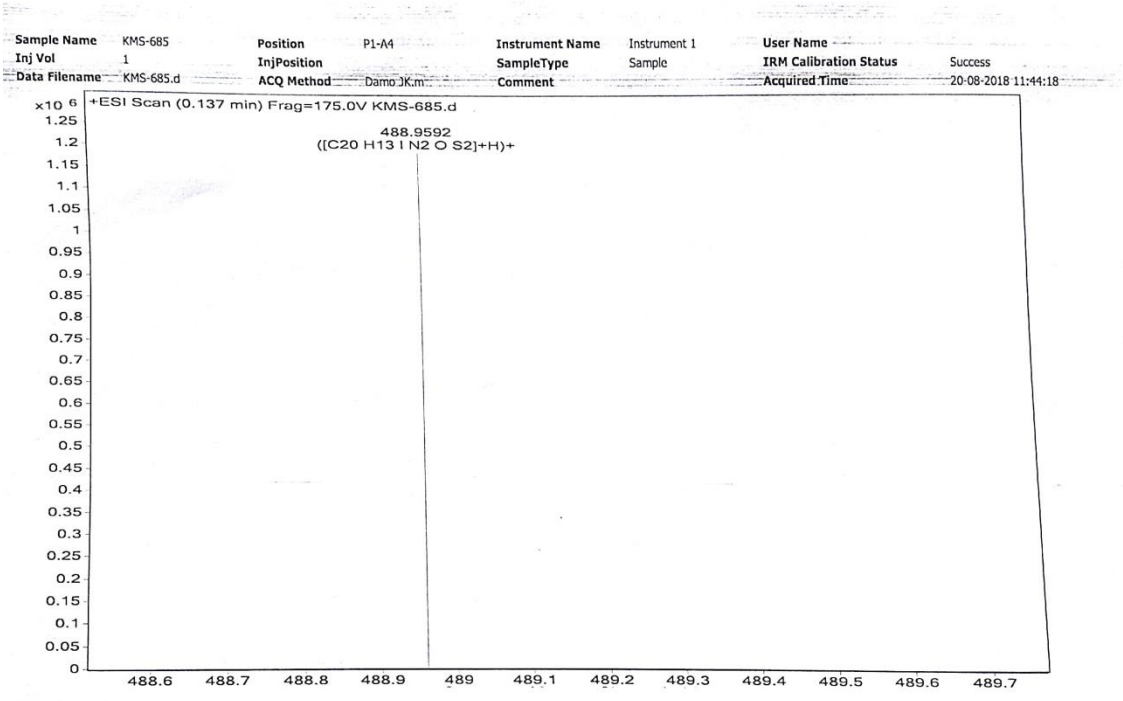
(Z)-N-((E)-4-(Iodo(thiophen-3-yl)methylene)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (3i)



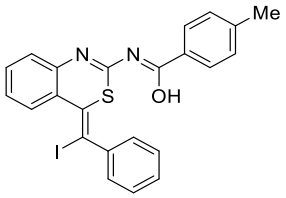
HRMS



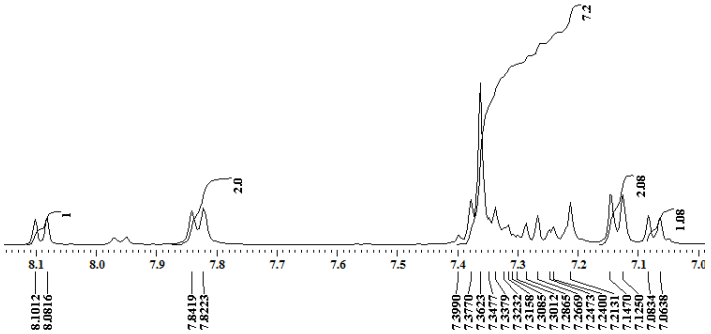
(Z)-N-((E)-4-(Iodo(thiophen-3-yl)methylene)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (3i)

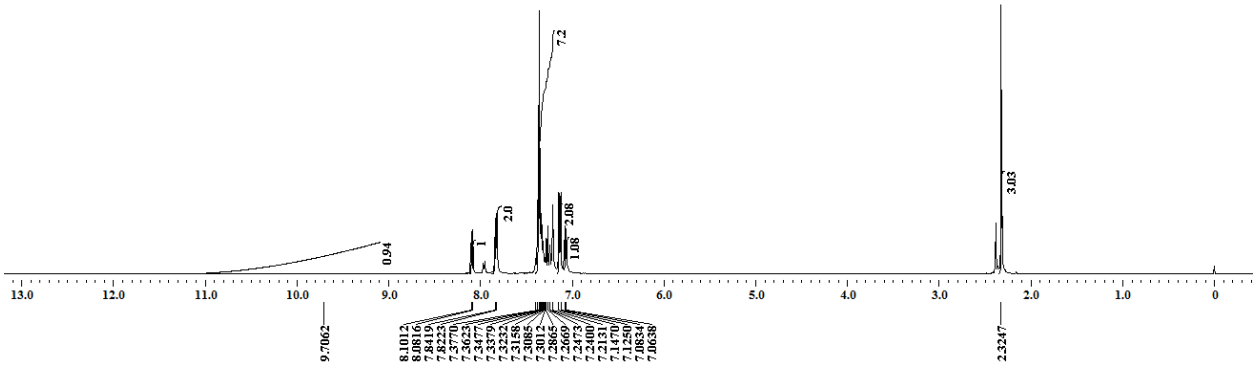


^{1}H NMR

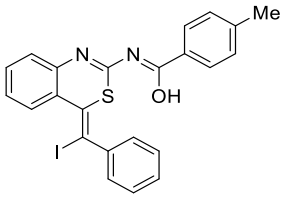


(Z)-N-((E)-4-(iodo(phenyl)methylene)-4H-benzo[d][1,3]thiazin-2-yl)-4-methylbenzimidic acid (3j)

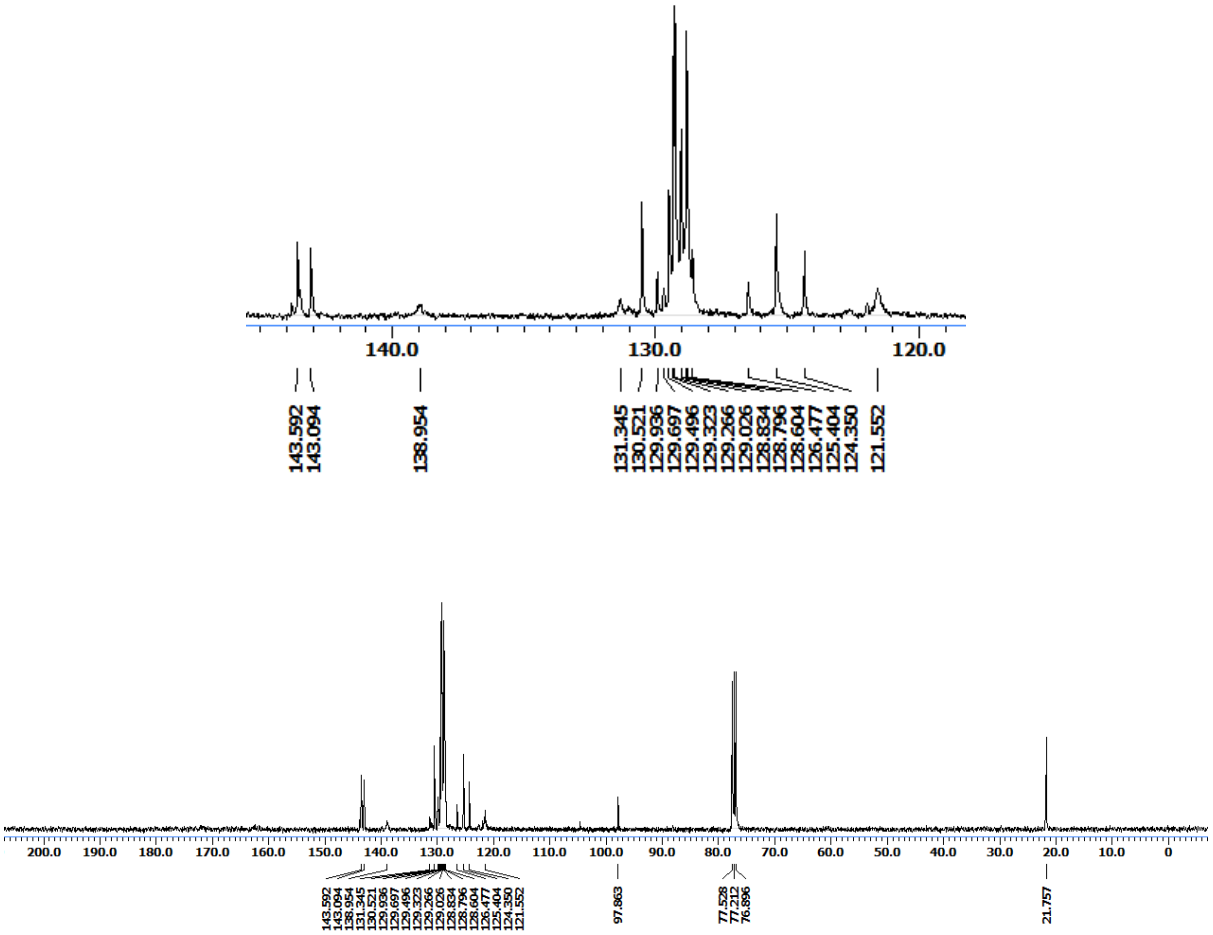




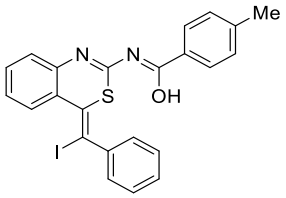
^{13}C NMR



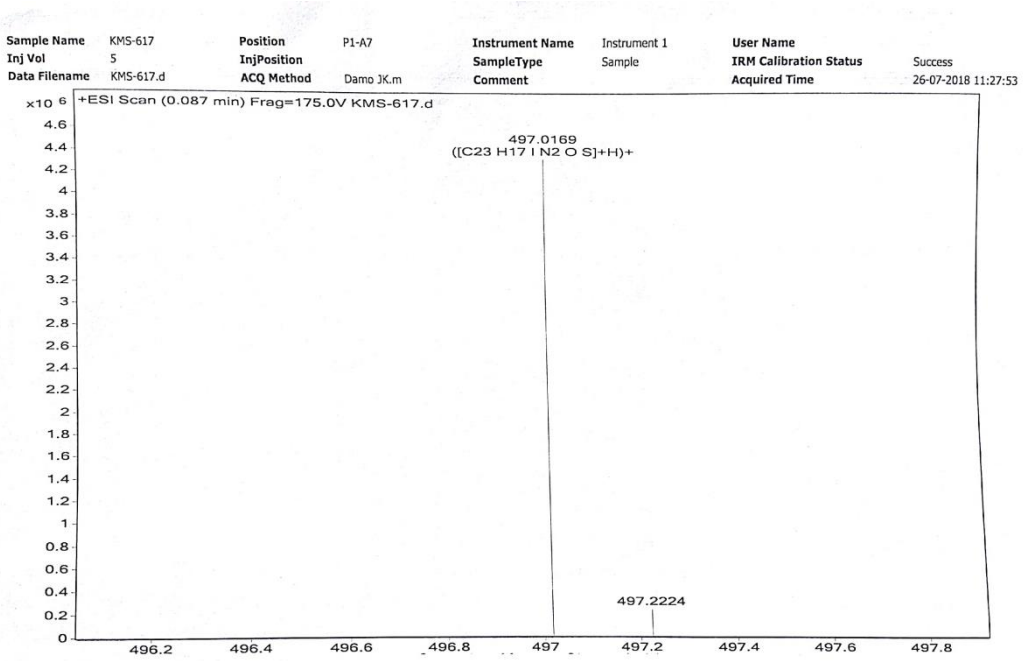
(Z)-N-((E)-4-(iodo(phenyl)methylene)-4H-benzo[d][1,3]thiazin-2-yl)-4-methylbenzimidic acid (3j)



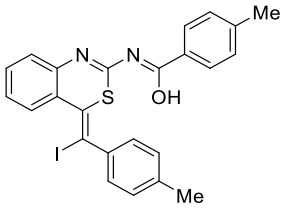
HRMS



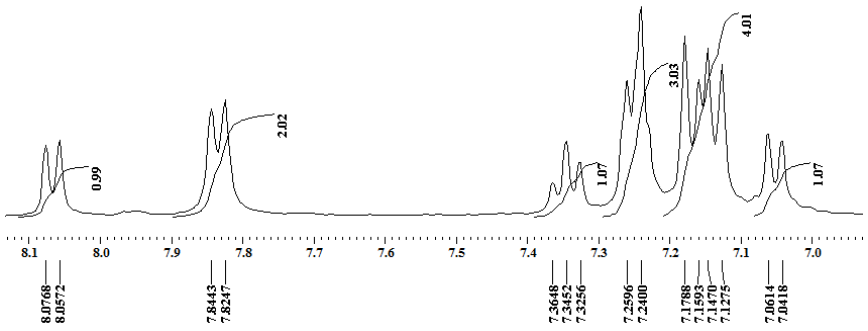
(Z)-N-((E)-4-(iodo(phenyl)methylene)-4H-benzo[d][1,3]thiazin-2-yl)-4-methylbenzimidic acid (3j)

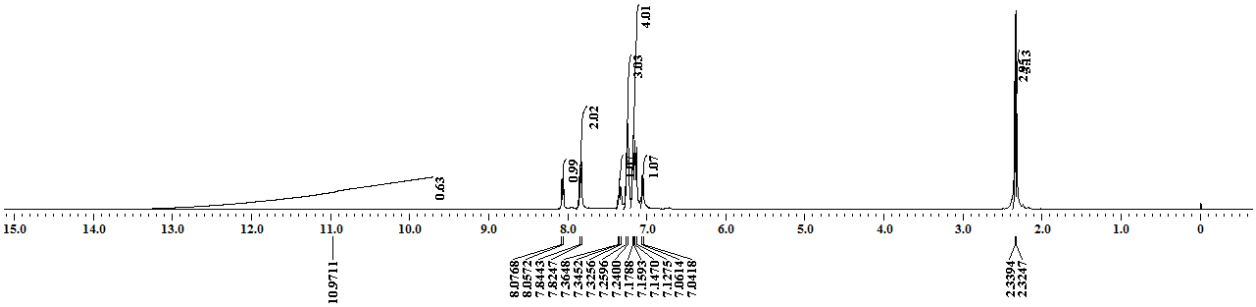


^{1}H NMR

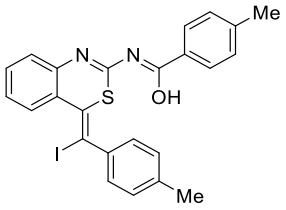


(Z)-N-((E)-4-(Iodo(*p*-tolyl)methylene)-4H-benzo[d][1,3]thiazin-2-yl)-4-methylbenzimidic acid (3k)

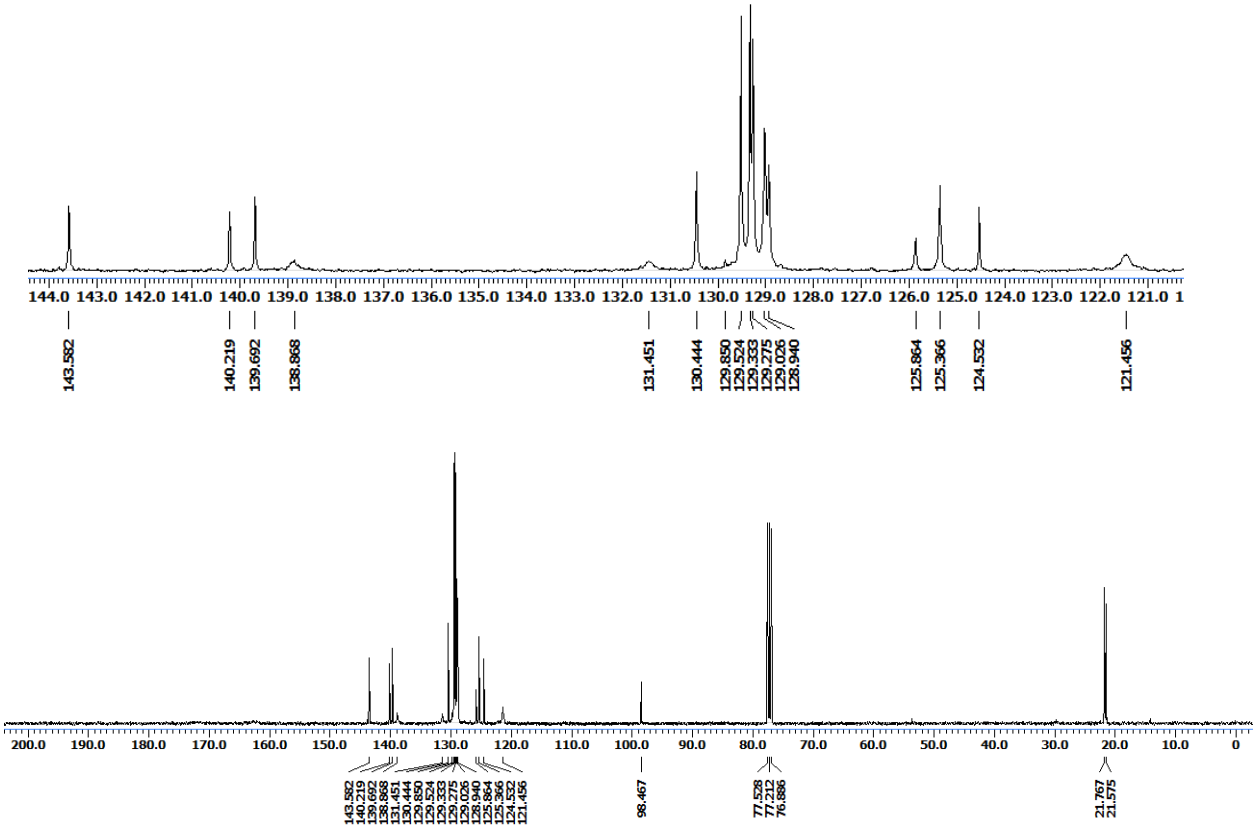




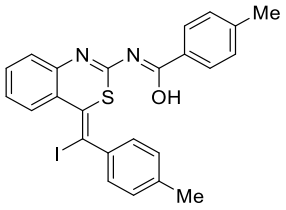
^{13}C NMR



(Z)-N-((E)-4-(Iodo(p-tolyl)methylene)-4H-benzo[d][1,3]thiazin-2-yl)-4-methylbenzimidic acid (3k)



HRMS



(Z)-N-((E)-4-(Iodo(p-tolyl)methylene)-4H-benzo[d][1,3]thiazin-2-yl)-4-methylbenzimidic acid (3k)

Qualitative Compound Report

Data File	KMS-621.d	Sample Name	KMS-621
Sample Type	Sample	Position	P1-A7
Instrument Name	Instrument 1	User Name	
Acq Method	Damo JK.m	Acquired Time	16-07-2018 12:40:12
IRM Calibration Status	Success	DA Method	Default.m
Comment			

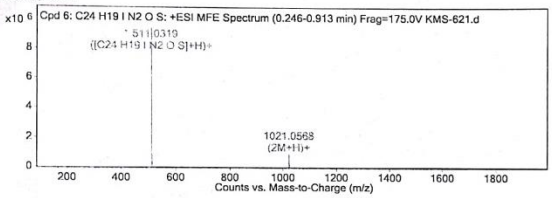
Sample Group	Info.
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.1)

Compound Table

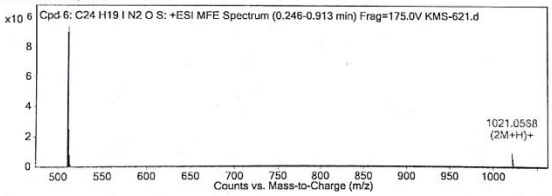
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 6: C24 H19 I N2 O S	0.308	510.0247	C24 H19 I N2 O S	C24 H19 I N2 O S	3.18	C24 H19 I N2 O S

Compound Label	m/z	RT	Algorithm	Mass
Cpd 6: C24 H19 I N2 O S	511.0319	0.308	Find by Molecular Feature	510.0247

MFE MS Spectrum



MFE MS Zoomed Spectrum

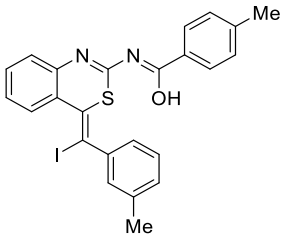


MS Spectrum Peak List

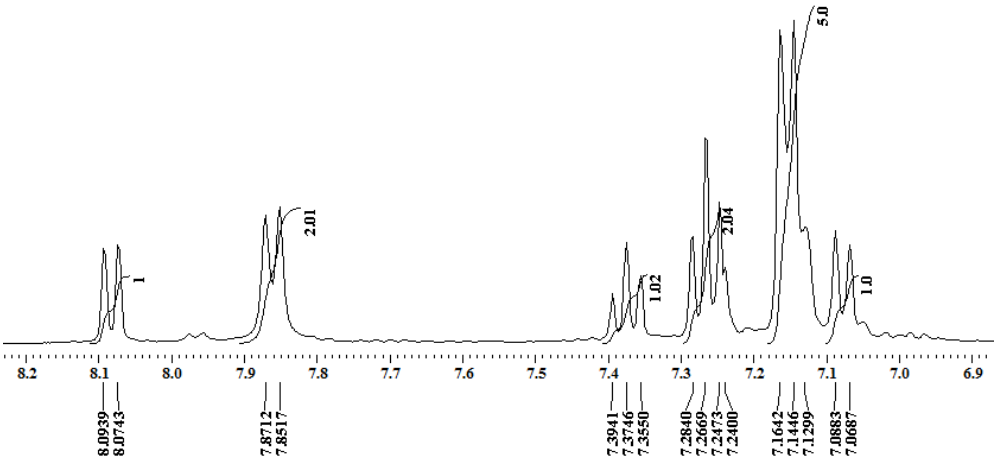
m/z	z	Abund	Formula	Ion
511.0319	1	9402933	C24 H19 I N2 O S	(M+H)+
512.0351	1	2018829.71	C24 H19 I N2 O S	(M+H)+
513.0333	1	786736.14	C24 H19 I N2 O S	(M+H)+
514.0336	1	114566.42	C24 H19 I N2 O S	(M+H)+
515.029	1	25103.82	C24 H19 I N2 O S	(M+H)+
1021.0568	1	883455.13		(2M+H)+
1022.0598	1	504005.46		(2M+H)+
1023.0587	1	210104.77		(2M+H)+
1024.0591	1	63927.27		(2M+H)+
1025.0577	1	17945.81		(2M+H)+

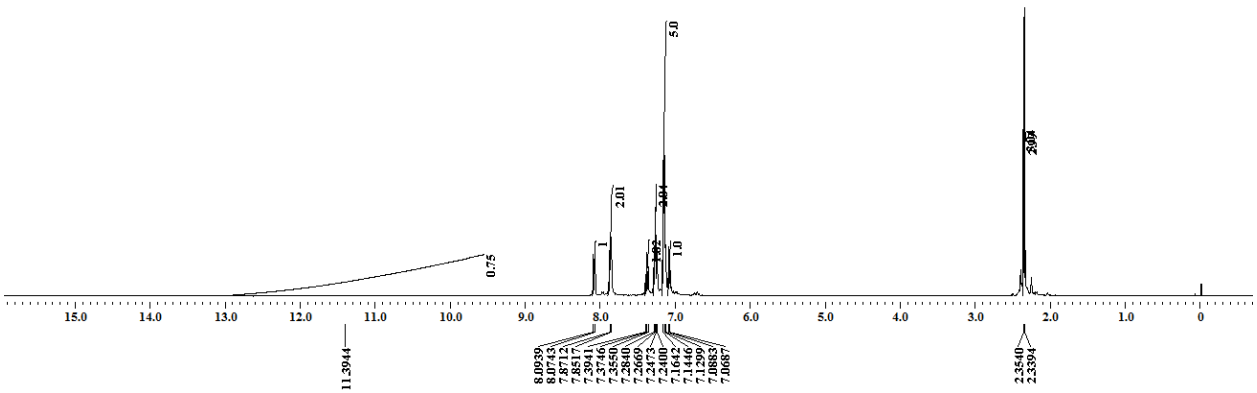
--- End Of Report ---

^{1}H NMR

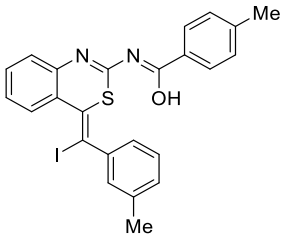


(Z)-N-((E)-4-(Iodo(m-tolyl)methylene)-4H-benzo[d][1,3]thiazin-2-yl)-4-methylbenzimidic acid (3l)

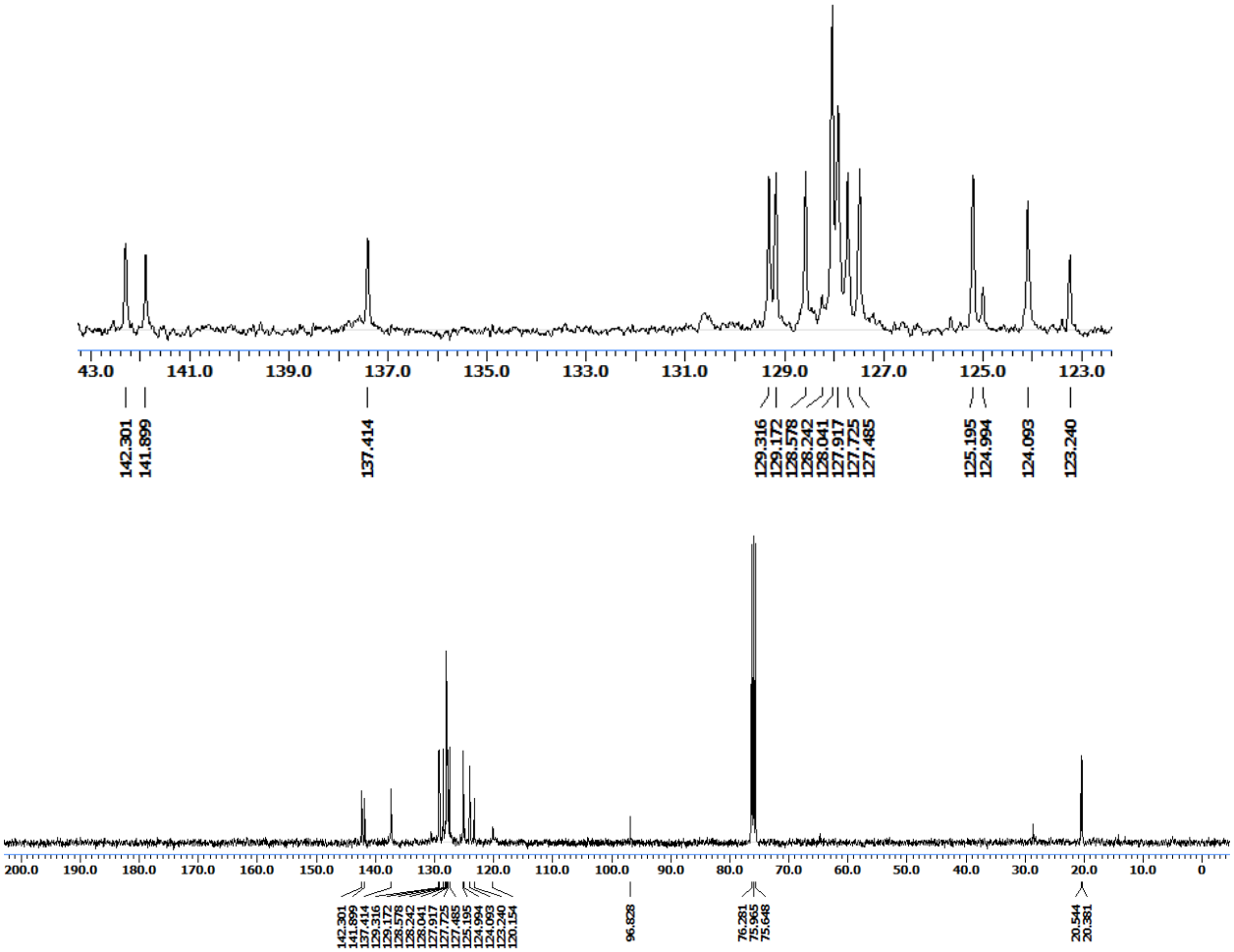




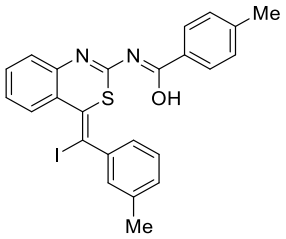
^{13}C NMR



(Z)-N-((E)-4-(Iodo(m-tolyl)methylene)-4H-benzo[d][1,3]thiazin-2-yl)-4-methylbenzimidic acid (3l)



HRMS



(Z)-N-((E)-4-(Iodo(m-tolyl)methylene)-4H-benzo[d][1,3]thiazin-2-yl)-4-methylbenzimidic acid (3l)

Qualitative Compound Report

Data File	KMS-687.d	**Sample Name**	KMS-687
Sample Type	Sample	**Position**	P1-A9
Instrument Name	Instrument 1	**User Name**	
Acq Method	Damo JK.m	**Acquired Time**	29-08-2018 11:31:50
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

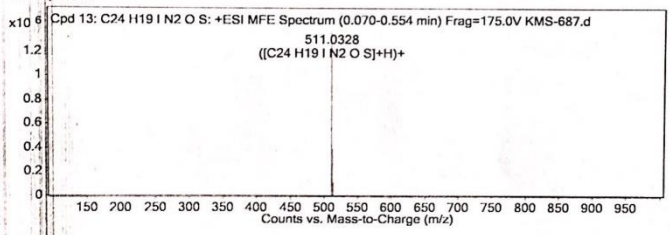
Sample Group **Info.**
Acquisition SW Version 6200 series TOF/6500 series Q-TOF B.05.01 (B5175.1)

Compound Table

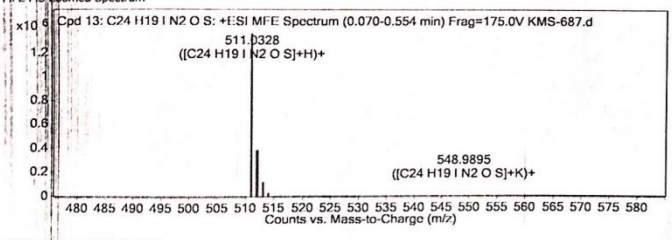
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 13: C24 H19 I N2 O S	0.124	510.0256	C24 H19 I N2 O S	C24 H19 I N2 O S	1.36	C24 H19 I N2 O S

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 13: C24 H19 I N2 O S	511.0328	0.124	Find by Molecular Feature	510.0256

MFE MS Spectrum



MFE MS Zoomed Spectrum

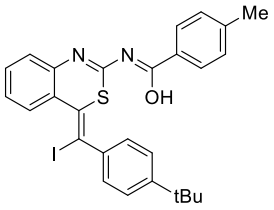


MS Spectrum Peak List

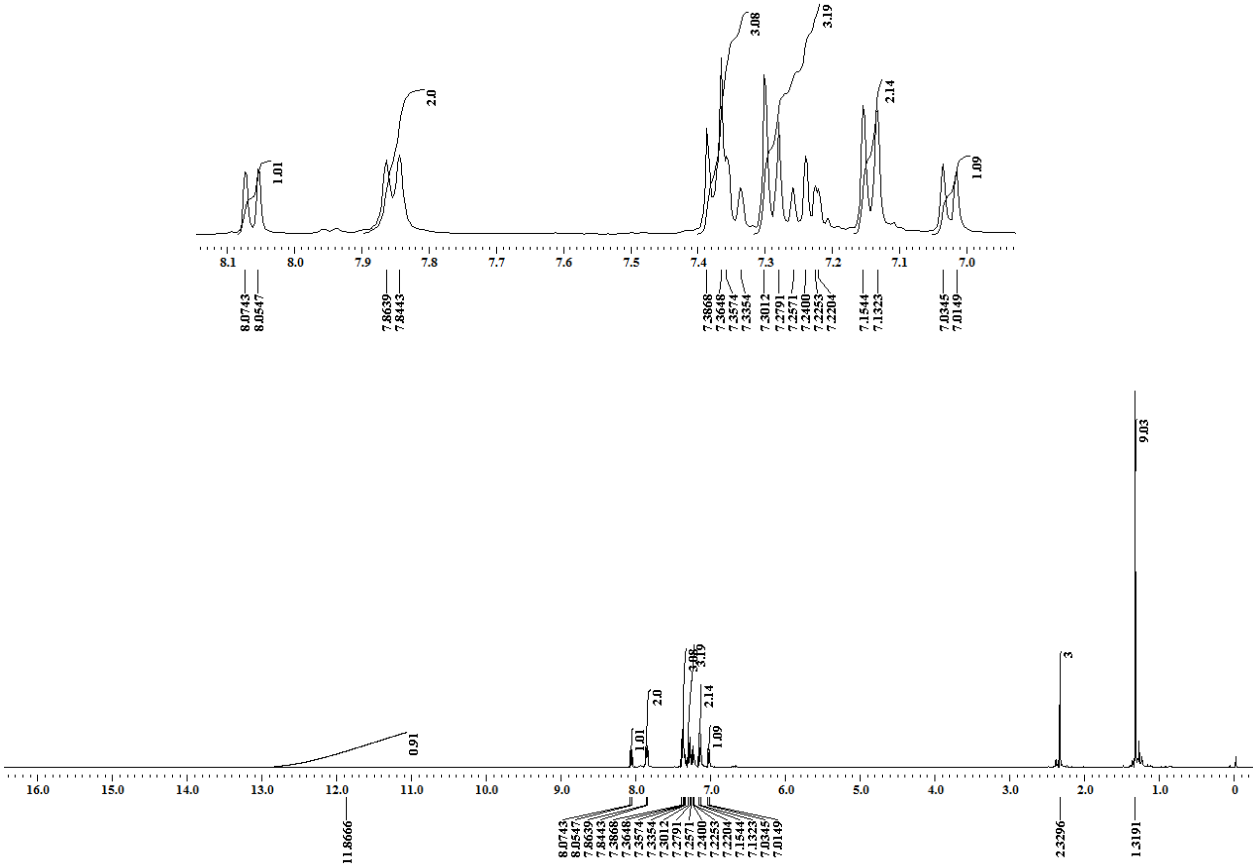
m/z	z	Abund	Formula	Ion
511.0328	1	1357682	C24 H19 I N2 O S	(M+H)+
512.0359	1	388667.93	C24 H19 I N2 O S	(M+H)+
513.0339	1	105644.27	C24 H19 I N2 O S	(M+H)+
514.0343	1	21985.59	C24 H19 I N2 O S	(M+H)+
515.0367	1	3402.11	C24 H19 I N2 O S	(M+H)+
516.0396	1	371.11	C24 H19 I N2 O S	(M+H)+
548.9895	1	1648.84	C24 H19 I N2 O S	(M+K)+
550.0018	1	391.78	C24 H19 I N2 O S	(M+K)+

--- End Of Report ---

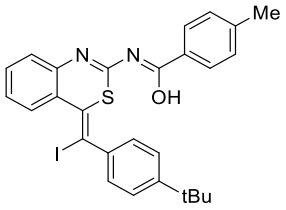
^{1}H NMR



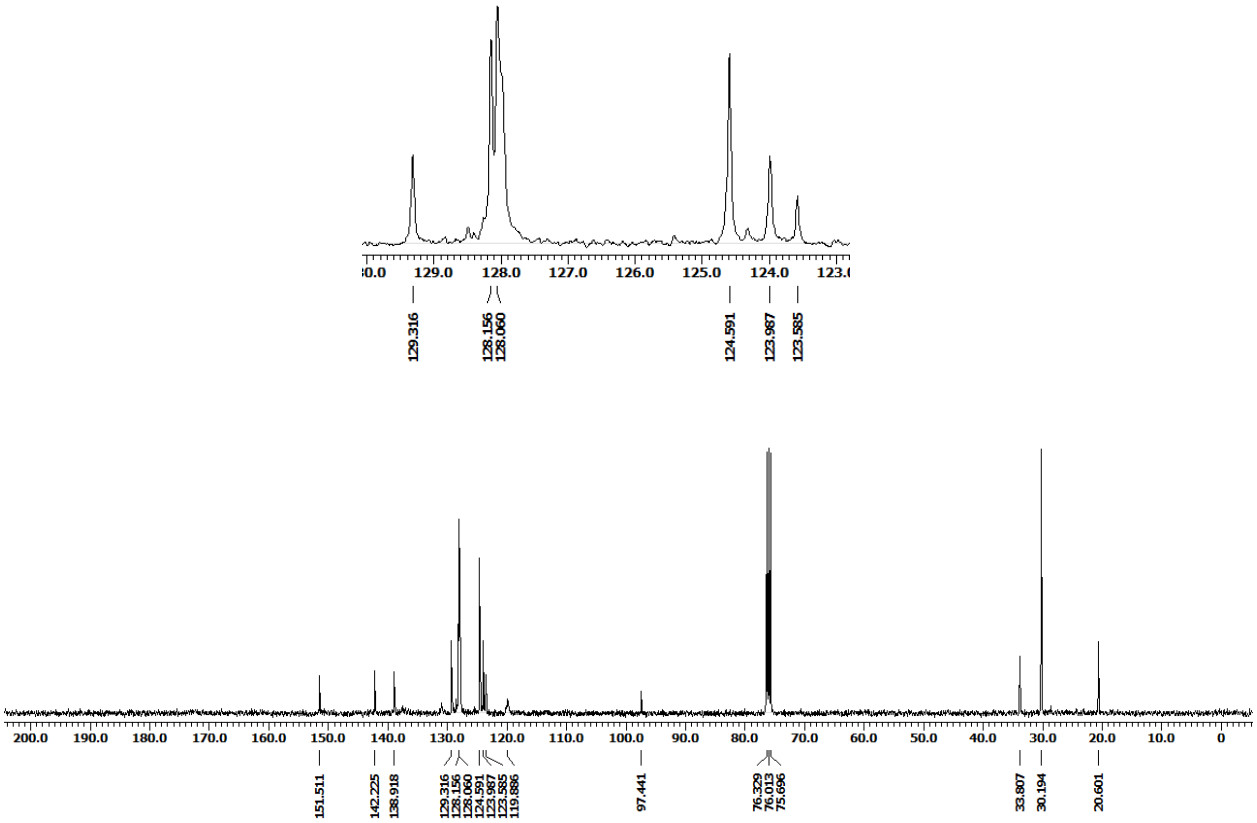
(Z)-N-((E)-4-((4-(tert-butyl)phenyl)iodomethylene)-4H-benzo[d][1,3]thiazin-2-yl)-4-methylbenzimidic acid (3m)



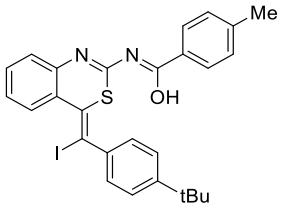
^{13}C NMR



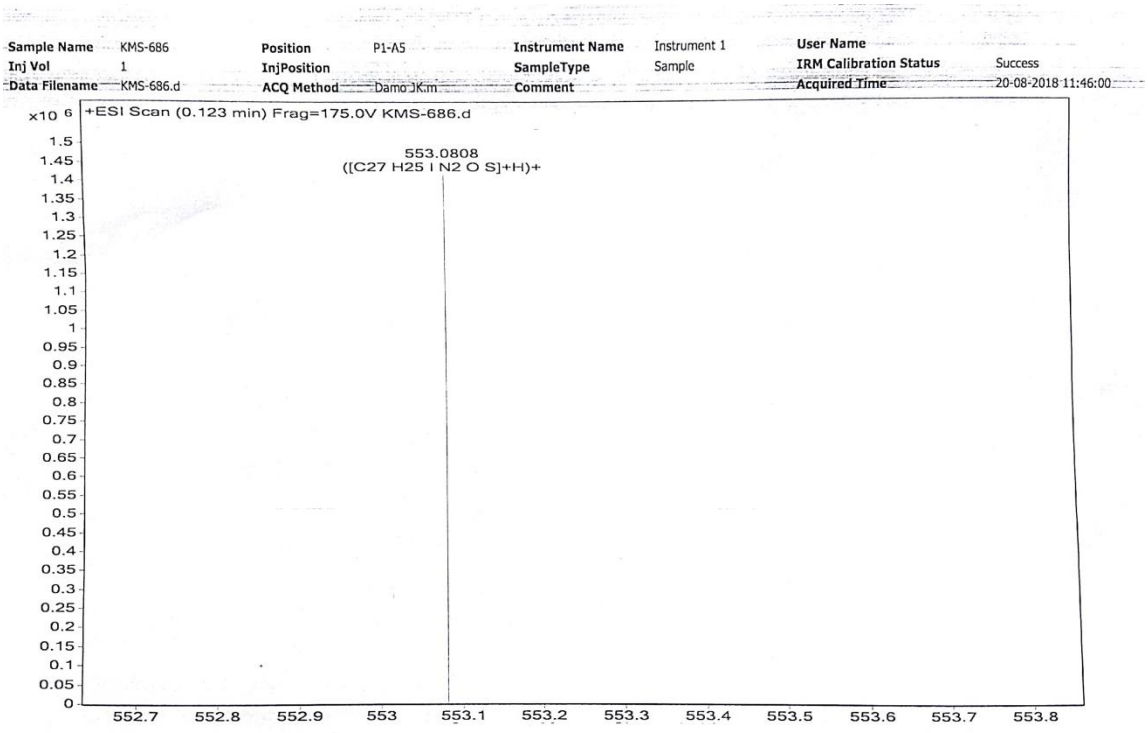
(Z)-N-((E)-4-((4-(tert-butyl)phenyl)iodomethylene)-4H-benzo[d][1,3]thiazin-2-yl)-4-methylbenzimidic acid (3m)



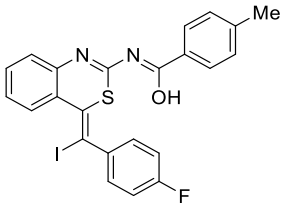
HRMS



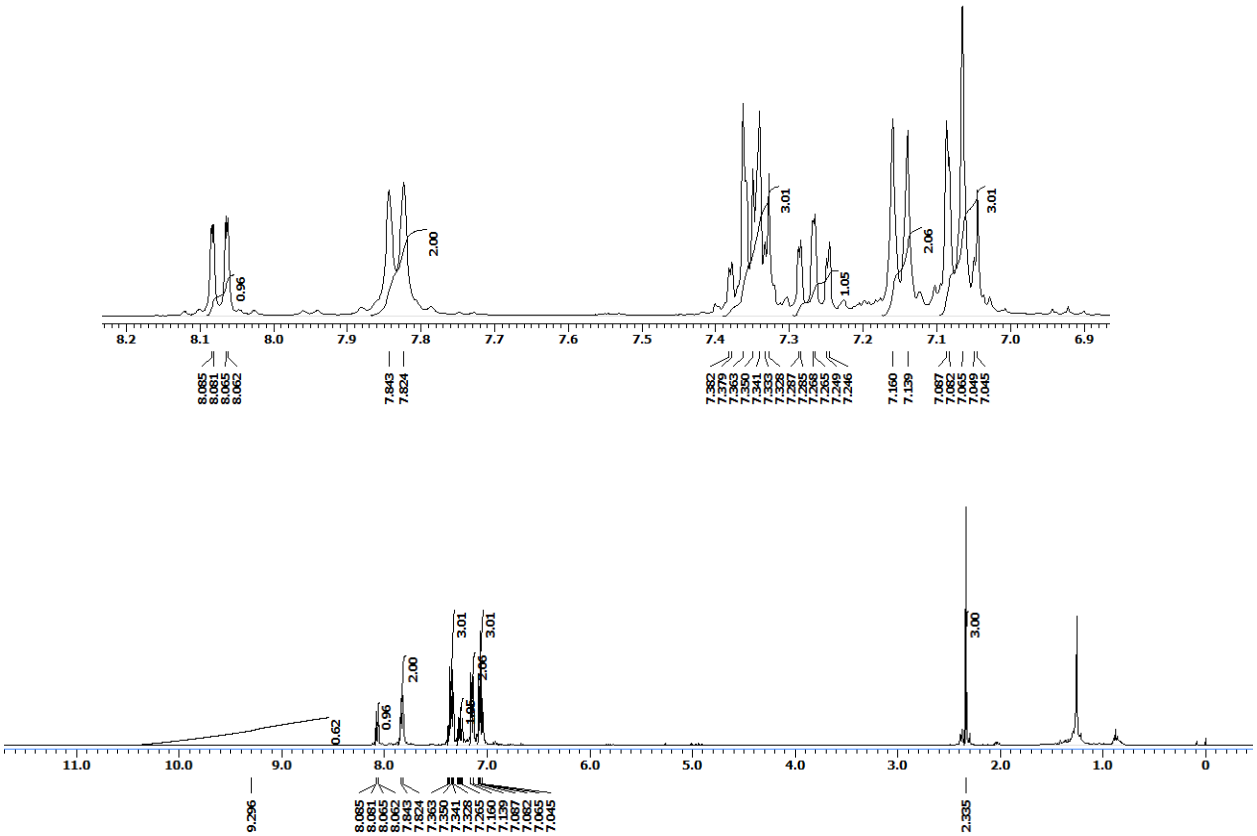
(Z)-N-((E)-4-((4-(tert-butyl)phenyl)iodomethylene)-4H-benzo[d][1,3]thiazin-2-yl)-4-methylbenzimidic acid (3m)



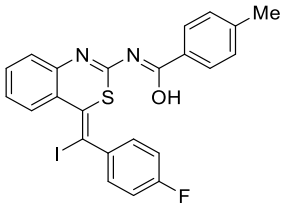
^{1}H NMR



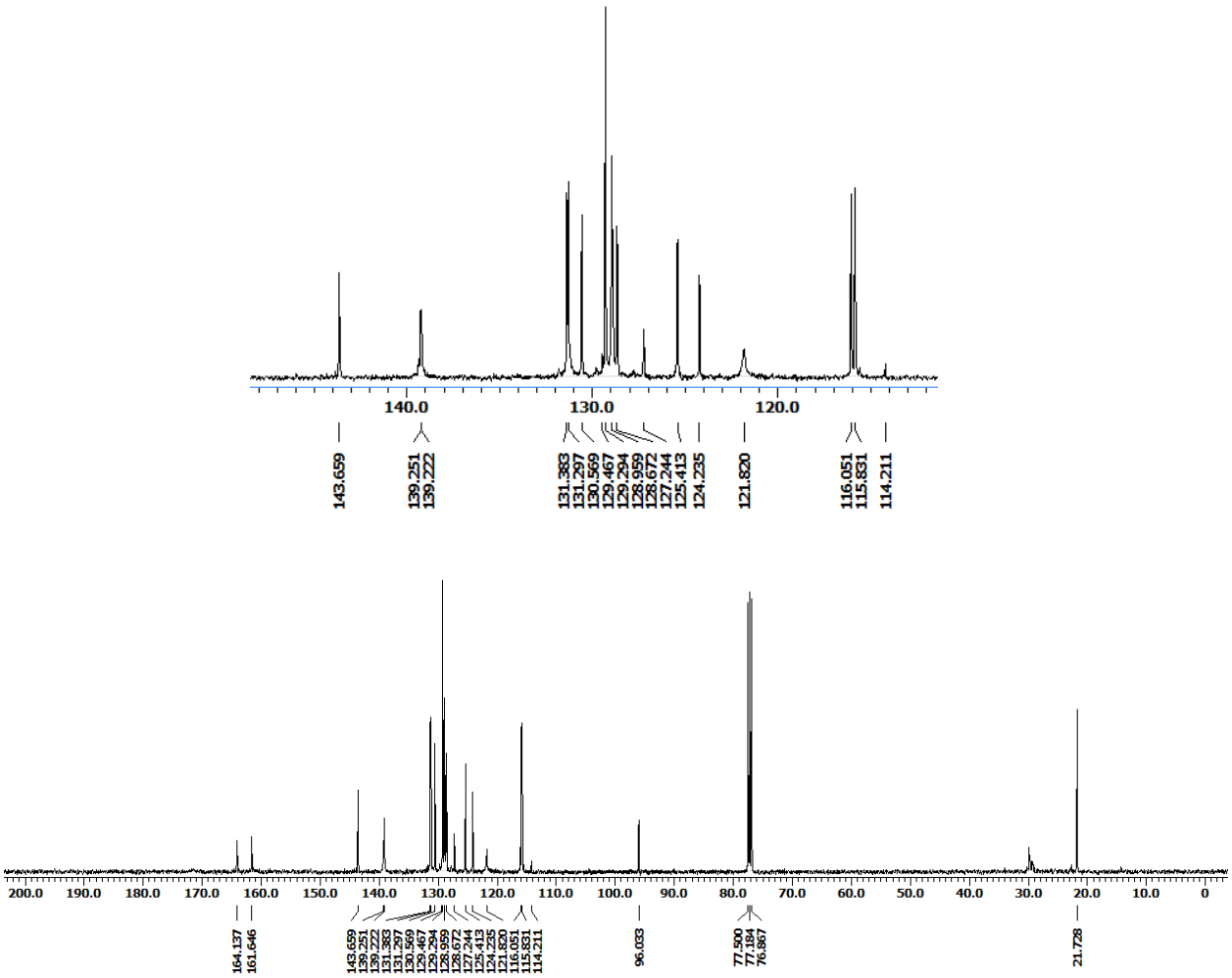
(Z)-N-((E)-4-((4-Fluorophenyl)iodomethylene)-4H-benzo[*d*][1,3]thiazin-2-yl)-4-methylbenzimidic acid (3n)



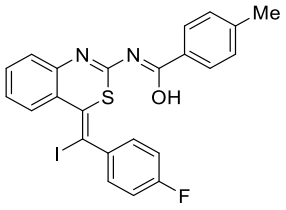
^{13}C NMR



(Z)-N-((E)-4-((4-Fluorophenyl)iodomethylene)-4*H*-benzo[d][1,3]thiazin-2-yl)-4-methylbenzimidic acid (3n)



HRMS



(Z)-N-((E)-4-((4-Fluorophenyl)iodomethylene)-4H-benzo[d][1,3]thiazin-2-yl)-4-methylbenzimidic acid (3n)

Qualitative Compound Report

Data File	KMS-618.d	**Sample Name**	KMS-618
Sample Type	Sample	**Position**	P1-A7
Instrument Name	Instrument 1	**User Name**	
Acq Method	Damo JK.m	**Acquired Time**	04-07-2018 11:28:22
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

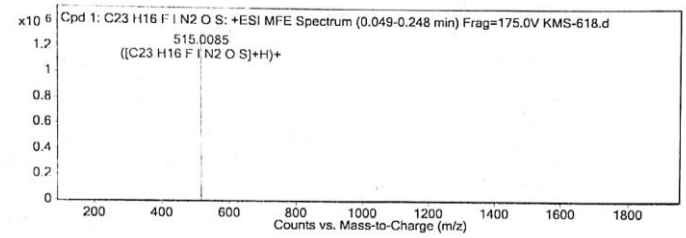
Sample Group **Info.**
Acquisition SW Version 6200 series TOF/6500 series Q-TOF B.05.01 (B5125.1)

Compound Table

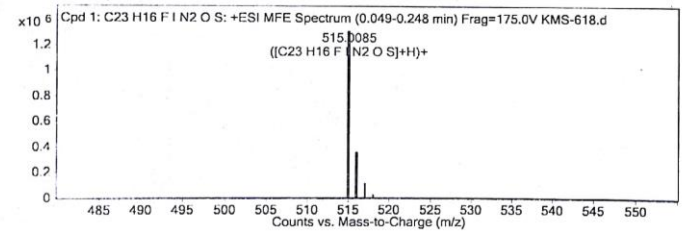
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 1: C23 H16 F I N2 O S	0.086	514.0015	C23 H16 F I N2 O S	C23 H16 F I N2 O S	-0.62	C23 H16 F I N2 O S

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: C23 H16 F I N2 O S	515.0085	0.086	Find by Molecular Feature	514.0015

MFE MS Spectrum



MFE MS Zoomed Spectrum

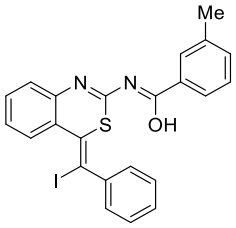


MS Spectrum Peak List

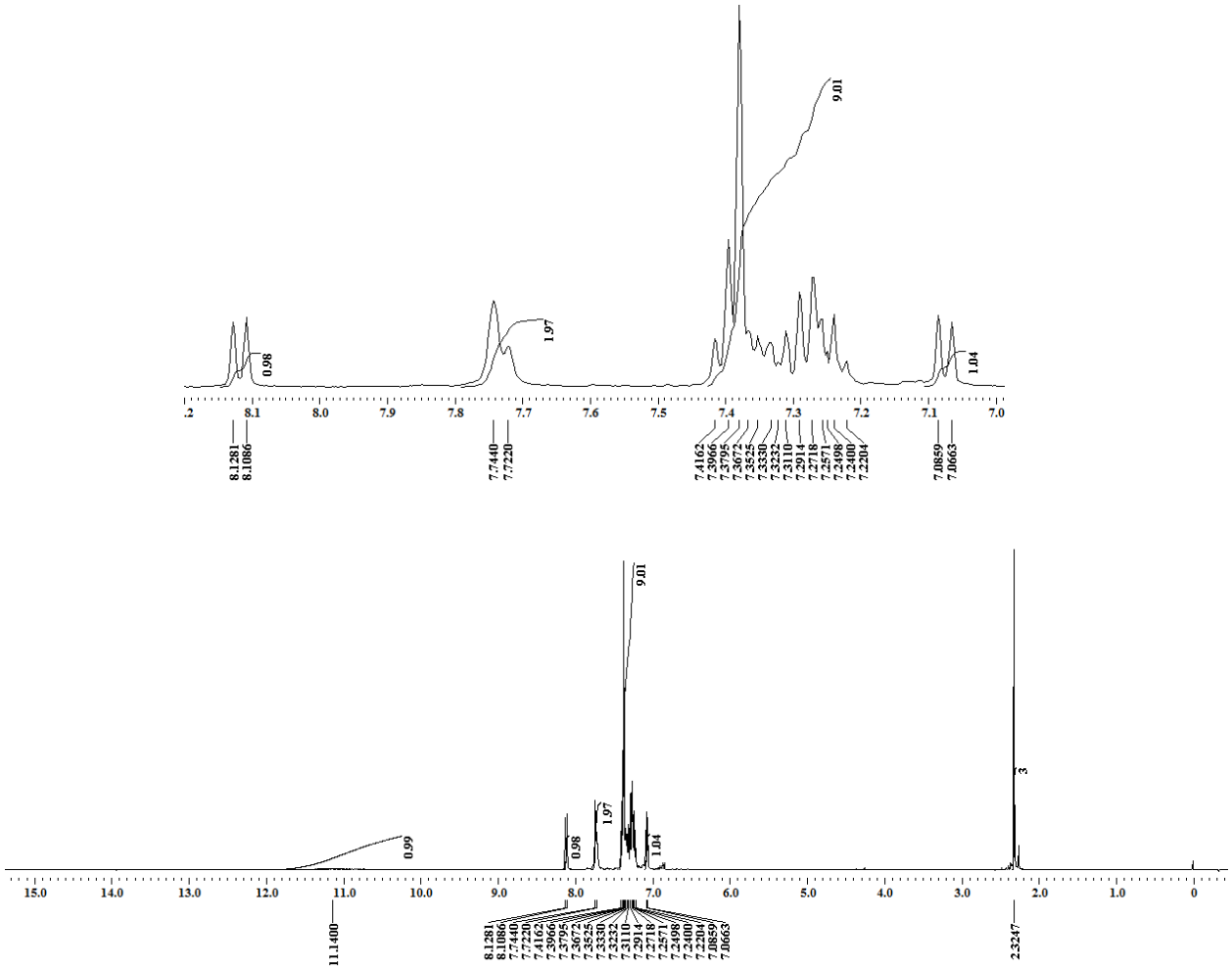
m/z	z	Abund	Formula	Ion
515.0085	1	1313651.75	C23 H16 F I N2 O S	(M+H)+
516.0117	1	347231.17	C23 H16 F I N2 O S	(M+H)+
517.0119	1	118802.53	C23 H16 F I N2 O S	(M+H)+
518.0144	1	17971.27	C23 H16 F I N2 O S	(M+H)+
519.0162	1	3263.72	C23 H16 F I N2 O S	(M+H)+
520.0234	1	963.95	C23 H16 F I N2 O S	(M+H)+

--- End Of Report ---

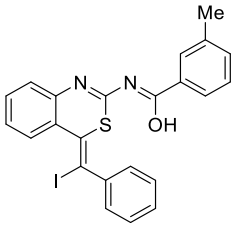
^{1}H NMR



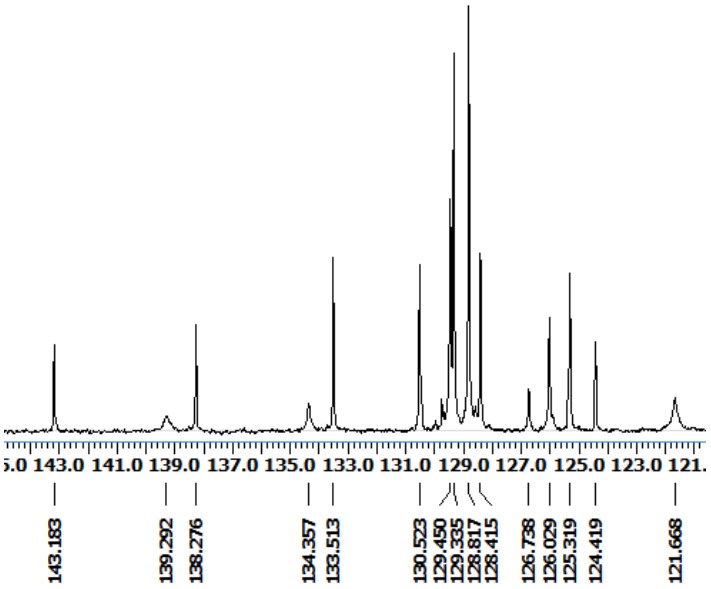
(Z)-N-((E)-4-(Iodo(phenyl)methylene)-4H-benzo[*d*][1,3]thiazin-2-yl)-3-methylbenzimidic acid (3o)

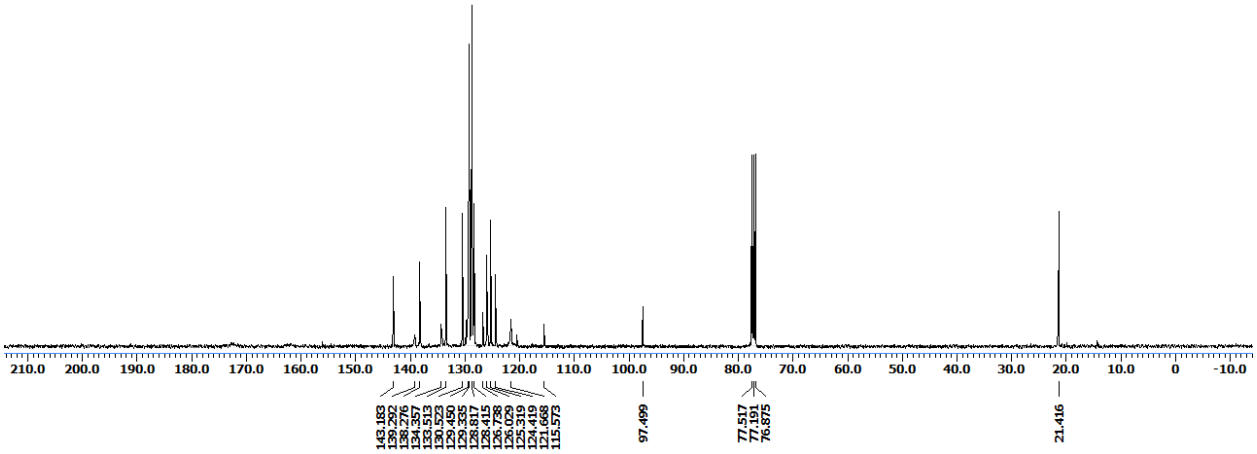


^{13}C NMR

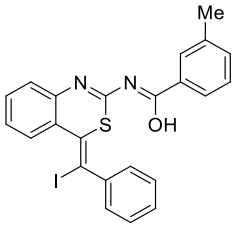


(Z)-N-((E)-4-(Iodo(phenyl)methylene)-4H-benzo[d][1,3]thiazin-2-yl)-3-methylbenzimidic acid (3o)

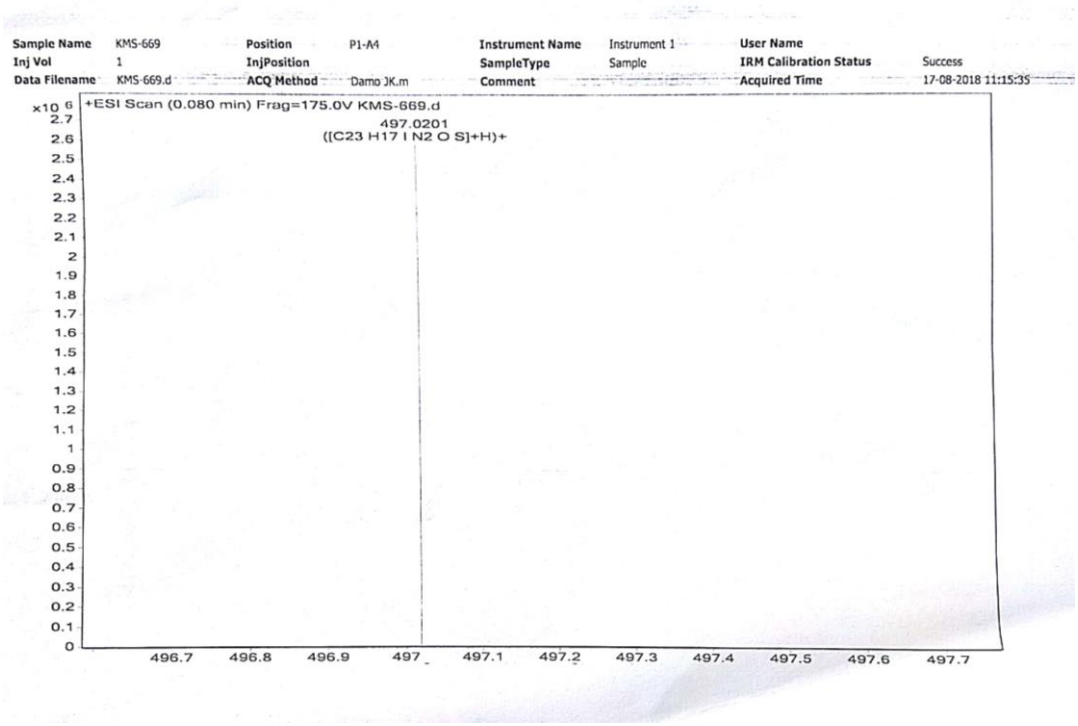




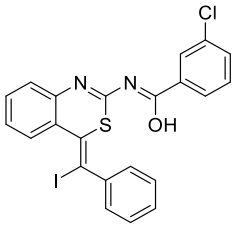
HRMS



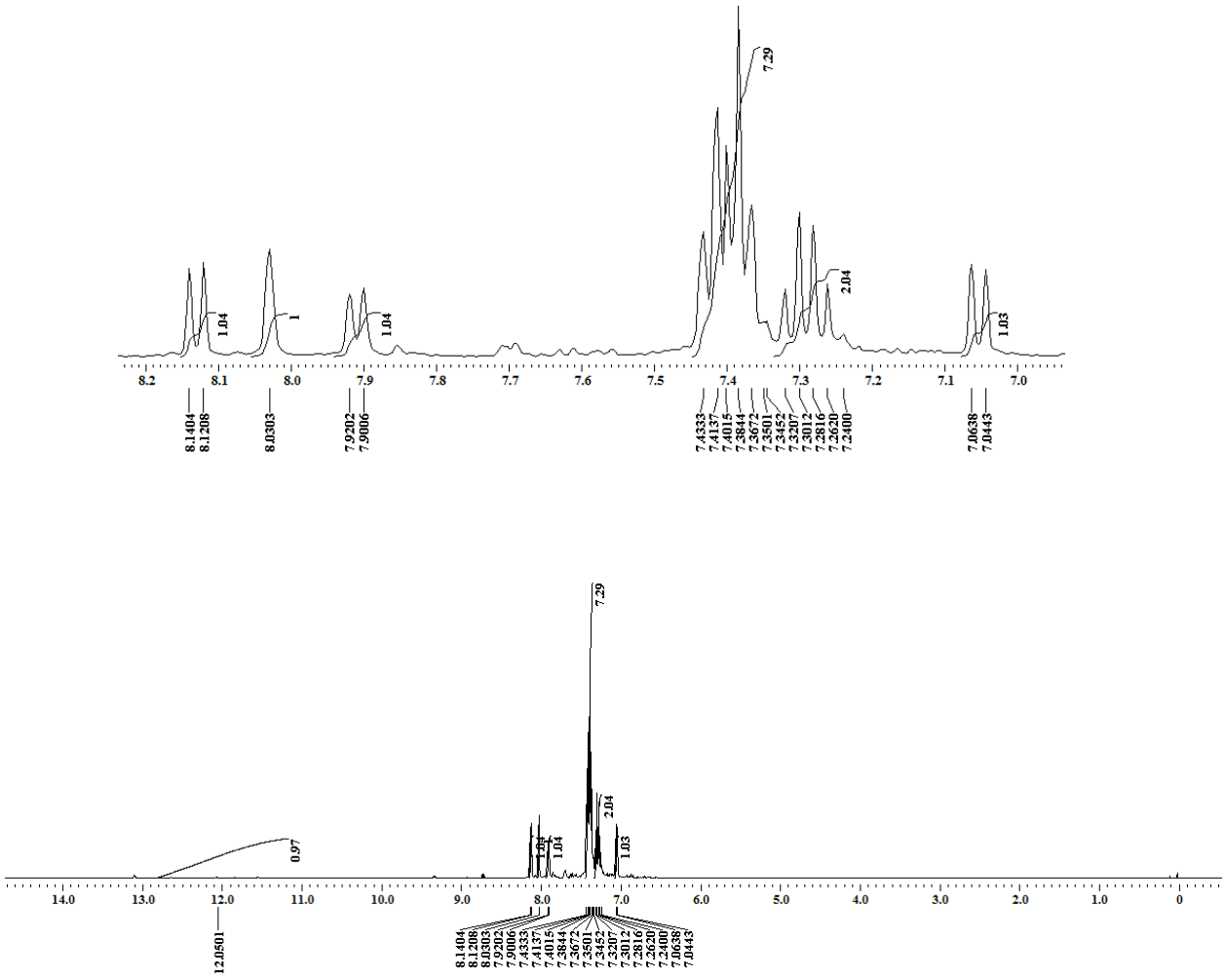
(Z)-N-((E)-4-(Iodo(phenyl)methylene)-4H-benzo[d][1,3]thiazin-2-yl)-3-methylbenzimidic acid (3o)



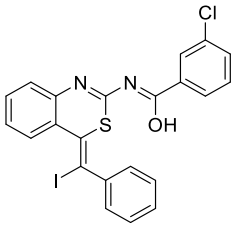
^{1}H NMR



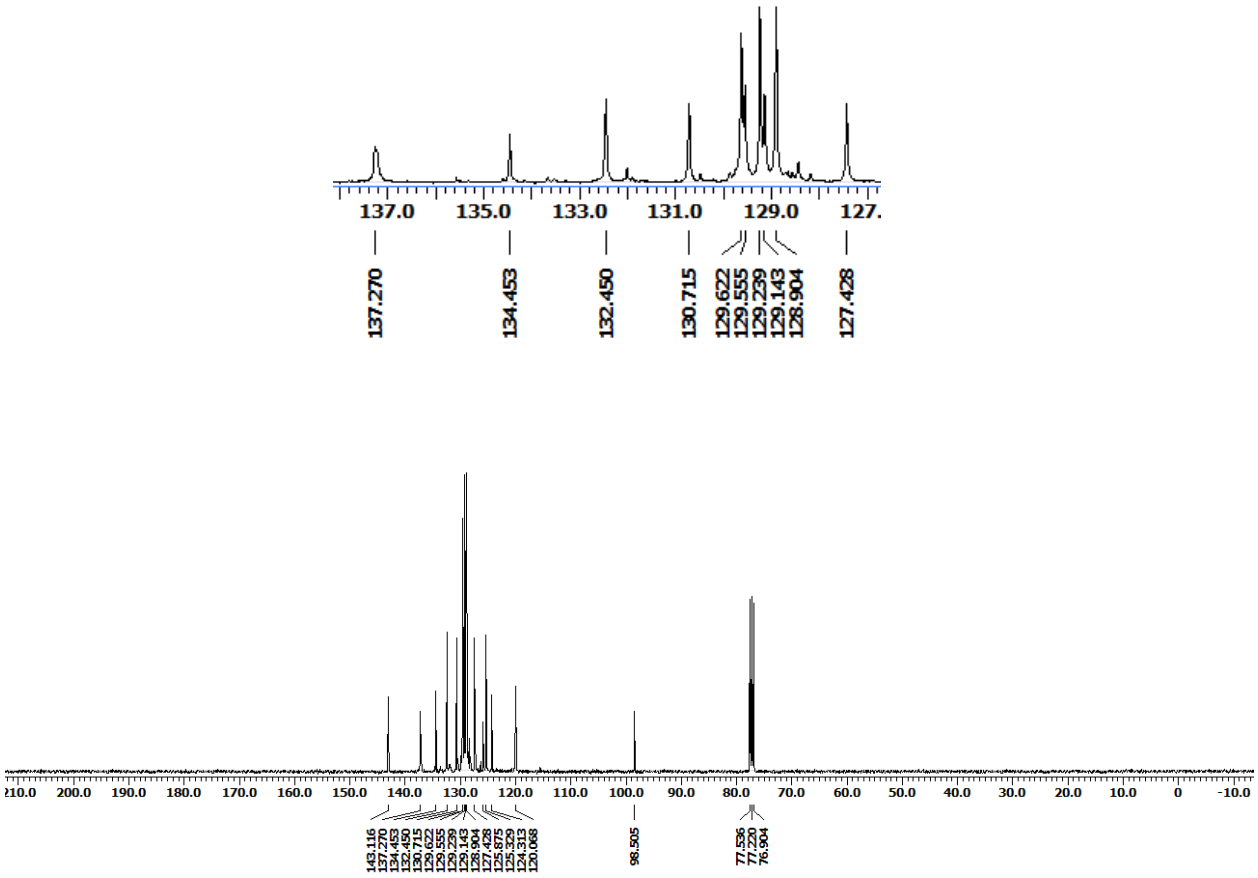
(Z)-3-Chloro-N-((E)-4-(iodo(phenyl)methylene)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (3p)



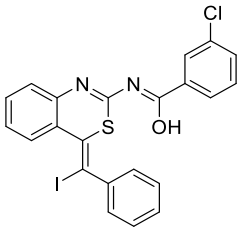
^{13}C NMR



(Z)-3-Chloro-N-((E)-4-(iodo(phenyl)methylene)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (3p)



HRMS



(Z)-3-Chloro-N-((E)-4-(iodo(phenyl)methylene)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (3p)

Qualitative Compound Report

Data File	KMS-670.d	**Sample Name**	KMS-670
Sample Type	Sample	**Position**	P1-B1
Instrument Name	Instrument 1	**User Name**	
Acq Method	Damo JK.m	**Acquired Time**	07-08-2018 10:55:12
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

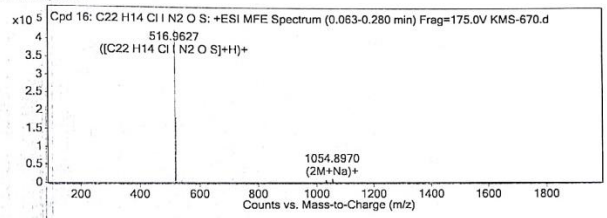
Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.1)

Compound Table

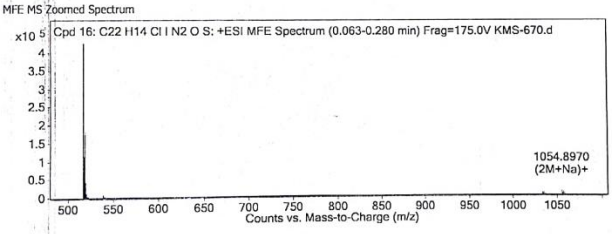
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 16: C22 H14 Cl I N2 O S	0.093	515.9557	C22 H14 Cl I N2 O S	C22 H14 Cl I N2 O S	0.67	C22 H14 Cl I N2 O S

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 16: C22 H14 Cl I N2 O S	516.9627	0.093	Find by Molecular Feature	515.9557

MFE MS Spectrum



MFE MS Zoomed Spectrum

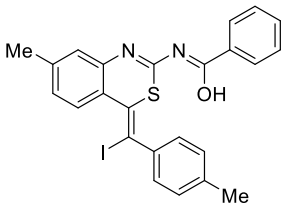


MS Spectrum Peak List

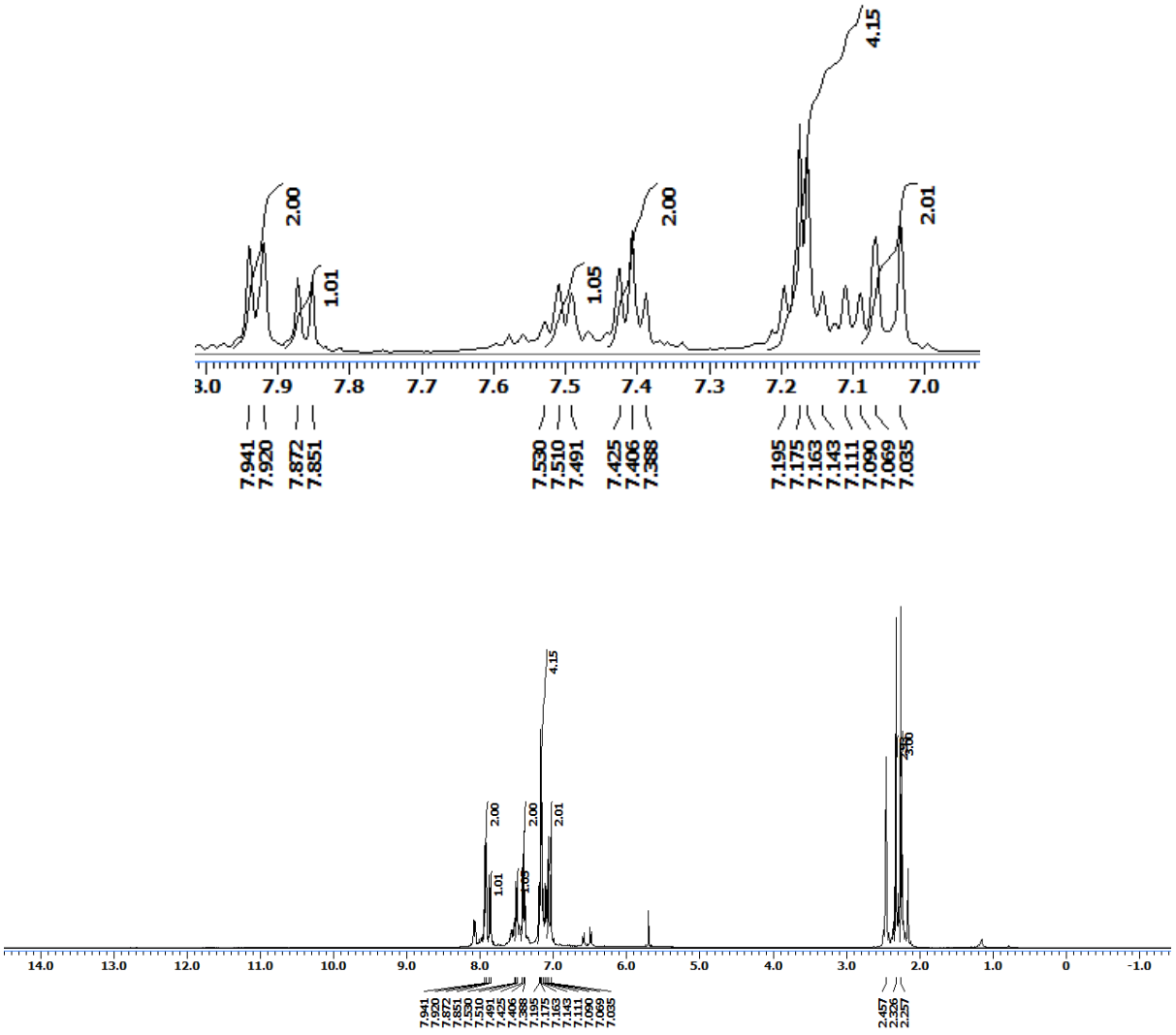
m/z	z	Abund	Formula	Ion
516.9627	1	427121.03	C22 H14 Cl I N2 O S	(M+H)+
517.9654	1	110056.21	C22 H14 Cl I N2 O S	(M+H)+
518.961	1	181640.4	C22 H14 Cl I N2 O S	(M+H)+
519.9635	1	40357.24	C22 H14 Cl I N2 O S	(M+H)+
520.9638	1	12932.19	C22 H14 Cl I N2 O S	(M+H)+
538.944	1	6406.47	C22 H14 Cl I N2 O S	(M+Na)+
1032.9168	1	6847.28		(2M+H)+
1034.9156	1	5854.63		(2M+H)+
1054.897	1	10694.32		(2M+Na)+
1056.8977	1	8806.92		(2M+Na)+

--- End Of Report ---

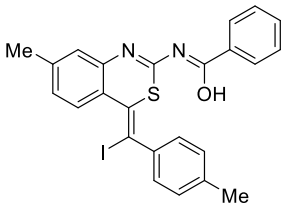
^{1}H NMR



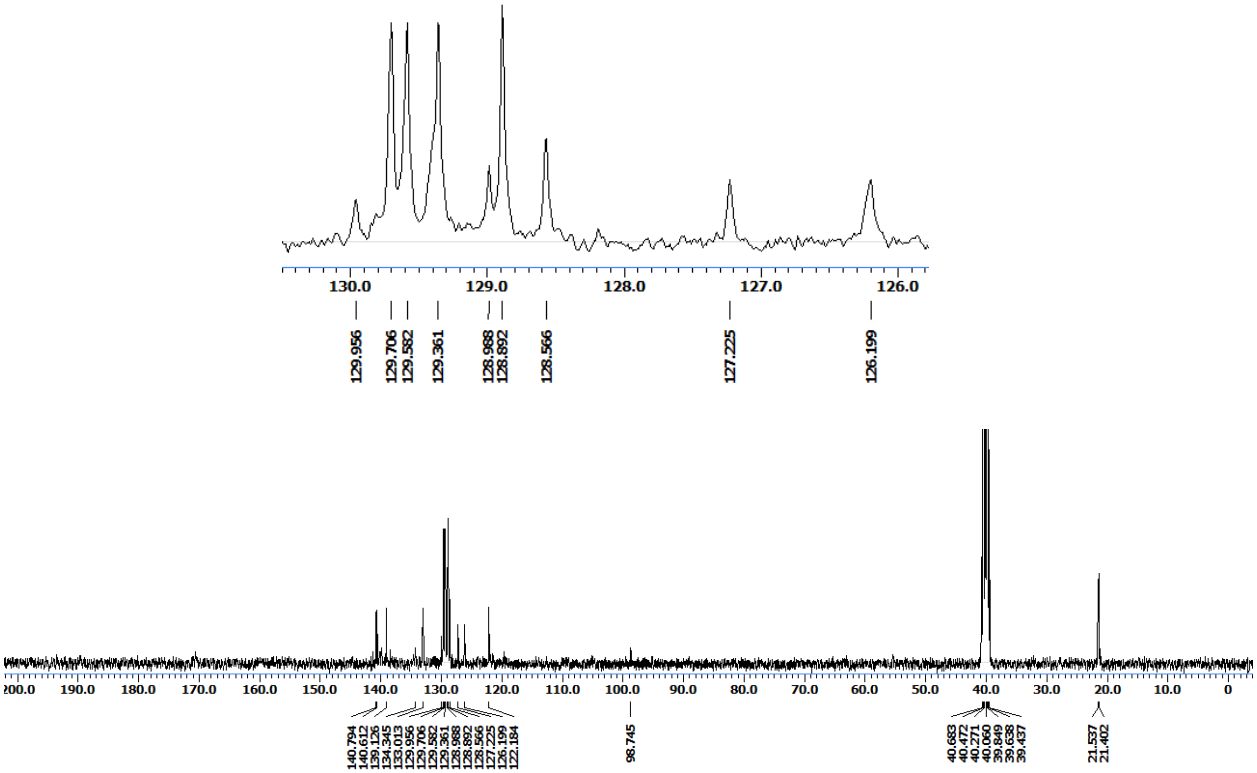
(Z)-N-((E)-4-(iodo(*p*-tolyl)methylene)-7-methyl-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (4a)



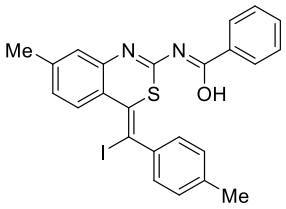
^{13}C NMR



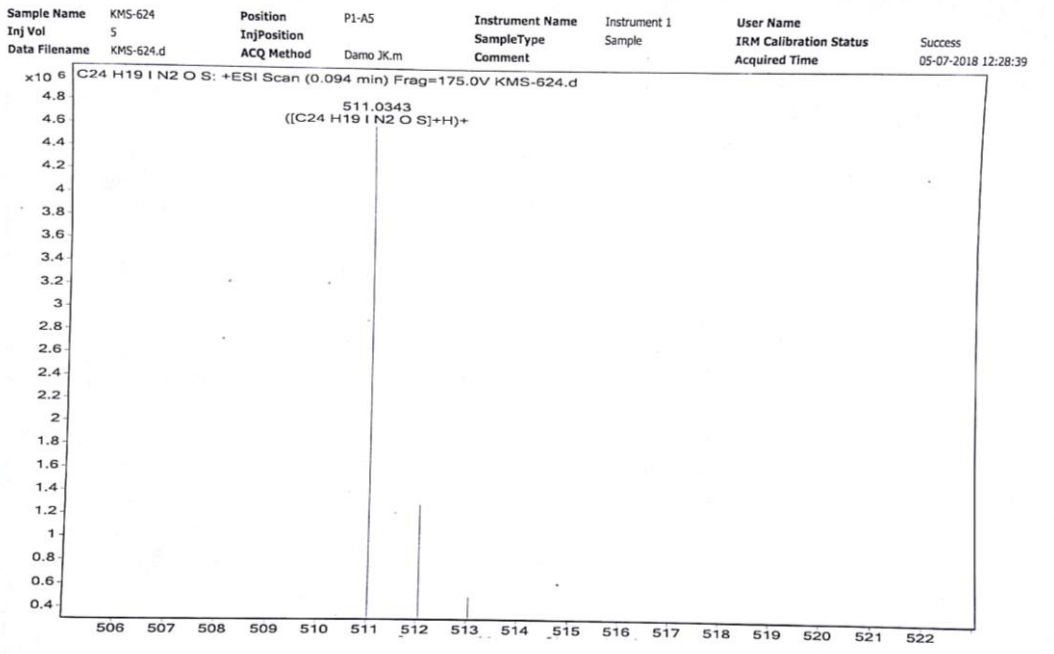
(Z)-N-((E)-4-(iodo(*p*-tolyl)methylene)-7-methyl-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (4a)



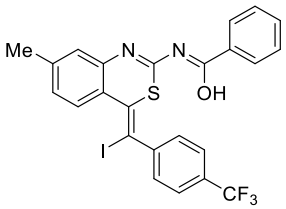
HRMS



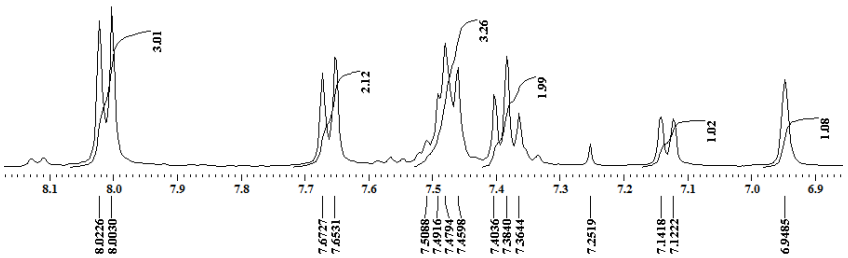
(Z)-N-((E)-4-(iodo(*p*-tolyl)methylene)-7-methyl-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (4a)

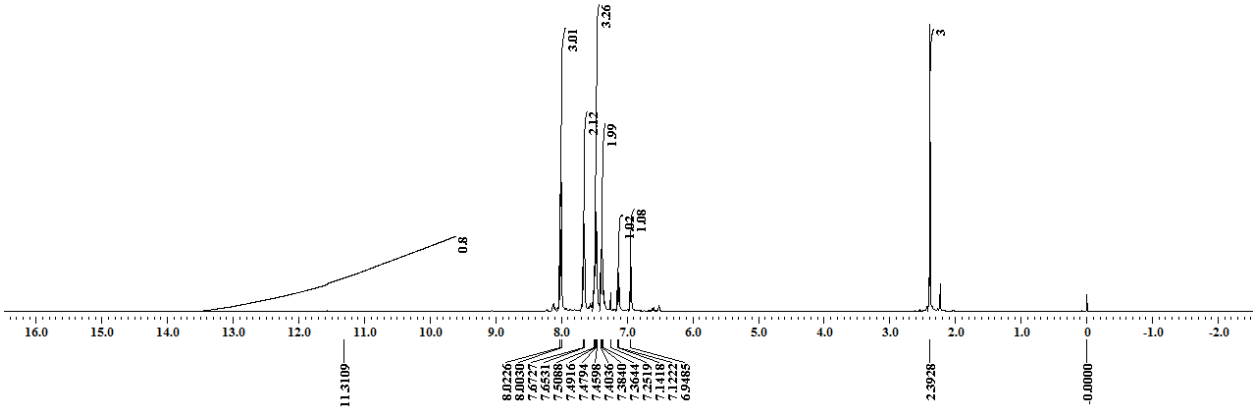


^{1}H NMR

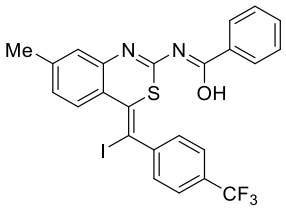


(Z)-N-((E)-4-(Iodo(4-(trifluoromethyl)phenyl)methylene)-7-methyl-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (4b)

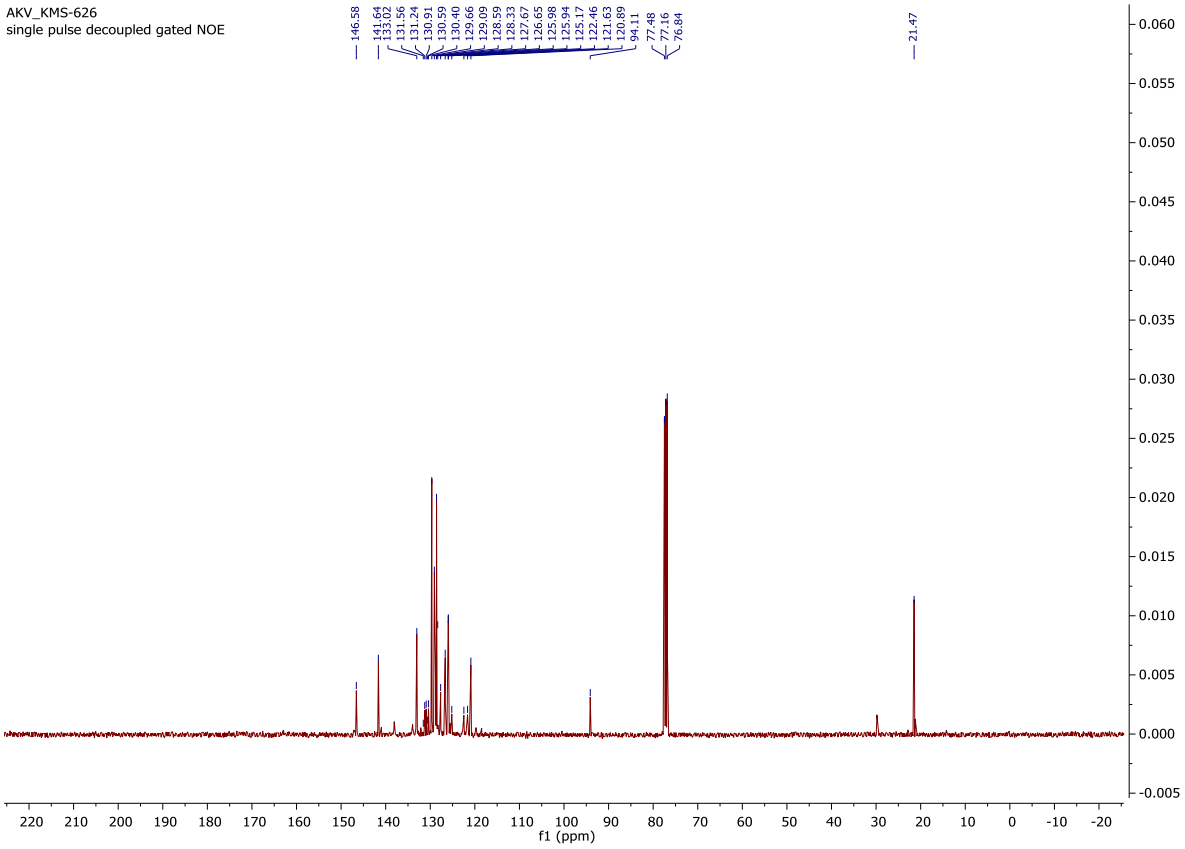




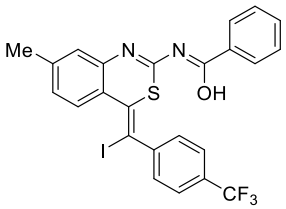
^{13}C NMR



(Z)-N-((E)-4-(Iodo(4-(trifluoromethyl)phenyl)methylene)-7-methyl-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (4b)



HRMS



(Z)-N-((E)-4-(Iodo(4-(trifluoromethyl)phenyl)methylene)-7-methyl-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (4b)

Qualitative Compound Report

Data File	KMS-626.d	**Sample Name**	KMS-626
Sample Type	Sample	**Position**	P1-A8
Instrument Name	Instrument 1	**User Name**	
Acq Method	Damo JK.m	**Acquired Time**	16-07-2018 12:41:57
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

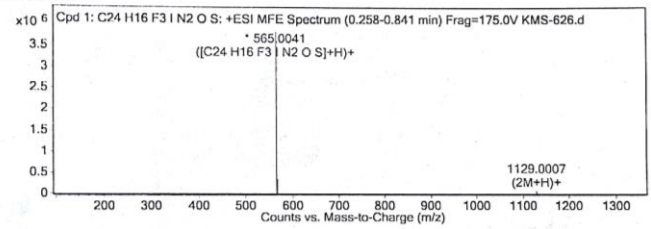
Sample Group **Info.**
Acquisition SW Version 6200 series TOF/6500 series Q-TOF B.05.01 (B5125.1)

Compound Table

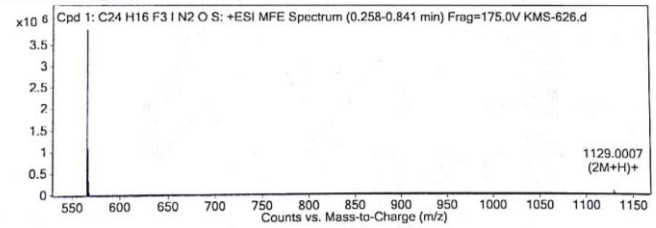
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 1: C24 H16 F3 I N2 O S	0.322	563.9972	C24 H16 F3 I N2 O S	C24 H16 F3 I N2 O S	1.52	C24 H16 F3 I N2 O S

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: C24 H16 F3 I N2 O S	565.0041	0.322	Find by Molecular Feature	563.9972

MFE MS Spectrum



MFE MS Zoomed Spectrum

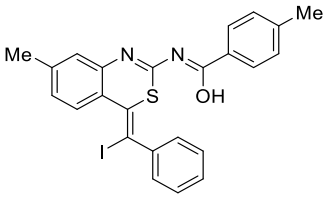


MS Spectrum Peak List

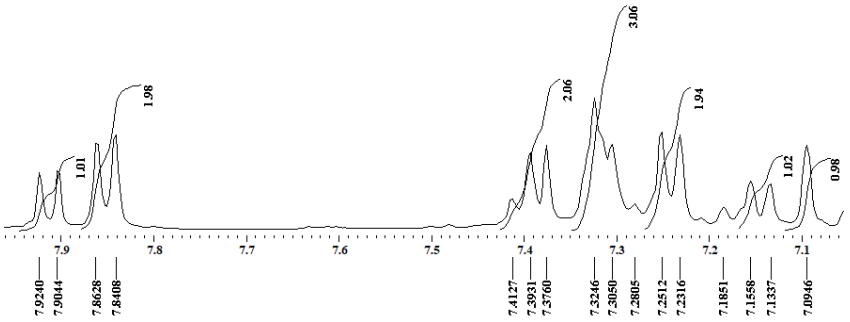
m/z	z	Abund	Formula	Ion
565.0041	1	3856949	C24 H16 F3 I N2 O S	(M+H)+
566.0076	1	1065826.02	C24 H16 F3 I N2 O S	(M+H)+
567.0075	1	347452.28	C24 H16 F3 I N2 O S	(M+H)+
568.0091	1	65159.12	C24 H16 F3 I N2 O S	(M+H)+
569.0119	1	9792.7	C24 H16 F3 I N2 O S	(M+H)+
586.988	1	5961.59	C24 H16 F3 I N2 O S	(M+Na)+
1129.0007	1	83425.64		(2M+H)+
1130.0028	1	47267.33		(2M+H)+
1131.004	1	20338.07		(2M+H)+
1132.0045	1	6722.34		(2M+H)+

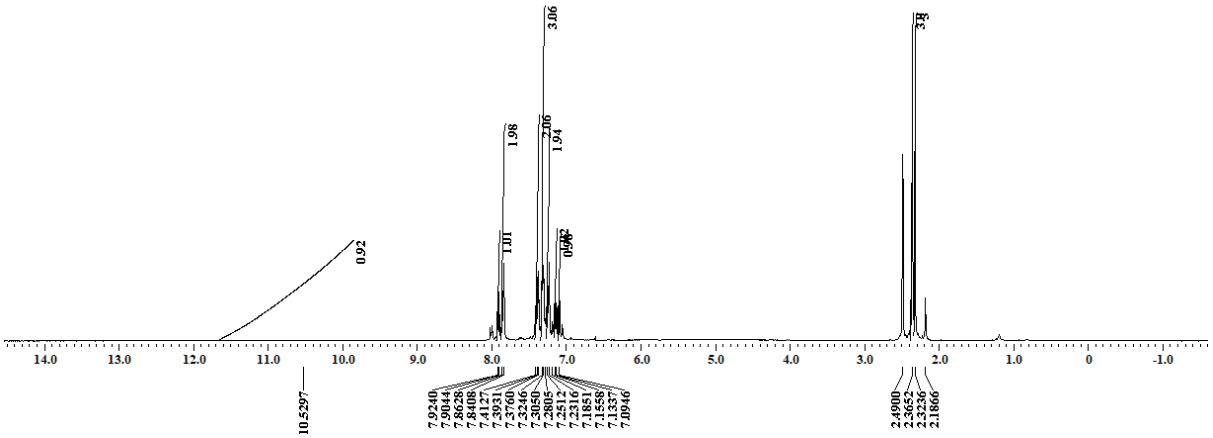
--- End Of Report ---

^{1}H NMR

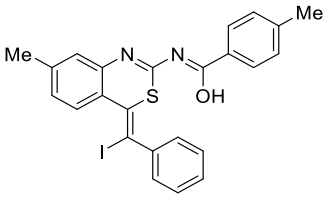


(Z)-N-((E)-4-(Iodo(phenyl)methylene)-7-methyl-4H-benzo[d][1,3]thiazin-2-yl)-4-methylbenzimidic acid (4c)

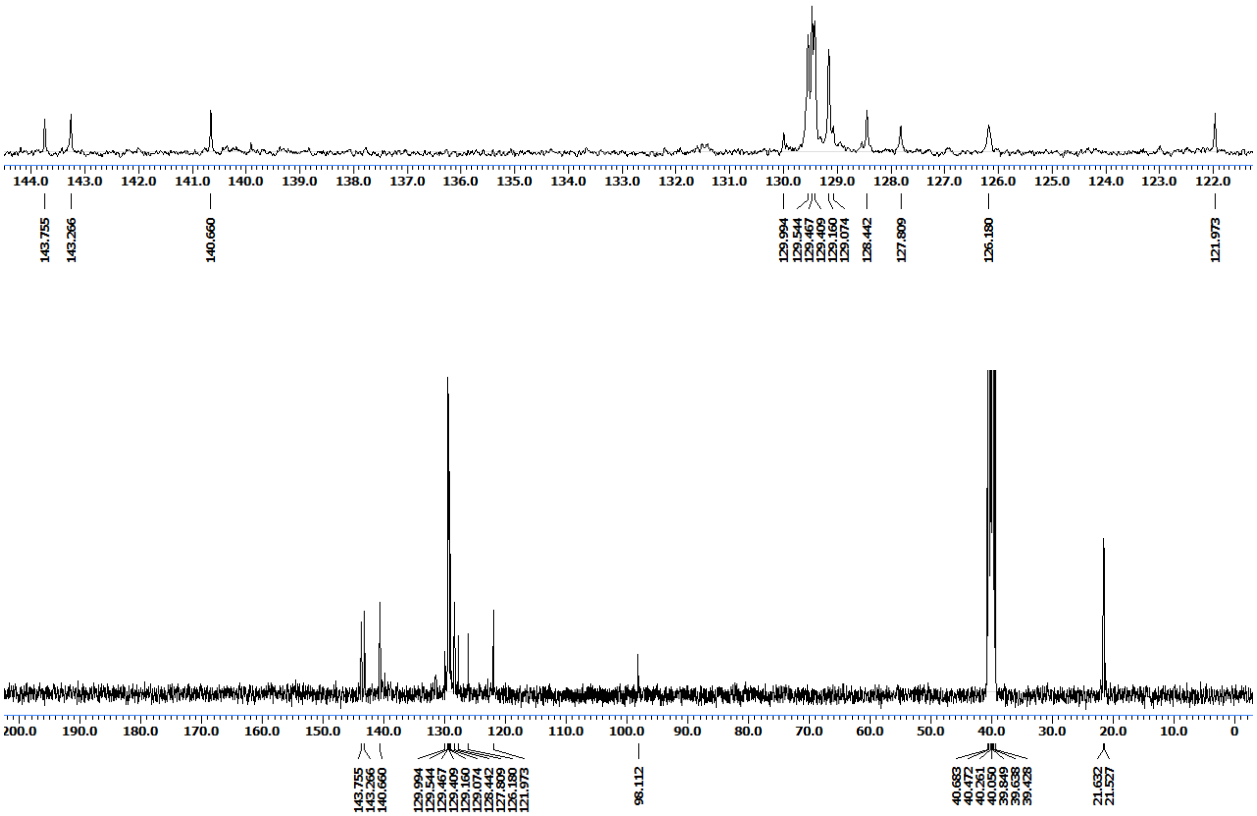




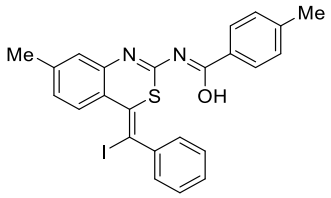
^{13}C NMR



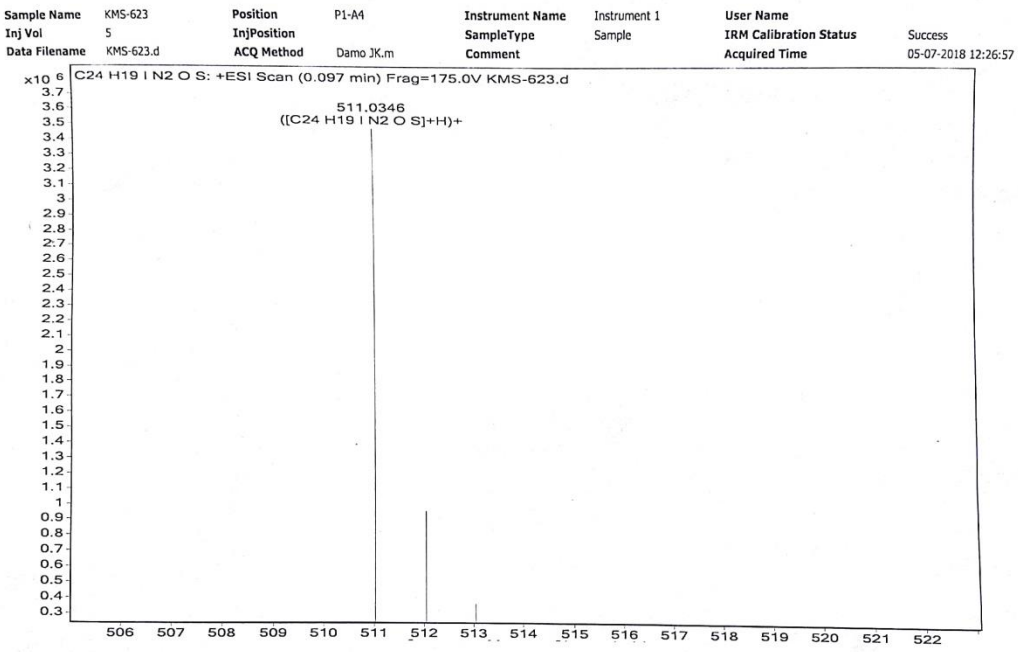
(Z)-N-((E)-4-(Iodo(phenyl)methylene)-7-methyl-4H-benzo[d][1,3]thiazin-2-yl)-4-methylbenzimidic acid (4c)



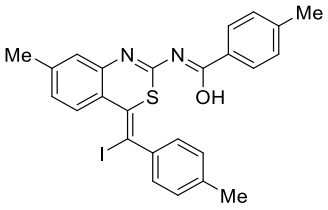
HRMS



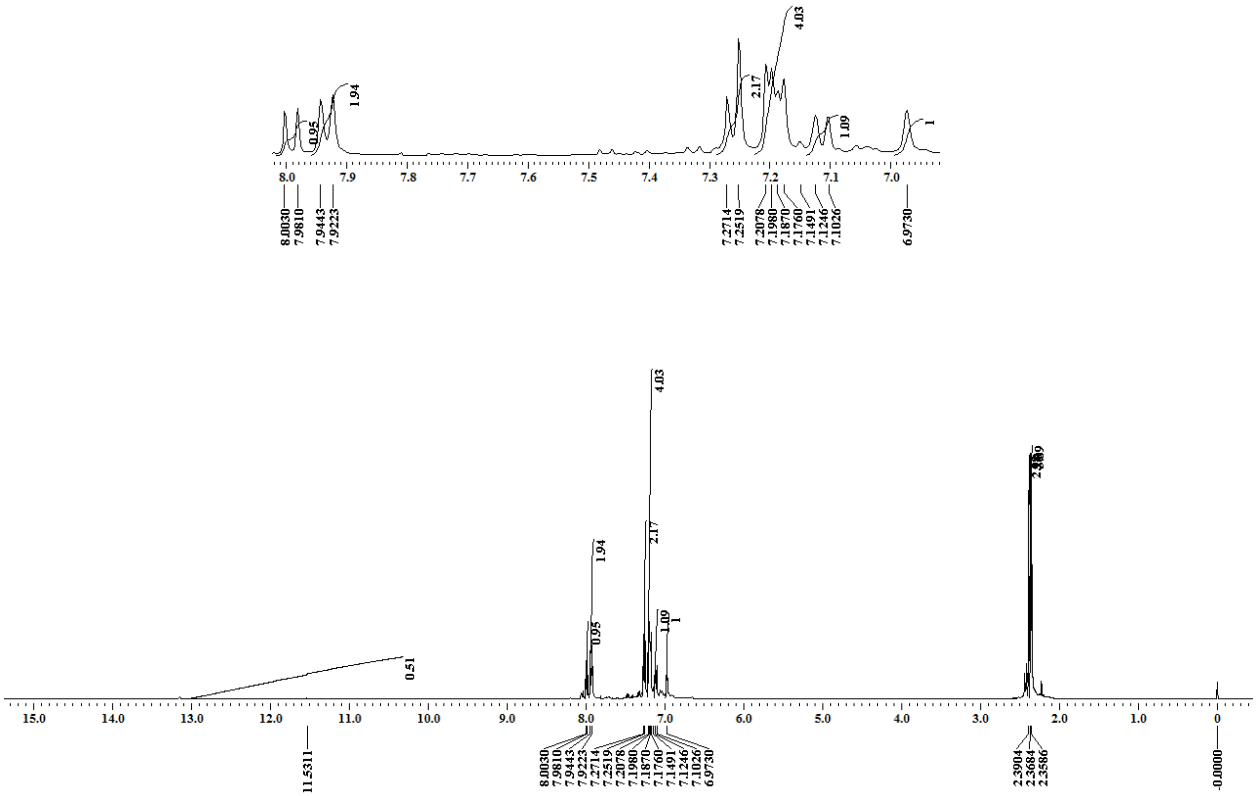
(Z)-N-((E)-4-(Iodo(phenyl)methylene)-7-methyl-4H-benzo[d][1,3]thiazin-2-yl)-4-methylbenzimidic acid (4c)



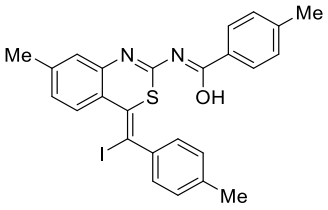
^{1}H NMR



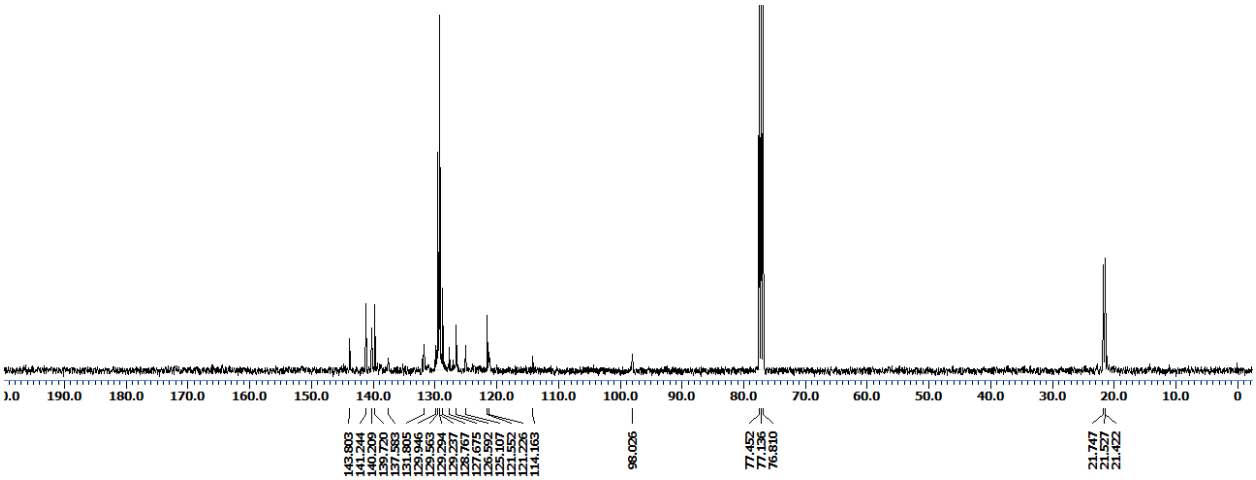
(Z)-N-((E)-4-(Iodo(p-tolyl)methylene)-7-methyl-4H-benzo[d][1,3]thiazin-2-yl)-4-methylbenzimidic acid (4d)



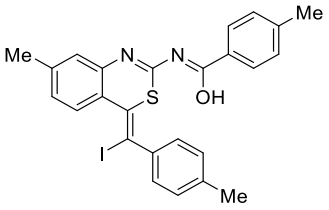
^{13}C NMR



(Z)-N-((E)-4-(Iodo(p-tolyl)methylene)-7-methyl-4H-benzo[d][1,3]thiazin-2-yl)-4-methylbenzimidic acid (4d)



HRMS



(Z)-N-((E)-4-(Iodo(p-tolyl)methylene)-7-methyl-4H-benzo[d][1,3]thiazin-2-yl)-4-methylbenzimidic acid (4d)

Qualitative Compound Report

Data File	KMS-625.d	**Sample Name**	KMS-625
Sample Type	Sample	**Position**	P1-A6
Instrument Name	Instrument 1	**User Name**	
Acq Method	Damo JK.m	**Acquired Time**	04-07-2018 11:26:42
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

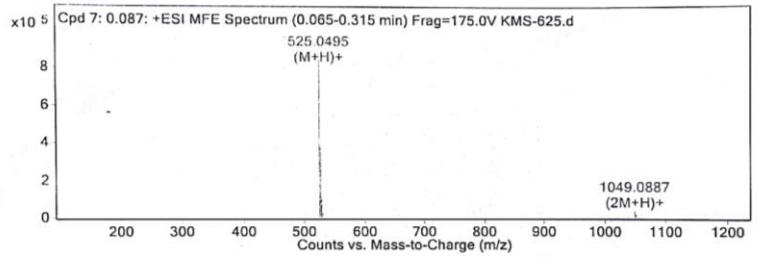
Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.1)

Compound Table

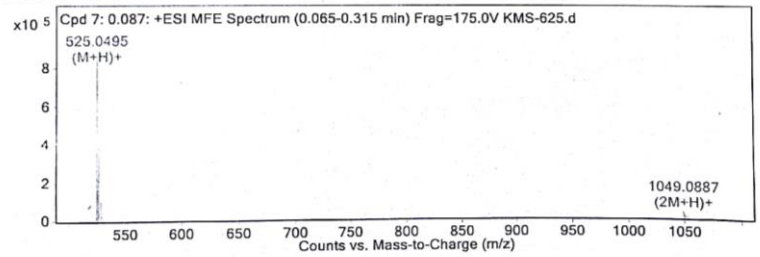
Compound Label	RT	Mass	MFG Formula
Cpd 7: 0.087	0.087	524.0421	<none>

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 7: 0.087	525.0495	0.087	Find by Molecular Feature	524.0421

MFE MS Spectrum



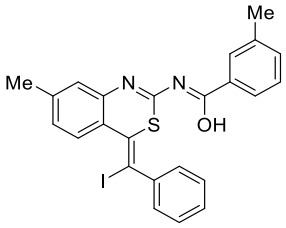
MFE MS Zoomed Spectrum



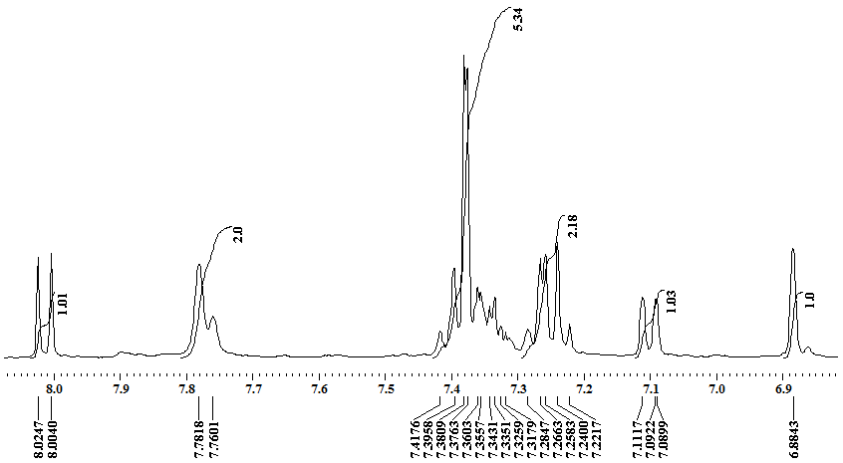
MS Spectrum Peak List

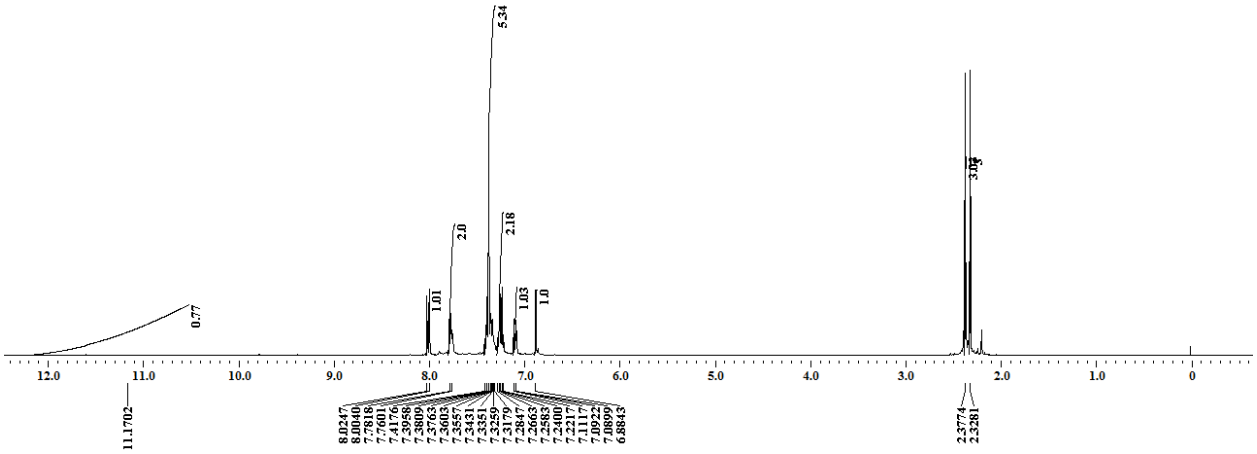
m/z	z	Abund	Ion
525.0495	1	847157.63	(M+H)+
526.0521	1	244738.9	(M+H)+
527.0632	1	384885.61	(M+H)+
528.0667	1	99465.73	(M+H)+
529.0652	1	26091.31	(M+H)+
530.0661	1	5565.09	(M+H)+

^{1}H NMR

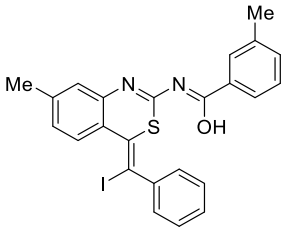


(Z)-N-((E)-4-(Iodo(phenyl)methylene)-7-methyl-4H-benzo[d][1,3]thiazin-2-yl)-3-methylbenzimidic acid (4e)

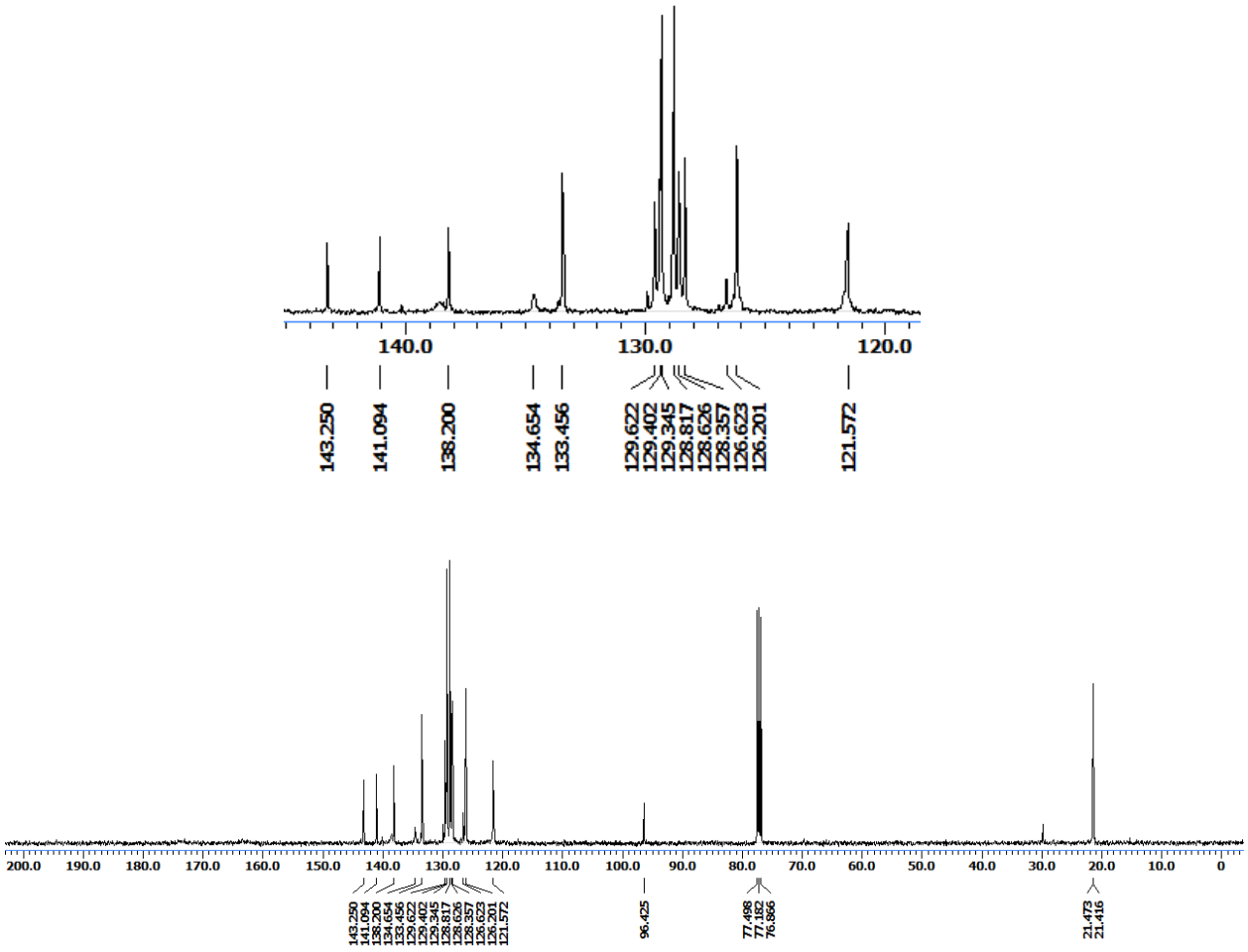




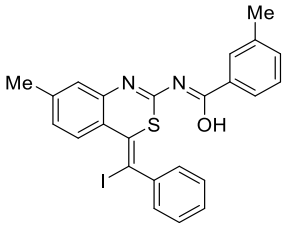
^{13}C NMR



(Z)-N-((E)-4-(Iodo(phenyl)methylene)-7-methyl-4H-benzo[d][1,3]thiazin-2-yl)-3-methylbenzimidic acid (4e)



HRMS



(Z)-N-((E)-4-(Iodo(phenyl)methylene)-7-methyl-4H-benzo[d][1,3]thiazin-2-yl)-3-methylbenzimidic acid (4e)

Qualitative Compound Report

Data File	KMS-671.d	Sample Name	KMS-671
Sample Type	Sample	Position	P1-B2
Instrument Name	Instrument 1	User Name	
Acq Method	Damo JK.m	Acquired Time	07-08-2018 10:56:54
IRM Calibration Status	Success	DA Method	Default.m
Comment			

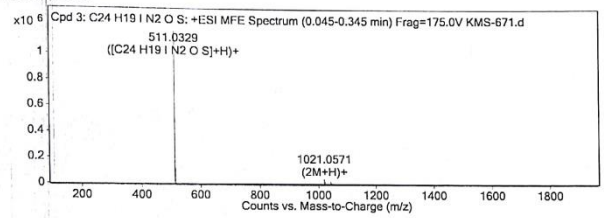
Sample Group — Info.
Acquisition SW Version: 6200 series TOF/6500 series Q-TOF B.05.01 (B5125.1)

Compound Table

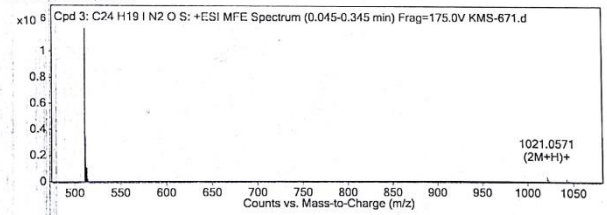
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 3: C24 H19 I N2 O S	0.089	510.0259	C24 H19 I N2 O S	C24 H19 I N2 O S	0.68	C24 H19 I N2 O S

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 3: C24 H19 I N2 O S	511.0329	0.089	Find by Molecular Feature	510.0259

MFE MS Spectrum



MFE MS Zoomed Spectrum

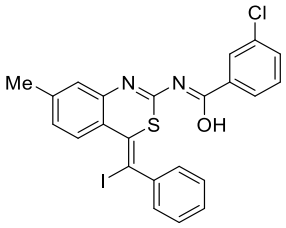


MS Spectrum Peak List

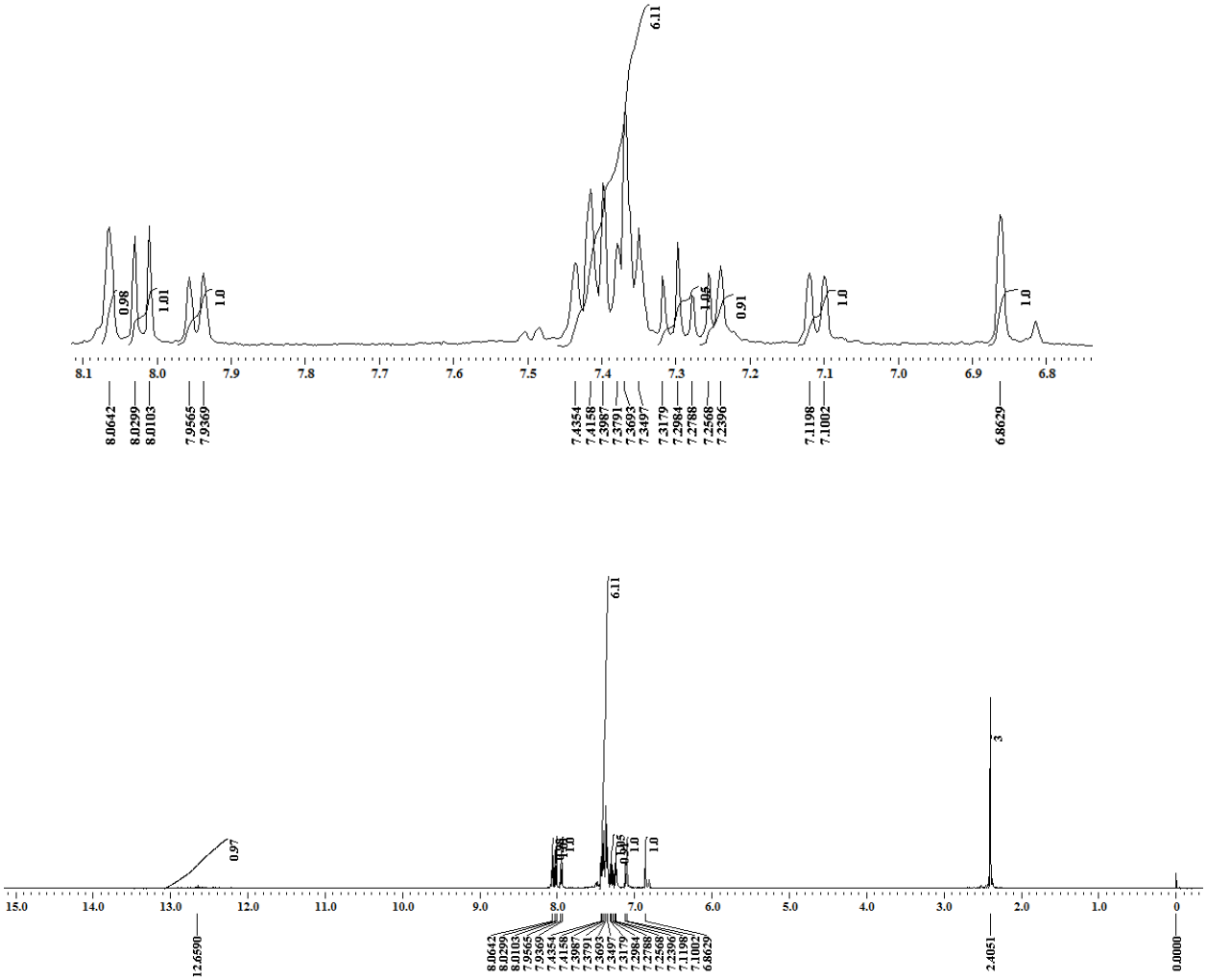
m/z	z	Abund	Formula	Ion
511.0329	1	1173545.88	C24 H19 I N2 O S	(M+H)+
512.036	1	356206.32	C24 H19 I N2 O S	(M+H)+
513.0368	1	113198.34	C24 H19 I N2 O S	(M+H)+
514.0386	1	22879.88	C24 H19 I N2 O S	(M+H)+
515.0421	1	4963.64	C24 H19 I N2 O S	(M+H)+
1021.0571	1	34360.81		(2M+H)+
1022.0603	1	20543.98		(2M+H)+
1023.0599	1	9863.86		(2M+H)+
1043.0388	1	16163.33		(2M+Na)+
1044.0427	1	8797.3		(2M+Na)+

--- End Of Report ---

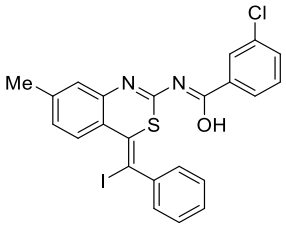
^{1}H NMR



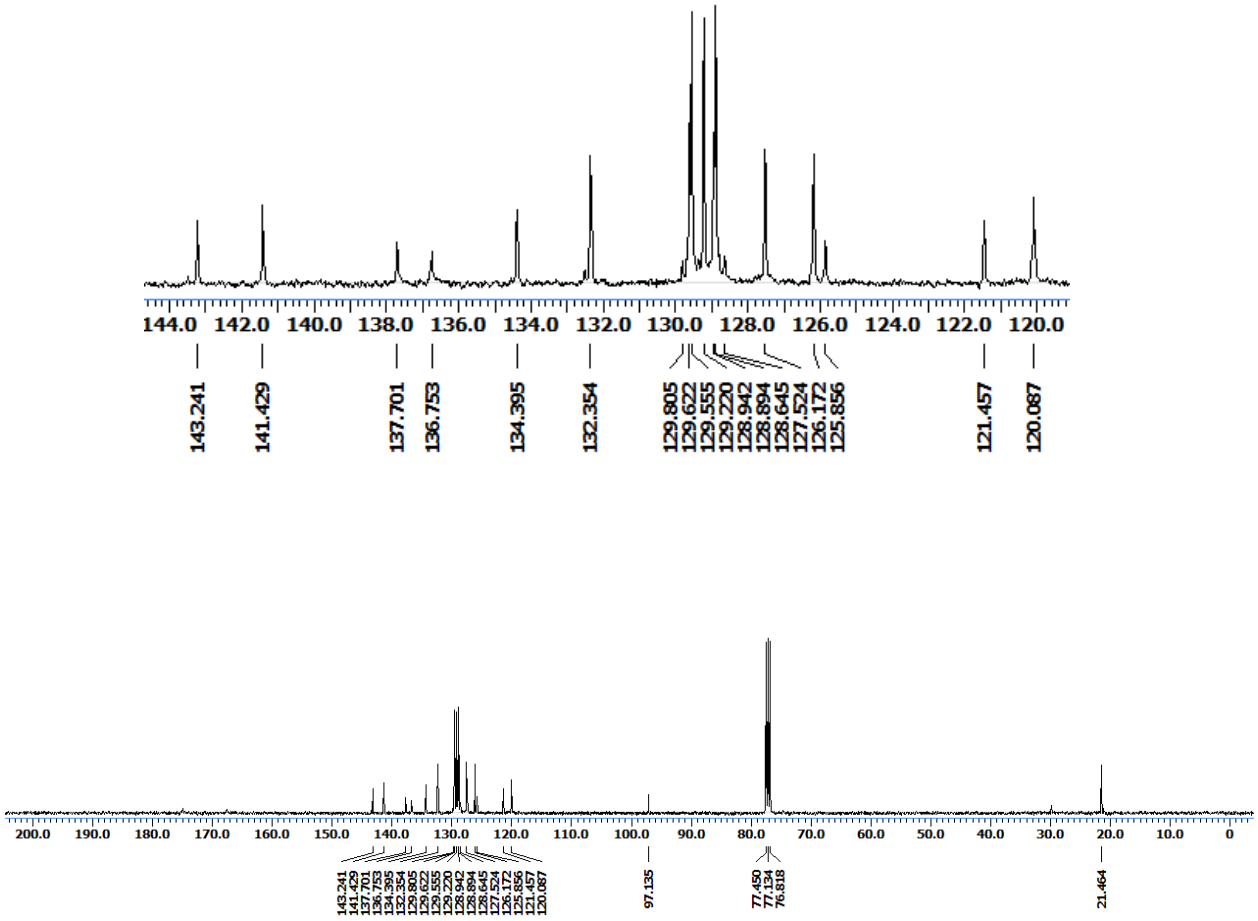
(Z)-3-Chloro-N-((E)-4-(iodo(phenyl)methylene)-7-methyl-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (4f)



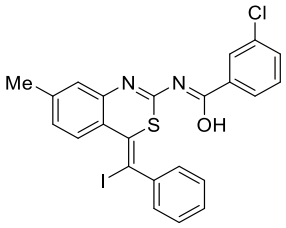
^{13}C NMR



(Z)-3-Chloro-N-((E)-4-(iodo(phenyl)methylene)-7-methyl-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (4f)



HRMS



(Z)-3-Chloro-N-((E)-4-(iodo(phenyl)methylene)-7-methyl-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (4f)

Qualitative Compound Report

Data File	KMS-672.d	**Sample Name**	KMS-672
Sample Type	Sample	**Position**	P1-B3
Instrument Name	Instrument 1	**User Name**	
Acq Method	Damo JK.m	**Acquired Time**	07-08-2018 10:58:35
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

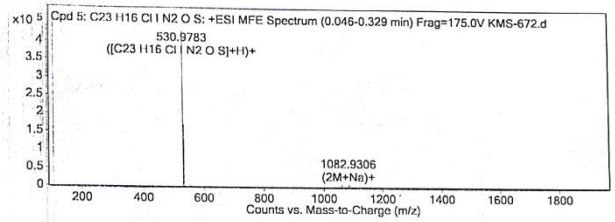
Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.1)

Compound Table

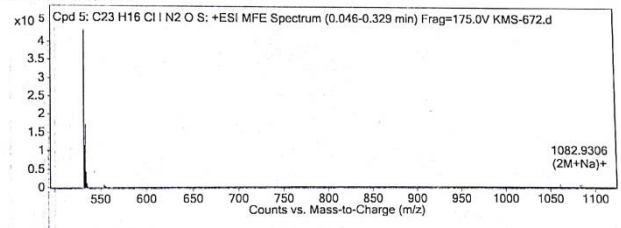
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 5: C23 H16 Cl I N2 O S	0.088	529.9713	C23 H16 Cl I N2 O S	C23 H16 Cl I N2 O S	0.6	C23 H16 Cl I N2 O S

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 5: C23 H16 Cl I N2 O S	530.9783	0.088	Find by Molecular Feature	529.9713

MFE MS Spectrum



MFE MS Zoomed Spectrum

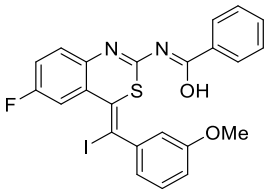


MS Spectrum Peak List

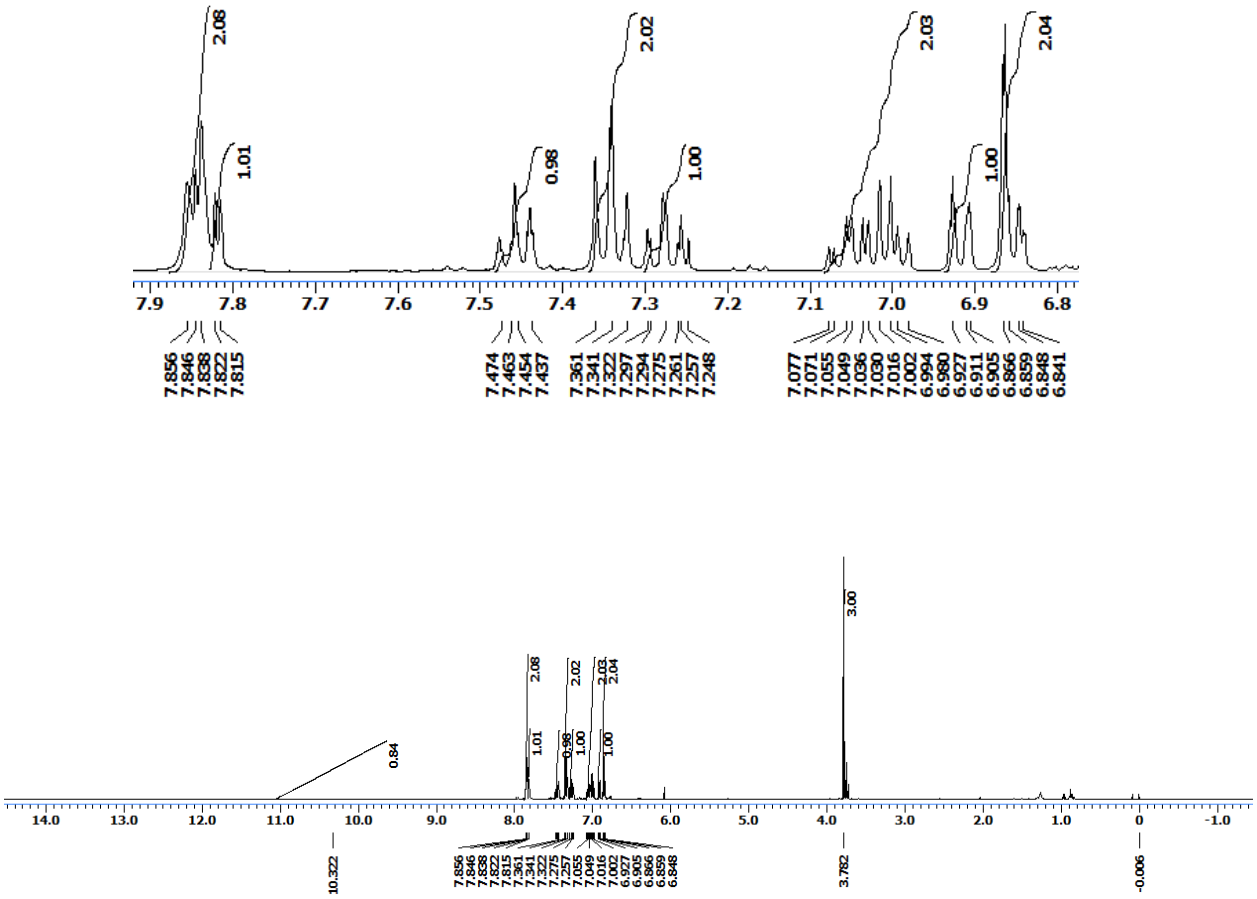
m/z	z	Abund	Formula	Ion
530.9783	1	433144.94	C23 H16 Cl I N2 O S	(M+H)+
531.9812	1	110834.56	C23 H16 Cl I N2 O S	(M+H)+
532.9771	1	171098.8	C23 H16 Cl I N2 O S	(M+H)+
533.979	1	39797.75	C23 H16 Cl I N2 O S	(M+H)+
534.9795	1	12264.52	C23 H16 Cl I N2 O S	(M+H)+
552.9597	1	6489.45	C23 H16 Cl I N2 O S	(M+Na)+
1060.9473	1	5974.71		(2M+H)+
1082.9306	1	7186.43		(2M+Na)+
1083.9331	1	3765.09		(2M+Na)+
1084.9292	1	5967.58		(2M+Na)+

--- End Of Report ---

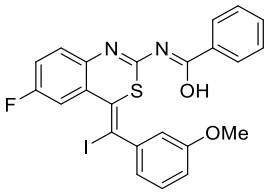
^{1}H NMR



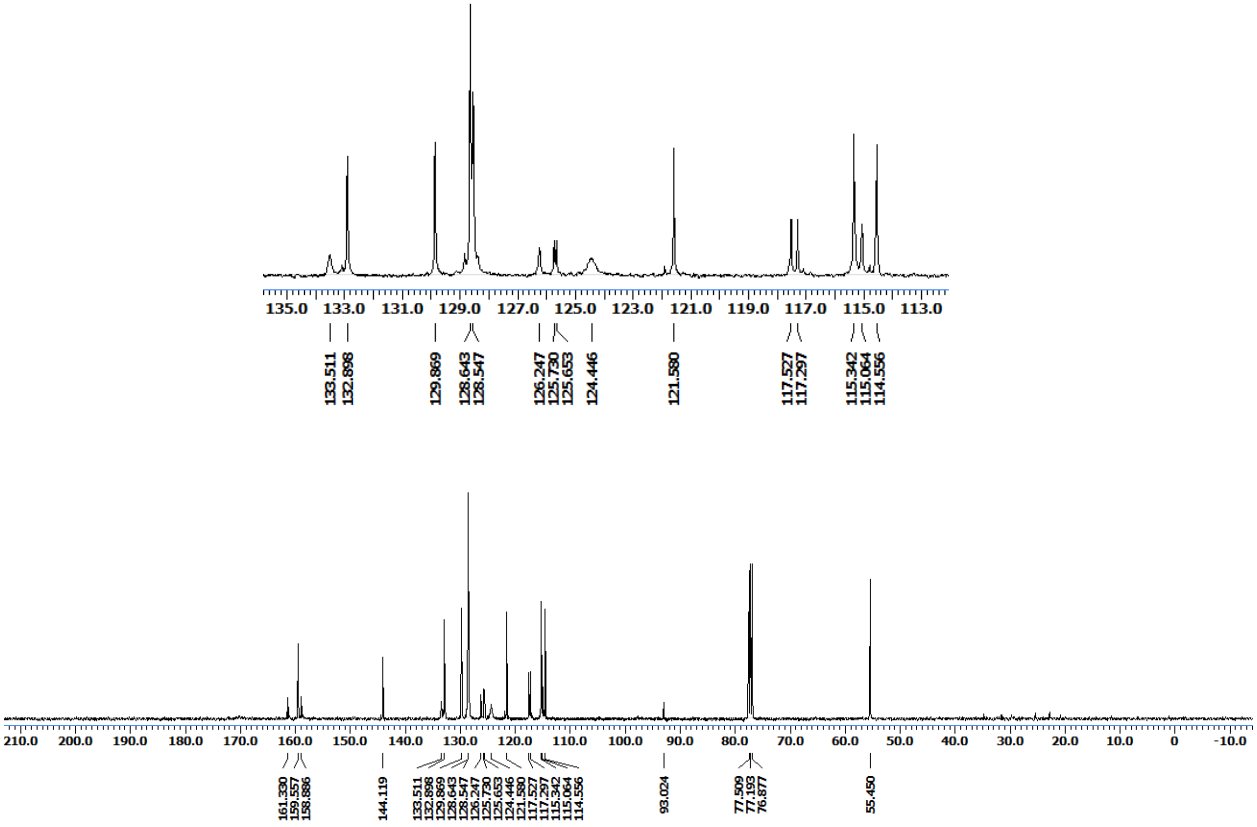
(Z)-N-((E)-6-fluoro-4-(iodo(3-methoxyphenyl)methylene)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (4g)



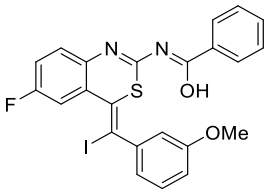
^{13}C NMR



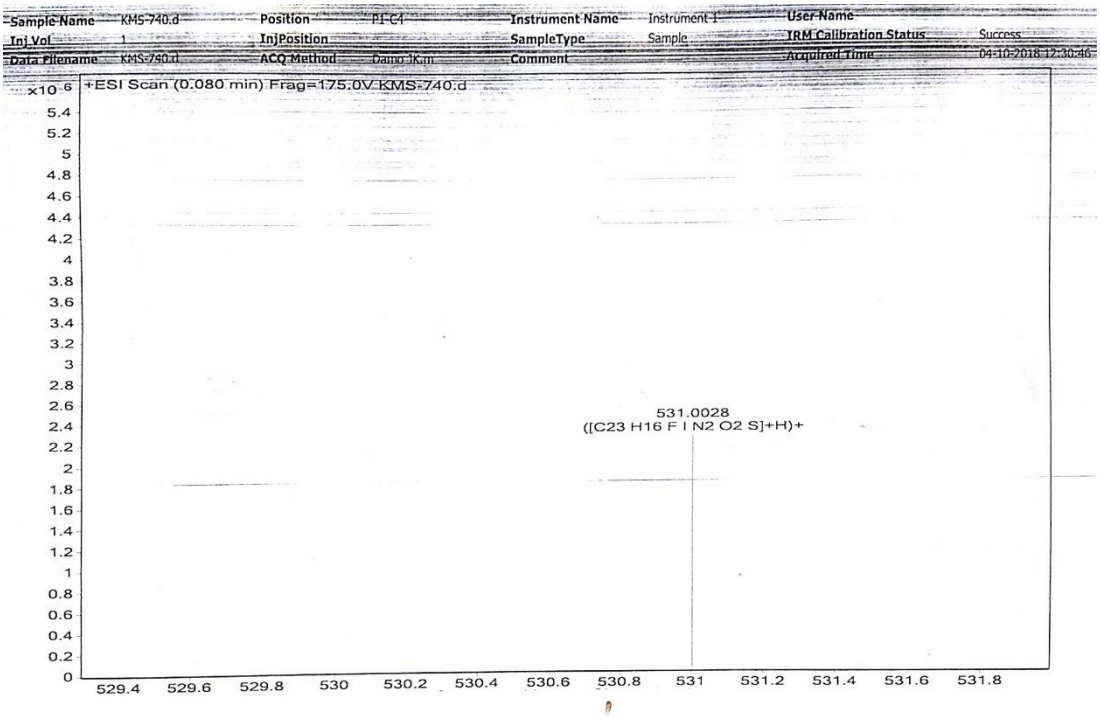
(Z)-N-((E)-6-fluoro-4-(iodo(3-methoxyphenyl)methylene)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (4g)



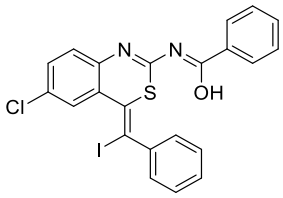
HRMS



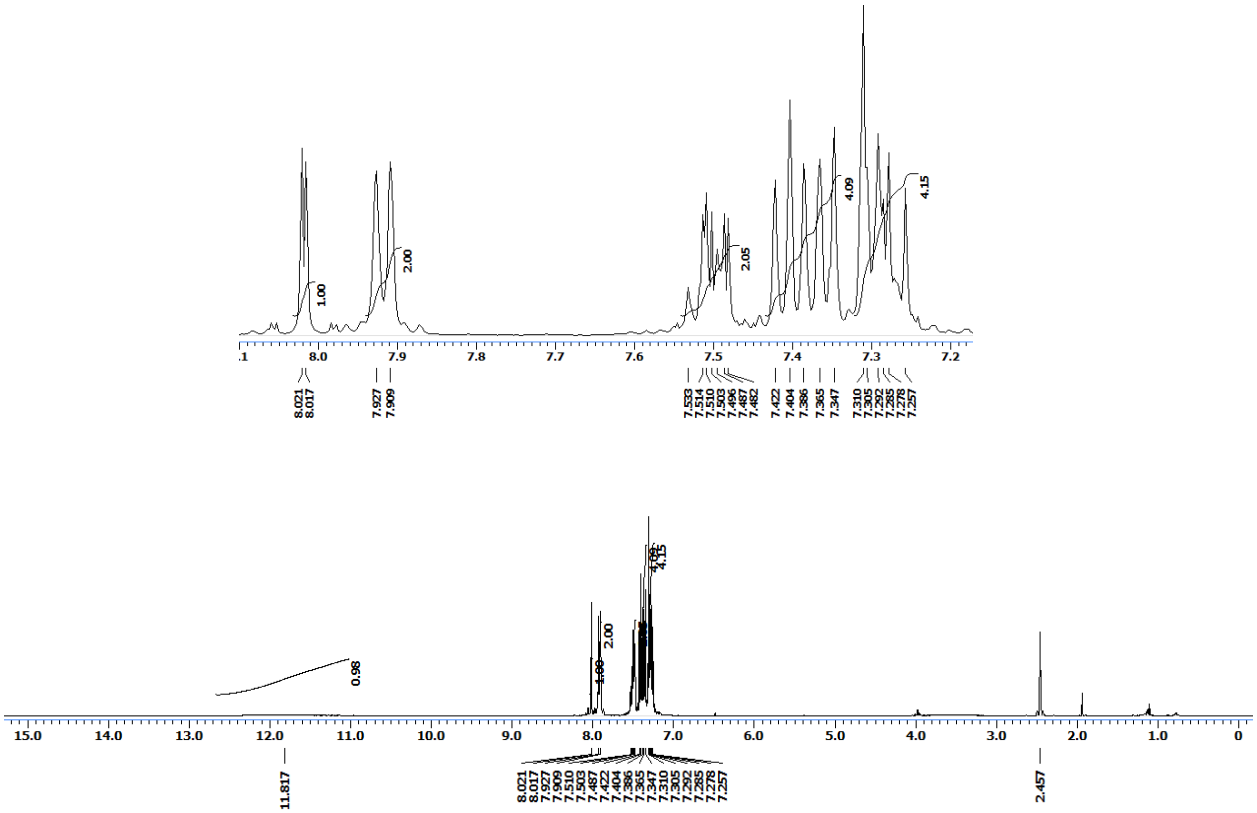
(Z)-N-((E)-6-fluoro-4-(iodo(3-methoxyphenyl)methylene)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (4g)



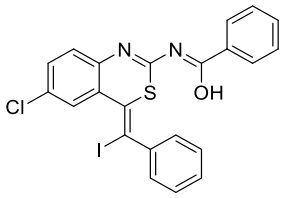
^{1}H NMR



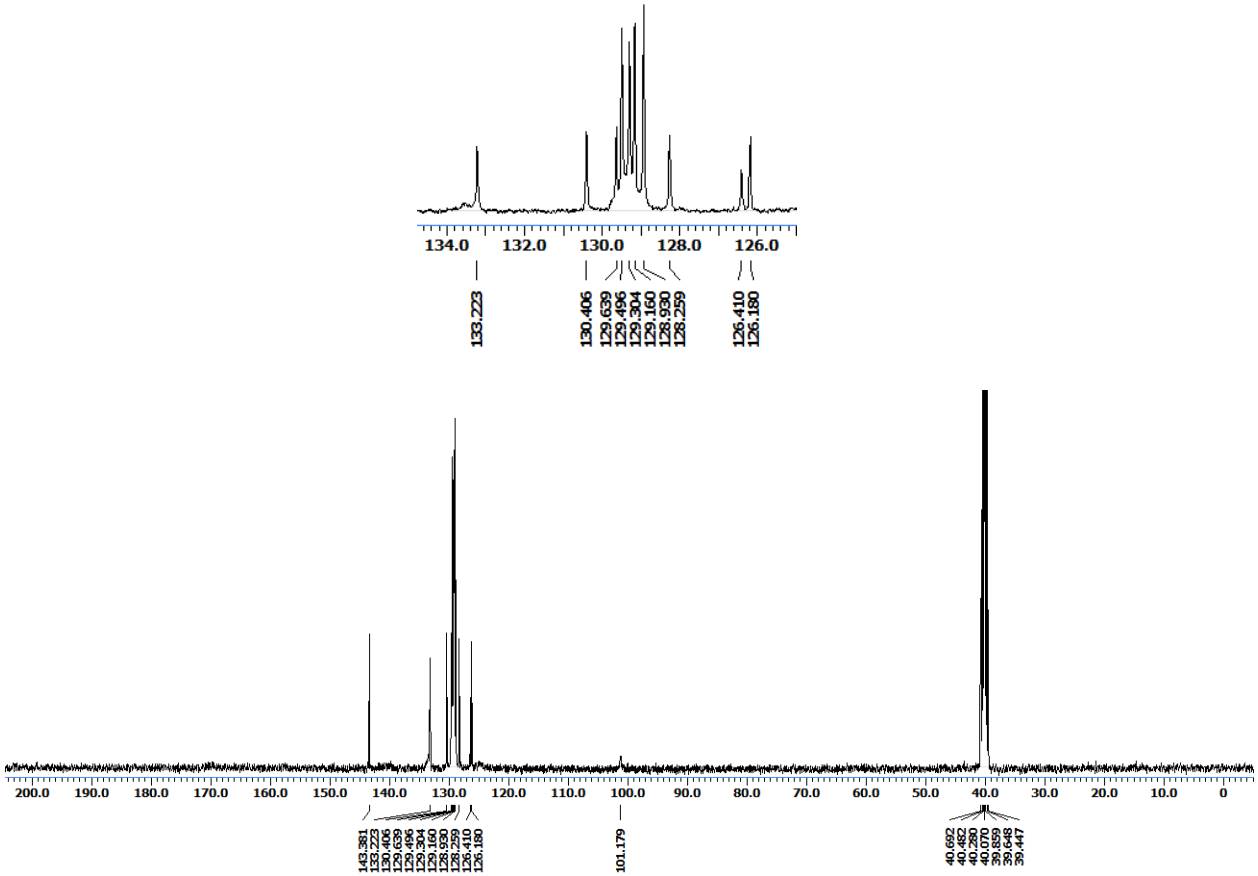
(Z)-N-((E)-6-Chloro-4-(iodo(phenyl)methylene)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (4h)



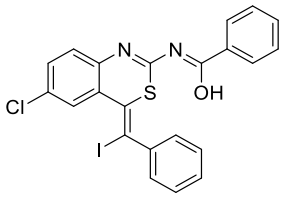
^{13}C NMR



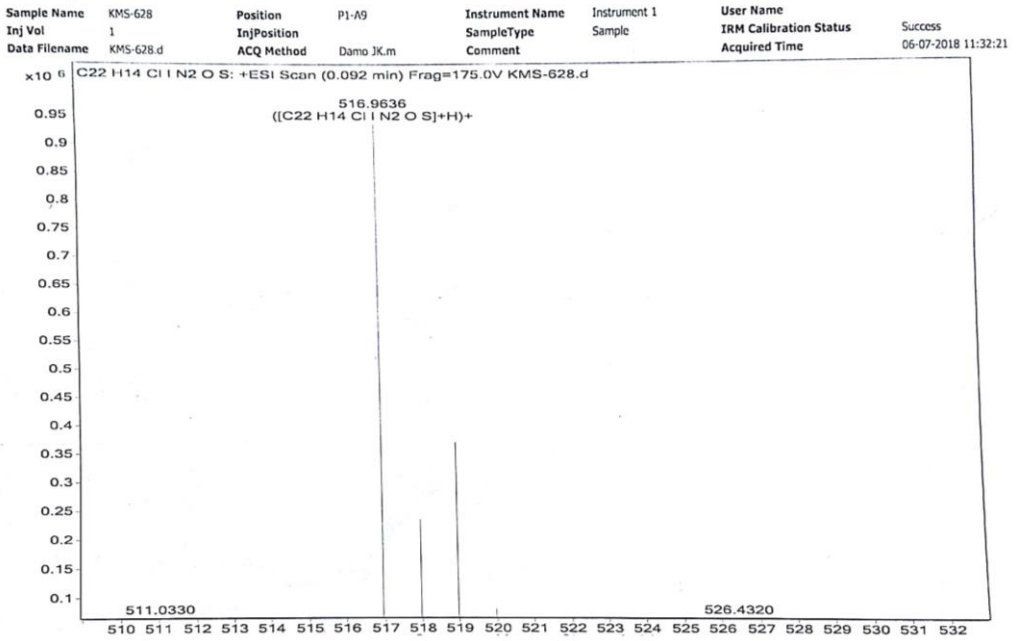
(Z)-N-((E)-6-Chloro-4-(iodo(phenyl)methylene)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (4h)



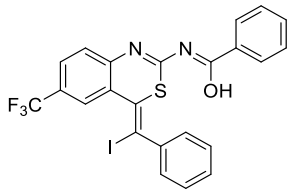
HRMS



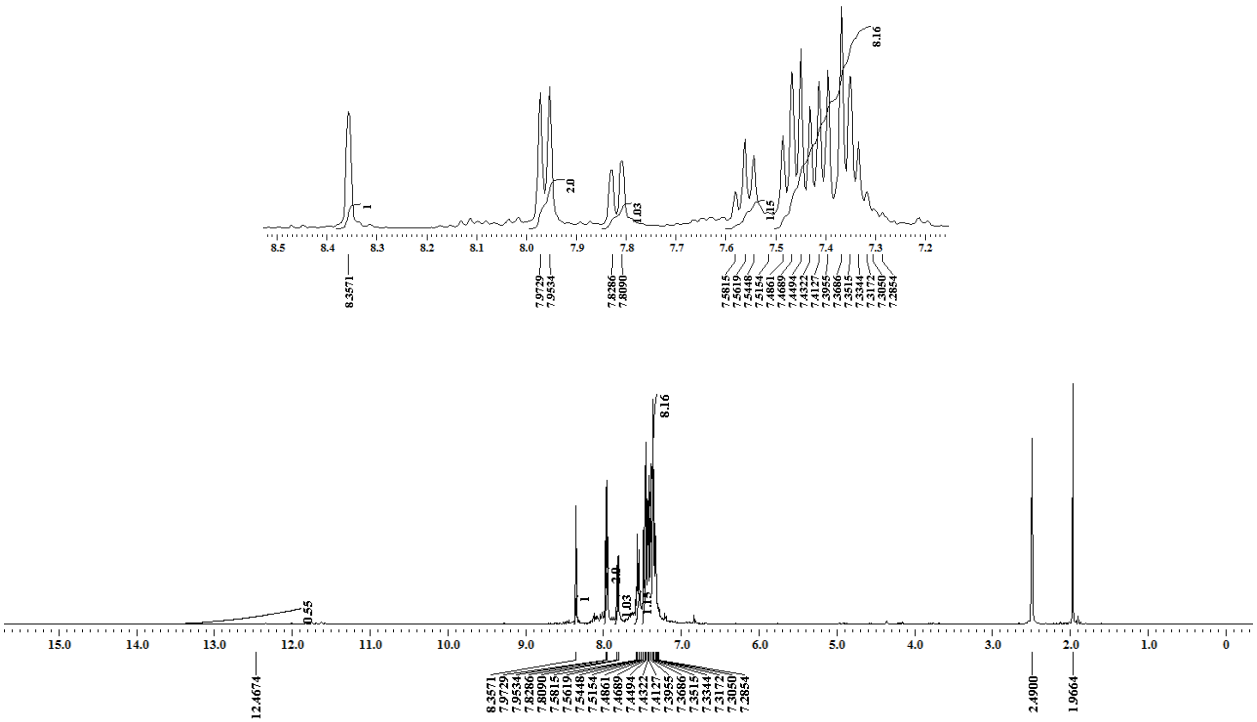
(Z)-N-((E)-6-Chloro-4-(iodo(phenyl)methylene)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (4h)



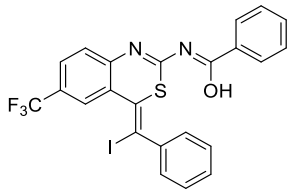
^{1}H NMR



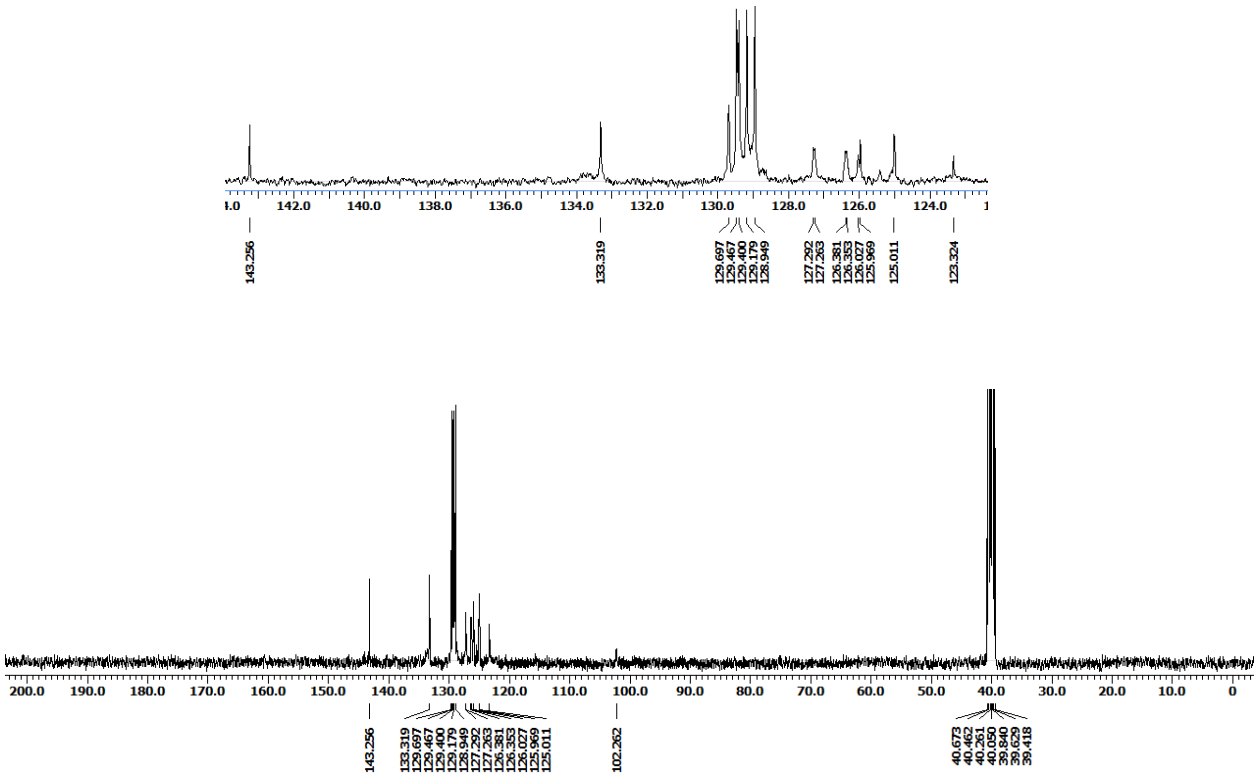
(Z)-N-((E)-4-(Iodo(phenyl)methylene)-6-(trifluoromethyl)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (4i)



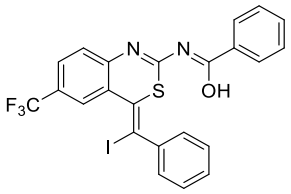
^{13}C NMR



(Z)-N-((E)-4-(Iodo(phenyl)methylene)-6-(trifluoromethyl)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (4i)



HRMS



(Z)-N-((E)-4-(Iodo(phenyl)methylene)-6-(trifluoromethyl)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (4i)

Qualitative Compound Report

Data File	KMS-630.d	Sample Name	KMS-630
Sample Type	Sample	Position	P1-A9
Instrument Name	Instrument 1	User Name	
Acq Method	Damo JK.m	Acquired Time	16-07-2018 14:41:11
IRM Calibration Status	Success	DA Method	Default.m
Comment			

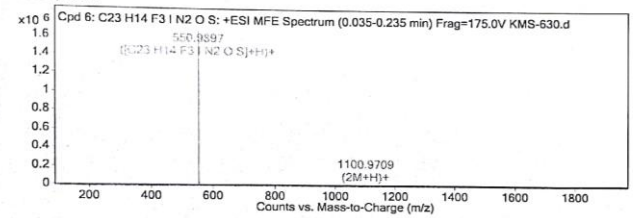
Sample Group	Info.
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.1)

Compound Table

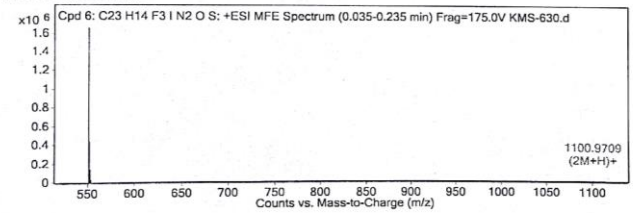
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 6: C23 H14 F3 I N2 O S	0.128	549.9824	C23 H14 F3 I N2 O S	C23 H14 F3 I N2 O S	-0.13	C23 H14 F3 I N2 O S

Compound Label	m/z	RT	Algorithm	Mass
Cpd 6: C23 H14 F3 I N2 O S	550.9897	0.128	Find by Molecular Feature	549.9824

MFE MS Spectrum



MFE MS Zoomed Spectrum

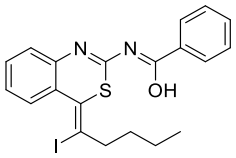


MS Spectrum Peak List

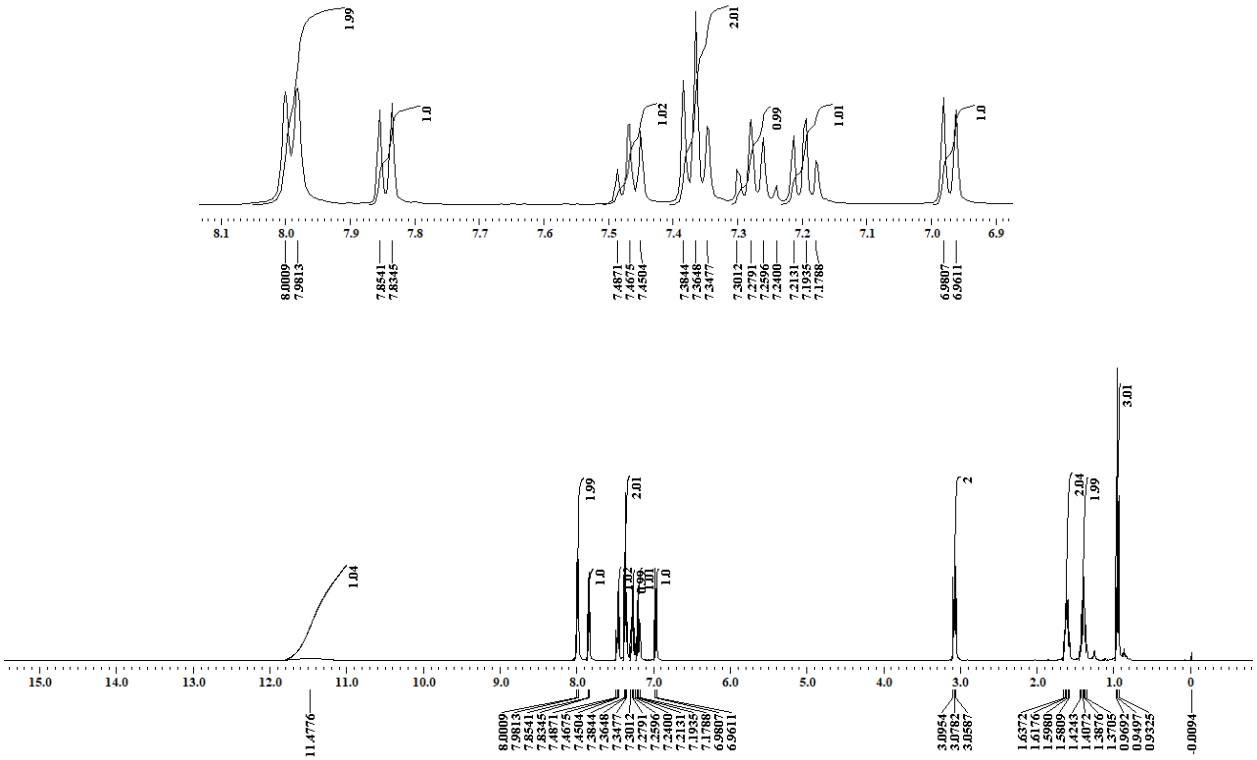
m/z	z	Abund	Formula	Ion
550.9897	1	1655826.5	C23 H14 F3 I N2 O S	(M+H)+
551.9929	1	456192.58	C23 H14 F3 I N2 O S	(M+H)+
552.9903	1	133032.87	C23 H14 F3 I N2 O S	(M+H)+
553.9906	1	22091.6	C23 H14 F3 I N2 O S	(M+H)+
554.9935	1	2872.89	C23 H14 F3 I N2 O S	(M+H)+
1100.9709	1	4644.42		(2M+H)+
1101.9737	1	2466.18		(2M+H)+
1102.9779	1	1096.55		(2M+H)+
1103.9701	1	485.3		(2M+H)+

--- End Of Report ---

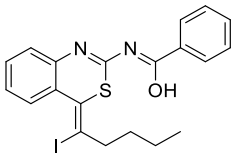
^{1}H NMR



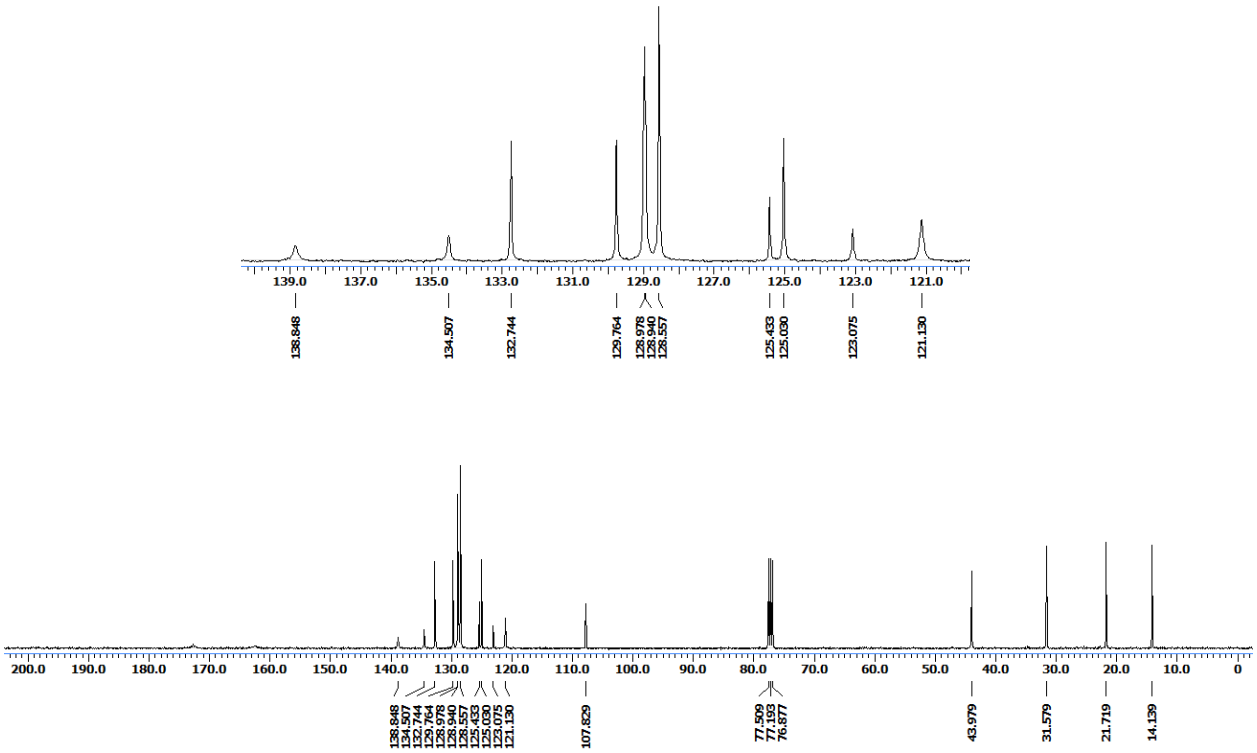
(Z)-N-((E)-4-(1-Iodopentylidene)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (5a)



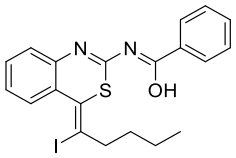
^{13}C NMR



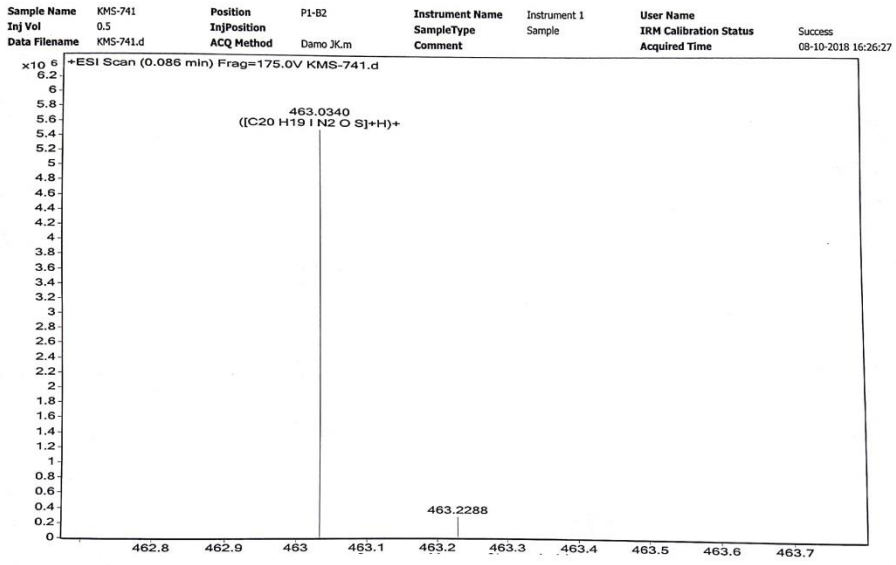
(Z)-N-((E)-4-(1-Iodopentylidene)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (5a)



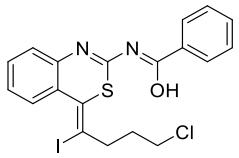
HRMS



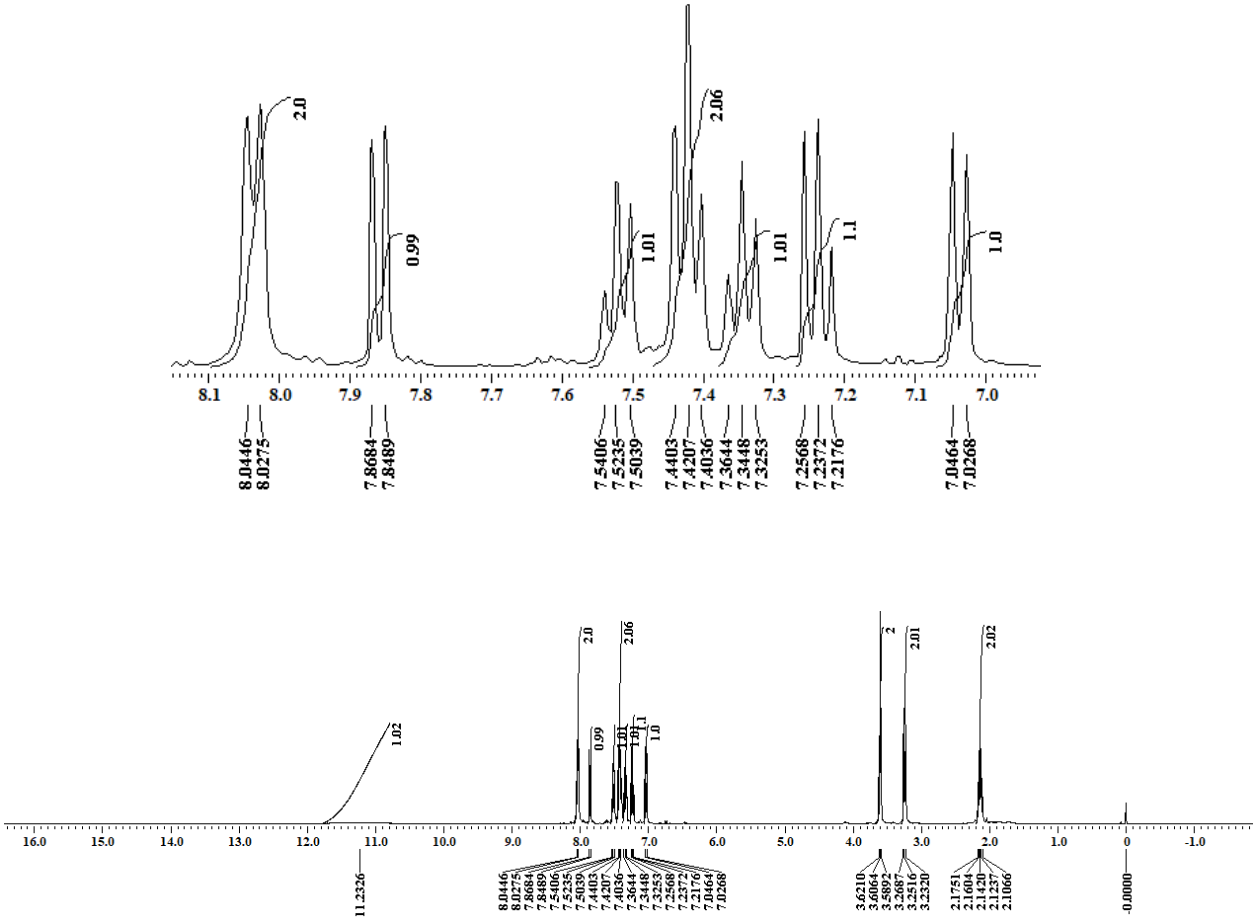
(Z)-N-((E)-4-(1-Iodopentylidene)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (5a)



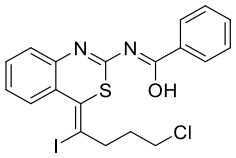
^{1}H NMR



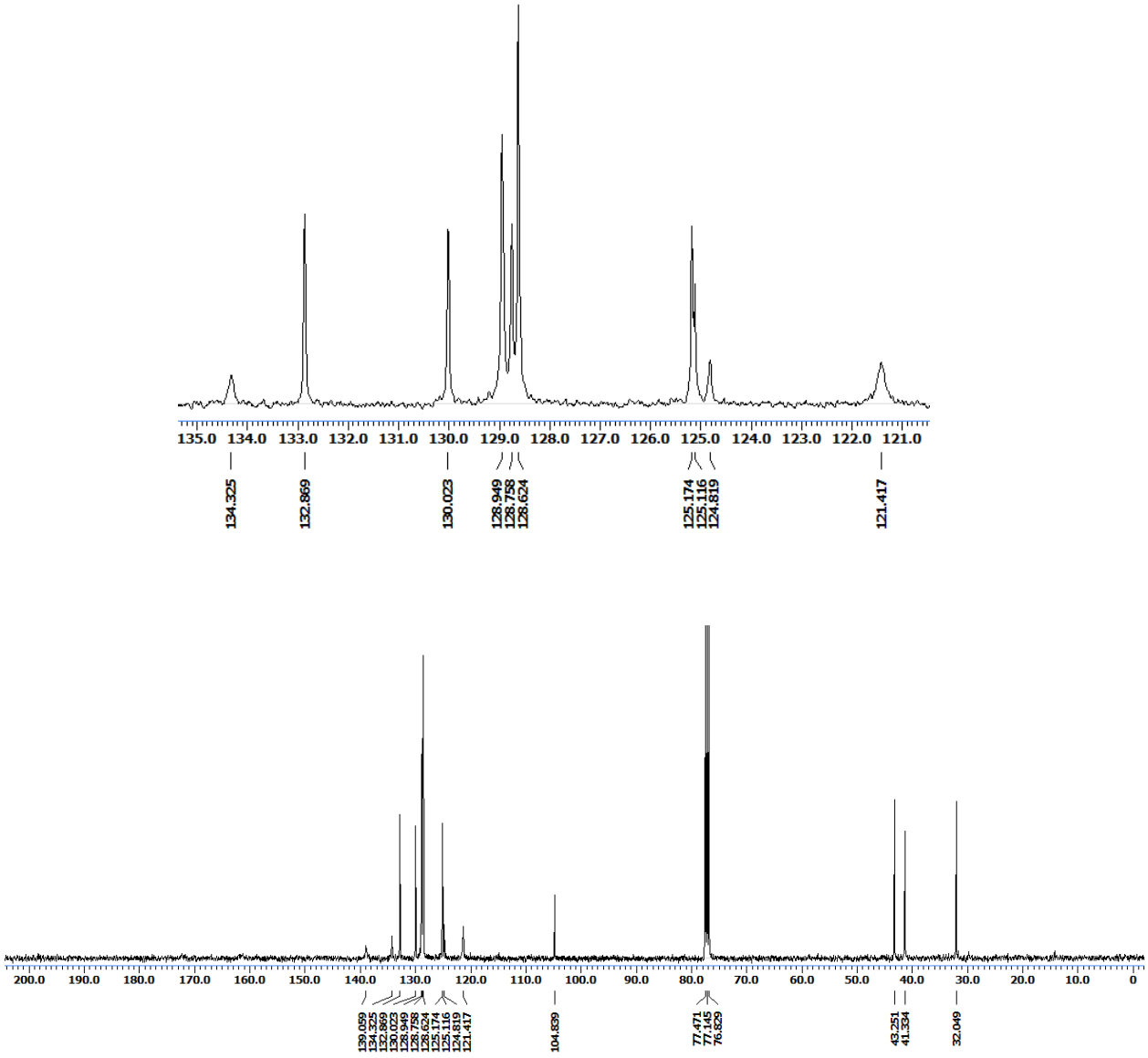
(Z)-N-((E)-4-(4-chloro-1-iodobutylidene)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (5b)



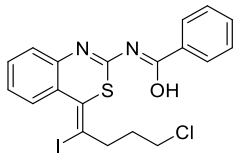
^{13}C NMR



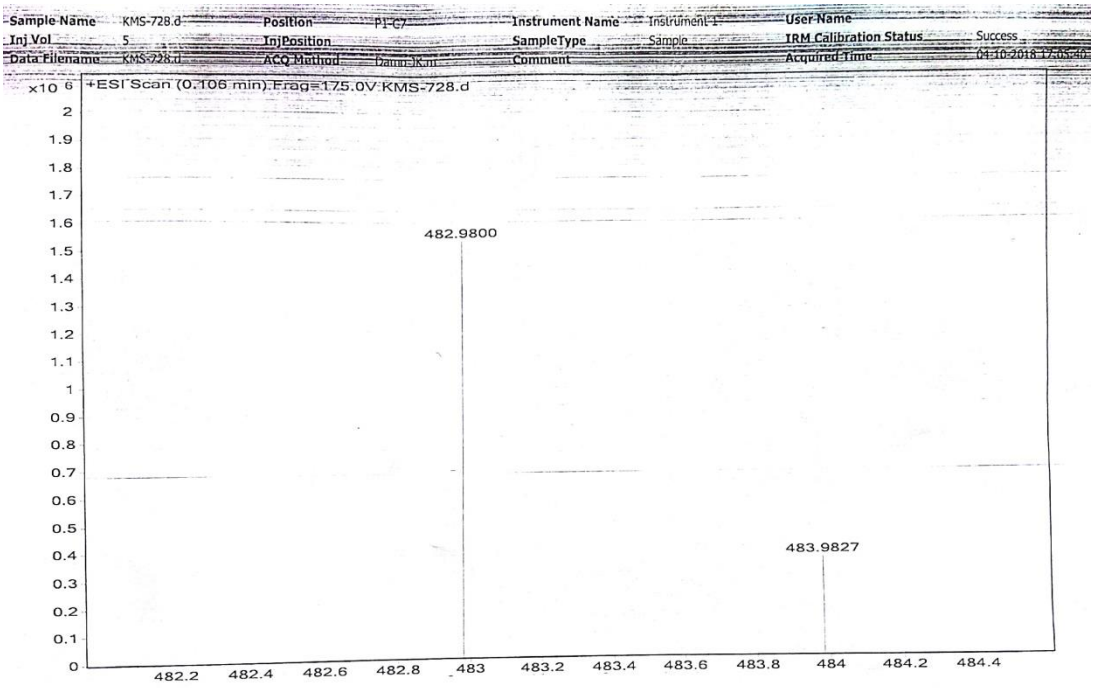
(Z)-N-((E)-4-(4-chloro-1-iodobutylidene)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (5b)



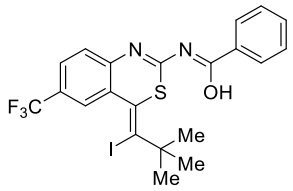
HRMS



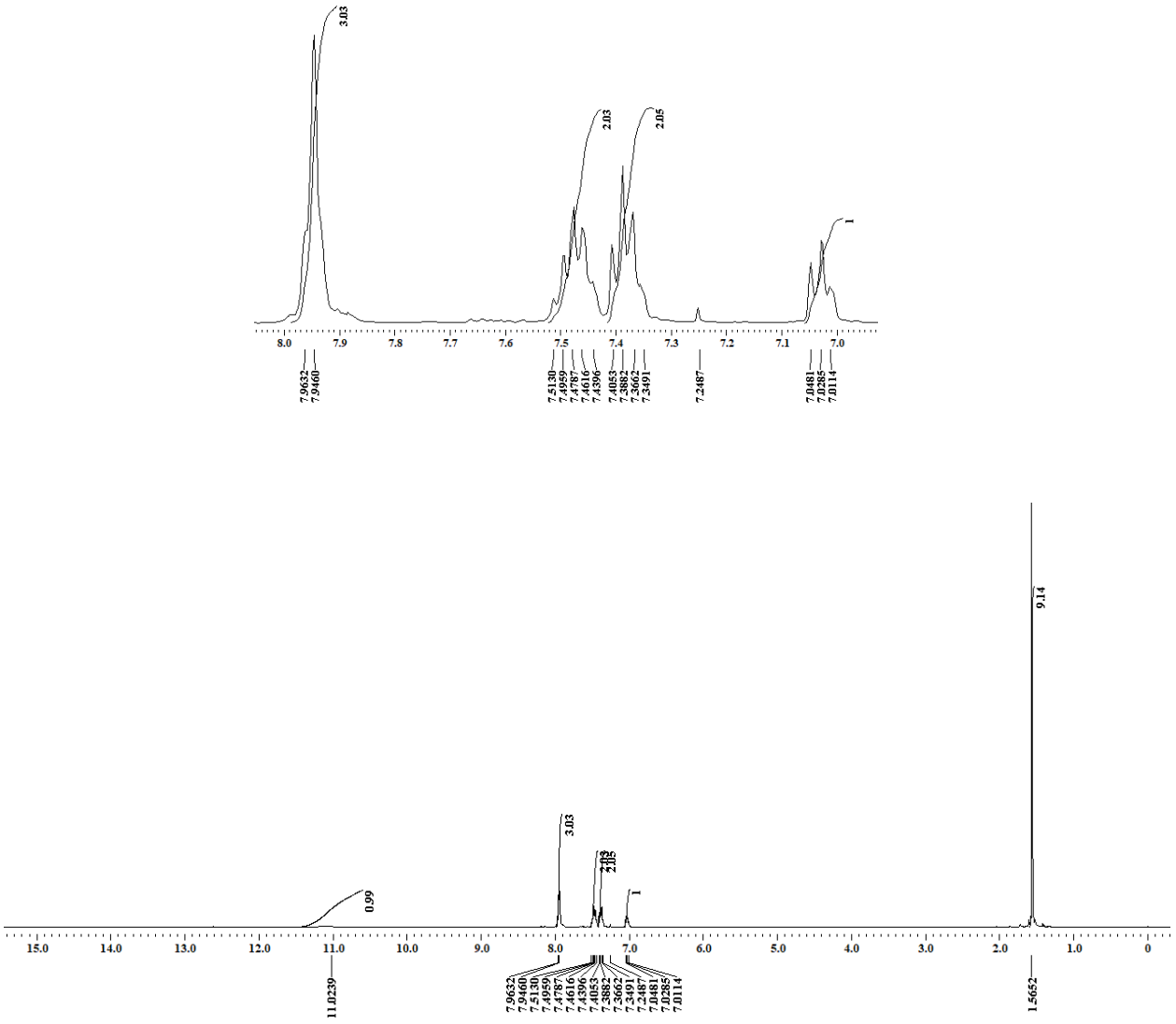
(Z)-N-((E)-4-(4-chloro-1-iodobutylidene)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (5b)



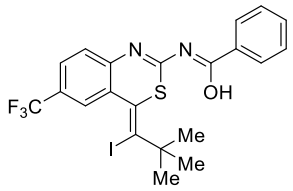
^{1}H NMR



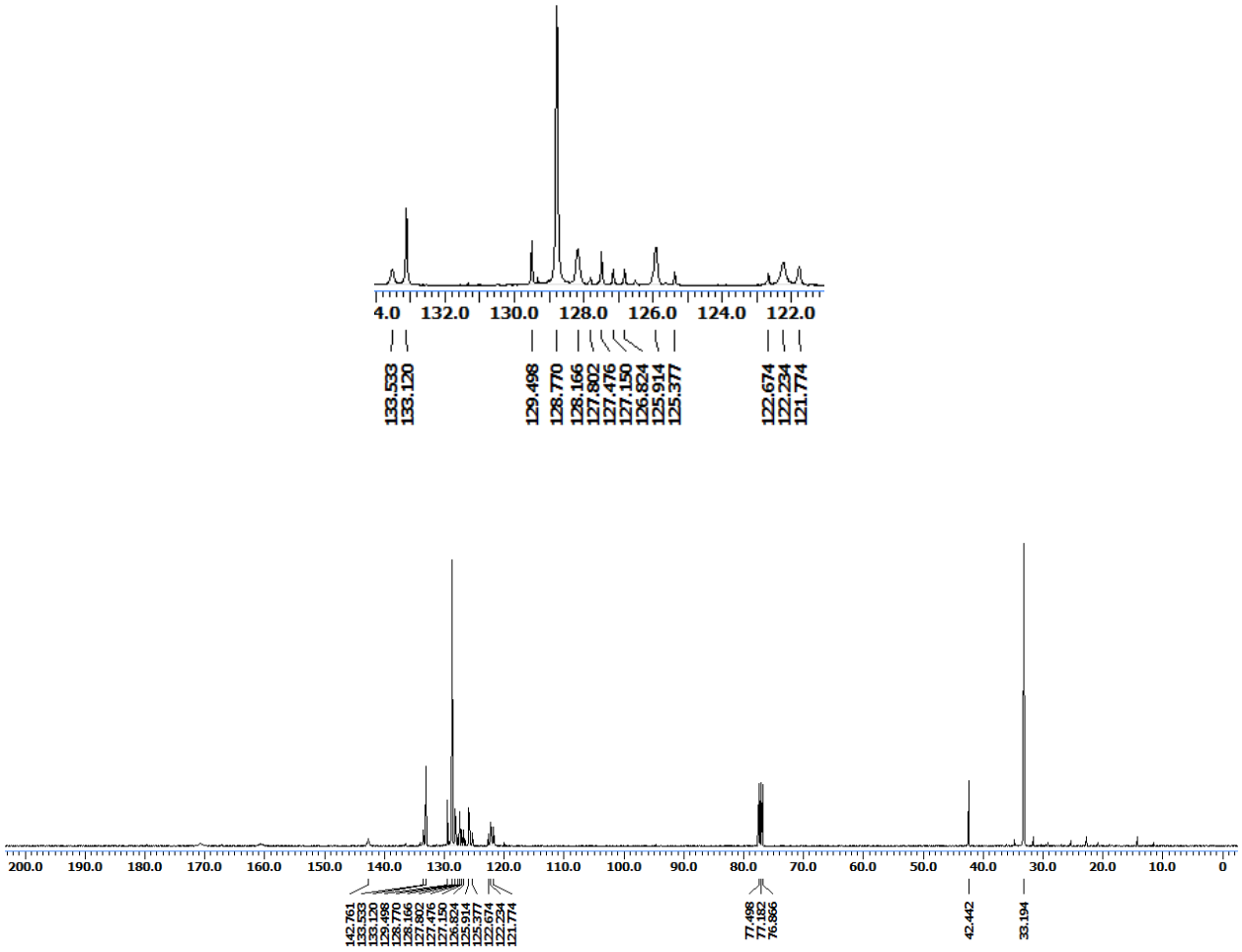
(Z)-N-((E)-4-(1-iodo-2,2-dimethylpropylidene)-6-(trifluoromethyl)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (5c)



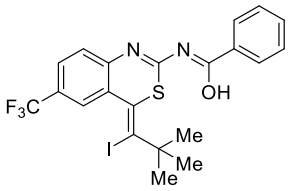
^{13}C NMR



(Z)-N-((E)-4-(1-iodo-2,2-dimethylpropylidene)-6-(trifluoromethyl)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (5c)



HRMS



(Z)-N-((E)-4-(1-iodo-2,2-dimethylpropylidene)-6-(trifluoromethyl)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (5c)

Qualitative Compound Report

Data File	PR-718.d	**Sample Name**	PR-718
Sample Type	Sample	**Position**	P1-A9
Instrument Name	Instrument 1	**User Name**	
Acq Method	Damo JK.m	**Acquired Time**	26-09-2018 12:30:27
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

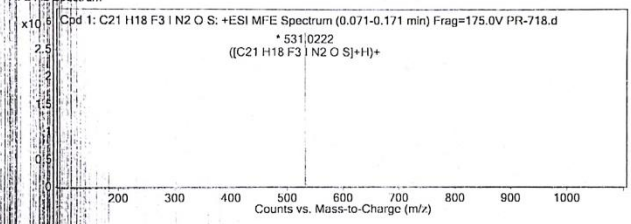
Sample Group **Info.**
Acquisition SW Version 6200 series TOF/6500 series Q-TOF B.05.01 (B5125.1)

Compound Table

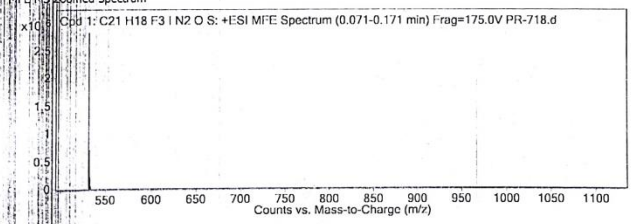
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 1: C21 H18 F3 I N2 O S	0.088	530.015	C21 H18 F3 I N2 O S	C21 H18 F3 I N2 O S	-2.46	C21 H18 F3 I N2 O S

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: C21 H18 F3 I N2 O S	531.0222	0.088	Find by Molecular Feature	530.015

MFE MS Spectrum



MFE MS Zoomed Spectrum

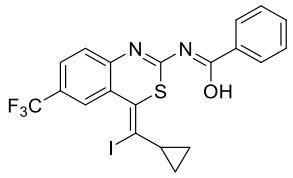


MS Spectrum Peak List

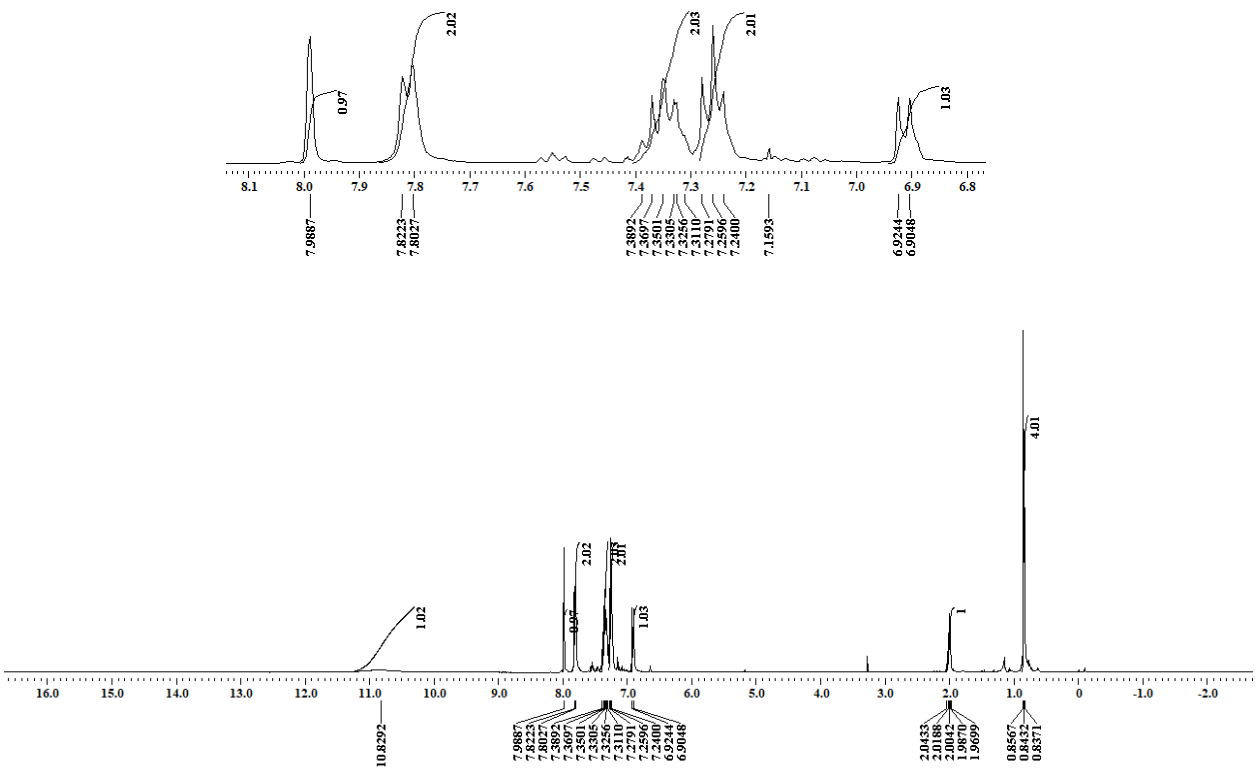
m/z	z	Abund	Formula	Ion
531.0222	1	2820691	C21 H18 F3 I N2 O S	(M+H)+
532.0254	1	712934.77	C21 H18 F3 I N2 O S	(M+H)+
533.0228	1	221016.35	C21 H18 F3 I N2 O S	(M+H)+
534.0228	1	38890.87	C21 H18 F3 I N2 O S	(M+H)+
535.024	1	9248.14	C21 H18 F3 I N2 O S	(M+H)+
568.9777	1	2984.26	C21 H18 F3 I N2 O S	(M+K)+
1098.9975	1	642.61		(2M+K)+

--- End Of Report ---

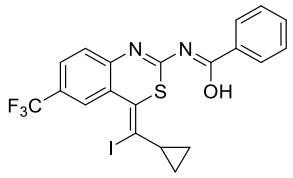
^{1}H NMR



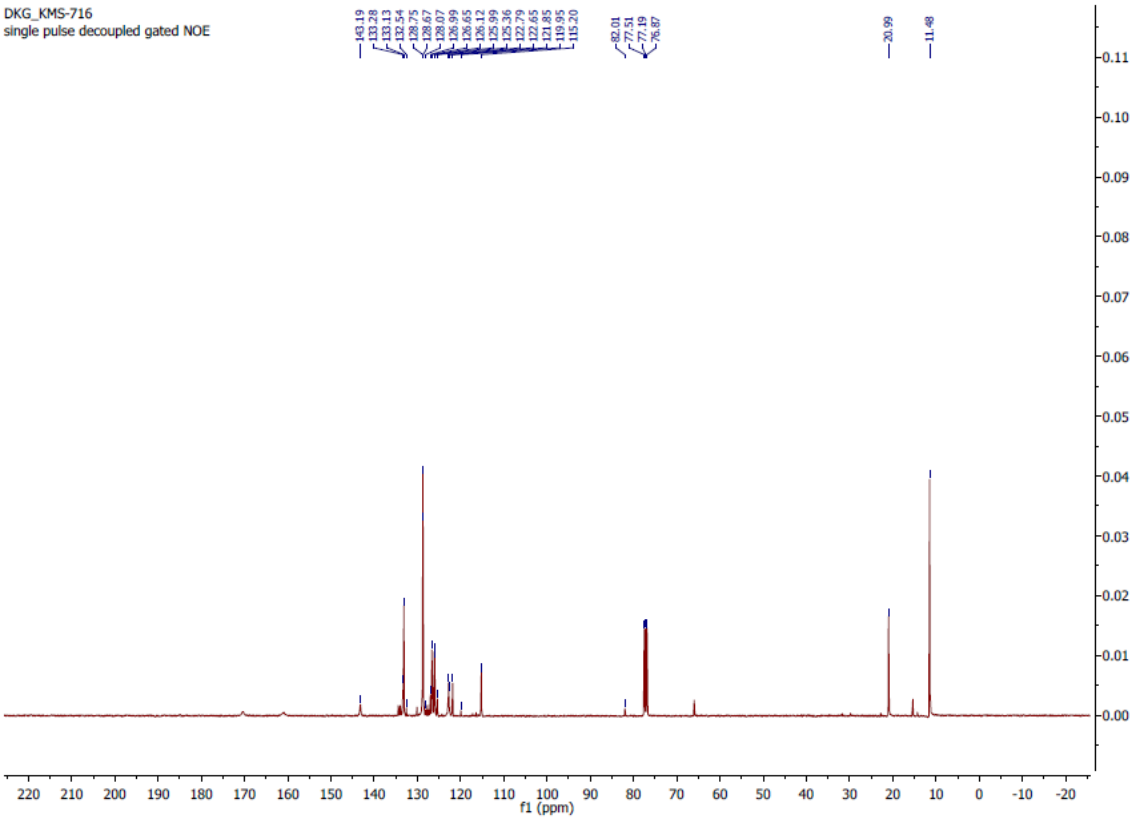
(Z)-N-((E)-4-(cyclopropyliodomethylene)-6-(trifluoromethyl)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (5d)



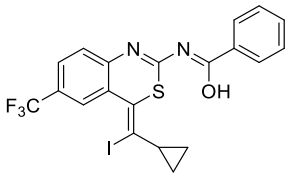
^{13}C NMR



(Z)-N-((E)-4-(cyclopropyliodomethylene)-6-(trifluoromethyl)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (5d)



HRMS



(Z)-N-((E)-4-(cyclopropyliodomethylene)-6-(trifluoromethyl)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (5d)

Qualitative Compound Report

Data File	KMS-716.d	**Sample Name**	KMS-716
Sample Type	Sample	**Position**	P1-D2
Instrument Name	Instrument 1	**User Name**	
Acq Method	Damo JK.m	**Acquired Time**	18-09-2018 14:07:45
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

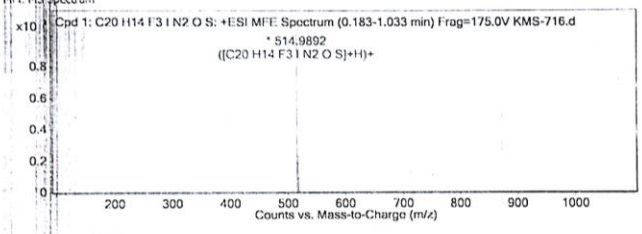
Sample Group Info.
Acquisition SW Version 6200 series TOF/6500 series Q-TOF B.05.01 (B5175.1)

Compound Table

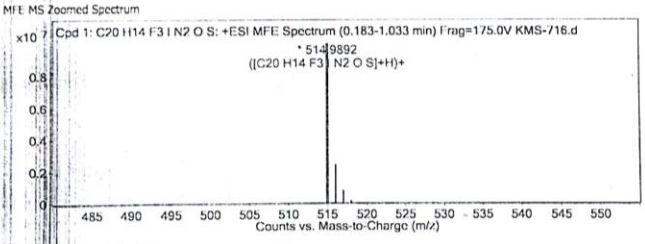
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 1: C20 H14 F3 I N2 O S	0.302	513.9822	C20 H14 F3 I N2 O S	C20 H14 F3 I N2 O S	0.22	C20 H14 F3 I N2 O S

Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: C20 H14 F3 I N2 O S	514.9892	0.302	Find by Molecular Feature	513.9822

MFE MS Spectrum



MFE MS Zoomed Spectrum

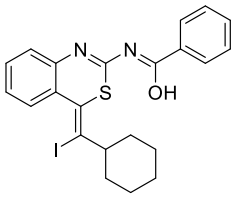


MS Spectrum Peak List

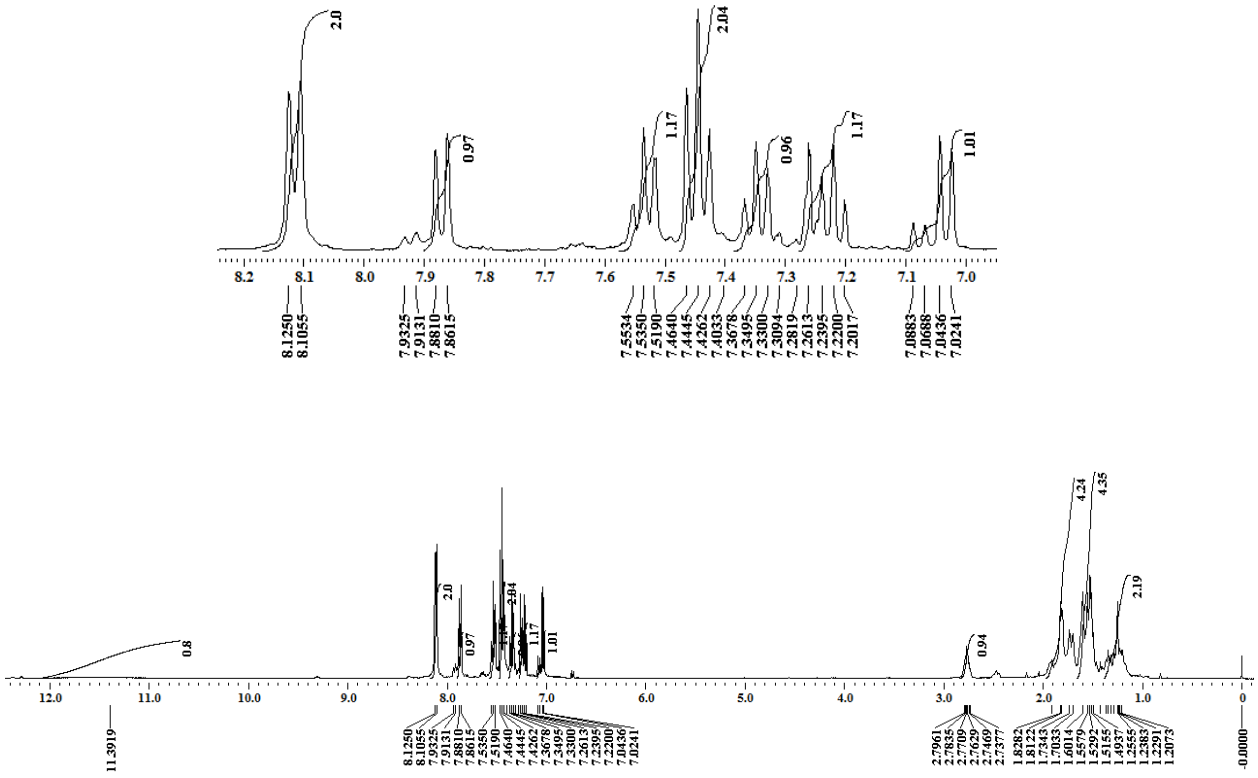
m/z	z	Abund	Formula	Ion
514.9892	1	10089115	C20 H14 F3 I N2 O S	(M+H)+
515.9923	1	2340695.93	C20 H14 F3 I N2 O S	(M+H)+
516.9936	1	899893.2	C20 H14 F3 I N2 O S	(M+H)+
517.9956	1	30336.06	C20 H14 F3 I N2 O S	(M+H)+
518.9987	1	29061.47	C20 H14 F3 I N2 O S	(M+H)+
520.0015	1	3864.66	C20 H14 F3 I N2 O S	(M+H)+

--- End Of Report ---

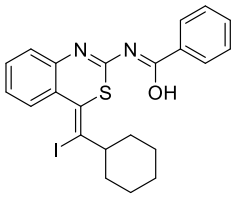
^{1}H NMR



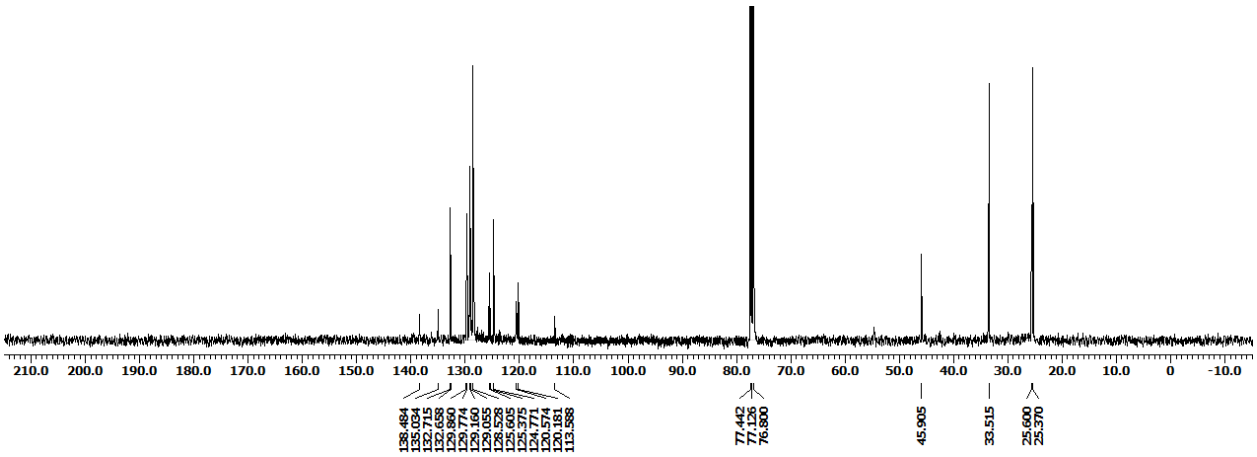
(Z)-N-((E)-4-(cyclohexyliodomethylene)-4H-benzo[*d*][1,3]thiazin-2-yl)benzimidic acid (5e)



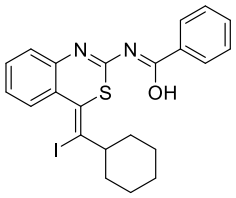
^{13}C NMR



(Z)-N-((E)-4-(cyclohexyliodomethylene)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (5e)



HRMS



(Z)-N-((E)-4-(cyclohexyliodomethylene)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (5e)

Qualitative Compound Report

Data File	KMS-531.d	Sample Name	KMS-531
Sample Type	Sample	Position	P1-A9
Instrument Name	Instrument 1	User Name	
Acq Method	Damo JK.m	Acquired Time	17-07-2018 11:14:27
IRM Calibration Status	Success	DA Method	Default.m
Comment			

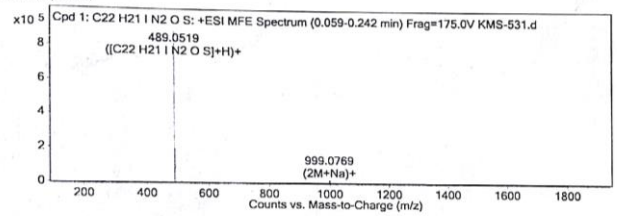
Sample Group	Info.
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.1)

Compound Table

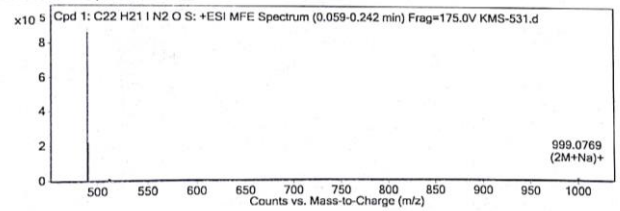
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 1: C22 H21 I N2 O S	0.087	488.0442	C22 H21 I N2 O S	C22 H21 I N2 O S	-4.68	C22 H21 I N2 O S

Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: C22 H21 I N2 O S	489.0519	0.087	Find by Molecular Feature	488.0442

MFE MS Spectrum



MFE MS Zoomed Spectrum

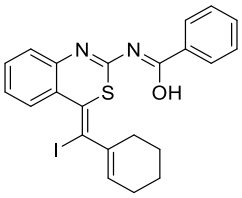


MS Spectrum Peak List

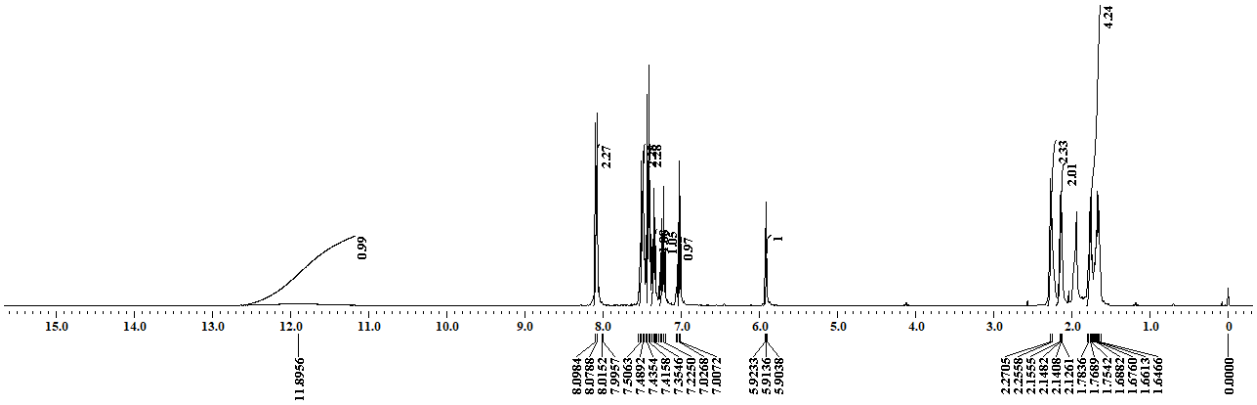
m/z	z	Abund	Formula	Ion
489.0519	1	886690.19	C22 H21 I N2 O S	(M+H)+
490.0547	1	198801.3	C22 H21 I N2 O S	(M+H)+
511.0333	1	11335.49	C22 H21 I N2 O S	(M+Na)+
512.0373	1	2412.74	C22 H21 I N2 O S	(M+Na)+
527.0077	1	1240.53	C28 H12 N2 O5 S	(M+K)+
528.0077	1	440.03	C28 H12 N2 O5 S	(M+K)+
999.0769	1	13757.61		(2M+Na)+
1000.0788	1	7649.42		(2M+Na)+
1001.0879	1	12452.67		(2M+Na)+
1002.0922	1	5826.1		(2M+Na)+

--- End Of Report ---

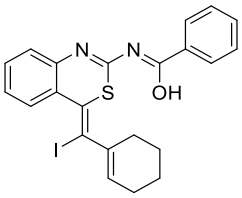
^{1}H NMR



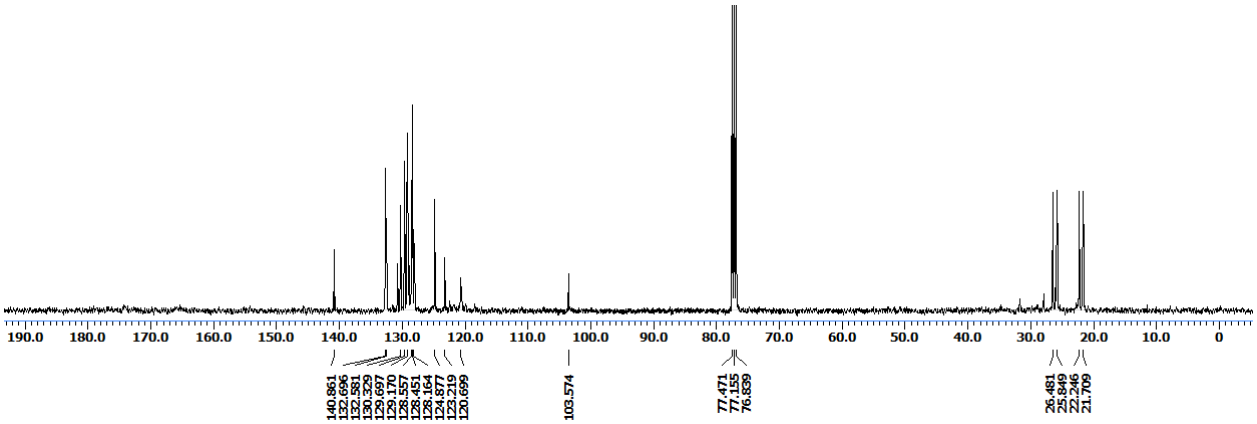
(Z)-N-((E)-4-(cyclohex-1-en-1-yliodomethylene)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (5f)



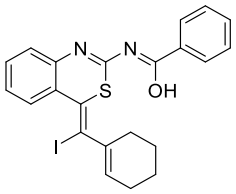
^{13}C NMR



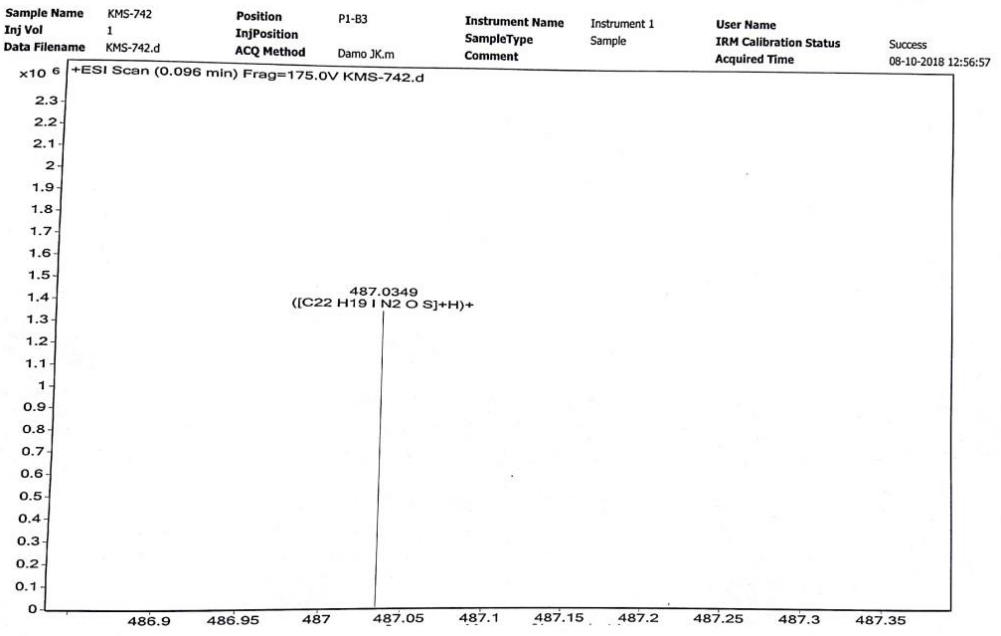
(Z)-N-((E)-4-(cyclohex-1-en-1-yliodomethylene)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (5f)



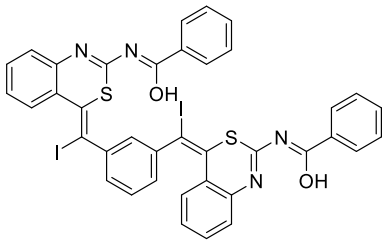
HRMS



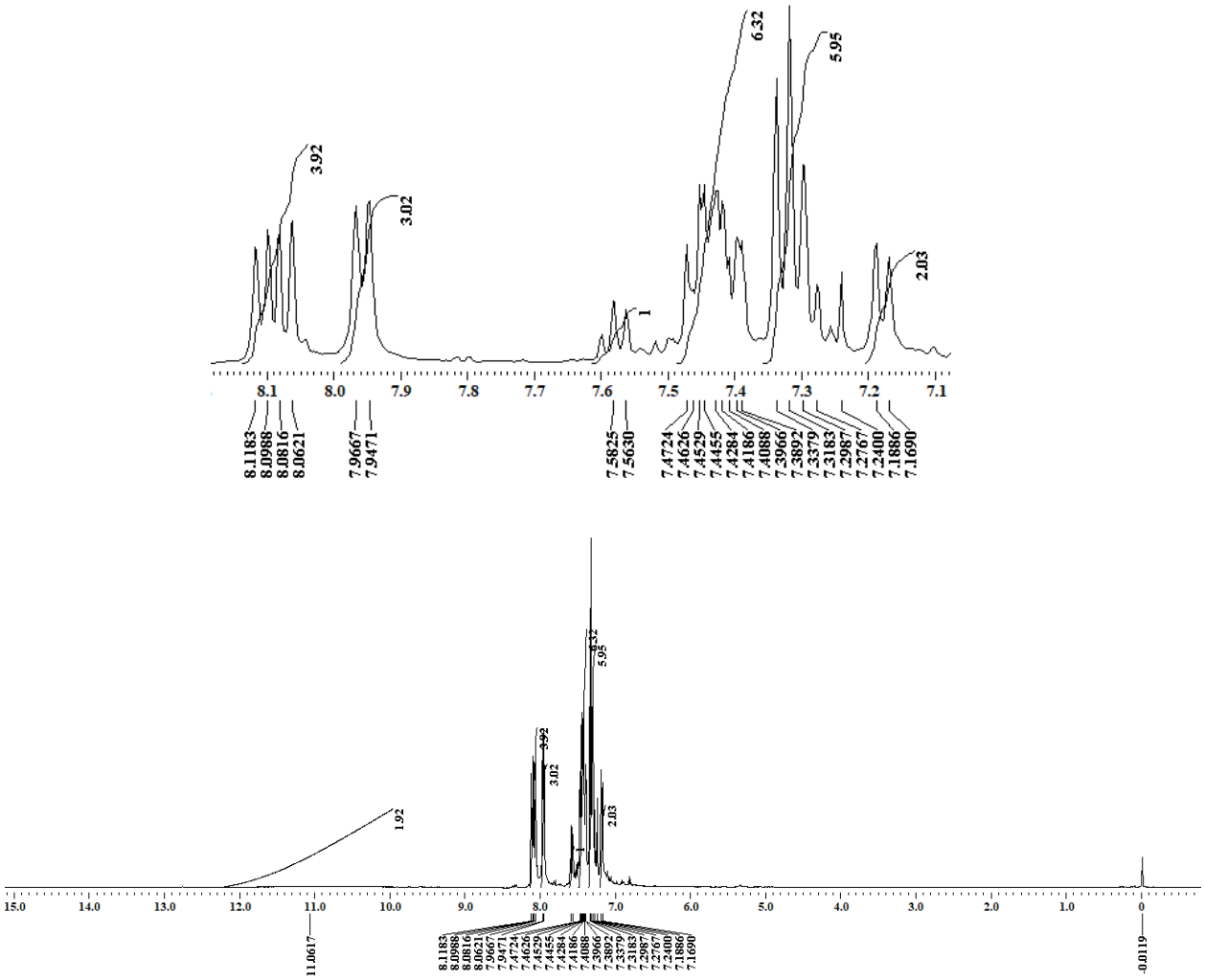
(Z)-N-((E)-4-(cyclohex-1-en-1-yliodomethylene)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (5f)



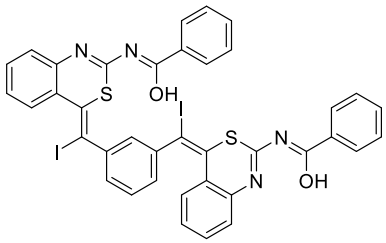
^{1}H NMR



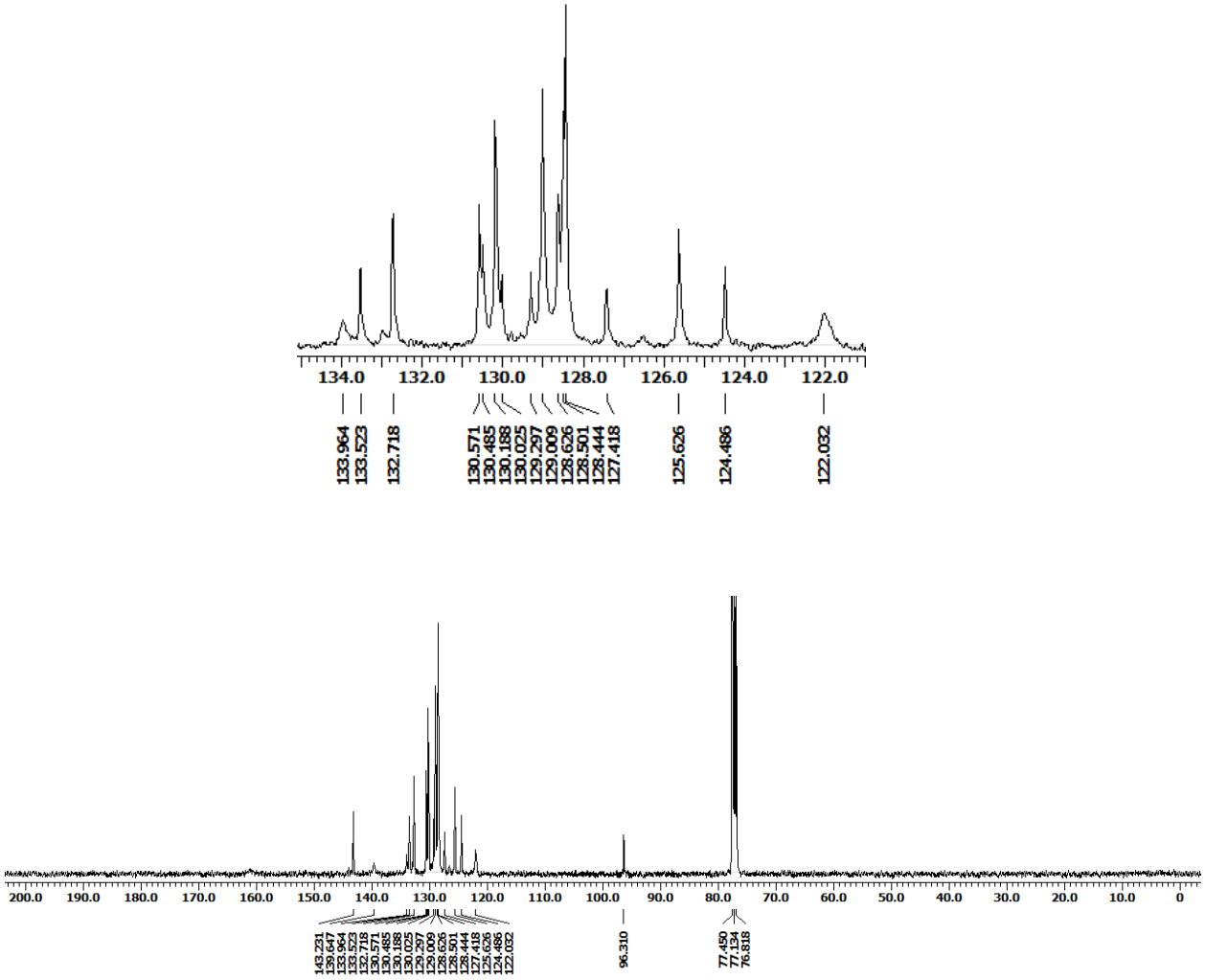
(1Z,1'Z)-N,N'-((4Z,4'E)-(1,3-phenylenebis(iodomethanylylidene))bis(4H-benzo[d][1,3]thiazine-2-yl-4-ylidene))dibenzimidic acid (7a)



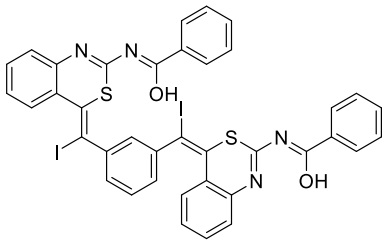
^{13}C NMR



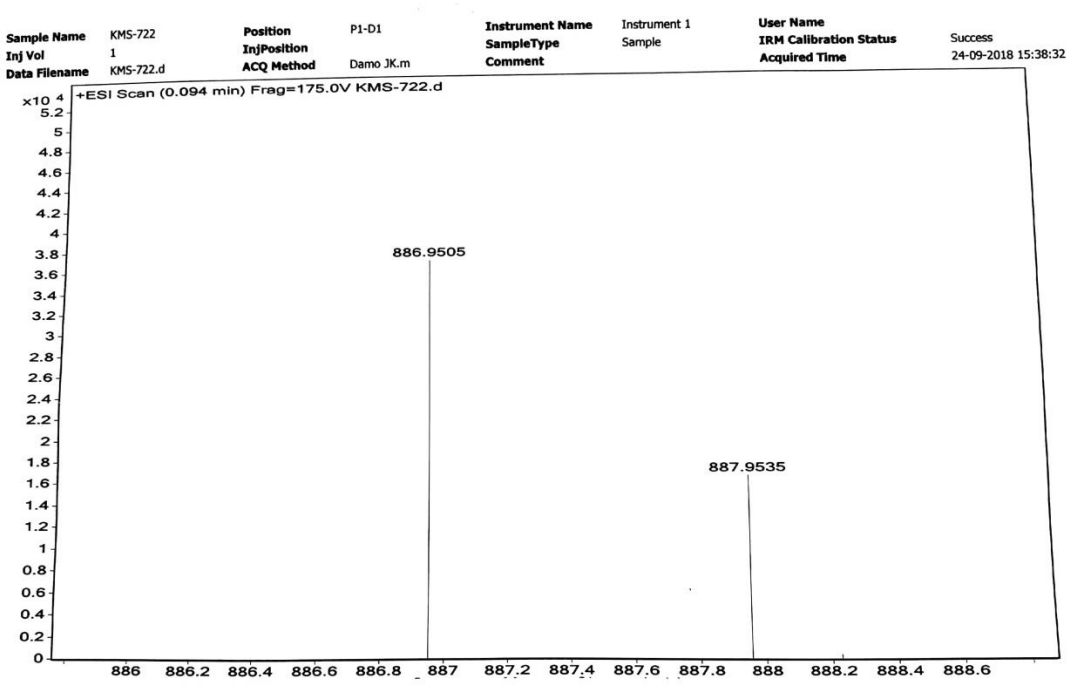
(1Z,1'Z)-N,N'-((4Z,4'E)-(1,3-phenylenebis(iodomethanylylidene))bis(4H-benzo[d][1,3]thiazine-2-yl-4-ylidene))dibenzimidic acid (7a)



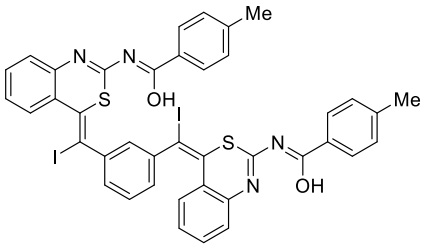
HRMS



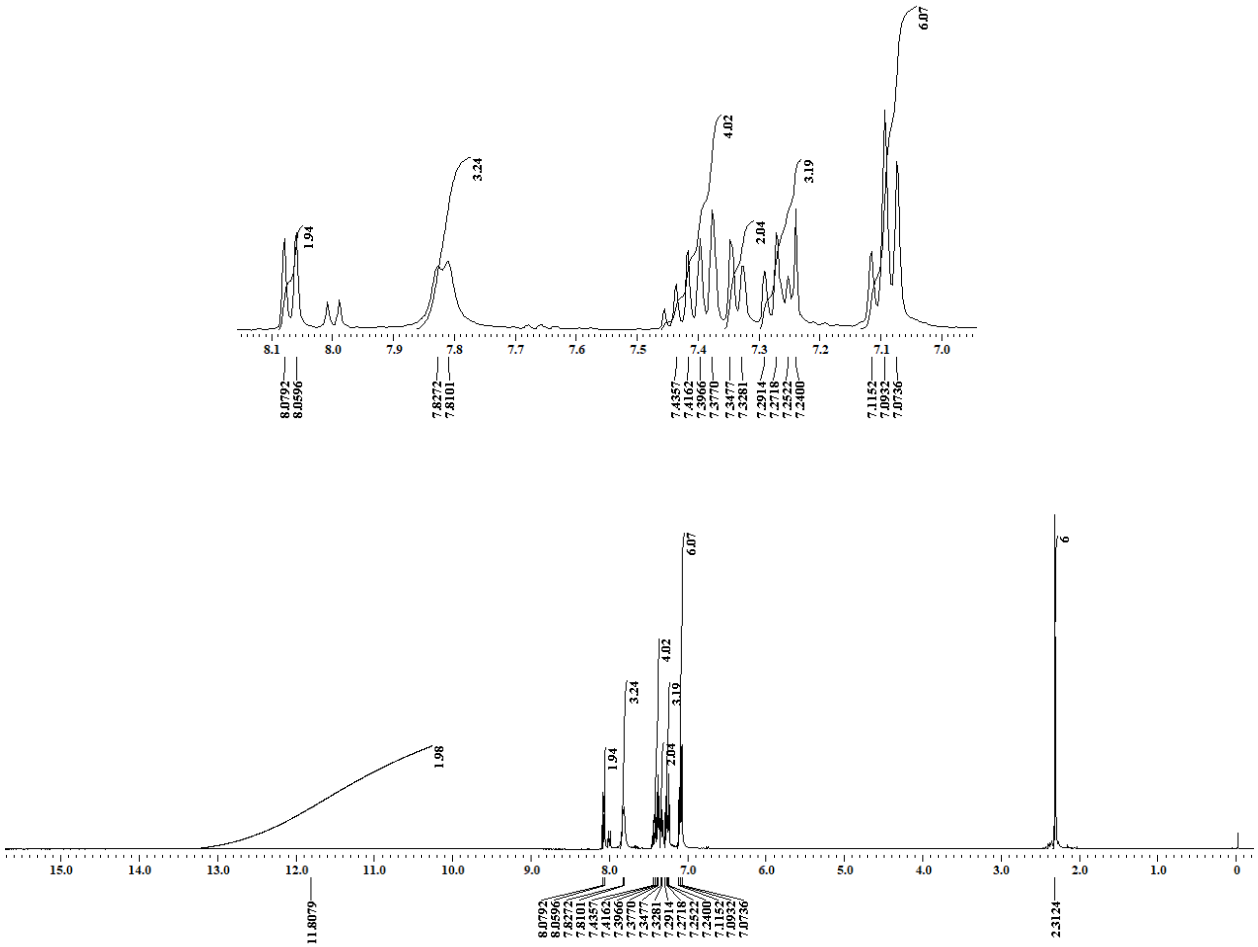
(1Z,1'Z)-N,N'-((4Z,4'E)-(1,3-phenylenebis(iodomethanylylidene))bis(4H-benzo[d][1,3]thiazine-2-yl-4-ylidene))dibenzimidic acid (7a)



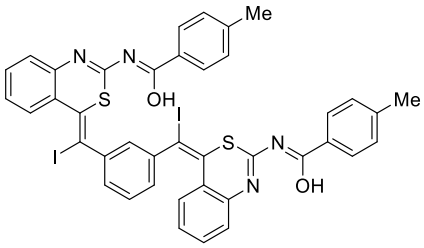
^{1}H NMR



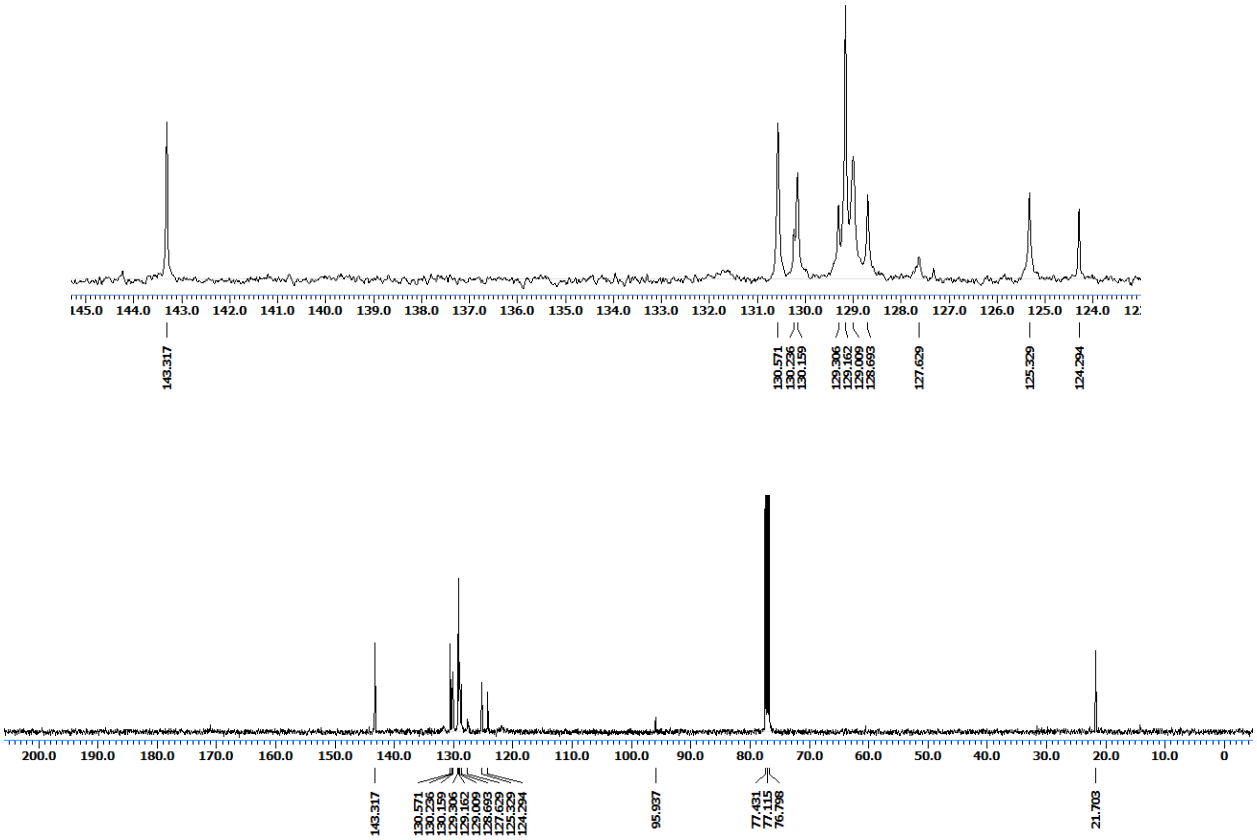
(1Z,1'Z)-N,N'-((4Z,4'E)-(1,3-phenylenebis(iodomethanylylidene))bis(4H-benzo[d][1,3]thiazine-2-yl-4-ylidene))bis(4-methylbenzimidic acid) (7b)



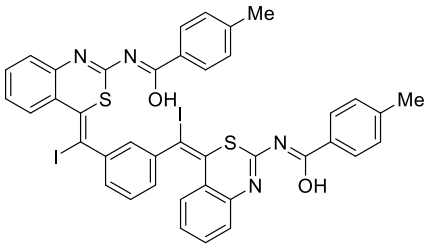
^{13}C NMR



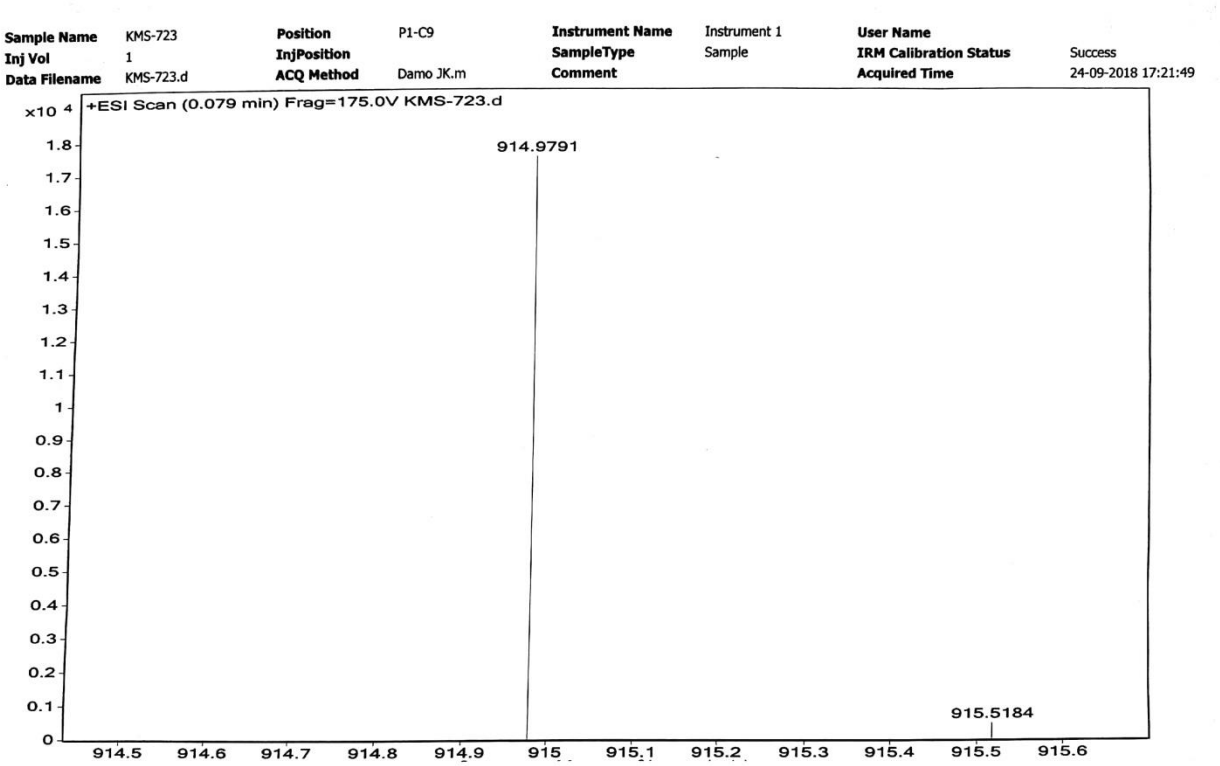
(1Z,1'Z)-N,N'-((4Z,4'E)-(1,3-phenylenebis(iodomethanylylidene))bis(4H-benzo[d][1,3]thiazine-2-yl-4-ylidene))bis(4-methylbenzimidic acid) (7b)



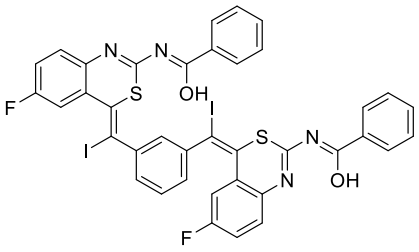
HRMS



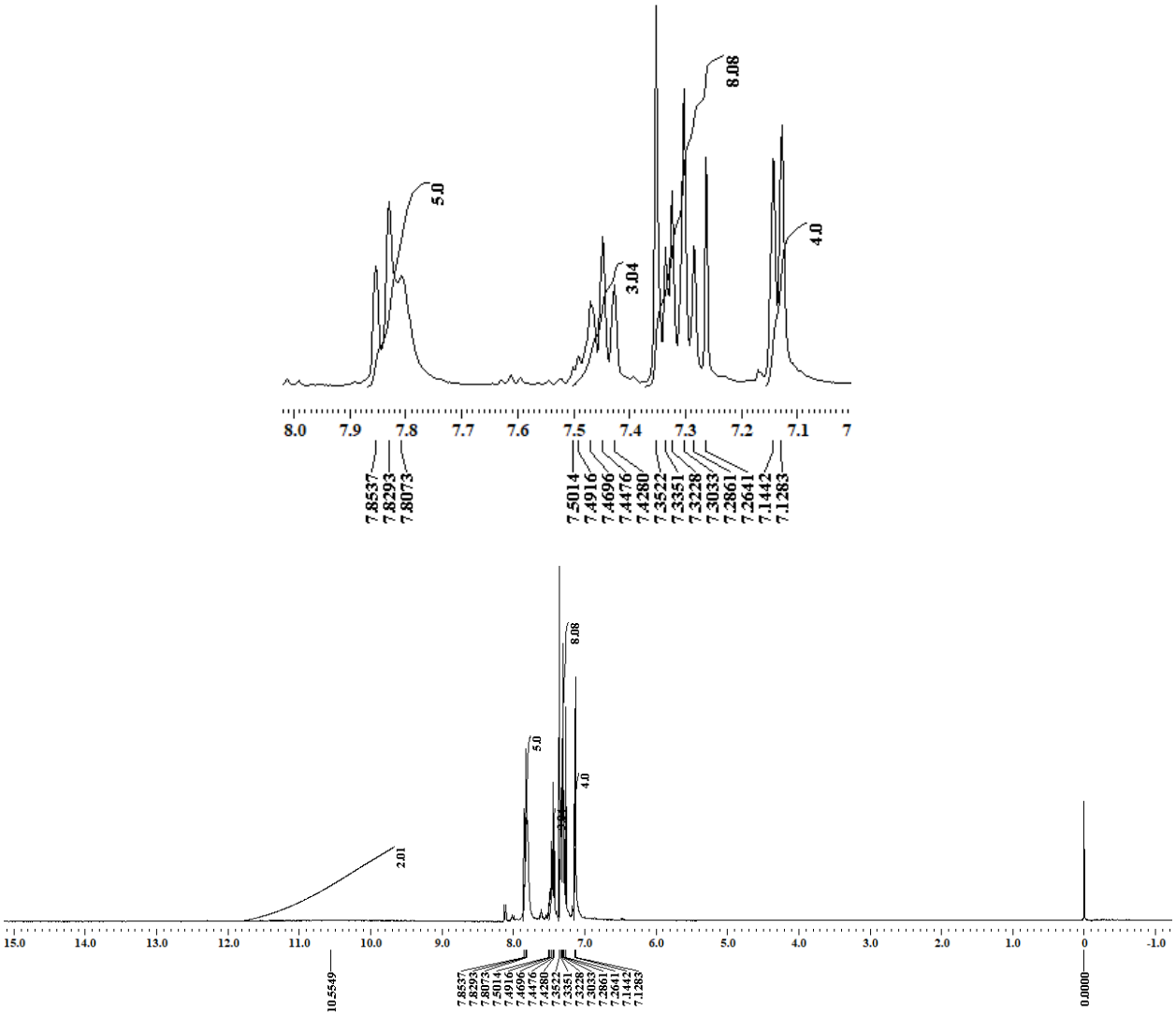
(1Z,1'Z)-N,N'-((4Z,4'E)-(1,3-phenylenebis(iodomethanylylidene))bis(4H-benzo[d][1,3]thiazine-2-yl-4-ylidene))bis(4-methylbenzimidic acid) (7b)



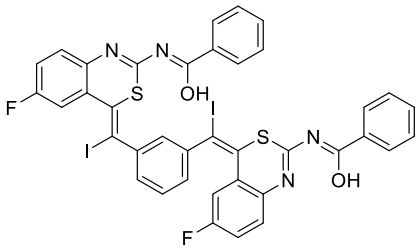
^{1}H NMR



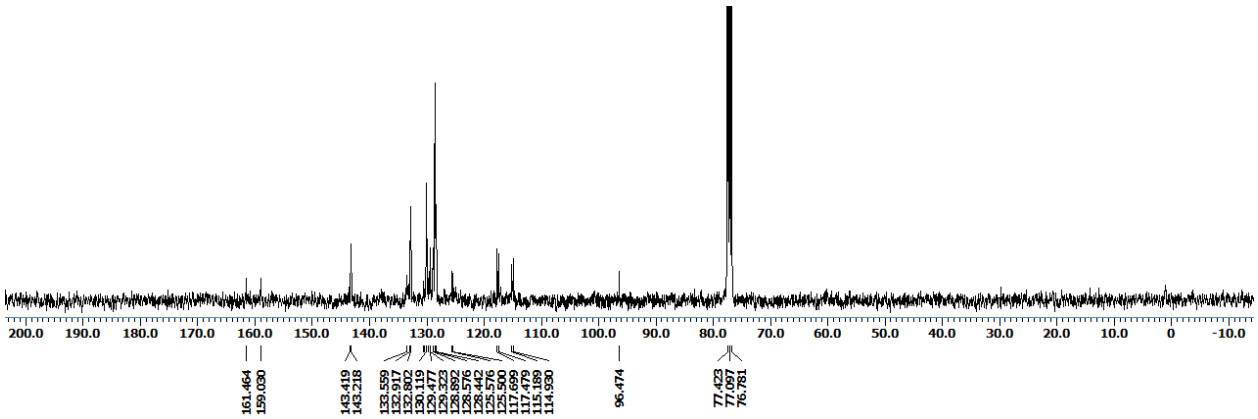
(1Z,1'Z)-N,N'-((4Z,4'E)-(1,3-phenylenebis(iodomethanylylidene))bis(6-fluoro-4H-benzo[d][1,3]thiazine-2-yl-4-ylidene))dibenzimidic acid (7c)



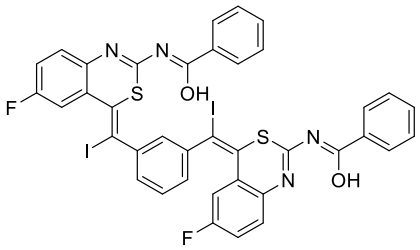
^{13}C NMR



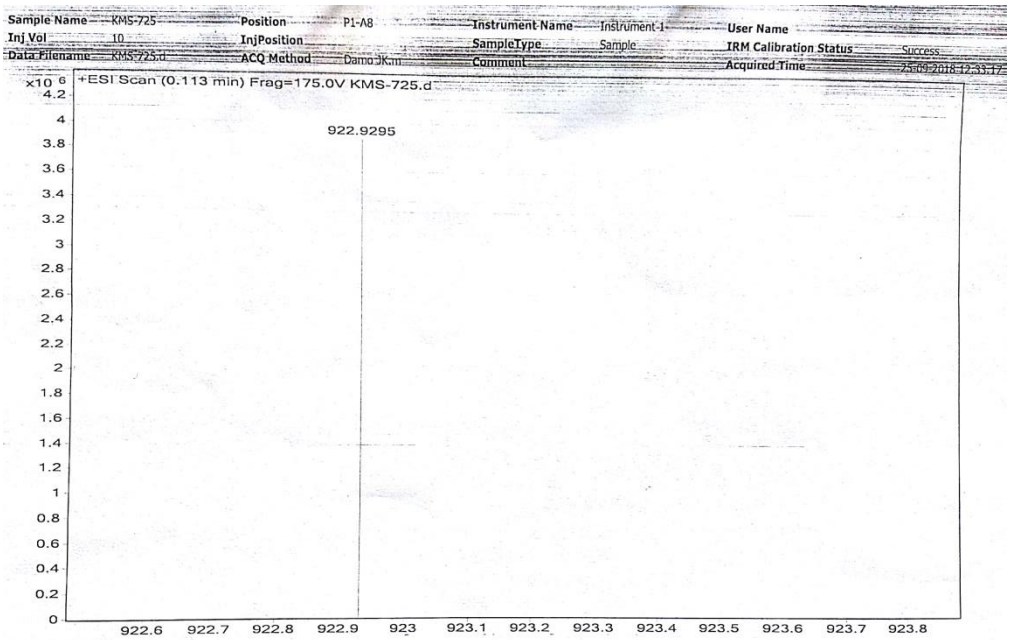
(1Z,1'Z)-N,N'-((4Z,4'E)-(1,3-phenylenebis(iodomethanylylidene))bis(6-fluoro-4H-benzo[d][1,3]thiazine-2-yl-4-ylidene))dibenzimidic acid (7c)



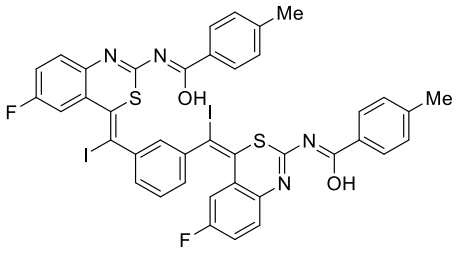
HRMS



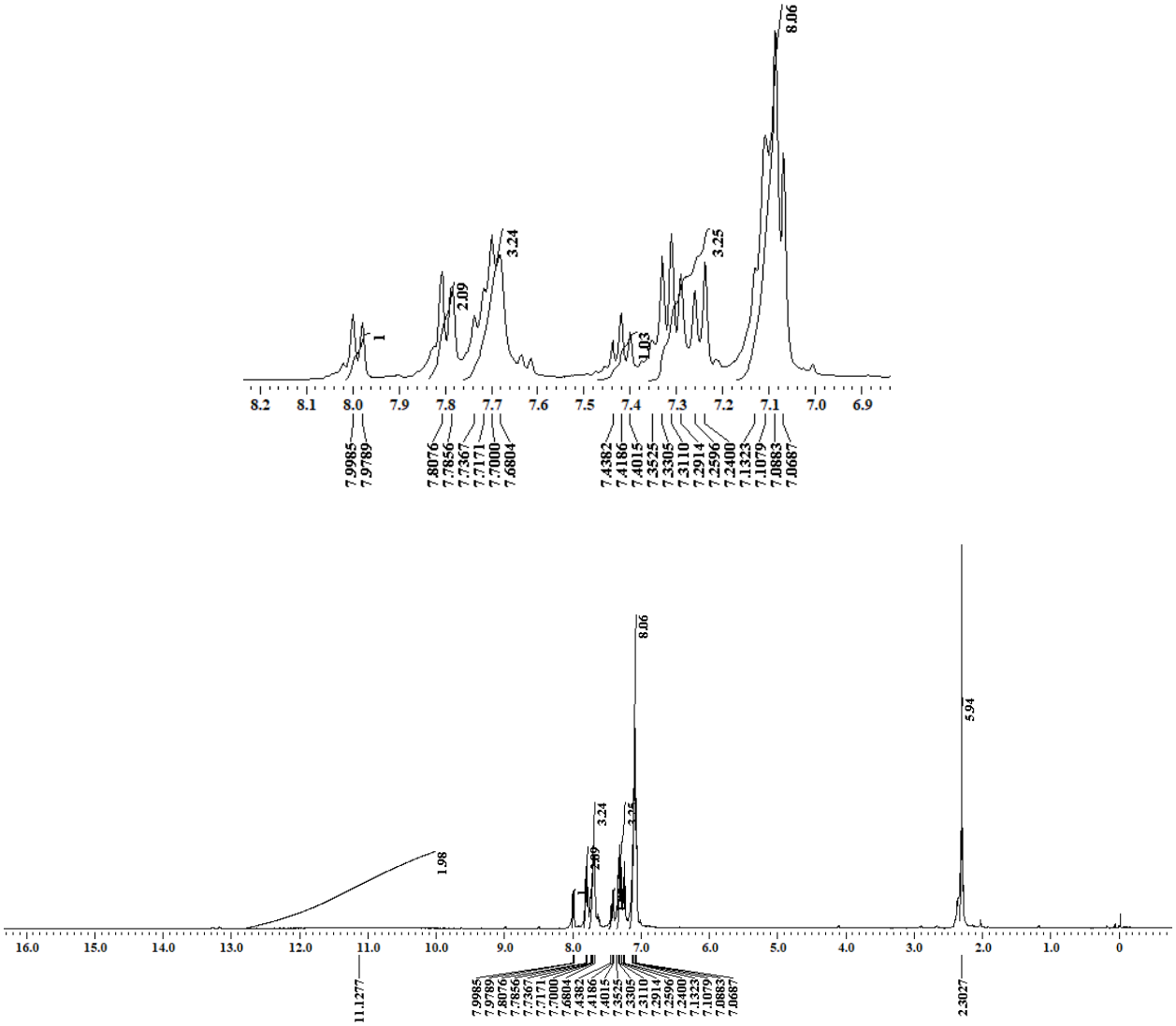
(1Z,1'Z)-N,N'-((4Z,4'E)-(1,3-phenylenebis(iodomethanylylidene))bis(6-fluoro-4H-benzo[d][1,3]thiazine-2-yl-4-ylidene))dibenzimidic acid (7c)



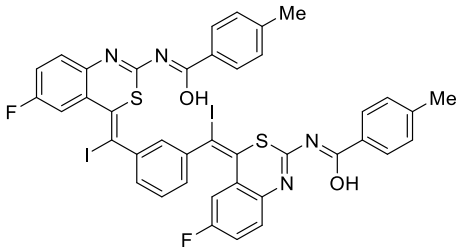
^{1}H NMR



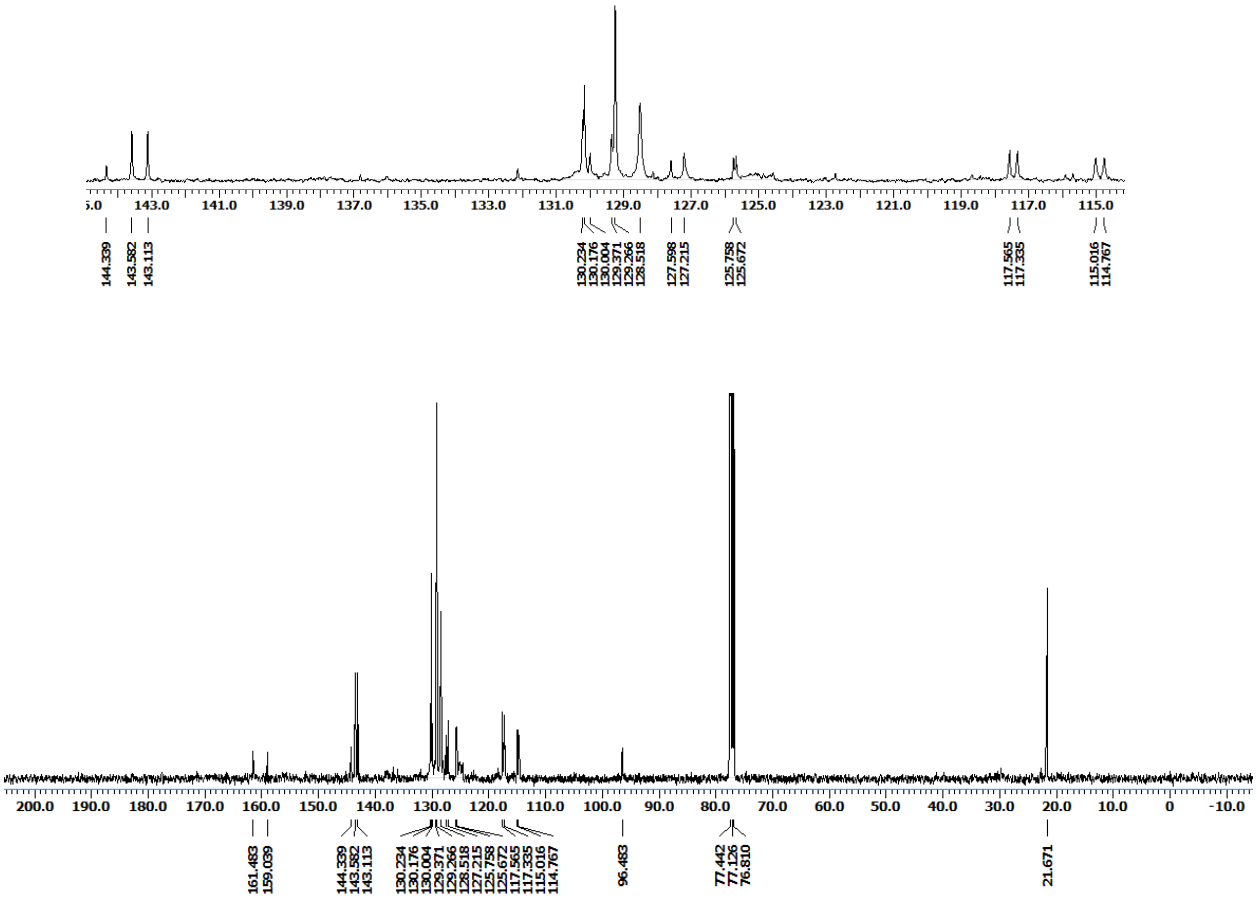
(1Z,1'Z)-N,N'-((4Z,4'E)-(1,3-phenylenebis(iodomethanylylidene))bis(6-fluoro-4H-benzo[d][1,3]thiazine-2-yl-4-ylidene))bis(4-methylbenzimidic acid) (7d)



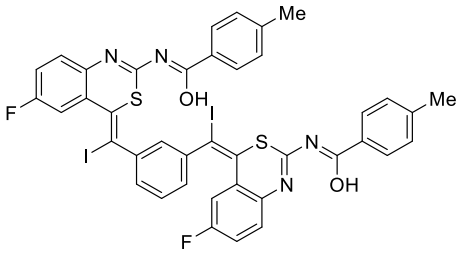
^{13}C NMR



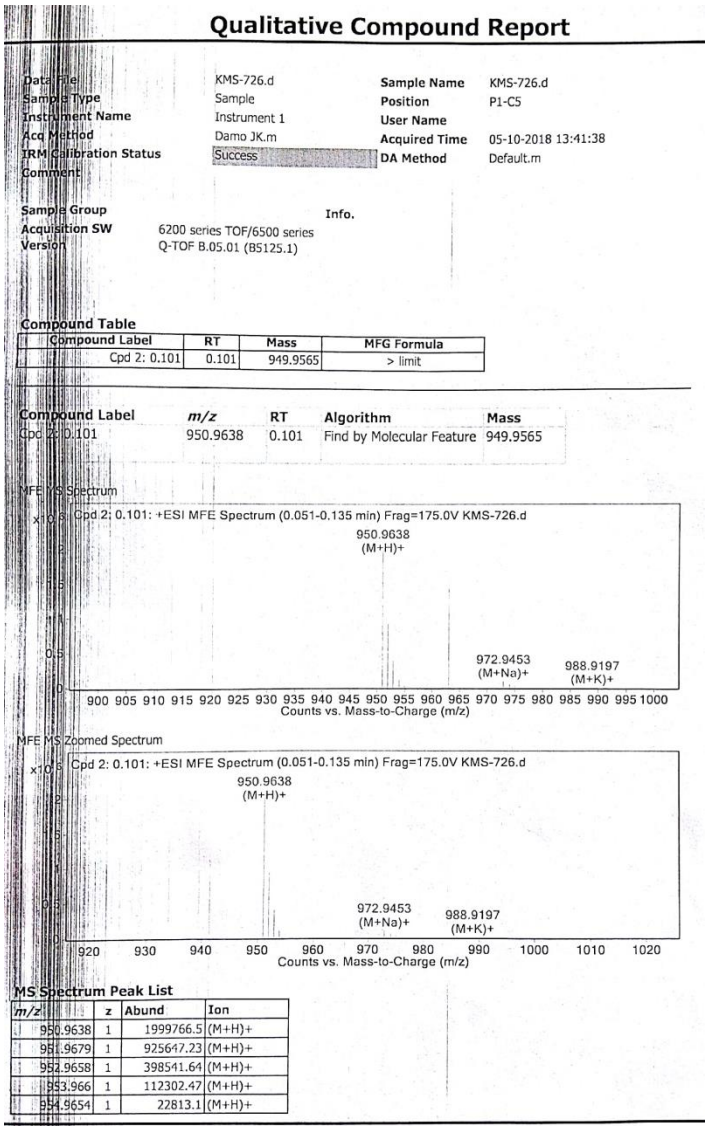
(1Z,1'Z)-N,N'-((4Z,4'E)-(1,3-phenylenebis(iodomethanylylidene))bis(6-fluoro-4H-benzo[d][1,3]thiazine-2-yl-4-ylidene))bis(4-methylbenzimidic acid) (7d)



HRMS



(1Z,1'Z)-N,N'-((4Z,4'E)-(1,3-phenylenebis(iodomethanylylidene))bis(6-fluoro-4H-benzo[d][1,3]thiazine-2-yl-4-ylidene))bis(4-methylbenzimidic acid) (7d)



Qualitative Compound Report

Data File	KMS-726.d	Sample Name	KMS-726.d
Sample Type	Sample	Position	P1-C5
Instrument Name	Instrument 1	User Name	
Acq Method	Damo JK.m	Acquired Time	05-10-2018 13:41:38
IRM Calibration Status	Success	DA Method	Default.m
Comment			

Sample Group — Info.
Acquisition SW Version: 6200 series TOF/6500 series Q-TOF B.05.01 (B5125.1)

Compound Table

Compound Label	RT	Mass	MFG Formula
Cpd 2: 0.101	0.101	949.9565	> limit

Compound Label	m/z	RT	Algorithm	Mass
Cpd 2: 0.101	950.9638	0.101	Find by Molecular Feature	949.9565

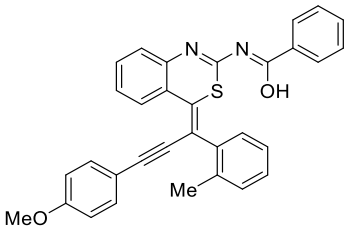
MFE MS Spectrum

MFE MS Zoomed Spectrum

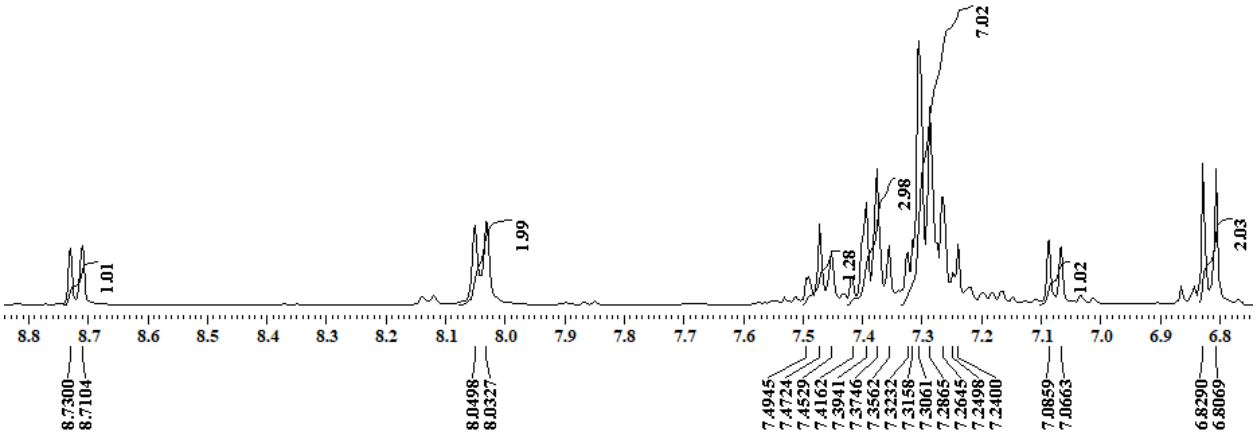
MS Spectrum Peak List

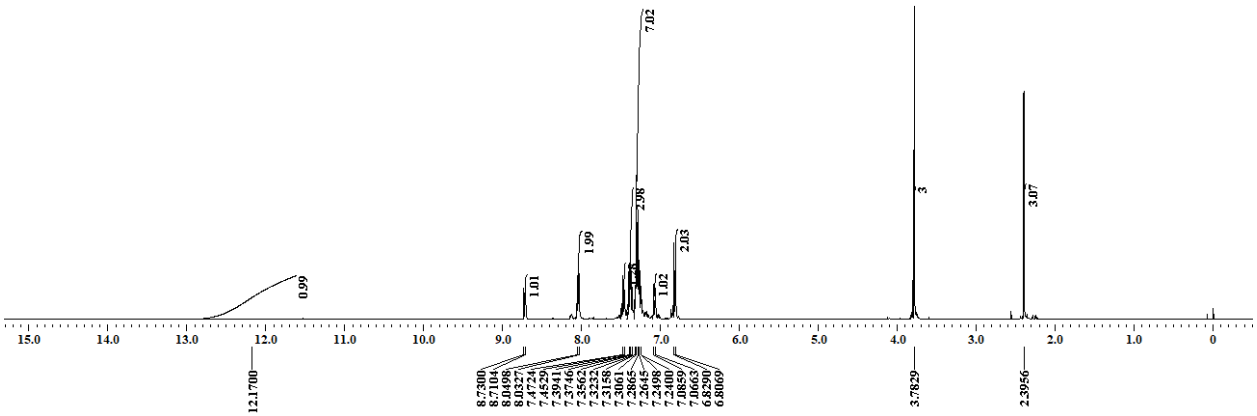
m/z	z	Abund	Ion
950.9638	1	1999766.5	(M+H)+
951.9679	1	925647.23	(M+H)+
952.9658	1	398541.64	(M+H)+
953.966	1	112302.47	(M+H)+
954.9654	1	22813.1	(M+H)+

^{1}H NMR

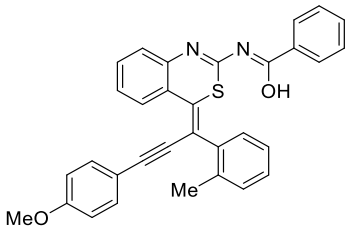


(Z)-N-((Z)-4-(3-(4-methoxyphenyl)-1-(*o*-tolyl)prop-2-yn-1-ylidene)-4H-benzo[*d*][1,3]thiazin-2-yl)benzimidic acid (9)

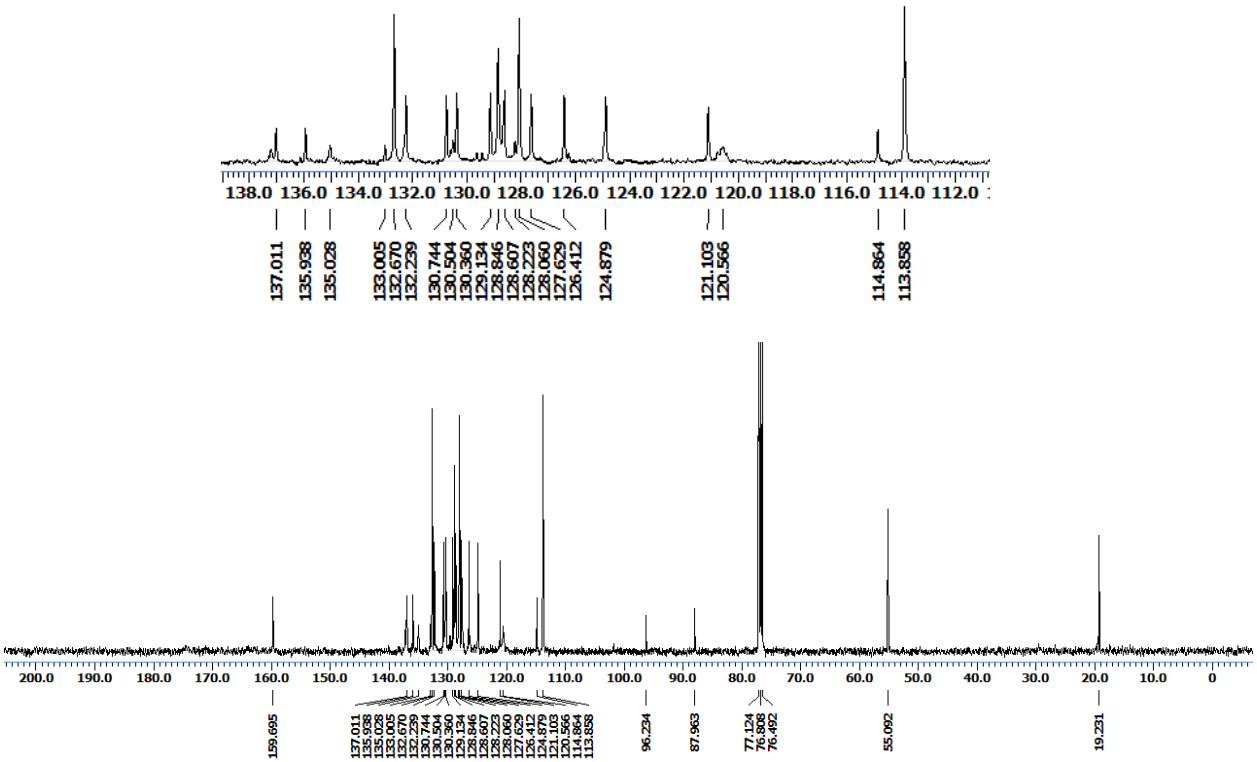




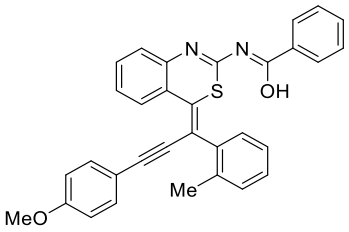
^{13}C NMR



(Z)-N-((Z)-4-(3-(4-methoxyphenyl)-1-(o-tolyl)prop-2-yn-1-ylidene)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (9)



HRMS



(Z)-N-((Z)-4-(3-(4-methoxyphenyl)-1-(o-tolyl)prop-2-yn-1-ylidene)-4H-benzo[d][1,3]thiazin-2-yl)benzimidic acid (9)

Qualitative Compound Report

Data File	KMS 698.d	**Sample Name**	KMS 698
Sample Type	Sample	**Position**	P1-C1
Instrument Name	Instrument 1	**User Name**	
Acq Method	Damo JK.m	**Acquired Time**	30-08-2018 14:05:55
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

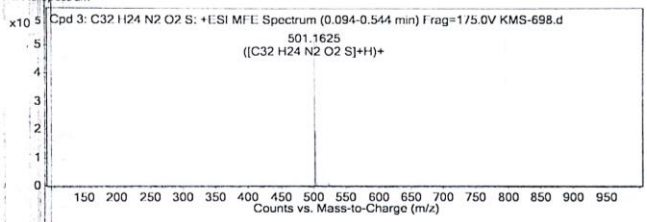
Sample Group **Info.**
Acquisition SW Version 6200 series TOF/6500 series Q-TOF B.05.01 (B5125.1)

Compound Table

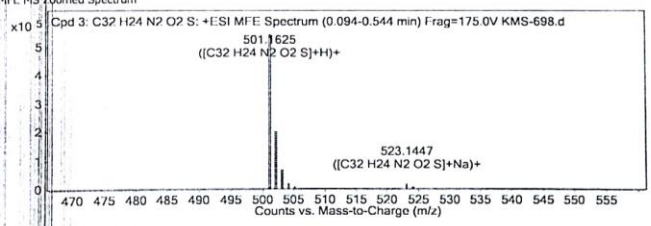
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 3: C32 H24 N2 O2 S	0.17	500.1552	C32 H24 N2 O2 S	C32 H24 N2 O2 S	1.21	C32 H24 N2 O2 S

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 3: C32 H24 N2 O2 S	501.1625	0.12	Find by Molecular Feature	500.1552

MFE MS Spectrum



MFE MS Zoomed Spectrum

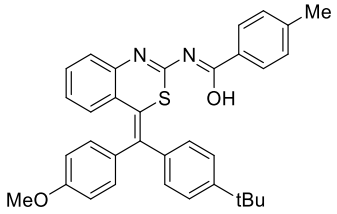


MS Spectrum Peak List

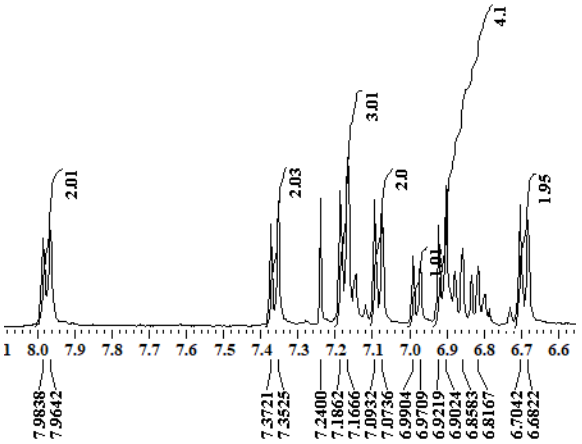
m/z	z	Abund	Formula	Ion
501.1625	1	547205.69	C32 H24 N2 O2 S	(M+H)+
502.1655	1	195714.98	C32 H24 N2 O2 S	(M+H)+
503.1652	1	56763.78	C32 H24 N2 O2 S	(M+H)+
504.1645	1	17501.47	C32 H24 N2 O2 S	(M+H)+
505.1675	1	2661.98	C32 H24 N2 O2 S	(M+H)+
523.1447	1	100917.61	C32 H24 N2 O2 S	(M+Na)+
524.1473	1	4088.72	C32 H24 N2 O2 S	(M+Na)+
525.1451	1	1324.56	C32 H24 N2 O2 S	(M+Na)+
526.1485	1	538.72	C32 H24 N2 O2 S	(M+Na)+

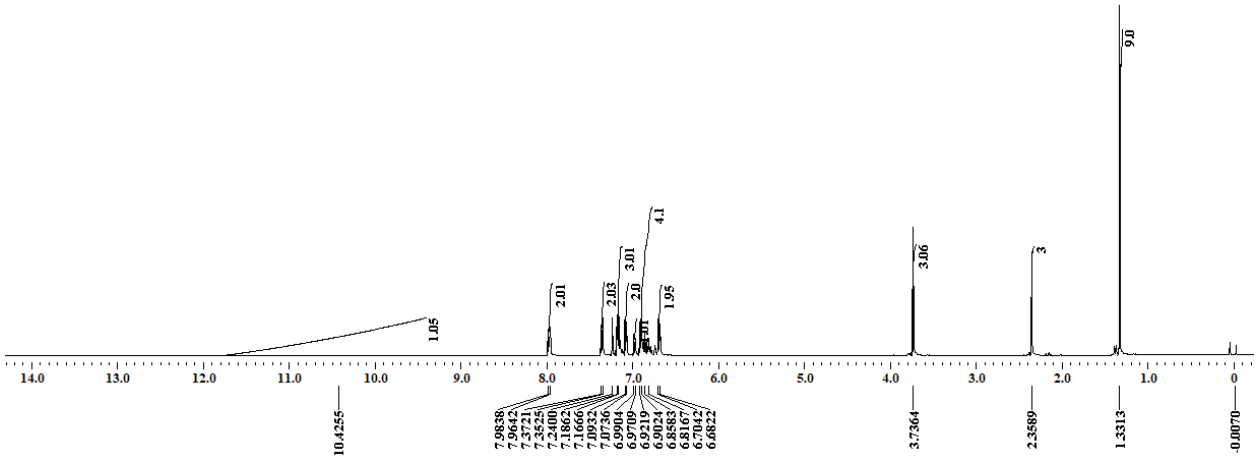
--- End Of Report ---

^{1}H NMR

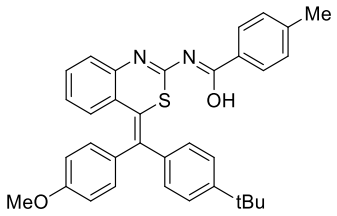


(Z)-N-((E)-4-((4-(tert-butyl)phenyl)(4-methoxyphenyl)methylene)-4H-benzo[d][1,3]thiazin-2-yl)-4-methylbenzimidic acid (11)

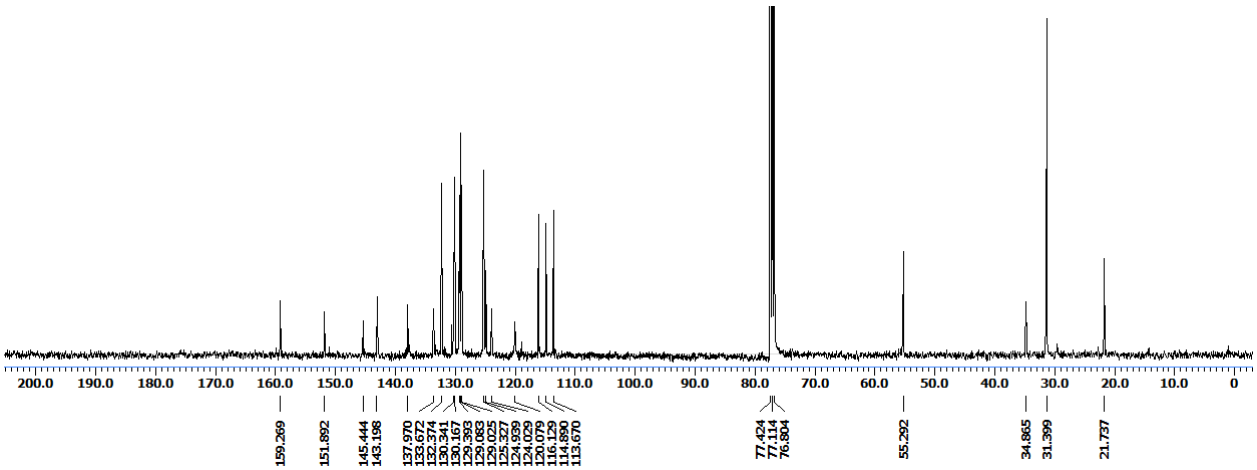




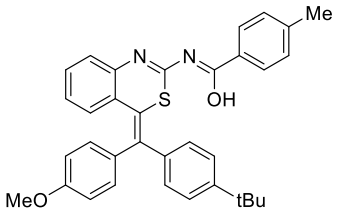
^{13}C NMR



(Z)-N-((E)-4-((4-(tert-butyl)phenyl)(4-methoxyphenyl)methylene)-4H-benzo[d][1,3]thiazin-2-yl)-4-methylbenzimidic acid (11)



HRMS



(Z)-N-((E)-4-((4-(tert-butyl)phenyl)(4-methoxyphenyl)methylene)-4H-benzo[d][1,3]thiazin-2-yl)-4-methylbenzimidic acid (11)

Qualitative Compound Report

Data File	KMS-702.d	**Sample Name**	KMS-702
Sample Type	Sample	**Position**	P1-D4
Instrument Name	Instrument 1	**User Name**	
Acq Method	Damo JK.m	**Acquired Time**	18-09-2018 14:09:37
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

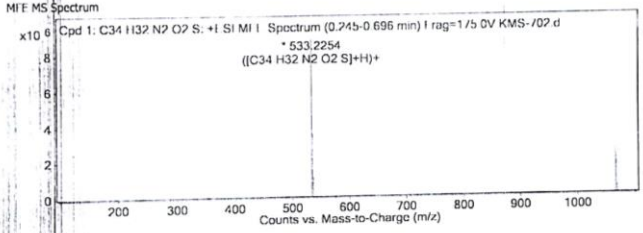
Sample Group **Info.**
Acquisition SW Version 6200 series TOF/6500 series Q-TOF B.05.01 (B5125.1)

Compound Table

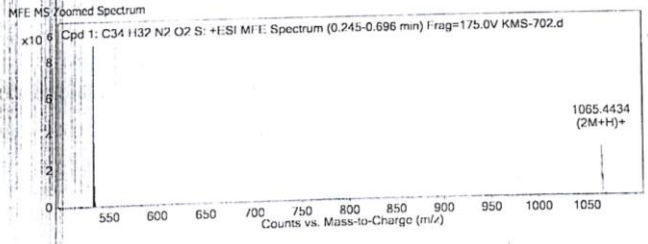
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 1: C34 H32 N2 O2 S	0.386	532.2182	C34 H32 N2 O2 S	C34 H32 N2 O2 S	0.46	C34 H32 N2 O2 S

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: C34 H32 N2 O2 S	533.2254	0.386	Find by Molecular Feature	532.2182

MFE MS Spectrum



MFE MS Zoomed Spectrum

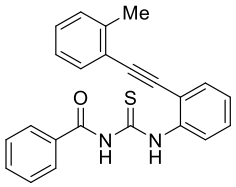


MS Spectrum Peak List

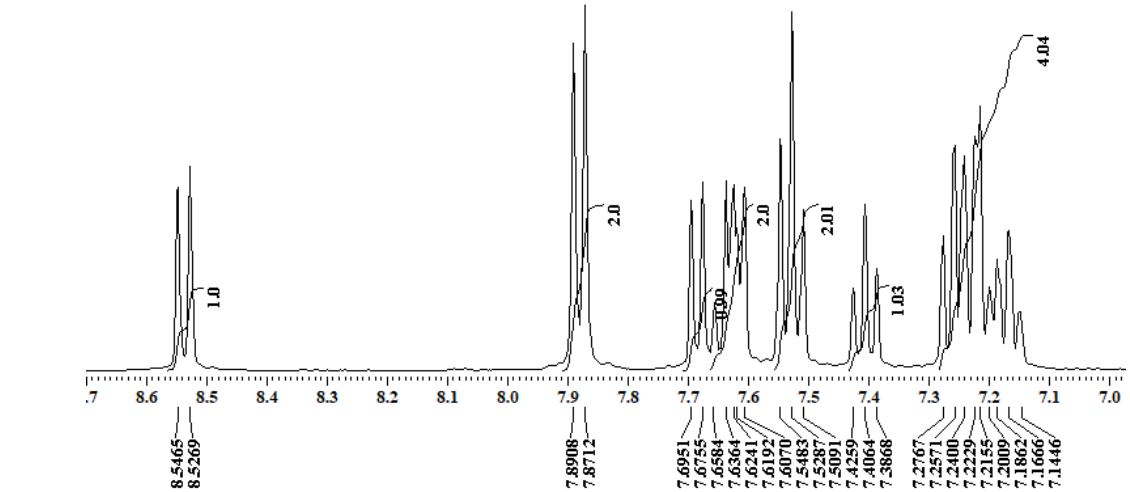
m/z	z	Abund	Formula	Ion
533.2254	1	8870890	C34 H32 N2 O2 S	(M+H)+
534.2287	1	3523160.78	C34 H32 N2 O2 S	(M+H)+
535.2286	1	1094062.46	C34 H32 N2 O2 S	(M+H)+
536.2287	1	234078.33	C34 H32 N2 O2 S	(M+H)+
1065.4434	1	27202/3.5		(2M+H)+
1066.4467	1	212/918.28		(2M+H)+
1067.448	1	1065978.04		(2M+H)+
1068.4484	1	399014.89		(2M+H)+
1069.4485	1	120309.67		(2M+H)+
1070.4485	1	28505.03		(2M+H)+

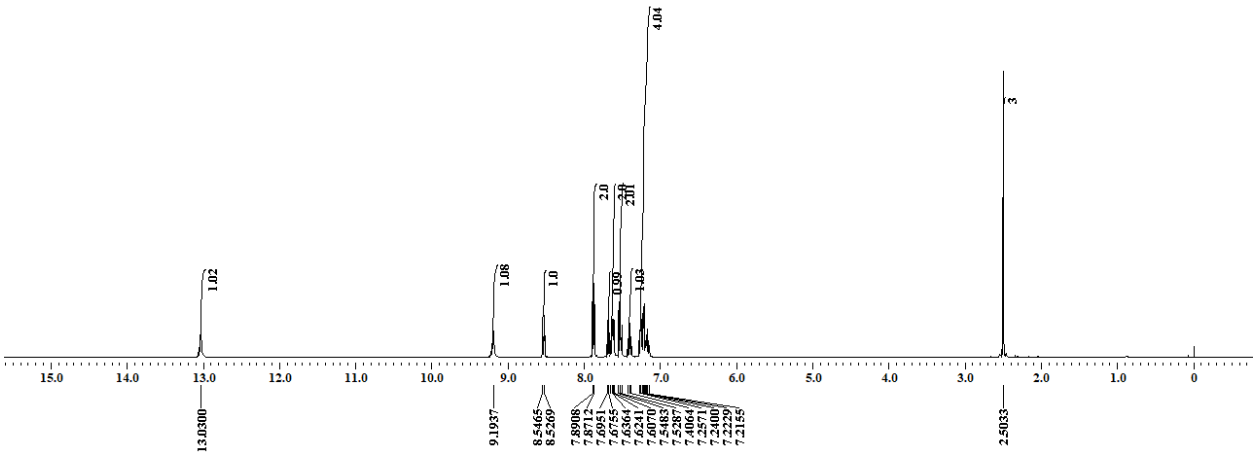
--- End Of Report ---

^{1}H NMR

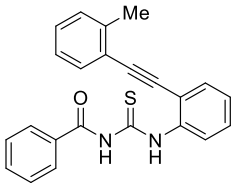


N-((2-(o-tolylethynyl)phenyl)carbamothioyl)benzamide (12a)

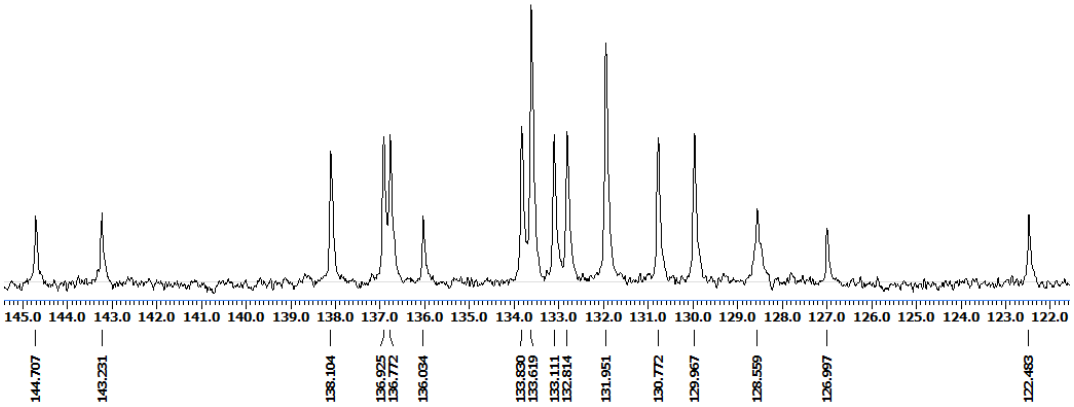


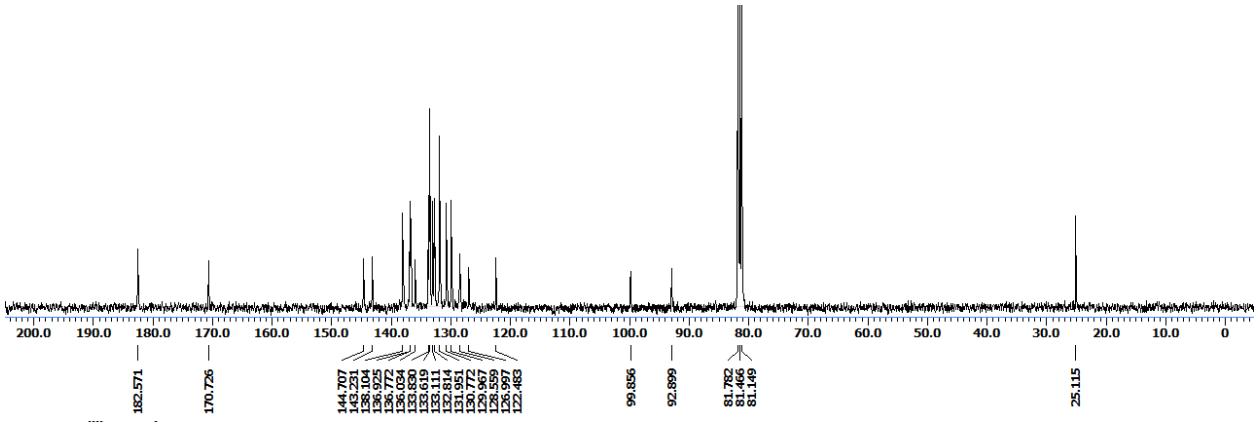


^{13}C NMR

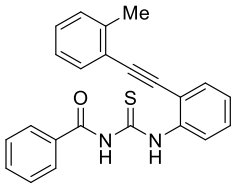


N-((2-(*o*-tolylethynyl)phenyl)carbamothioyl)benzamide (12a)





HRMS



N-((2-(*o*-tolylethynyl)phenyl)carbamothioyl)benzamide (12a)

Qualitative Compound Report

Data File	KMS-689C.d	**Sample Name**	KMS-689C
Sample Type	Sample	**Position**	P1-C3
Instrument Name	Instrument 1	**User Name**	
Acq Method	Damo JK.m	**Acquired Time**	30-08-2018 14:55:45
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

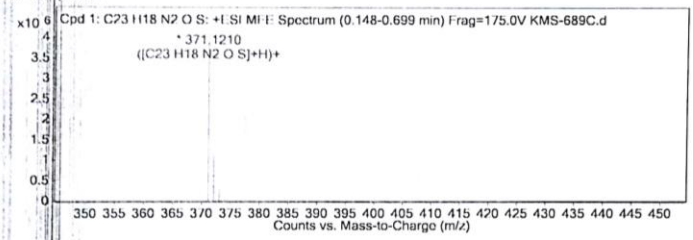
Sample Group **Info.**
Acquisition SW Version 6200 series TOF/6500 series Q-TOF B.05.01 (B5125.1)

Compound Table

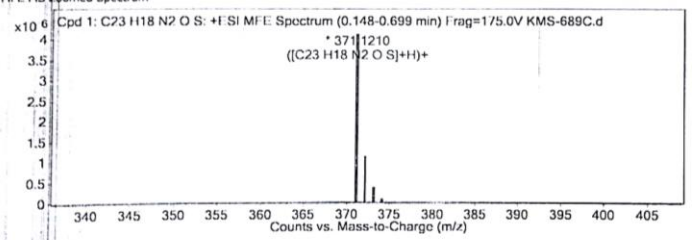
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 1: C23 H18 N2 O S	0.219	370.1138	C23 H18 N2 O S	C23 H18 N2 O S	0.44	C23 H18 N2 O S

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: C23 H18 N2 O S	371.121	0.219	Find by Molecular Feature	370.1138

MFE MS Spectrum



MFE MS Zoomed Spectrum

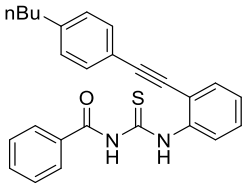


MS Spectrum Peak List

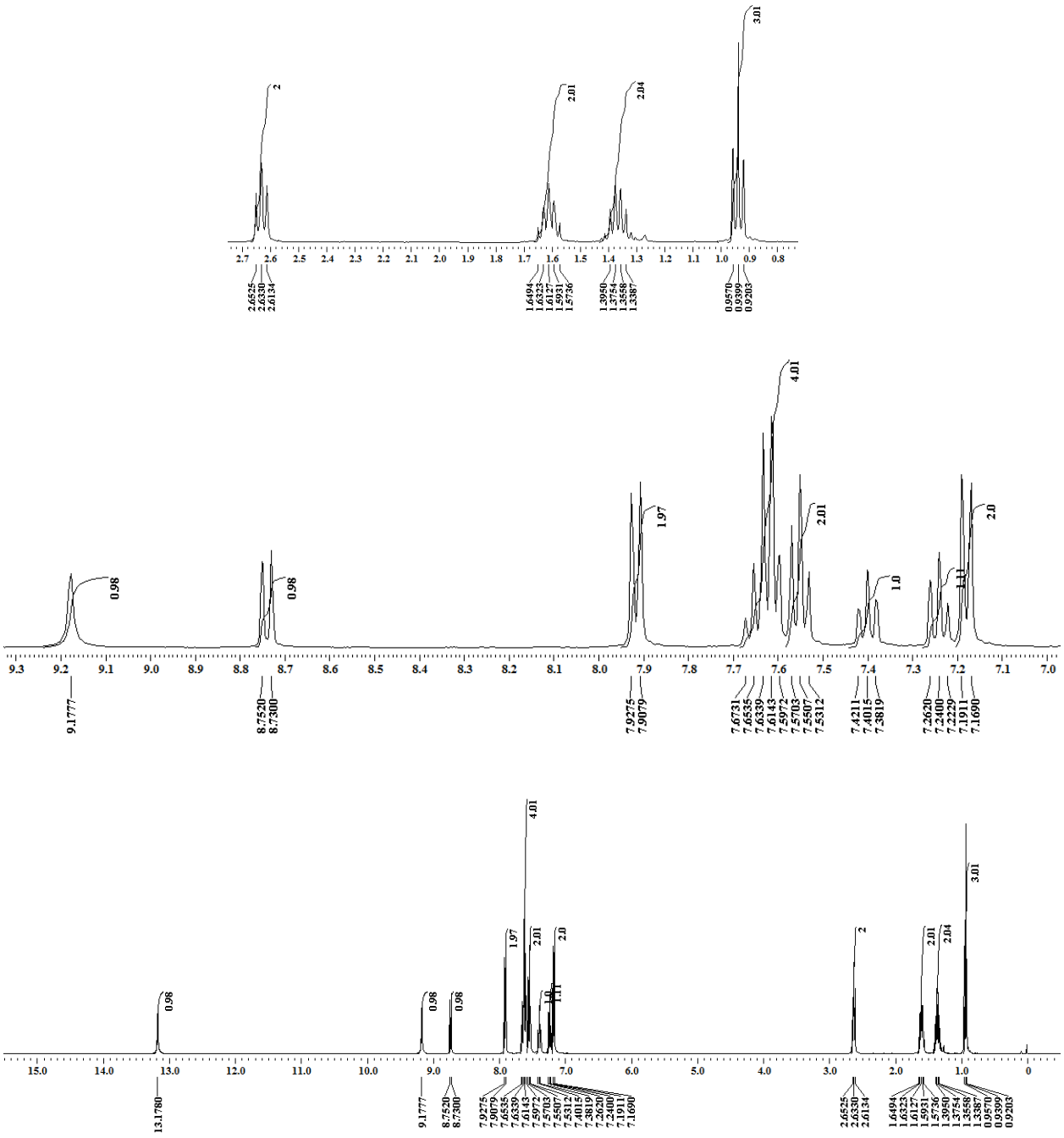
m/z	z	Abund	Formula	Ion
371.1211	1	4128963	C23 H18 N2 O S	(M+H)+
372.1244	1	1109807.9	C23 H18 N2 O S	(M+H)+
373.1221	1	324489.56	C23 H18 N2 O S	(M+H)+
374.1223	1	57873.47	C23 H18 N2 O S	(M+H)+

--- End Of Report ---

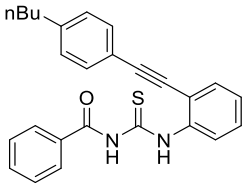
^{1}H NMR



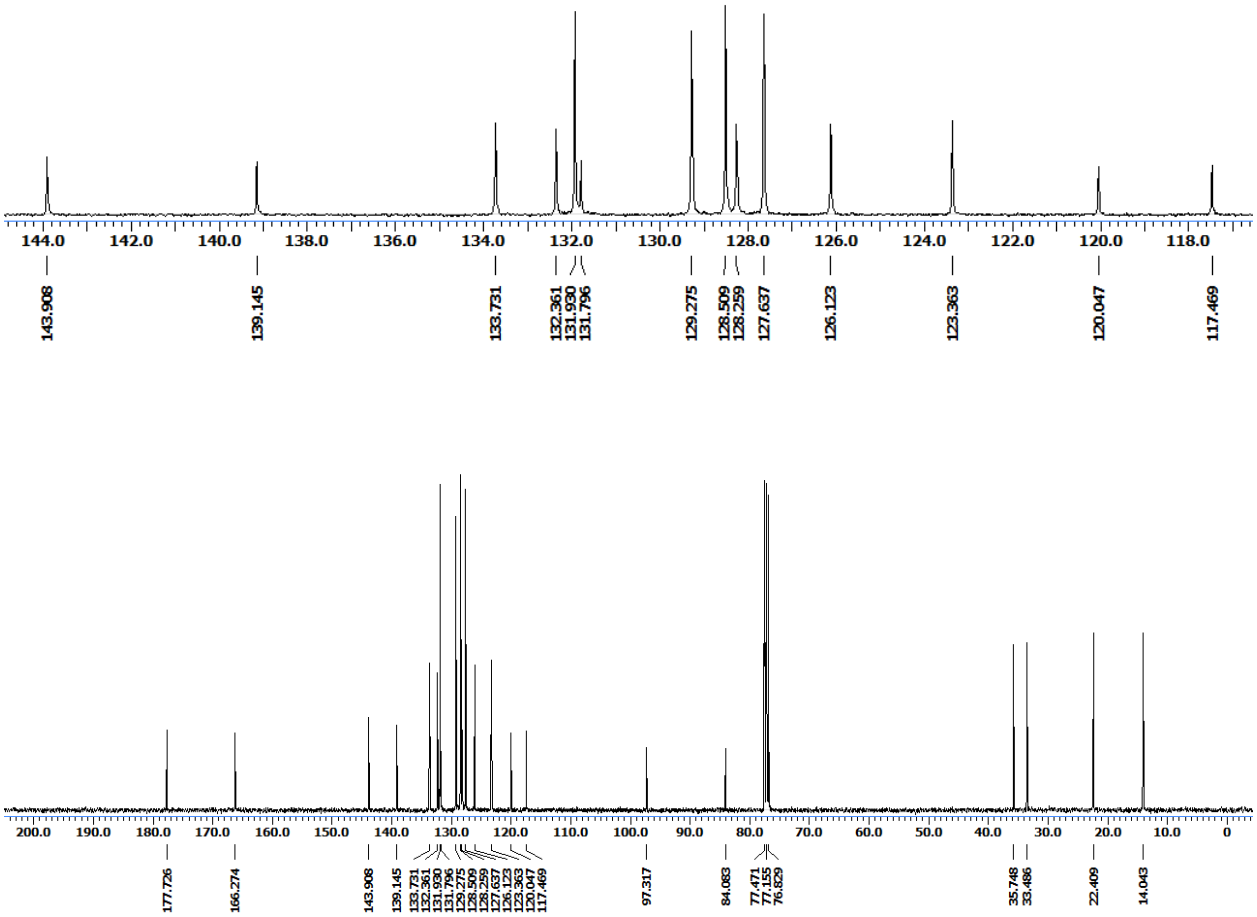
N-((2-((4-Butylphenyl)ethynyl)phenyl)carbamothioyl)benzamide (12b)



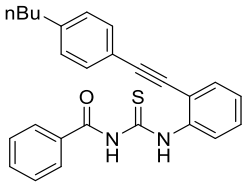
^{13}C NMR



N-((2-((4-Butylphenyl)ethynyl)phenyl)carbamothioyl)benzamide (12b)



HRMS



N-((2-((4-Butylphenyl)ethynyl)phenyl)carbamothioyl)benzamide (12b)

Qualitative Compound Report

Data File	KMS-613.d	**Sample Name**	KMS-613
Sample Type	Sample	**Position**	P1-B1
Instrument Name	Instrument 1	**User Name**	
Acq Method	Damo JK.m	**Acquired Time**	09-10-2018 13:32:20
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

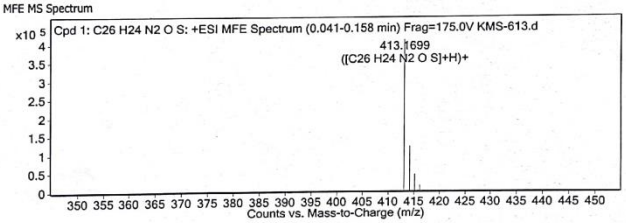
Sample Group **Info.**
Acquisition SW 6200 series TOF/6500 series
Version Q-TOF B.05.01 (B5125.1)

Compound Table

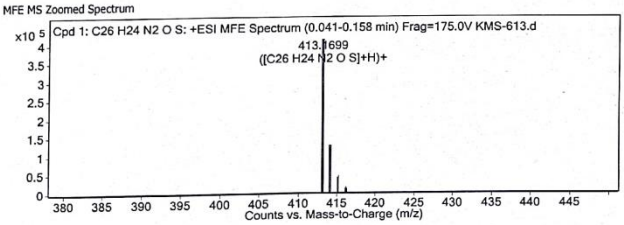
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 1: C26 H24 N2 O S	0.087	412.1633	C26 H24 N2 O S	C26 H24 N2 O S	-5.75	C26 H24 N2 O S

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: C26 H24 N2 O S	413.1699	0.087	Find by Molecular Feature	412.1633

MFE MS Spectrum



MFE MS Zoomed Spectrum

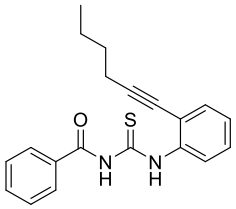


MS Spectrum Peak List

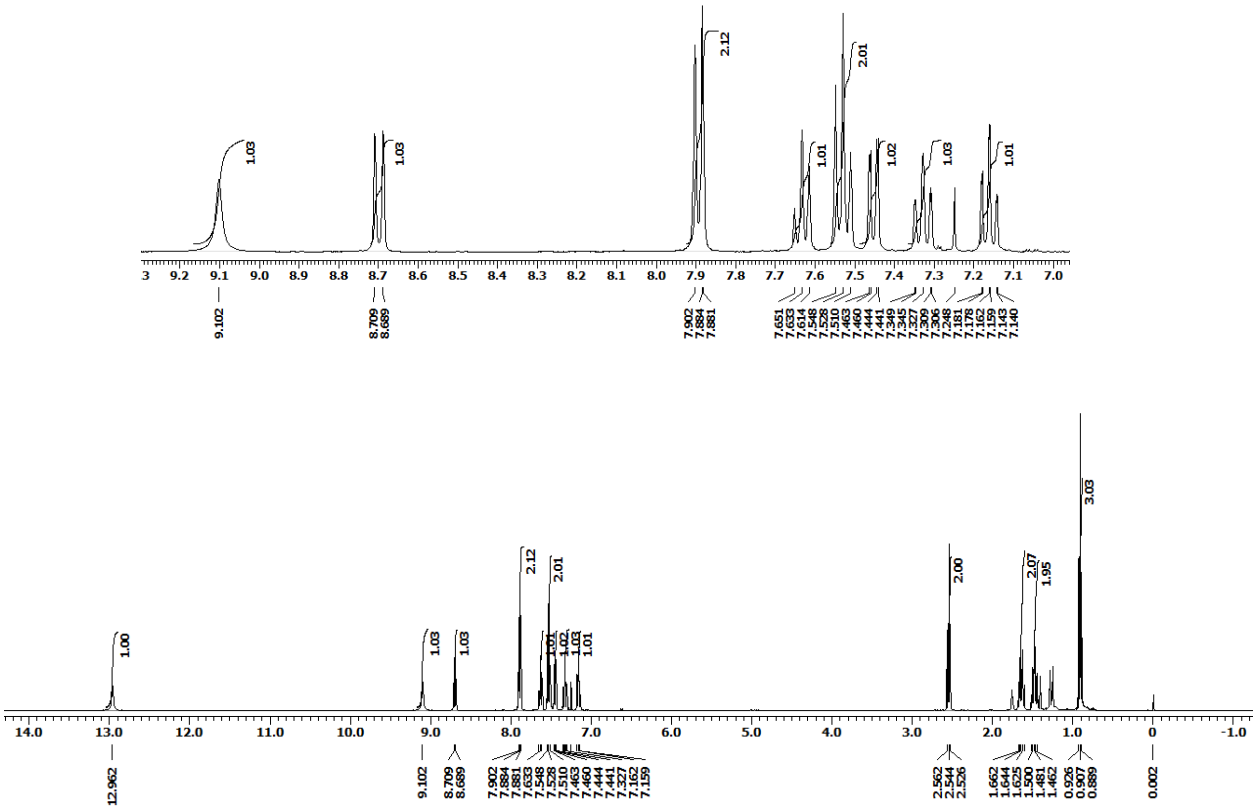
m/z	z	Abund	Formula	Ion
413.1699	1	412458	C26 H24 N2 O S	(M+H)+
414.1726	1	121180.21	C26 H24 N2 O S	(M+H)+
415.1779	1	43768.91	C26 H24 N2 O S	(M+H)+
416.1816	1	14651.67	C26 H24 N2 O S	(M+H)+

--- End Of Report ---

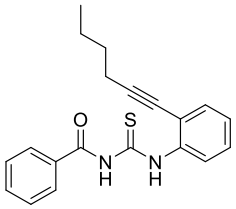
^{1}H NMR



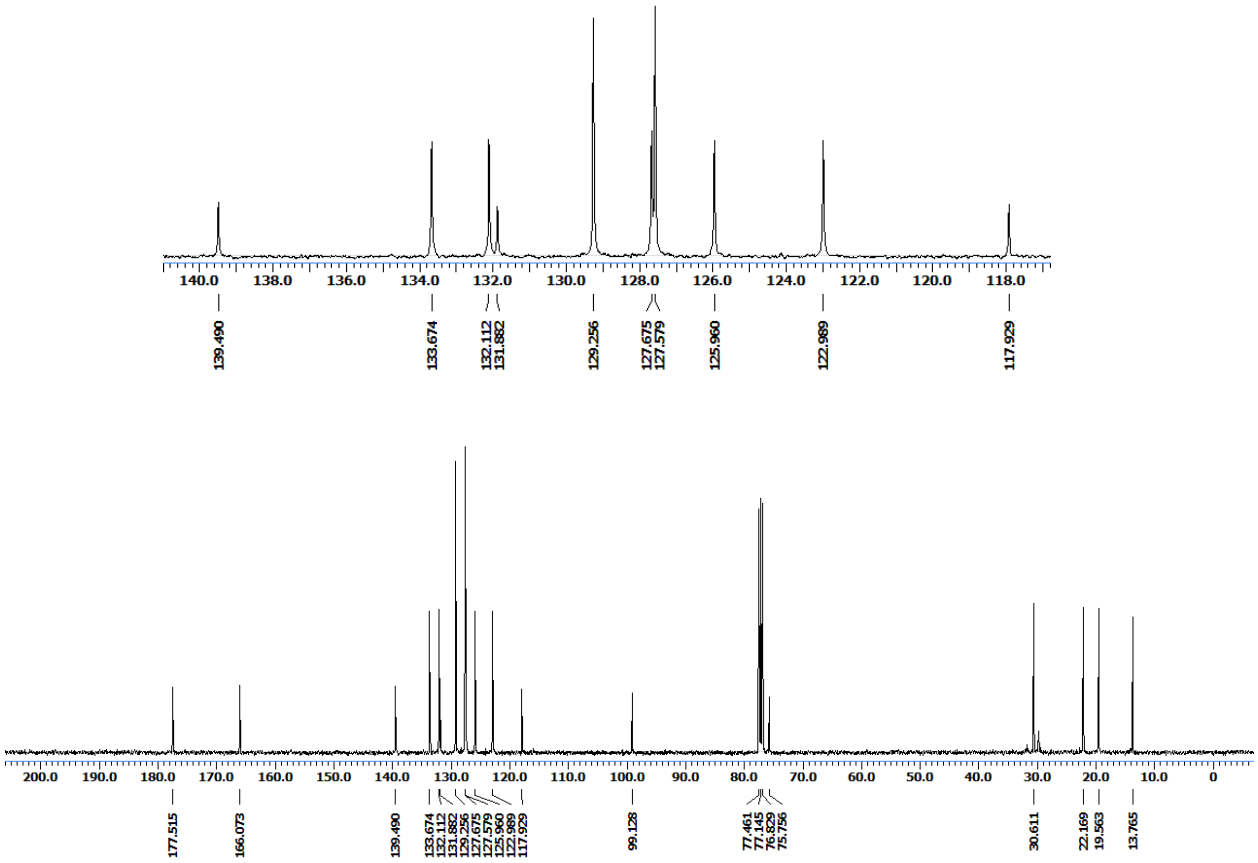
N-((2-(hex-1-yn-1-yl)phenyl)carbamothioyl)benzamide (12c)



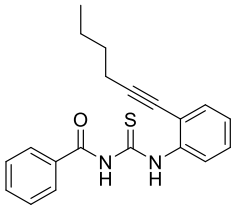
^{13}C NMR



N-((2-(hex-1-yn-1-yl)phenyl)carbamothioyl)benzamide (12c)



HRMS



N-((2-(hex-1-yn-1-yl)phenyl)carbamothioyl)benzamide (12c)