Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Ruthenium catalyzed chemo and site-selective C–H amidation of oxobenzoxazine derivatives with sulfonyl azides

Manickam Bakthadoss,*[a] Polu Vijay Kumar[a], Ravan Kumar[a], Manickam Surendar[a] and Duddu S. Sharada[b]
[a]*Department of Chemistry, Pondicherry University, Pondicherry-605 014, India*
[b]*Department of Chemistry, Indian Institute of Technology, Hyderabad, Kandi,Telangana-502285, India*
E-mail: bhakthadoss@yahoo.com

Electronic Supplementary Information

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EXPERIMENTAL SECTION

General Information and Materials

Commercial reagents were used without further purification. Melting points are uncorrected. IR spectra were recorded on a Perkin Elmer-FTIR spectrometer using solid samples as KBr plates. For compounds ^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (100 MHz, $CDCl_3$) spectra were recorded in deuterochloroform ($CDCl_3$) as well as DMSO-D_6 on a Bruker 400 MHz spectrometer using tetramethylsilane (TMS, $\delta = 0$) as an internal standard at room temperature. Mass spectra were recorded on Agilent 1200 LC/MS-6110 mass spectrometer. Spectral data and copy of ^{1}H, ^{13}C NMR and ESI-HRMS spectra of all compounds (**5a-v, 5aa, 9, 10, 11 & 12**) are listed below.

General Procedure for the Synthesis of Starting Materials:

Based on literature procedure[1], all substituted 2-aryl-benzoxazinones were synthesized from the corresponding benzoyl chlorides and anthranilic acids.

General synthetic procedure for the [$RuCl_2$(*p*-cymene)$_2$] catalyzed chemo and siteselective *ortho*-C-H amidation of 2-aryl-benzoxazinones (3) with sulfonyl azides (4)

To an oven dried single neck test tube employed with 2-aryl-benzoxazinones (**3**) (0.3 mmol), sulfonyl azides (**4**) (0.45 mmol), [$RuCl_2$(*p*-cymene)]$_2$ (5 mol-%), $AgSbF_6$ (20 mol-%) and $Cu(OAc)_2$ (100 mol %) was added DCE (3mL). The test tube was purged with nitrogen gas three times. The reaction mixture was stirred at reflux temperature for 24 h. After completion of the reaction as shown by TLC, the crude reaction mixture was diluted with CH_2Cl_2, filtered over celite pad. The filtrate was concentrated under reduced pressure and purified by column chromatography (10%, EtOAc / hexanes) to provide the desired pure products (**5a-v**) in good yields.

Typical synthetic procedure for the 2-(2-(phenylsulfonamido) benzamido) benzoic acid 5aa

A compound (**5a**) dissolved (50 mg, 0.162 mmol) in acetone (2 mL) was added dropwise slowly to a stirred solution of 4N NaOH (1 mL) at 0 °C and the reaction mixture was allowed to stirr at room temperature until completion of the reaction. The crude mixture was poured into ice water (10 mL), acidified with AcOH and acetone was removed in vacuo. The crude reaction

mixture was filtered off to afford the desired cleavage product (**5aa)** as white amorphorous solid in excellent yield (95 %) without further purification.

Typical synthetic procedure for the 2-(2-(phenylsulfonamido) benzamido) benzoic acid 5aa

A compound (**5a**) dissolved (50 mg, 0.162 mmol) in *t*-butanol (2 mL) was added dropwise slowly to KO*t*-Bu (0.162 mmol.) at 0 °C and the reaction mixture was allowed to stirr at reflux temperature until completion of the reaction. The crude mixture was poured into ice water (10 mL), acidified with 2N dil. HCl. The crude reaction mixture was filtered off to afford the desired cleavage product (**5aa)** as white amorphorous solid in excellent yield (94 %) without further purification.

Typical synthetic procedure for the 2-(2-(phenylsulfonamido) benzamido) benzoic acid 5aa

A compound (**5a**) (50 mg, 0.162 mmol) was added slowly to a stirred solution of HBr in AcOH (0.648 mmol) at 0 °C and the reaction mixture was allowed to stirr at room temperature until completion of the reaction. The crude mixture was poured into ice water (10 mL). The crude reaction mixture was filtered off to afford the desired cleavage product (**5aa)** as white amorphorous solid in excellent yield (92 %) without further purification.

Typical synthetic procedure for the 2-(2-(phenylsulfonamido) benzamido) benzoic acid 5aa

A compound (**5a**) dissolved (50 mg, 0.162 mmol) in TFE : DCE (1:1 ratio, 2 mL) was added dropwise slowly to a stirred solution of $Na_2S_2O_8$ (0.162 mmol) at 0 °C and the reaction mixture was allowed to stirr at reflux temperature until completion of the reaction. The crude mixture was poured into ice water (10 mL) and TFE : DCE mixture was removed in vacuo. The crude reaction mixture was filtered off to afford desired cleavage product (**5aa)** as white amorphorous solid in excellent yield (96 %) without further purification.

Typical synthetic procedure for the 2-(2-(2-((4-methylphenyl)sulfonamido)-4-nitrophenyl)-4-oxoquinazolin-3(4H)-yl)benzoic acid 9

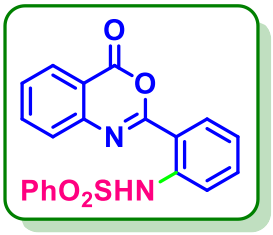
A mixture of compound (**5m**) (50 mg, 0.114 mmol) and anthranilic acid (**6**) dissolved (16 mg, 0.114 mmol) in pyridine (3 mL) at 0 °C and the reaction mixture was allowed to stirr at reflux temperature until completion of the reaction. The crude mixture was poured into ice water (10 mL), acidified with 2N dil. HCl. The crude reaction mixture was filtered off to afford desired

cleavage product (**9)** as white amorphorous solid in excellent yield (87%) without further purification.

Typical synthetic procedure for the removal of directing group (DG) to be used for post-synthetic functionalization:[2]

A compound (**5f, 5r & 5t**) dissolved (50 mg, 0.162 mmol) in MeOH (2 mL) was added dropwise slowly to a stirred solution of NaOMe (0.324 mmol) at 0 °C and the reaction mixture was allowed to stirr at reflux temperature until completion of the reaction. The crude mixture was poured into ice water (10 mL), acidified with 2N dil. HCl. The crude reaction mixture was filtered off to afford desired cleavage products (**10, 11 & 12)** as white amorphorous solids in excellent yields (93%, 91% & 96 % respectively) without further purification.

***N*-(2-(4-oxo-4*H*-benzo[d][1,3]oxazin- yl)phenyl)benzenesulfonamide (5a)**



Physical state: White solid

Reaction Time: 24 h

Yield: 86 % (98 mg)

M.P : 205-210°C

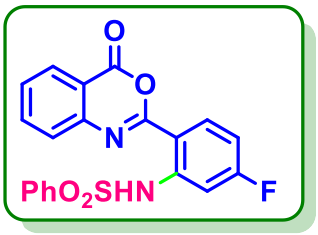
IR (KBr) ν_{max} cm^{-1}: 3492, 1823, 1760, 1579

^{1}H NMR (400 MHz, $CDCl_3$): **δ** 12.3 (s, NH), 8.24 (dd, *J* = 15.6 Hz, 1H), 7.67 (t, *J* = 16 Hz, 1H), 7.65 – 7.48 (m, 3H), 7.39-7.11 (m, 6H), 7.13-7.17 (m, *J* = 15.6 Hz, 1H).

^{13}C NMR (100 MHz, $CDCl_3$): **δ** 157.2, 146.5, 145.0, 139.8, 139.5, 137.3, 134.2, 133.2, 129.9, 129.3, 129.2, 129.0, 127.2, 126.8, 123.6, 119.8, 116.7, 115.7

HRMS (ESI): Calc. for $[(C_{20}H_{14}N_2SO_4)]$ $(M+H)^+$ 379.0753, measured 379.0757

***N*-(5-fluoro-2-(4-oxo-4H-benzo[d][1,3]oxazin-2-yl)phenyl)benzenesulfonamide (5b)**



Physical state: White solid

Reaction Time: 24 h

Yield: 87% (103 mg)

M.P : 151-155 °C

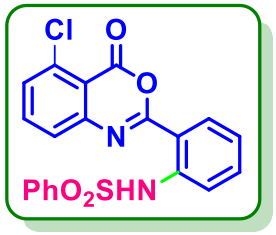
IR (KBr) ν_{max} cm^{-1}: 3461, 1793, 1686, 1636

^{1}H NMR (400 MHz, $CDCl_3$): **δ** 12.65 (s, NH), 8.18-8.26 (m, 2H), 7.88-7.94 (m, 3H), 7.76 (t, *J* = 7.6Hz, 1H), 7.41-7.62 (m, 5H), 6.81-6.85 (m, 1H);

^{13}C NMR (100 MHz, $CDCl_3$): **δ** 157.9, 156.7, 144.7, 139.3, 137.4, 133.5, 132.3, 132.2, 129.4, 129.3, 129.1, 127.3, 126.6, 116.7, 110.9, 110.7, 106.4, 106.1.

HRMS (ESI): Calc. for [($C_{20}H_{14}FSN_2O_4$)] $(M+H)^+$ 397.0658 measured 397.0682.

***N*-(2-(5-chloro-4-oxo-4H-benzo[d][1,3]oxazin-2-yl)phenyl)benzenesulfonamide (5c)**



Physical state: White solid

Reaction Time: 24 h

Yield: 78 % (96 mg)

M.P : 194-199 °C

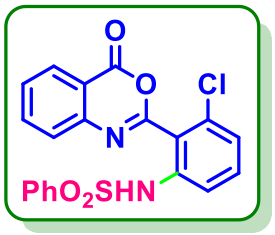
IR (KBr) ν_{max} cm^{-1}: 3473, 1801, 1760, 1637

^{1}H NMR (400 MHz, $CDCl_3$): **δ** 12.14(s, NH), 8.17 (dd, *J* = 6.4, 1.6 Hz, 1H), 7.64-7.84 (m, 6H), 7.36-7.52 (m, 4H), 7.14-7.18 (m, 1H)

^{13}C NMR (100 MHz, $CDCl_3$): **δ** 165.8, 157.9, 147.3, 139.9, 139.5, 136.7, 136.6, 134.6, 133.3, 131.7, 131.0, 129.2, 127.2, 125.7, 123.6, 119.6, 115.1, 114.5

HRMS (ESI): Calc. for [($C_{20}H_{14}ClN_2SO_4$)] $(M+H)^+$ 413.0363, measured 413.0368.

***N*-(3-chloro-2-(4-oxo-4H-benzo[d][1,3]oxazin-2-yl)phenyl)benzenesulfonamide (5d)**



Physical state: White solid

Reaction Time: 24h

Yield: 79 % (98 mg)

M.P : 151-155 ^{o}C

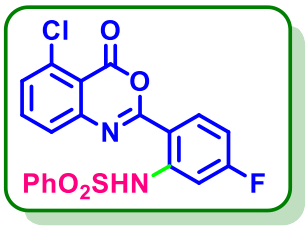
IR (KBr) ν_{max} cm^{-1}: 3432, 1809, 1767, 1634

^{1}H NMR (400 MHz, $CDCl_3$): **δ** 13.01 (s, NH), 9.00 (d, *J* = 8.4 Hz, 1H), 8.34 (dd, *J* = 6.4, 1.6 Hz, 1H), 8.23 (dd, *J* = 6.8, 1.2 Hz, 1H), 7.42-7.77(m, 7H), 7.28(d, *J* = 1.2 Hz, 1H), 7.20 (d, *J* = 8, 0.8 Hz, 1H)

^{13}C NMR (100 MHz, $CDCl_3$): **δ** 165.5, 158.3, 157.4, 145.3, 140.6, 137.0, 134.6, 131.8, 131.4, 130.8, 129.7, 129.0, 127.2, 126.1, 123.6, 120.9, 116.8, 115.0

HRMS (ESI): Calc. for $[(C_{20}H_{13}N_2SClO_4)]$ $(M+H)^+$ 413.0363, measured 413.0368.

***N*-(2-(5-chloro-4-oxo-4H-benzo[d][1,3]oxazin-2-yl)-5-fluorophenyl) benzenesulfonamide (5e)**



Physical state: White Solid

Reaction Time: 24 h

Yield: 89% (115 mg)

M.P : 210-215 ^{o}C

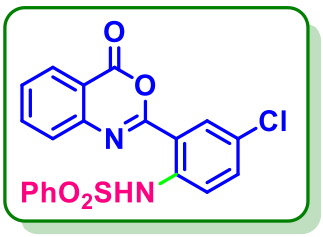
IR (KBr) ν_{max} cm^{-1}: 3457, 1793, 1640

^{1}H NMR (400 MHz, $CDCl_3$): **δ** 12.47 (s, NH), 8.19 (dd, *J* = 6.4, 2.8 Hz, 1H), 7.75 – 7.90 (m, 2H), 7.43-7.66 (m, 7H), 6.81-6.86 (m, 1H)

^{13}C NMR (100 MHz, $CDCl_3$): **δ** 165.8, 157.9, 147.3, 139.9, 139.5, 136.7, 136.6, 134.6, 133.3, 131.7, 130.1, 129.2, 127.2, 125.7, 123.6, 119.6, 115.1, 114.5

HRMS (ESI): Calc. for $[(C_{20}H_{13}ClFN_2SO_4)]$ $(M+H)^+$ 444.0300, measured 444.0412.

***N*-(4-chloro-2-(4-oxo-4H-benzo[d][1,3]oxazin-2-yl)phenyl)benzenesulfonamide (5f)**



Physical state: White solid

Reaction Time: 24h

Yield: 77 % (95 mg)

M.P : 189-205 ^{o}C

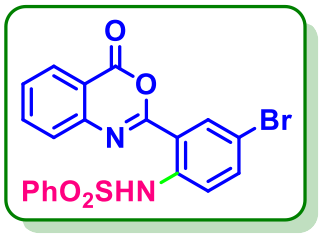
IR (KBr) ν_{max} cm^{-1}: 3414, 1801, 1760, 1637

^{1}H NMR (400 MHz, $CDCl_3$): **δ** 13.1 (s, NH), 9.00 (d, *J* = 1.2Hz, 1H), 8.27-8.98 (m, 2H), 8.10 (s, 1H), 8.00-8.09 (m, 1H), 7.86-8.00 (m, 1H), 7.27-7.69 (m, 5H), 7.23-7.25 (m, 1H)

^{13}C NMR (100 MHz, $CDCl_3$): **δ** 165.0, 158.2, 157.8, 145.3, 140.8, 137.8, 137.2, 134.9, 132.3, 130.5, 129.9, 129.2, 127.4, 126.5, 123.6, 120.8, 116.8, 115.2

HRMS (ESI): Calc. for $[(C_{20}H_{13}N_2SClO_4)]$ $(M+H)^+$ 413.0363, measured 413.2690.

***N*-(4-bromo-2-(4-oxo-4H-benzo[d][1,3]oxazin-2yl)phenyl)benzenesulfonamide(5g)**



Physical state: White solid

Reaction Time: 24 h

Yield: 87 % (119 mg)

M.P : 198-199 ^{o}C

IR (KBr) ν_{max} cm^{-1}: 3442, 1804, 1765, 1633

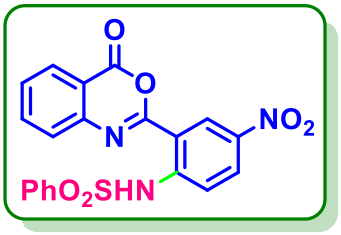
^{1}H NMR (400 MHz, $CDCl_3$): **δ** 12.23(s, NH), 8.24-8.27 (m, 2H), 7.91– 7.93 (m, 1H), 7.76 – 7.82 (m, 3H), 7.54-7.65 (m, 4H), 7.36-7.50 (m, 2H)

^{13}C NMR (100 MHz, $CDCl_3$): **δ** 157.6, 156.0, 144.7, 139.2, 138.7, 137.4, 136.9, 133.4, 132.2, 129.7, 129.3, 129.1, 127.2, 126.9, 121.2, 117.1, 116.8, 116.4

HRMS (ESI): Calc. for $[(C_{20}H_{14}BrN_2SO_4)]$ $(M+H)^+$ 455.9858, measured 456.9864 & 458.9844

***N*-(4-nitro-2-(4-oxo-4*H*-benzo[d][1,3]oxazin-2-yl)phenyl)benzenesulfonamide (5h)**

Physical state: White solid



Reaction Time: 24 h

Yield: 76 % (96 mg)

M.P : 151-155 ^{o}C

IR (KBr) ν_{max} cm^{-1}: 3542, 1824, 1764, 1653

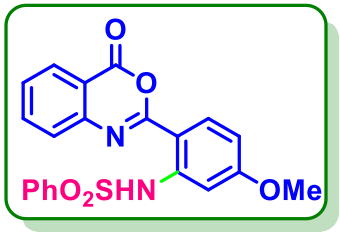
^{1}H NMR (400 MHz, $CDCl_3$): **δ** 13.05 (s, NH), 9.1 (d, *J* = 2.8 Hz, 1H), 8.30 (dd, *J* = 4.8, 2.4Hz, 2H), 7.48-7.84 (m, 9H)

^{13}C NMR (100 MHz, $CDCl_3$): **δ** 144.9, 139.0, 137.6, 134.0, 130.2, 129.4, 128.8, 127.4, 126.9, 125.9, 117.9, 114.4

HRMS (ESI): Calc. for $[(C_{20}H_{14}N_3SO_6)]$ $(M+H)^+$ 424.0603, measured 424.0596.

***N*-(5-methoxy-2-(4-oxo-4H-benzo[d][1,3]oxazin-2-yl)phenyl) benzenesulfonamide (5i)**

Physical state: White Solid



Reaction Time: 24 h

Yield: 85 % (104 mg)

M.P : 132-134 ^{o}C

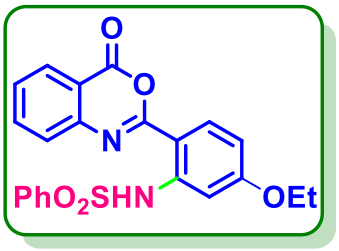
IR (KBr) ν_{max} cm^{-1}: 3442, 1812, 1746, 1637

^{1}H NMR (400 MHz, $CDCl_3$): **δ** 12.59 (s, 1H), 8.21 (dd, *J* = 6.8, 1.2 Hz, 1H), 8.08 (d, *J* = 9.2 Hz, 1H), 7.85-7.89 (m, 3H), 7.37-7.56 (m, 5H), 7.24 (d, *J* = 6.4 Hz, 1H), 6.64 (dd, *J* = 6.8, 2.4Hz, 1H), 3.84 (s, 3H);

^{13}C NMR (100 MHz, $CDCl_3$): **δ** 164.2, 158.3, 157.4, 145.4, 141.9, 139.5, 137.2, 133.3, 131.5, 129.2, 128.9, 128.6, 127.3, 126.4, 116.4, 110.1, 107.9, 104.0, 55.8.

HRMS (ESI): Calc. for $[(C_{21}H_{16}N_2SO_5)]$ $(M+H)^+$ 409.0858, measured 409.0856.

***N*-(5-ethoxy-2-(4-oxo-4H-benzo[d][1,3]oxazin-2-yl)phenyl)benzenesulfonamide (5j)**



Physical state: White Solid

Reaction Time: 24 h

Yield: 89 % (112 mg)

M.P : 168-170°C

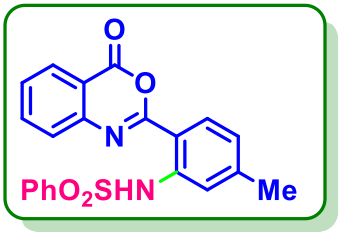
IR (KBr) ν_{max} cm^{-1}: 3469, 1800, 1753, 1625

^{1}H NMR (400 MHz, $CDCl_3$): **δ** 12.57 (s, NH), 8.21 (dd, *J* = 6.4, 1.2 Hz, 1H), 8.07 (d, *J* = 8.8 Hz, 1H), 7.84-7.87 (m, 3H), 7.70-7.72 (m, 1H), 7.24-7.56(m,5H), 6.63 (dd, *J* = 6.4, 2.4 Hz, 1H), 4.07 (q, *J* = 7.6, 6.8 Hz, 2H), 1.42 (t, *J* = 6.8 Hz, 3H)

^{13}C NMR (100 MHz, $CDCl_3$): **δ** 163.6, 158.4, 157.4, 145.4, 141.9, 139.6, 137.2, 133.2, 131.5, 129.2, 128.9, 128.6, 127.3, 126.6, 116.4, 110.7, 107.8, 104.4, 64.2, 14.7

HRMS (ESI): Calc. for $[(C_{22}H_{18}N_2SO_5)]$ $(M+H)^+$ 423.1015, measured 423.1001.

***N*-(5-methyl-2-(4-oxo-4H-benzo[d][1,3]oxazin-2-yl)phenyl) benzenesulfonamide (5k)**



Physical state: White Solid

Reaction Time: 24 h

Yield: 80 % (94 mg)

M.P : 112-114 °C

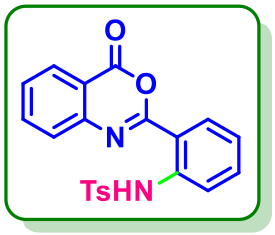
IR (KBr) ν_{max} cm^{-1}: 3452, 1803, 1765, 1637;

^{1}H NMR (400 MHz, $CDCl_3$): **δ** 12.27 (s, NH), 8.23 (dd, *J* = 16, 6.8 Hz, 1H), 8.03 (d, *J* = 8.4 Hz, 1H), 7.73-7.89 (m, 4H), 7.34-7.59 (m, 5H), 6.95 (dd, *J* = 0.8 Hz, 1H), 2.38 (s, 3H)

^{13}C NMR (100 MHz, $CDCl_3$): **δ** 158.2, 157.4, 145.6, 145.2, 139.7, 139.6, 137.3, 133.1, 129.7, 129.1, 129.0, 128.9, 127.2, 126.6, 124.7, 120.3, 116.7, 113.1, 22.2

HRMS (ESI): Calc. for $[(C_{21}H_{17}N_2SO_4)]$ $(M+H)^+$ 393.0909, measured 393.0907

4-Methyl-*N*-(2-(4-oxo-4H-benzo[d][1,3]oxazin-2-yl)phenyl) benzenesulfonamide (5l)



Physical state: White solid

Reaction Time: 24 h

Yield: 82 % (96 mg)

M.P : 201-203 °C

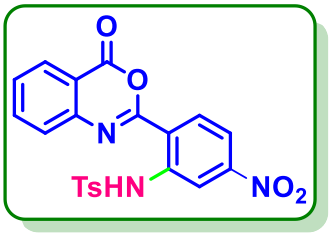
IR (KBr) ν_{max} cm^{-1}: 3346, 1829, 1774, 1654

^{1}H NMR (400 MHz, $CDCl_3$): **δ** 12.21 (s, NH), 8.23-8.25 (m, 1H), 8.15 (dd, *J* = 6. 8, 1.2 Hz, 1H), 7.89-7.93 (m, 1H), 7.68-7.78 (m, 4H), 7.58-7.62 (m, 1H), 7.47-7.49 (m, 1H), 7.12-7.16 (m, 3H), 2.32 (s, 3H)

^{13}C NMR (100 MHz, $CDCl_3$): **δ** 158.1, 157.2, 145.1, 144.1, 139.8, 137.3, 136.5, 134.1, 129.8, 129.8, 129.3, 128.9, 127.3, 126.8, 123.5, 119.8, 116.7, 115.7, 21.6

HRMS (ESI): Calc. for $[(C_{21}H_{17}O_4SN_2)]$ $(M+H)^+$ 393.0909, measured 393.0906.

4-Methyl-*N*-(5-nitro-2- (4-oxo-4H-benzo [d][1,3] oxazin-2-yl)phenyl) benzenesulfonamide (5m)



Physical state: White solid

Reaction Time: 24h

Yield: 79 % (104 mg)

M.P : 241-243 °C

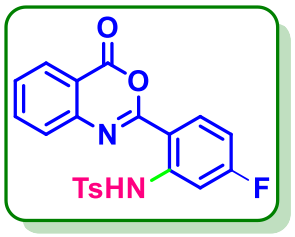
IR (KBr) ν_{max} cm^{-1}: 3512, 1822, 1766, 1665

^{1}H NMR (400 MHz, $CDCl_3$): **δ** 12.51 (s, NH), 8.54 (d, *J* = 2 Hz, 1H), 8.36 (d, *J* = 8.4 Hz, 1H), 8.29 (dd, *J* = 6.4, 1.2 Hz, 1H), 7.66-7.99 (m, 7H), 7.25 (d, *J* = 9.2 Hz, 1H), 2.36 (s, 3H)

^{13}C NMR (100 MHz, $CDCl_3$): **δ** 157.3, 155.8, 150.6, 145.0, 144.4, 140.9, 137.6, 135.9, 134.7, 133.6, 131.1, 130.3, 130.2, 129.2, 127.6, 127.2, 119.3, 113.3, 21.7

HRMS (ESI): Calc. for $[(C_{21}H_{16}N_3SO_6)]$ $(M+H)^+$ 438.0760, measured 438.0770.

***N*-(5-fluoro-2-(4-oxo-4H-benzo[d][1,3]oxazin-2-yl)phenyl)-4-methyl benzene sulfonamide (5n)**



Physical state: White solid

Reaction Time: 24 h

Yield: 81 % (100 mg)

M.P : 198-199 ^oC

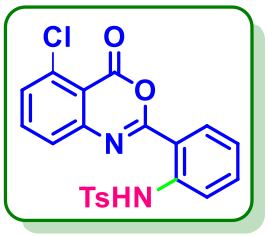
IR (KBr) ν_{max} cm^{-1}: 3490, 1810, 1723, 1645

^1H NMR (400 MHz, $CDCl_3$): **δ** 12.57 (s, NH), 8.17-8.26 (m, *2*H), 7.89-7.93 (m, 1H), 7.75 (dd, *J* = 4.8, 1.6 Hz, 3H), 7.45-7.62 (m, 2H), 7.21 (d, *J* = 8.4 Hz, 2H), 6.80-6.84 (m, 1H), 2.35 (s, 3H)

^{13}C NMR (100 MHz, $CDCl_3$): **δ** 157.9, 156.7, 145.0, 137.4, 136.3, 132.2, 130.0, 129.3, 129.0, 127.3, 126.9, 126.7, 116.7, 111.3, 110.8, 110.6, 106.4, 106.1, 21.7

HRMS (ESI): Calc. for $[(C_{21}H_{16}N_2FSO_4)]$ $(M+H)^+$ 411.0815, measured 411.0841.

***N*-(2-(5-chloro-4-oxo-4H-benzo[d][1,3]oxazin-2-yl)phenyl)-4-methyl benzene sulfonamide (5o)**



Physical state: White solid

Reaction Time: 24 h

Yield: 80% (102 mg)

M.P : 180-181 ^oC

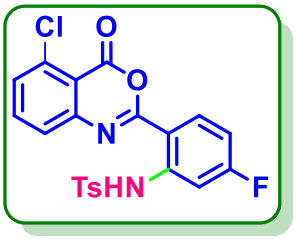
IR (KBr) ν_{max} cm^{-1}: 3512, 1812, 1737, 1680

^1H NMR (400 MHz, $CDCl_3$): **δ** 12.03 (s, NH), 8.14 (d, *J* = 8 Hz, 1H), 7.47 – 7.79 (m, 7H), 7.15 (m, 3H), 2.33 (s, 3H)

^{13}C NMR (100 MHz, $CDCl_3$): **δ** 158.0, 154.7, 147.4, 144.3, 140.0, 136.7, 136.6, 136.5, 134.5, 131.6, 130.0, 129.8, 127.3, 125.8, 123.5, 119.8, 115.2, 114.5, 21.7

HRMS (ESI): Calc. for $[(C_{21}H_{16}ClN_2SO_4)]$ $(M+H)^+$ 427.0519, measured 427.0514.

***N*-(2-(5-chloro-4-oxo-4H-benzo[d][1,3]oxazin-2-yl)-5-fluorophenyl)-4-methylbenzene sulfonamide (5p)**



Physical state: White solid

Reaction Time: 24 h

Yield: 81 % (108 mg)

M.P : 240-242 ^oC

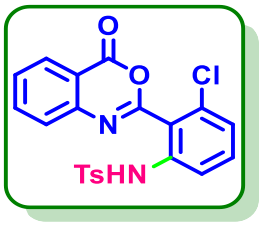
IR (KBr) ν_{max} cm^{-1}: 3381, 1787, 1634

^1H NMR (400 MHz, $CDCl_3$): **δ** 12.4 (s, NH), 8.61-8.57 (d, *J* = 16 Hz, 1H), 7.58-7.79 (m, 5H), 7.45(dd, *J* = 8.0, 2.8 Hz, 1H), 7.22 (d, *J* = 8 Hz, 2H), 6.80 – 6.85(m, 1H), 2.36 (s, 3H)

^{13}C NMR (100 MHz, $CDCl_3$): **δ** 157.7, 154.6, 147.2, 144.8, 136.8, 136.2, 132.5, 131.6, 130.0, 127.3, 125.6, 114.6, 113.9, 111.0, 110.6, 106.6, 106.1, 104.1, 21.7

HRMS (ESI): Calc. for $[(C_{21}H_{15}ClFN_2SO_4)]$ $(M+H)^+$ 445.0425, measured 445.0444.

3-chloro-2-(4-oxo-4*H*-benzo[d][1,3]oxazin-2-yl)phenyl)-4-methylbenzenesulfonamide (5q)



Physical state: White solid

Reaction Time: 24 h

Yield: 71 % (91 mg)

M.P : 185-187 ^oC

IR (KBr) ν_{max} cm^{-1}: 3452, 1802, 1743, 1624

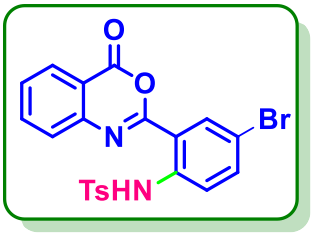
^1H NMR (400 MHz, $CDCl_3$): **δ** 8.89 (s, NH), 8.21 (dd, *J* = 6.8, 1.2 Hz, 1H), 7.91–7.95 (m, 1H), 7.64-7.72 (m, 3H), 7.36 – 7.50 (m, 4H), 7.15 (dd, *J* = 5.2, 1.6 Hz, 1H), 6.89 (d, *J* = 8 Hz, 2H), 2.31 (s, 3H)

^{13}C NMR (100 MHz, $CDCl_3$): **δ** 158.0, 155.3, 152.6, 145.1, 144.8, 137.6, 137.2, 135.4, 134.2, 132.6, 130.0, 129.9, 128.8, 127.1, 126.5, 125.6, 123.7, 117.0, 21.6

HRMS (ESI): Calc. for $[(C_{21}H_{16}ClN_2SO_4)]$ $(M+H)^+$ 427.0519, measured 427.0530.

***N*-(4-bromo-2-(4-oxo-4H-benzo[d][1,3]oxazin-2-yl)phenyl)-4-methylbenzene sulfonamide (5r)**

Physical state: White solid



Reaction Time: 24 h

Yield: 82 % (116 mg)

M.P : 195-196 °C

IR (KBr) ν_{max} cm^{-1}: 3456, 1804, 1732, 1637

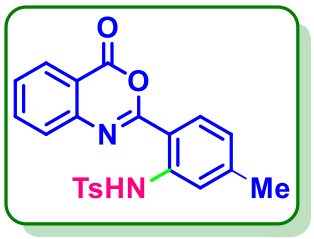
^{1}H NMR (400 MHz, $CDCl_3$): **δ** 12.10 (s, NH), 8.24-8.28 (m, 2H), 7.54-7.95 (m, 7H), 7.15-7.17 (m, 2H), 2.33 (s, 3H)

^{13}C NMR (100 MHz, $CDCl_3$): **δ** 157.8, 156.2, 144.8, 144.4, 138.9, 137.4, 136.9, 132.2, 131.8, 130.6, 129.9, 129.7, 129.1, 127.3, 126.9, 121.3, 116.8, 116.3, 21.7.

HRMS (ESI): Calc. for $[(C_{21}H_{16}BrN_2SO_4)]$ $(M+H)^+$ 471.0014, measured 471.0021 & 473.003.

***N*-(5-methyl-2-(4-oxo-4*H*-benzo[d][1,3]oxazin-2-yl)phenyl)-4-methylbenzene sulfonamide (5s)**

Physical state: White solid



Reaction Time: 24 h

Yield: 77 % (94 mg)

M.P : 155-156 °C

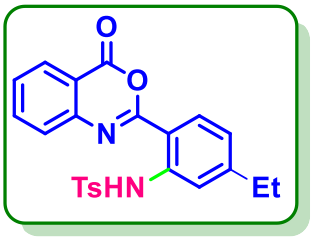
IR (KBr) ν_{max} cm^{-1}: 3410, 1803, 1725, 1613

^{1}H NMR (400 MHz, $CDCl_3$): **δ** 12.18 (s, 1H), 8.22 (dd, *J* = 6.8, 1.2 Hz, 1H), 8.02 (d, *J* = 8Hz, 1H), 7.39-7.91 (m, 6H), 7.13 (d, *J* = 8 Hz, 2H), 6.95 (dd, *J* = 7.2, 0.8 Hz, 1H), 2.37 (s, 3H), 2.32 (s, 3H)

^{13}C NMR (100 MHz, $CDCl_3$): **δ** 158.3, 157.4, 145.5, 145.2, 144.0, 139.8, 137.2, 136.6, 130.4, 129.7, 129.0, 128.9, 127.7, 126.6, 124.6, 120.3, 116.6, 113.2, 22.2, 21.6

HRMS (ESI): Calc. for $[(C_{22}H_{19}N_2SO_4)]$ $(M+H)^+$ 407.1066, measured 407.1039.

***N*-(5-ethyl-2-(4-oxo-4H-benzo[d][1,3]oxazin-2-yl)phenyl)-4-methylbenzene sulfonamide (5t)**



Physical state: White Solid

Reaction Time: 24 h

Yield: 75 % (95 mg)

M.P : 200-201°C

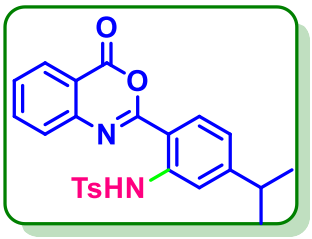
IR (KBr) ν_{max} cm^{-1}: 3432, 1801, 1751, 1627

^{1}H NMR (400 MHz, $CDCl_3$): **δ** 12.21 (s, NH), 8.23 (dd, *J* = 6.4, 1.6 Hz, 1H), 8.04 (d, *J* = 8.4 Hz, 1H), 7.87-7.91 (m, 1H), 7.55-7.76 (m, 5H), 7.13 (d, *J* = 8Hz, 2H), 6.96 (dd, *J* = 6.8, 1.6 Hz, 1H), 2.66 (q, *J* = 7.6, 7.6 Hz, 2H), 2.32(s, 3H), 1.22 (t, *J* = 7.6 Hz, 3H)

^{13}C NMR (100 MHz, $CDCl_3$): **δ** 158.3, 157.4, 151.6, 145.3, 144.1, 139.9, 137.2, 136.5, 129.8, 129.7, 129.0, 128.9, 127.3, 126.7, 123.4, 119.0, 116.6, 113.2, 29.3, 21.6, 15.0

HRMS (ESI): Calc. for $[(C_{23}H_{21}N_2SO_4)]$ $(M+H)^+$ 421.1222, measured 421.1234

***N*-(5-isopropyl-2-(4-oxo-4*H*-benzo[d][1,3]oxazin-2-yl)phenyl)-4-methylbenzene sulfonamide (5u)**



Physical state: White Solid

Reaction Time: 24 h

Yield: 74 % (96 mg)

M.P : 108-110 °C

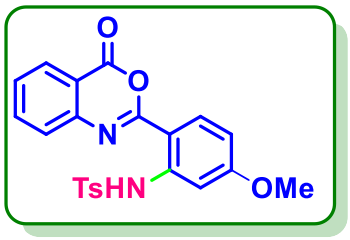
IR (KBr) ν_{max} cm^{-1}: 3421, 1810, 1732, 1662

^{1}H NMR (400 MHz, $CDCl_3$): **δ** 12.2 (s, NH), 8.22-8.24 (m, 1H), 8.05 (d, *J* = 8.4Hz, 1H), 7.55-7.91 (m, 6H), 6.97-7.14 (m, 3H), 2.88-2.95 (m, 1H), 2.32 (s, 3H), 1.23 (d, *J* = 7.2Hz, 6H)

^{13}C NMR (100 MHz, $CDCl_3$): **δ** 158.4, 157.4, 156.1, 145.3, 144.1, 140.0, 137.2, 136.5, 129.8, 129.7, 129.0, 128.9, 127.4, 126.7, 121.9, 117.7, 116.7, 113.3, 34.5, 23.5, 21.6.

HRMS (ESI): Calc. for $[(C_{24}H_{23}N_2O_4S)]$ $(M+H)^+$ 435.1379, measured 435.1393.

***N*-(5-methoxy-2-(4-oxo-4*H*-benzo[d][1,3]oxazin-2-yl)phenyl)-4-methylbenzenesulfonamide (5v)**



Physical state: White solid

Reaction Time: 24 h

Yield: 85 % (108 mg)

M.P : 215-217 ^oC

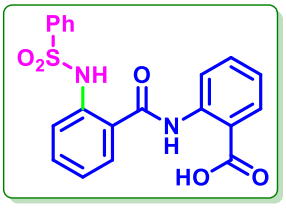
IR (KBr) ν_{max} cm^{-1}: 3448, 1801, 1764, 1643

^{1}H NMR (400 MHz, $CDCl_3$): **δ** 12.52 (s, NH), 8.21 (dd, *J* = 6.8, 1.2 Hz, 1H), 8.05 (d, *J* = 9.2Hz, 1H), 7.85-7.89 (m, 3H), 7.71-7.75 (m, 1H), 7.52-7.56 (m, 1H), 7.17-7.26 (m, 3H), 6.64 (dd, *J* = 6.8, 2.4 Hz, 1H), 3.85 (s, 3H), 2.34 (s, 3H)

^{13}C NMR (100 MHz, $CDCl_3$): **δ** 164.2, 158.4, 157.4, 145.5, 144.2, 142.0, 137.2, 136.6, 131.5, 129.8, 128.9, 128.6, 127.4, 126.4, 116.5, 110.1, 107.9, 103.9, 55.9, 22.7.

HRMS (ESI): Calc. for $[(C_{22}H_{19}N_2SO_5)]$ $(M+H)^+$ 423.1015, measured 423.1037.

2-(2-(phenylsulfonamido)benzamido)benzoic acid (5aa)



Physical state: White solid

Reaction Time : 6 h

Yield: 94 % (60 mg)

M.P : 234-236 ^oC

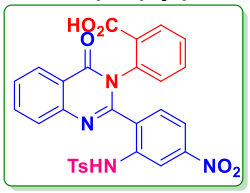
IR (KBr) ν_{max} cm^{-1}: 3654, 3541, 3479, 1715, 1678, 1486

^{1}H NMR (400 MHz, $CDCl_3$): **δ** 12.15 (s, 1H), 10.68(s, 1H), 8.57 (s, 1H), 8.02(m, 1H), 7.11-7.62 (m, 12H)

^{13}C NMR (100 MHz, $CDCl_3$): **δ** 169.8, 166.5, 140.2, 138.7, 137.1, 134.4, 133.6, 133.1, 131.6, 131.3, 129.6, 128.5, 127.1, 125.6, 124.1, 122.7, 121.3, 118.1,

HRMS (ESI): Calc. for $[(C_{20}H_{17}N_2O_5S)]$ $(M+H)^+$ 397.0858, measured 397.0855

2-(2-(2-((4-methylphenyl)sulfonamido)-4-nitrophenyl)-4-oxoquinazolin-3(4H)-yl)benzoic acid (9)



Physical state: White solid

Yield: 87 % (55mg)

M.P : 276-278 ^oC

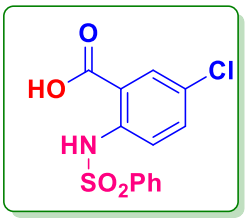
IR (KBr) ν_{max} cm^{-1}: 3631, 3529, 3418, 1725, 1683, 1472,

^{1}H NMR (400 MHz, $CDCl_3$): **δ** 12.21 (s, 1H), 11.63 (s, 1H), 8.71-8.94 (m, 3H), 8.18-8.39 (m, 3H), 7.62-7.84(m, 4H), 7.25 (s, 1H), 2.34 (s, 3H)

^{13}C NMR (100 MHz, $CDCl_3$): **δ** 168.1, 167.1, 140.2, 139.4, 139.3, 134.8, 133.3, 132.9, 129.0, 128.4, 127.4, 127.3, 127.1, 124.9, 124.5, 124.1, 122.5, 122.2, 122.1, 121.8, 120.0, 22.8.

HRMS (ESI): Calc. for $[(C_{28}H_{21}N_4O_7S)]$ $(M+H)^+$ 557.1131, measured 557.1123

5-chloro-2-(phenylsulfonamido)benzoic acid (10)



Physical state: White solid

Reaction Time : 12 h

Yield: 93 % (49 mg)

M.P : 163-164 ^oC

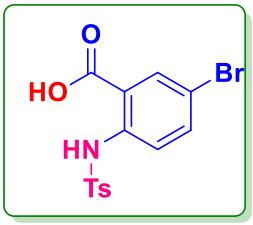
IR (KBr) ν_{max} cm^{-1}: 3632, 3511, 3437, 1731, 1651, 1479

^{1}H NMR (400 MHz, DMSO-D_6): **δ** 9.91 (s, 1H), 8.50 (s, 1H), 8.26 (s, 1H), 8.07 (dd, J = 39.8, 2.5 Hz, 1H), 7.51(m, 2H), 7.22 (m, 3H)

^{13}C NMR (100 MHz, DMSO-D_6): **δ** 167.0, 136.1, 124.6, 123.7, 122.3, 121.1, 119.9, 118.5, 114.8, 113.1, 113.0.

HRMS (ESI): Calc. for $[(C_{13}H_{11}ClNO_4S)]$ $(M+H)^+$ 312.0097, measured 312.0414

5-bromo-2-((4-methylphenyl)sulfonamido)benzoic acid (11)



Physical state: White solid

Reaction Time : 12 h

Yield: 91 % (36 mg)

M.P : 171-172 °C

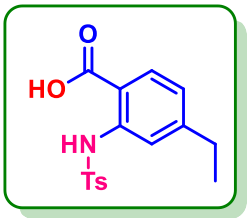
IR (KBr) ν_{max} cm^{-1}: 3629, 3492, 3444, 1730, 1641, 1463

^{1}H NMR (400 MHz, $CDCl_3$+DMSO-D_6): **δ** 10.92 (s, 1H), 7.91 (dd, J = 39.8, 2.5 Hz, 1H), 7.61 (d, J = 8.0 Hz, 1H), 7.47 – 7.37 (m, 2H), 7.27 (d, J = 3.5 Hz, 1H), 7.19 – 7.11 (m, 2H), 6.49 (dd, J = 8.7, 3.2 Hz, 1H), 2.27 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$): **δ** 169.1, 144.1, 139.8, 136.4, 133.8, 129.7, 127.2, 119.9, 118.2, 112.4, 106.8, 21.3

HRMS (ESI): Calc. for $[(C_{14}H_{13}BrNO_4S)]$ $(M+H)^+$ 369.9749, measured 369.9753, 371.9733.

4-ethyl-2-((4-methylphenyl)sulfonamido)benzoic acid (12)



Physical state: White solid

Reaction Time : 12 h

Yield: 96 % (35 mg)

M.P : 156-157 °C

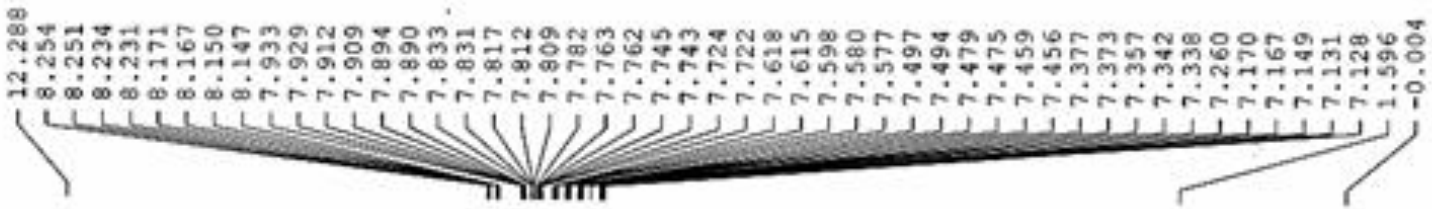
IR (KBr) ν_{max} cm^{-1}: 3648, 3501, 3429, 1728, 1647, 1456

^{1}H NMR (400 MHz, $CDCl_3$): **δ** 10.42 (s, 1H), 7.94 (d, J = 8.1 Hz, 1H), 7.78 (d, J = 8.3 Hz, 2H), 7.56 (s, 1H), 7.25 (d, J = 8.1 Hz, 2H), 6.92

	(dd, J = 8.2, 1.4 Hz, 1H), 2.67 (q, J = 7.6 Hz, 2H), 2.38 (s, 3H), 1.22 (t, J = 7.6 Hz, 3H).
^{13}C NMR (100 MHz, $CDCl_3$):	**δ** 172.6, 153.1, 144.1, 141.2, 136.2, 132.3, 129.7, 127.4, 122.9, 118.1, 112.2, 29.2, 21.5, 14.8
HRMS (ESI):	Calc. for $[(C_{16}H_{18}NO_4S)]$ $(M+H)^+$ 320.0957, measured 320.0962

References

[1]. S. Thakral, D. Saini, A. Kumar, N. Jain, S. Jain, *Med. Chem. Res* **2017**, 26, 1595–1604.
[2]. K. Raghuvanshi, L. Ackermann and K. Koszinowski, Dissertation, 2017, https://dnb.info/1125713054/34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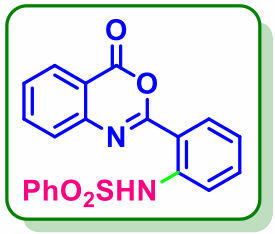
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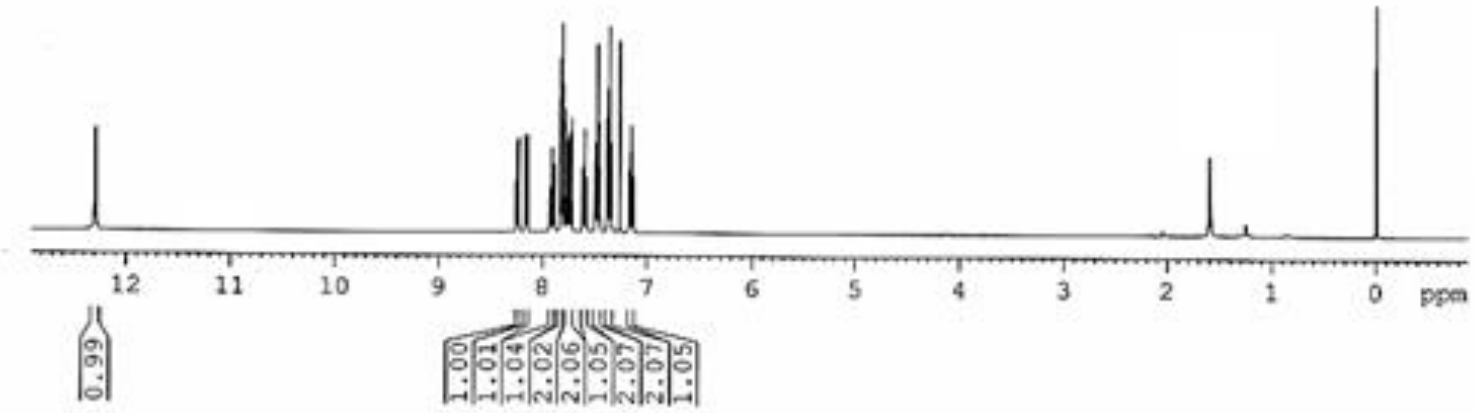
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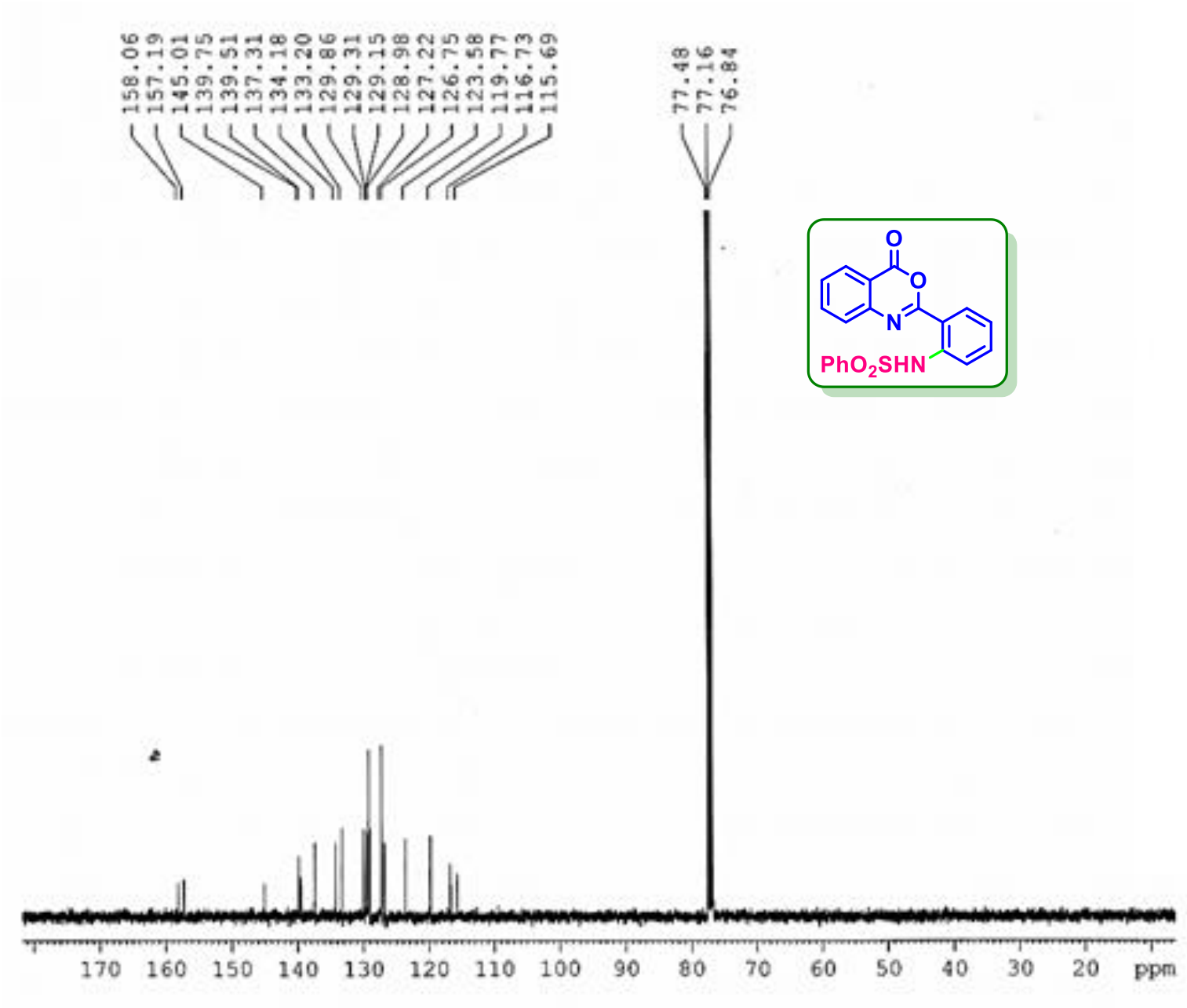
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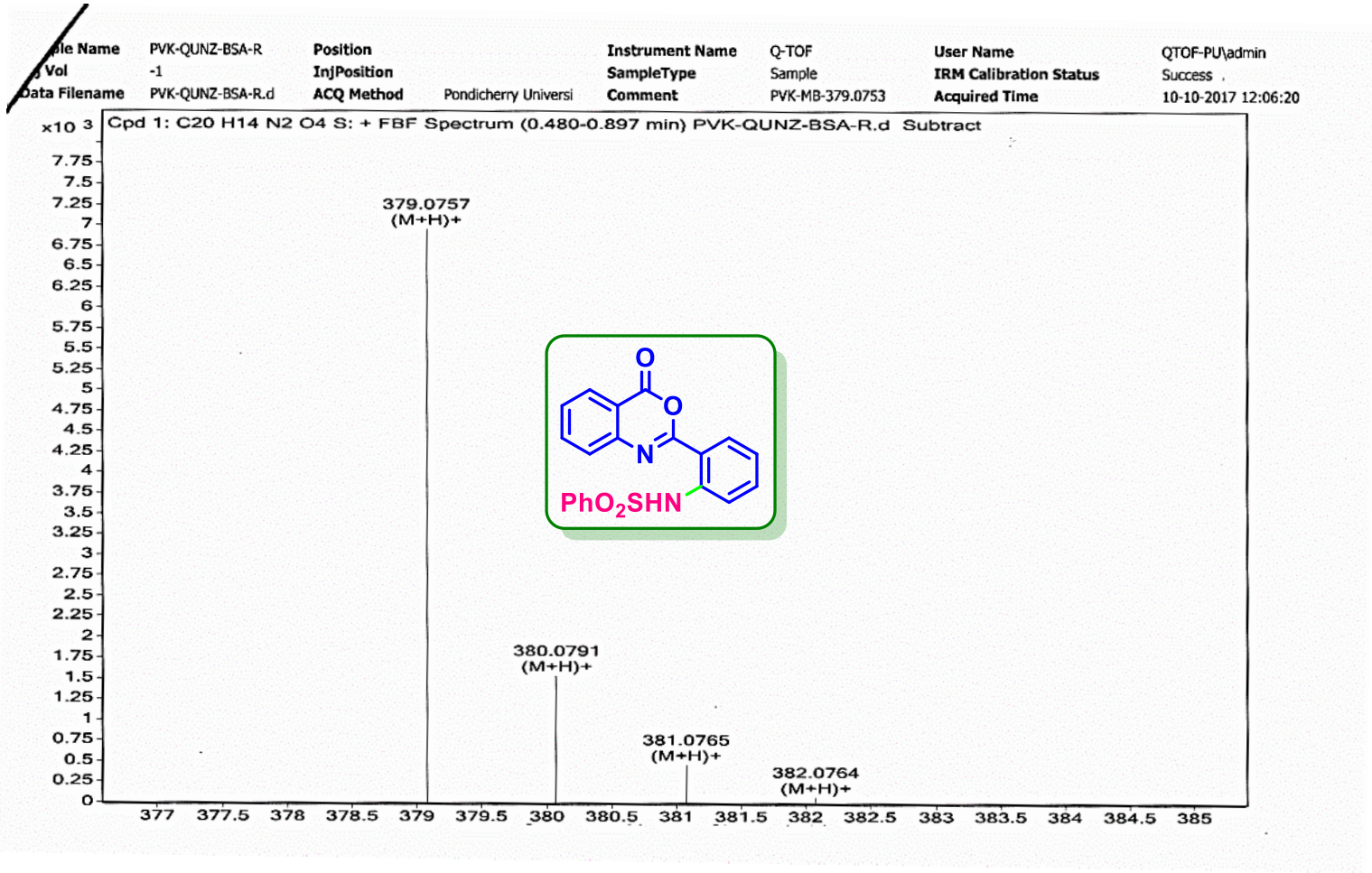
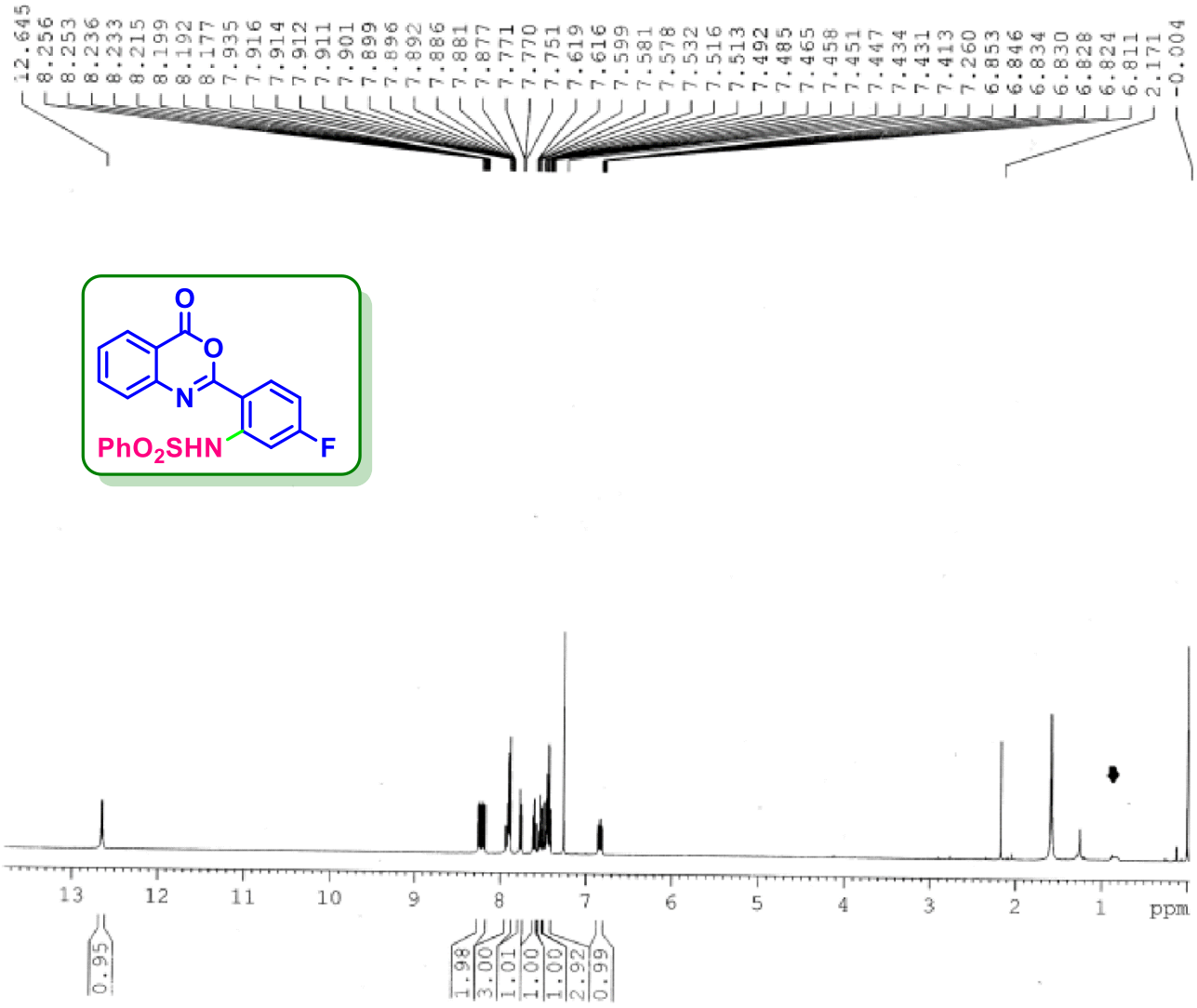
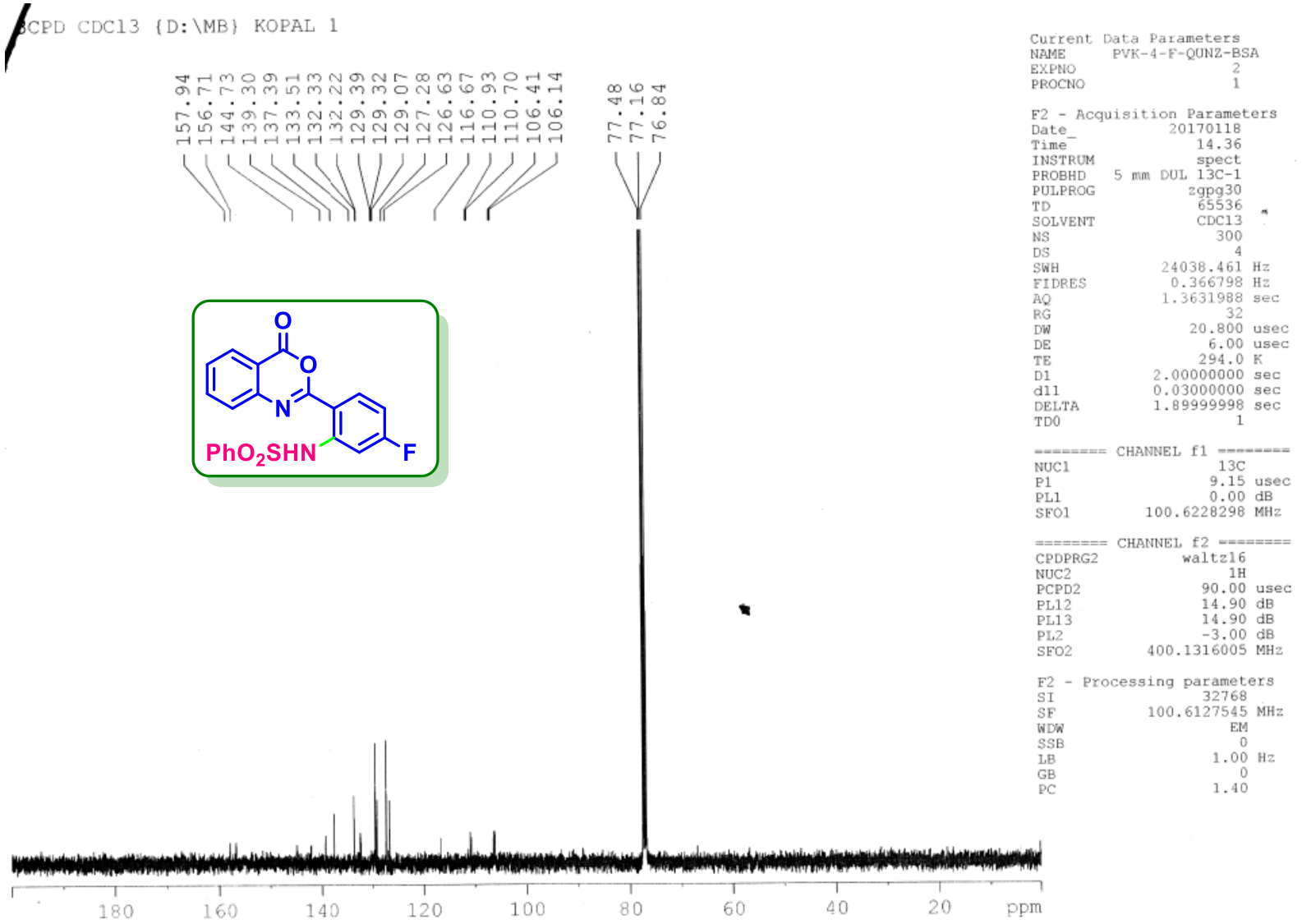
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm


ble Name PVK-QUNZ-BSA-R
Position
Instrument Name Q-TOF
User Name QTOF-PU\admin
g Vol -1
InjPosition
SampleType Sample
IRM Calibration Status Success
Data Filename PVK-QUNZ-BSA-R.d
ACQ Method Pondicherry Universi
Comment PVK-MB-379.0753
Acquired Time 10-10-2017 12:06:20
Cpd 1: C20 H14 N2 O4 S: + FBF Spectrum (0.480-0.897 min) PVK-QUNZ-BSA-R.d Subtract
x10 3
379.0757
(M+H)+
380.0791
(M+H)+
381.0765
(M+H)+
382.0764
(M+H)+
PhO2SHN

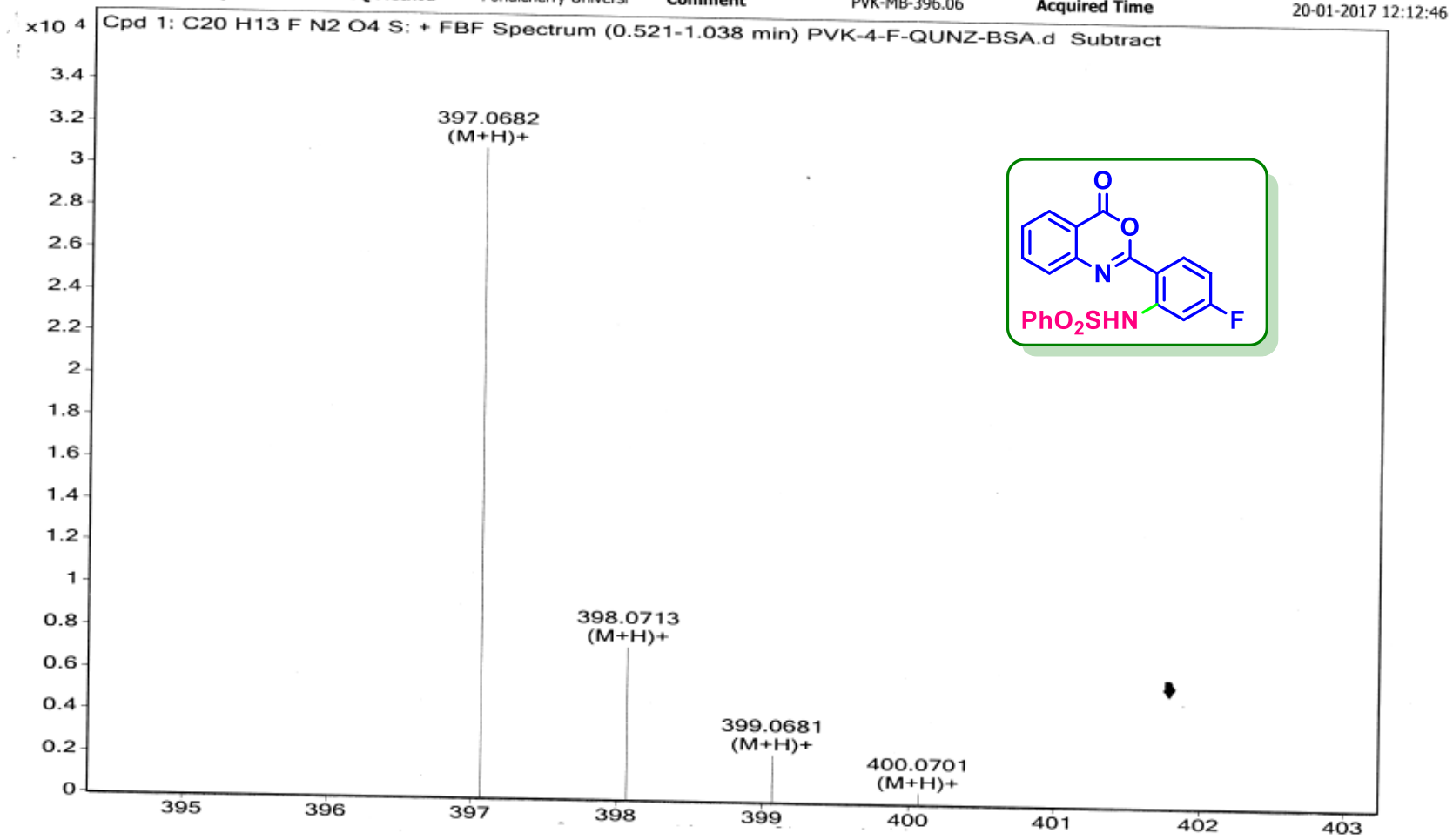


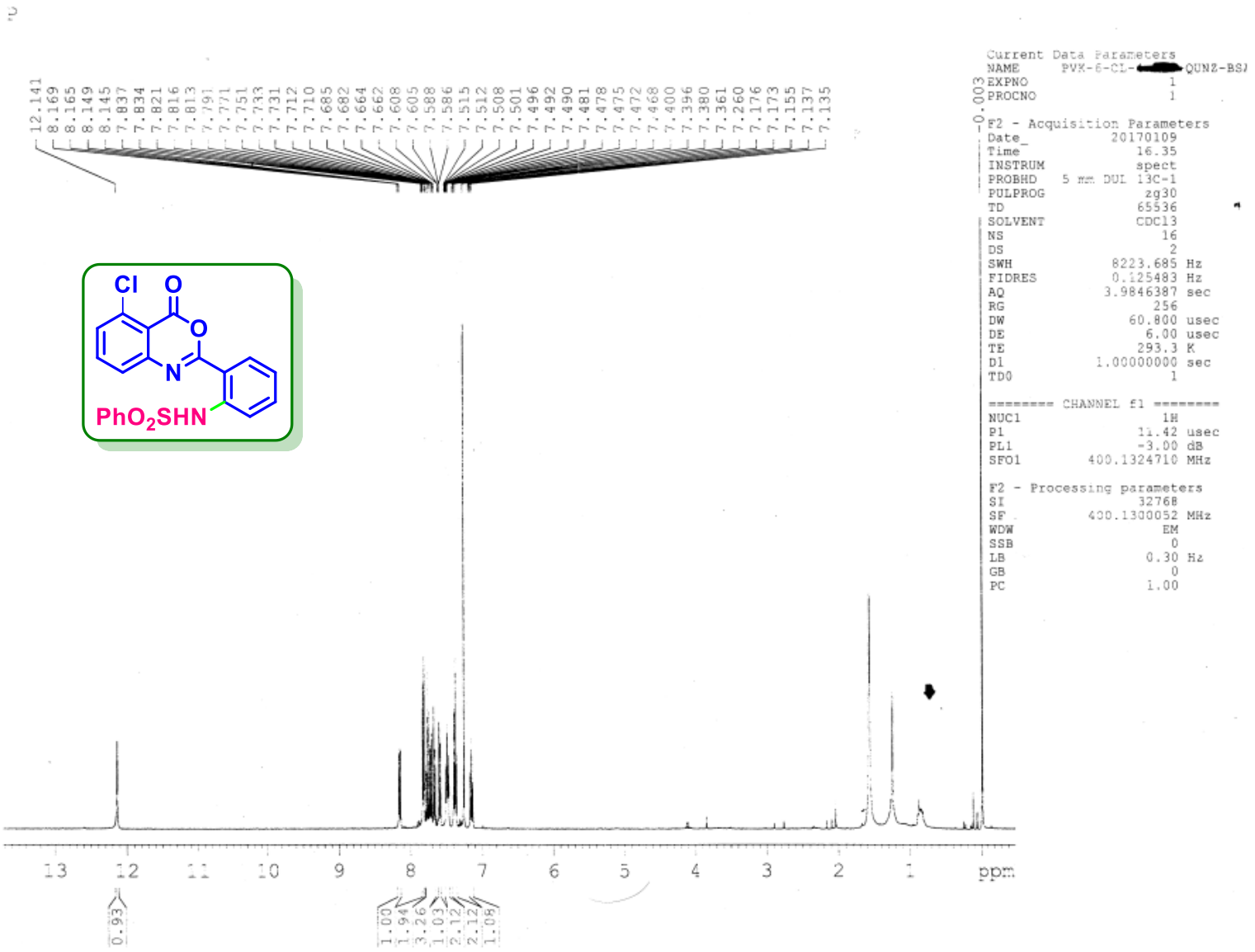

```
Current Data Parameters
NAME      PVK-4-F-QUNZ-BSA
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_              20170118
Time                 14.27
INSTRUM              spect
PROBHD   5 mm DUL 13C-1
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                     16
DS                      2
SWH             8223.685 Hz
FIDRES          0.125483 Hz
AQ              3.9846387 sec
RG                    322
DW                60.800 usec
DE                 6.00 usec
TE                293.3 K
D1             1.00000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                   1H
P1                 11.42 usec
PL1                -3.00 dB
SFO1        400.1324710 MHz

F2 - Processing parameters
SI                  32768
SF          400.1300051 MHz
WDW                    EM
SSB                     0
LB                 0.30 Hz
GB                      0
PC                   1.00
```

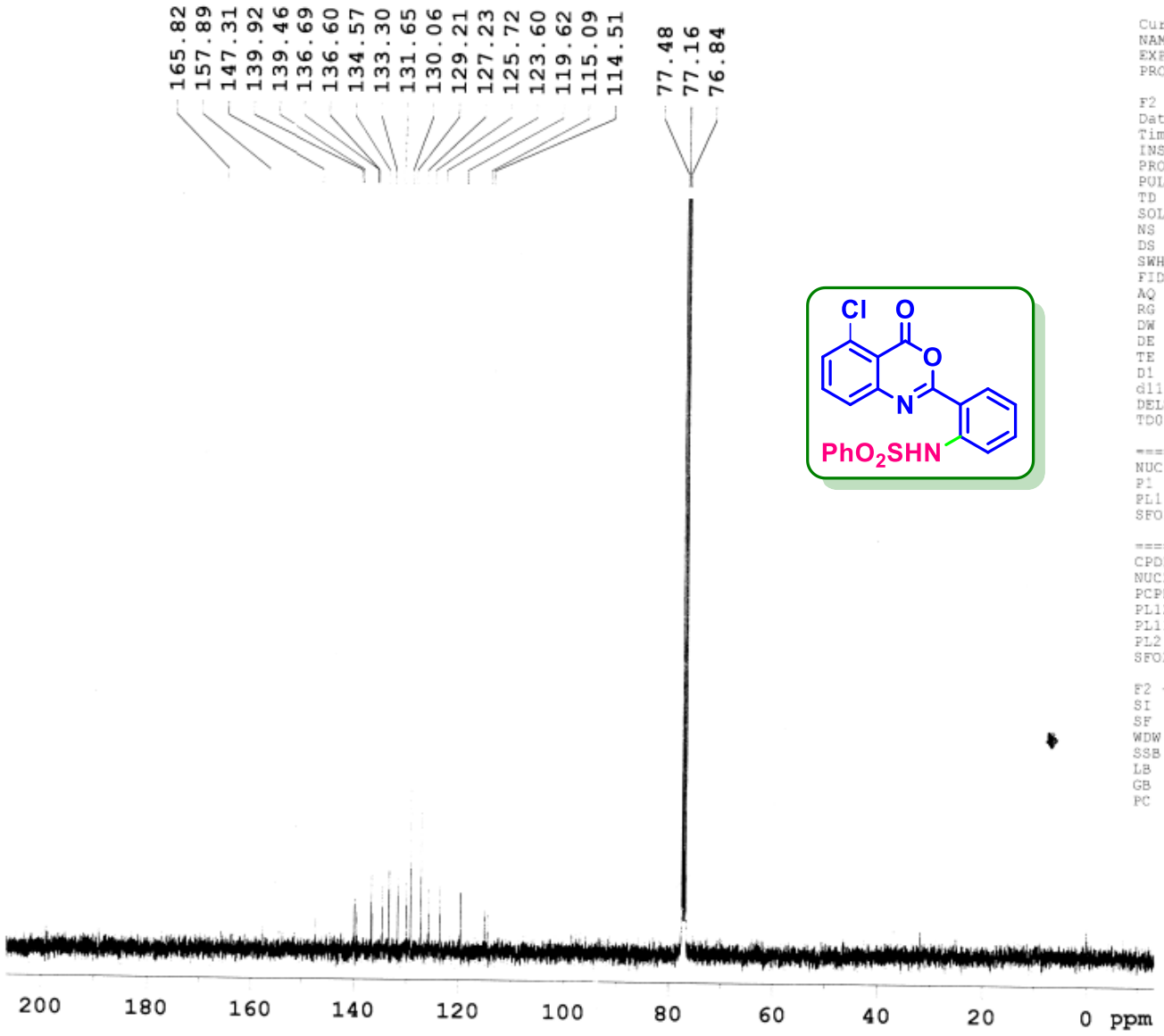



```
Current Data Parameters
NAME      PVK-4-F-QUNZ-BSA
EXPNO                    2
PROCNO                   1

F2 - Acquisition Parameters
Date_             20170118
Time                 14.36
INSTRUM              spect
PROBHD   5 mm DUL 13C-1
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   300
DS                     4
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ              1.3631988 sec
RG                    32
DW                20.800 usec
DE                 6.00 usec
TE                294.0 K
D1             2.00000000 sec
d11            0.03000000 sec
DELTA          1.89999998 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 13C
P1                9.15 usec
PL1                0.00 dB
SFO1         100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2             90.00 usec
PL12              14.90 dB
PL13              14.90 dB
PL2               -3.00 dB
SFO2         400.1316005 MHz

F2 - Processing parameters
SI                 32768
SF          100.6127545 MHz
WDW                   EM
SSB                    0
LB                1.00 Hz
GB                     0
PC                 1.40
```

Sample Name	PVK-4-F-QUNZ-BSA	**Position**		**Instrument Name**	Q-TOF	**User Name**	QTOF-PU\admin
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	PVK-4-F-QUNZ-BSA.d	**ACQ Method**	Pondicherry Universi	**Comment**	PVK-MB-396.06	**Acquired Time**	20-01-2017 12:12:46

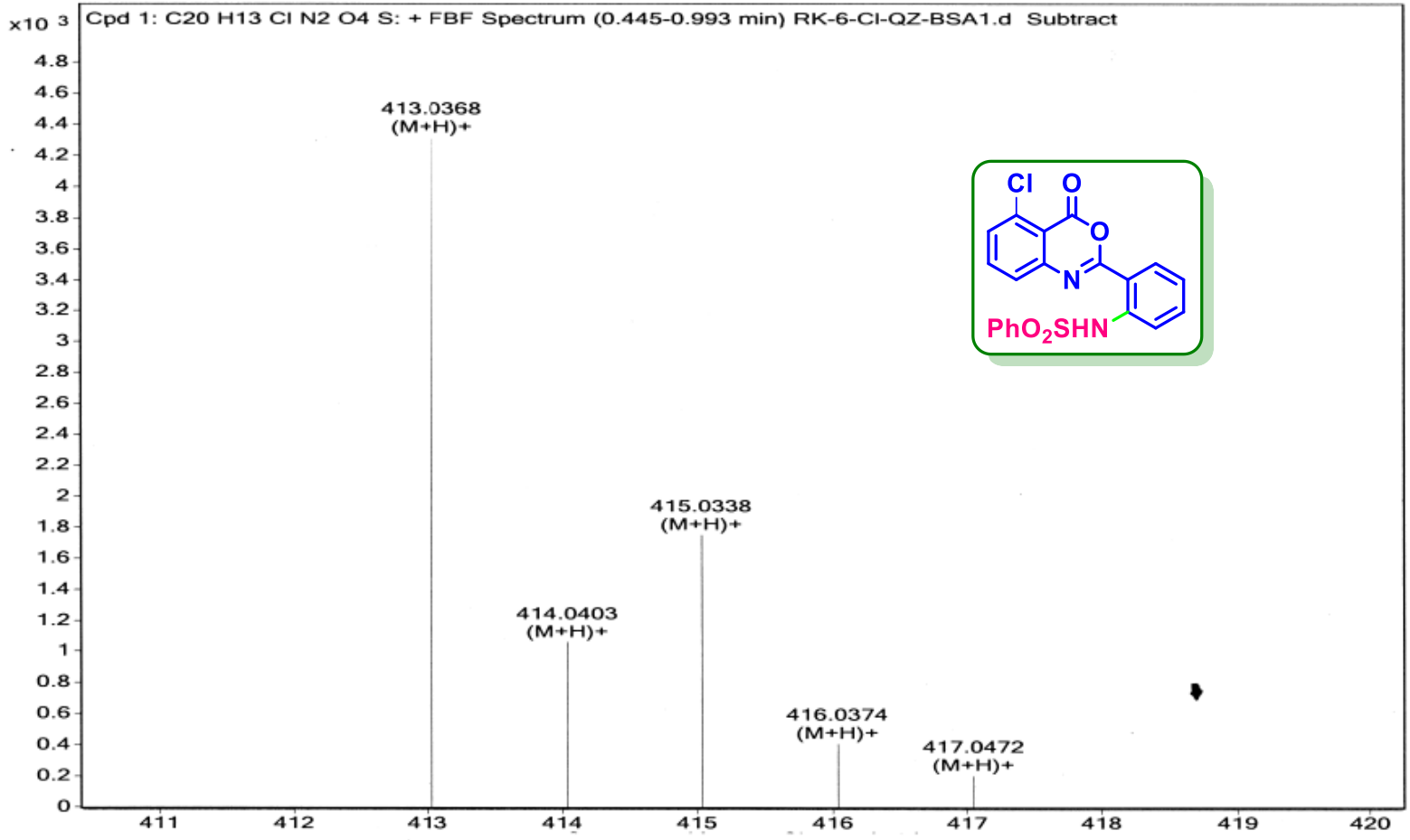


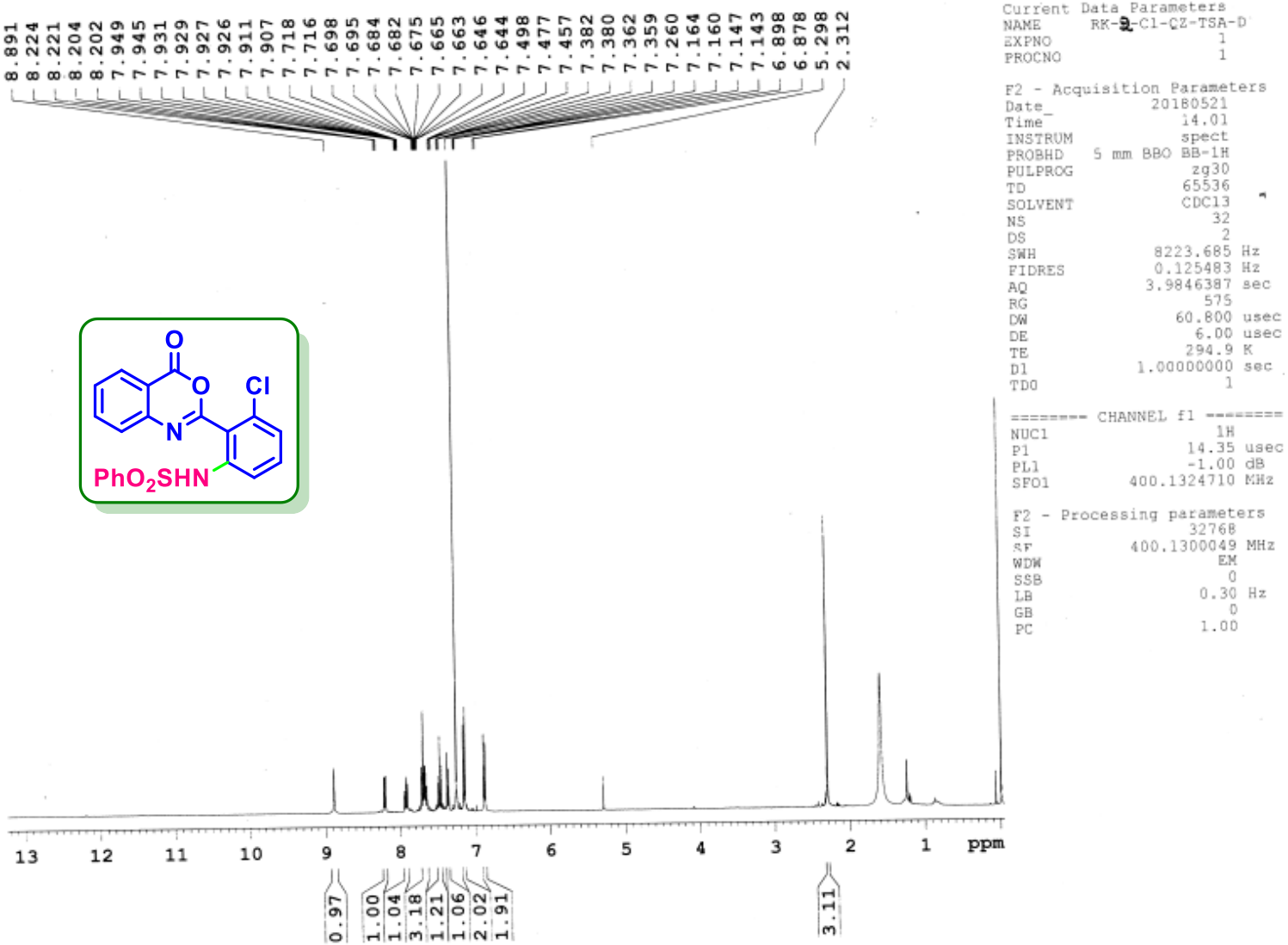

12.141
8.169
8.165
8.149
8.145
7.837
7.834
7.821
7.816
7.813
7.791
7.771
7.751
7.733
7.731
7.712
7.710
7.685
7.682
7.664
7.662
7.608
7.605
7.588
7.586
7.515
7.512
7.508
7.501
7.496
7.492
7.490
7.481
7.478
7.475
7.472
7.468
7.400
7.396
7.380
7.361
7.260
7.176
7.173
7.155
7.137
7.135
Cl
O
O
N
PhO2SHN
13
12
11
10
9
8
7
6
5
4
3
2
1
ppm
0.93
1.00
1.94
3.26
1.03
2.12
2.12
1.08
Current Data Parameters
NAME PVK-6-Cl-[redacted]QUNZ-BS
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170109
Time 16.35
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 256
DW 60.800 usec
DE 6.00 usec
TE 293.3 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 11.42 usec
PL1 -3.00 dB
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 32768
SF 400.1300052 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



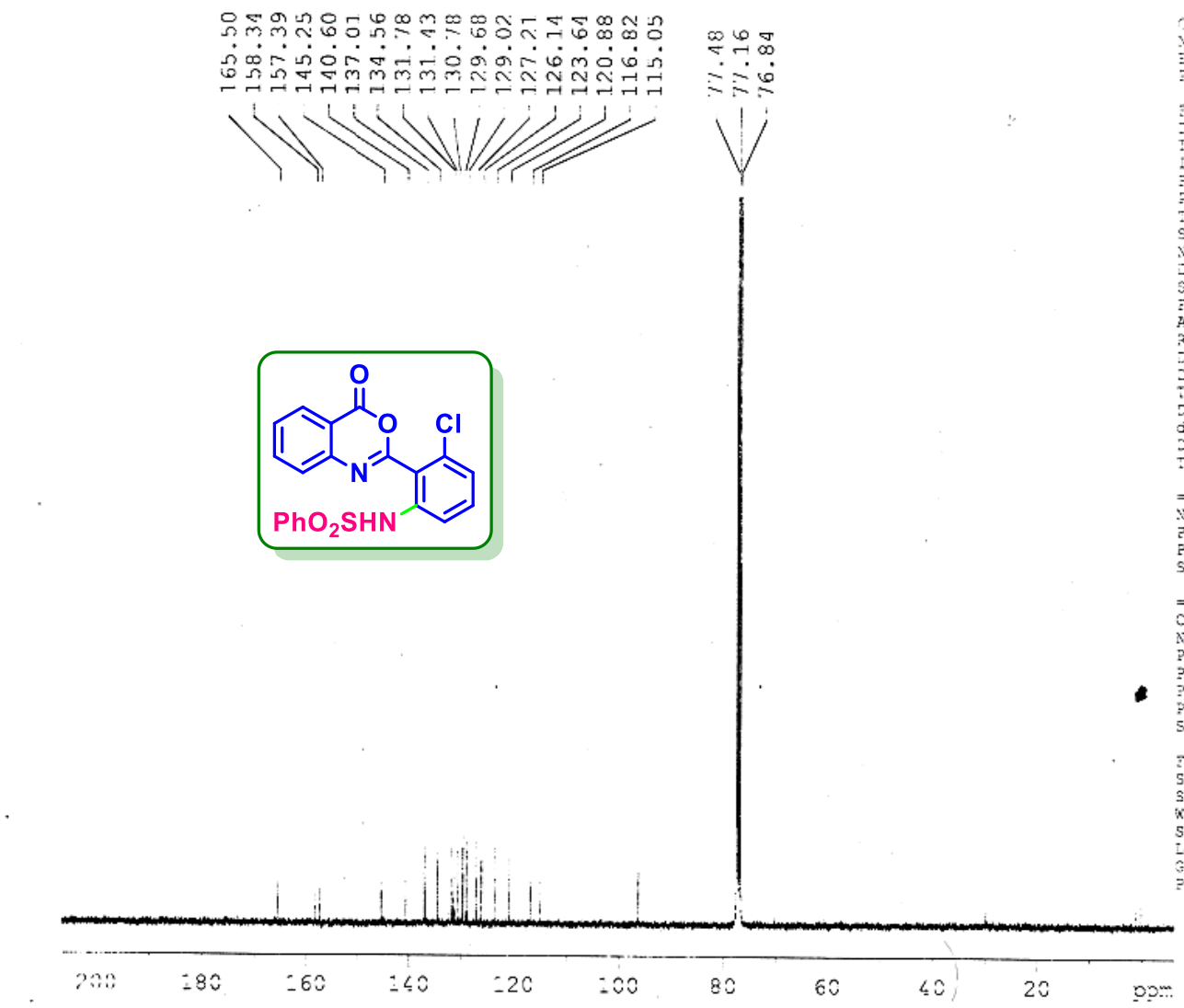

```
Current Data Parameters
NAME      PVK-6-Cl-4-NO2-QUNZ-35A
EXPNO                           4
PROCNO                          1

F2 - Acquisition Parameters
Date_                    20170109
Time                        23.26
INSTRUM                     spect
PROBHD    5 mm DUL 13C-1
PULPROG                  zgpg30
TD                            65536
SOLVENT                     CDCl3
NS                             1024
DS                                4
SWH                   24038.461 Hz
FIDRES                0.366798 Hz
AQ                    1.3631988 sec
RG                           28.5
DW                        20.800 usec
DE                         6.00 usec
TE                          293.8 K
D1                    2.00000000 sec
d11                   0.03000000 sec
DELTA                 1.89999998 sec
TD0                            1

======== CHANNEL f1 ========
NUC1                         13C
P1                          9.15 usec
PL1                         0.00 dB
SFO1                100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2                  waltz16
NUC2                         1H
PCPD2                      90.00 usec
PL12                       14.90 dB
PL13                       14.90 dB
PL2                        -3.00 dB
SFO2                400.1316005 MHz

F2 - Processing parameters
SI                            32768
SF                  100.6127538 MHz
WDW                            EM
SSB                             0
LB                           1.00 Hz
GB                              0
PC                           1.40
```

Sample Name	RK-6-Cl-QZ-BSA	**Position**		**Instrument Name**	Q-TOF	**User Name**	QTOF-PU\admin
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	RK-6-Cl-QZ-BSA1.d	**ACQ Method**	Pondicherry Universi	**Comment**	RK-MB-412.0285	**Acquired Time**	25-05-2018 13:16:52



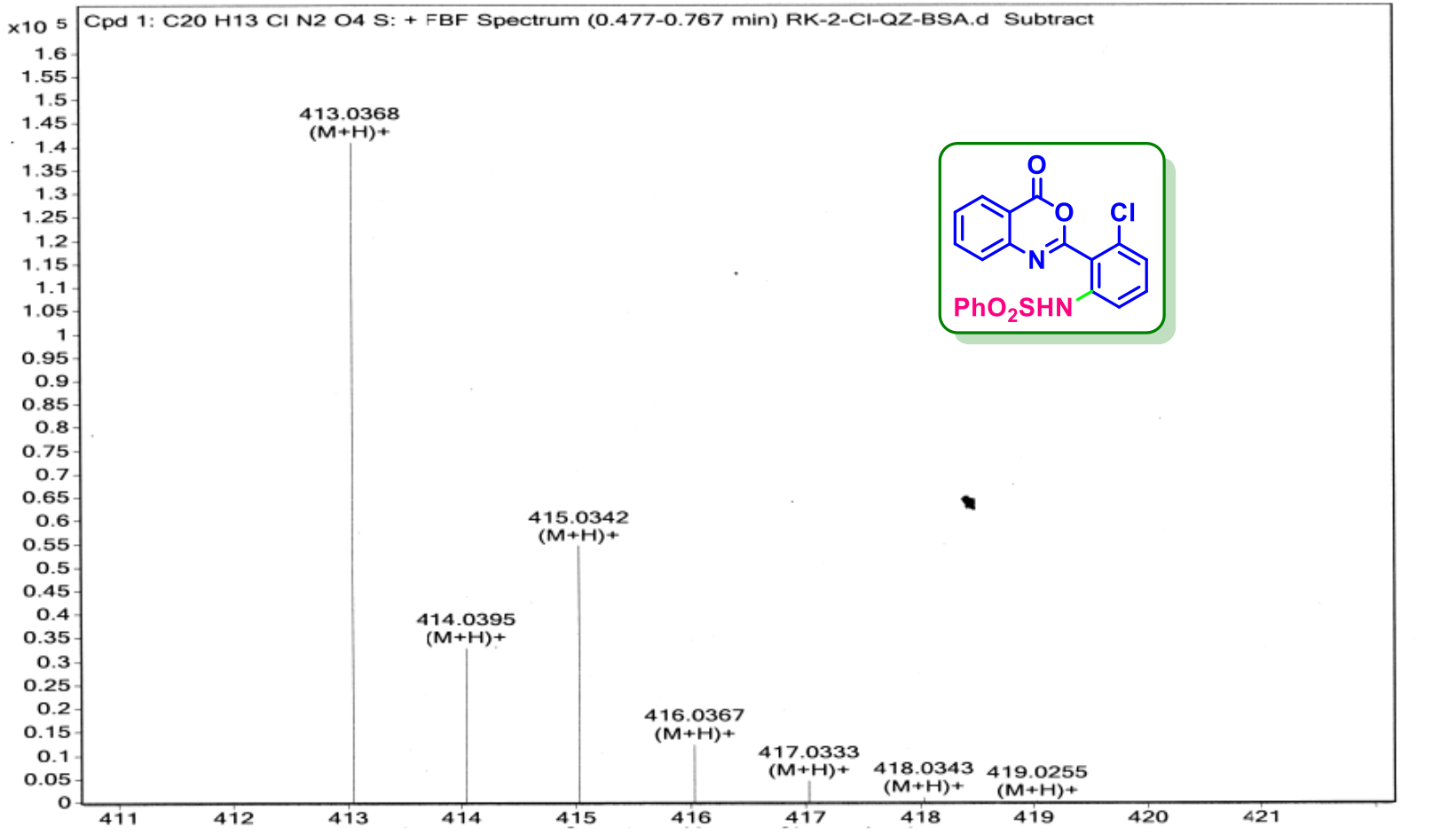


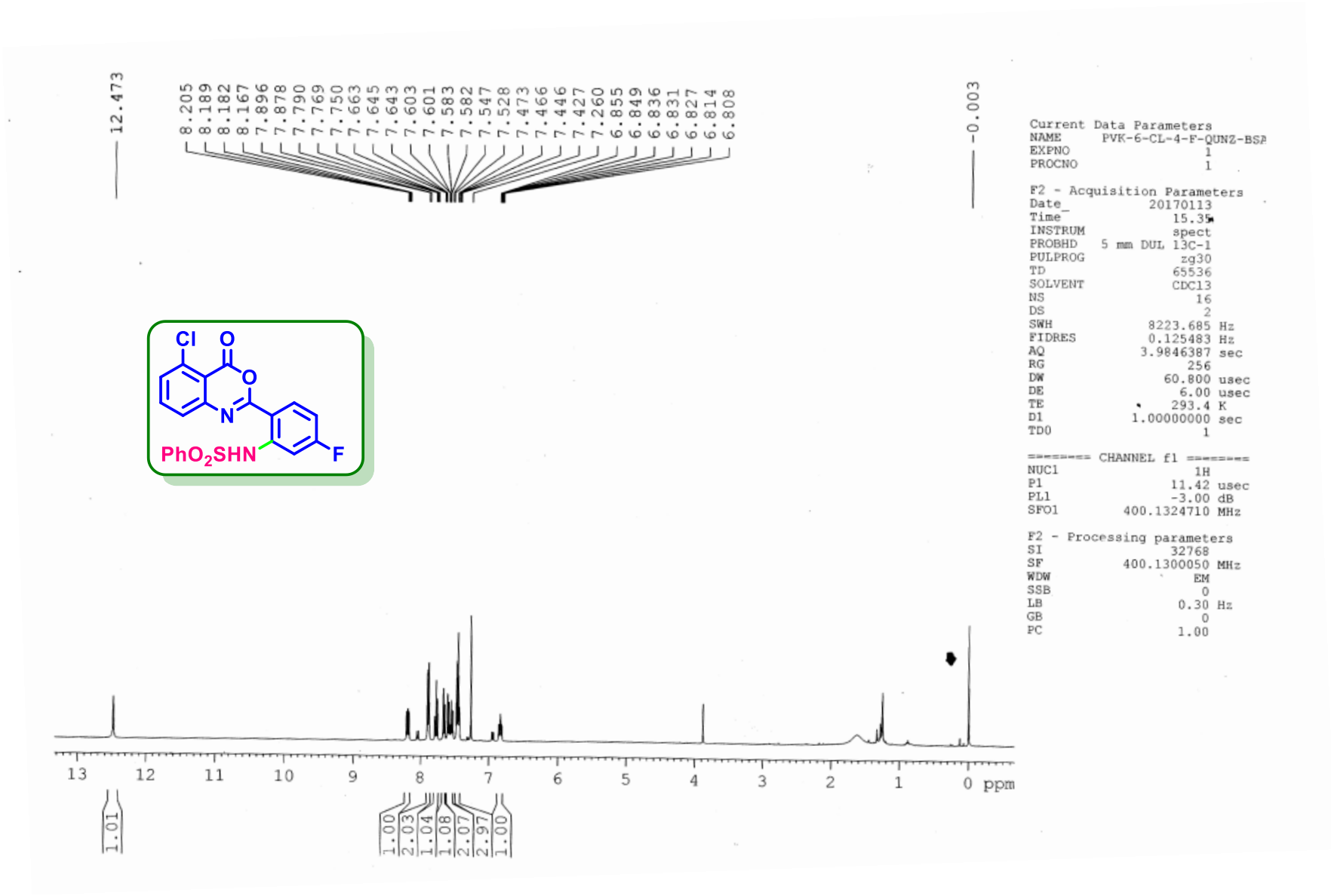

```
Current Data Parameters
NAME      RK-[illegible]-Cl-CZ-TSA-D
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_            20180521
Time                14.01
INSTRUM             spect
PROBHD   5 mm BBO BB-1H
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    32
DS                     2
SWH             8223.685 Hz
FIDRES          0.125483 Hz
AQ              3.9846387 sec
RG                   575
DW                60.800 usec
DE                 6.00 usec
TE                294.9 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 14.35 usec
PL1                -1.00 dB
SFO1          400.1324710 MHz

F2 - Processing parameters
SI                 32768
SF            400.1300049 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

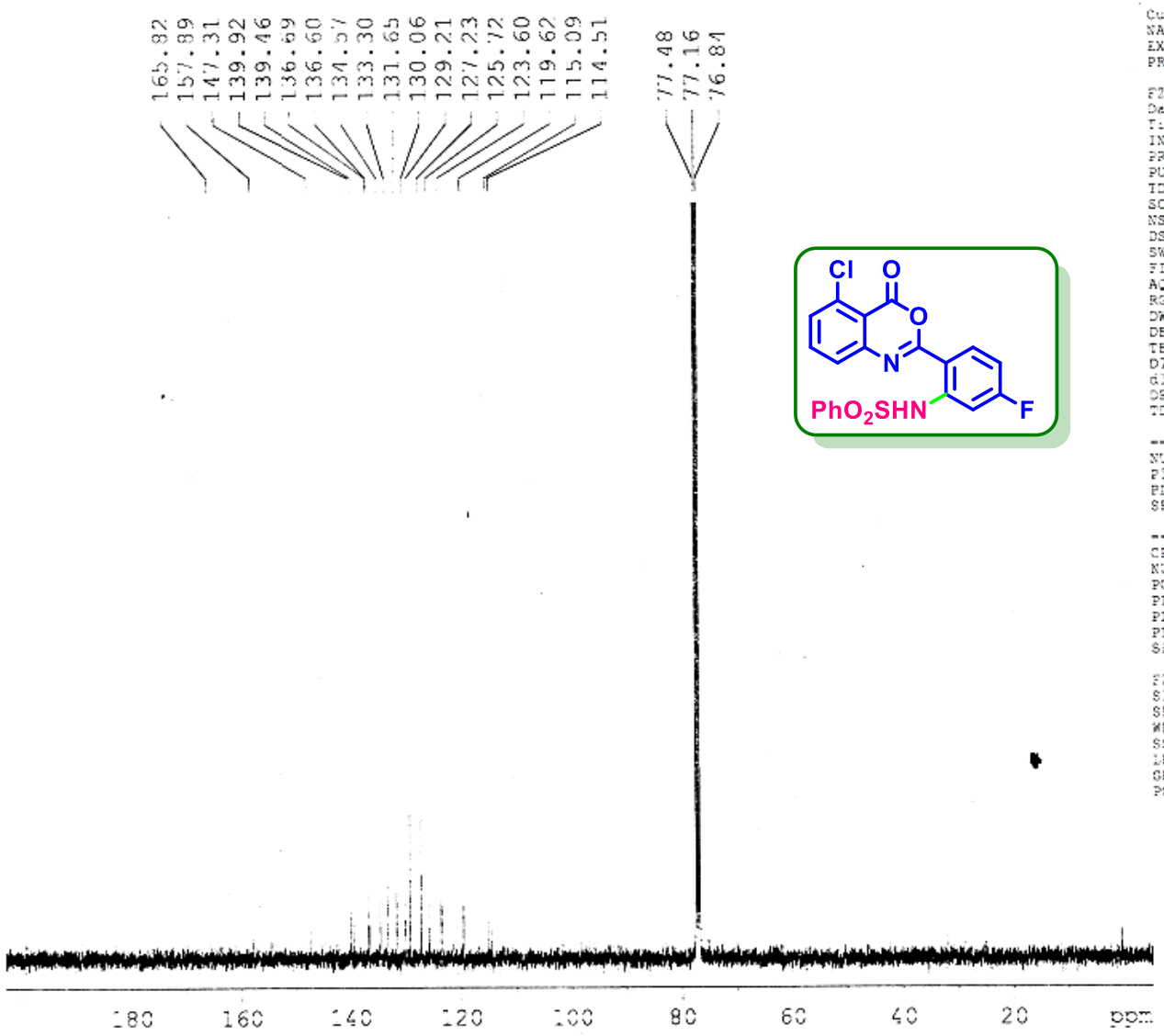



```
Current Data Parameters
NAME      PVK-2-CL-QUNZ-TSA
EXPNO                     2
PROCNO                    1

F2 - Acquisition Parameters
Date_           20171118
Time                7.27
INSTRUM            spect
PROBHD   5 mm DUL 13C-1
PULPROG          zgpg30
TD                 65536
SOLVENT            CDCl3
NS                  8000
DS                     4
SWH            24038.461 Hz
FIDRES         0.366798 Hz
AQ             1.3631988 sec
RG                    57
DW                20.800 usec
DE                 6.00 usec
TE                292.0 K
D1             2.00000000 sec
d11            0.03000000 sec
DELTA          1.89999998 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  13C
P1                  9.15 usec
PL1                 0.00 dB
SFO1          100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2              90.00 usec
PL12               14.90 dB
PL13               14.90 dB
PL2                -3.00 dB
SFO2          400.1316005 MHz

F2 - Processing parameters
SI                 32768
SF            100.6127548 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

Sample Name	RK-2-Cl-QZ-BSA	**Position**		**Instrument Name**	Q-TOF	**User Name**	QTOF-PU\admin
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	RK-2-Cl-QZ-BSA.d	**ACQ Method**	Pondicherry Universi	**Comment**	RK-MB-412.0285	**Acquired Time**	24-05-2018 12:54:27

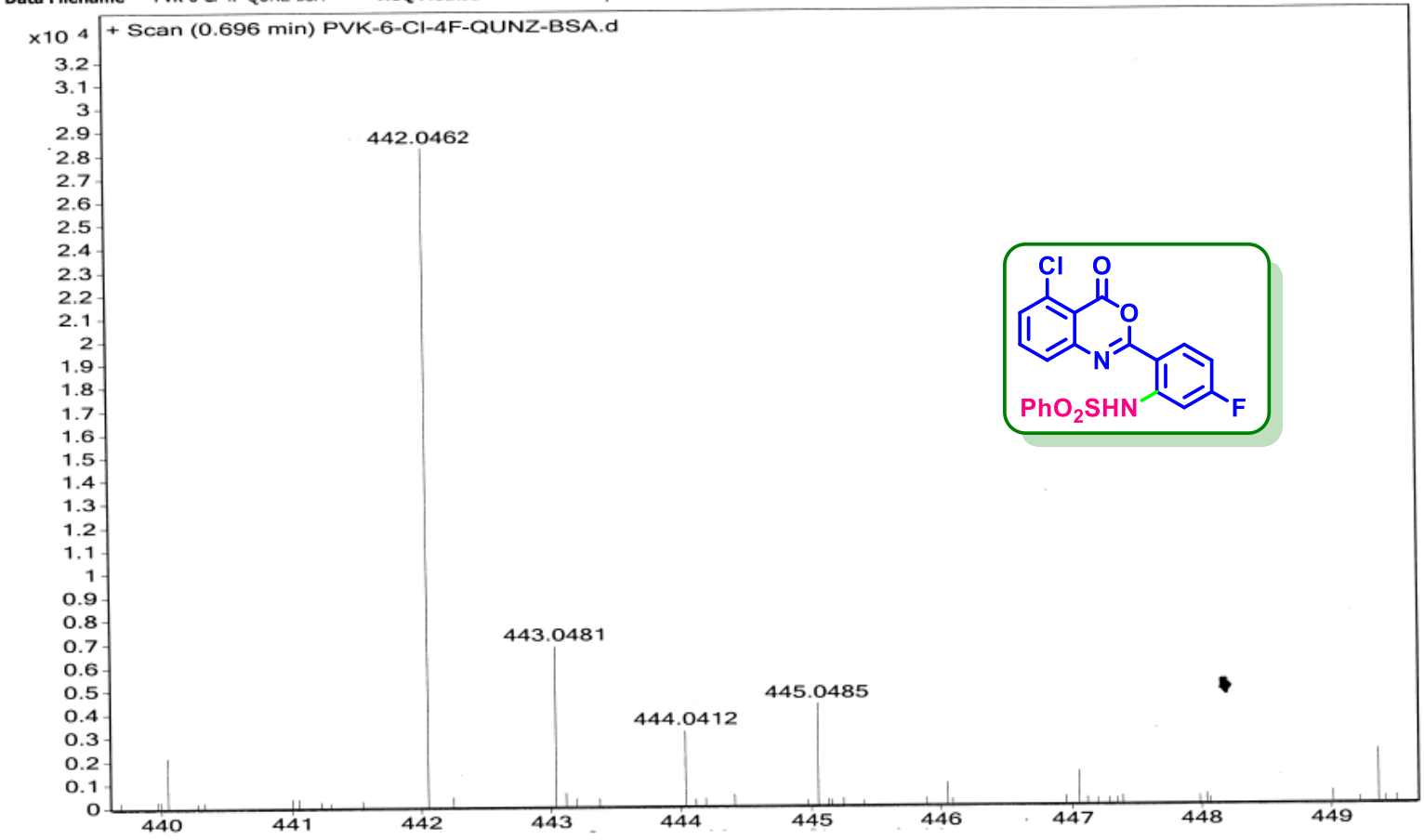


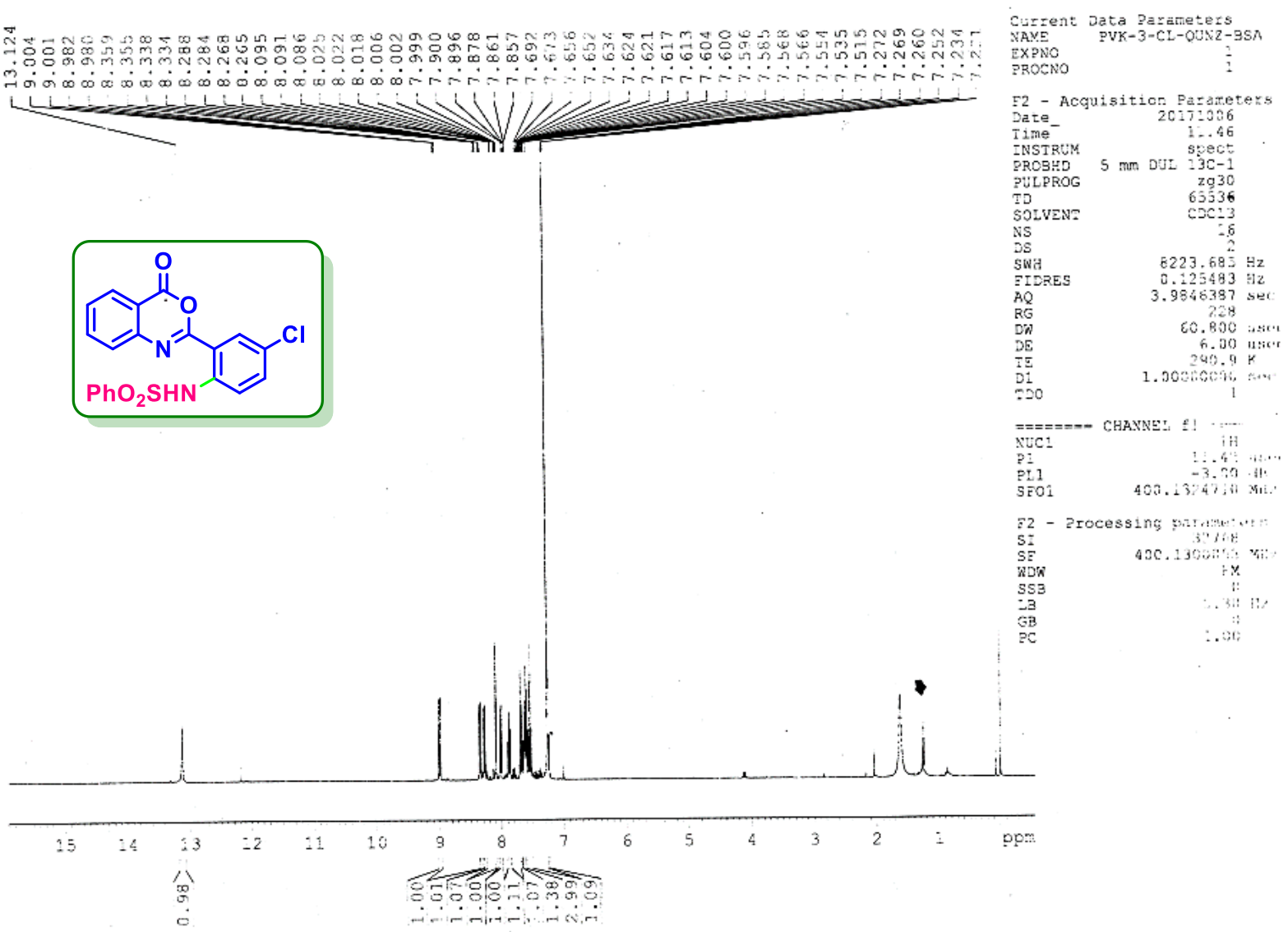

12.473
8.205
8.189
8.182
8.167
7.896
7.878
7.790
7.769
7.750
7.663
7.645
7.643
7.603
7.601
7.583
7.582
7.547
7.528
7.473
7.466
7.446
7.427
7.260
6.855
6.849
6.836
6.831
6.827
6.814
6.808
-0.003
Cl
O
O
N
PhO2SHN
F
13
12
11
10
9
8
7
6
5
4
3
2
1
0 ppm
1.01
1.00
2.03
1.04
1.08
2.07
2.97
1.00
Current Data Parameters
NAME PVK-6-CL-4-F-QUNZ-BSP
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170113
Time 15.35
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 256
DW 60.800 usec
DE 6.00 usec
TE 293.4 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 11.42 usec
PL1 -3.00 dB
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 32768
SF 400.1300050 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



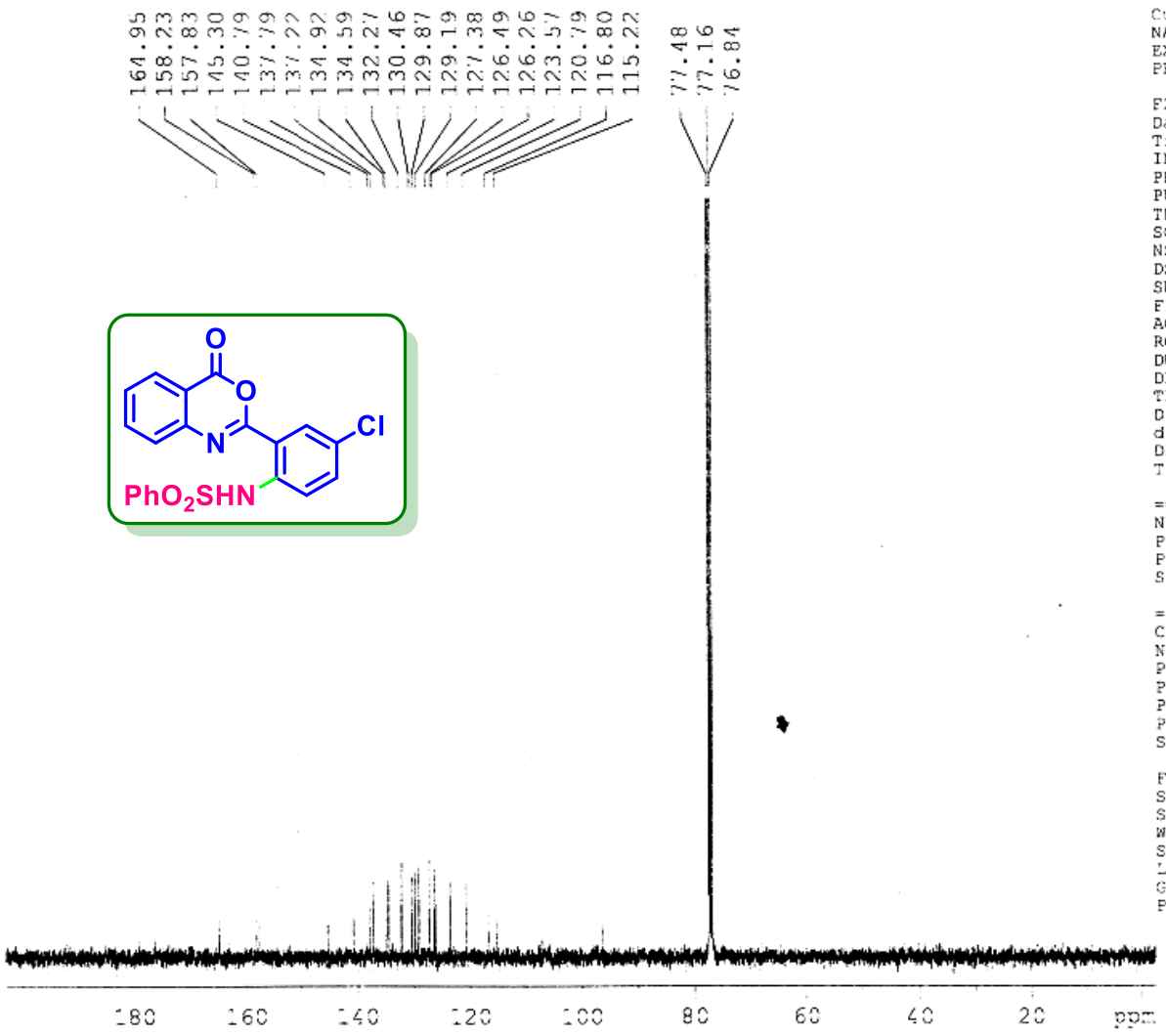

```
Current Data Parameters
NAME      PVK-6-CL-4-NO2-2UN2-A
EXPNO                         4
PROCNO                        1

F2 - Acquisition Parameters
Date_               20170109
Time                   23.26
INSTRUM                spect
PROBHD     5 mm DUL 13C-1
PULPROG             zgpg30
TD                     65536
SOLVENT                CDCl3
NS                      1024
DS                         4
SWH                24038.461 Hz
FIDRES             0.366798 Hz
AQ                 1.3631988 sec
RG                      28.5
DW                    20.800 usec
DE                     6.00 usec
TE                    293.8 K
D1                 2.00000000 sec
d11                0.03000000 sec
DELTA              1.89999998 sec
TD0                        1

======== CHANNEL f1
NUC1                      13C
P1                      9.10 usec
PL1                     1.00 dB
SFO1             100.6130000 MHz

======== CHANNEL f2
CPDPRG2                 waltz16
NUC2                       1H
PCPD2                   90.00 usec
PL12                    14.00 dB
PL13                    14.00 dB
PL2                     -3.00 dB
SFO2             400.1324005 MHz

F2 - Processing parameters
SI                        32768
SF               100.6127638 MHz
WDW                        EM
SSB                         0
LB                      1.00 Hz
GB                          0
PC                      1.40
```

Sample Name	PVK-6-Cl-4F-QUNZ-BSA	**Position**		**Instrument Name**	Q-TOF	**User Name**	QTOF-PU\admin
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	PVK-6-Cl-4F-QUNZ-BSA	**ACQ Method**	Pondicherry Universi	**Comment**	PVK-MB-444.03	**Acquired Time**	13-01-2017 13:52:53

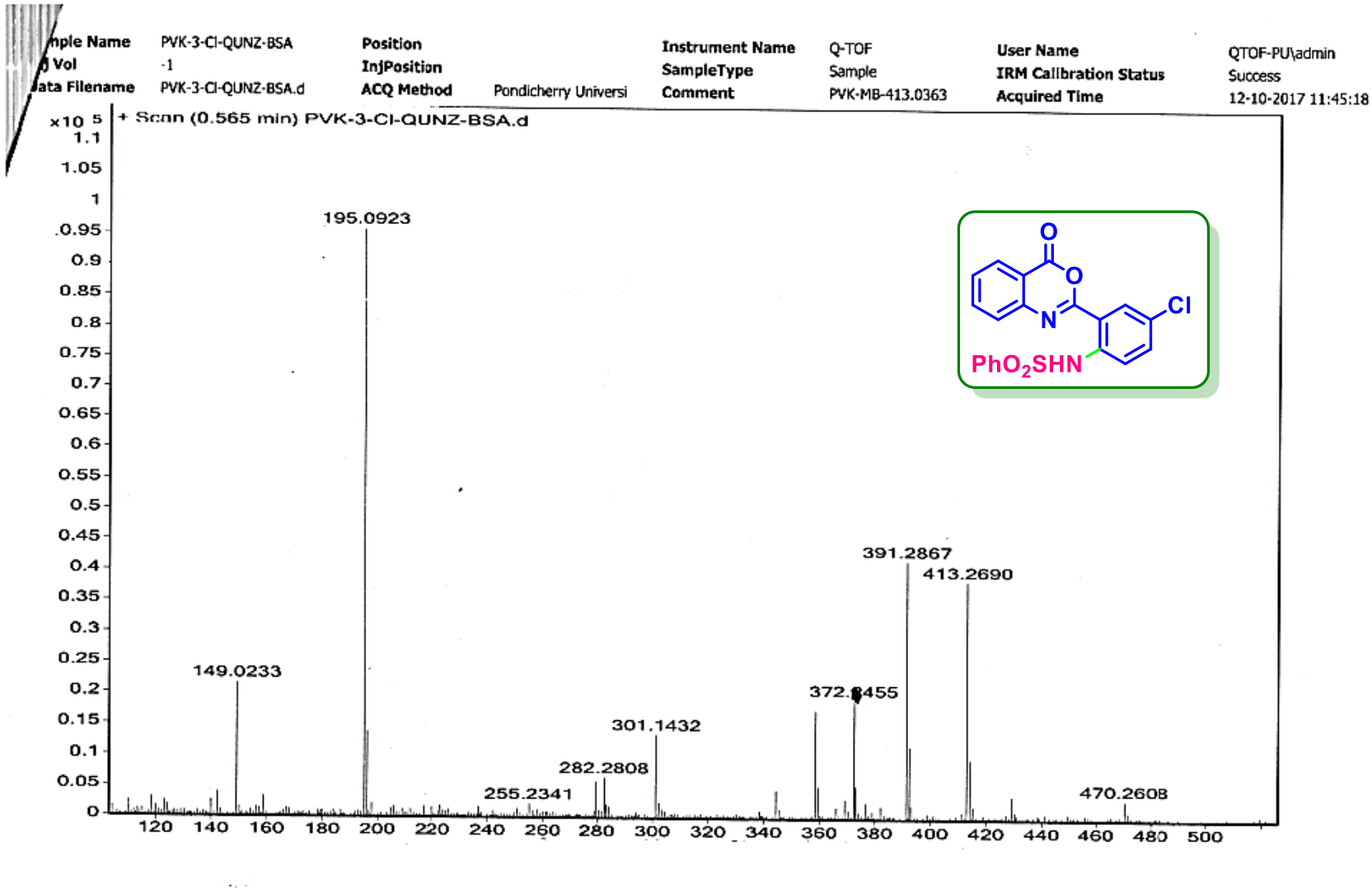


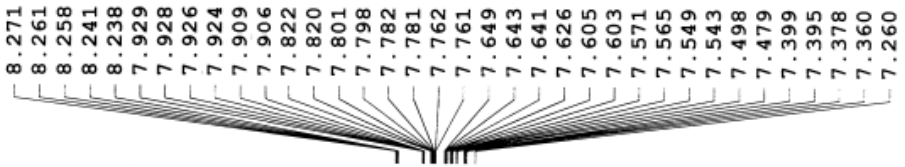


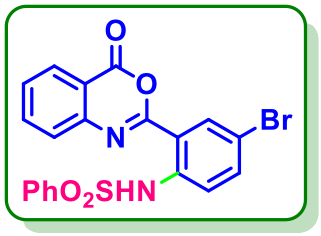

```
Current Data Parameters
NAME      PVK-3-CL-QUNZ-BSA
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_             20171006
Time                 11.46
INSTRUM              spect
PROBHD    5 mm DUL 13C-1
PULPROG               zg30
TD                   65536
SOLVENT              CDCl3
NS                      16
DS                       2
SWH               6223.685 Hz
FIDRES            0.125483 Hz
AQ                3.9846387 sec
RG                     228
DW                  60.800 usec
DE                   6.00 usec
TE                  240.9 K
D1                1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                     1H
P1                   11.45 usec
PL1                  -3.00 dB
SFO1          400.1324710 MHz

F2 - Processing parameters
SI                   65768
SF            400.1300000 MHz
WDW                      EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.00
```

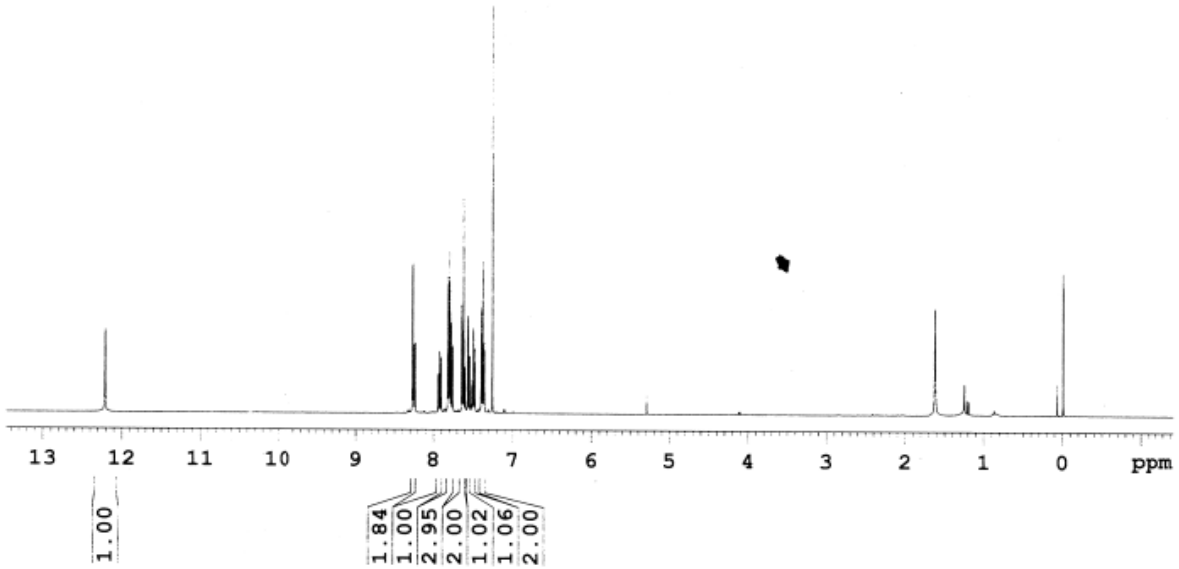



```
Current Data Parameters
NAME      PVK-3-CL-QUNZ-BSA
EXPNO                     2
PROCNO                    1

F2 - Acquisition Parameters
Date_           20171006
Time               12.31
INSTRUM            spect
PROBHD   5 mm DUL 13C-1
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  512
DS                    4
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3631988 sec
RG                   32
DW                20.800 usec
DE                 6.00 usec
TE                292.0 K
D1           2.00000000 sec
d11          0.03000000 sec
DELTA        1.89999998 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                  9.15 usec
PL1                 0.00 dB
SFO1         100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2              90.00 usec
PL12               14.90 dB
PL13               14.90 dB
PL2                -3.00 dB
SFO2         400.1316005 MHz

F2 - Processing parameters
SI                  32768
SF           100.6127552 MHz
WDW                    EM
SSB                     0
LB                   1.00 Hz
GB                      0
PC                   1.40
```

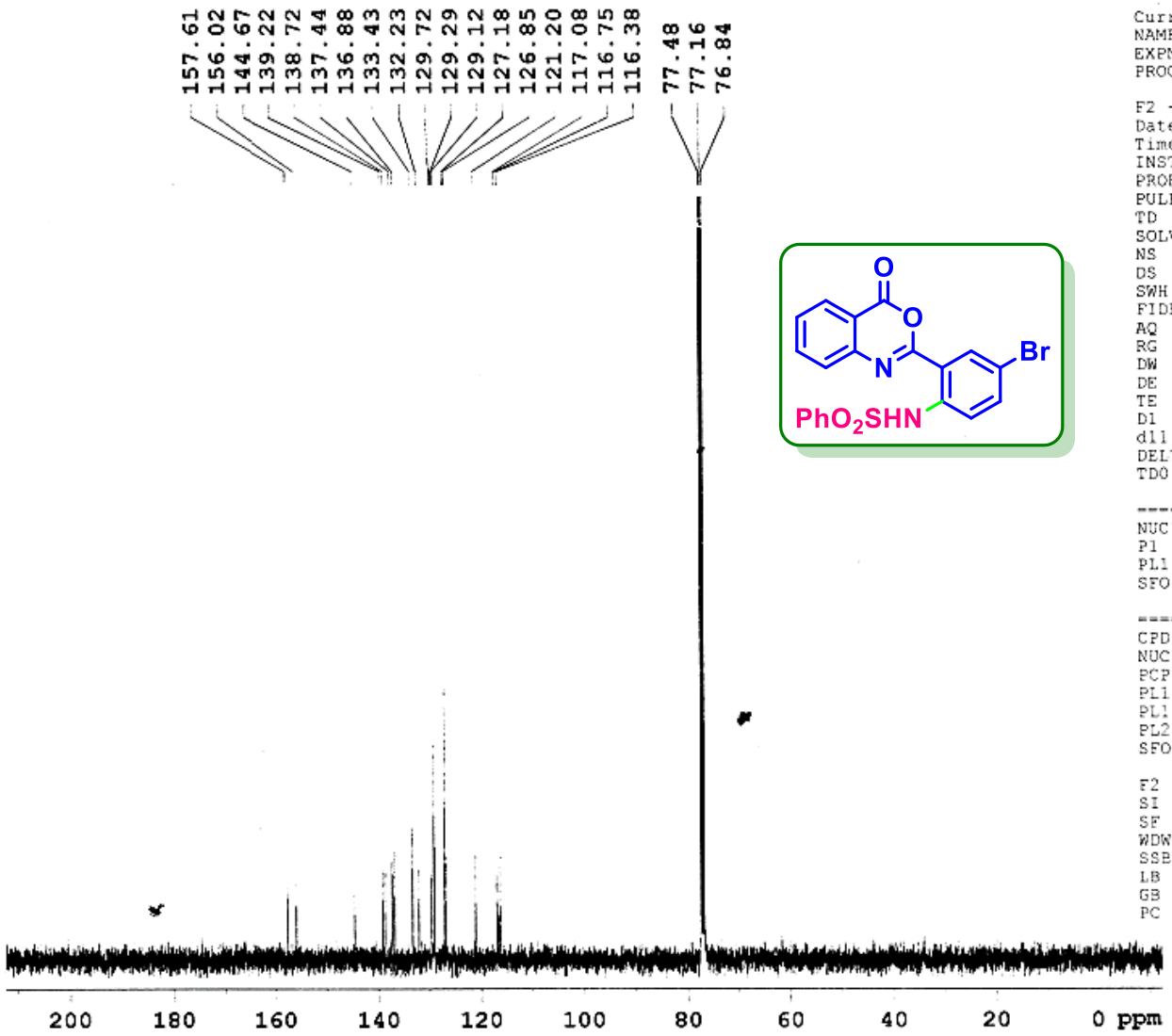

mple Name PVK-3-Cl-QUNZ-BSA
Position
Instrument Name Q-TOF
User Name QTOF-PU\admin
Vol -1
InjPosition
SampleType Sample
IRM Calibration Status Success
Data Filename PVK-3-Cl-QUNZ-BSA.d
ACQ Method Pondicherry Universi
Comment PVK-MB-413.0363
Acquired Time 12-10-2017 11:45:18
x10 5
+ Scan (0.565 min) PVK-3-Cl-QUNZ-BSA.d
195.0923
149.0233
255.2341
282.2808
301.1432
372.2455
391.2867
413.2690
470.2608
PhO2SHN
Cl
O
N





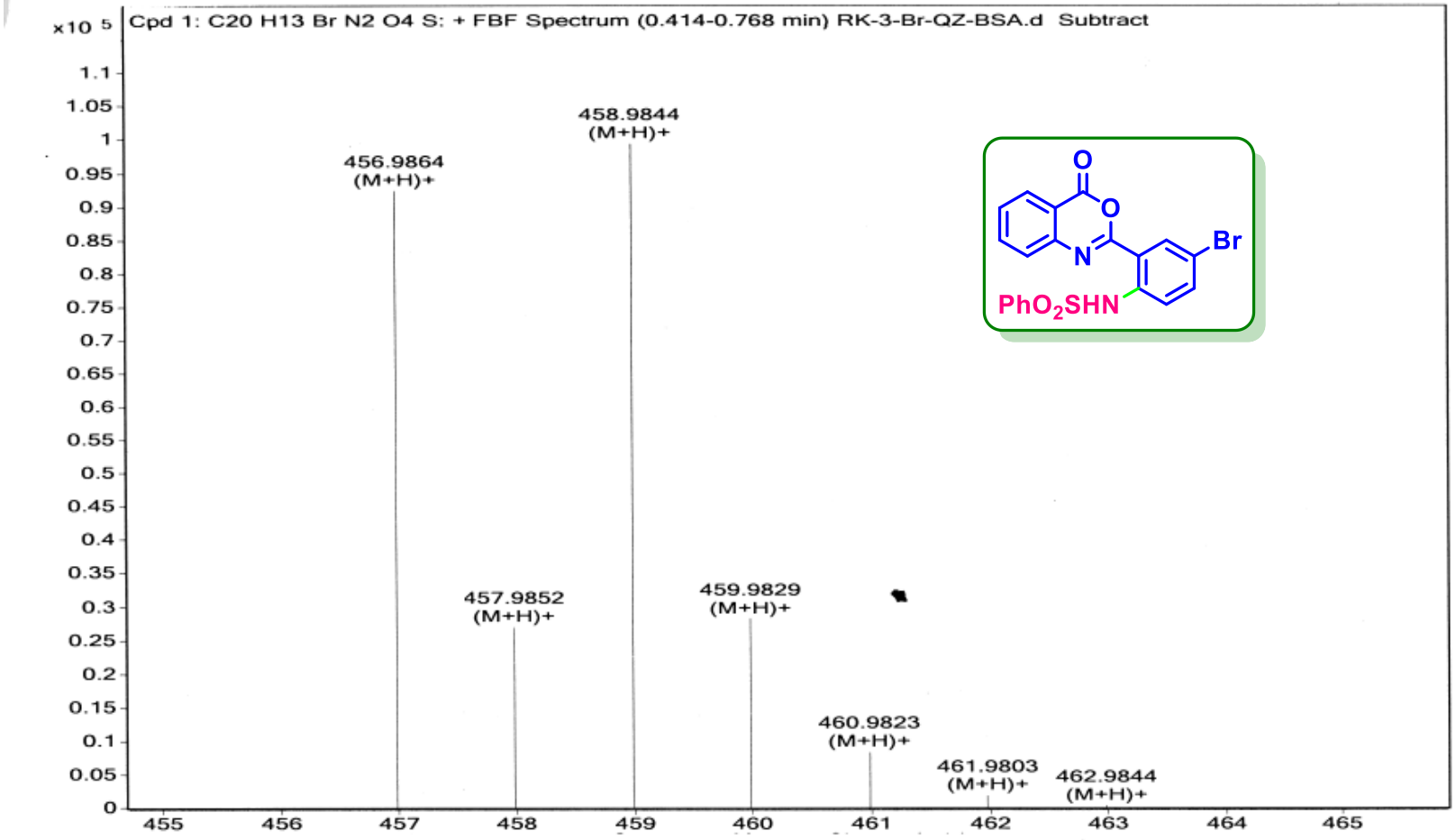


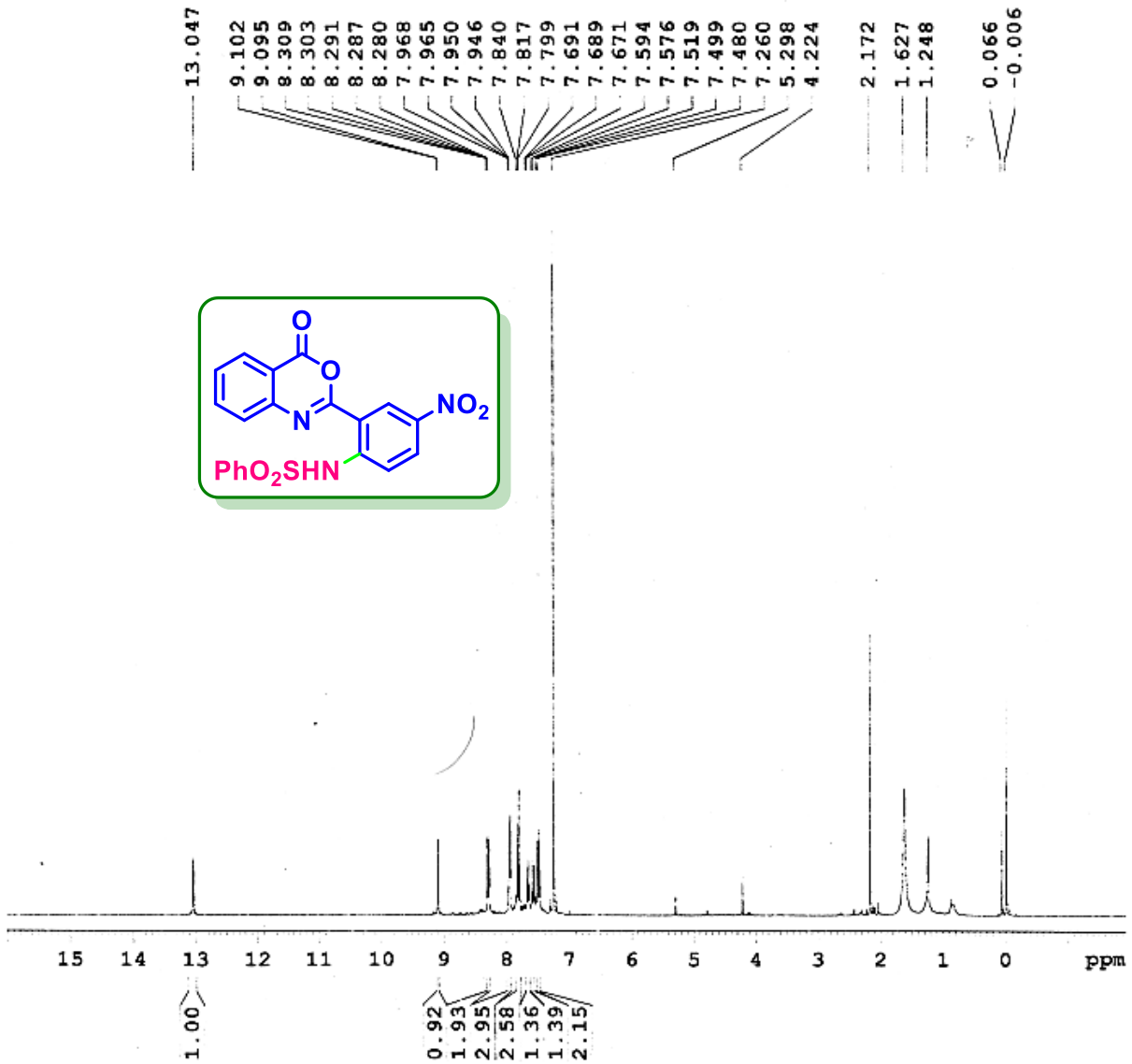

```
Current Data Parameters
NAME      RK-3-Br-QZ-BSA
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20180518
Time               15.42
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8223.685 Hz
FIDRES          0.125483 Hz
AQ              3.9846387 sec
RG                   287
DW                60.800 usec
DE                 6.00 usec
TE                294.2 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 14.35 usec
PL1                -1.00 dB
SFO1        400.1324710 MHz

F2 - Processing parameters
SI                 32768
SF          400.1300048 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```



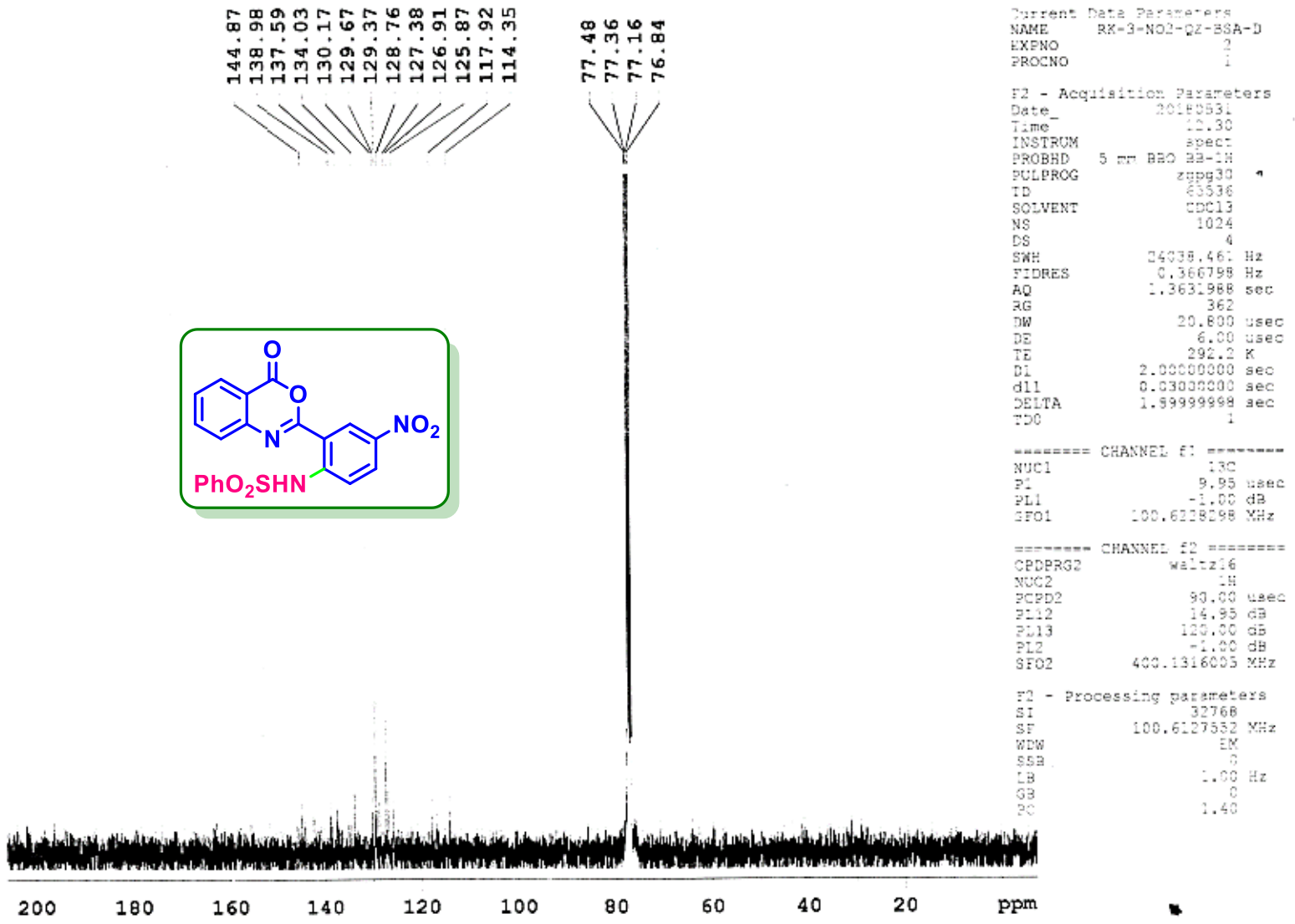

```
Current Data Parameters
NAME      RK-3-Br-QZ-BSA
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20180518
Time              15.58
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG         zgpg30
TD               65536
SOLVENT          CDCl3
NS                 256
DS                   4
SWH          24038.461 Hz
FIDRES        0.366798 Hz
AQ            1.3631988 sec
RG                 406
DW              20.800 usec
DE               6.00 usec
TE              294.7 K
D1           2.00000000 sec
d11          0.03000000 sec
DELTA        1.89999998 sec
TD0                  1

======== CHANNEL f1 ========
NUC1                 1H
P1                9.00 usec
PL1               -1.00 dB
SFO1        100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2            90.00 usec
PL12              14.00 dB
PL13              20.00 dB
PL2               -1.00 dB
SFO2        400.1316005 MHz

F2 - Processing parameters
SI                 32768
SF          100.6127690 MHz
WDW                  EM
SSB                  0
LB                1.00 Hz
GB                   0
PC                1.40
```

Sample Name	RK-3-Br-QZ-BSA	**Position**		**Instrument Name**	Q-TOF	**User Name**	QTOF-PU\admin
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	RK-3-Br-QZ-BSA.d	**ACQ Method**	Pondicherry Universi	**Comment**	RK-MB-455.9779	**Acquired Time**	21-05-2018 12:57:31



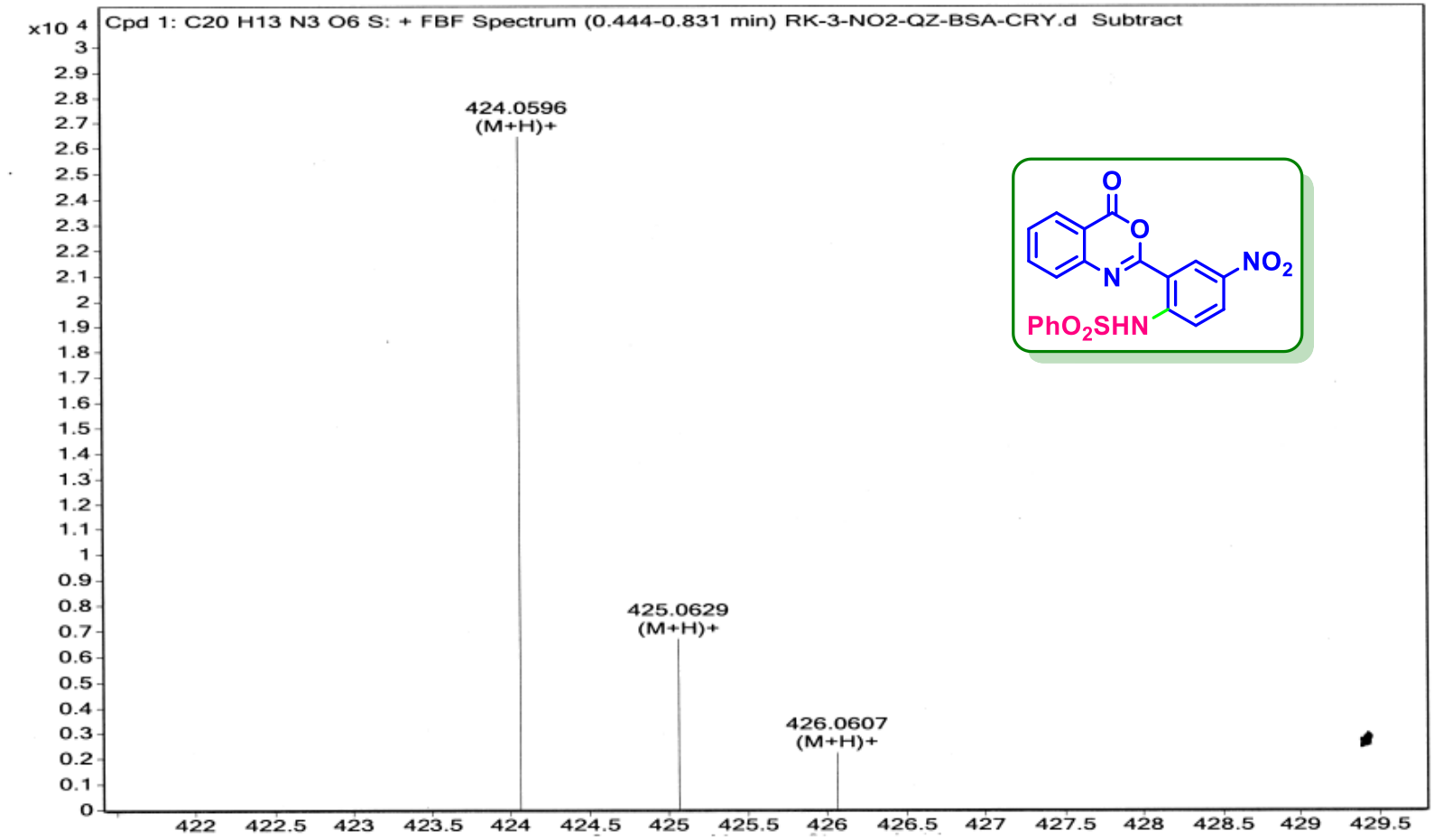


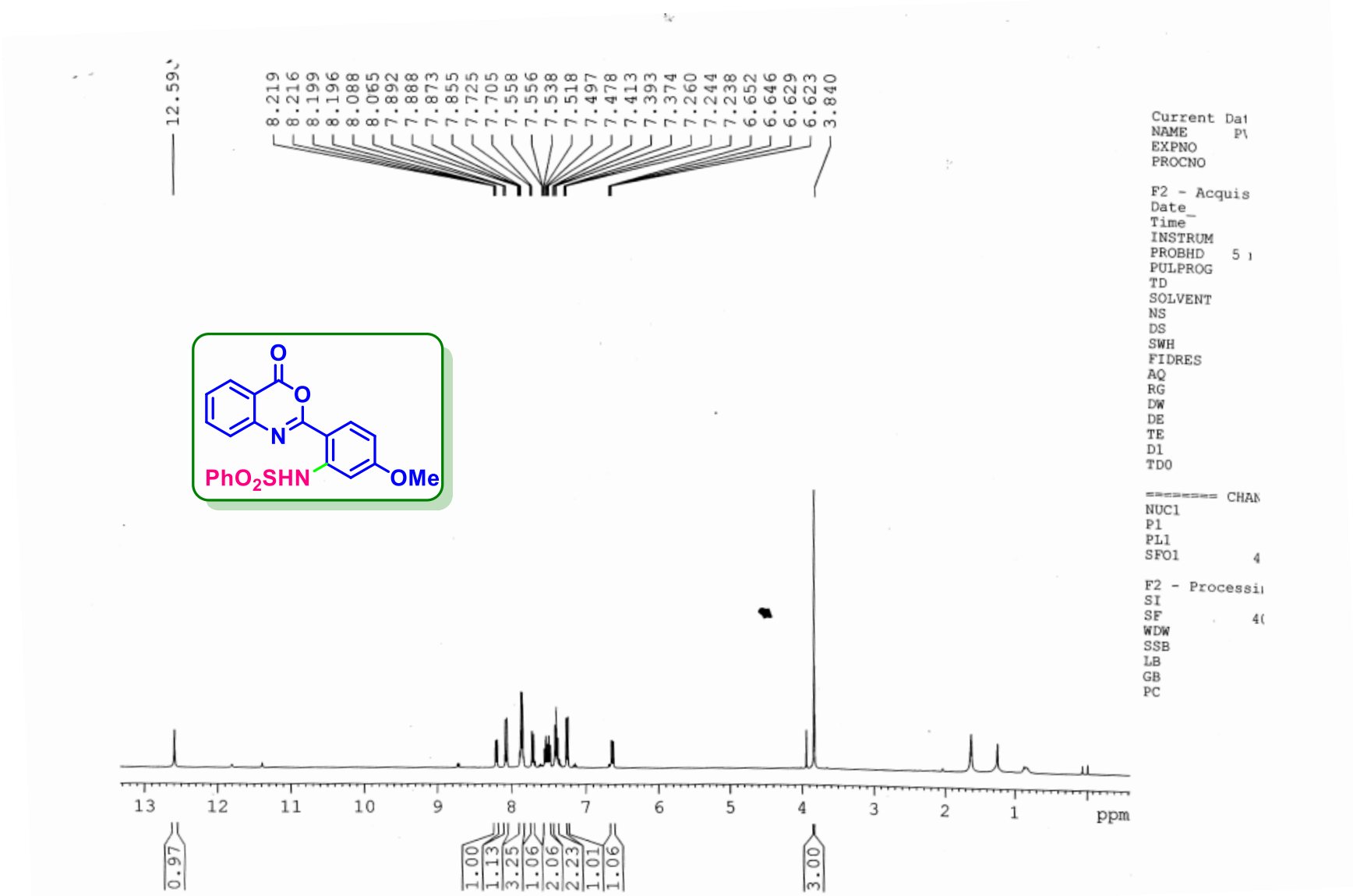

```
Current Data Parameters
NAME      RK-3-NO2-Q2-BSA-D
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_             20180528
Time                 11.23
INSTRUM              spect
PROBHD   5 mm BBO BB-1H
PULPROG              zg30
TD                  65536
SOLVENT              CDCl3
NS                      32
DS                       2
SWH               8223.685 Hz
FIDRES            0.125483 Hz
AQ                3.9846387 sec
RG                     512
DW                  60.800 usec
DE                   6.00 usec
TE                  291.7 K
D1                1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                    1H
P1                   14.35 usec
PL1                  -1.00 dB
SFO1          400.1324710 MHz

F2 - Processing parameters
SI                   32768
SF            400.1300048 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.00
```

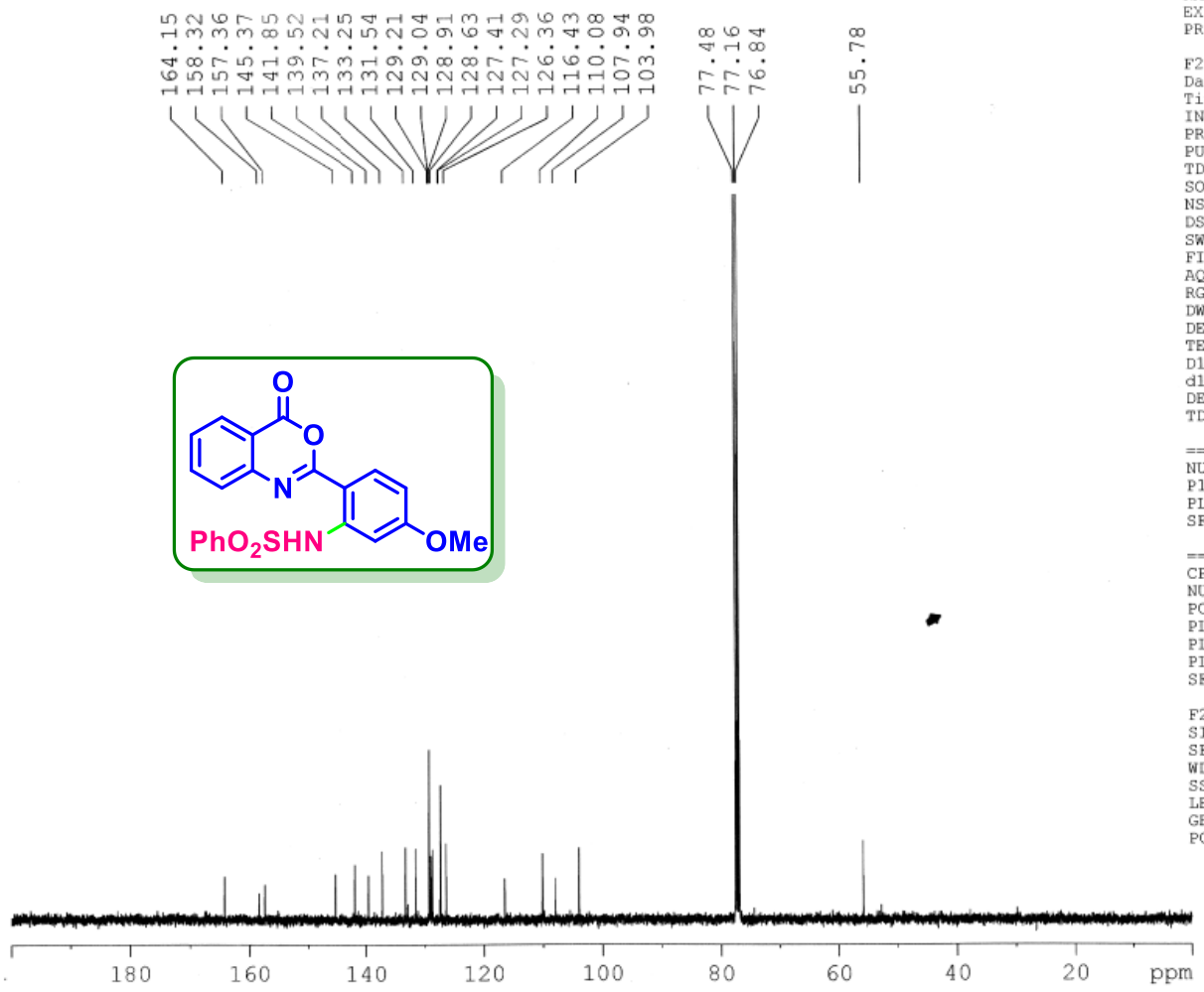



```
Current Data Parameters
NAME      RK-3-NO2-QZ-BSA-D
EXPNO                     2
PROCNO                    1

F2 - Acquisition Parameters
Date_           20180531
Time                12.30
INSTRUM             spect
PROBHD   5 mm BBO BB-1H
PULPROG          zgpg30
TD                 65536
SOLVENT              CDCl3
NS                    1024
DS                       4
SWH              24038.461 Hz
FIDRES           0.366798 Hz
AQ               1.3631988 sec
RG                     362
DW                20.800 usec
DE                 6.00 usec
TE                292.2 K
D1             2.00000000 sec
d11            0.03000000 sec
DELTA          1.89999998 sec
TD0                       1

========== CHANNEL f1 =========
NUC1                    13C
P1                   9.95 usec
PL1                 -1.00 dB
SFO1          100.6228298 MHz

========= CHANNEL f2 =========
CPDPRG2            waltz16
NUC2                    1H
PCPD2                90.00 usec
PL12                14.95 dB
PL13                120.00 dB
PL2                 -1.00 dB
SFO2          400.1316005 MHz

F2 - Processing parameters
SI                   32768
SF            100.6127532 MHz
WDW                     EM
SSB                      0
LB                    1.00 Hz
GB                       0
PC                    1.40
```

Sample Name	RK-3-NO2-QZ-BSA-CRY	**Position**		**Instrument Name**	Q-TOF	**User Name**	QTOF-PU\admin
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	RK-3-NO2-QZ-BSA-CRY.	**ACQ Method**	Pondicherry Universi	**Comment**	RK-MB-423.0525	**Acquired Time**	30-05-2018 11:55:53

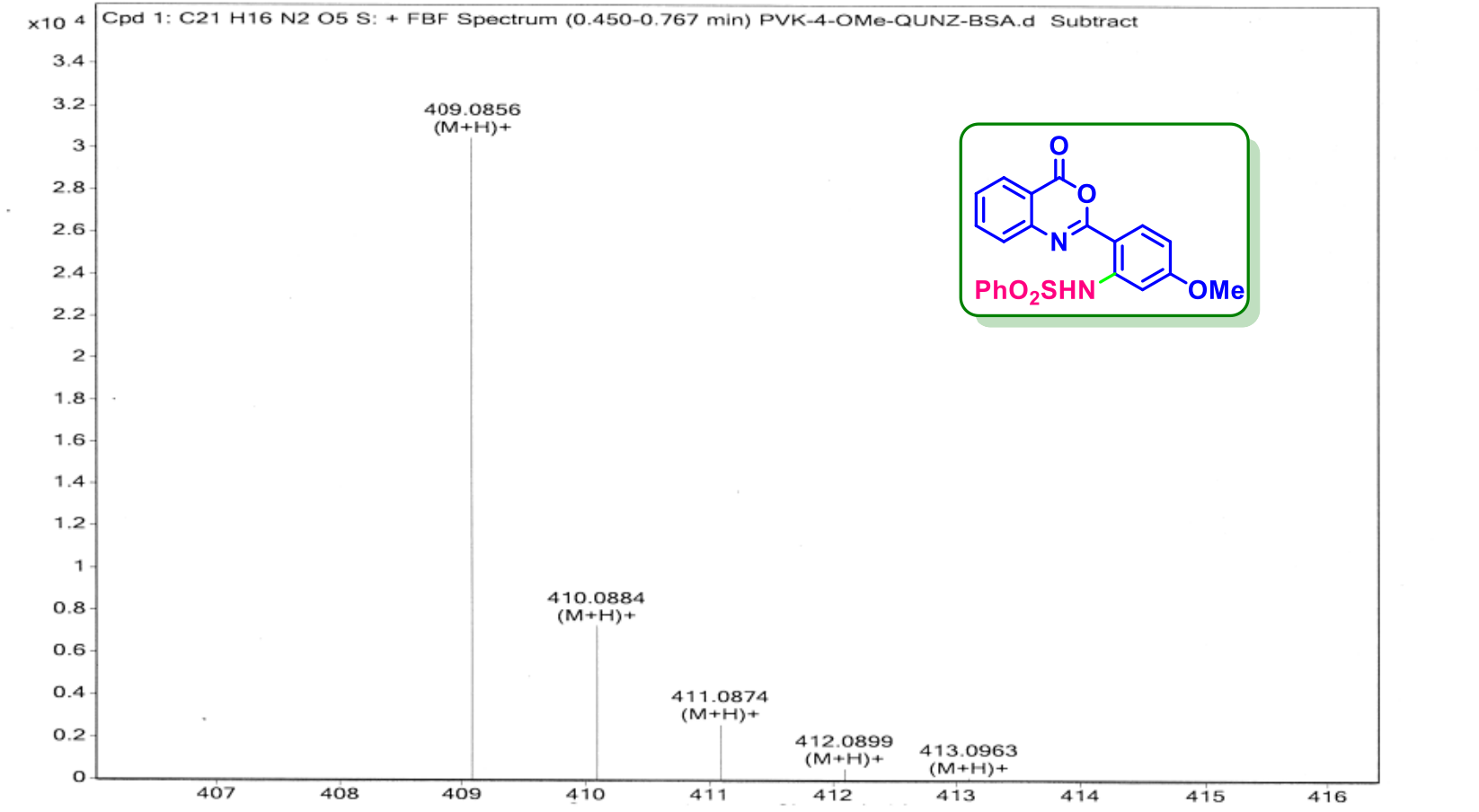


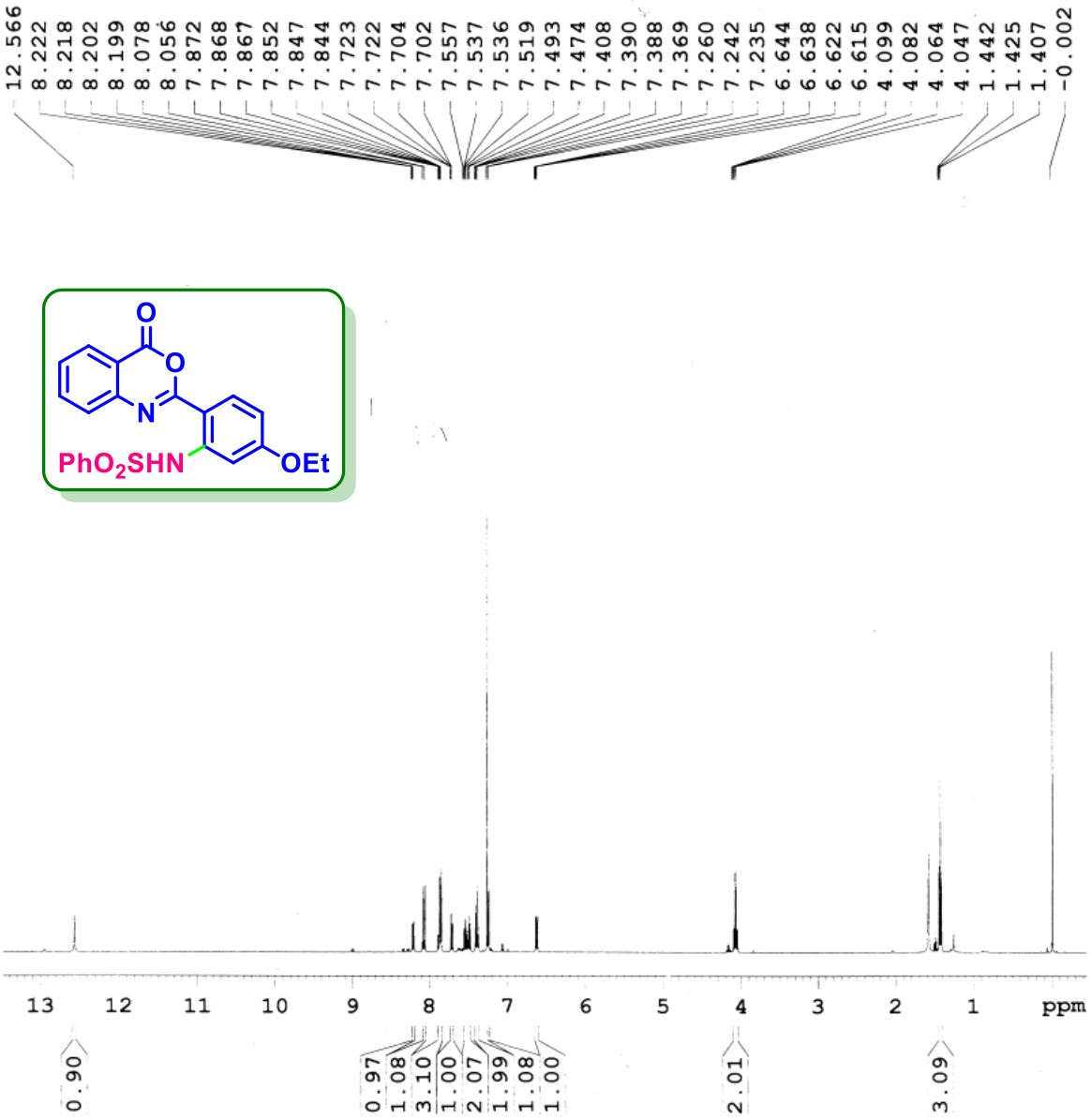

12.59
8.219
8.216
8.199
8.196
8.088
8.065
7.892
7.888
7.873
7.855
7.725
7.705
7.558
7.556
7.538
7.518
7.497
7.478
7.413
7.393
7.374
7.260
7.244
7.238
6.652
6.646
6.629
6.623
3.840
O
O
N
PhO2SHN
OMe
Current Da
NAME P\
EXPNO
PROCNO
F2 - Acquis
Date_
Time
INSTRUM
PROBHD 5
PULPROG
TD
SOLVENT
NS
DS
SWH
FIDRES
AQ
RG
DW
DE
TE
D1
TDO
====== CHAN
NUC1
P1
PL1
SFO1 4
F2 - Processi
SI
SF 4(
WDW
SSB
LB
GB
PC
13
12
11
10
9
8
7
6
5
4
3
2
1
ppm
0.97
1.00
1.13
3.25
1.06
2.06
2.23
1.01
1.06
3.00



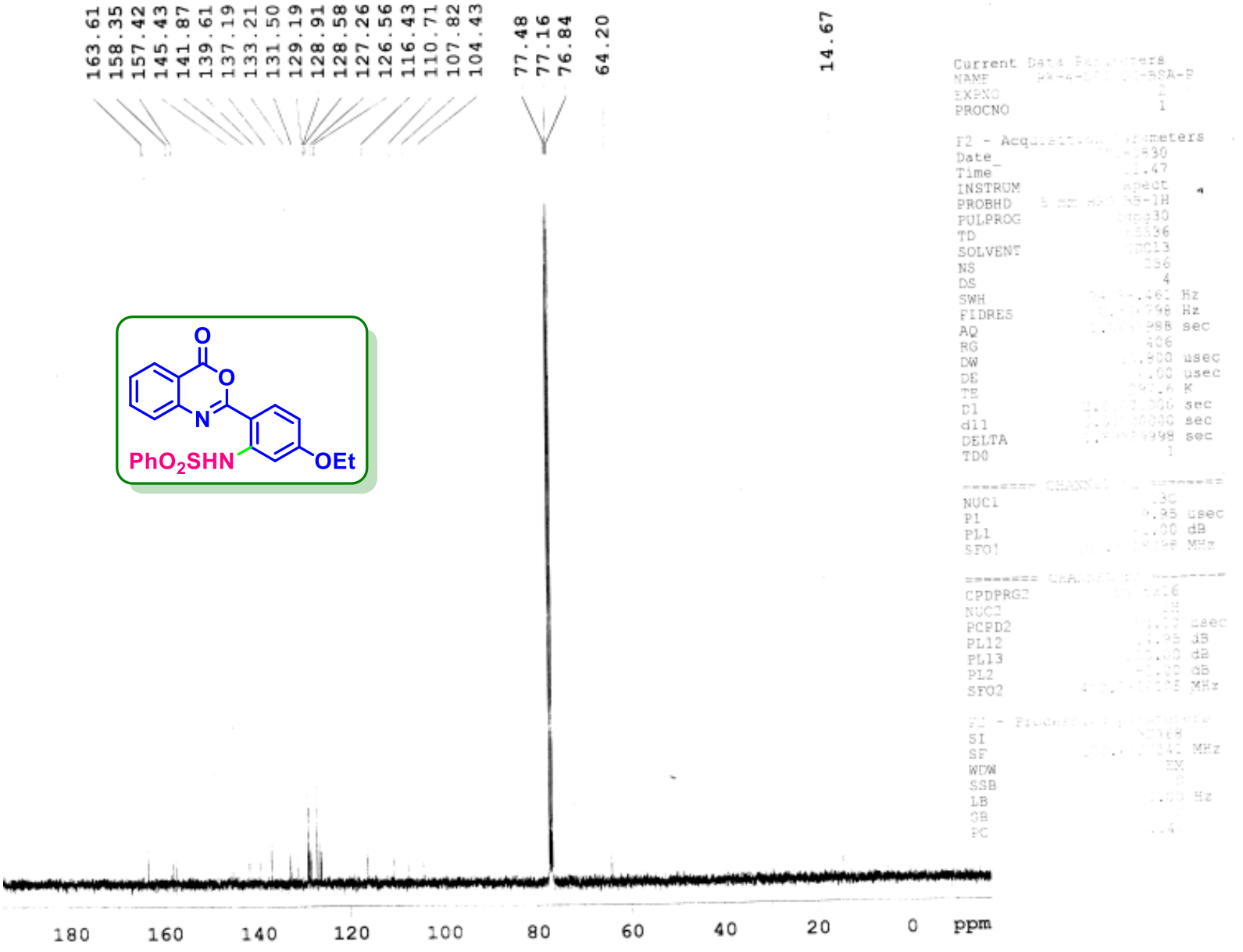

```
Current Data Parameters
NAME      PVK-4-OME-QUNZ-BSA
EXPNO                      5
PROCNO                     1

F2 - Acquisition Parameters
Date_              20170102
Time                 16.55
INSTRUM              spect
PROBHD   5 mm DUL 13C-1
PULPROG            zgpg30
TD                  65536
SOLVENT             CDCl3
NS                    300
DS                      4
SWH             24038.461 Hz
FIDRES          0.366798 Hz
AQ              1.3631988 sec
RG                   28.5
DW                20.800 usec
DE                 6.00 usec
TE                294.1 K
D1             2.00000000 sec
d11            0.03000000 sec
DELTA          1.89999998 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  13C
P1                  9.15 usec
PL1                 0.00 dB
SFO1          100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                  1H
PCPD2              90.00 usec
PL12               14.90 dB
PL13               14.90 dB
PL2                -3.00 dB
SFO2          400.1316005 MHz

F2 - Processing parameters
SI                   32768
SF            100.6127556 MHz
WDW                     EM
SSB                      0
LB                  1.00 Hz
GB                       0
PC                    1.40
```

Sample Name	PVK-4-OMe-QUNZ-BSA	**Position**		**Instrument Name**	Q-TOF	**User Name**	QTOF-PU\admin
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	PVK-4-OMe-QUNZ-BSA.d	**ACQ Method**	Pondicherry Universi	**Comment**	PVK-MB-408.0780	**Acquired Time**	19-04-2018 14:40:41

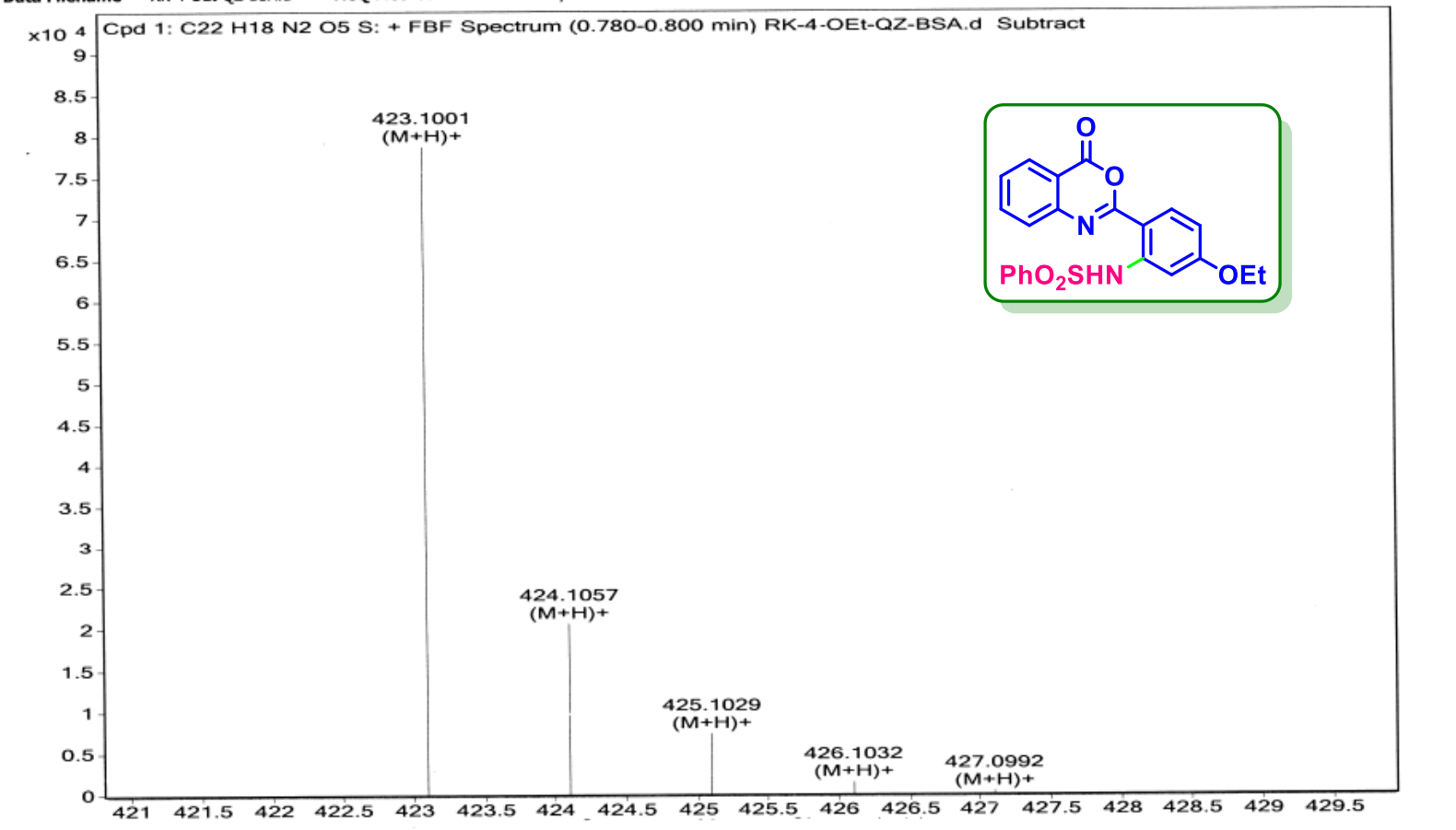


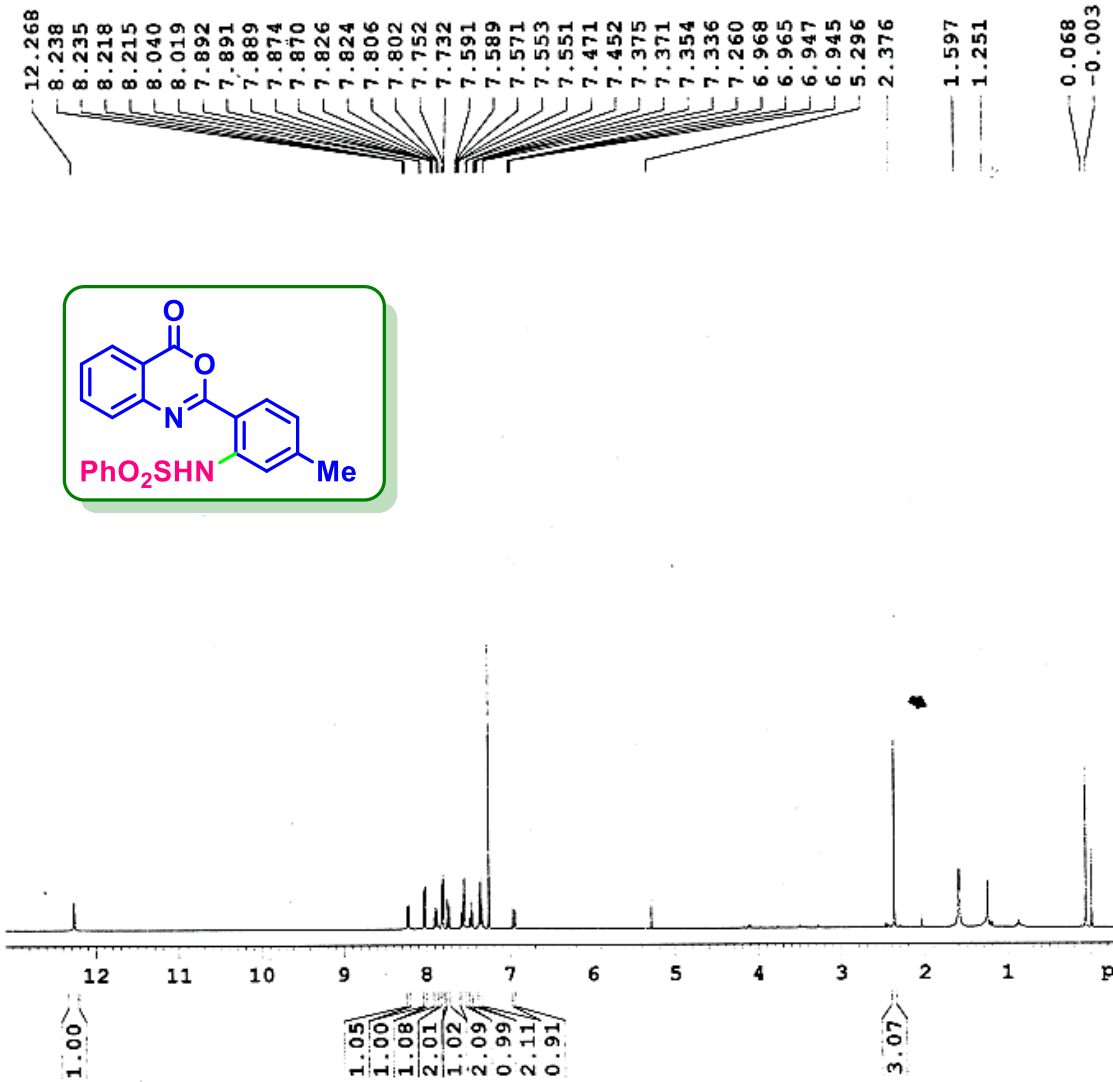



```
Current Data Parameters
NAME      RK-4-OEt-Qz-BSA
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_           20180828
Time               12.06
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8223.685 Hz
FIDRES          0.125483 Hz
AQ              3.9846367 sec
RG                   362
DW                60.800 usec
DE                 6.00 usec
TE                295.8 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 14.35 usec
PL1                -1.00 dB
SFO1         400.1324710 MHz

F2 - Processing parameters
SI                 32768
SF          400.1300048 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

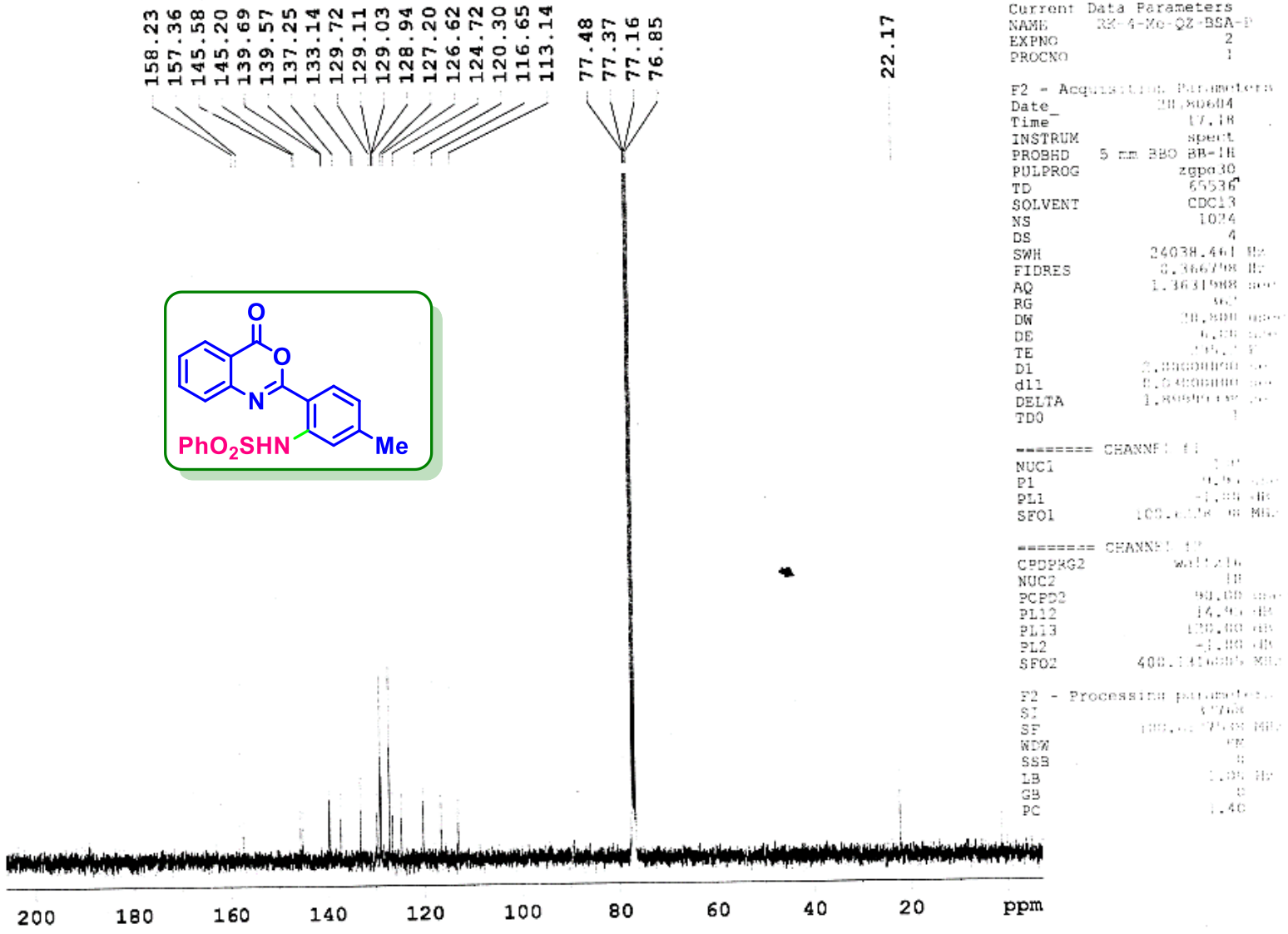

163.61
158.35
157.42
145.43
141.87
139.61
137.19
133.21
131.50
129.19
128.91
128.58
127.26
126.56
116.43
110.71
107.82
104.43
77.48
77.16
76.84
64.20
14.67
O
O
N
PhO2SHN
OEt
180
160
140
120
100
80
60
40
20
0
ppm

Sample Name	RK-4-OEt-QZ-BSA	**Position**		**Instrument Name**	Q-TOF	**User Name**	QTOF-PU\admin
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	RK-4-OEt-QZ-BSA.d	**ACQ Method**	Pondicherry Universi	**Comment**	RK-MB-422.0936	**Acquired Time**	11-09-2018 12:16:03






```
Current Data Parameters
NAME      RK-4-Me-QZ-BSA-P
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_             20180604
Time                 16.18
INSTRUM              spect
PROBHD   5 mm BBO BB-1H
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                     32
DS                      2
SWH               8223.685 Hz
FIDRES            0.125483 Hz
AQ                3.9846387 sec
RG                    456
DW                 60.800 usec
DE                  6.00 usec
TE                 296.1 K
D1              1.00000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                   1H
P1                  14.35 usec
PL1                 -1.00 dB
SFO1          400.1324710 MHz

F2 - Processing parameters
SI                  32768
SF            400.1300049 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   1.00
```



Current Data Parameters
NAME RX-4-Me-QZ-BSA-P
EXPNO 2
PROCNO 1

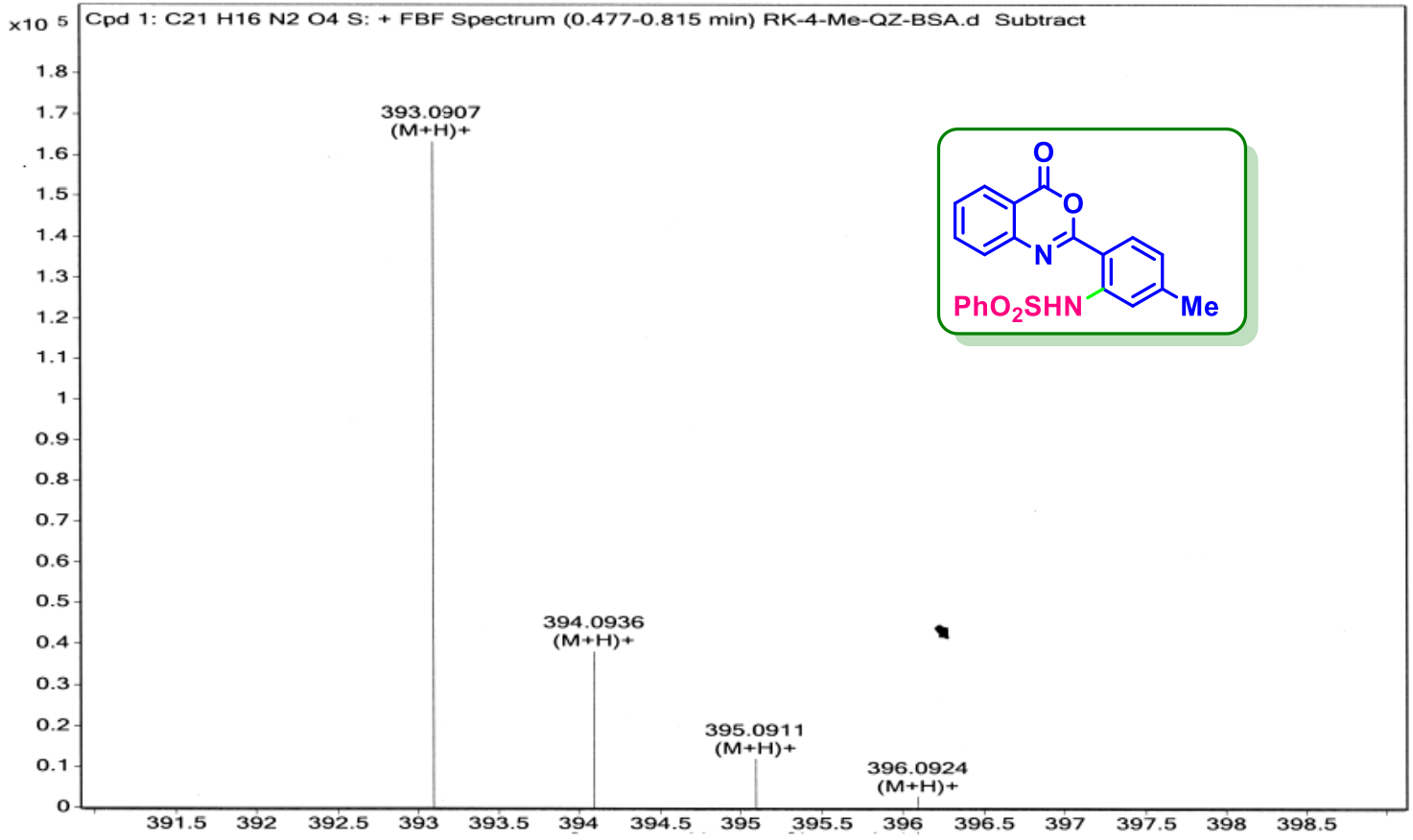
F2 - Acquisition Parameters
Date_ 20180604
Time 17.18
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 362
DW 20.800 usec
DE 6.00 usec
TE 295.1 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.80000000 sec
TD0 1

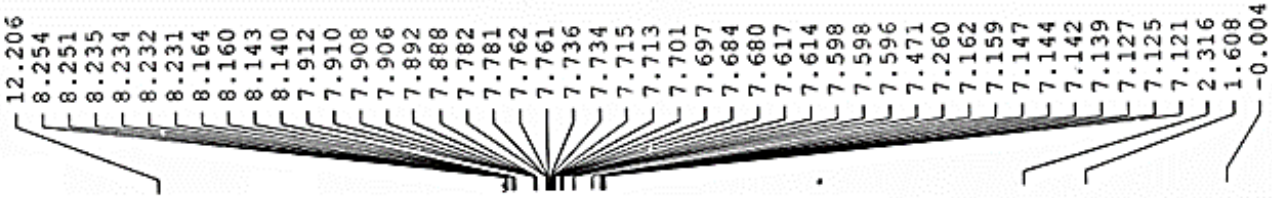
======== CHANNEL f1
NUC1 1H
P1 9.50 usec
PL1 -1.05 dB
SFO1 400.1316005 MHz

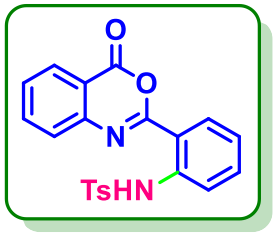
======== CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL12 14.90 dB
PL13 120.00 dB
PL2 -1.00 dB
SFO2 400.1316005 MHz

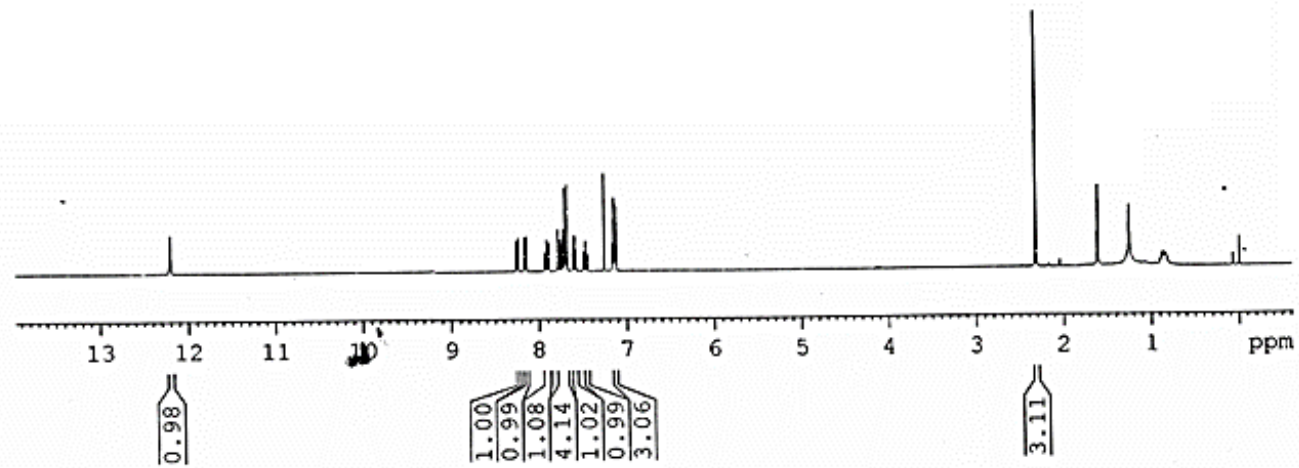
F2 - Processing parameters
SI 65536
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

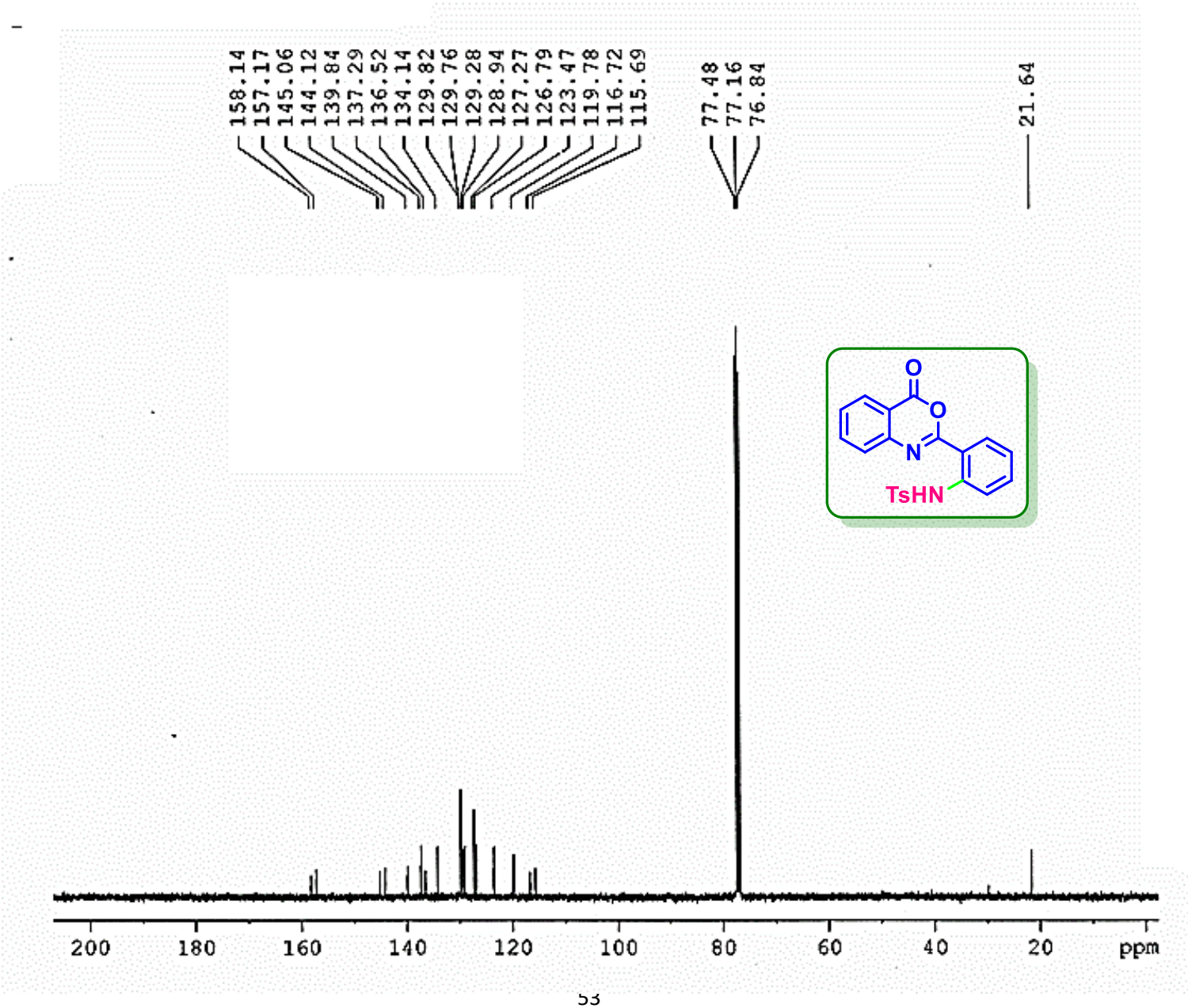
Sample Name	RK-4-Me-QZ-BSA	**Position**		**Instrument Name**	Q-TOF	**User Name**	QTOF-PU\admin
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	RK-4-Me-QZ-BSA.d	**ACQ Method**	Pondicherry Universi	**Comment**	RK-MB-392.0831	**Acquired Time**	06-06-2018 15:31:19

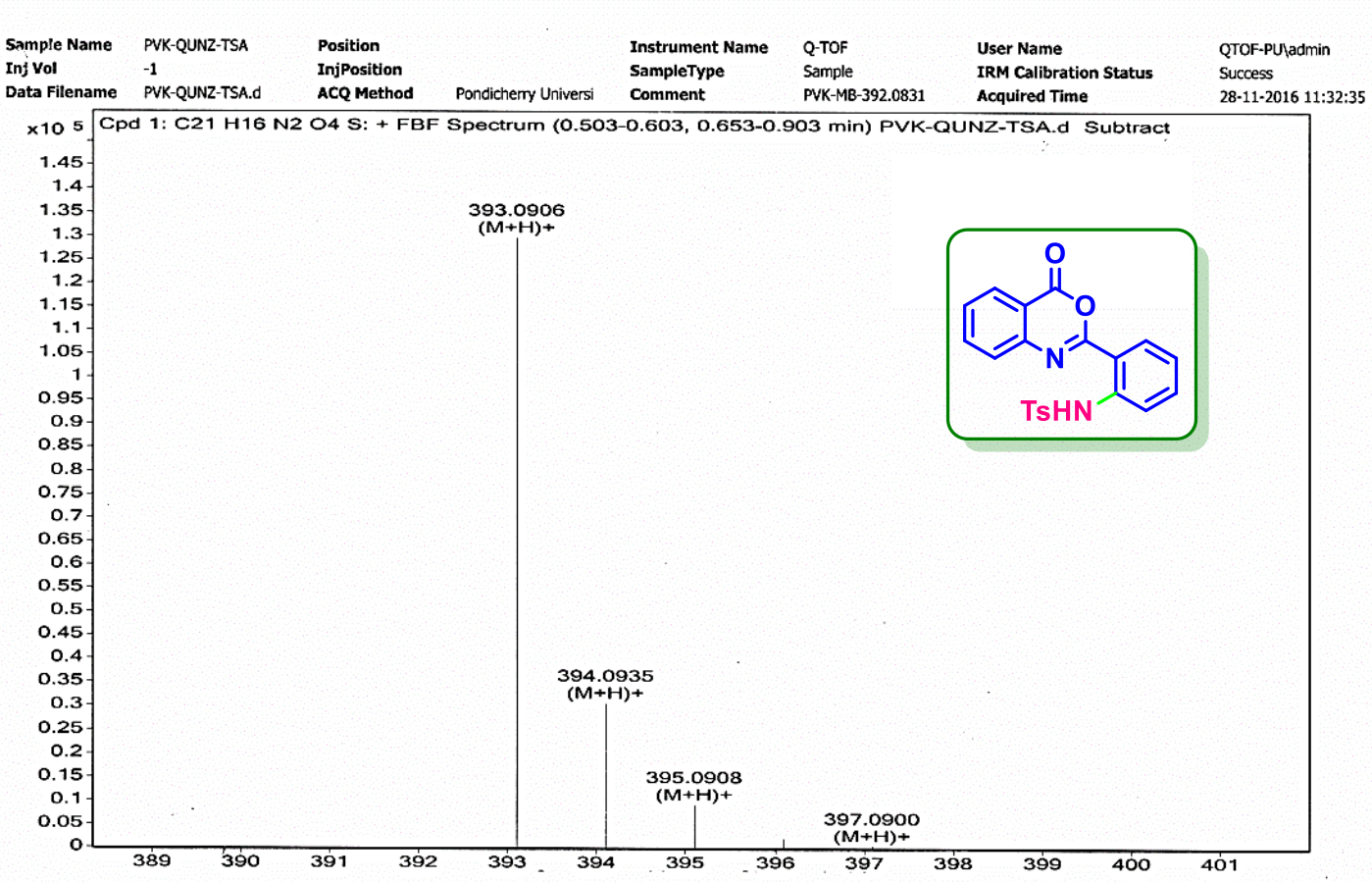


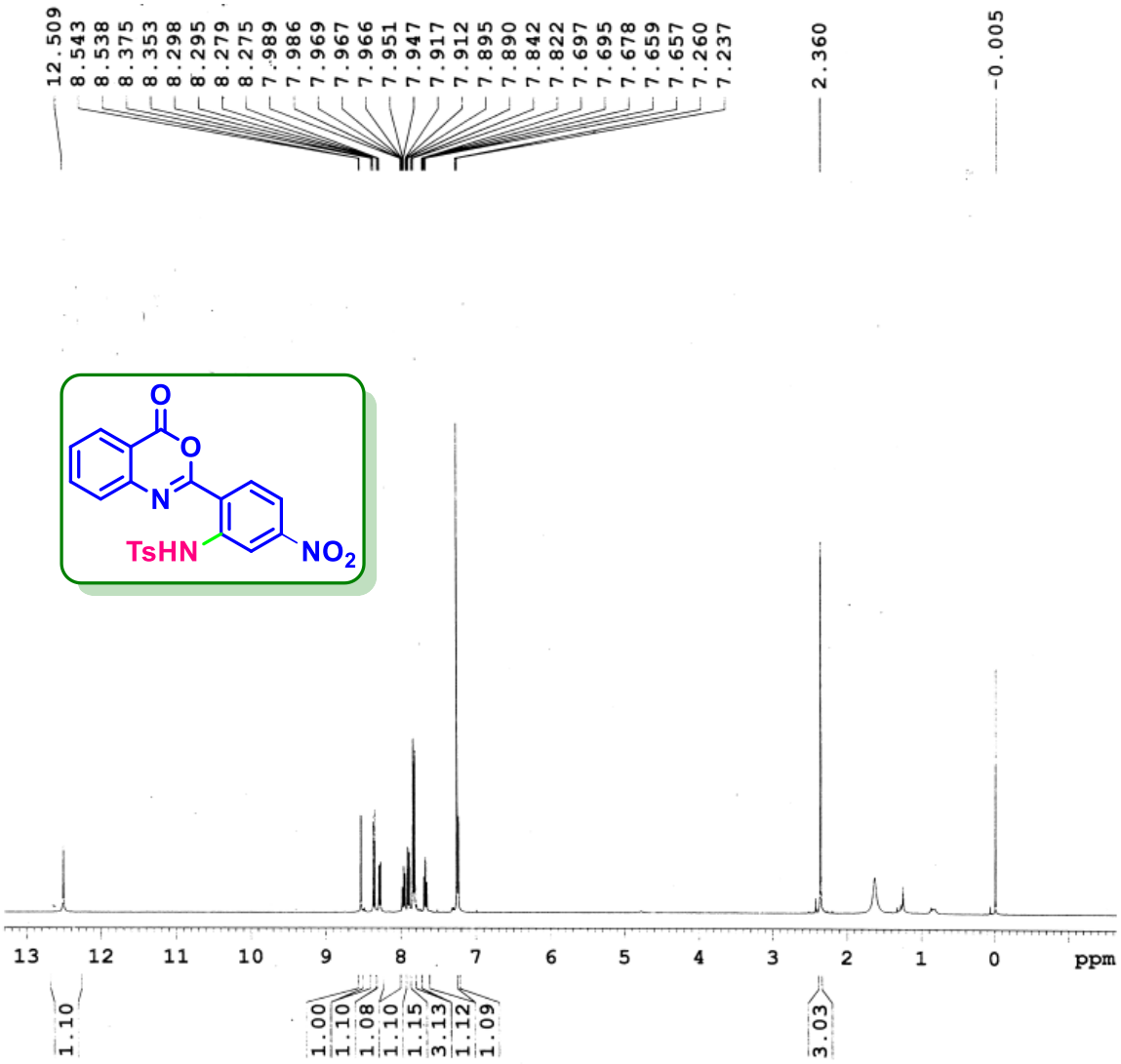

12.206
8.254
8.251
8.235
8.234
8.232
8.231
8.164
8.160
8.143
8.140
7.912
7.910
7.908
7.906
7.892
7.888
7.782
7.781
7.762
7.761
7.736
7.734
7.715
7.713
7.701
7.697
7.684
7.680
7.617
7.614
7.598
7.598
7.596
7.471
7.260
7.162
7.159
7.147
7.144
7.142
7.139
7.127
7.125
7.121
2.316
1.608
-0.004


O
O
N
TsHN

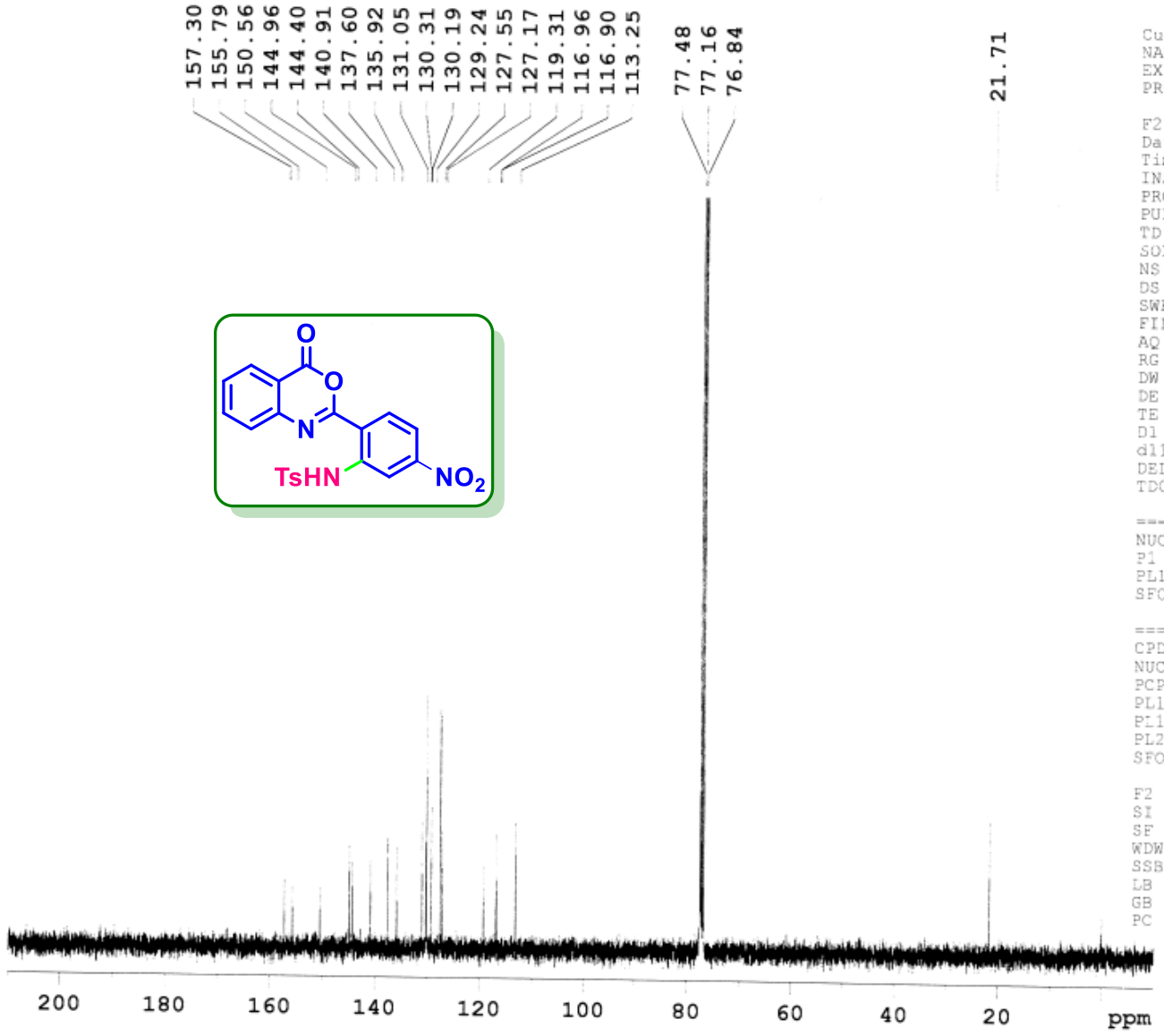

13
12
11
10
9
8
7
6
5
4
3
2
1
ppm
0.98
1.00
0.99
1.08
4.14
1.02
0.99
3.06
3.11


158.14
157.17
145.06
144.12
139.84
137.29
136.52
134.14
129.82
129.76
129.28
128.94
127.27
126.79
123.47
119.78
116.72
115.69
77.48
77.16
76.84
21.64
O
O
N
TsHN
200
180
160
140
120
100
80
60
40
20
ppm


Sample Name PVK-QUNZ-TSA
Position
Instrument Name Q-TOF
User Name QTOF-PU\admin
Inj Vol -1
InjPosition
SampleType Sample
IRM Calibration Status Success
Data Filename PVK-QUNZ-TSA.d
ACQ Method Pondicherry Universi
Comment PVK-MB-392.0831
Acquired Time 28-11-2016 11:32:35
Cpd 1: C21 H16 N2 O4 S: + FBF Spectrum (0.503-0.603, 0.653-0.903 min) PVK-QUNZ-TSA.d Subtract
x10 5
393.0906
(M+H)+
394.0935
(M+H)+
395.0908
(M+H)+
397.0900
(M+H)+
TsHN

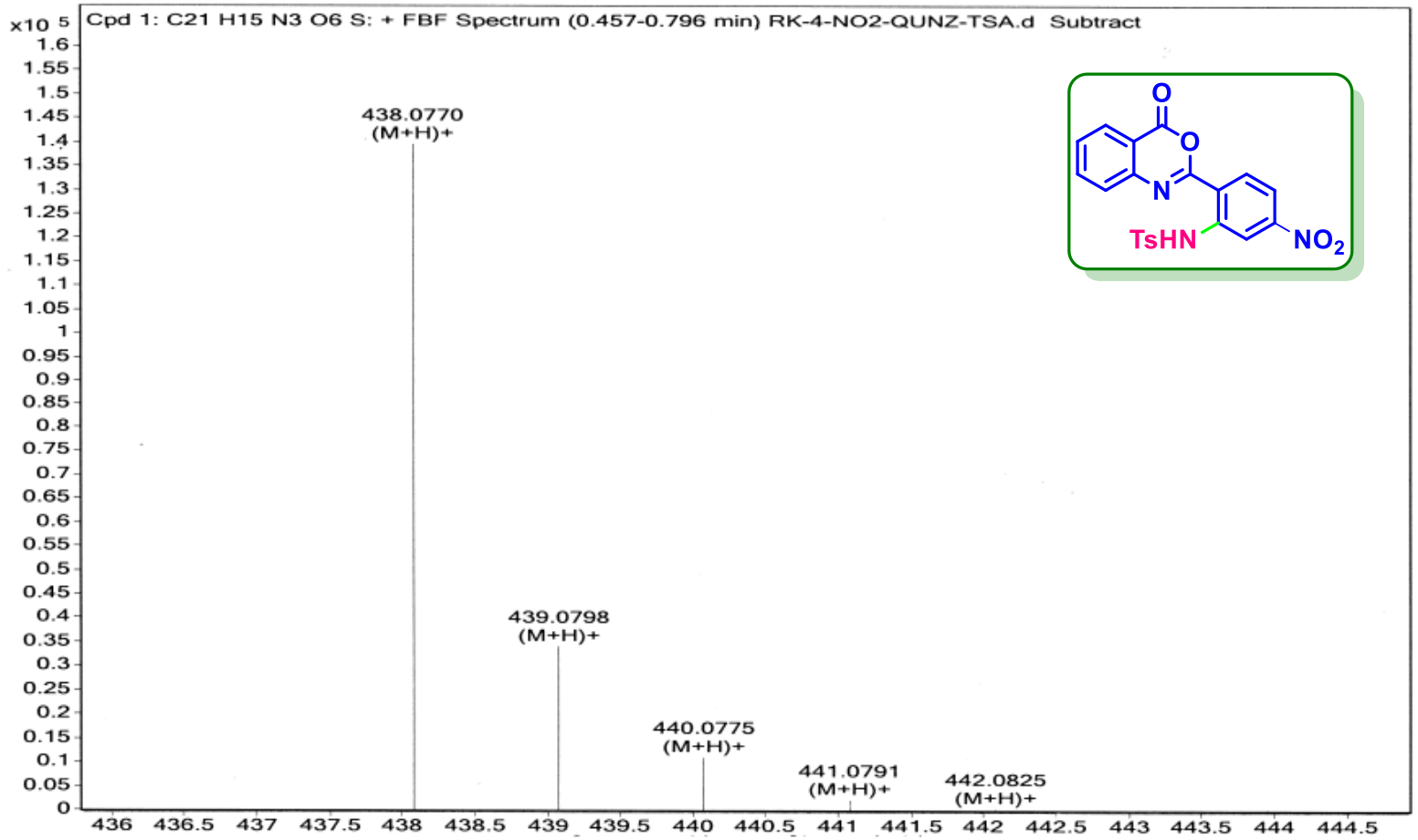


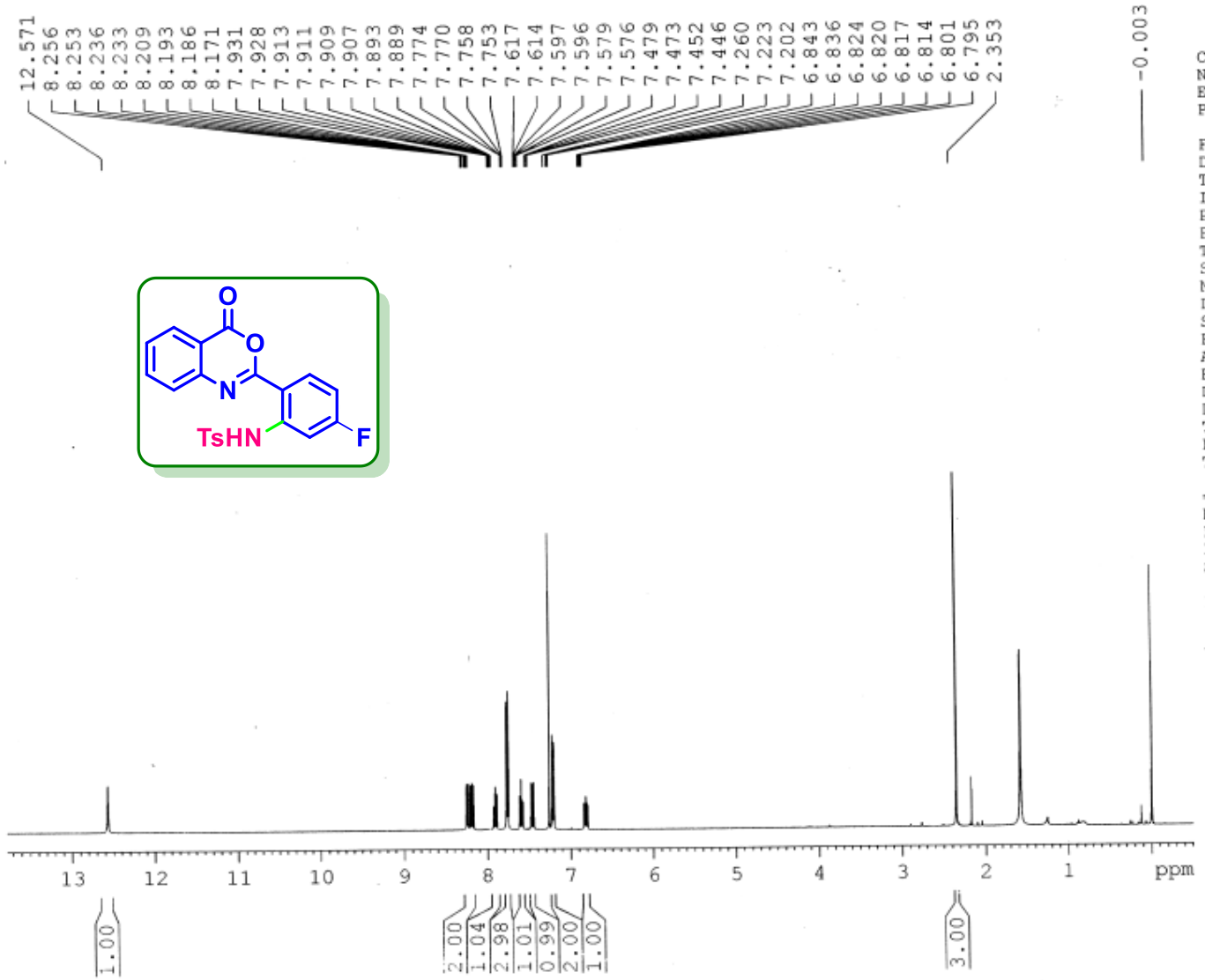

```
Current Data Parameters
NAME      RK-4-NO2-QZ-TSA
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_           20180518
Time              23.33
INSTRUM           spect
PROBHD   5 mm BBO BB-1H
PULPROG             zg30
TD                65536
SOLVENT           CDCl3
NS                   16
DS                    2
SWH            8223.685 Hz
FIDRES        0.125483 Hz
AQ            3.9846387 sec
RG                  456
DW               60.800 usec
DE                6.00 usec
TE               293.6 K
D1            1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 1H
P1                14.35 usec
PL1               -1.00 dB
SFO1       400.1324710 MHz

F2 - Processing parameters
SI                32768
SF         400.1300048 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 1.00
```



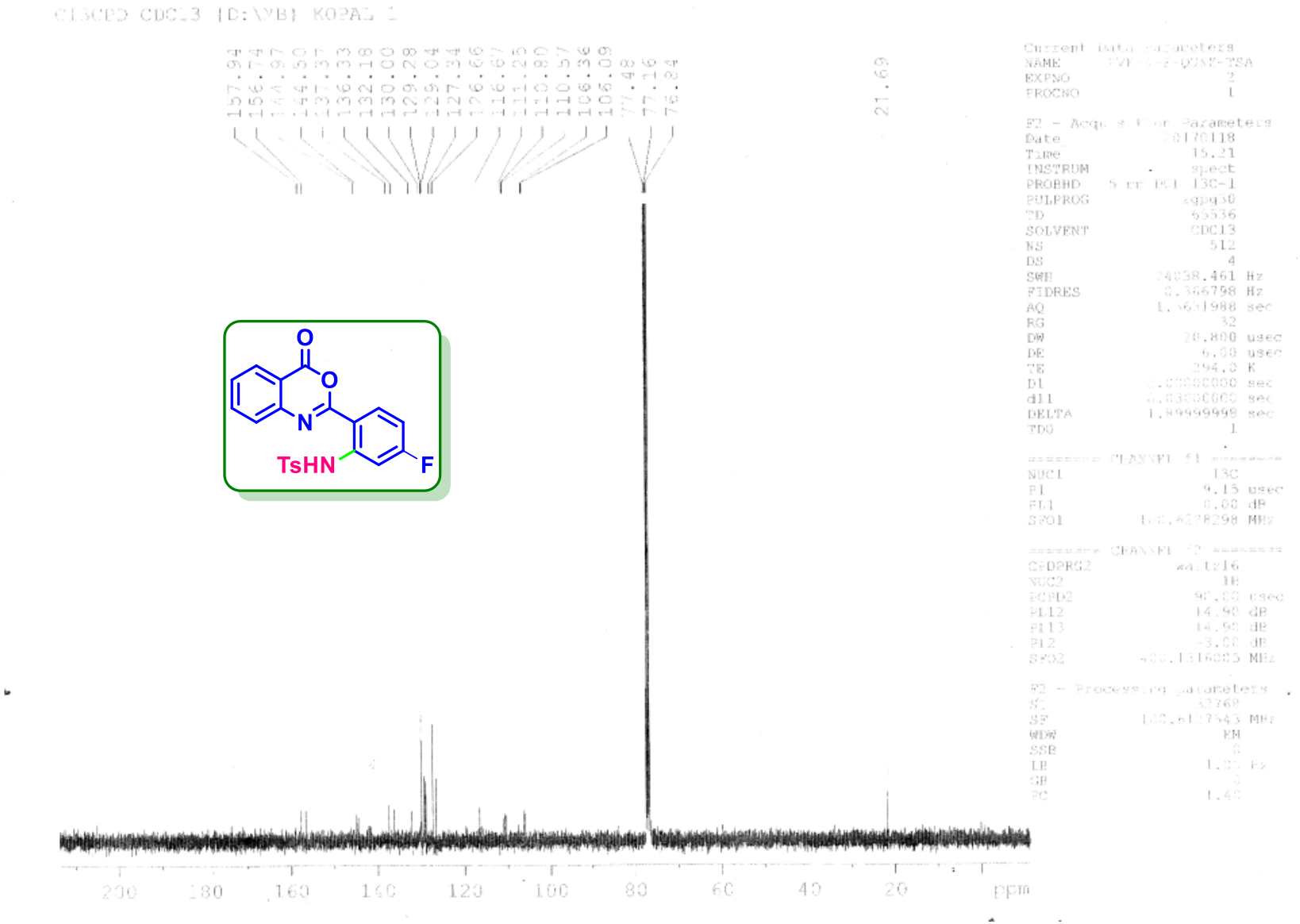

```
Current Data Parameters
NAME      RK-4-NO2-Q2-TSA
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_            20180522
Time               13.28
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  512
DS                    4
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ             1.3631988 sec
RG                  322
DW               20.800 usec
DE                6.00 usec
TE               294.4 K
D1            1.00000000 sec
d11           0.03000000 sec
DELTA         0.89999998 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                 9.95 usec
PL1               -1.00 dB
SFO1        100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2             90.00 usec
PL12              14.95 dB
PL13             120.00 dB
PL2               -1.00 dB
SFO2        400.1316005 MHz

F2 - Processing parameters
SI                  32768
SF          100.6127552 MHz
WDW                    EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

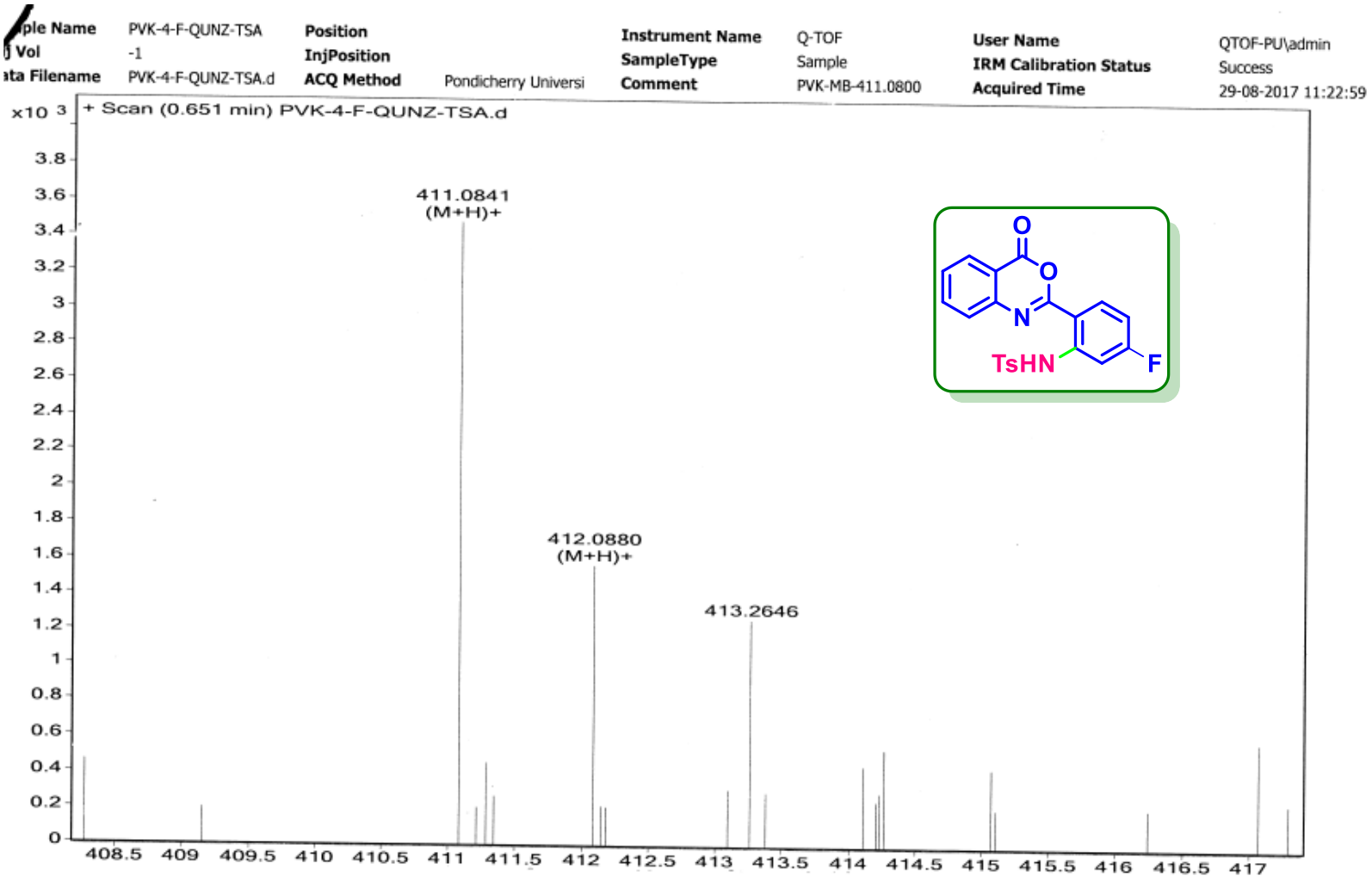
Sample Name	RK-4-NO2-QUNZ-TSA	**Position**		**Instrument Name**	Q-TOF	**User Name**	QTOF-PU\admin
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	RK-4-NO2-QUNZ-TSA.d	**ACQ Method**	Pondicherry Universi	**Comment**	RK-MB-437.0682	**Acquired Time**	21-05-2018 12:49:58

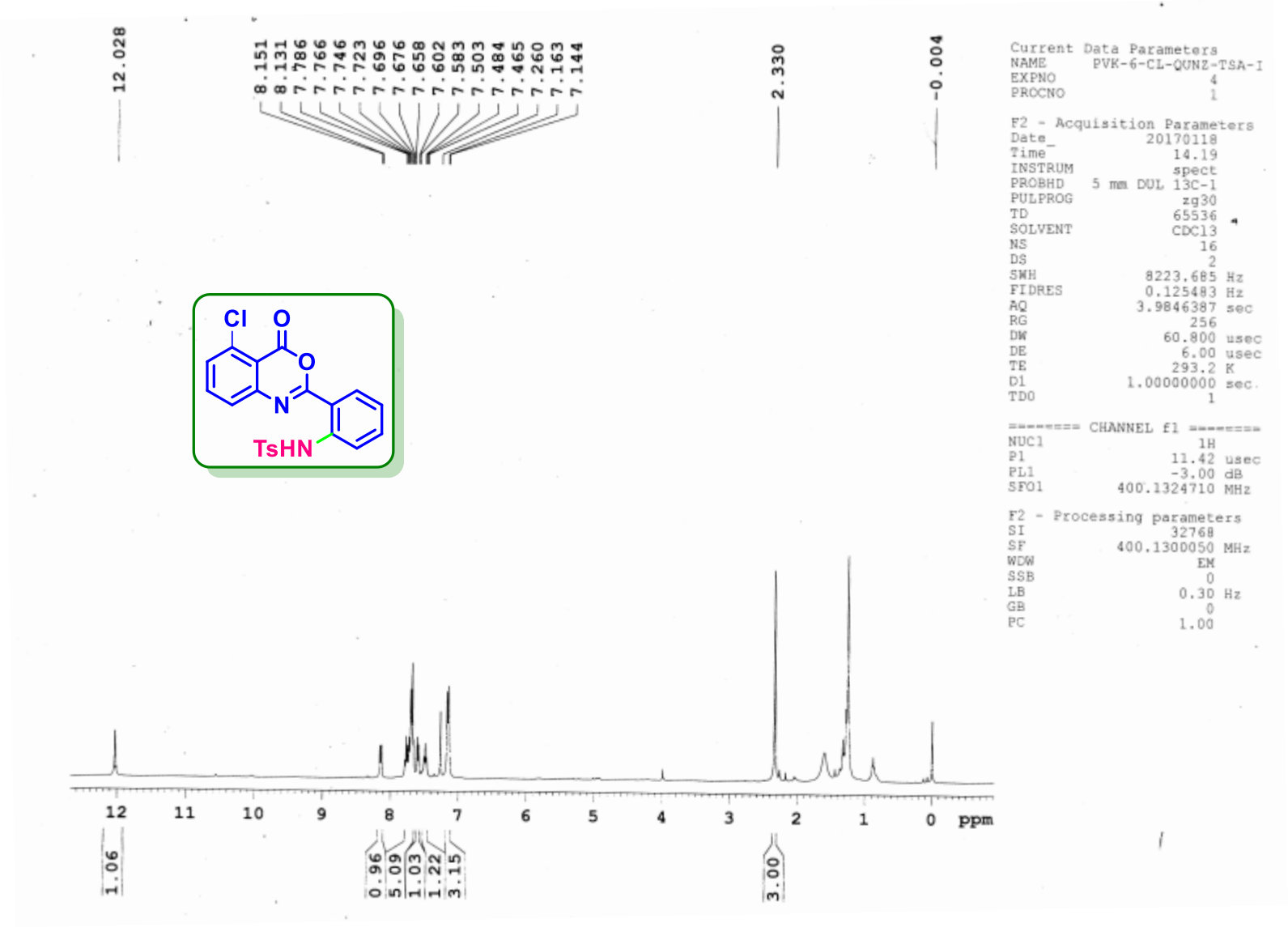




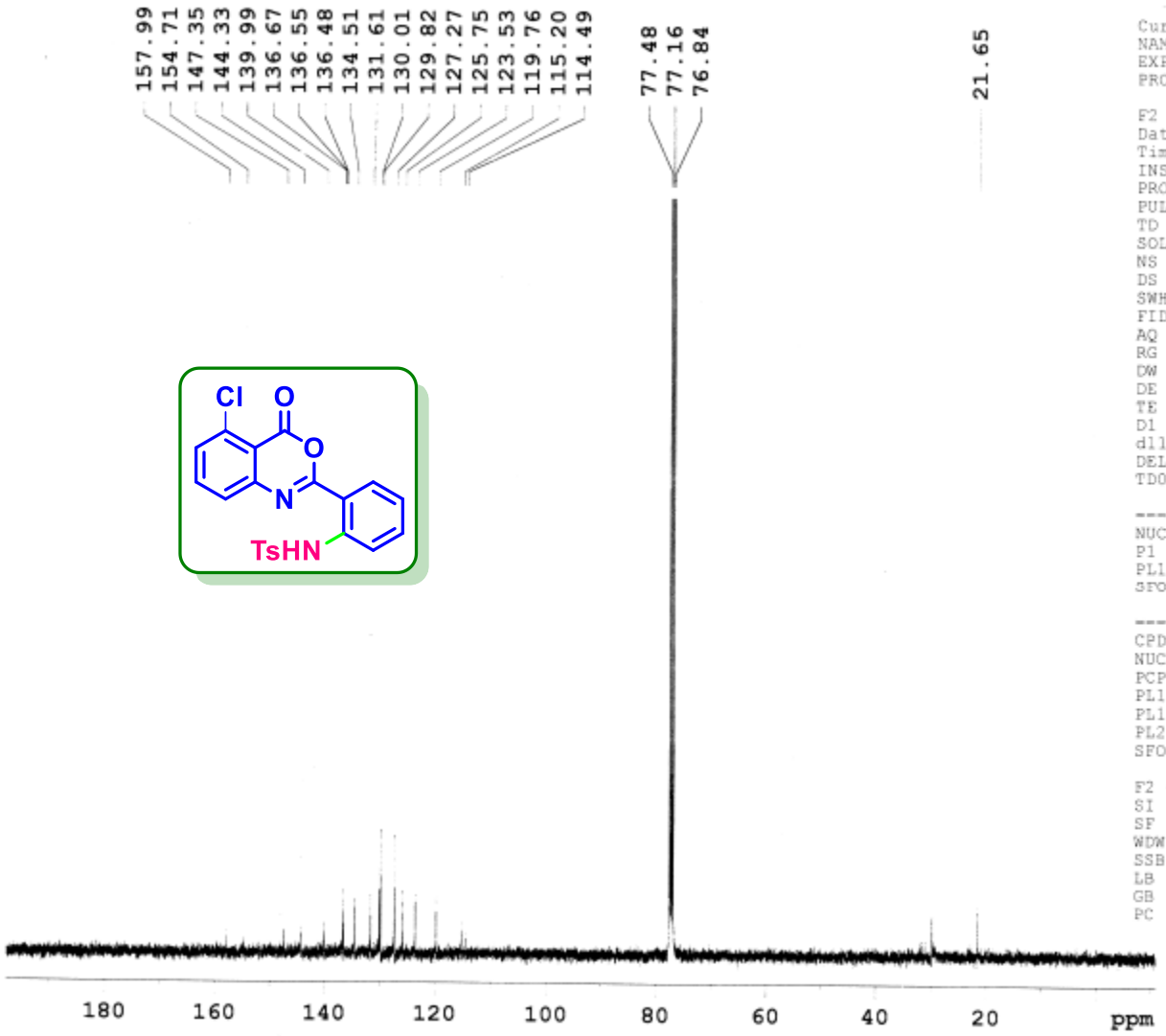

```
Current Data Parameters
NAME      PVK-4-F-QUNZ-TSA
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_             20170118
Time                 14.23
INSTRUM              spect
PROBHD   5 mm DUL 13C-1
PULPROG               zg30
TD                   65536
SOLVENT              CDCl3
NS                      16
DS                       2
SWH               8223.685 Hz
FIDRES            0.125483 Hz
AQ                3.9846387 sec
RG                     287
DW                  60.800 usec
DE                   6.00 usec
TE                  293.1 K
D1             1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                    1H
P1                   11.42 usec
PL1                  -3.00 dB
SFO1          400.1324710 MHz

F2 - Processing parameters
SI                   32768
SF            400.1300051 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.00
```


O
O
N
TsHN
F
21.69
200
180
160
140
120
100
80
60
40
20
ppm


ple Name PVK-4-F-QUNZ-TSA
Vol -1
ta Filename PVK-4-F-QUNZ-TSA.d
Position
InjPosition
ACQ Method
Pondicherry Universi
Instrument Name Q-TOF
SampleType Sample
Comment PVK-MB-411.0800
User Name QTOF-PU\admin
IRM Calibration Status Success
Acquired Time 29-08-2017 11:22:59
x10 3
+ Scan (0.651 min) PVK-4-F-QUNZ-TSA.d
411.0841
(M+H)+
412.0880
(M+H)+
413.2646
O
O
N
TsHN
F
3.8
3.6
3.4
3.2
3
2.8
2.6
2.4
2.2
2
1.8
1.6
1.4
1.2
1
0.8
0.6
0.4
0.2
0
408.5
409
409.5
410
410.5
411
411.5
412
412.5
413
413.5
414
414.5
415
415.5
416
416.5
417

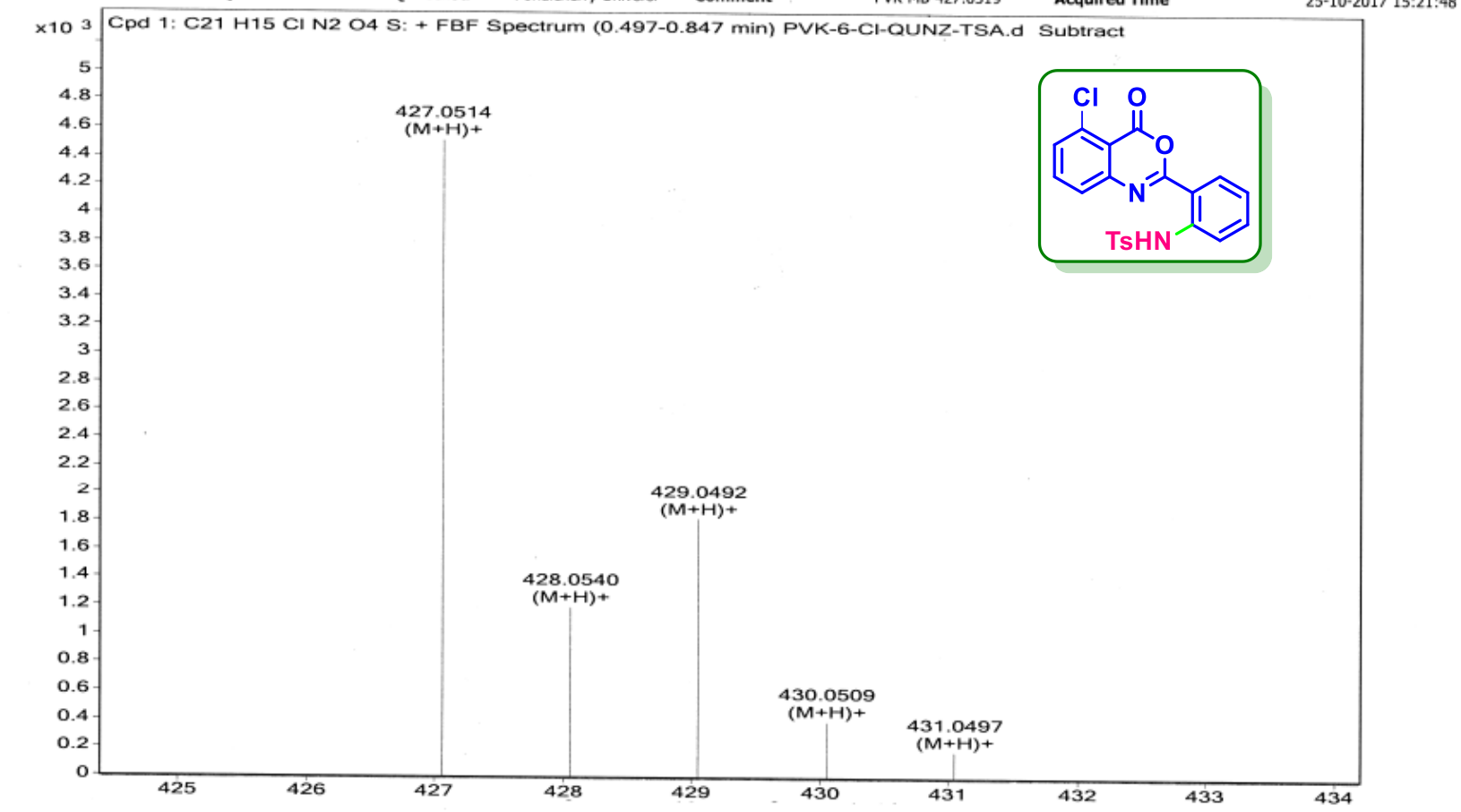


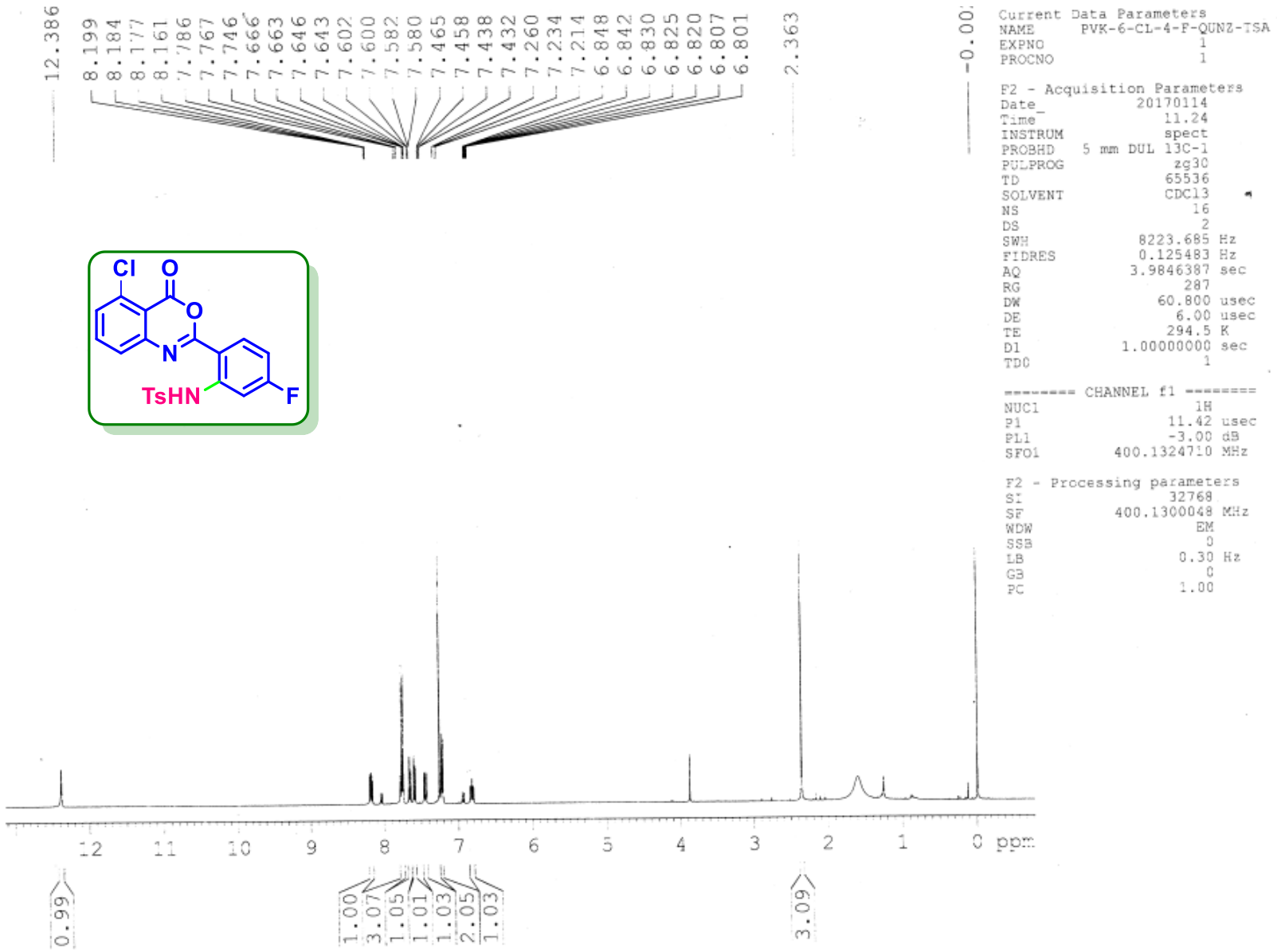

```
Current Data Parameters
NAME      PVK-6-CL-QUNZ-TSA-I
EXPNO                   4
PROCNO                  1

F2 - Acquisition Parameters
Date_            20170118
Time                14.19
INSTRUM             spect
PROBHD    5 mm DUL 13C-1
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                     16
DS                      2
SWH              8223.685 Hz
FIDRES           0.125483 Hz
AQ               3.9846387 sec
RG                    256
DW                 60.800 usec
DE                  6.00 usec
TE                 293.2 K
D1              1.00000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                   1H
P1                  11.42 usec
PL1                 -3.00 dB
SFO1          400.1324710 MHz

F2 - Processing parameters
SI                  32768
SF            400.1300050 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   1.00
```

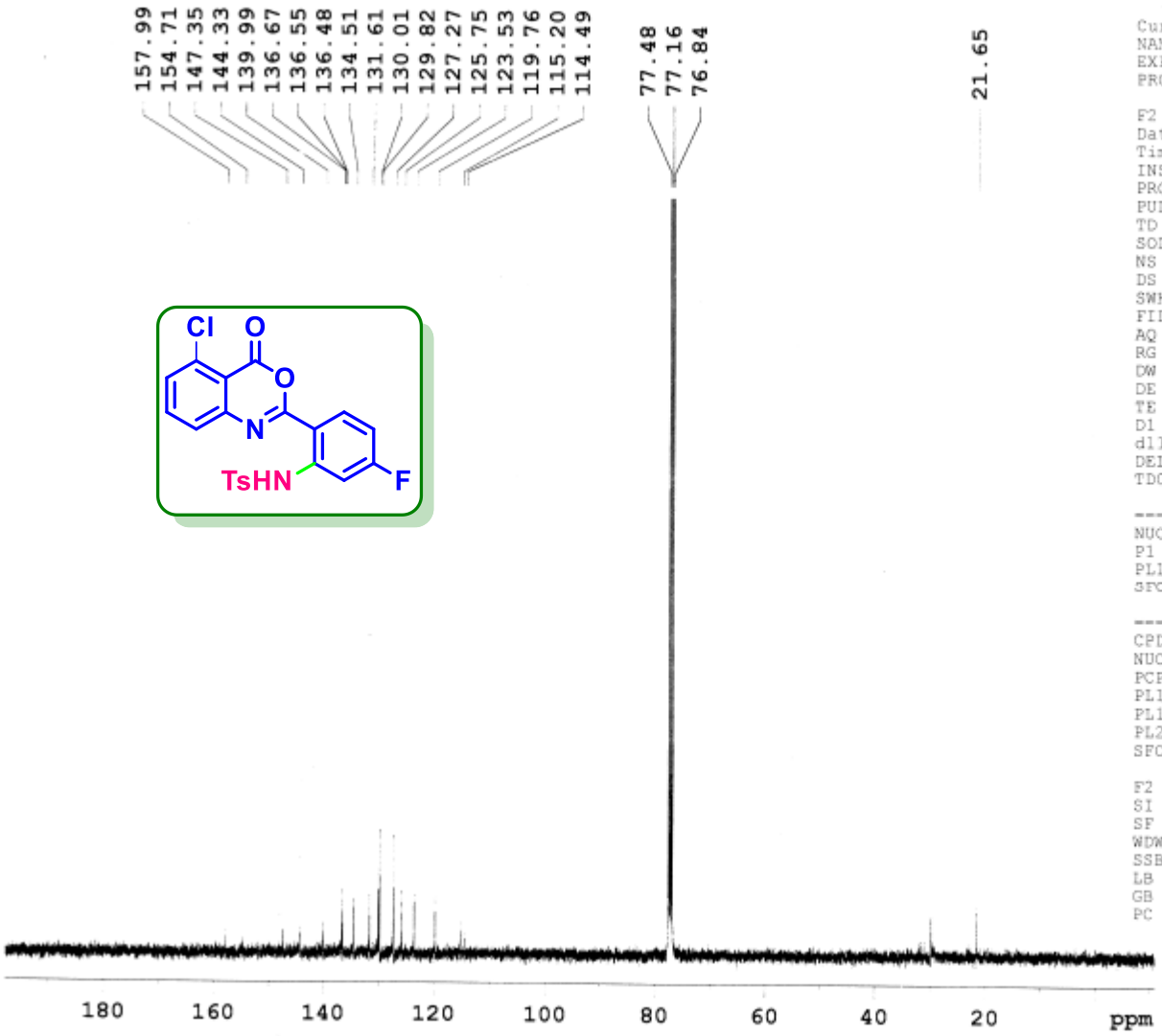



```
Current Data Parameters
NAME      PVK-6-CL-QUNZ-TSA-I
EXPNO                       5
PROCNO                      1

F2 - Acquisition Parameters
Date_              20170119
Time                  10.58
INSTRUM                spect
PROBHD   5 mm DUL 13C-1
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                    1024
DS                       4
SWH              24038.461 Hz
FIDRES           0.366798 Hz
AQ               1.3631988 sec
RG                      32
DW                 20.800 usec
DE                  6.00 usec
TE                 294.2 K
D1              2.00000000 sec
d11             0.03000000 sec
DELTA           1.89999998 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                   13C
P1                    9.15 usec
PL1                   0.00 dB
SFO1          100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2            waltz16
NUC2                   1H
PCPD2                90.00 usec
PL12                 14.90 dB
PL13                 14.90 dB
PL2                  -3.00 dB
SFO2          400.1316005 MHz

F2 - Processing parameters
SI                    32768
SF            100.6127542 MHz
WDW                      EM
SSB                       0
LB                     1.00 Hz
GB                        0
PC                     1.40
```

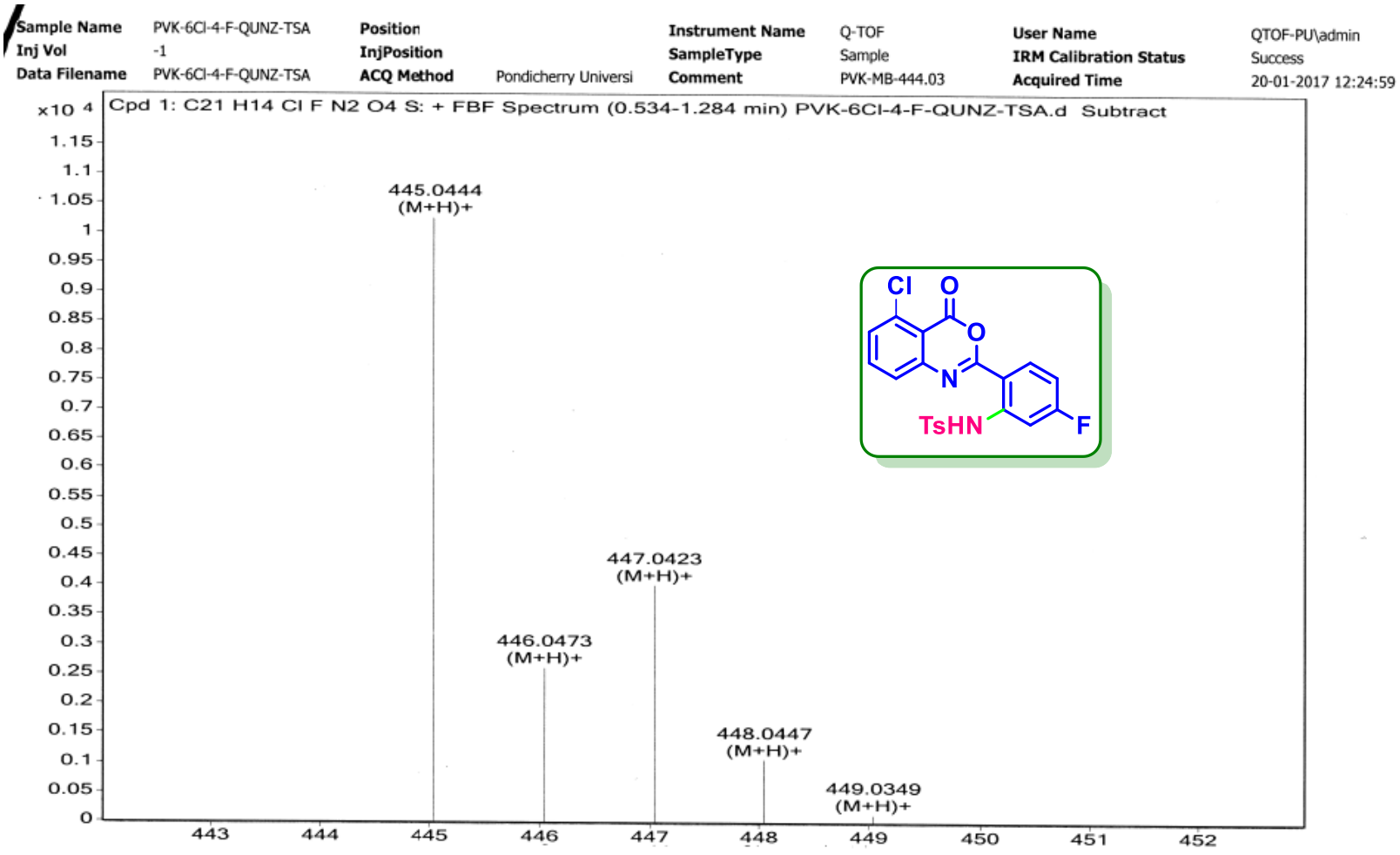
Sample Name	PVK-6-Cl-QUNZ-TSA	**Position**		**Instrument Name**	Q-TOF	**User Name**	QTOF-PU\admin
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	PVK-6-Cl-QUNZ-TSA.d	**ACQ Method**	Pondicherry Universi	**Comment**	PVK-MB-427.0519	**Acquired Time**	25-10-2017 15:21:48

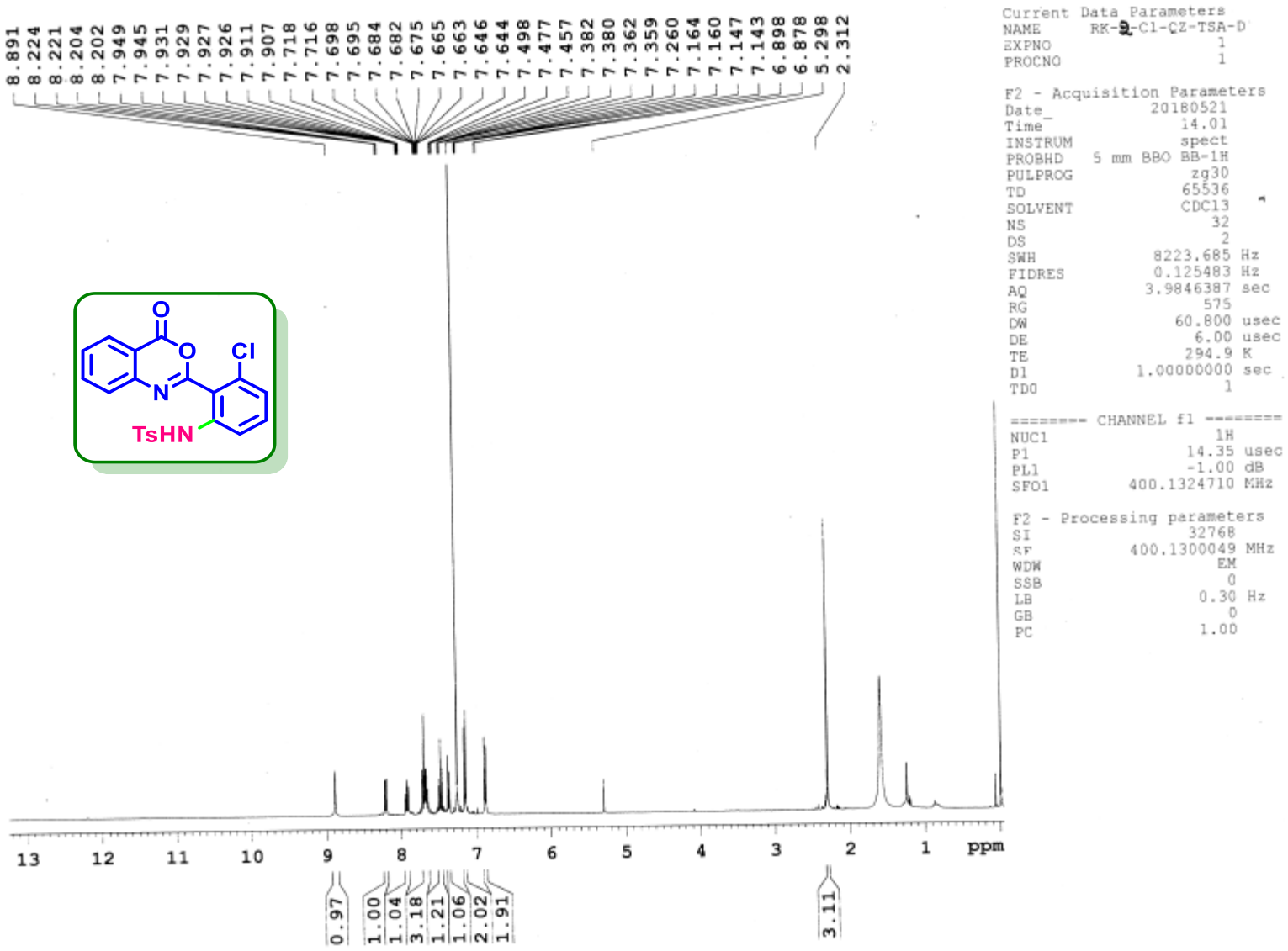



12.386
8.199
8.184
8.177
8.161
7.786
7.767
7.746
7.666
7.663
7.646
7.643
7.602
7.600
7.582
7.580
7.465
7.458
7.438
7.432
7.260
7.234
7.214
6.848
6.842
6.830
6.825
6.820
6.807
6.801
2.363
-0.00
Cl
O
O
N
TsHN
F
Current Data Parameters
NAME PVK-6-CL-4-F-QUNZ-TSA
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170114
Time 11.24
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 287
DW 60.800 usec
DE 6.00 usec
TE 294.5 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 11.42 usec
PL1 -3.00 dB
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 32768
SF 400.1300048 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
12
11
10
9
8
7
6
5
4
3
2
1
0 ppm
0.99
1.00
3.07
1.05
1.01
1.03
2.05
1.03
3.09

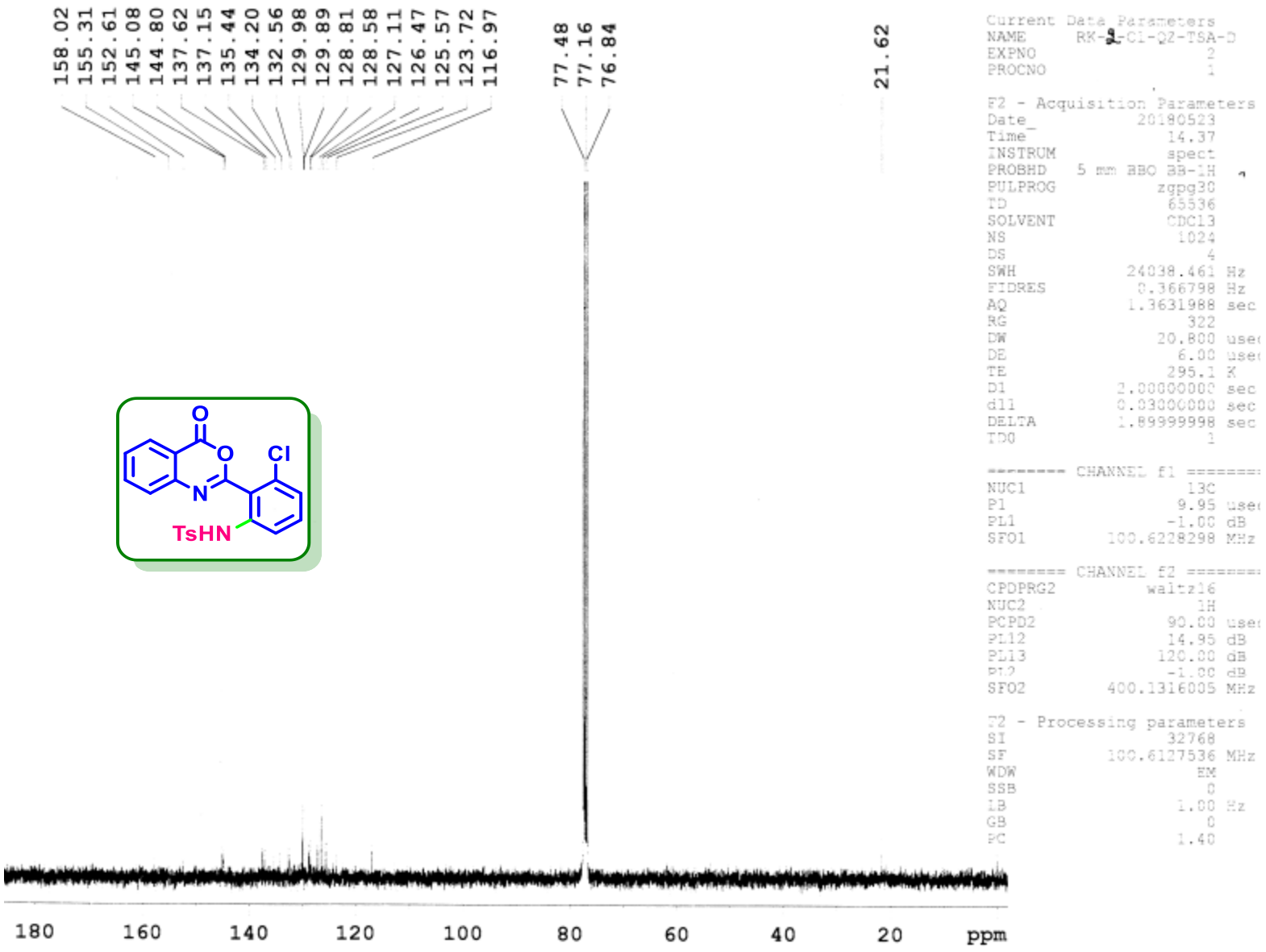



```
Current Data Parameters
NAME      PVK-6-CL-QUNZ-TSA-I
EXPNO                       5
PROCNO                      1

F2 - Acquisition Parameters
Date_              20170119
Time                  10.58
INSTRUM                spect
PROBHD    5 mm DUL 13C-1
PULPROG             zgpg30
TD                    65536
SOLVENT               CDCl3
NS                     1024
DS                        4
SWH              24038.461 Hz
FIDRES           0.366798 Hz
AQ               1.3631988 sec
RG                       32
DW                  20.800 usec
DE                   6.00 usec
TE                  294.2 K
D1               2.00000000 sec
d11              0.03000000 sec
DELTA            1.89999998 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                    13C
P1                   9.15 usec
PL1                  0.00 dB
SFO1          100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2            waltz16
NUC2                    1H
PCPD2               90.00 usec
PL12                14.90 dB
PL13                14.90 dB
PL2                 -3.00 dB
SFO2          400.1316005 MHz

F2 - Processing parameters
SI                     32768
SF            100.6127542 MHz
WDW                       EM
SSB                        0
LB                   1.00 Hz
GB                         0
PC                      1.40
```


Sample Name PVK-6Cl-4-F-QUNZ-TSA
Position
Instrument Name Q-TOF
User Name QTOF-PU\admin
Inj Vol -1
InjPosition
SampleType Sample
IRM Calibration Status Success
Data Filename PVK-6Cl-4-F-QUNZ-TSA
ACQ Method Pondicherry Universi
Comment PVK-MB-444.03
Acquired Time 20-01-2017 12:24:59
Cpd 1: C21 H14 Cl F N2 O4 S: + FBF Spectrum (0.534-1.284 min) PVK-6Cl-4-F-QUNZ-TSA.d Subtract
x10 4
445.0444 (M+H)+
447.0423 (M+H)+
446.0473 (M+H)+
448.0447 (M+H)+
449.0349 (M+H)+
Cl
O
O
N
TsHN
F

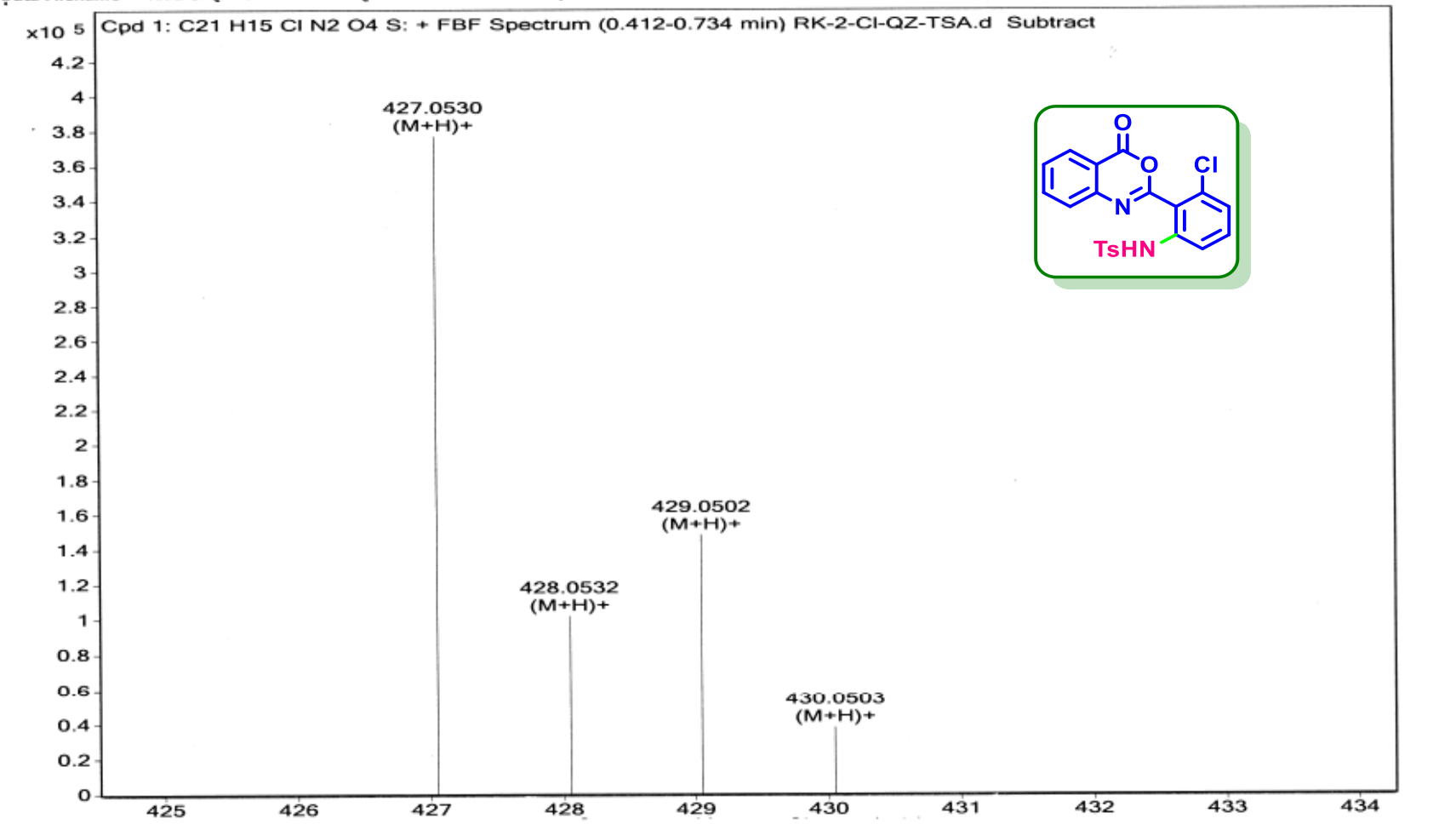


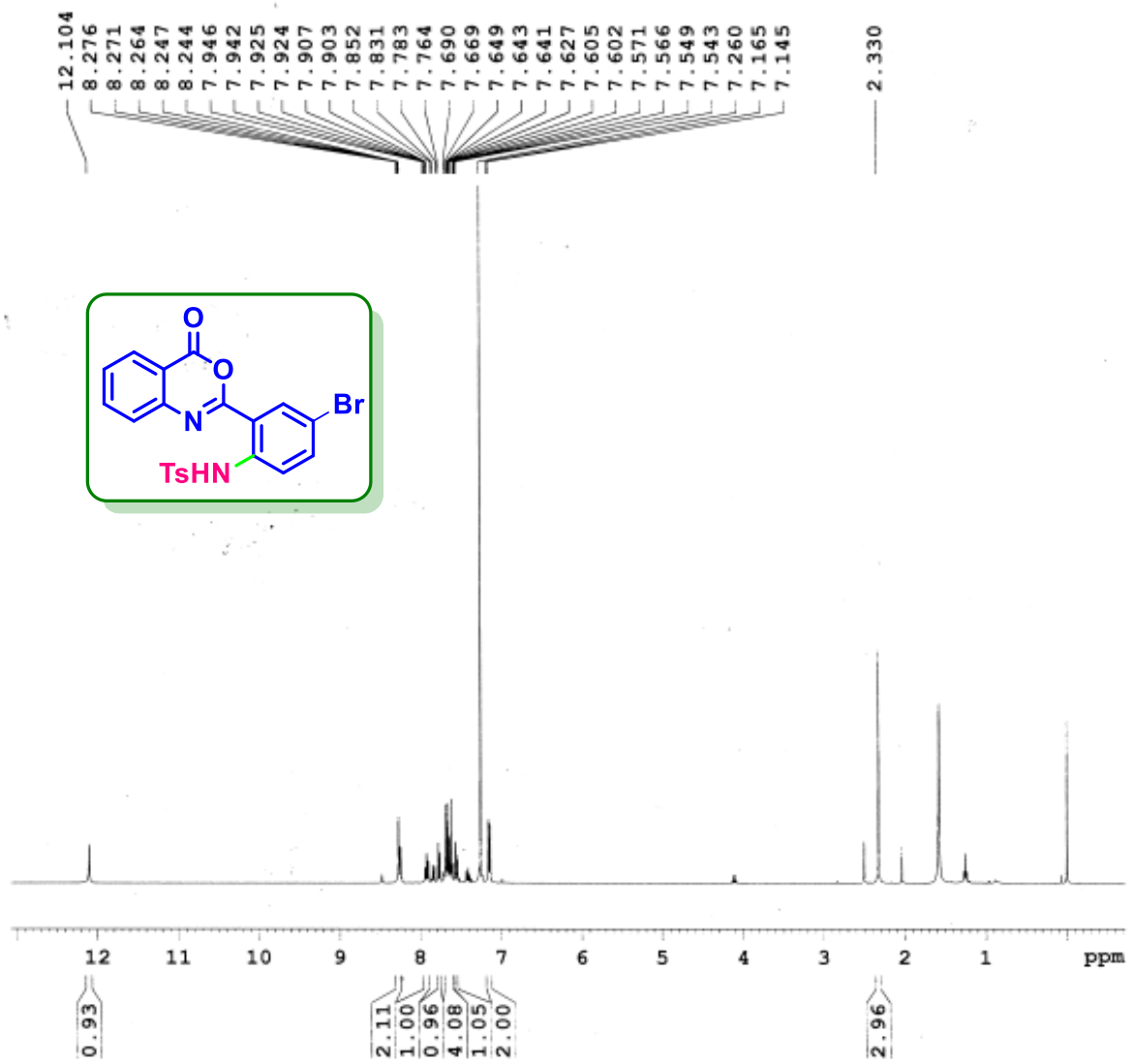

```
Current Data Parameters
NAME      RK-[illegible]-Cl-QZ-TSA-D
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20180521
Time              14.01
INSTRUM           spect
PROBHD   5 mm BBO BB-1H
PULPROG           zg30
TD               65536
SOLVENT          CDCl3
NS                  32
DS                   2
SWH           8223.685 Hz
FIDRES       0.125483 Hz
AQ           3.9846387 sec
RG                 575
DW              60.800 usec
DE               6.00 usec
TE              294.9 K
D1          1.00000000 sec
TD0                  1

======== CHANNEL f1 ========
NUC1                1H
P1             14.35 usec
PL1            -1.00 dB
SFO1      400.1324710 MHz

F2 - Processing parameters
SI                32768
SF        400.1300049 MHz
WDW                  EM
SSB                   0
LB             0.30 Hz
GB                    0
PC                 1.00
```



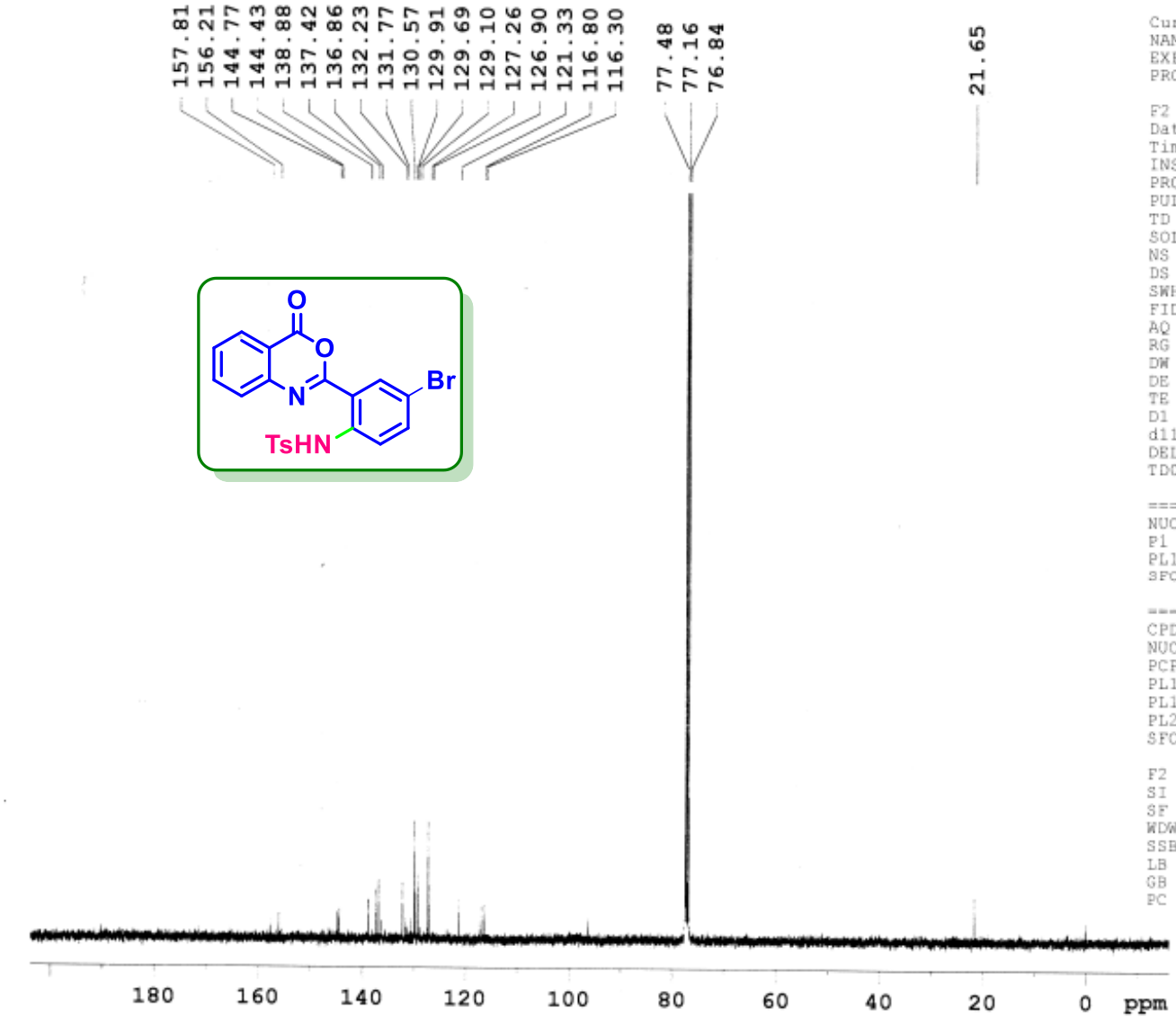

```
Current Date_Parameters
NAME      RK-3-Cl-Q2-TSA-D
EXPNO                    2
PROCNO                   1

F2 - Acquisition Parameters
Date_             20180523
Time                 14.37
INSTRUM              spect
PROBHD   5 mm BBO BB-1H
PULPROG            zgpg30
TD                  65536
SOLVENT             CDCl3
NS                   1024
DS                      4
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ             1.3631988 sec
RG                    322
DW                20.800 use
DE                 6.00 use
TE                295.1 K
D1             2.00000000 sec
d11            0.03000000 sec
DELTA          1.89999998 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                  13C
P1                   9.95 use
PL1                 -1.00 dB
SFO1         100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                  1H
PCPD2              90.00 use
PL12               14.95 dB
PL13              120.00 dB
PL2                -1.00 dB
SFO2         400.1316005 MHz

F2 - Processing parameters
SI                   32768
SF           100.6127536 MHz
WDW                     EM
SSB                      0
LB                    1.00 Hz
GB                       0
PC                    1.40
```

Sample Name	RK-2-Cl-QZ-TSA	**Position**		**Instrument Name**	Q-TOF	**User Name**	QTOF-PU\admin
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	RK-2-Cl-QZ-TSA.d	**ACQ Method**	Pondicherry Universi	**Comment**	RK-MB-426.0441	**Acquired Time**	24-05-2018 12:50:51



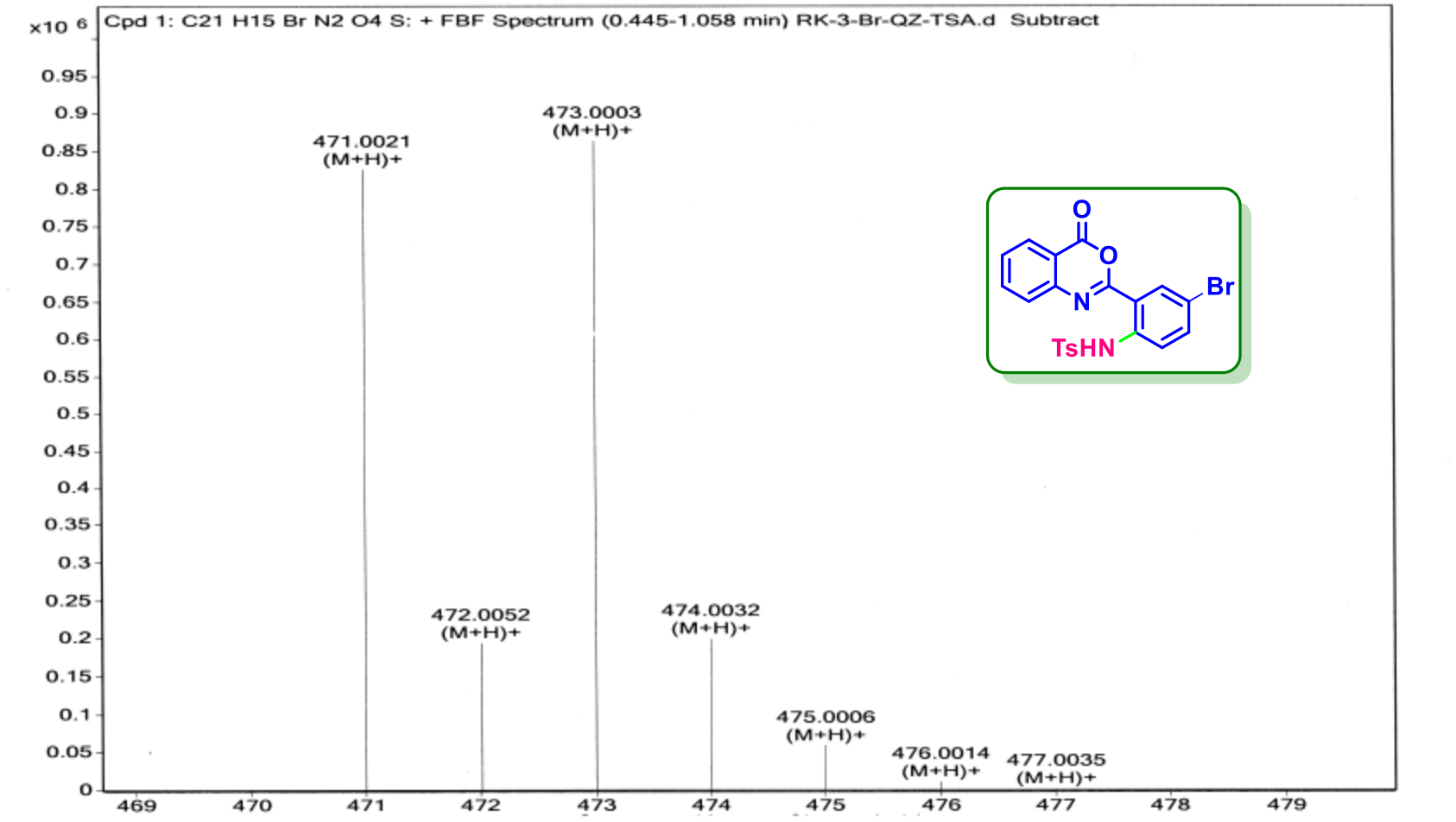


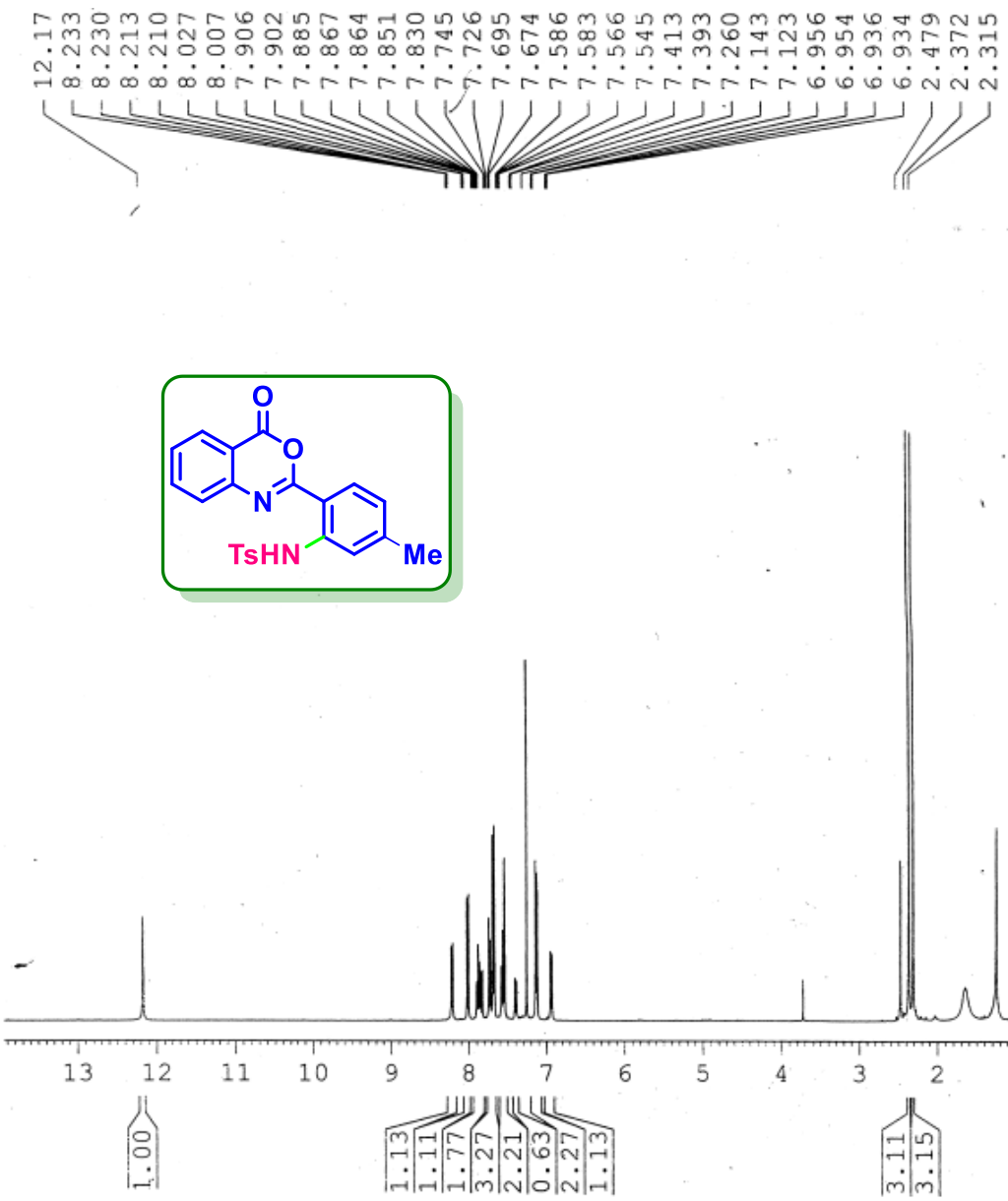

```
Current Data Parameters
NAME      PVK-3-Br-QUNZ-TSA
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_              20171105
Time                 13.44
INSTRUM              spect
PROBHD    5 mm DUL 13C-1
PULPROG               zg30
TD                   65536
SOLVENT              CDCl3
NS                      16
DS                       2
SWH               8223.685 Hz
FIDRES           0.125483 Hz
AQ               3.9846387 sec
RG                     228
DW                60.800 usec
DE                 6.00 usec
TE                 300.1 K
D1             1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                    1H
P1                  11.42 usec
PL1                 -3.00 dB
SFO1          400.1324710 MHz

F2 - Processing parameters
SI                   32768
SF            400.1300049 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.00
```



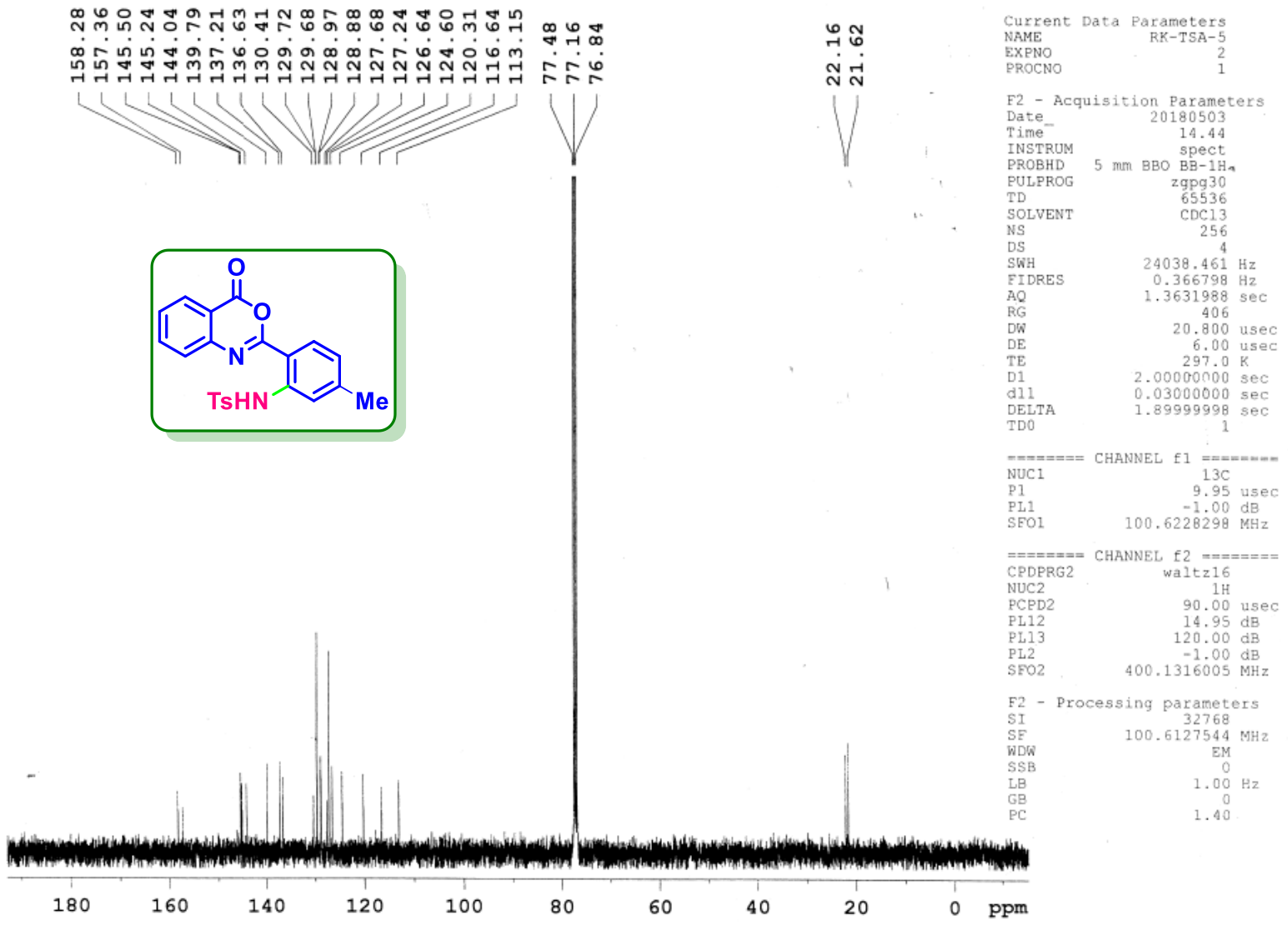

```
Current Data Parameters
NAME      PVK-3-Br-QUNZ-TSA
EXPNO                     2
PROCNO                    1

F2 - Acquisition Parameters
Date_              20171105
Time                  14.26
INSTRUM               spect
PROBHD   5 mm DUL 13C-1 
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                    1024
DS                       4
SWH              24038.461 Hz
FIDRES           0.366798 Hz
AQ               1.3631988 sec
RG                      57
DW                 20.800 usec
DE                  6.00 usec
TE                 297.5 K
D1              1.00000000 sec
d11             0.03000000 sec
DELTA           0.89999998 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                   13C
P1                  9.15 usec
PL1                 0.00 dB
SFO1         100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2            waltz16
NUC2                    1H
PCPD2              90.00 usec
PL12               14.90 dB
PL13               14.90 dB
PL2                -3.00 dB
SFO2         400.1316005 MHz

F2 - Processing parameters
SI                    32768
SF           100.6127530 MHz
WDW                      EM
SSB                       0
LB                  1.00 Hz
GB                        0
PC                  1.40
```

mple Name	RK-3-Br-QZ-TSA	**Position**		**Instrument Name**	Q-TOF	**User Name**	QTOF-PU\admin
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	RK-3-Br-QZ-TSA.d	**ACQ Method**	Pondicherry Universi	**Comment**	RK-MB-412.0283	**Acquired Time**	01-06-2018 12:54:45



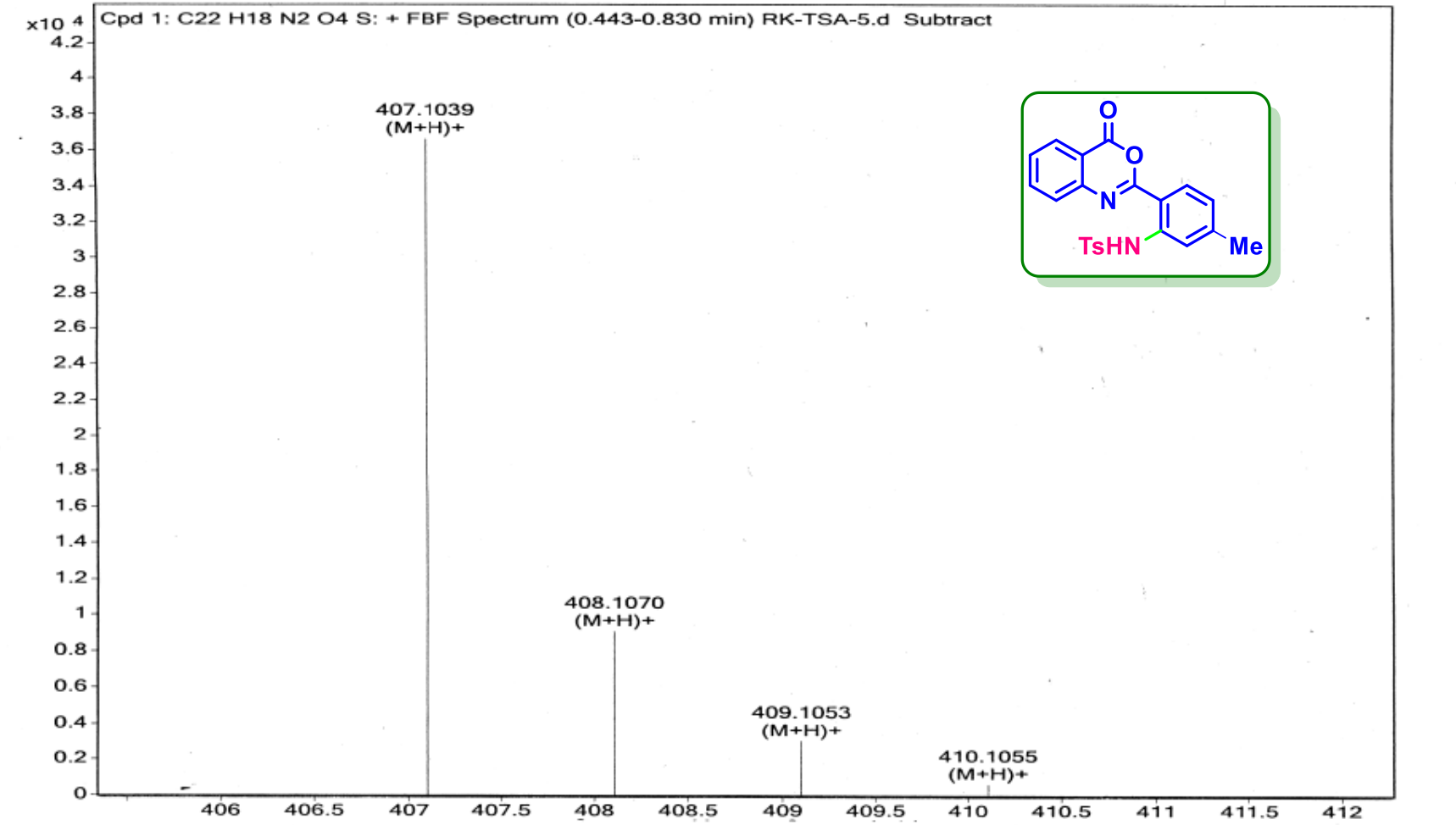


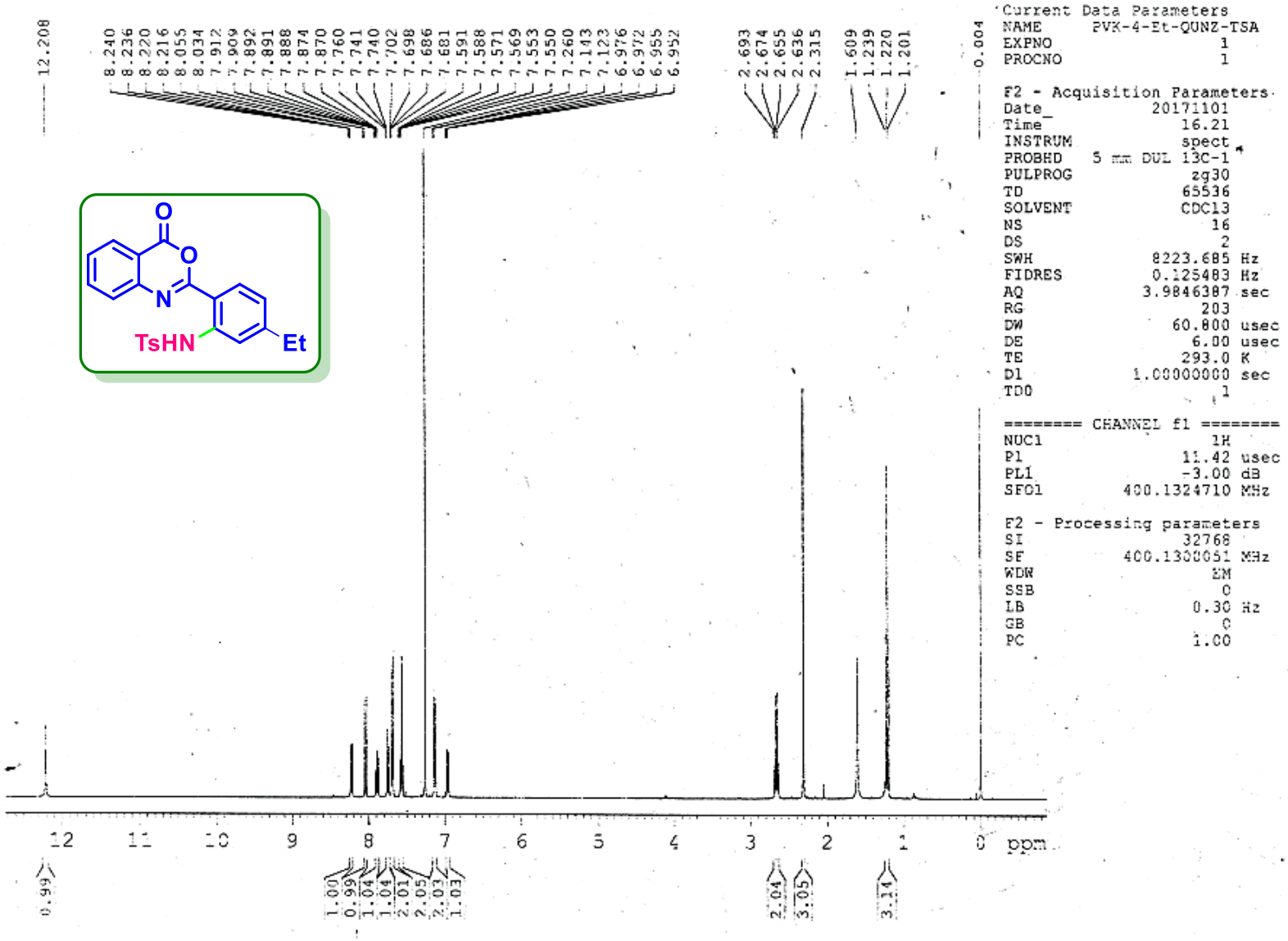

```
Current Data Parameters
NAME                  RK-TSA-5
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20180503
Time                     14.42
INSTRUM                  spect
PROBHD    5 mm BBO BB-1H
PULPROG                  zg30
TD                      65536
SOLVENT                 CDCl3
NS                         16
DS                          2
SWH                  8223.685 Hz
FIDRES               0.125483 Hz
AQ                   3.9846387 sec
RG                        287
DW                       60.800 usec
DE                        6.00 usec
TE                       296.8 K
D1                1.00000000 sec
TD0                          1

======== CHANNEL f1 ========
NUC1                        1H
P1                       14.35 usec
PL1                      -1.00 dB
SFO1              400.1324710 MHz

F2 - Processing parameters
SI                       32768
SF                400.1300046 MHz
WDW                         EM
SSB                          0
LB                        0.30 Hz
GB                           0
PC                        1.00
```

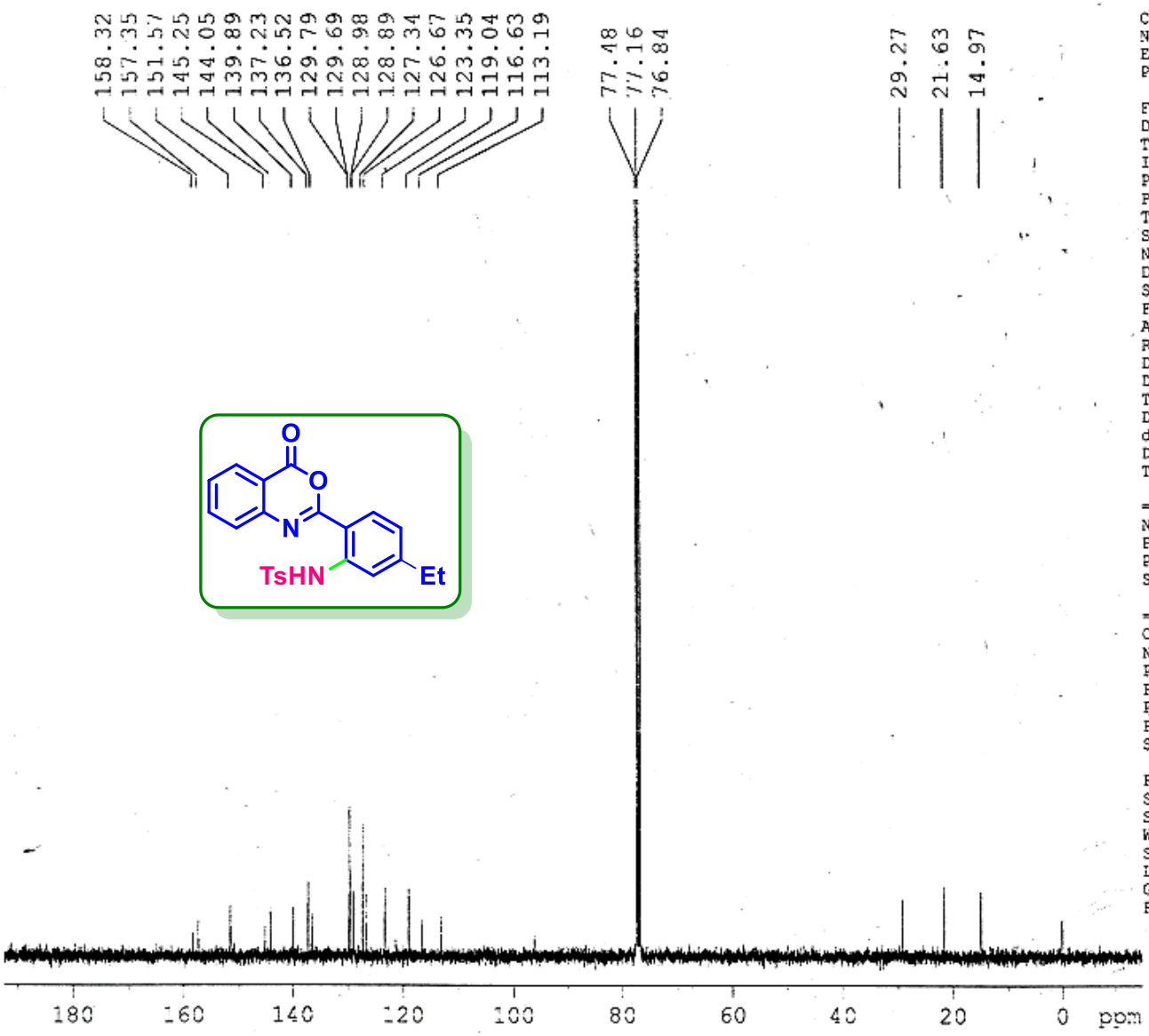



```
Current Data Parameters
NAME                  RK-TSA-5
EXPNO                        2
PROCNO                       1

F2 - Acquisition Parameters
Date_              20180503
Time                 14.44
INSTRUM              spect
PROBHD    5 mm BBO BB-1H
PULPROG              zgpg30
TD                   65536
SOLVENT              CDCl3
NS                     256
DS                       4
SWH              24038.461 Hz
FIDRES           0.366798 Hz
AQ               1.3631988 sec
RG                     406
DW                20.800 usec
DE                 6.00 usec
TE                 297.0 K
D1             2.00000000 sec
d11            0.03000000 sec
DELTA          1.89999998 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                   13C
P1                  9.95 usec
PL1                -1.00 dB
SFO1         100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2            waltz16
NUC2                   1H
PCPD2              90.00 usec
PL12               14.95 dB
PL13              120.00 dB
PL2                -1.00 dB
SFO2         400.1316005 MHz

F2 - Processing parameters
SI                   32768
SF           100.6127544 MHz
WDW                    EM
SSB                     0
LB                 1.00 Hz
GB                      0
PC                   1.40
```

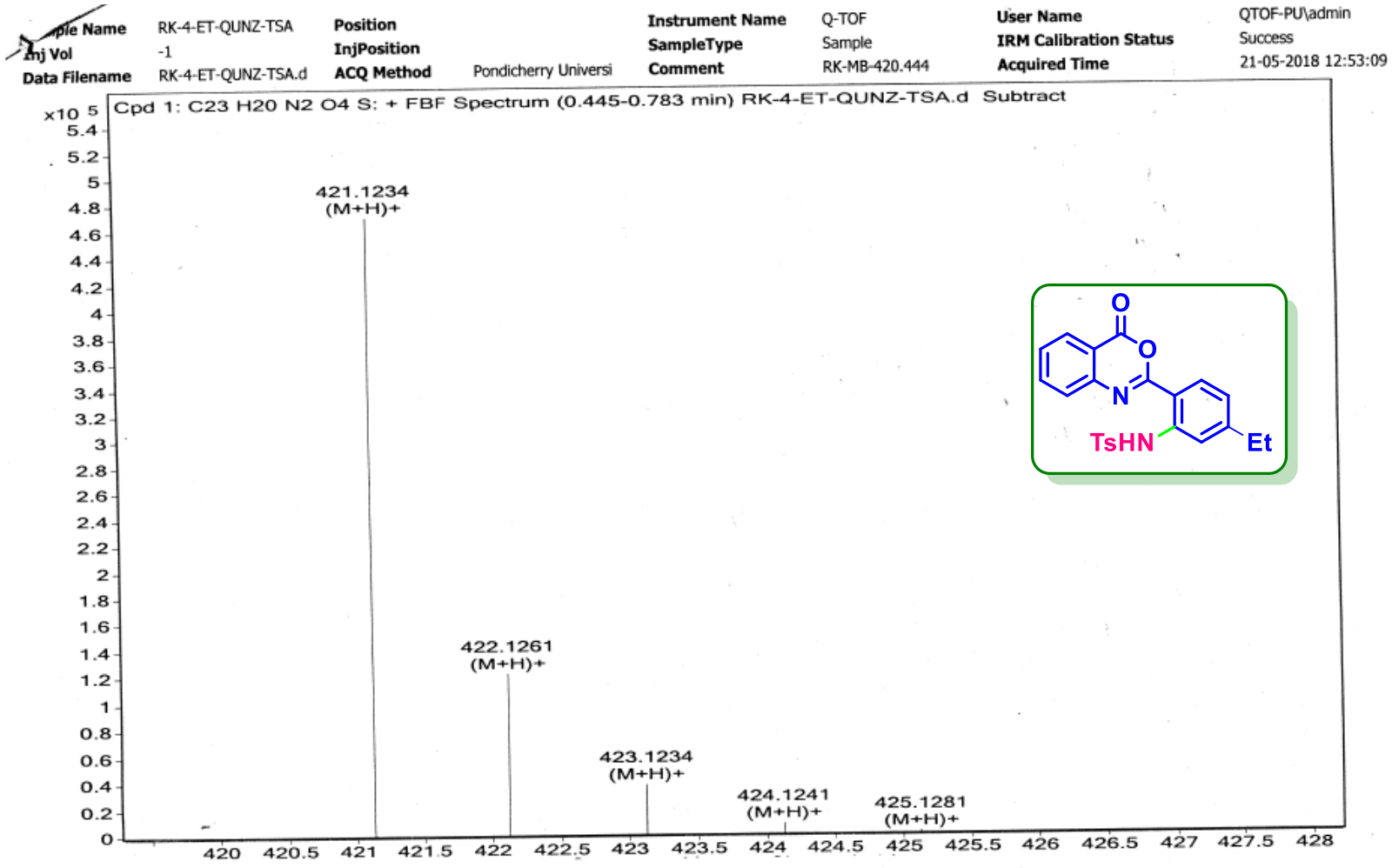
Sample Name	RK-TSA-5	**Position**		**Instrument Name**	Q-TOF	**User Name**	QTOF-PU\admin
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	RK-TSA-5.d	**ACQ Method**	Pondicherry Universi	**Comment**	RK-MB-406.0987	**Acquired Time**	07-05-2018 12:53:37

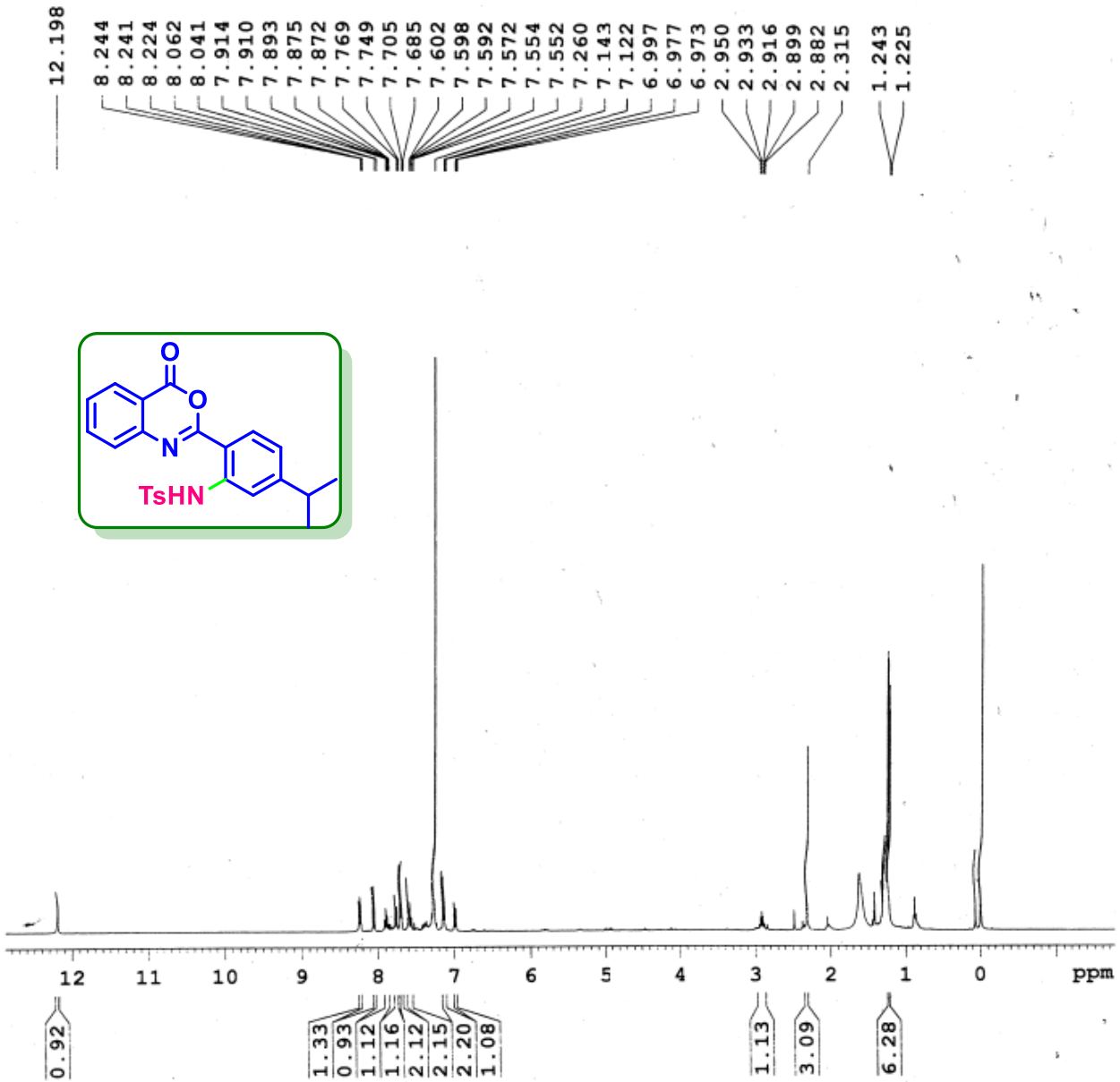



12.208
8.240
8.236
8.220
8.216
8.055
8.034
7.912
7.909
7.892
7.891
7.888
7.874
7.870
7.760
7.741
7.740
7.702
7.698
7.686
7.681
7.591
7.588
7.571
7.569
7.553
7.550
7.260
7.143
7.123
6.976
6.972
6.955
6.952
2.693
2.674
2.655
2.636
2.315
1.609
1.239
1.220
1.201
0.004
O
O
N
TsHN
Et
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
0.99
1.00
0.99
1.04
1.04
2.01
2.05
2.03
1.03
2.04
3.05
3.14
Current Data Parameters
NAME PVK-4-Et-QUNZ-TSA
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20171101
Time 16.21
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 203
DW 60.800 usec
DE 6.00 usec
TE 293.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 11.42 usec
PL1 -3.00 dB
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 32768
SF 400.1300051 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

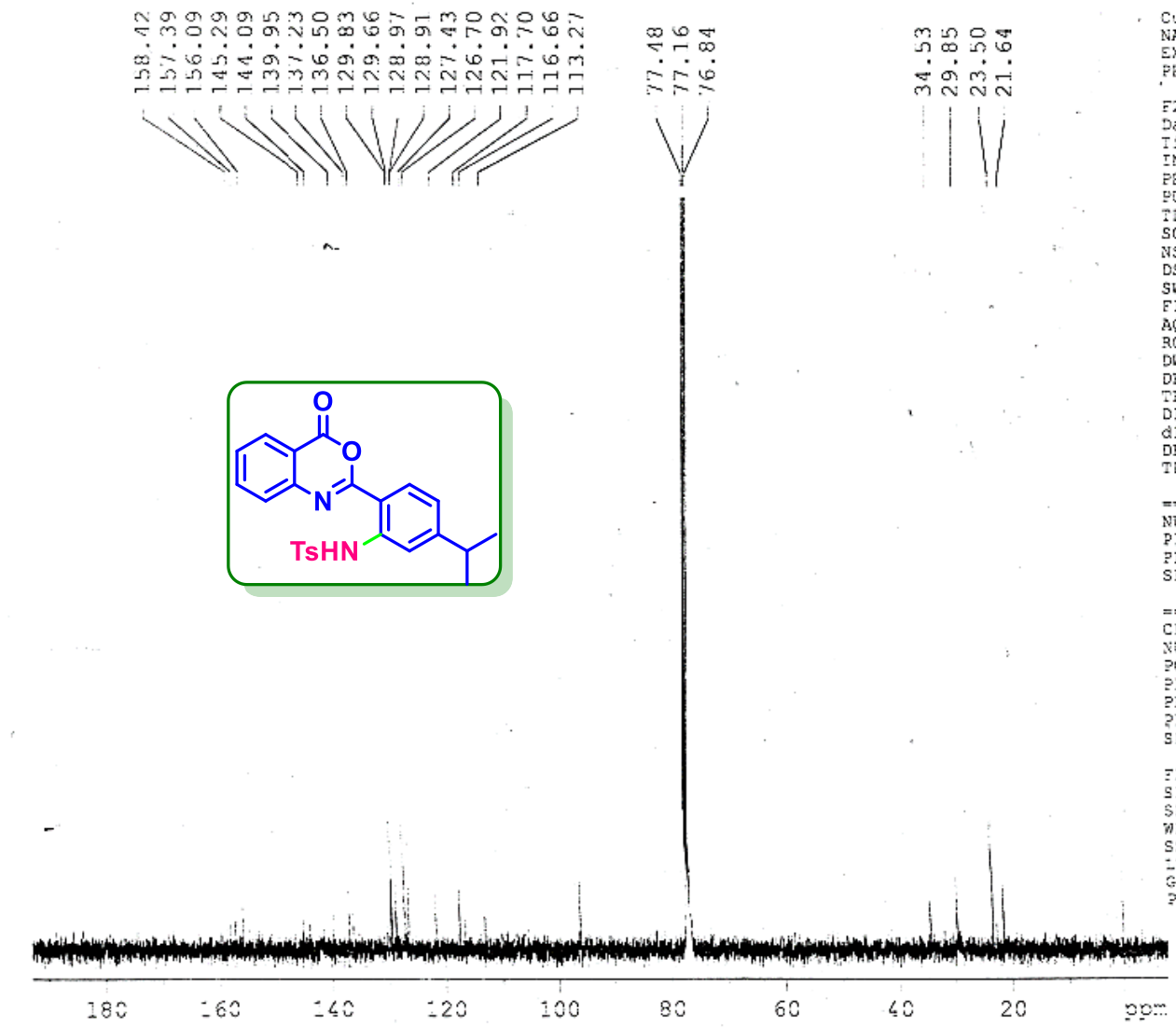



```
Current Data Parameters
NAME      PVK-4-Et-QUNZ-TSA
EXPNO                     2
PROCNO                    1

F2 - Acquisition Parameters
Date_              20171101
Time                  22.45
INSTRUM                spect
PROBHD   5 mm DUL 13C-1
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                     238
DS                       4
SWH             24038.461 Hz
FIDRES           0.366798 Hz
AQ              1.3631988 sec
RG                      57
DW                20.800 usec
DE                 6.00 usec
TE                293.3 K
D1           2.00000000 sec
d11          0.03000000 sec
DELTA        1.89999998 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                   13C
P1                  9.15 usec
PL1                 0.00 dB
SFO1         100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2            waltz16
NUC2                    1H
PCPD2              90.00 usec
PL12               14.90 dB
PL13               14.90 dB
PL2                -3.00 dB
SFO2         400.1316005 MHz

F2 - Processing parameters
SI                   32768
SF          100.6127551 MHz
WDW                     EM
SSB                      0
LB                  1.00 Hz
GB                       0
PC                    1.40
```


Sample Name RK-4-ET-QUNZ-TSA
Inj Vol -1
Data Filename RK-4-ET-QUNZ-TSA.d
Position
InjPosition
ACQ Method
Pondicherry Universi
Instrument Name Q-TOF
SampleType Sample
Comment RK-MB-420.444
User Name QTOF-PU\admin
IRM Calibration Status Success
Acquired Time 21-05-2018 12:53:09
Cpd 1: C23 H20 N2 O4 S: + FBF Spectrum (0.445-0.783 min) RK-4-ET-QUNZ-TSA.d Subtract
x10 5
421.1234 (M+H)+
422.1261 (M+H)+
423.1234 (M+H)+
424.1241 (M+H)+
425.1281 (M+H)+
TsHN
Et

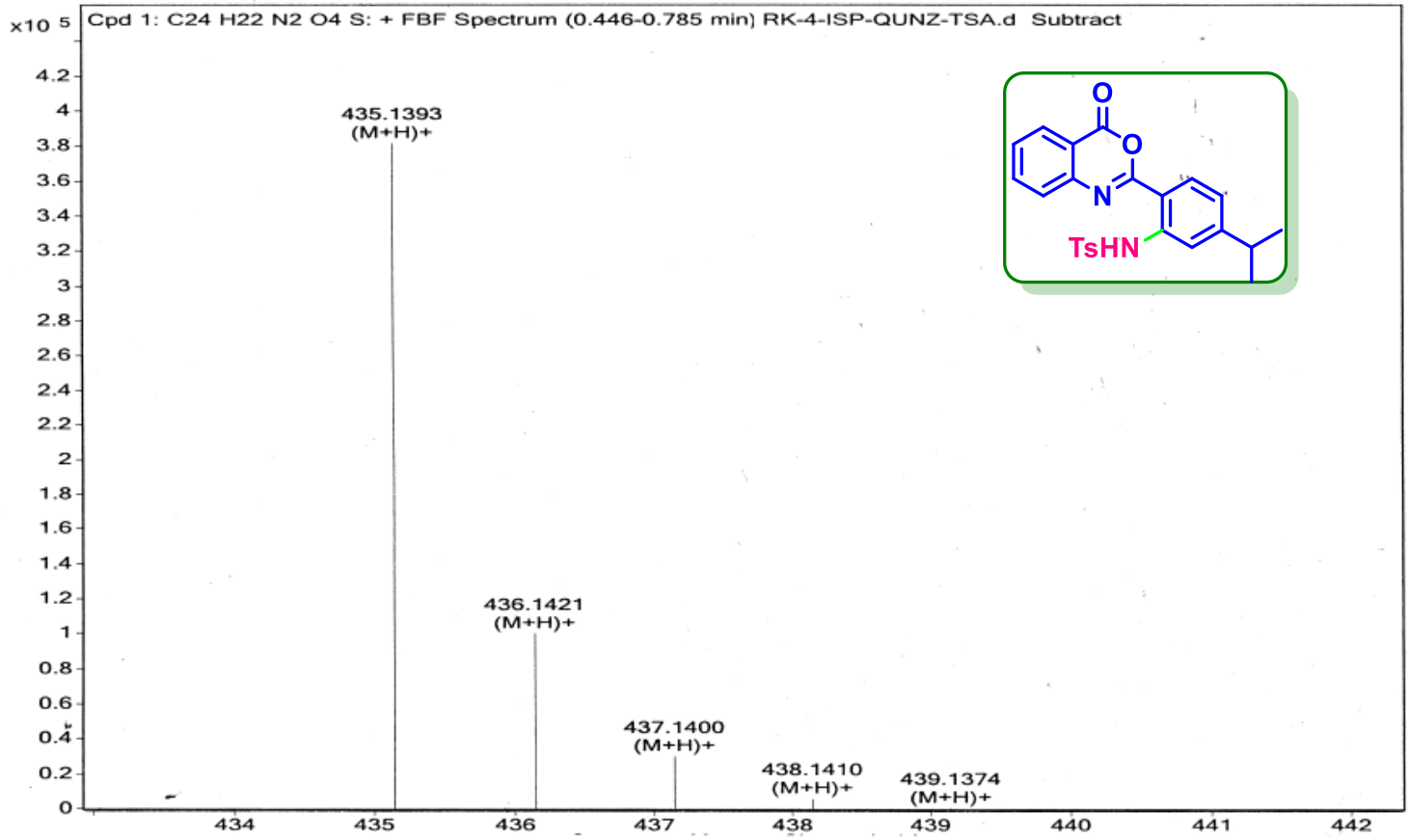


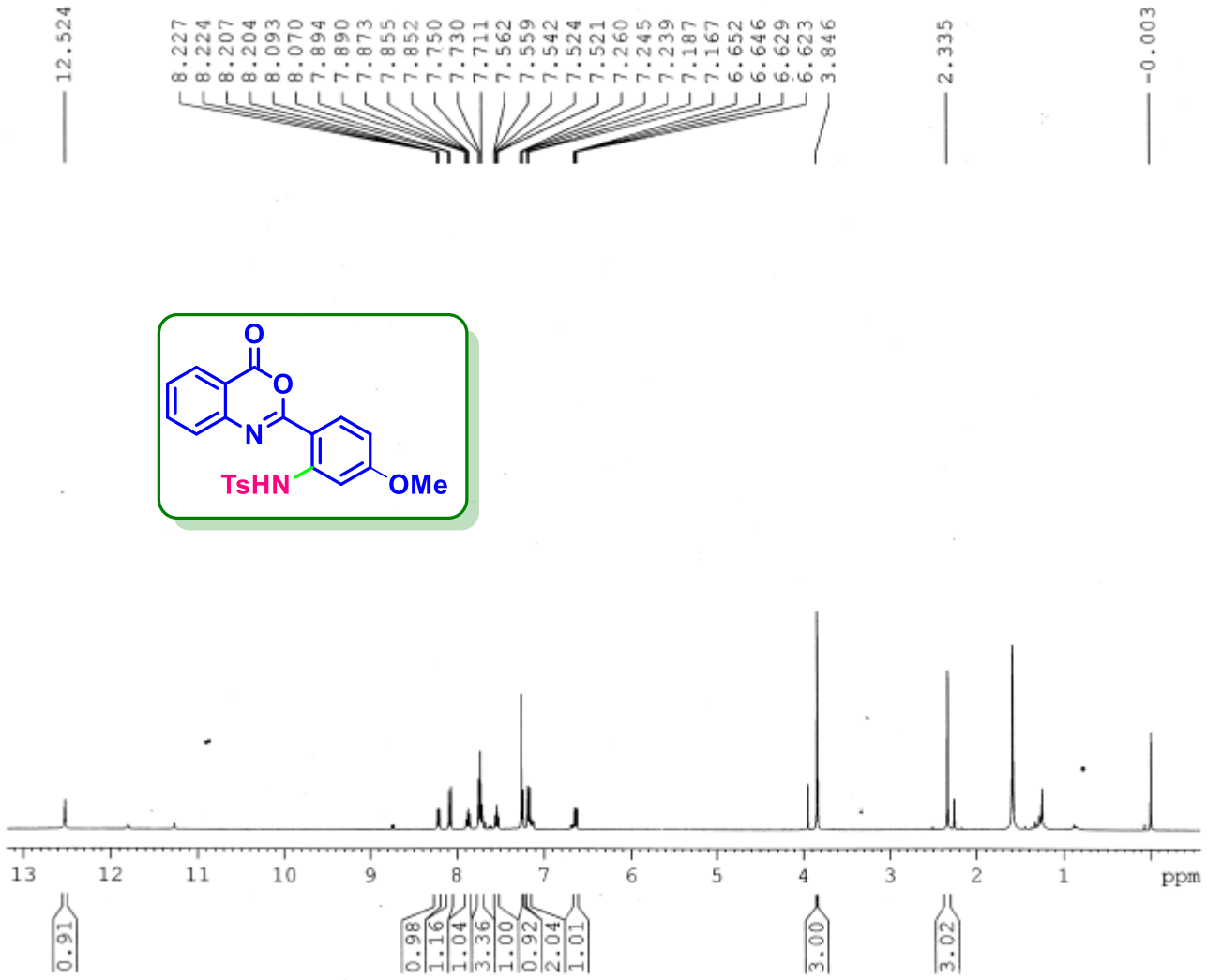

```
Current Data Parameters
NAME      PVK-4-ISP-QUNZ-TSA
EXPNO                      1
PROCNO                     1

F2 - Acquisition Parameters
Date_              20171106
Time                  16.02
INSTRUM               spect
PROBHD   5 mm DUL 13C-1
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        2
SWH                8223.685 Hz
FIDRES             0.125483 Hz
AQ                 3.9846387 sec
RG                      256
DW                   60.800 usec
DE                    6.00 usec
TE                   295.4 K
D1                 1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                      1H
P1                     11.42 usec
PL1                    -3.00 dB
SFO1          400.1324710 MHz

F2 - Processing parameters
SI                        32768
SF             400.1300051 MHz
WDW                       EM
SSB                        0
LB                      0.30 Hz
GB                         0
PC                      1.00
```



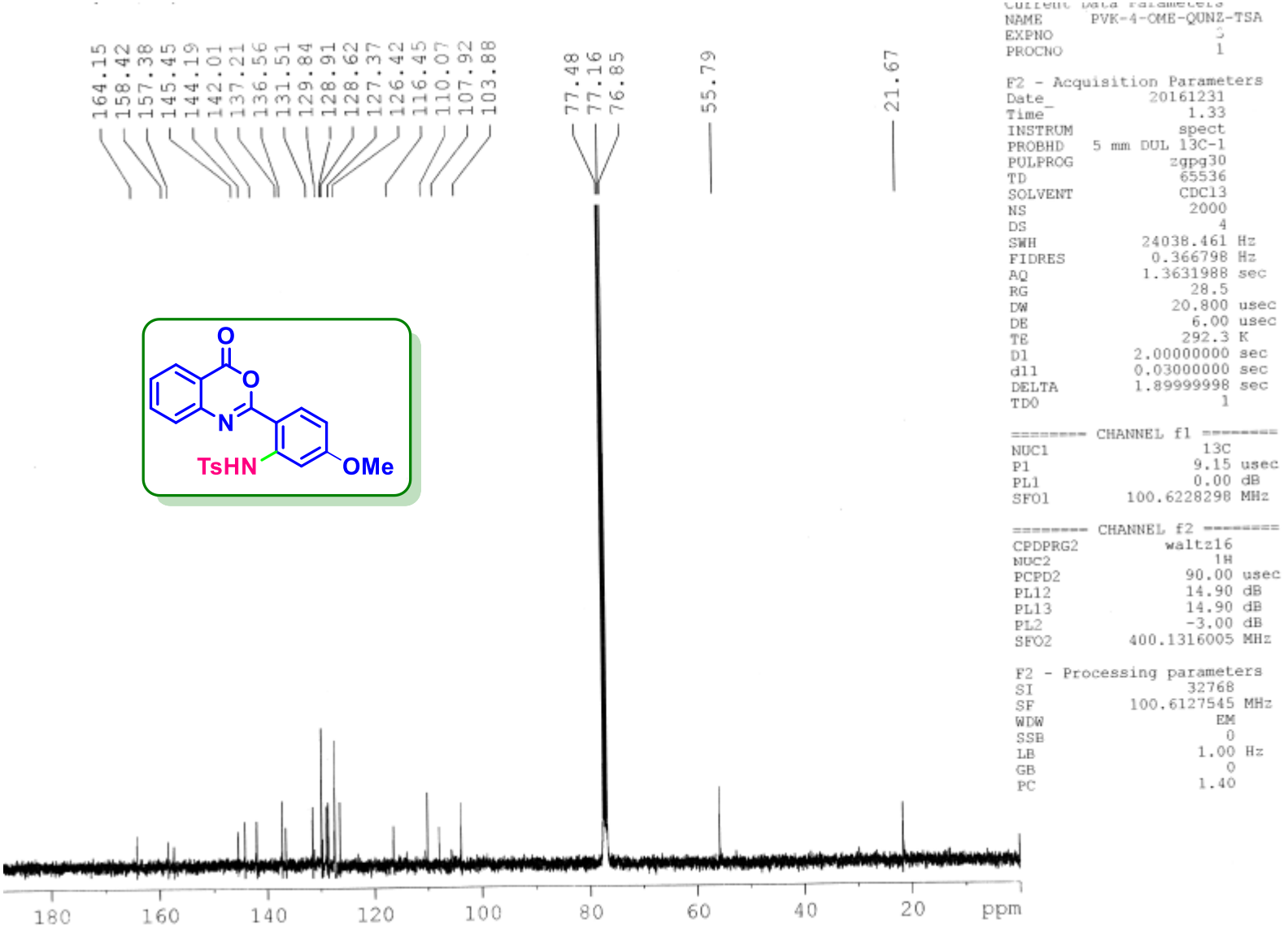

```
Current Data Parameters
NAME      PVK-U-ISP-QUN2-TSA
EXPNO                      1
PROCNO                     1

F2 - Acquisition Parameters
Date_            20171113
Time                 13.27
INSTRUM                spect
PROBHD   5 mm DUL 13C-1
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                    1024
DS                       4
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3631988 sec
RG                      64
DW               20.800 usec
DE                6.00 usec
TE               294.6 K
D1            2.00000000 sec
d11           0.03000000 sec
DELTA         1.89999998 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                    13C
P1                   9.15 usec
PL1                  0.00 dB
SFO1         100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2             waltz16
NUC2                    1H
PCPD2               90.00 usec
PL12                14.90 dB
PL13                14.90 dB
PL2                 -3.00 dB
SFO2         400.1316005 MHz

F2 - Processing parameters
SI                   32768
SF           100.6127539 MHz
WDW                     EM
SSB                      0
LB                    1.00 Hz
GB                       0
PC                    1.40
```

Sample Name	RK-4-ISP-QUNZ-TSA	**Position**		**Instrument Name**	Q-TOF	**User Name**	QTOF-PU\admin
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	RK-4-ISP-QUNZ-TSA.d	**ACQ Method**	Pondicherry Universi	**Comment**	RK-MB-434.1300	**Acquired Time**	21-05-2018 12:46:05



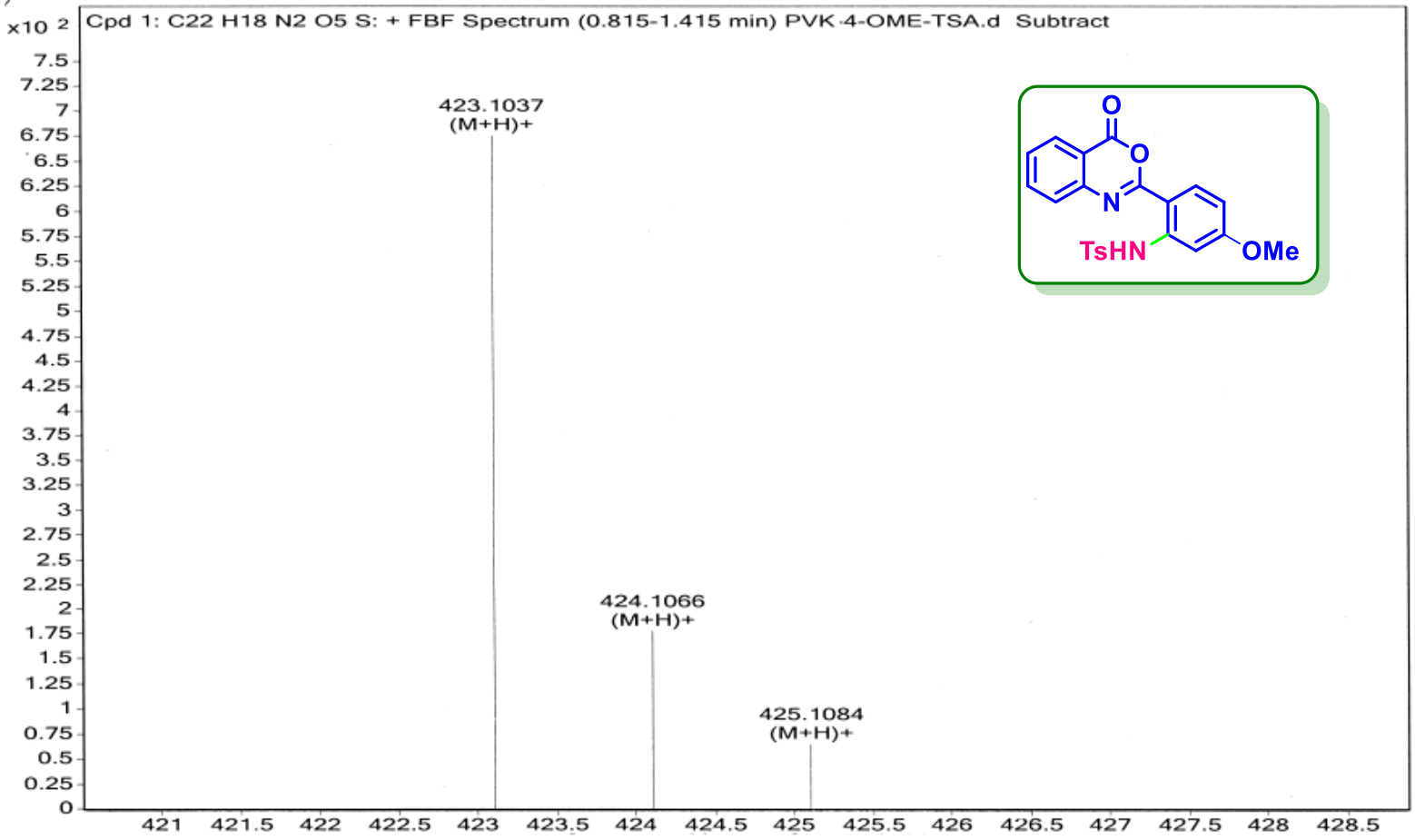


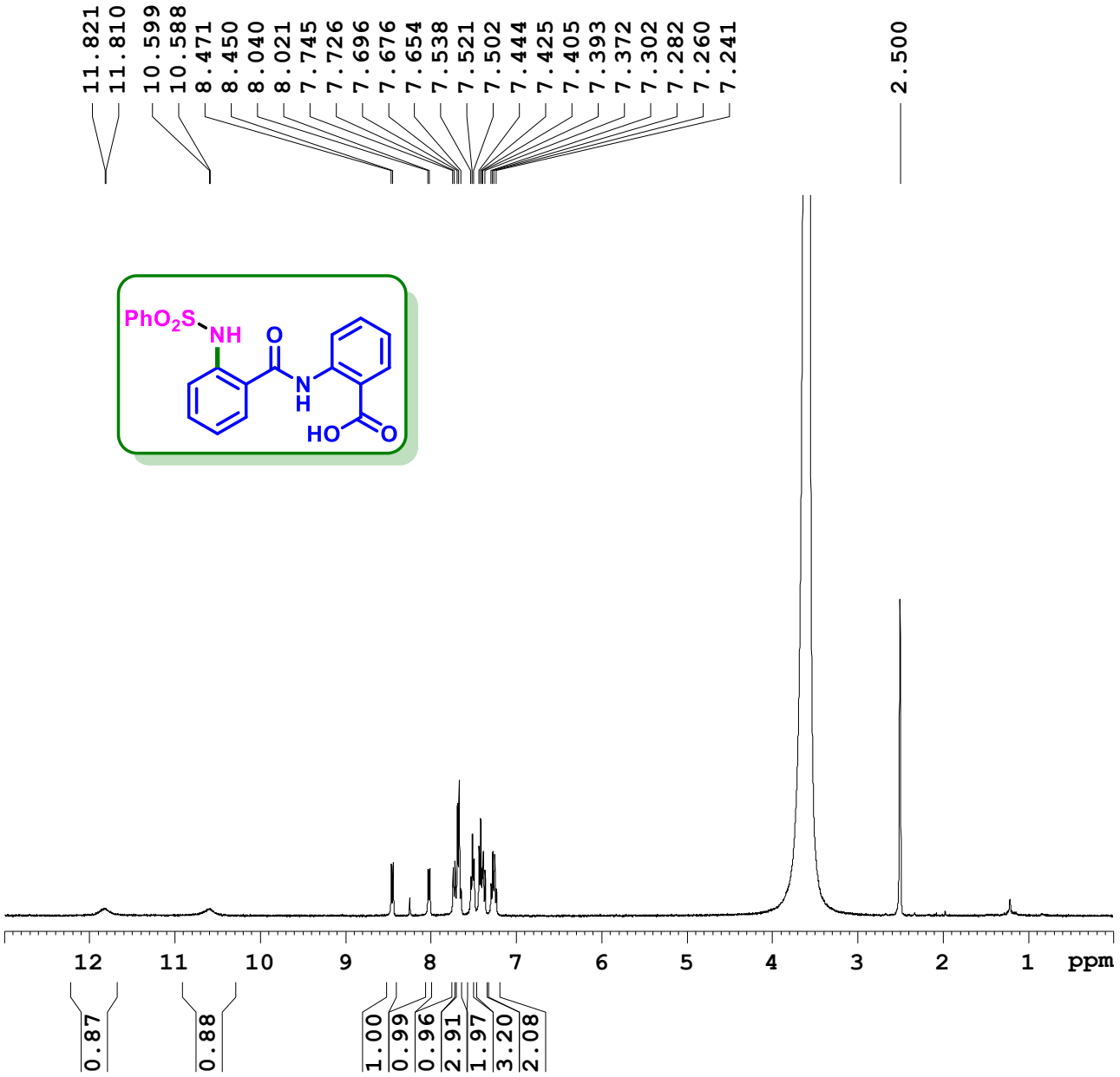

```
Current Data Parameters
NAME      PVK-4-OME-QUNZ-TSA
EXPNO                      1
PROCNO                     1

F2 - Acquisition Parameters
Date_               20161230
Time                   10.10
INSTRUM                spect
PROBHD    5 mm DUL 13C-1
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        2
SWH                8223.685 Hz
FIDRES            0.125483 Hz
AQ                3.9846387 sec
RG                      228
DW                   60.800 usec
DE                    6.00 usec
TE                   293.5 K
D1              1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                      1H
P1                     11.42 usec
PL1                    -3.00 dB
SFO1           400.1324710 MHz

F2 - Processing parameters
SI                        32768
SF             400.1300050 MHz
WDW                       EM
SSB                        0
LB                      0.30 Hz
GB                         0
PC                      1.00
```



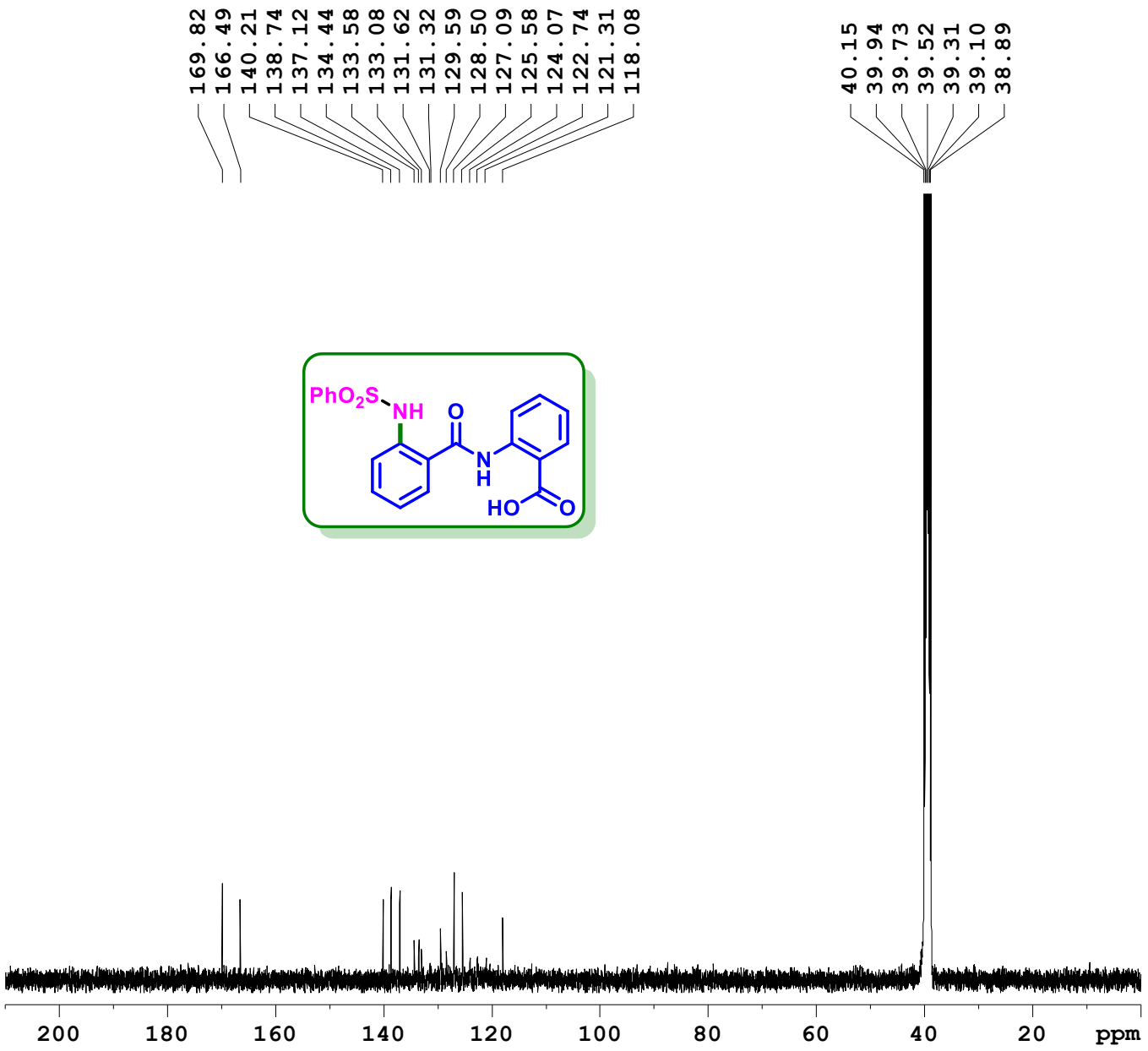

```
NAME            PVK-4-OME-QUNZ-TSA
EXPNO                            5
PROCNO                           1

F2 - Acquisition Parameters
Date_                     20161231
Time                          1.33
INSTRUM                      spect
PROBHD     5 mm DUL 13C-1
PULPROG                    zgpg30
TD                          65536
SOLVENT                     CDCl3
NS                           2000
DS                              4
SWH                     24038.461 Hz
FIDRES                   0.366798 Hz
AQ                       1.3631988 sec
RG                            28.5
DW                          20.800 usec
DE                           6.00 usec
TE                          292.3 K
D1                      2.00000000 sec
d11                     0.03000000 sec
DELTA                   1.89999998 sec
TD0                              1

======== CHANNEL f1 ========
NUC1                           13C
P1                            9.15 usec
PL1                           0.00 dB
SFO1                100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2                   waltz16
NUC2                           1H
PCPD2                        90.00 usec
PL12                         14.90 dB
PL13                         14.90 dB
PL2                          -3.00 dB
SFO2                400.1316005 MHz

F2 - Processing parameters
SI                            32768
SF                  100.6127545 MHz
WDW                              EM
SSB                               0
LB                            1.00 Hz
GB                                0
PC                             1.40
```

ame	PVK-4-OME-TSA	Position		Instrument Name	Q-TOF	User Name	QTOF-PU\admin
	-1	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Filename	PVK-4-OME-TSA.d	ACQ Method	Pondicherry Universi	Comment	PVK-MB-422.08	Acquired Time	13-01-2017 13:48:54



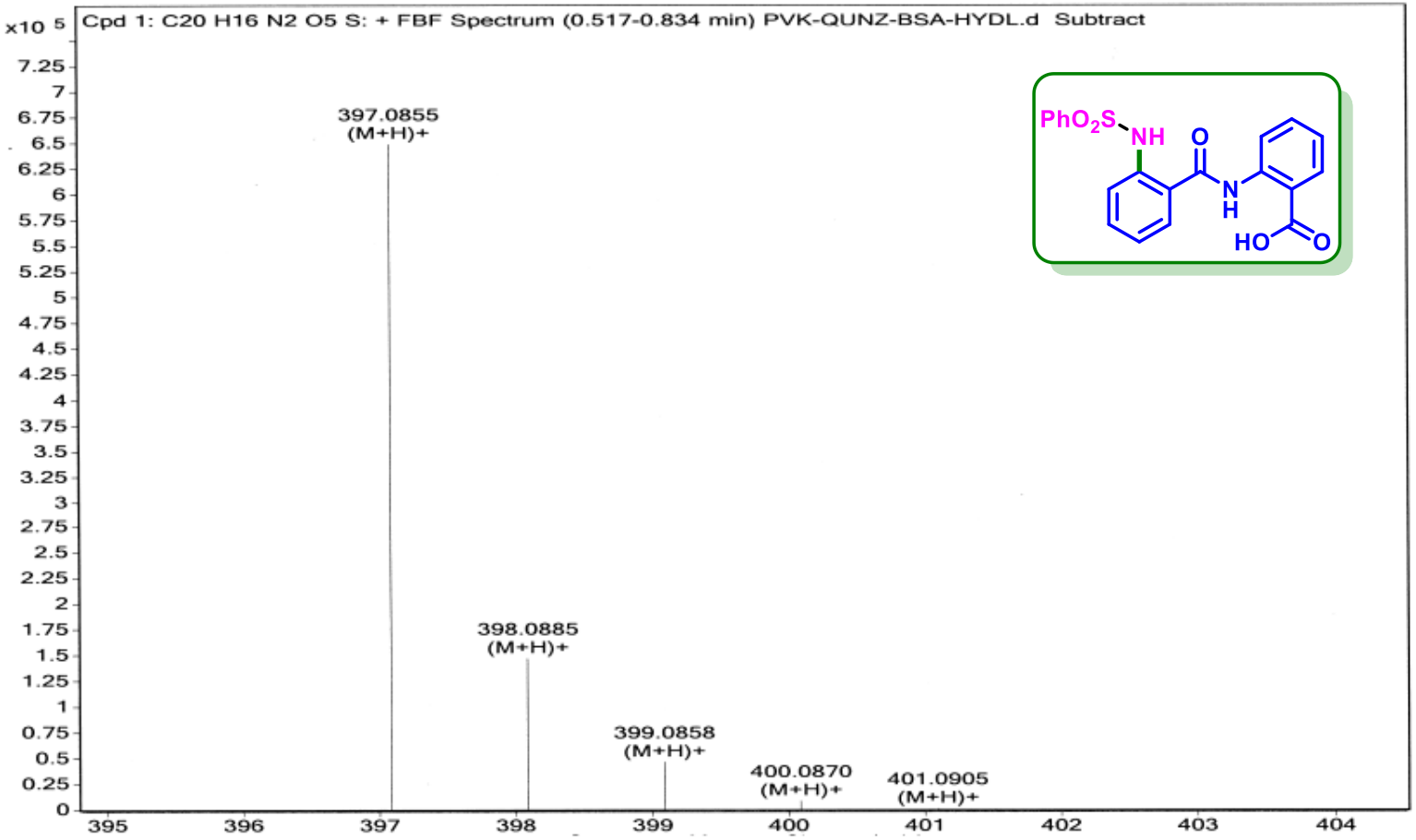


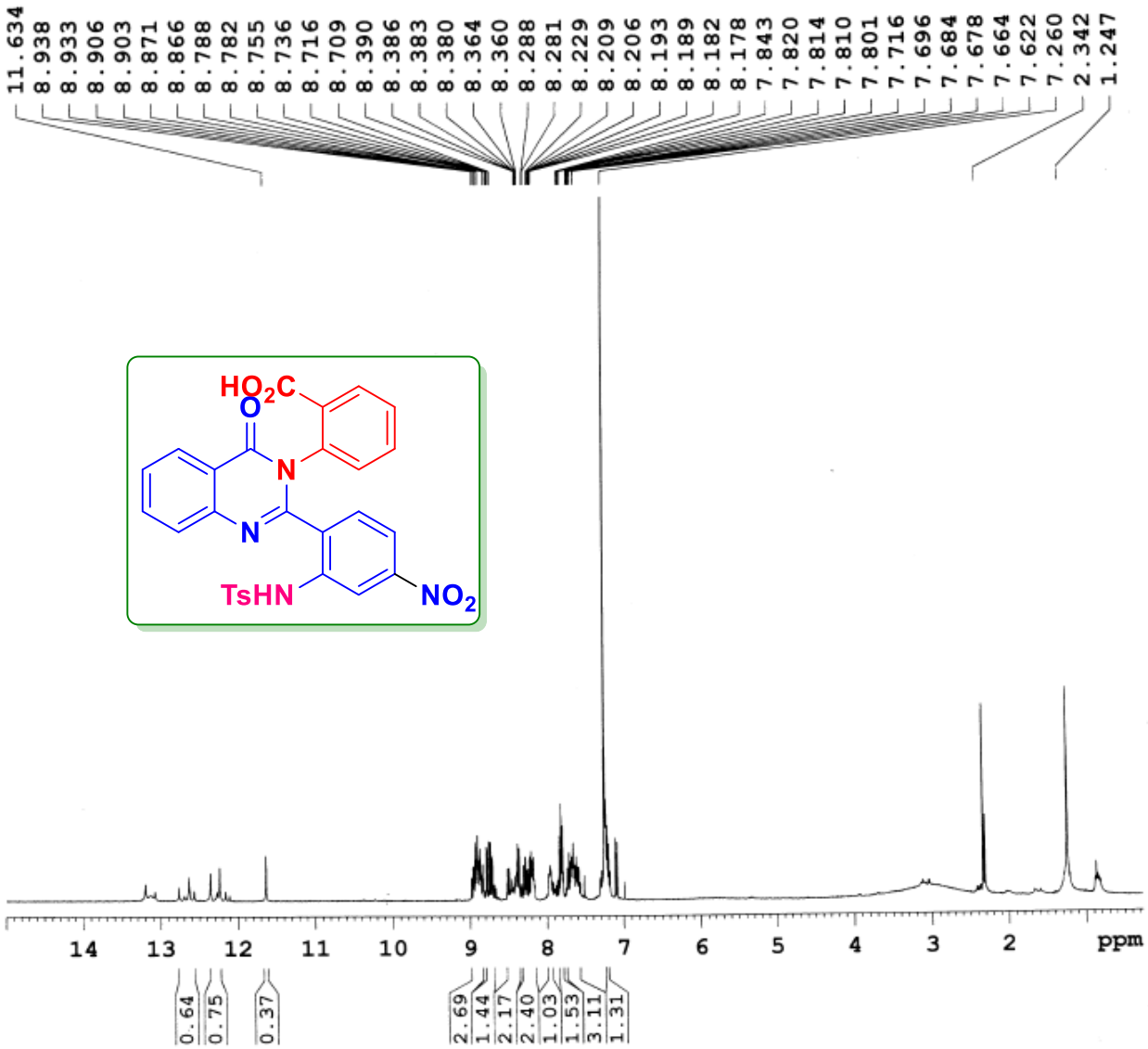

```
Current Data Parameters
NAME      RK-QZ-BSA-HYDRL
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_           20190214
Time              16.52
INSTRUM           spect
PROBHD   5 mm BBO BB-1H
PULPROG             zg30
TD                65536
SOLVENT            DMSO
NS                   16
DS                    2
SWH            8223.685 Hz
FIDRES        0.125483 Hz
AQ            3.9846387 sec
RG                  322
DW               60.800 usec
DE                6.00 usec
TE                296.1 K
D1           1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                  1H
P1                14.35 usec
PL1               -1.00 dB
SFO1        400.1324710 MHz

F2 - Processing parameters
SI                32768
SF          400.1300023 MHz
WDW                  EM
SSB                   0
LB                0.30 Hz
GB                    0
PC                1.00
```



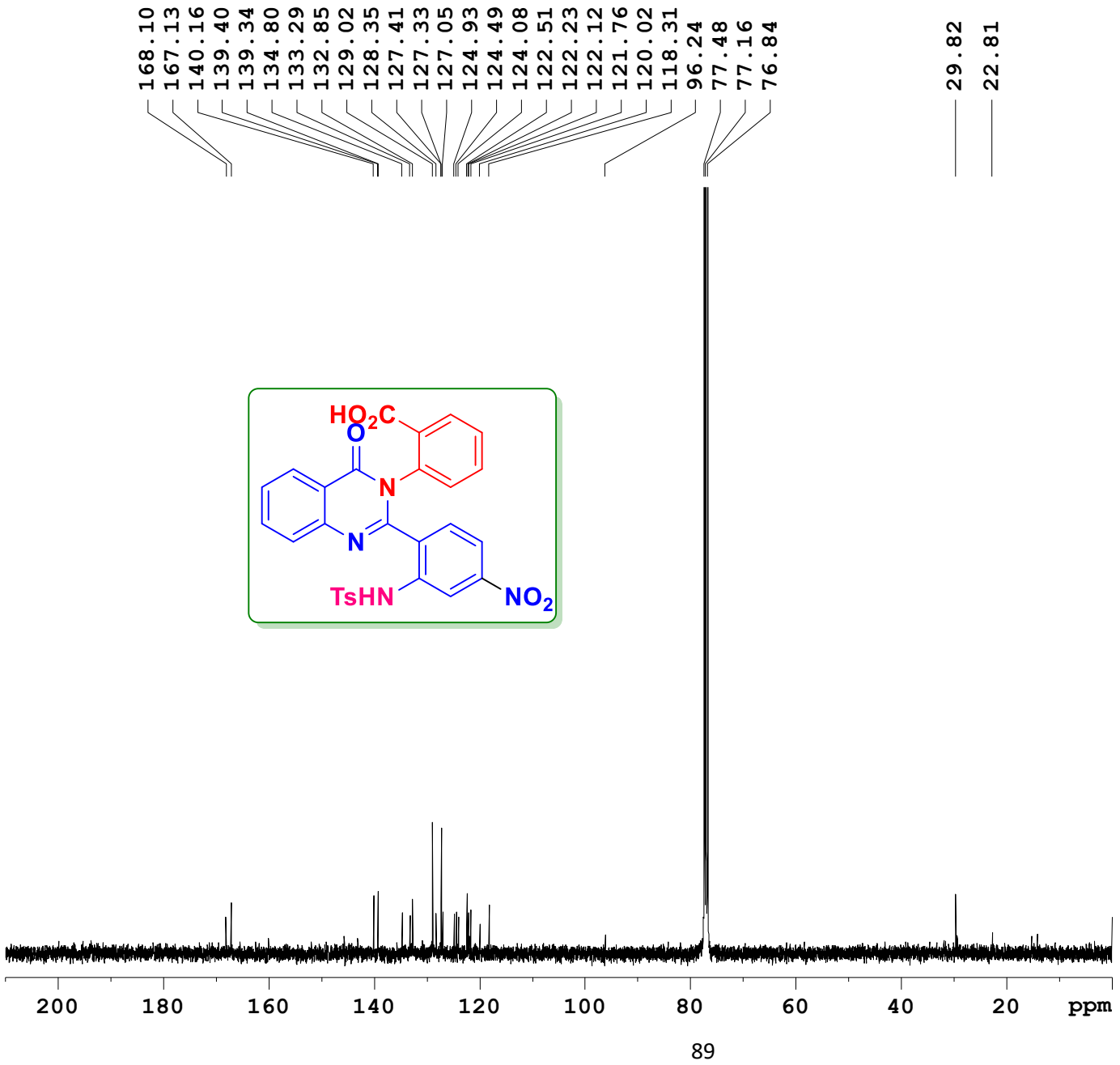

```
Current Data Parameters
NAME      PVK-Qz-BSA-HYDRL
EXPNO                    2
PROCNO                   1

F2 - Acquisition Parameters
Date_             20190225
Time                 6.16
INSTRUM             spect
PROBHD   5 mm BBO BB-1H
PULPROG             zgpg30
TD                   65536
SOLVENT               DMSO
NS                    7000
DS                       4
SWH             24038.461 Hz
FIDRES           0.366798 Hz
AQ               1.3631988 sec
RG                     322
DW                  20.800 usec
DE                   6.00 usec
TE                  291.4 K
D1             2.00000000 sec
d11            0.03000000 sec
DELTA          1.89999998 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                   13C
P1                    9.95 usec
PL1                  -1.00 dB
SFO1          100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2            waltz16
NUC2                    1H
PCPD2                90.00 usec
PL12                 14.95 dB
PL13                120.00 dB
PL2                  -1.00 dB
SFO2          400.1316005 MHz

F2 - Processing parameters
SI                     32768
SF            100.6127833 MHz
WDW                       EM
SSB                        0
LB                    1.00 Hz
GB                         0
PC                    1.40
```

Sample Name	PVK-QUNZ-BSA-HYDL	**Position**		**Instrument Name**	Q-TOF	**User Name**	QTOF-PU\admin
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	PVK-QUNZ-BSA-HYDL.d	**ACQ Method**	Pondicherry Universi	**Comment**	PVK-MB-396.0780	**Acquired Time**	27-07-2018 14:32:46



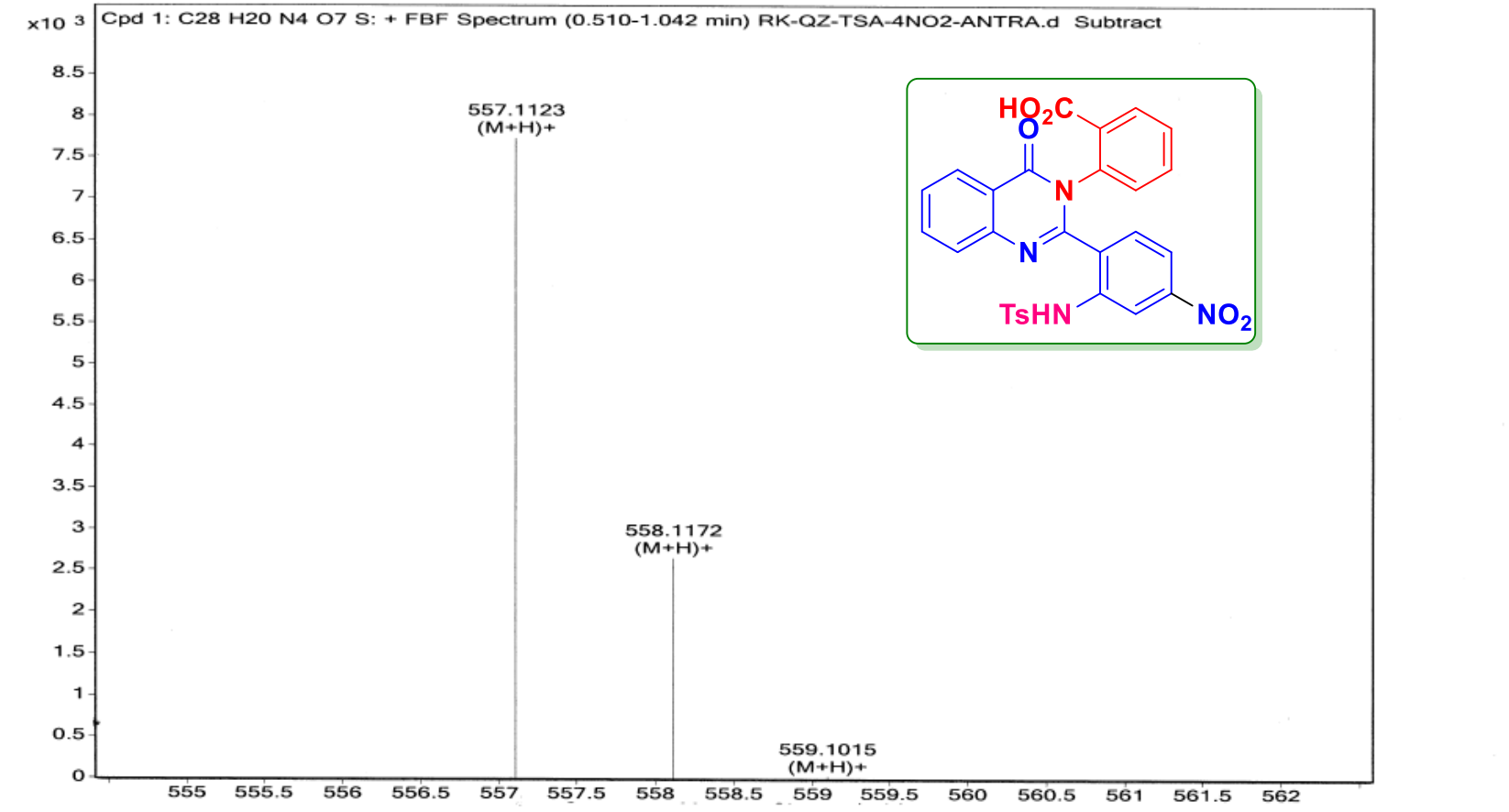


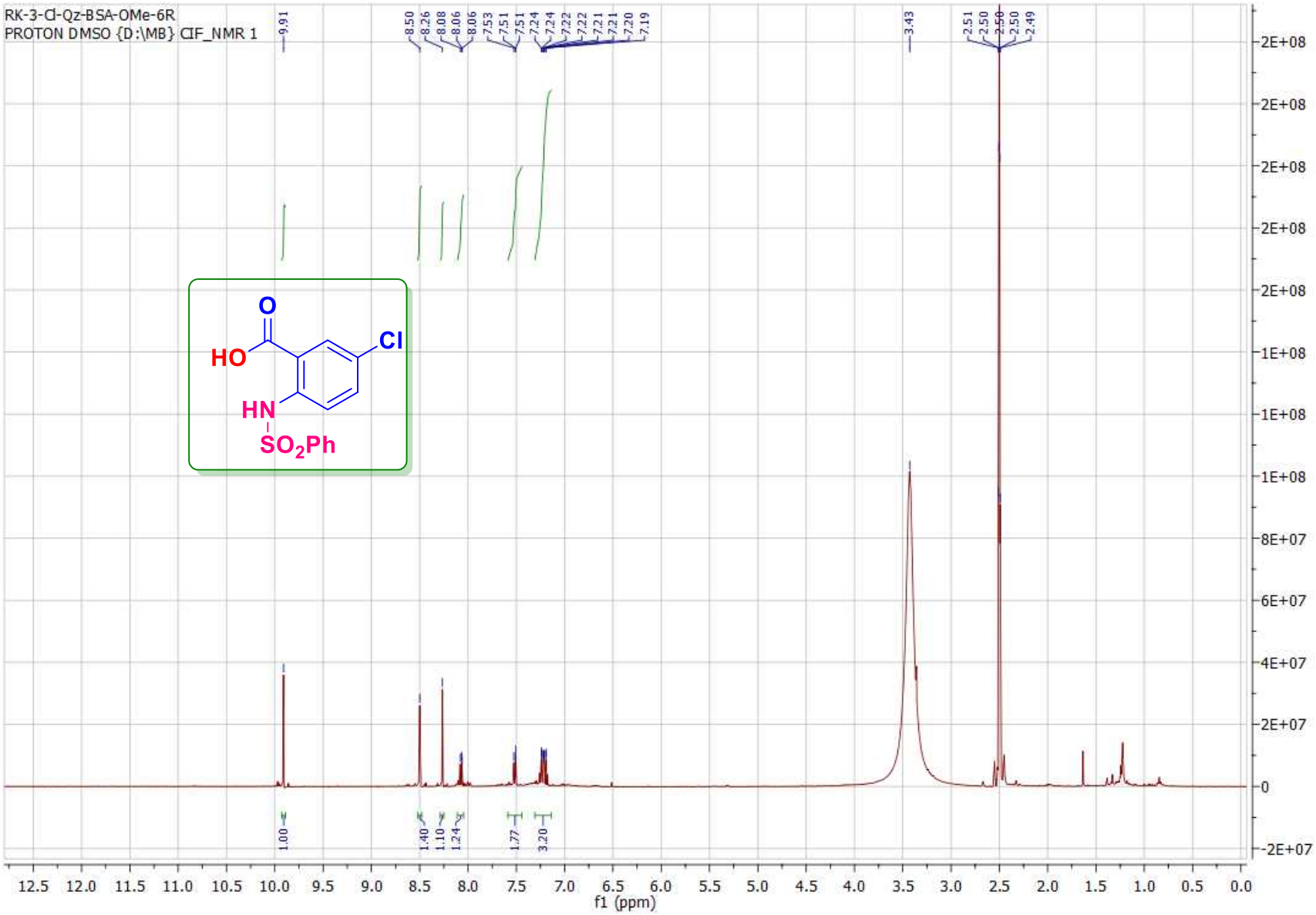

```
Current Data Parameters
NAME      RK-4-NO2-QZ-TSA-ANTRA
EXPNO                         1
PROCNO                        1

F2 - Acquisition Parameters
Date_                  20190422
Time                      16.40
INSTRUM                   spect
PROBHD    5 mm BBO BB-1H
PULPROG                   zg30
TD                       65536
SOLVENT                   CDCl3
NS                           16
DS                            2
SWH                    8223.685 Hz
FIDRES                 0.125483 Hz
AQ                     3.9846387 sec
RG                          512
DW                       60.800 usec
DE                        6.00 usec
TE                       293.1 K
D1                     1.00000000 sec
TD0                           1

======== CHANNEL f1 ========
NUC1                         1H
P1                       14.35 usec
PL1                      -1.00 dB
SFO1                400.1324710 MHz

F2 - Processing parameters
SI                        32768
SF                 400.1300094 MHz
WDW                          EM
SSB                           0
LB                       0.30 Hz
GB                            0
PC                         1.00
```

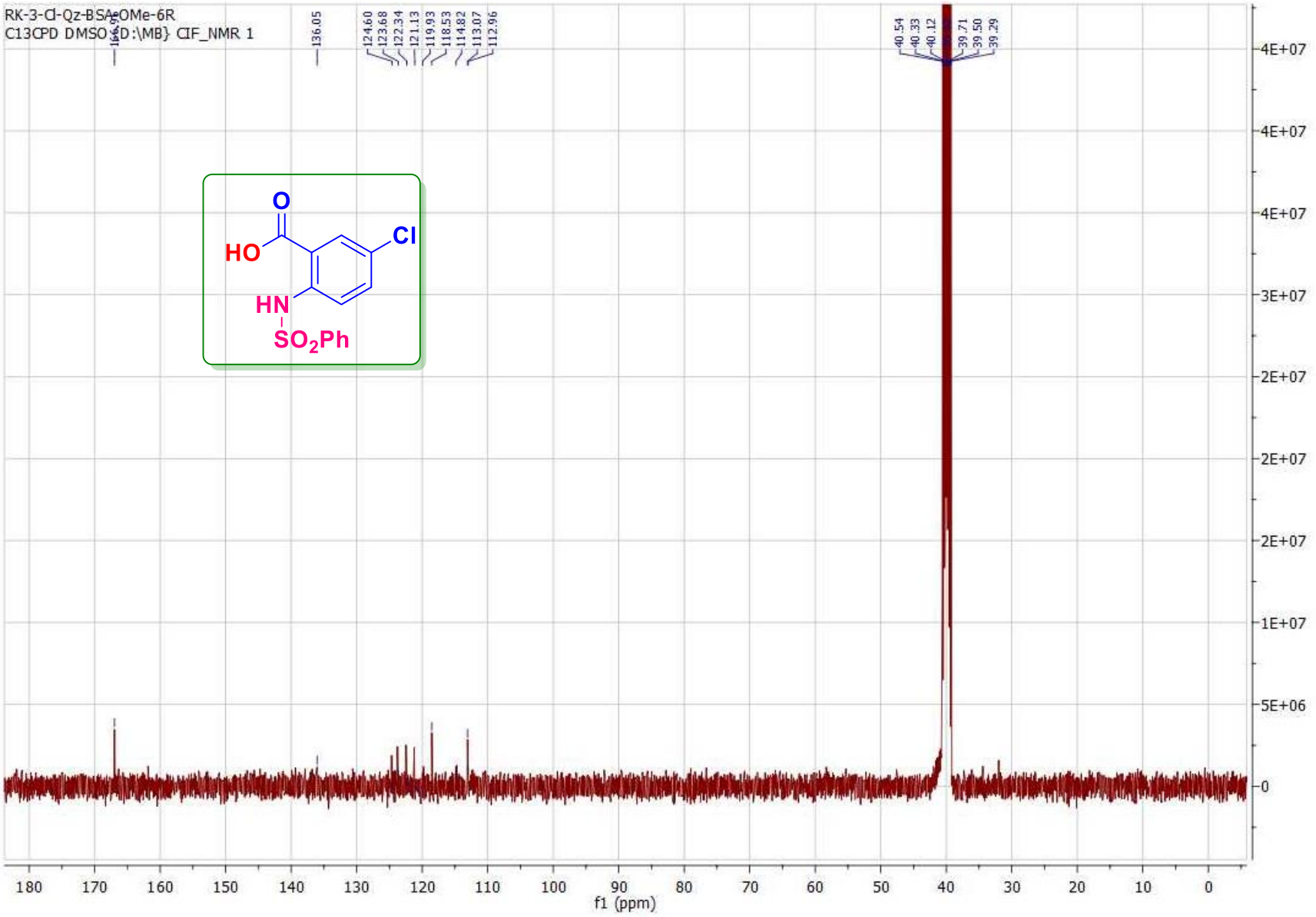



```
Current Data Parameters
NAME      RK-Qz-BSA-ANTRA
EXPNO                   2
PROCNO                  1

F2 - Acquisition Parameters
Date_            20190324
Time                15.58
INSTRUM             spect
PROBHD    5 mm BBO BB-1H
PULPROG            zgpg30
TD                  65536
SOLVENT             CDCl3
NS                   3551
DS                      4
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3631988 sec
RG                   40.3
DW                20.800 usec
DE                 6.00 usec
TE                295.5 K
D1           2.00000000 sec
d11          0.03000000 sec
DELTA        1.89999998 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                  13C
P1                 9.95 usec
PL1               -1.00 dB
SFO1        100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2              90.00 usec
PL12               14.95 dB
PL13              120.00 dB
PL2                -1.00 dB
SFO2        400.1316005 MHz

F2 - Processing parameters
SI                 32768
SF          100.6127576 MHz
WDW                   EM
SSB                    0
LB                 1.00 Hz
GB                     0
PC                  1.40
```

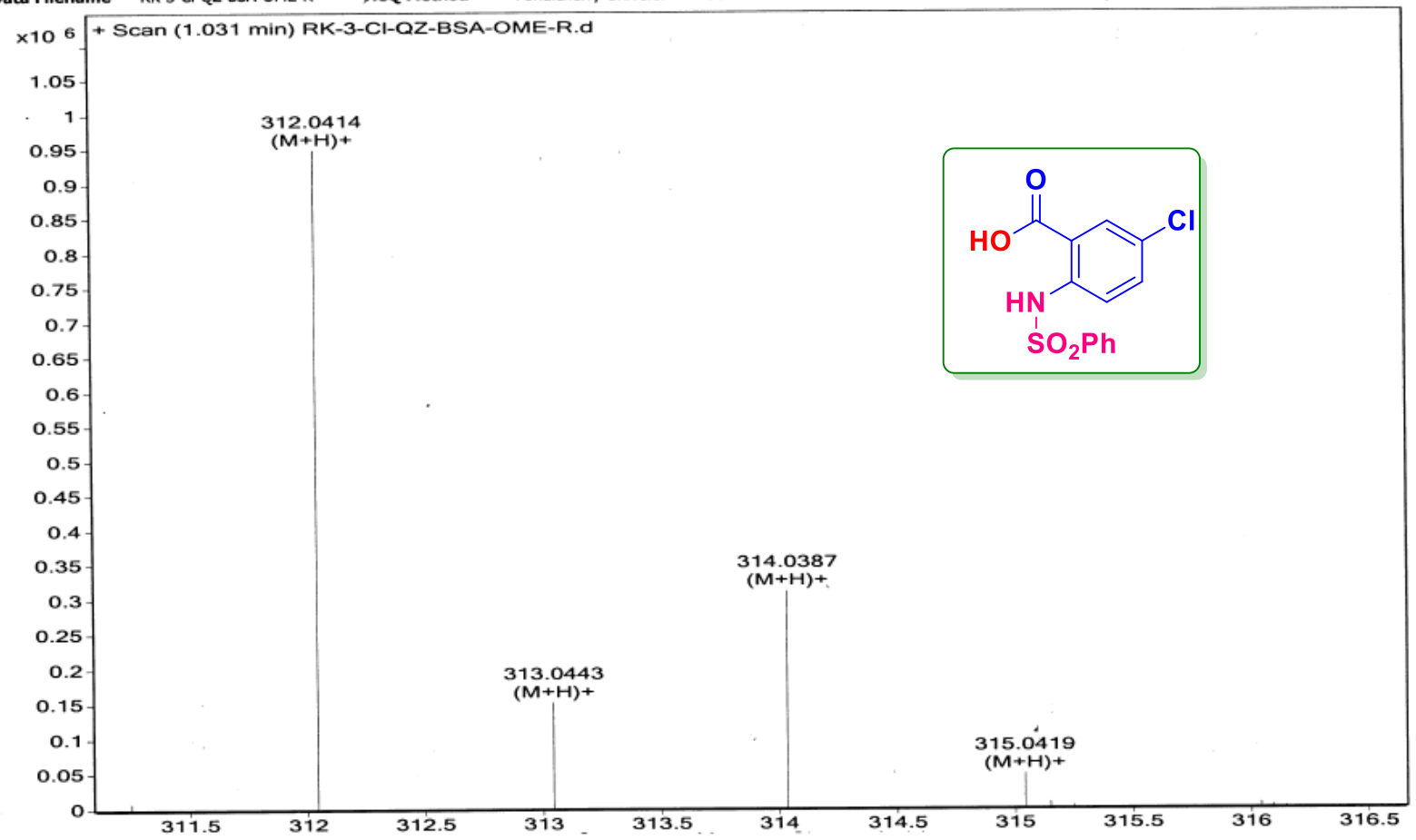
Sample Name	RK-QZ-TSA-4NO2-ANTRA	**Position**		**Instrument Name**	Q-TOF	**User Name**	QTOF-PU\admin
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	RK-QZ-TSA-4NO2-ANTRA	**ACQ Method**	Pondicherry Universi	**Comment**	RK-MB-556.1053	**Acquired Time**	23-04-2019 14:29:53

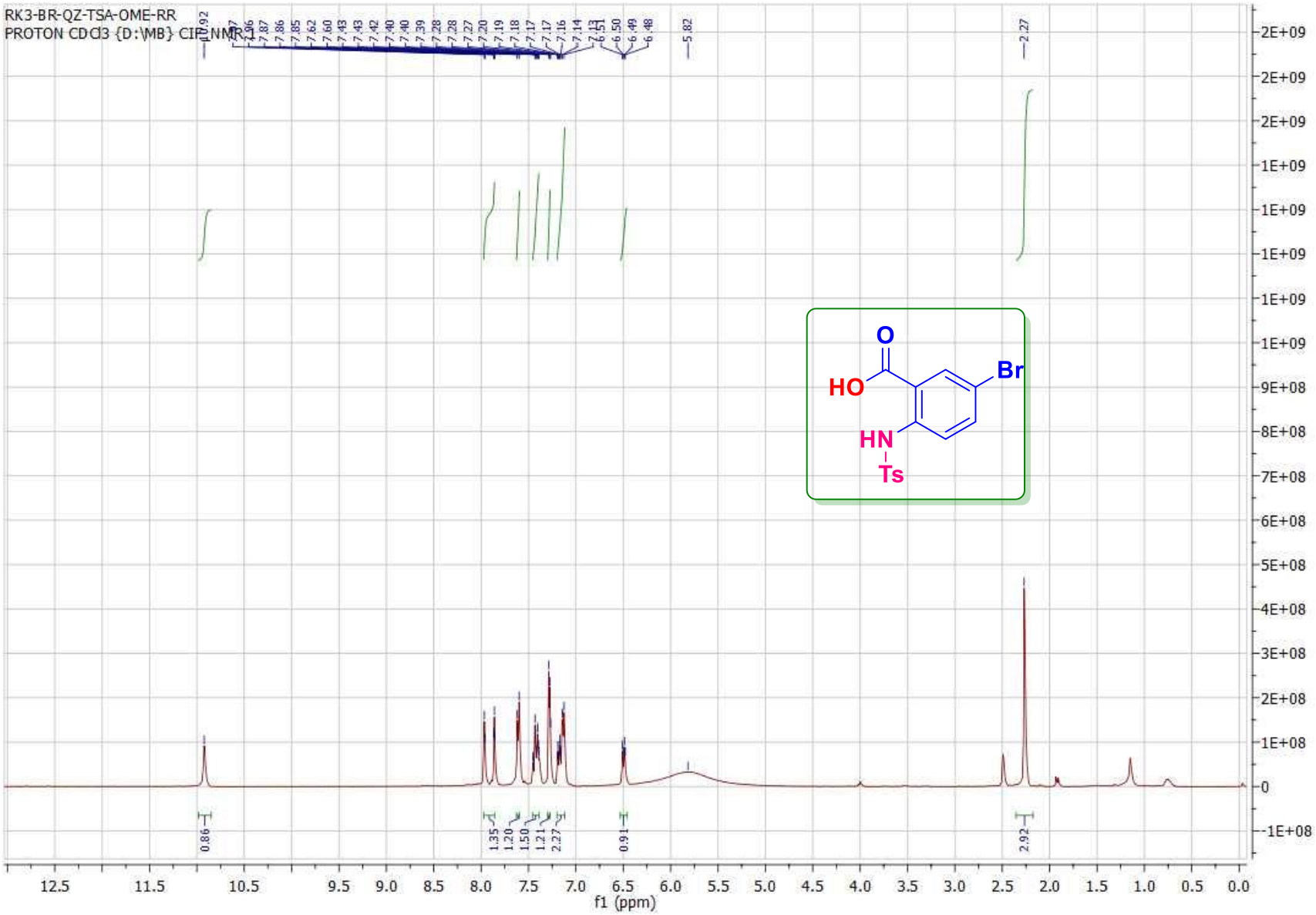


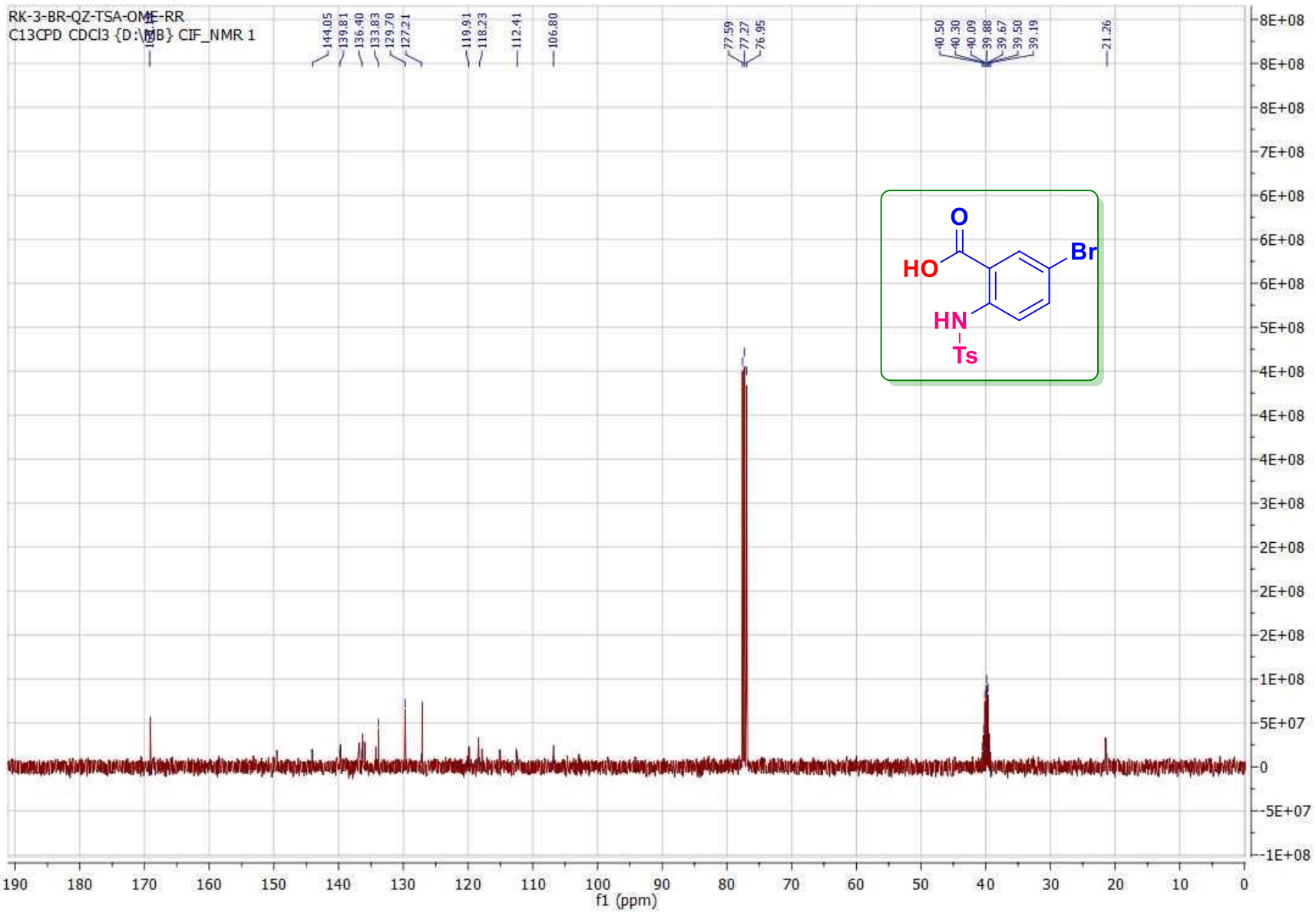

RK-3-Cl-Qz-BSA-OMe-6R
PROTON DMSO {D:\MB} CIF_NMR 1
9.91
8.50
8.26
8.08
8.06
8.06
7.53
7.51
7.51
7.24
7.24
7.22
7.21
7.21
7.20
7.19
3.43
2.51
2.50
2.50
2.50
2.49
O
HO
Cl
HN
SO2Ph
1.00
1.40
1.10
1.24
1.77
3.20
2E+08
2E+08
2E+08
2E+08
2E+08
1E+08
1E+08
1E+08
8E+07
6E+07
4E+07
2E+07
0
-2E+07
12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


RK-3-Cl-Qz-BSAeOMe-6R
C13CPD DMSO-D:\MB} CIF_NMR 1
166.95
136.05
124.60
123.68
122.34
121.13
119.93
118.53
114.82
113.07
112.96
40.54
40.33
40.12
39.71
39.50
39.29
O
HO
Cl
HN
SO2Ph
4E+07
4E+07
4E+07
3E+07
2E+07
2E+07
2E+07
1E+07
5E+06
0
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

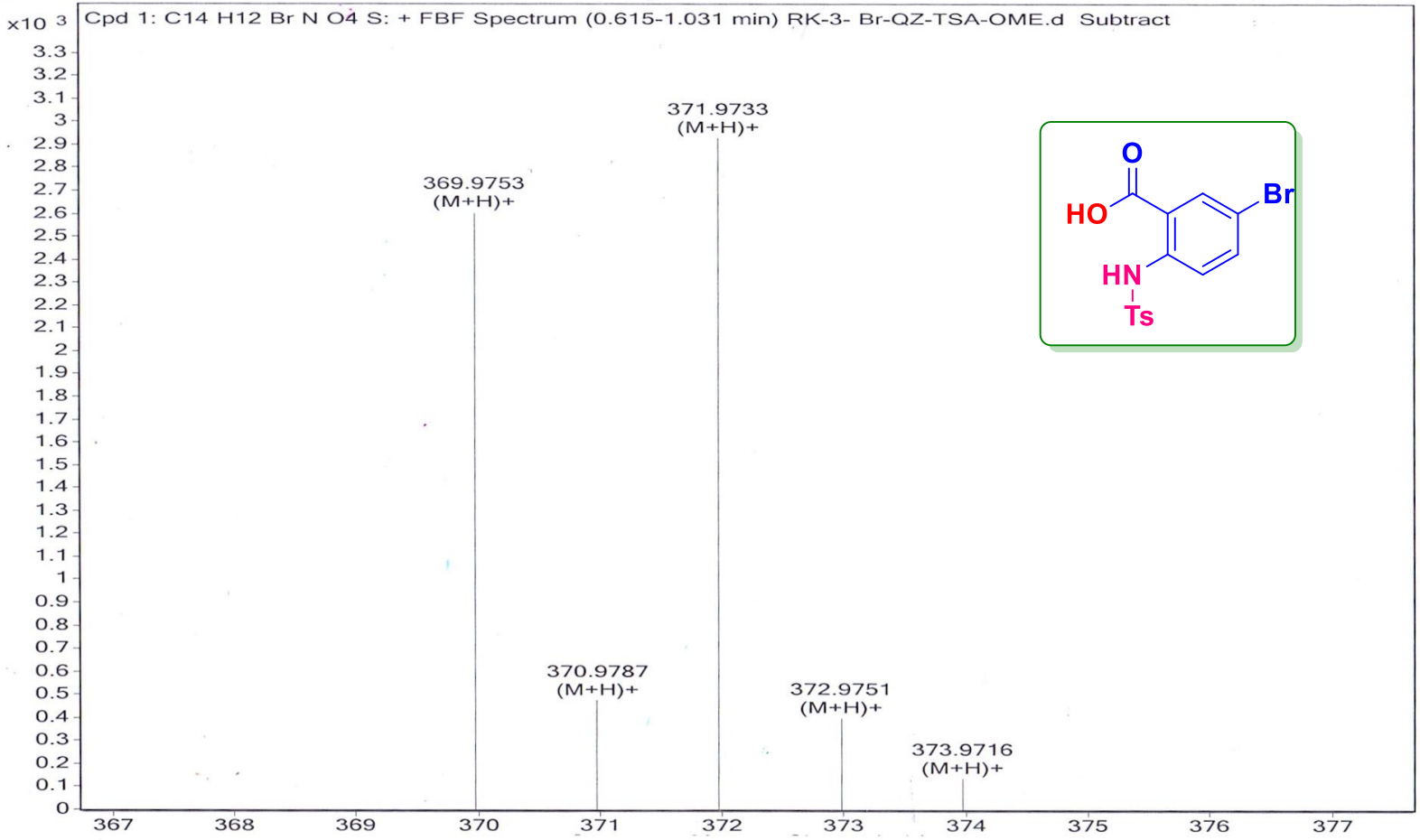
Sample Name	RK-3-Cl-QZ-BSA-OME-R	**Position**		**Instrument Name**	Q-TOF	**User Name**	QTOF-PU\admin
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	RK-3-Cl-QZ-BSA-OME-R	**ACQ Method**	Pondicherry Universi	**Comment**	RK-MB-311.0019	**Acquired Time**	24-07-2019 13:30:58

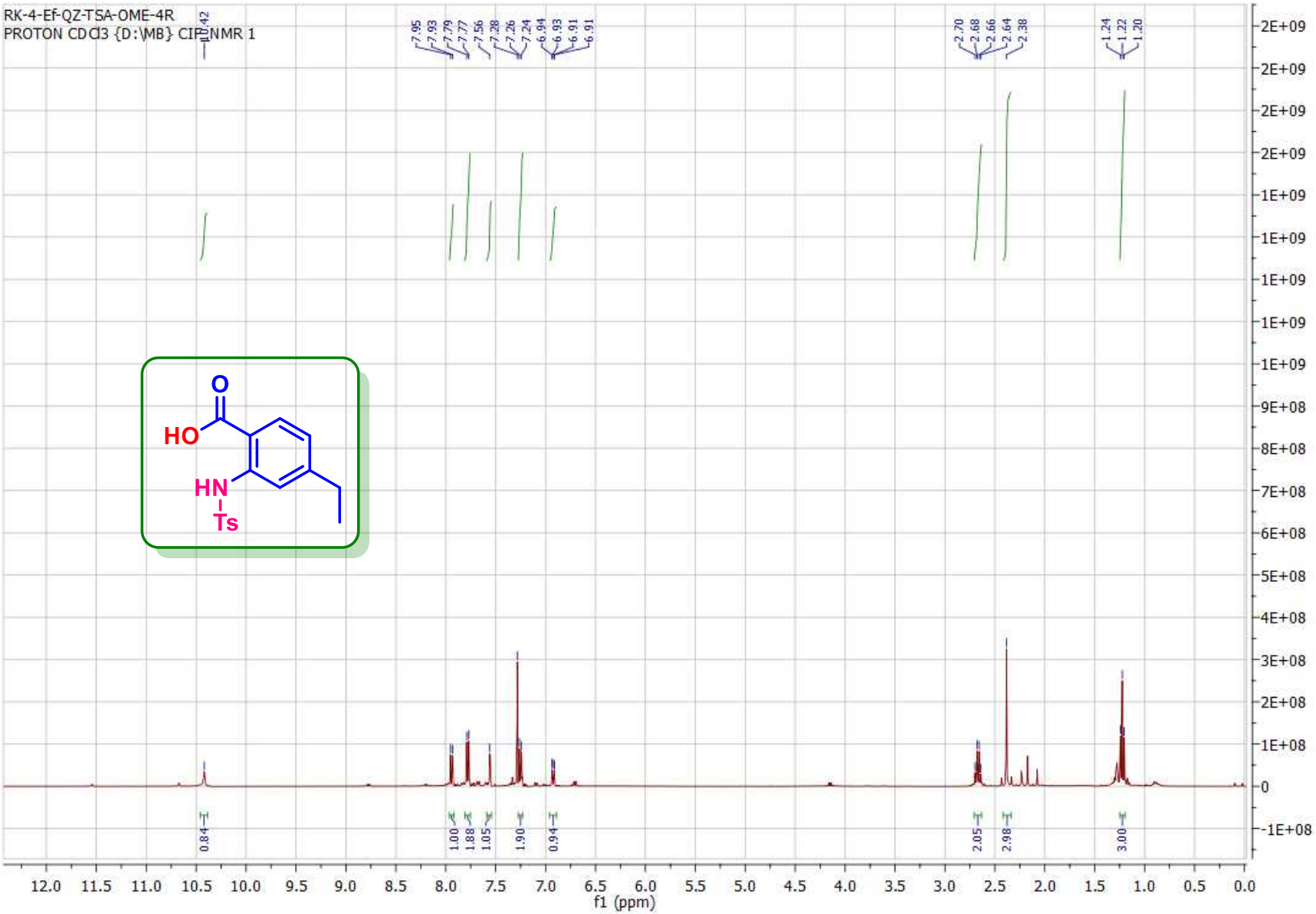


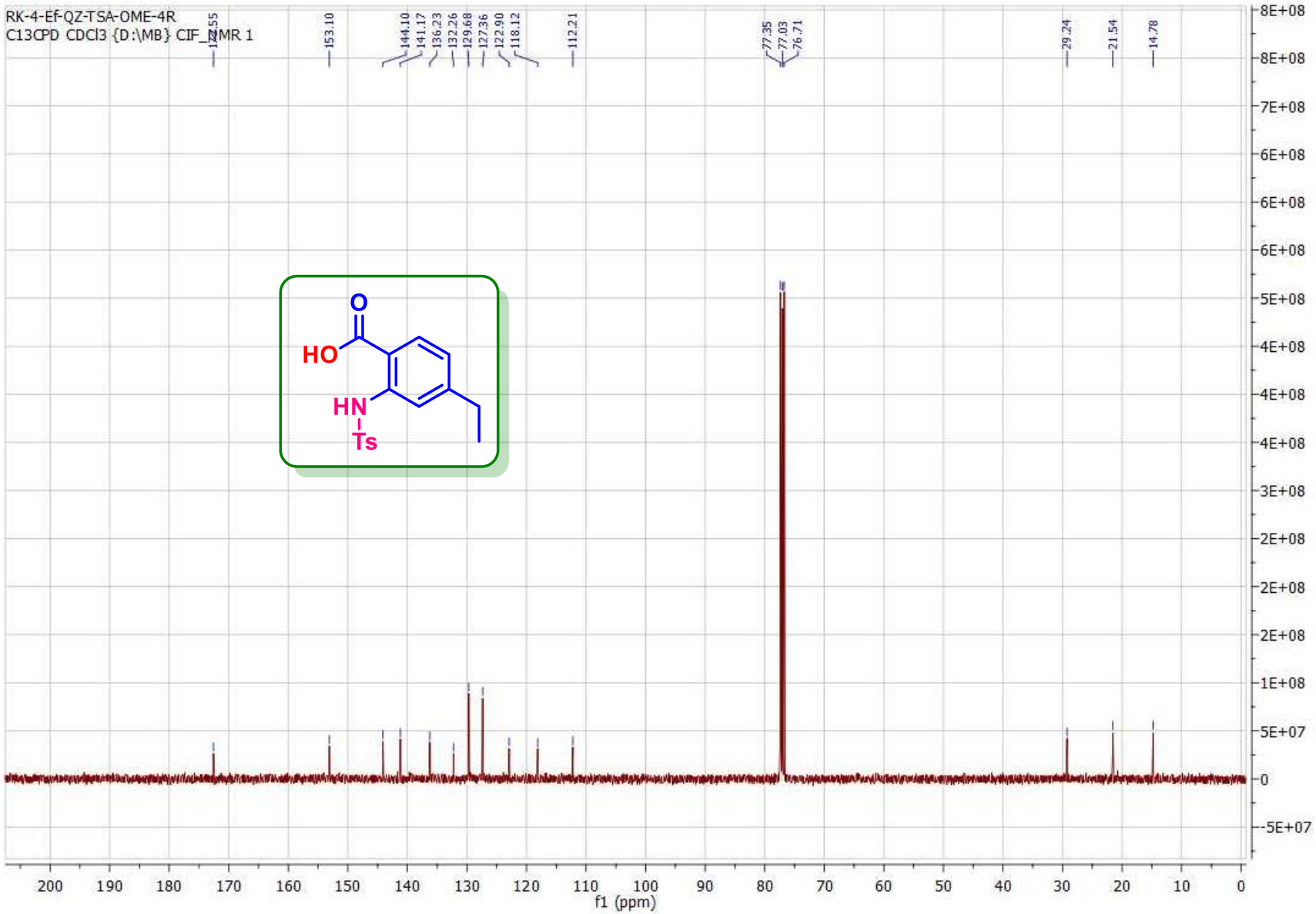

RK3-BR-QZ-TSA-OME-RR
PROTON CDCl3 {D:\MB} CIF NMR
10.92
7.87
7.86
7.85
7.62
7.60
7.43
7.43
7.42
7.40
7.40
7.39
7.28
7.27
7.20
7.19
7.18
7.17
7.17
7.16
7.14
6.51
6.50
6.49
6.48
5.82
2.27
O
HO
Br
HN
Ts
0.86
1.35
1.20
1.50
1.21
2.27
0.91
2.92
f1 (ppm)


RK-3-BR-QZ-TSA-OME-RR
C13CPD CDCl3 {D:\MB} CIF_NMR 1
169.41
144.05
139.81
136.40
133.83
129.70
127.21
119.91
118.23
112.41
106.80
77.59
77.27
76.95
40.50
40.30
40.09
39.88
39.67
39.50
39.19
21.26
O
HO
Br
HN
Ts
8E+08
7E+08
6E+08
5E+08
4E+08
3E+08
2E+08
1E+08
5E+07
0
-5E+07
-1E+08
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

Sample Name	RK-3- Br-QZ-TSA-OME	**Position**		**Instrument Name**	Q-TOF	**User Name**	QTOF-PU\admin
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	RK-3- Br-QZ-TSA-OME.	**ACQ Method**	Pondicherry Universi	**Comment**	RK-MB-368.9670	**Acquired Time**	21-06-2019 13:54:06




RK-4-Ef-QZ-TSA-OME-4R
PROTON CDCl3 {D:\MB} CIPL NMR 1
7.95
7.93
7.79
7.77
7.56
7.28
7.26
7.24
6.94
6.93
6.91
6.91
2.70
2.68
2.66
2.64
2.38
1.24
1.22
1.20
HO
O
HN
Ts
0.84
1.00
1.88
1.05
1.90
0.94
2.05
2.98
3.00
f1 (ppm)


RK-4-Ef-QZ-TSA-OME-4R
C13CPD CDCl3 {D:\MB} CIF_13MR 1
153.10
144.10
141.17
136.23
132.26
129.68
127.36
122.90
118.12
112.21
77.35
77.03
76.71
29.24
21.54
14.78
HO
O
HN
Ts
f1 (ppm)

Sample Name	RK-4-ET-QZ-TSA-OME	**Position**		**Instrument Name**	Q-TOF	**User Name**	QTOF-PU\admin
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	RK-4-ET-QZ-TSA-OME.d	**ACQ Method**	Pondicherry Universi	**Comment**	RK-MB	**Acquired Time**	21-06-2019 13:58:11