Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Palladium catalyzed chemo- and siteselective C-H acetoxylation and hydroxylation of oxobenzoxazine derivatives

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Electronic Supplementary Information

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General Information

Commercial reagents were used without further purification. 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 ($CDCl_3$) 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 of ^{1}H, ^{13}C NMR and ESI-HRMS of all compounds **4a-w**, **5a-i** & **5aa** are listed below.

General Procedure for the Synthesis of Starting Materials:

Based on literature procedure[1], 2-aryl-4*H*-benzo[d][1,3]oxazin-4-ones **3a-w** were prepared from substituted 2-aminobenzoic acids and benzoyl chlorides.

General procedure for the synthesis of 2-(4-oxo-4*H*-benzo[d][1,3]oxazin-2-yl)aryl acetate derivatives (4a-w):

A mixture of 2-aryl-4*H*-benzo[d][1,3]oxazin-4-ones **3** (0.3 mmol), $Pd(OAc)_2$ (5 mol%), $PhI(OAc)_2$ (3 equiv.) in a mixture of Ac_2O & AcOH (1:1) was placed in a round bottom flask and stirred under reflux condition for 12h. After completion of the reaction as monitored by TLC, the crude mass was purified through column chromatography using hexane: ethylacetate (9:1) which successfully led to the desired pure products **4a-w** in excellent yields.

Typical synthetic procedure for the 2-(2-hydroxybenzamido) benzoic acid 5aa *via* functional group transformation strategy.

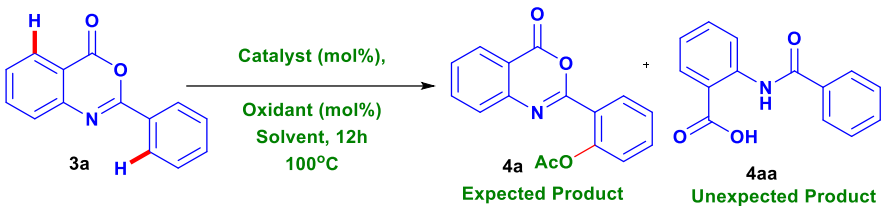
A compound (**4a**) / (**5a**) dissolved (50 mg, 0.162 mmol) in acetone (2 mL) was added dropwise slowly to a stirred solution of 4N NaOH (1 mL) at 0 °C and the reaction mixture was allowed to stir at room temperature. After completion of the reaction, the crude mixture was poured into ice water (10 mL), acidified with AcOH and acetone was removed in vacuo. The crude reaction mixture was filtered off to afford desired cleavage product (**5aa**) as white amorphous solid in excellent yields (94% / 96%) without further purification.

General procedure for the synthesis of 2-(2-hydroxyaryl)-4H-benzo[d][1,3]oxazin-4-one derivatives (5a-i):

A mixture of 2-aryl-4*H*-benzo[d][1,3]oxazin-4-ones (**3**, 0.25 mmol), $Pd(OAc)_2$ (0.1 equiv.), Oxone (3 equiv.) and DIAD (1.5 equiv.) was placed in an oven dried test tube dissolved in a mixture of DCE:TFE (3:1) solvent and stirred under reflux condition for 16h. After

completion of the reaction as indicated by TLC, the crude mass was purified through column chromatography using 10 % ethylacetate and hexane mixture which successfully led to the desired pure products **(5a-i)** in excellent yields.

Table 1. Optimization conditions for the selective *ortho*-C-H acetoxylated 2-phenyl-4-oxobenzoxazine[a,b, c]



S.N.	Catalyst (mol %)	Oxidant (mol %)	Additive (mol %)	Base (1equiv.)	Solvent	Yield%[b] 4a	Yield%[b] 4aa
1[a]	$Cu(OAc)_2$ (10)	O_2	-	-	$CH_3CN : H_2O$(1:1)	NR	NR
2[a]	$Cu(OAc)_2$ (10)	O_2	-	-	$AcOH:Ac_2O$(1:1)	NR	NR
3[a]	$Cu(OAc)_2$(10)	O_2	$AgSbF_6$ (20)	-	Ac_2O	NR	NR
4[a]	$Cu(OAc)_2$(10)	O_2	CH_3COCl(20)	^tBuOK	Toluene	NR	NR
5[a]	$Cu(OAc)_2$(10)	TBHP(200)	-	-	AcOH/PhCl(1:1)	0	95
6[a]	$Cu(OTf)_2$(10)	$K_2S_2O_8$(200)	-	NaOAc	$PhCH_3$	NR	NR
7[a]	$Cu(OTf)_2$(10)	$K_2S_2O_8$(200)	$AgSbF_6$ (20)	NaOAc	$PhCH_3$	NR	NR
8[a]	$Co(OAc)_2$(10)	$PhI(OAc)_2$(200)	Ag_2CO_3 (100)	Na_2CO_3	$AcOH/PhCH_3$(1:1)	NR	NR
9[a]	$Pd(OAc)_2$ (5)	CuI / $ArCO_2H$ (20/20)	Ag_2CO_3(100)	-	DCE	NR	NR
10[a]	$Pd(OAc)_2$(5)	$PhI(OAc)_2$(300)	-	-	DCE/ $PhCH_3$(1:1)	trace	NR
11[a]	**$Pd(OAc)_2$** (5)	**$PhI(OAc)_2$**(300)	**-**	**-**	**AcOH/Ac_2O**(1:1)	**81**	**0**
12[c]	$Pd(OAc)_2$ (10)	$PhI(OAc)_2$(300)	-	-	AcOH/Ac_2O(1:1)	82	0
13[a]	$Pd(OAc)_2$(5)	-	-	-	AcOH/Ac_2O(1:1)	NR	NR
14[a]	$Pd(OAc)_2$(5)	$K_2S_2O_8$ (200)	-	-	AcOH/DCE(1:1)	42	0
15[a]	$Rh_2(OAc)_4$(2)	$PhI(OAc)_2$(300)	$AgSbF_6$(20)	-	AcOH/Ac_2O(1:1)	59	0

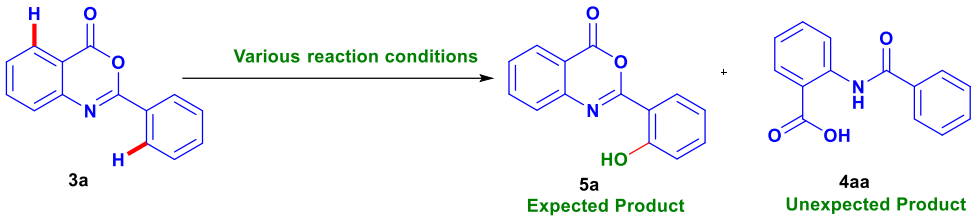
Reaction conditions[a]: **3a** (0.3 mmol), metal catalyst (5-10 mol %), oxidant (3 equiv.), Ag salt (0.2-1.0 equiv.) in various solvents at 100°C for 12 h; [b]Isolated yield of the pure products; [c] **3a** (0.3 mmol), $Pd(OAc)_2$ (10 mol %), $PhI(OAc)_2$ (3 equiv.), in AcOH/ Ac_2O (1:1) at 100°C for 12 h.

In order to test the possibility for Pd (II) catalyzed *ortho*-acetoxylation of 2-phenyl-4-oxobenzoxazines (**3a**), we first carried out *ortho*-acetoxylation reaction of **3a** by screening the different combination of catalysts, oxidants and solvents. At first, the reaction was tried by using different copper salts for obtaining the desired product **4a**. Accordingly, we have performed the reaction by using our substrate 2-phenyl-4-oxobenzoxazine (**3a**) with 10 mol% $Cu(OAc)_2$ (which acts as catalyst, oxidant and acetate source) in a mixture of H_2O

and CH_3CN (1:3) under oxygen balloon atmosphere (O_2) at 100°C for 24h. Unfortunately, we did not observe the anticipated product (**4a**) (Table 1, entry 1). When the reaction was carried out by changing the solvent system to AcOH : Ac_2O in place of mixture of H_2O and CH_3CN, we could not obtain the desired product (**4a**) (Table 1, entry 2). The reaction again failed to afford the expected product when it was carried out in presence of 10 mol % $Cu(OAc)_2$, 20 mol % $AgSbF_6$ (additive) in Ac_2O (Table 1, entry 3). Next, the same reaction was performed by altering some additional parameters such as additive (CH_3COCl), solvent (toluene) in presence of base (*t*-BuOK), no product formation was detected (Table 1, entry 4). Further, the reaction was carried out by using 70 % aq. TBHP (5 equiv.) as an oxidant in place of O_2 in a mixture of AcOH & PhCl at 100°C, surprisingly, we have observed the formation of oxidative cleavage of substrate as product (**4aa**) rather than the desired coupled product (**4a**) (Table 1, entry 5). After getting these results, we attempted the same reaction with the combination of different oxidants such as $K_2S_2O_8$, $PhI(OAc)_2$, additives such as $AgSbF_6$, Ag_2CO_3, bases such as NaOAc, Na_2CO_3 in toluene and mixture of toluene and AcOH solvent system catalysed by $Cu(OTf)_2$ and $Co(OAc)_2$, we did not find any desired product in these cases also (Table 1, entry 6, 7 and 8). Then, we hypothesized that the reaction may work well with heavier transition metals such as Pd & Rh. Accordingly, we have tried the reaction of **3a** with $Pd(OAc)_2$ (5 mol%), CuI (10 mol %), benzoic acid (20 mol %) and Ag_2CO_3 (1.0 equiv.) in DCE at 100°C for 16 h did not provide the desired product **4a** (Table 1, entry 9). When same reaction was carried out in presence of $Pd(OAc)_2$, (5 mol %) and $PhI(OAc)_2$ in mixture of DCE and toluene (1:1), interestingly, trace amount of desired product **4a** was obtained (Table 1, entry 10). To improve the yield of the reaction, we changed the solvent system from DCE and toluene (1:1) to Ac_2O & AcOH (1:1) by keeping remaining parameters constant (Table 1, entry 11). To our delight, we have obtained the anticipated *ortho*-acetoxylated-2-phenyl-4-oxobenzoxazine (**4a**) in 81 % yield (Table 1, entry 11).). Then, to check the catalyst loading efficiency, we increased the amount of $Pd(OAc)_2$ from 5 mol % to 10 mol % by keeping the remaining parameters constant, but, there was no significant improvement in yield of the desired product (82 %) observed (Table 1, entry 12). Furthermore to check the role of $PhI(OAc)_2$, the same reaction was conducted in absence of $PhI(OAc)_2$ which did not provide the desired product (**4a**) (Table 1, entry 13). In order to increase the yield, we replaced the oxidant with 3 equiv. $K_2S_2O_8$ instead of 3 equiv. $PhI(OAc)_2$ in Ac_2O & AcOH (1:1) giving only 42 % yield (Table 1, entry 14). This clearly indicates that diacetoxyiodobenzene acts as an effective oxidant as well as acetate source for the reaction to take place smoothly. In order to improve the yield further, the same reaction was conducted in presence of 2 mol % $Rh_2(OAc)_4$, 20 mol % $AgSbF_6$, 3 equiv. $PhI(OAc)_2$ in Ac_2O & AcOH (1:1) affording the desired product **4a** in 59 % yield only (Table 1, entry 15). Based on these observations, we found that the optimized condition was achieved when the reaction was carried out in presence

of 5 mol % $Pd(OAc)_2$, 3 equiv. $PhI(OAc)_2$ in Ac_2O & AcOH (1:1) at 100°C for 12h with 81% yield of the desired product (**4a**).

Table 2. Optimization conditions for the selective mono *ortho*-C-H hydroxylation of 2-phenyl-4-oxobenzoxazine (**3a**) [a,b]



S. No.	Catalyst (mol %)	Oxidant (equiv.)	Additive / Base (mol %)	Solvent	Yield % 5a[b]	Yield % 4aa[b]
1[a]	$PdCl_2$ (10)	O_2	NHPI (20)	Toluene	NR	NR
2[a]	$PdCl_2$ (10)	TBHP (5)	-	DCE	0	95
3[a]	$Pd(OAc)_2$ (10)	TBHP(5)	-	DCE	0	94
4[a]	$PdCl_2$ (10)	O_2	^{i}PrCHO (5)	DCE: CH_3CN (1:1)	76	0
5[a]	$Pd(OAc)_2$ (10)	O_2	^{i}PrCHO (5)	DCE	59	0
6[a]	$Pd(OAc)_2$(10)	$PhI(OAc)_2$(3)	-	AcOH / H_2O(1:1)	NR	NR
7[a]	$Pd(OAc)_2$(10)	$Na_2S_2O_8$(1.5)	-	Dioxane	82	0
8[a]	$Pd(OAc)_2$(10)	$Na_2S_2O_8$/ Oxone(1.5/3)	-	Dioxane	83	0
9[a]	$Pd(OAc)_2$(10)	Oxone(3)	-	Dioxane	trace	0
10[a]	$Pd(OAc)_2$(10)	Oxone(3)	PPh_3(20)	DCE	NR	NR
11[a]	$Pd(OAc)_2$(10)	Oxone	-	*t*-amyl-OH / PEG-400(1:1)	0	92
12[a]	$Pd(OAc)_2$(10)	Oxone/ $K_2S_2O_8$ (3/3)	NHPI(20)	DCE	0	94
13[a]	$Pd(OAc)_2$(10)	$(NH_4)_2S_2O_8$(3)	NHPI(20)	Dioxane	0	95
14[a]	$Pd(OAc)_2$(10)	Oxone(3)	AIBN(20)	DCE	NR	NR
15[a]	$Pd(OAc)_2$(10)	Oxone(3)	TBPB(200)	DCE	NR	NR
16[a]	$Pd(OAc)_2$(10)	Oxone(3)	DTBP(200)	DCE	NR	NR
17[a]	$Pd(OAc)_2$(10)	Oxone(3)	DIAD(150)	DCE	84	0
18[a]	$Pd(OAc)_2$(10)	Oxone(3)	DIAD(150)	TFE	87	0
19[a]	**$Pd(OAc)_2$(10)**	**Oxone(3)**	**DIAD(150)**	**TFE : DCE(1:1)**	**89**	**0**
20[c]	$Pd(OAc)_2$(5)	Oxone(3)	DIAD(150)	TFE : DCE(1:1)	66	0
21[d]	$Pd(OAc)_2$(10)	Oxone(3)	DIAD(120)	TFE : DCE(1:1)	69	0
22[d]	$Pd(OAc)_2$(10)	Oxone(3)	DIAD(100)	TFE : DCE(1:1)	60	0
23[d]	$Pd(OAc)_2$(10)	Oxone(3)	DIAD(50)	TFE : DCE(1:1)	57	0
24[d]	$Pd(OAc)_2$(10)	Oxone(3)	DIAD(20)	TFE : DCE(1:1)	48	0
25[a]	$Pd(OAc)_2$(10)	$(NH_4)_2S_2O_8$(3)	-	AcOH/DCE(1:1)	NR	NR
26[a]	$Pd(OAc)_2$(10)	$K_2S_2O_8$(3)	-	TFA/TFAA(1:1)	0	95
27[a]	[Ru(*p*-cymene)Cl_2]$_2$(5)	$K_2S_2O_8$(3)	-	TFA/TFAA(1:1)	0	96
28[a]	[Ru(*p*-cymene)Cl_2]2(5)	$K_2S_2O_8$(3)	KPF_6(20)	Acetone/DCE(1:1)	NR	NR
29[a]	$Rh_2(OAc)_4$(5)	$PhI(OAc)_2$(3)	$AgSbF_6$(20)	AcOH/Ac_2O/H_2O (1:1:1)	NR	NR

Reaction conditions[a]: **3a** (0.25 mmol), metal catalyst (5-10 mol %), oxidant (3 equiv.), Ag salt (0.2-1.0 equiv.) in various solvents under reflux condition for 16 -24h. [b]Isolated yield of the pure products. [c]**3a** (0.25 mmol), metal catalyst (5 mol %), Oxone (3 equiv.), DIAD (1.5 equiv.) in TFE: DCE (1:3) under reflux condition for 16h.

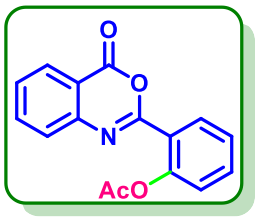
[d]**3a** (0.25 mmol), metal catalyst (10 mol %), Oxone (3 equiv.), DIAD (20-120 mol %) in TFE: DCE (1:3) under reflux condition for 16h.

In order to test the possibility for Pd (II) catalyzed *ortho*-hydroxylation of 2-phenyl-4-oxobenzoxazines (**3a**), the reaction of **3a** with hydroxyl radical source such as NHPI (20 mol %) was performed in presence of 10 mol % $PdCl_2$ catalyst, additive and oxygen balloon in toluene under reflux condition for 16 h, unfortunately we did not obtain the desired *ortho*-hydroxylated product (**5a**) (Table 2, entry 1). Further the reaction was performed with different Pd catalysts such as $PdCl_2$ / $Pd(OAc)_2$ (10 mol %) in 70 % aq. TBHP (5 equiv.) and DCE, surprisingly, we have observed the formation of oxidative cleavage of the substrate **4aa** rather than expected *ortho*-hydroxylated product (**5a**) (Table 1, entry 2-3). Similarly, when the reaction was performed in presence of 10 mol % $PdCl_2$ / $Pd(OAc)_2$ using isobutyraldehyde (5 equiv.) as an additive as well as hydroxyl source under O_2 atmosphere in DCE as well as a combination of DCE & CH_3CN solvent system under reflux condition for 16 h, the desired *ortho*-hydroxylated-2-phenyl-4-oxobenzoxazine (**5a**) was obtained in 76 % & 59 % yields respectively (Table 1, entry 4-5). In order to improve the yield of the desired product, we changed the oxidant to $PhI(OAc)_2$ (3 equiv.) in a mixture of AcOH / H_2O and $Pd(OAc)_2$ (10 mol %) was used as a catalyst. However, we did not observe the desired product **5a** (Table 1, entry 6). Further, treatment of **3a** with 10 mol % $Pd(OAc)_2$, 1.5 equiv. $Na_2S_2O_8$ in dioxane at 100°C for 16h, smoothly led to the desired coupled product **5a** in 82% yield (Table 1, entry 7). Additionally, 3 equiv. oxone was added to the same reaction, but there is no substantial improvement in the yield (Table 1, entry 8). When the same reaction was proceeded in absence of $Na_2S_2O_8$, only trace amount of product (**5a**) was observed (Table 1, entry 9). In continuation for the improvement in yield, 20 mol % PPh_3 was added to the reaction by altering the solvent to DCE, surprisingly, we did not attain the desired product (**5a**) (Table 1, entry 10). Therefore, in order to overcome this probem, the reaction conditions was tuned by using the combination of different oxidants such as $K_2S_2O_8$ & $(NH_4)_2S_2O_8$, additive such as NHPI and solvents such as DCE & dioxane, but unfortunately, again the oxidative cleavage of the substrate **4aa** was observed (Table 1, entry 11-13). Further, we changed the additives such as AIBN, TBPB & DTBP in combination with 10 mol % $Pd(OAc)_2$ and 3 equiv. oxone in DCE, none of them gave us fruitful results (Table 1, entry 14-16). However, when we replaced the additives with DIAD to the same reaction system in DCE, TFE solvents alone as well as a mixture of DCE & TFE system, the desired product was obtained in excellent yields (84-89%) (Table 1, entry 17-19). Then, to check the catalyst loading efficiency, we reduced the amount of $Pd(OAc)_2$ from 10 mol % to 5 mol % by keeping the remaining parameters constant, unfortunately, we have obtained only 66 % yield of the desired product (Table 1, entry 20). Further, to examine the ligand as well as additive loading efficiency, we have reduced

gradually the amount of DIAD from 120 mol % to 20 mol % by keeping the remaining factors persistent, surprisingly, we have observed the decrease in the yields range (48-69 %) of the desired product (Table 1, entry 21-24). To improve the yield further, the reaction of **3a** was performed in presence of 10 mol % $Pd(OAc)_2$ and 3 equiv. $(NH_4)_2S_2O_8$ in a mixture of AcOH & H_2O, but unfortunately no anticipated product was detected (Table 1, entry 25). The reaction was also performed with different catalysts such as $Pd(OAc)_2$ & $[Ru(p\text{-cym})Cl_2]_2$ with the combination of TFA / TFAA solvent system using 3 equiv. $K_2S_2O_8$, but in this case also, we have obtained only the oxidative cleavage of the substrate **4aa** (Table 1, entry 26-27). The reaction was also tried in presence of 5 mol % $[Ru(p\text{-cym})Cl_2]_2$ & $Rh(cp^*)Cl_2$ catalysts using the oxidants $K_2S_2O_8$, $PhI(OAc)_2$ and additives such as KPF_6 & $AgSbF_6$ in a combination of different solvent system such as acetone / DCE and Ac_2O / AcOH / H_2O under reflux condition for 24h, in these cases also we could not detect formation of the desired product (Table 1, entry 28-29). After screening various standardization reaction conditions on *ortho*-hydroxylation of compound **3a**, we conclude that the reaction performed well in presence of 10 mol % $Pd(OAc)_2$, 3 equiv. oxone, 1.5 equiv. DIAD in a mixture of DCE : TFE (3:1) under reflux condition for 16 h with a maximum yield (89%) of product (**5a**).

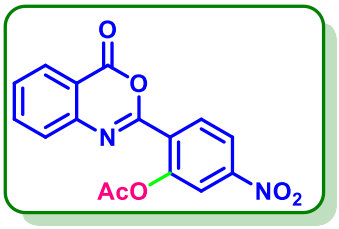
^{1}H, ^{13}C NMR and ESI-HRMS spectral data for the compounds (4a-w)

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



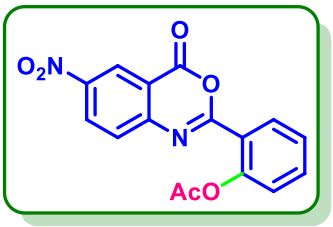
White solid; Reaction time: 12 h; Yield: 81 % (68 mg); M.P.: 152-153°C; IR (KBr) ν_{max} cm^{-1}: 1803, 1765, 1632; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.23-8.29 (m, 1H), 7.82-7.86 (m, 1H), 7.40 – 7.65 (m, 4H), 7.20 (dd, *J*= 0.8 Hz, 1.2 Hz, 2H), 2.64 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 170.0, 159.2, 155.3, 150.3, 150.0, 146.7, 136.7, 128.7, 127.3, 126.5, 124.5, 123.5, 117.1, 21.3; HRMS (ESI): Calc. for $[(C_{16}H_{12}NO_4)]$ $(M+H)^+$ 282.0766, measured 282.0769.

5-nitro-2-(4-oxo-4H-benzo[d][1,3]oxazin-2-yl)phenyl acetate (4b)



White Solid; Reaction Time: 12 h; Yield: 78 % (76 mg); M. P.: 190-193°C; IR (KBr) ν_{max} cm^{-1}: 1815, 1728, 1653; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.35-8.49 (m, 2H), 8.23-8.28 (m, 1H), 8.07 (d, *J*= 2.4Hz, 1H), 7.87-7.91 (m, 1H), 7.59-7.69 (m, 2H), 2.50 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 169.4, 158.4, 150.4, 146.2, 137.1, 132.3, 129.8, 129.5, 129.4, 129.0, 127.7, 124.1, 121.1, 121.3, 117.2, 21.1; HRMS (ESI): Calc. for $[C_{16}H_{11}N_2O_6]$ $(M+H)^+$ 327.0617, measured 327.0621.

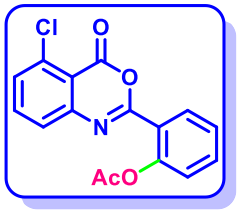
2-(6-nitro-4-oxo-4*H*-benzo[d][1,3]oxazin-2-yl)phenyl acetate (4c)



White Solid; Reaction Time: 12 h; Yield: 74 % (72 mg); M.P.: 198 °C; IR (KBr) ν_{max} cm^{-1}: 1807, 1715, 1693; ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.08 (d, *J* = 2.4Hz, 1H), 8.63 (dd, *J* = 2.8 Hz, 2.4 Hz, 1H), 8.32 (dd, *J* = 1.6 Hz, 1.6 Hz, 1H), 7.78 (d, *J* = 8.8Hz, 1H), 7.64-7.79 (m, 1H), 7.42-7.47 (m, 1H), 7.22 (d, *J* = 0.8 Hz, 1H), 2.47 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 169.9,

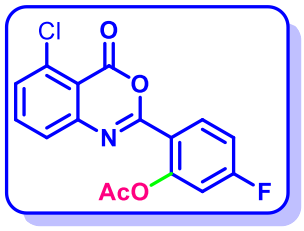
158.4, 157.4, 151.1, 150.5, 146.9, 134.9, 131.7, 130.9, 128.9, 126.8, 124.9, 124.8, 122.7, 117.5, 21.3; HRMS (ESI): Calc. [($C_{16}H_{11}N_2O_6$)] $(M+H)^+$ 327.0617, measured 327.0634.

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



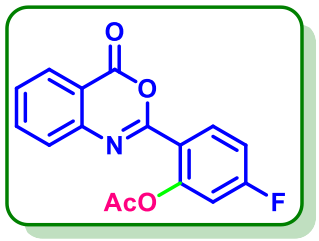
White Solid; Reaction Time: 12 h; Yield: 88 % (83 mg); M.P.: 135-137°C; IR (KBr) ν_{max} cm^{-1}: 1816, 1719, 1653; ^1H NMR (400 MHz, $CDCl_3$): δ 8.25 (dd, *J* = 6.4, 1.6Hz, 1H), 7.69 – 7.57 (m, 1H), 7.53 (t, J=0.8Hz, 2H), 7.51 – 7.16 (m, 2H), 4.95 (s, 1H), 2.45 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 169.9, 156.2, 155.7, 150.1, 149.1, 136.1, 136.1, 133.9, 131.3, 131.2, 126.5, 126.4, 124.6, 123.0, 114.8, 21.2; HRMS (ESI): Calc. for [$C_{16}H_{10}NClO_4$] $(M+H)^+$ 316.0377, measured 316.0375.

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



White Solid; Reaction Time: 12 h; Yield: 93% (93 mg); M.P: 135-137 °C; IR (KBr) ν_{max} cm^{-1}: 1816,1719, 1653; ^1H NMR (400 MHz, $CDCl_3$): δ 8.30 (dd, *J* = 9.2Hz, 6.4Hz, 1H), 7.69 (t, *J* = 8Hz, 1H), 7.50-7.55 (m, 2H), 7.10-7.15 (m, 1H), 6.94 (dd, *J* = 8.8 Hz, 2.8 Hz, 1H), 2.47 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 169.5, 155.6, 155.5, 149.0, 136.2, 136.2, 133.2, 133.1, 131.2, 126.3, 114.7, 114.2, 114.0, 112.7, 112.5, 21.2; HRMS (ESI): Calc. for [$C_{16}H_{10}NFClO_4$] $(M+H)^+$ 334.0282, measured 334.0322.

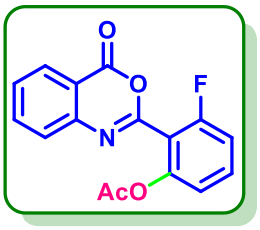
5-fluoro-2-(4-oxo-4*H*-benzo[d][1,3]oxazin-2-yl)phenyl acetate (4f)



White Solid; Reaction Time: 12 h; Yield: 83 % (74 mg); M.P.: 163-165°C; IR (KBr) ν_{max} cm^{-1}:1719, 1678, 1553; ^1H NMR (400 MHz, $CDCl_3$): δ 8.22-8.32 (m, 2H), 7.81-7.86 (m, 1H), 7.53-7.63 (m, 2H), 7.10-7.15 (m, 1H), 6.94 (dd, *J* = 8.8 Hz, 2.4Hz, 1H), 2.47 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 169.6, 159.0, 154.6, 151.6, 146.7, 136.8, 133.0, 128.8, 128.3, 120.0,

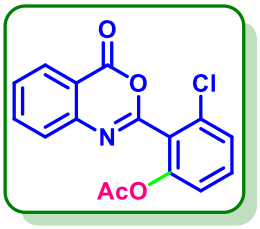
117.0, 114.1, 113.9, 112.7, 112.4, 21.3; HRMS (ESI): Calc. for $[C_{16}H_{11}NFO_4]$ $(M+H)^+$ 300.0672, measured 300.0670.

3-fluoro-2-(4-oxo-4*H*-benzo[d][1,3]oxazin-2-yl)phenyl acetate (4g)



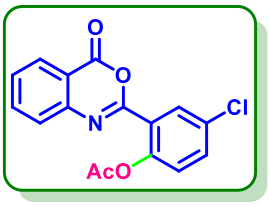
White Solid; Reaction Time: 12 h; Yield: 83 % (74 mg); M.P.: 165-166°C; IR (KBr) ν_{max} cm^{-1}: 1804, 1740, 1693; ^1H NMR (400 MHz, $CDCl_3$): δ 8.27 (dd, *J* = 6.8 Hz, 1.2Hz, 1H), 7.84-7.88 (m, 1H), 7.50-7.69 (m, 3H), 7.05-7.16 (m, 2H), 2.28 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 169.9, 162.6, 160.0, 159.8, 146.4, 136.9, 132.9, 132.8, 129.4, 128.8, 127.4, 119.7, 117.3, 114.4, 114.2, 20.9; HRMS (ESI): Calc. for $[C_{16}H_{11}NFO_4]$ $(M+H)^+$ 300.0672, measured 300.0673.

3-chloro-2-(4-oxo-4*H*-benzo[d][1,3]oxazin-2-yl)phenyl acetate(4h)



White solid; Reaction Time: 12 h; Yield: 70 % (66 mg); M.P. : 185-186°C; IR (KBr) ν_{max} cm^{-1}: 1801, 1768, 1651; ^1H NMR (400 MHz, $CDCl_3$): δ 8.29 (d, *J* = 8Hz, 1H), 7.86-7.90 (m, 1H), 7.71(d, *J* = 8Hz, 1H), 7.62 (t, *J* = 8Hz, 1H), 7.40-7.50 (m, 2H), 7.20 (dd, *J* = 0.8Hz, 0.8Hz, 1H), 2.19 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 168.7, 159.2, 153.7, 150.1, 146.2, 136.9, 134.4, 132.0, 129.6, 128.9, 127.8, 127.5, 125.1, 122.1, 117.3, 20.9; HRMS (ESI): Calc. for $[C_{16}H_{11}NClO_4]$ $(M+H)^+$ 316.0377, measured 316.0378.

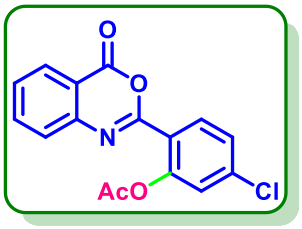
4-chloro-2-(4-oxo-4*H*-benzo[d][1,3]oxazin-2-yl)phenyl acetate (4i)



White Solid; Reaction Time: 12 h; Yield: 78 % (74 mg); M.P: 156-157°C; IR (KBr) ν_{max} cm^{-1}:1809, 1764, 1678; ^1H NMR (400 MHz, $CDCl_3$): δ 8.23-8.28(m, 2H), 7.83-7.88 (m, 1H), 7.64-7.66 (m, 1H), 7.53-.7.59 (m, 2H), 7.14 (d, *J* = 8.4 Hz, 1H), 2.46 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 193.10, 156.61, 151.17, 149.29, 142.75, 132.75, 130.80, 128.36, 125.49, 123.13,

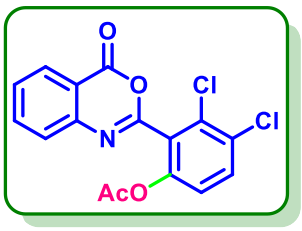
120.88, 114.46, 111.20, 109.74, 56.08, 22.27; HRMS (ESI): Calc. for $[C_{16}H_{11}NClO_4]$ $(M+H)^+$ 316.0377, measured 316.0396.

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



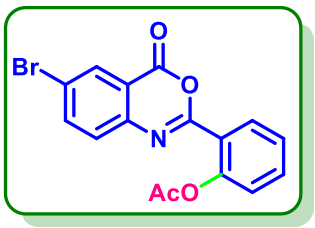
White Solid; Reaction Time: 12 h; Yield: 85 % (80 mg); M.P.: 130-131°C; IR (KBr) ν_{max} cm^{-1}: 1802, 1763, 1656; ^1H NMR (400 MHz, $CDCl_3$): δ 8.23 (dd, *J* = 8.4Hz, 1.6Hz, 2H), 7.82-7.86 (m, 1H), 7.54-7.64 (m, 2H), 7.38-7.41 (m, 1H), 7.22 (d, *J* = 2Hz, 1H), 2.47 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 169.6, 150.5, 146.6, 139.3, 136.9, 134.9, 132.1, 129.0, 128.8, 127.4, 127.0, 125.1, 124.5, 122.2, 117.1, 21.2; HRMS (ESI): Calc. for $[C_{16}H_{11}NClO_4]$ $(M+H)^+$ 316.0377, measured 316.0377.

3, 4-dichloro-2-(4-oxo-4*H*-benzo[d][1,3]oxazin-2-yl)phenyl acetate (4k)



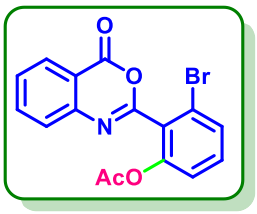
White solid; Reaction Time: 12 h; Yield: 87 % (91 mg); M.P.: 159-161°C; IR (KBr) ν_{max} cm^{-1}: 1758, 1640; ^1H NMR (400 MHz, $CDCl_3$): δ 8.29 (d, *J* =7.6, 1H), 7.88 (dd, *J* = 7.6Hz, 1.2Hz, 1H), 7.61-7.71 (m, 3H), 7.19 (d, *J* = 8.8Hz, 1H), 2.17 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 168.4, 158.9, 153.1, 148.3, 146.0, 137.0, 132.8, 132.4, 131.3, 139.7, 138.9, 127.5, 126.7, 122.9, 117.3, 20.8; HRMS (ESI): Calc. for $[(C_{16}H_{10}NCl_2O_4)]$ $(M+H)^+$ 349.9987, measured 350.0000.

2-(6-bromo-4-oxo-4*H*-benzo[d][1,3]oxazin-2-yl)phenyl acetate (4l)



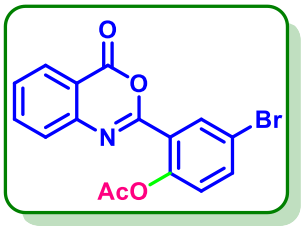
White Solid; Reaction Time: 12 h; Yield: 88% (95 mg); M.P.: 140-141°C; IR (KBr) ν_{max} cm^{-1}: 1804, 1769, 1642; ^1H NMR (400 MHz, $CDCl_3$): δ 8.35 (d, *J* = 2Hz, 1H), 8.25 (dd, *J* = 6.4, 1.6 Hz, 1H), 7.91 (dd, *J* = 6.4, 2 Hz, 1H), 7.63-7.59 (m, 1H), 7.51 (d, *J* = 8.8 Hz, 1H), 7.50-7.39 (m, 1H), 7.19 (dd, *J* = 7.2, 0.8Hz, 1H), 2.45 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 170.2, 157.9, 154.8, 150.1, 147.3, 145.7, 139.9, 133.9, 131.3, 129.0, 126.6, 124.6, 123.2, 122.1, 118.4, 21.3; HRMS (ESI): Calc. for $[C_{16}H_{11}NBrO_4]$ $(M+H)^+$ 359.9871, measured 359.9873.

3-bromo-2-(4-oxo-4*H*-benzo[d][1,3]oxazin-2-yl)phenylacetate (4m)



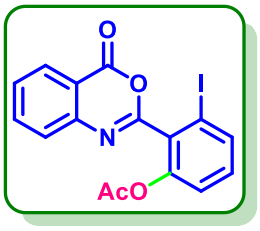
White solid; Reaction Time: 12 h; Yield: 79 % (85 mg); M.P.:143-142°C; IR (KBr) ν_{max} cm^{-1}: 1811, 1763, 1633; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.28-8.30 (m, 1H), 7.86-7.90 (m, 1H), 7.57-7.72 (m, 3H), 7.40 (t, *J* = 8Hz, 1H), 7.25 (d, *J* = 9.2 Hz, 1H), 2.17 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 168.6, 159.1, 154.5, 150.0, 146.1, 136.9, 132.2, 130.8, 129.5, 128.9, 127.5, 127.0, 122.7, 122.6, 117.2, 20.8; HRMS (ESI): Calc. for $[(C_{16}H_{11}BrNO_4)]$ $(M+H)^+$ 359.9871, measured 359.9874, 360.9950.

4-bromo-2-(4-oxo-4*H*-benzo[d][1,3]oxazin-2-yl)phenyl acetate (4n)



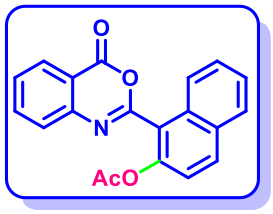
White Solid; Reaction Time: 12 h; Yield: 89 % (96 mg); M.P.:172-173°C; IR (KBr) ν_{max} cm^{-1}: 1806, 1737, 1637; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.41 (s, 1H), 8.24 (dd, *J* = 6.8, 1.2Hz, 1H), 7.84 (dd, *J* = 6.8, 0.4Hz, 1H), 7.70-7.64 (m, 2H), 7.59-7.55 (m, 1H), 7.04 (d, *J* = 8.4Hz, 1H), 2.46 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 169.8, 158.8, 154.1, 149.0, 146.5, 136.9, 136.4, 133.8, 129.2, 128.8, 127.5, 126.3, 125.2, 119.7, 117.1, 21.2; HRMS (ESI): Calc. for $[C_{16}H_{11}NBrO_4]$ $(M+H)^+$ 359.9871, measured 359.9867.

3-iodo-2-(4-oxo-4*H*-benzo[d][1,3]oxazin-2-yl)phenyl acetate (4o)



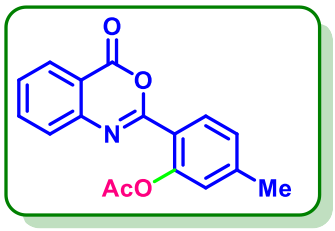
White Solid; Reaction Time: 12 h; Yield: 87 % (106 mg); M.P.: 147-148°C; IR (KBr) ν_{max} cm^{-1}: 1805, 1685, 1638; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.21-8.25 (m, 2H), 7.82-7.85 (m, 1H), 7.53-7.65 (m, 2H), 7.39-7.43 (m, 1H), 7.20 (dd, *J* = 1.2Hz, 0.8Hz, 1H), 2.46 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 170.0, 159.2, 150.0, 146.8, 136.8, 133.6, 131.2, 128.9, 128.8, 127.4, 126.6, 124.5, 134.7 123.5, 117.1, 21.3; HRMS (ESI): Calc. for $[(C_{16}H_{10}NaINO_4)]$ $(M+Na)^+$ 429.9552, measured 429.3189.

1-(4-oxo-4H-benzo[d][1,3]oxazin-2-yl)naphthalen-2-yl acetate (4p)



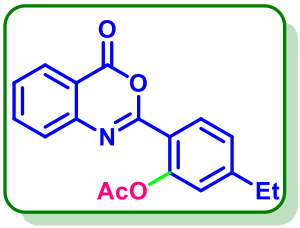
White Solid; Reaction Time: 12 h; Yield: 84 % (83 mg); M.P: 198-199°C; IR (KBr) ν_{max} cm^{-1}: 1804, 1762, 1643; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8. 33 (dd, *J* = 8Hz, 1.2Hz, 1H), 8.21-8.23 (m, 1H), 8.04 (d, *J* = 9.2 Hz, 1H), 7.90-7.93 (m, 2H), 7.89 (d, *J* = 1.6Hz, 1H), 7.52-7.77 (m, 3H), 7.37 (d, *J* = 9.2Hz, 1H), 2.31 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 168.7, 161.1, 159.5, 146.9, 145.4, 137.1, 135.3, 131.7, 129.8, 129.1, 128.7, 127.3, 126.7, 126.6, 126.5, 125.4, 123.8, 121.2, 116.9, 20.8; HRMS (ESI): Calc. for [($C_{20}H_{14}O_4$)] $(M+H)^+$ 332.0923, measured 332.0926.

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



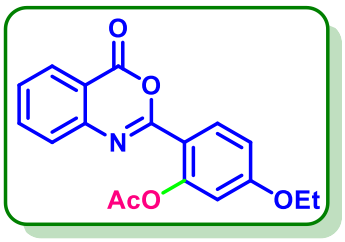
White solid; Reaction Time:12 h; Yield: 86 % (76 mg); M.P.: 129-130°C; IR (KBr) ν_{max} cm^{-1}: 1809, 1757, 1690; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.16-8.24 (m, 2H), 7.80-7.84 (m, 1H), 7.50-7.62 (m, 2H), 7.21 (d, *J* = 8 Hz, 1H), 7.00 (s, 1H), 2.46 (s, 3H), 2.44 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 170.1, 159.7, 155.4, 150.0, 146.9, 145.0, 136.7, 131.0, 128.7, 128.6, 127.5, 127.2, 125.1, 120.6, 117.1, 21.6, 21.4; HRMS (ESI): Calc. for [($C_{17}H_{14}NO_4$)] $(M+H)^+$ 296.0923, measured 296.0976.

5-ethyl-2-(4-oxo-4*H*-benzo[d][1,3]oxazin-2-yl)phenyl acetate (4r)



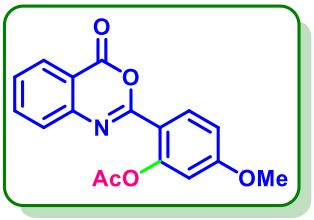
White Solid; Reaction Time: 12 h; Yield: 73 % (68 mg); M.P : 134-136°C; IR (KBr) ν_{max} cm^{-1}: 1801, 1776, 1629, ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.21 (dd, *J* = 12.8 Hz, 8Hz, 2H), 7.80-7.83 (m, 1H), 7.50-7.62 (m, 1H), 7.22-7.31 (m, 2H), 7.02 (s, 1H), 4.74 (q, *J* = 7.2Hz, 2H), 2.46 (s, 3H), 1.30 (t, *J* = 1.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 170.1, 159.3, 155.4, 151.1, 150.1, 146.9, 136.7, 131.1, 128.7, 128.6, 127.2, 126.2, 123.8, 120.7, 117.1, 28.8, 21.4, 14.8
HRMS (ESI): Calc. for [($C_{18}H_{16}NO_4$)] $(M+H)^+$ 310.1079, measured 310.1103.

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



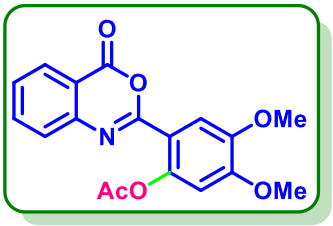
White solid; Reaction Time: 12 h; Yield: 89 % (87 mg); M.P.: 140-143°C; IR (KBr) ν_{max} cm^{-1}: 1810, 1764, 1637; ^{1}H NMR (400 MHz, $CDCl_3$):δ 8.19-8.24 (m, 2H), 7.79-7.82(m, 1H), 7.47-7.59 (m, 2H), 6.90 (dd, *J* = 2.4 Hz, 2.4 Hz, 1H), 6.68 (d, *J* = 2.4 Hz, 1H), 4.11 (q, *J* = 6.8 Hz, 2H), 2.47 (s, 3H), 1.45 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 169.9, 162.5, 159.4, 155.3, 151.7, 147.2, 136.6, 132.5, 128.7, 128.3, 127.1, 116.9, 115.4, 112.9, 110.4, 62.3, 21.4, 14.7; HRMS (ESI): Calc. for [($C_{18}H_{16}NO_5$)] $(M+H)^+$ 326.1028, measured 326.1022.

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



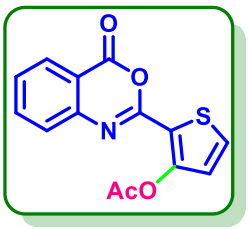
White solid; Reaction Time: 12 h; Yield: 71% (66 mg); M. P : 138-139°C; IR (KBr) ν_{max} cm^{-1}: 1821, 1767,1651; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.19-8.25 (m, 2H), 7.77 -7.82 (m, 2H), 7.47-7.59 (m, 1H), 6.91 (dd, *J* = 2.8 Hz, 2.4 Hz 1H), 6.69 (d, *J* = 2.8 Hz, 1H), 2.48 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 169.9, 163.9, 159.4, 155.2, 151.7, 147.1, 136.6, 132.5, 128.7, 128.3, 127.1, 116.9, 115.6, 112.5, 110.0, 55.9, 21.4; HRMS (ESI): Calc. for [($C_{17}H_{14}NO_5$)] $(M+H)^+$ 312.0872, measured 312.0868.

4, 5-dimethoxy-2-(4-oxo-4*H*-benzo[d][1,3]oxazin-2-yl)phenyl acetate (4u)



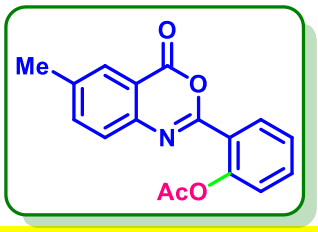
White solid; Reaction Time: 12 h; Yield: 81 % (83 mg); M.P :182-183°C; IR (KBr) ν_{max} cm^{-1}: 1813, 1763, 1643; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.21 (dd, *J* = 1.6 Hz, 1.6Hz, 1H), 7.79-7.83 (m, 1H), 7.73 (s, 1H), 7.60 (d, *J* = 8Hz, 1H), 7.48-7.52 (m, 1H), 6.67 (m, 1H), 3.99 (s, 3H), 3.94 (s, 3H), 2.47 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 170.4, 159.3, 155.2, 153.2, 147.1, 147.1, 145.0, 136.7, 128.7, 128.4, 127.1, 116.8, 114.7, 112.1, 107.6, 21.3; HRMS (ESI): Calc. for [($C_{18}H_{16}NO_6$)] $(M+H)^+$ 342.0978, measured 342.0995.

2-(4-oxo-4*H*-benzo[d][1,3]oxazin-2-yl)thiophen-3-yl acetate (4v)



White solid; Reaction Time: 12 h; Yield: 79 % (68 mg); M.P.: 144-145°C; IR (KBr) ν_{max} cm^{-1}: 1795, 1749, 1624; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.18 (d, *J* = 7.6 Hz, 1H), 7.74-7.81 (m, 2H), 7.60 (d, *J* = 0.4 Hz, 1H), 7.44-7.59 (m, 1H), 6.77 (d, *J* = 7.6 Hz, 1H), 2.37 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 166.73, 159.26, 156.9, 153.7, 147.3, 136.8, 128.9, 128.8, 127.9, 126.9, 126.0, 116.8, 114.2, 20.9; HRMS (ESI): Calc. for [($C_{14}H_{10}SNO_4$)] $(M+H)^+$ 288.0331, measured 288.0352.

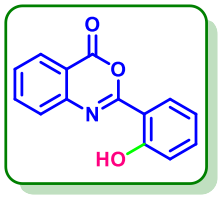
2-(6-methyl-4-oxo-4H-benzo[d][1,3]oxazin-2-yl)phenyl acetate (4w)



White solid; Reaction Time:12 h; Yield: 84% (74 mg); M.P.: 139-141°C; IR (KBr) ν_{max} cm^{-1}: 1814, 1759, 1697; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.82 (dd, J = 5.6 Hz, J = 0.8Hz,1H), 7.80 (d, J = 1.2 Hz, 1H), 7.61 (dd, J = 7.6 Hz, J = 0.4Hz,1H), 7.50-7.54 (m, 2H), 7.20-7.22 (m, 1H), 7.00 (s, 1H), 2.46 (s, 3H), 2.44 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 170.1, 159.3, 155.4, 150.0, 146.9, 145.0, 136.7, 131.0, 128.7, 128.6, 127.5, 127.2, 125.1, 120.5, 117.1, 22.6, 21.4; HRMS (ESI): Calc. for [($C_{17}H_{14}NO_4$)] $(M+H)^+$ 296.0923, measured 296.0907.

^{1}H, ^{13}C NMR and ESI-HRMS spectral data for the compounds (5a-i)

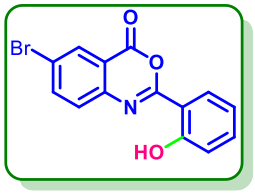
2-(2-hydroxyphenyl)-4*H*-benzo[d][1,3]oxazin-4-one (5a)



White solid; Reaction Time: 16 h; Yield: 89 % (53 mg); M. P.: 163°C; IR (KBr) ν_{max} cm^{-1}; 3657, 1875, 1756, 1625, 1482; ^{1}H NMR (400 MHz, $CDCl_3$): δ 12.44 (s, 1H), 8.23-8.26 (m, 1H), 8.08 (dd, *J* = 6.4, 1.6 Hz, 1H), 7.82 – 7.86 (m, 1H), 7.46-7.63 (m, 3H), 6.96-7.07 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 161.1, 159.3, 158.1, 145.0, 137.1, 135.4, 129.1, 128.7, 128.5,

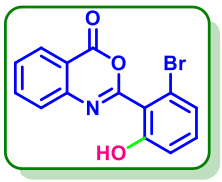
125.9, 119.6, 118.1, 116.8, 112.2; HRMS (ESI): Calc. for [($C_{14}H_{10}NO_3$)] $(M+H)^+$ 240.0661, measured 240.0769.

6-bromo-2-(2-hydroxyphenyl)-4*H*-benzo[d][1,3]oxazin-4-one (5b)



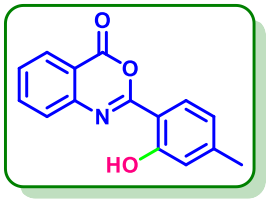
White solid; Reaction Time: 16h; Yield: 87 % (69 mg); M.P : 147°C ; IR (KBr) ν_{max} cm^{-1}: 3389, 1889, 1773, 1749, 1631; ^1H NMR (400 MHz, $CDCl_3$):δ 12.22 (s, OH), 8.36 (d, *J* = 2.4Hz, 1H), 8.060 (dd, *J* = 6.4, 1.6 Hz, 1H), 7.93 (dd, *J* = 6.4, 2.4 Hz, 1H), 7.47-7.52 (m, 2H), 6.97-7.07 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 161.2, 159.5, 156.9, 143.9, 140.3, 135.7, 131.6, 128.5, 127.5, 121.9, 119.8, 118.2, 118.1, 111.9; HRMS (ESI): Calc. for [($C_{14}H_9BrNO_3$)] $(M+H)^+$ 317.9800, measured 317.9770, 319.9752.

2-(2-bromo-6-hydroxyphenyl)-4*H*-benzo[d][1,3]oxazin-4-one (5c)



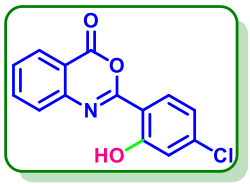
White solid; Reaction Time: 16 h; Yield: 72 % (57 mg); M.P.:153 °C; IR (KBr) ν_{max} cm^{-1}: 3371, 1829, 1763, 1729, 1633; ^1H NMR (400 MHz, $CDCl_3$): δ 12.45 (s, 1H), 8.25 (dd, *J* = 6.4, 1.2 Hz, 1H), 8.08 (dd, *J* = 6.4, 1.6 Hz, 1H), 7.83-7.87 (m, 1H), 7.46-7.64 (m, 2H), 6.96-7.08 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 161.2, 159.3, 158.1, 145.0, 137.1, 135.4, 129.2, 128.7, 128.5, 125.9, 119.7, 118.1, 116.8, 112.2; HRMS (ESI): Calc. for [($C_{14}H_8BrNO_3$)] $(M+H)^+$ 316.9888, measured 316.2854.

2-(2-hydroxy-4-methylphenyl)-4*H*-benzo[d][1,3]oxazin-4-one (5d)



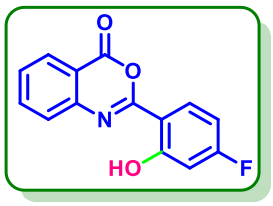
White solid; Reaction Time: 16 h; Yield: 71 % (45mg); M. P:149°C; IR (KBr) ν_{max} cm^{-1}: 3703, 1848, 1740, 1612; ^1H NMR (400 MHz, $CDCl_3$): δ 13.19 (s, 1H), 8.26 (dd, *J* = 6.4, 1.2Hz, 1H), 8.25 (s, 1H), 7.86-7.8.04 (m, 2H), 7.57-7.62 (m, 3H), 2.57 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 158.0, 157.4, 155.3, 144.3, 142.1, 137.4, 129.4, 129.3, 127.9, 125.9, 125.5, 124.0, 116.7, 111.1, 18.8; HRMS (ESI): Calc. for [($C_{15}H_{11}NO_3$)] $(M+H)^+$ 254.0817, measured 254.0826.

2-(4-chloro-2-hydroxyphenyl)-4*H*-benzo[d][1,3]oxazin-4-one (5e)



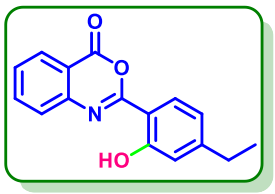
White solid; Reaction Time: 16 h; Yield: 82 % (56 mg); M.P.:159°C; IR (KBr) ν_{max} cm^{-1}: 3890, 1843, 1776, 1446, 1425; ^{1}H NMR (400 MHz, $CDCl_3$): δ 12.62 (s, 1H), 8.25(dd, *J* = 6.8, 1 2Hz, 1H), 8.12 (d, *J* = 8.4 Hz, 1H), 7.84-7.88 (m, 1H), 7.54-7.63 (m, 2H), 7.09 (s, 1H), 6.96-7.09 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 161.6, 158.7, 157.7, 144.7, 141.2, 137.3, 129.4, 129.3, 128.9, 125.9, 120.4, 118.3, 116.8, 110.9; HRMS (ESI): Calc. for [($C_{14}H_8ClNO_3$)] $(M+H)^+$ 274.0271, measured 274.0250.

2-(4-fluoro-2-hydroxyphenyl)-4H-benzo[d][1,3]oxazin-4-one (5f)



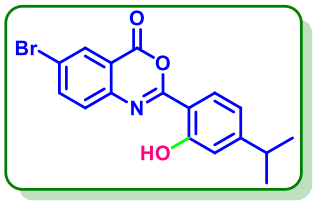
White solid; Reaction Time: 16 h; Yield: 84 % (54 mg); M.P.:155°C; IR (KBr) ν_{max} cm^{-1}: 3878, 1841, 1766, 1439, 1418; ^{1}H NMR (400 MHz, $CDCl_3$): δ 12.76 (s, 1H), 8.24 (dd, *J* = 6.8, 1 2Hz, 1H), 8.09 (dd, *J* = 6.4, 2.4Hz, 1H), 7.83-7.87 (m, 1H), 7.53-7.62 (m, 1H), 7.09 (s, 1H), 6.69-6.78 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 163.2, 158.8, 157.8, 144.8, 137.2, 130.7, 129.2, 128.7, 125.7, 116.7, 108.0, 107.8, 105.9, 104.9; HRMS (ESI): Calc. for [($C_{14}H_8FNO_3$)] $(M+H)^+$ 258.0566, measured 258.0553.

2-(2-hydroxy-4-ethylphenyl)-4*H*-benzo[d][1,3]oxazin-4-one (5g)



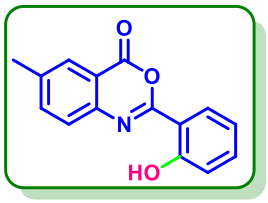
White solid; Reaction Time: 16 h; Yield: 88 % (59 mg); M.P : 168°C; IR (KBr) ν_{max} cm^{-1}: 3703, 1848, 1740, 1612; ^{1}H NMR (400 MHz, $CDCl_3$):δ 12.39 (s, 1H), 8.22 (d, *J* = 7.6, 1H), 7.96 (d, *J* = 7.6, 1H), 7.80-7.84 (m, 1H), 7.59 (d, *J* = 8 Hz, 1H), 7.49-7.53 (m, 1H), 6.89 (s, 1H), 6.81 (d, *J* =8.4 Hz, 1H), 2.67 (q, *J* = 7.6, 7.6, 2H), 1.27 (t, *J* = 7.6, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 164.9, 162.5, 153.9, 147.2, 145.5, 136.7, 132.2, 131.5, 129.8, 128.6, 124.9, 124.8, 124.1, 123.0, 21.8, 14.5; HRMS (ESI): Calc. for [($C_{16}H_{13}NO_3$)] $(M+H)^+$ 268.0974, measured 268.0950.

6-bromo-2-(2-hydroxy-4-isopropylphenyl)-4*H*- benzo[d][1,3]oxazin-4-one (5h)



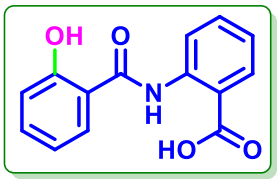
White solid; Reaction Time: 16 h; Yield:78 % (70mg); M.P.: 178 °C; IR (KBr) ν_{max} cm^{-1}: 3571, 1899, 1763, 1739, 1631; ^{1}H NMR (400 MHz, $CDCl_3$): δ 12.17 (s, OH), 8.35 (d, *J* = 2.4 Hz, 1H), 7.90-7.98 (m, 2H), 7.49 (d, 8.4 Hz, 1H), 6.93 (s, 1H), 6.85-6.93(m, 1H), 2.89-2.96 (m, 1H), 1.27 (d, *J* = 7.2 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 161.3, 159.6, 158.1, 157.1, 144.1, 140.2, 131.6 128.5, 127.4, 121.5, 118.7, 118.0, 115.7, 109.6, 34.6, 23.5; HRMS (ESI): Calc. for [($C_{17}H_{14}BrNO_3$)] $(M+H)^+$ 360.0235, measured 360.0206.

2-(2-hydroxyphenyl)-6-methyl-4H-benzo[d][1,3]oxazin-4-one (5i)



White solid; Reaction Time: 16 h; Yield: 80 % (50mg); M. P:158-160°C; IR (KBr) ν_{max} cm^{-1}: 3714, 1833, 1735, 1609; ^{1}H NMR (400 MHz, $CDCl_3$): δ 12.40 (s, 1H), 8.22-8.24 (m, 1H), 7.95 (d, *J* =8.4Hz, 1H), 7.81-7.85 (m, 1H), 7.49-7.60 (m, 2H), 6.88 (s, 1H), 6.79-6.81 (m, 1H), 2.38 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 161.1, 159.4, 158.3, 146.9, 145.2, 137.1, 129.1, 128.4, 128.3, 125.7, 121.0, 118.3, 116.7, 109.6, 22.1; HRMS (ESI): Calc. for [($C_{15}H_{11}NO_3$)] $(M+H)^+$ 254.0817, measured 254.0808.

2-(2-hydroxybenzamido) benzoic acid (5aa)

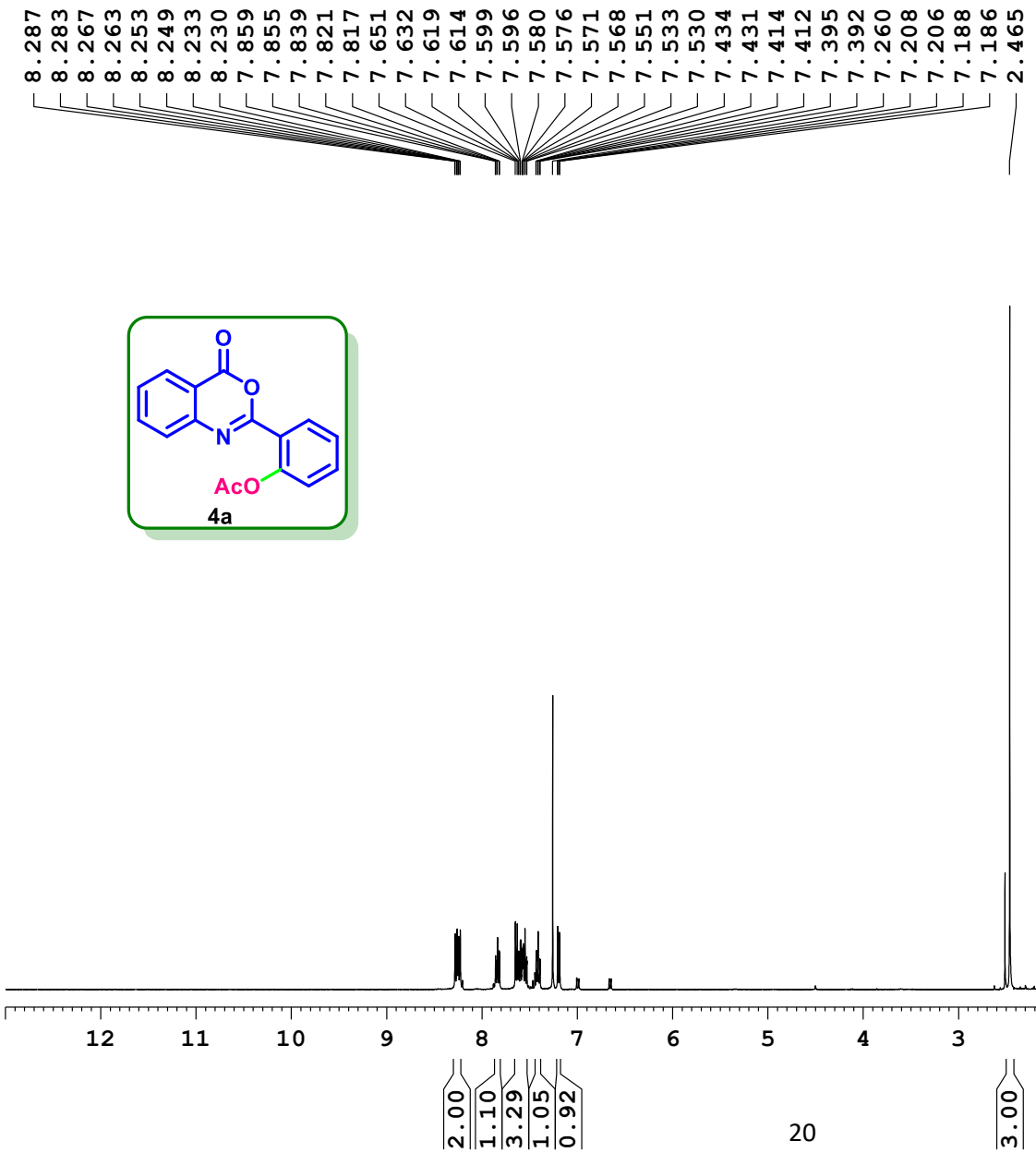


White solid; Reaction Time: 6 h; Yield: 96% (40mg); M. P.: 198 °C; IR (KBr) ν_{max} cm^{-1}: 3831, 3615, 3555, 1790, 1485, 1282; ^{1}H NMR (400 MHz, $CDCl_3$): δ 12.54 (s, 1H), 12.30 (s, 1H), 12.05 (s, 1H), 8.78 (d, *J* = 8.4 Hz, 1H), 8.66 (d, *J* = 8.4 Hz, 1H), 8.03-8.06 (m, 1H), 7.75 (t, 1H), 7.33-7.54(m, 2H), 7.05-711 (m, 1H), 6.86-6.90 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 170.1, 166.4, 140.3, 138.4, 138.3, 133.9, 132.4, 131.1, 128.5, 126.5, 122.4, 121.5, 119.8, 116.0; HRMS (ESI): Calc. for [($C_{14}H_{11}NO_4$)] $(M+H)^+$ 258.0766, measured 258.0757.

4. References

[1]. S. Thakral, D. Saini, A. Kumar, N. Jain, S. Jain, *Med. Chem. Res* 2017, **26**, 1595–1604.

PROTON CDCl3 {D:\MB} KOPAL 1

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FIDRES           0.125483 Hz
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TE                 293.4 K
D1            1.00000000 sec
TD0                    1

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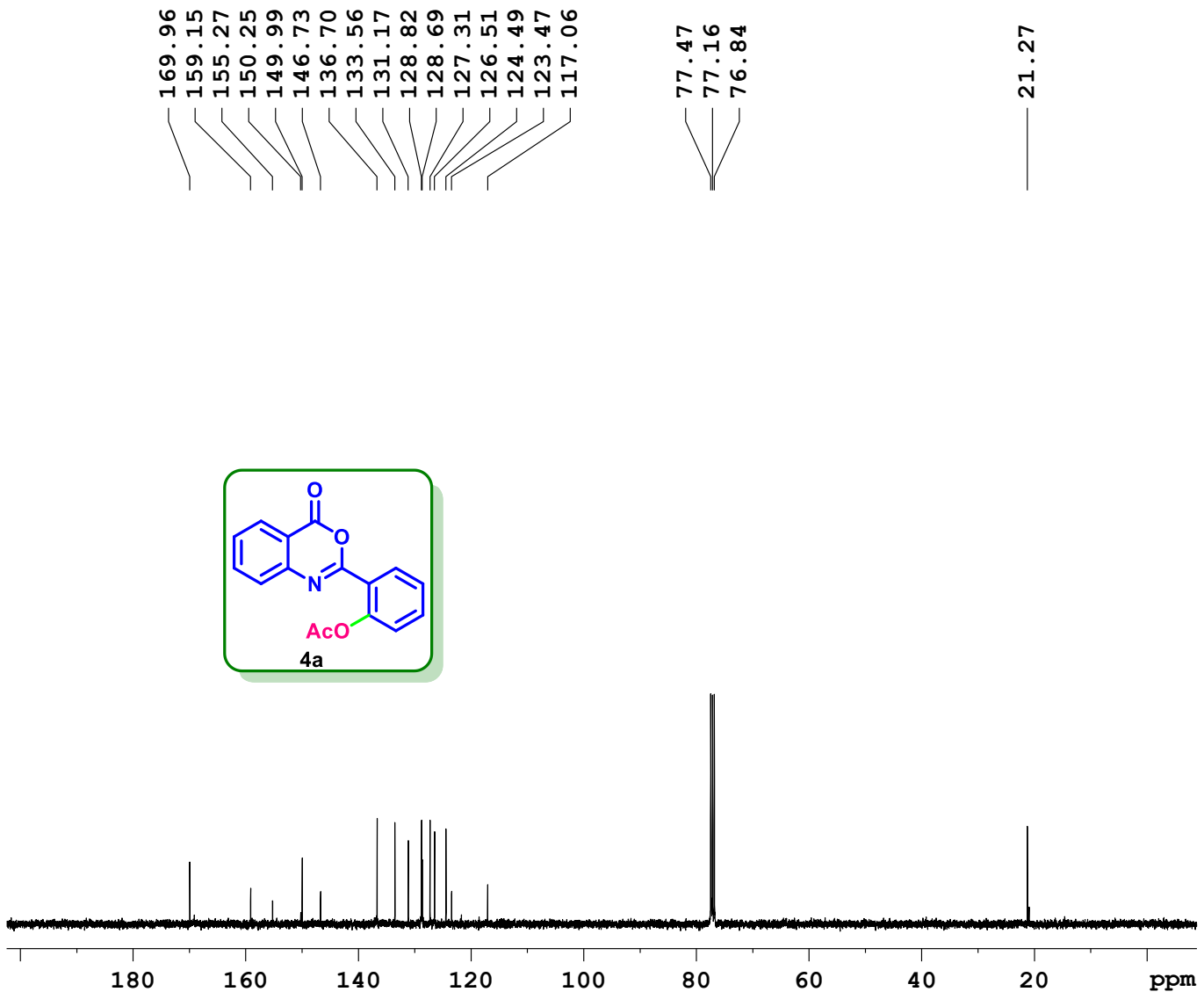


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DW                20.800 usec
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SFO2        400.1316005 MHz

F2 - Processing parameters
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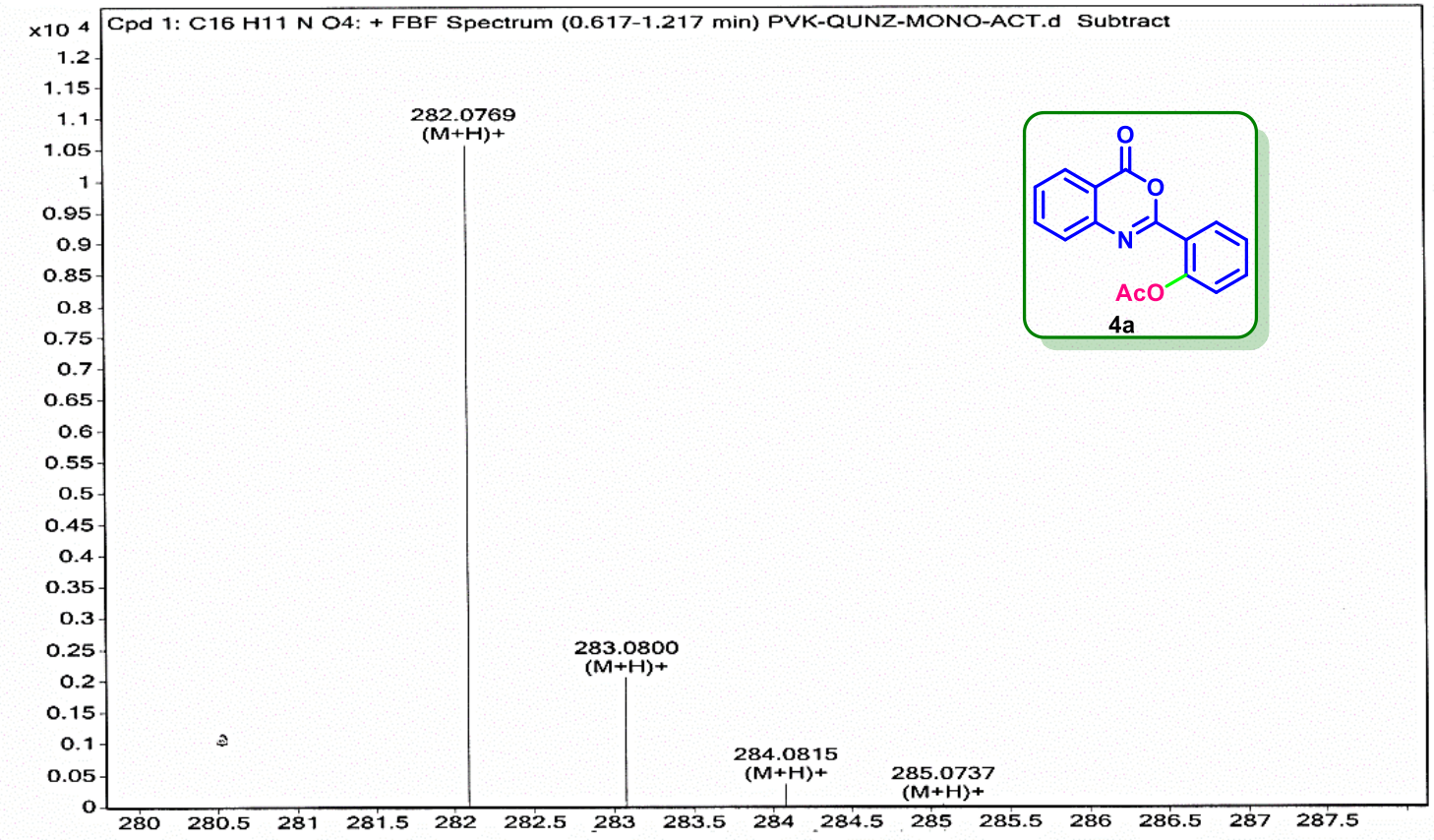

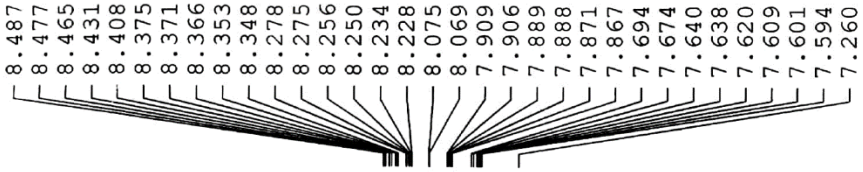

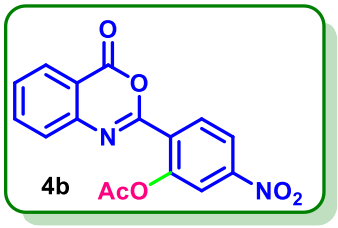


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FIDRES             0.125483 Hz
AQ                 3.9846387 sec
RG                      256
DW                   60.800 usec
DE                    6.00 usec
TE                   293.4 K
D1                1.00000000 sec
TD0                       1

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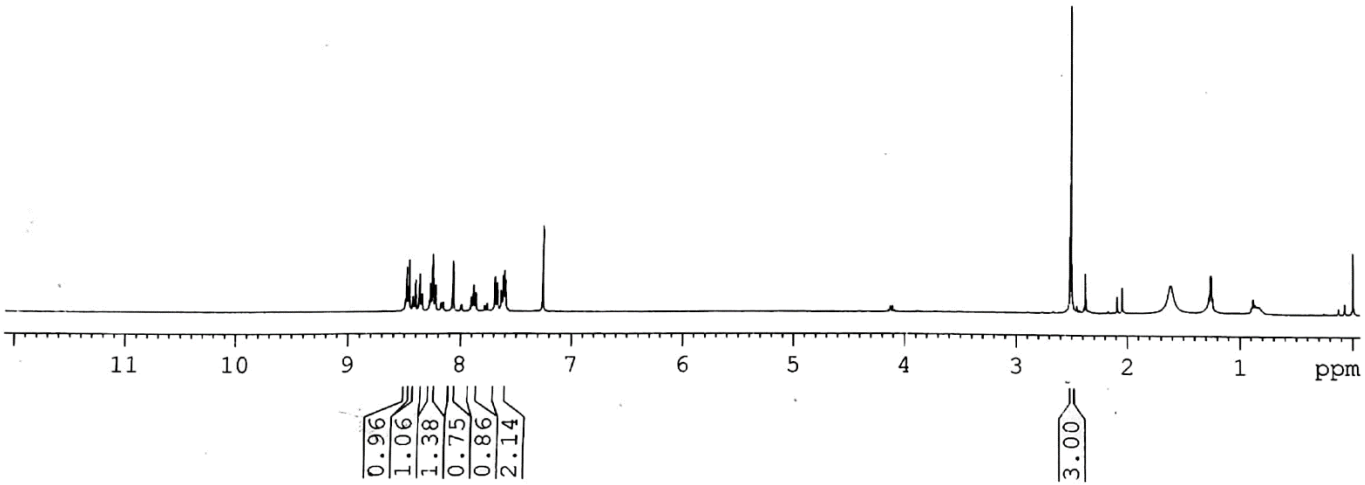
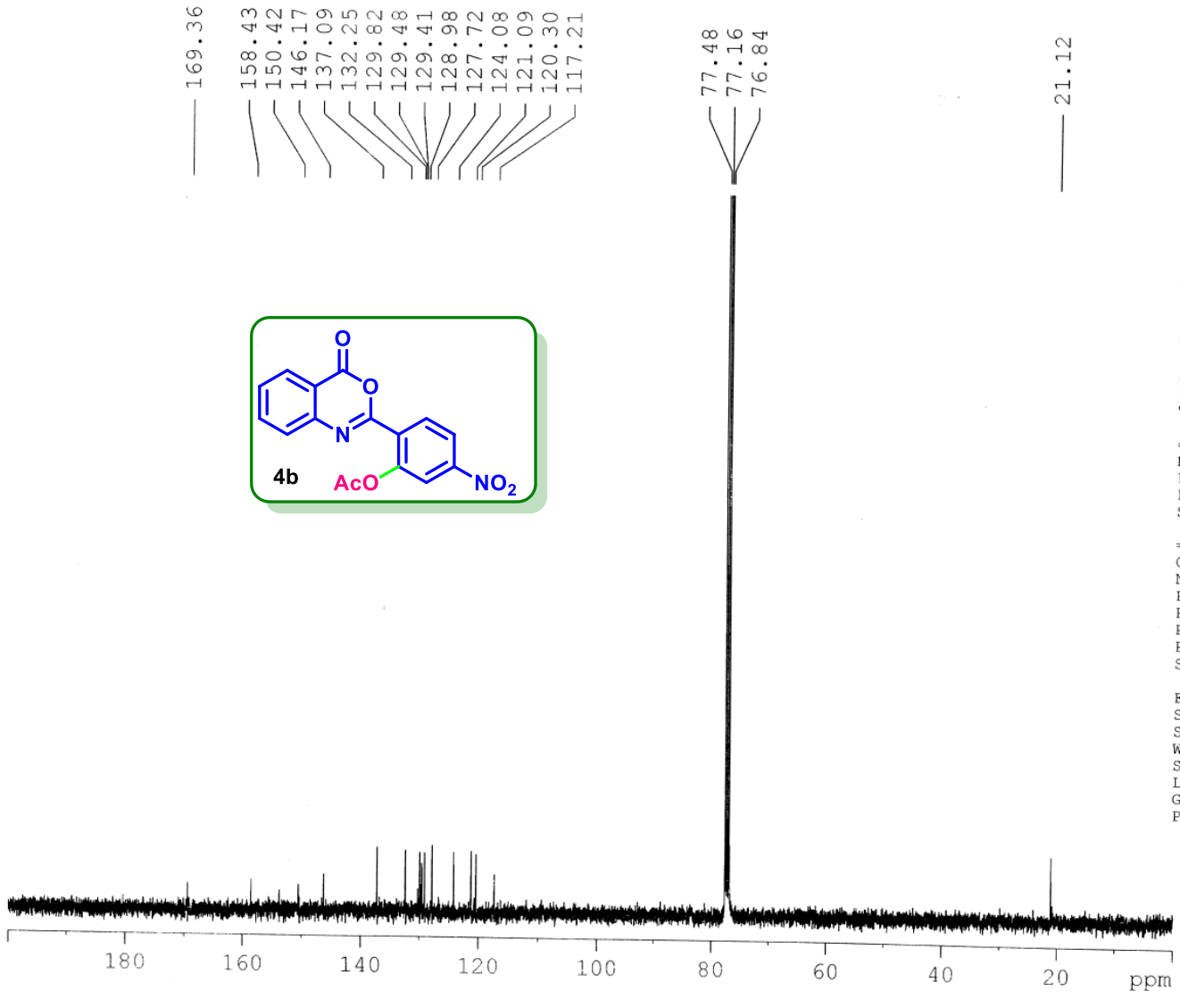


C13CPD CDCl3 {D:\MB} KOPAL 1



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DELTA 1.89999998 sec
TD0 1

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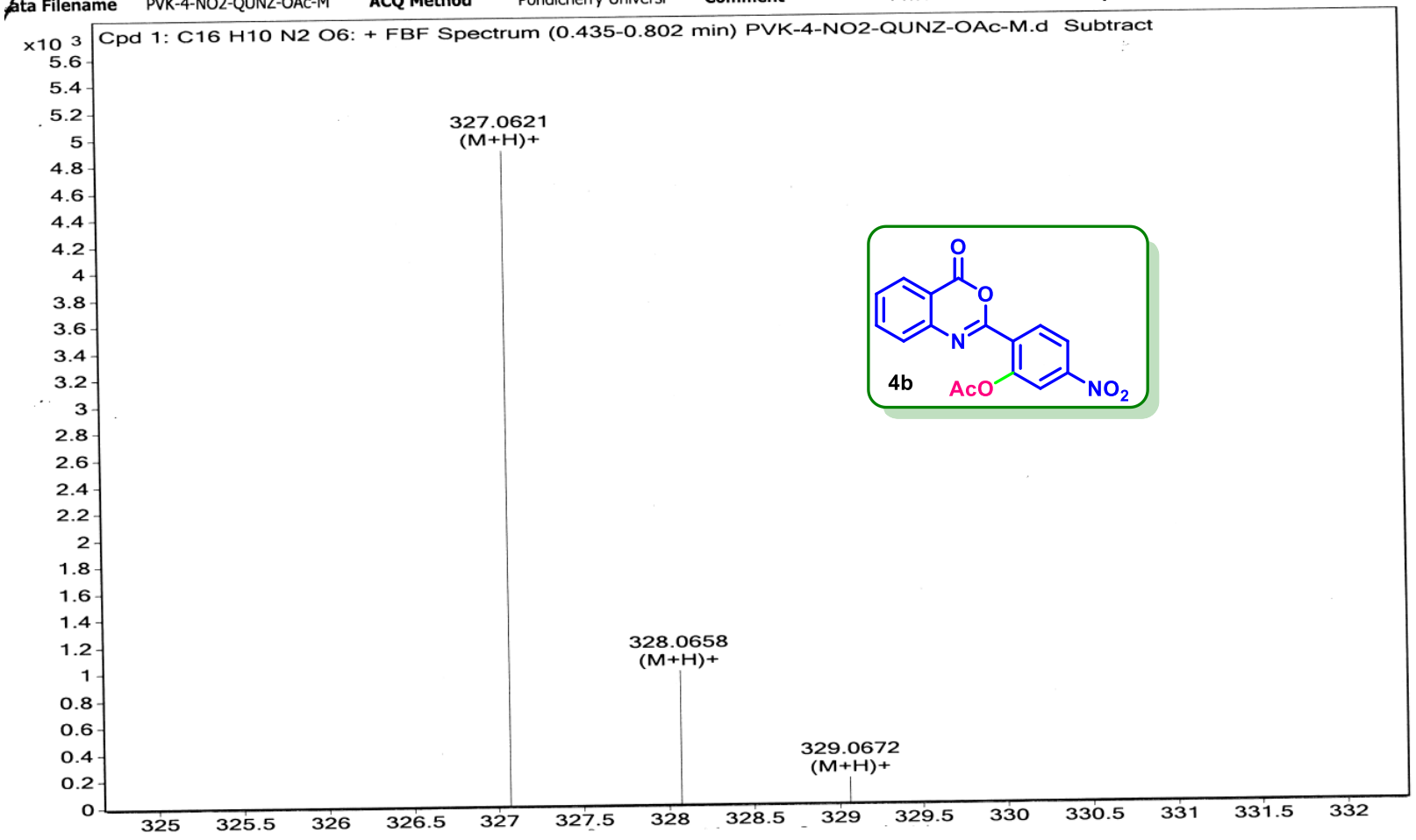
PL1 0.00 dB
SFO1 100.6228298 MHz

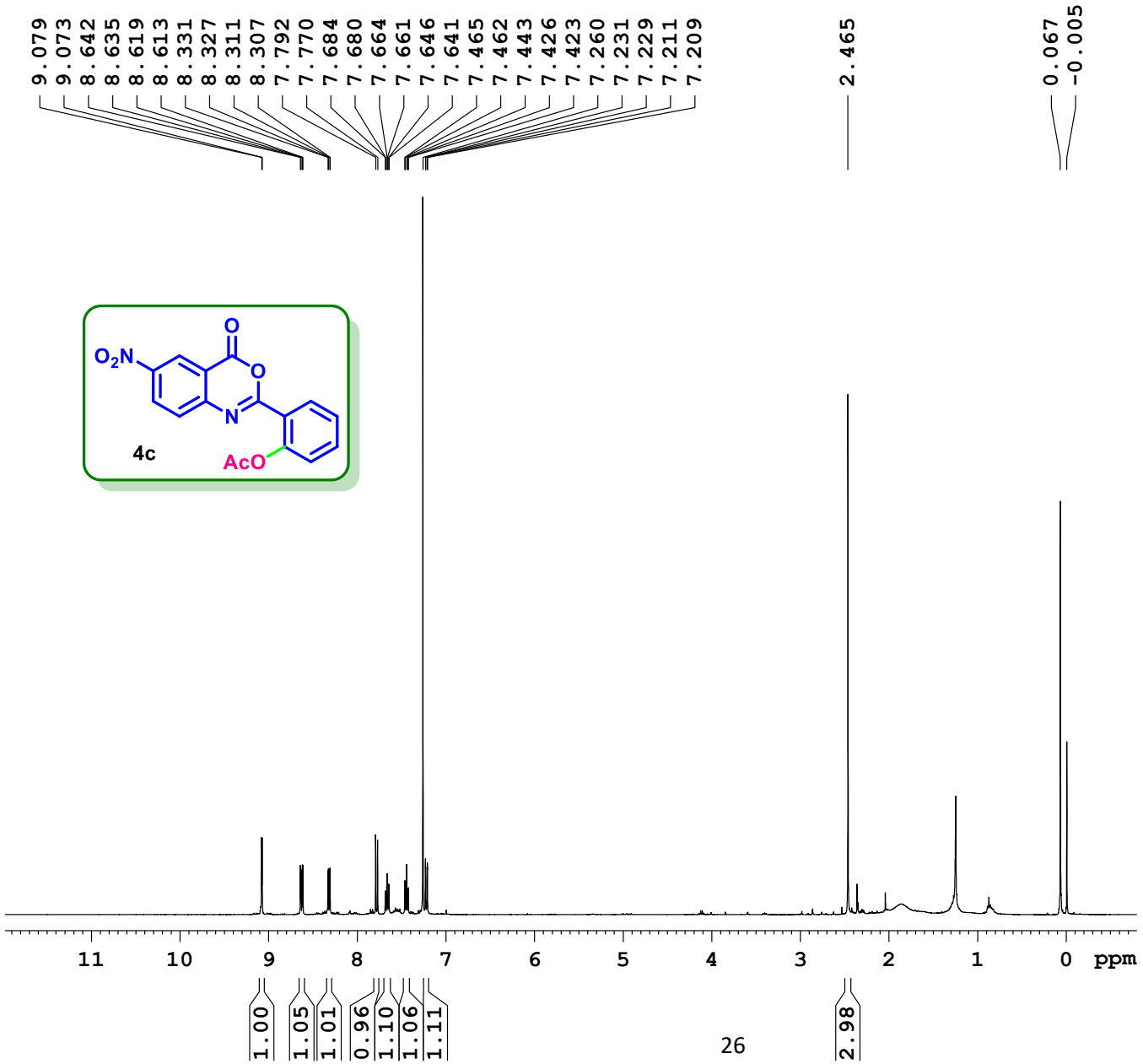
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL12 14.90 dB
PL13 14.90 dB
PL2 -3.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127546 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

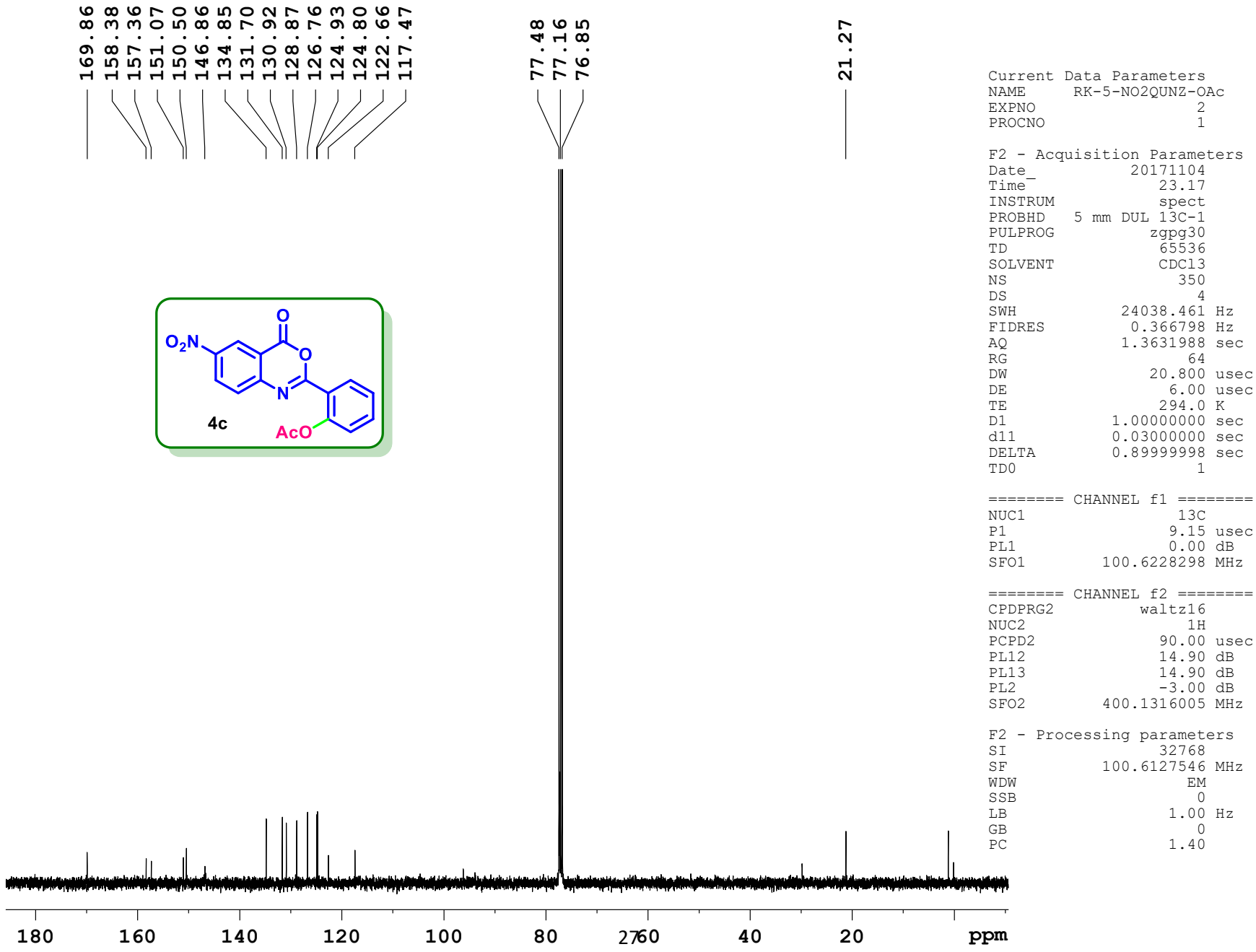
ple Name	PVK-4-NO2-QUNZ-OAc-M	Position		Instrument Name	Q-TOF	User Name	QTOF-PU\admin
Vol	-1	InjPosition		SampleType	Sample	IRM Calibration Status	Success
ata Filename	PVK-4-NO2-QUNZ-OAc-M	ACQ Method	Pondicherry Universi	Comment	PVK-MB-327.0627	Acquired Time	03-10-2017 11:42:13



PROTON CDCl3 D:MB KOPAL 1

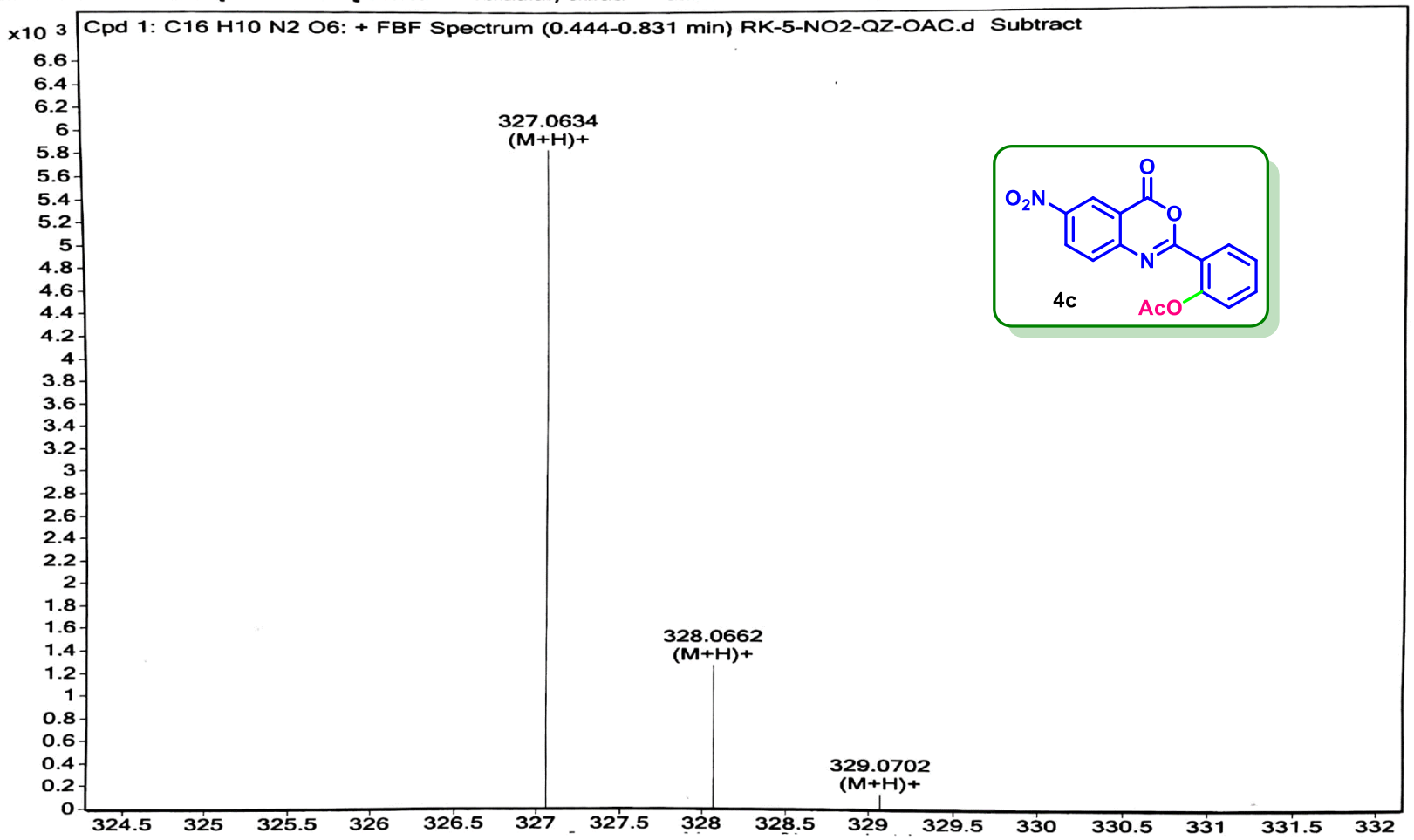


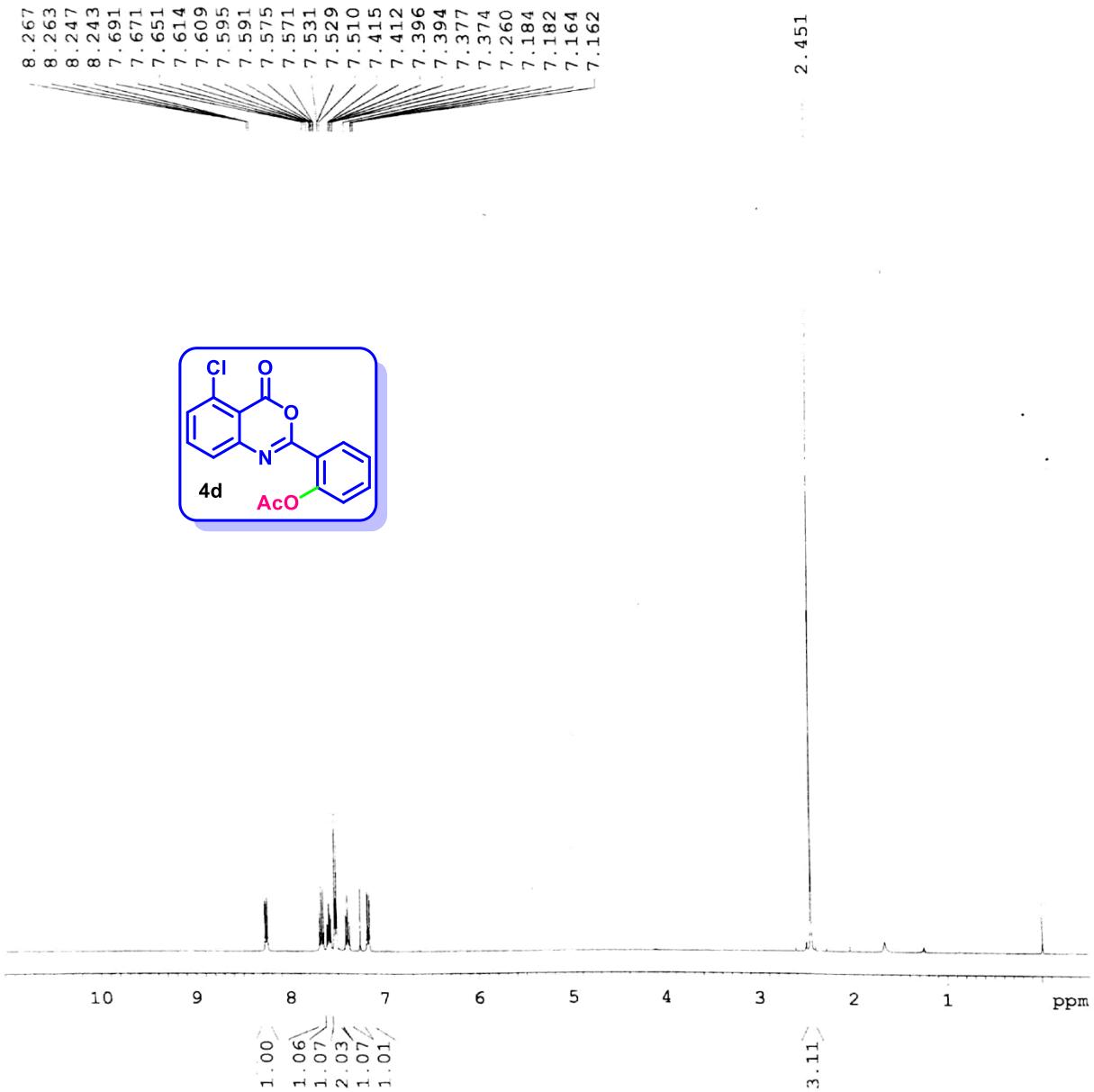

```
Current Data Parameters
NAME      RK-5-NO2QUNZ-OAc
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_             20171104
Time                 23.02
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                     181
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            400.1300054 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.00
```



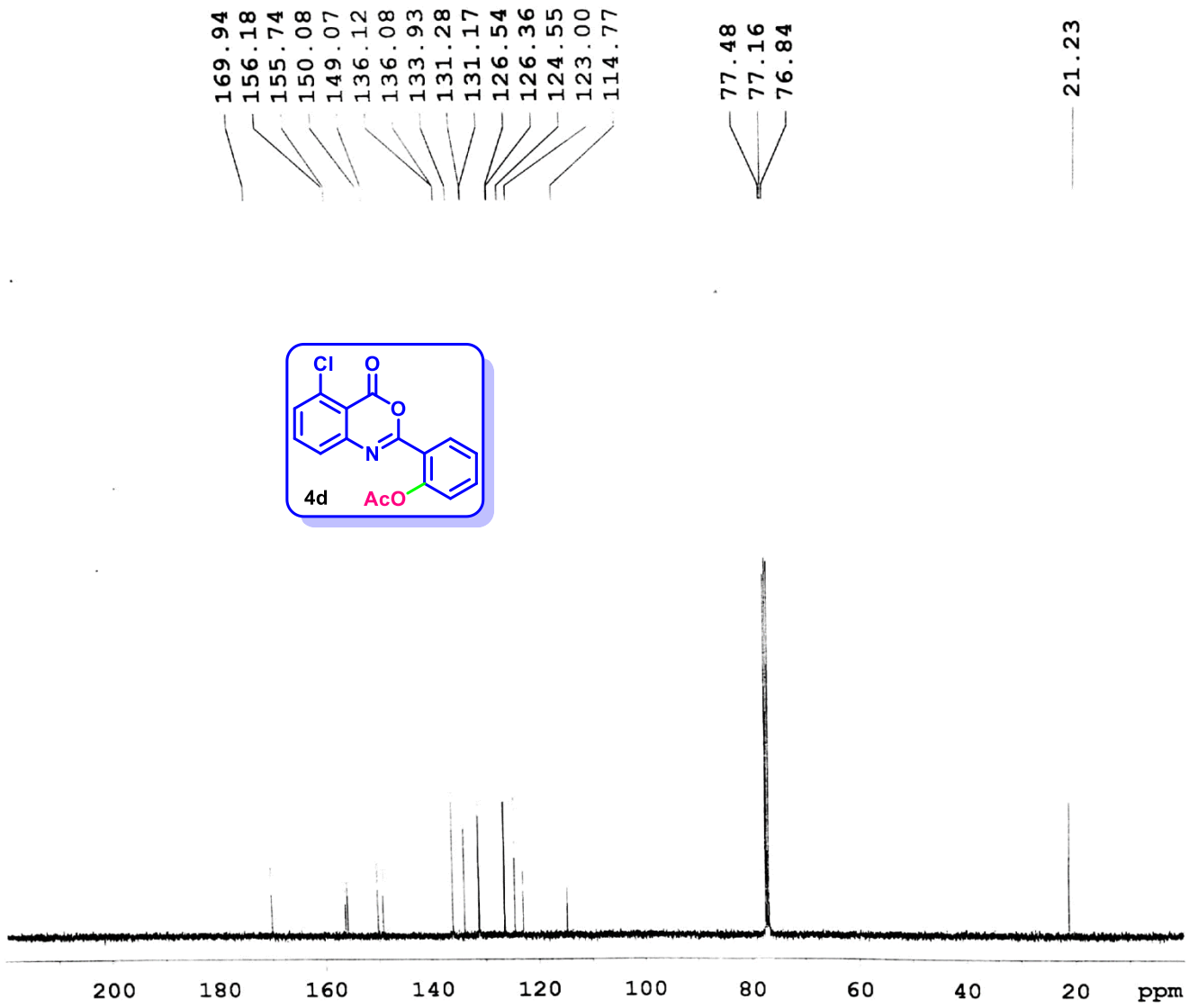

```
Current Data Parameters
NAME      RK-5-NO2QUNZ-OAc
EXPNO                    2
PROCNO                   1

F2 - Acquisition Parameters
Date_           20171104
Time              23.17
INSTRUM           spect
PROBHD   5 mm DUL 13C-1
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  350
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                294.0 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          100.6127546 MHz
WDW                 EM
SSB                  0
LB                1.00 Hz
GB                   0
PC                1.40
```

Sample Name	RK-5-NO2-QZ-OAC	**Position**		**Instrument Name**	Q-TOF	**User Name**	QTOF-PU\admin
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	RK-5-NO2-QZ-OAC.d	**ACQ Method**	Pondicherry Universi	**Comment**	RK-MB-326.0539	**Acquired Time**	03-05-2018 12:41:55



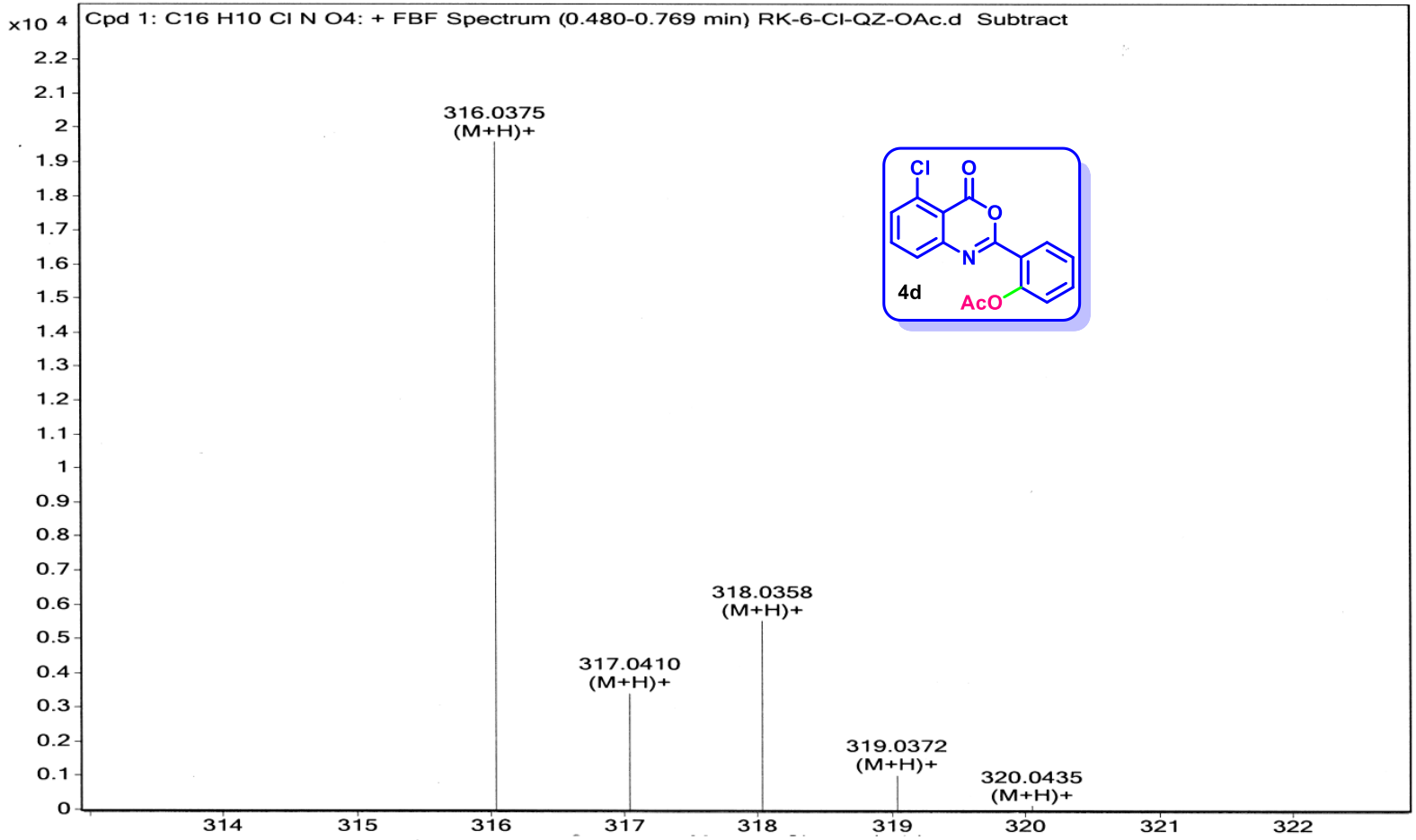


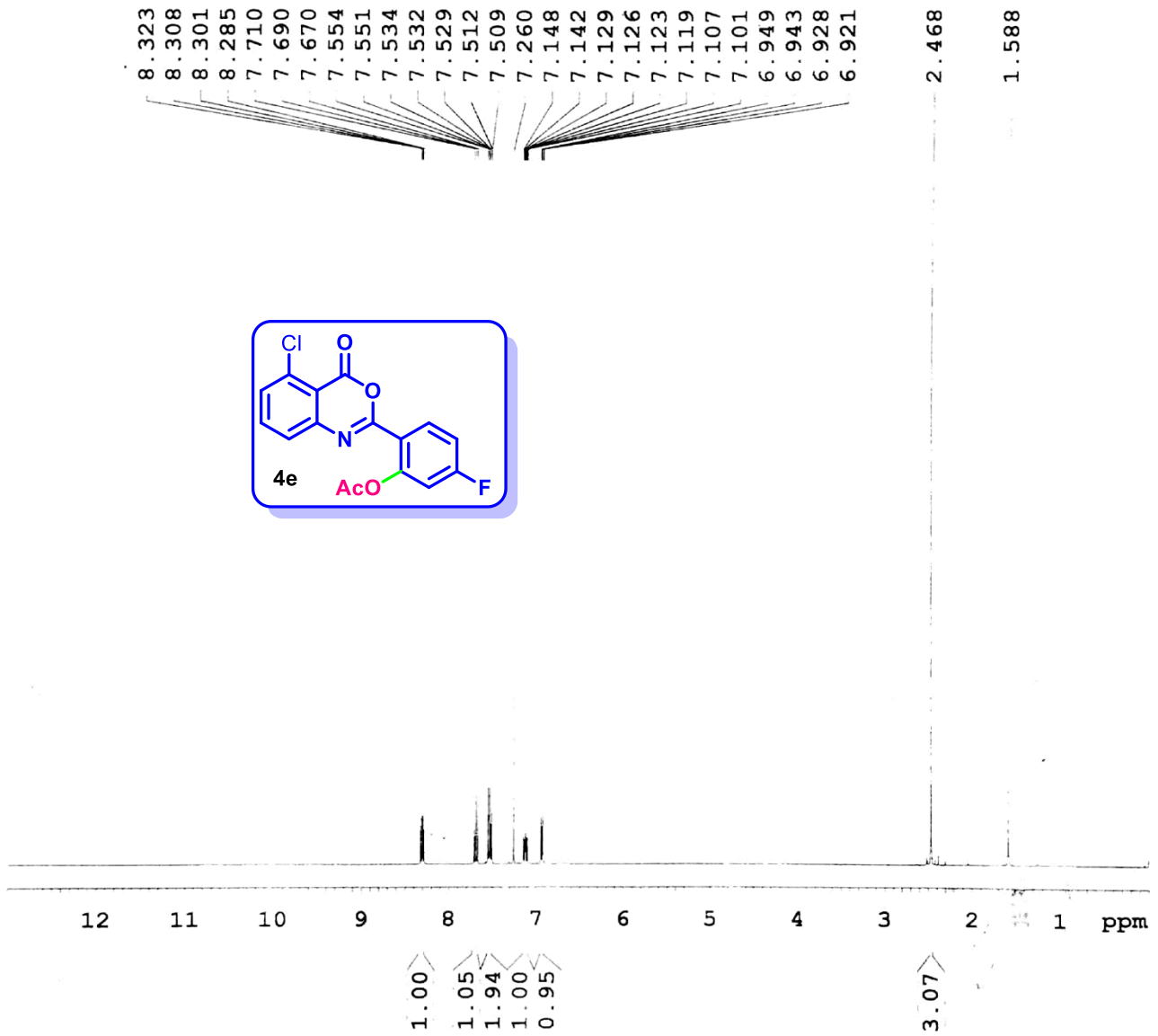

```
Current Data Parameters
NAME      RK-6-Cl-Qz-OAc
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20180921
Time               17.05
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                   181
DW                60.800 usec
DE                 6.00 usec
TE                290.9 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          400.1300048 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```



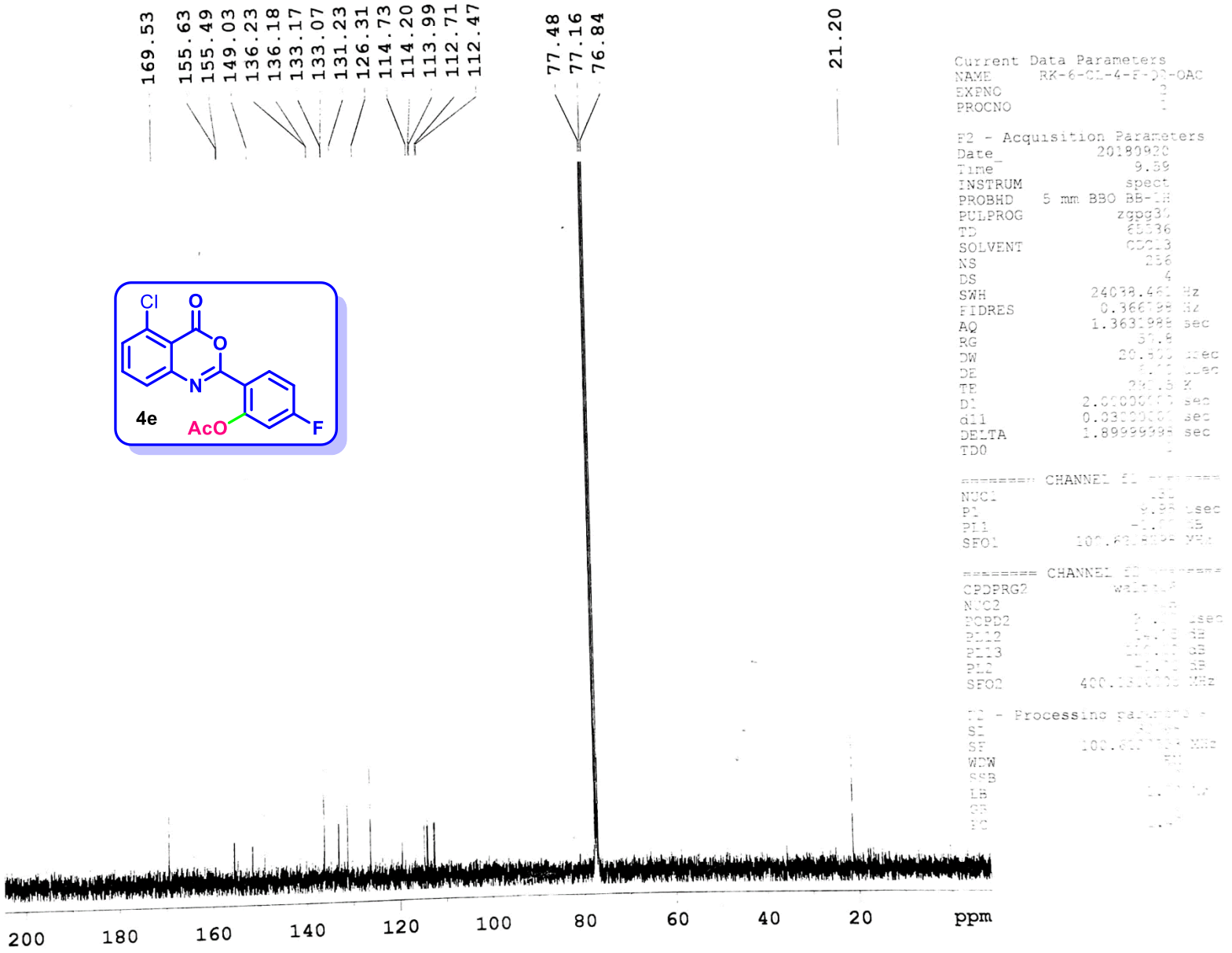

```
Current Data Parameters
NAME      RK-6-Cl-Qz-OAc
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20180922
Time              21.56
INSTRUM           spect
PROBHD   5 mm BBO BB-1H
PULPROG         zgpg30
TD                65536
SOLVENT           CDC13
NS                  229
DS                    4
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3631988 sec
RG                  456
DW               20.800 usec
DE                6.00 usec
TE               294.5 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          100.6127578 MHz
WDW                EM
SSB                 0
LB               1.00 Hz
GB                  0
PC               1.40
```

Sample Name	RK-6-Cl-QZ-OAc	**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-OAc.d	**ACQ Method**	Pondicherry Universi	**Comment**	RK-MB-315.0298	**Acquired Time**	10-10-2018 13:02:24






```
Current Data Parameters
NAME      RK-6-CL-4-F-Q2-OAC
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_              20180920
Time                   9.43
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                  292.0 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-6-Cl-4-F-OAc
EXPNO 2
PROCNO 1

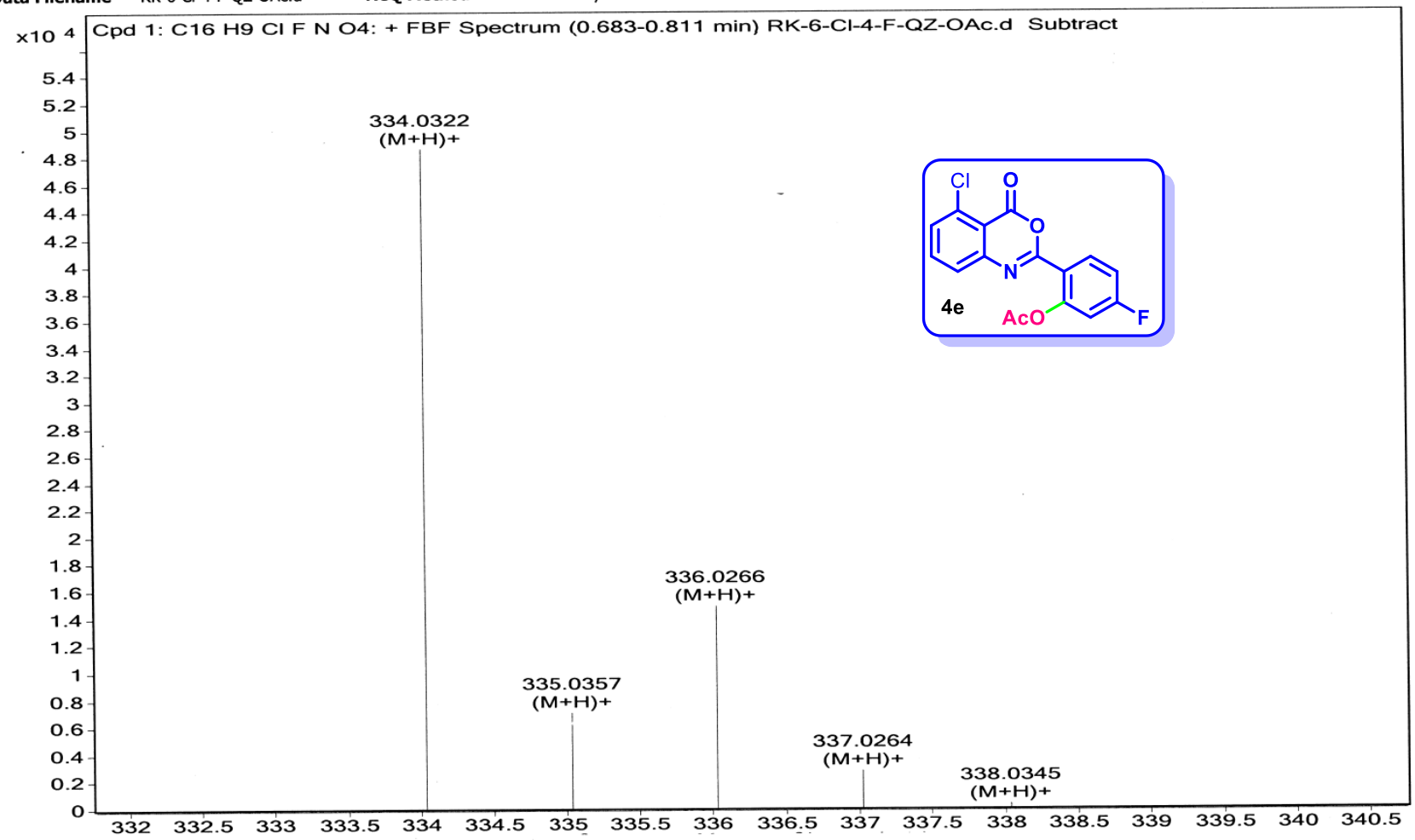
F2 - Acquisition Parameters
Date_ 20180920
Time 9.59
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 256
DS 4
SWH 24038.461 Hz
FIDRES 0.366799 Hz
AQ 1.3631988 sec
RG 36.8
DW 20.800 usec
DE 6.00 usec
TE 296.5 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

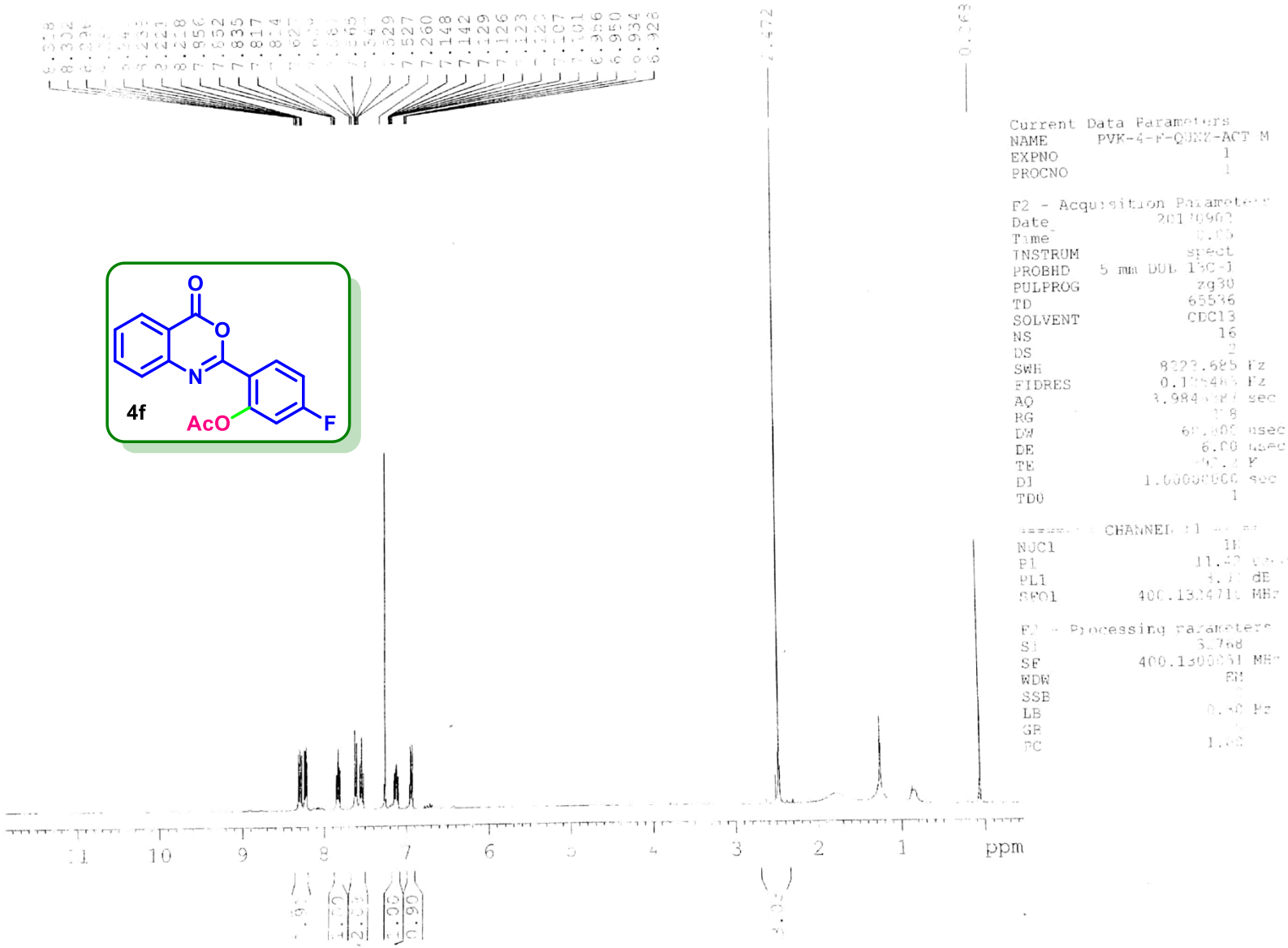
======== CHANNEL f1 ========
NUC1 13C
P1 9.95 usec
PL1 -1.00 dB
SFO1 100.6314892 MHz

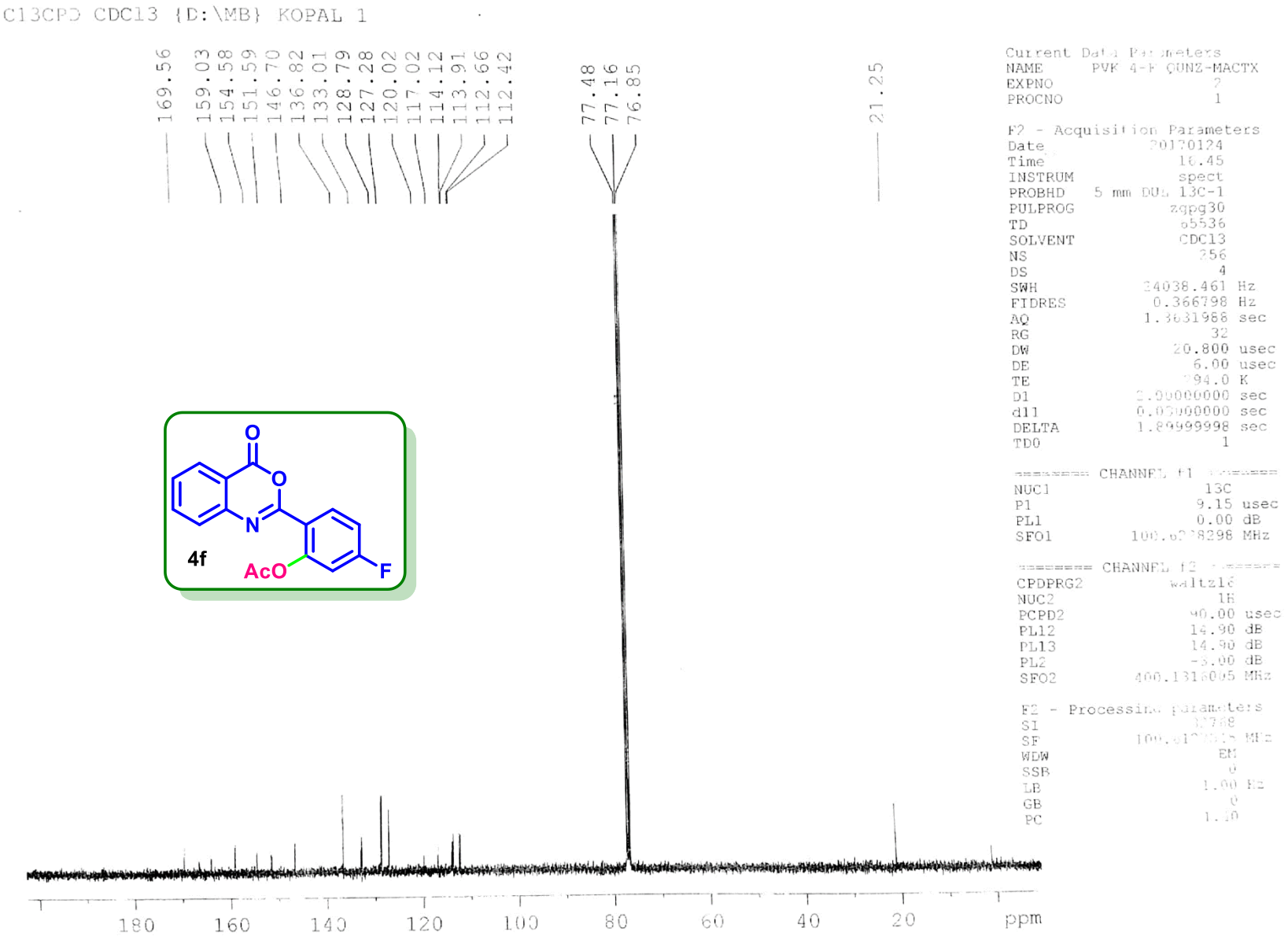
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 9.70 usec
PL12 15.18 dB
PL13 22.41 dB
PL2 -1.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127754 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

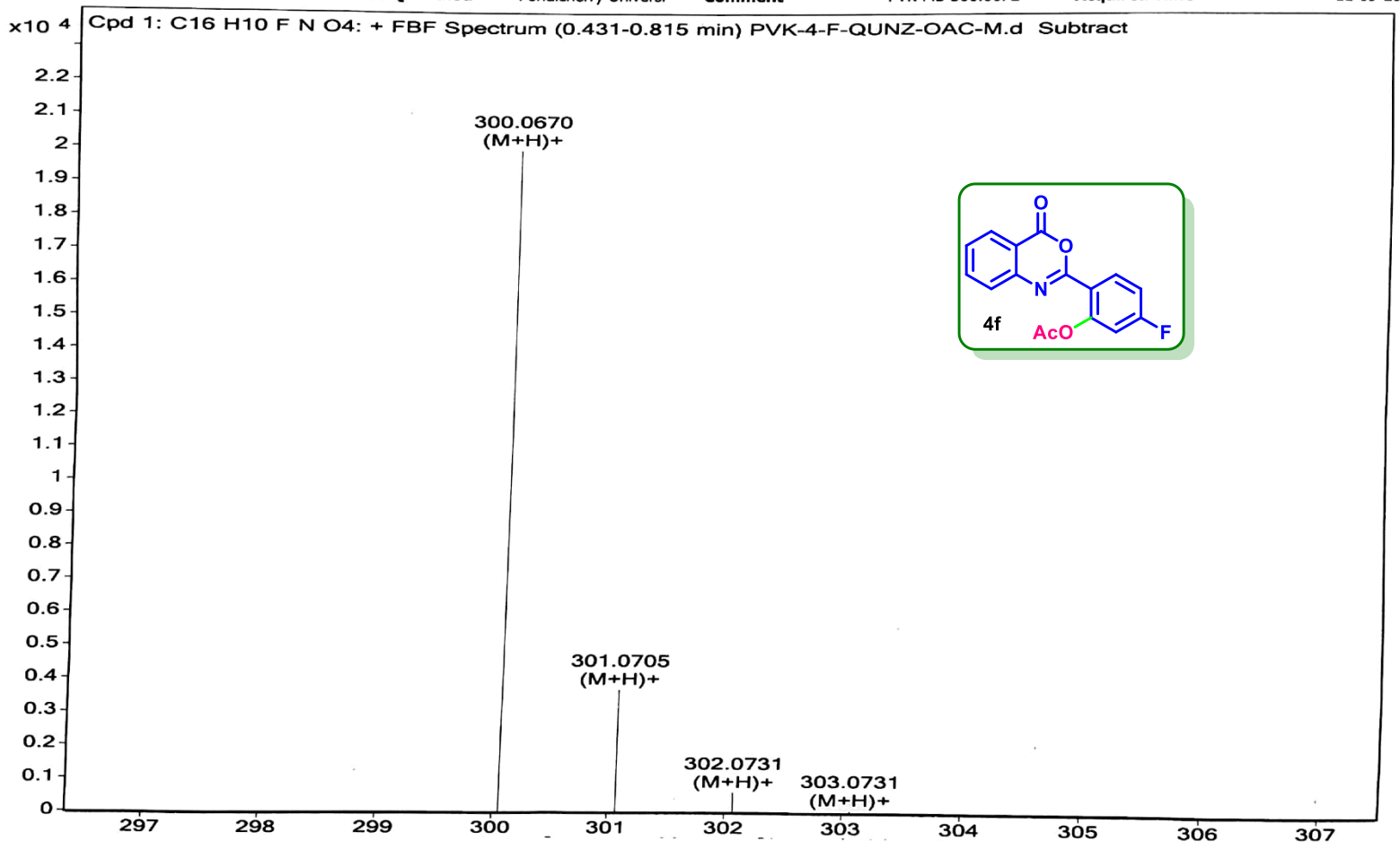
Sample Name	RK-6-Cl-4-F-QZ-OAc	**Position**		**Instrument Name**	Q-TOF	**User Name**	QTOF-PU\admin
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	RK-6-Cl-4-F-QZ-OAc.d	**ACQ Method**	Pondicherry Universi	**Comment**	RK-MB-333.0204	**Acquired Time**	20-09-2018 12:35:54



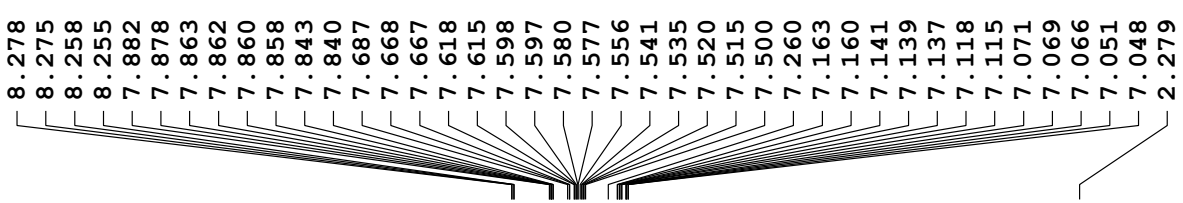

8.318
8.332
8.344
7.652
7.835
7.817
7.814
7.148
7.142
7.129
7.126
6.956
6.950
6.934
6.928
2.472
0.263
4f
AcO
F
O
O
N
11
10
9
8
7
6
5
4
3
2
1
ppm
Current Data Parameters
NAME PVK-4-F-QUNZ-ACT M
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date 20110902
Time 8.05
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125465 Hz
AQ 3.9845287 sec
RG 228
DW 60.800 usec
DE 6.00 usec
TE 302.2 K
D1 1.00000000 sec
TD0 1
CHANNEL f1
NUC1 1H
P1 11.40 usec
PL1 3.71 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

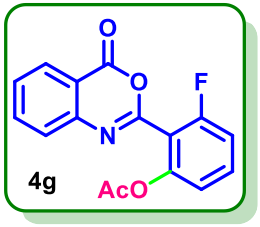

C13CPD CDCl3 (D:\MB) KOPAL 1
169.56
159.03
154.58
151.59
146.70
136.82
133.01
128.79
127.28
120.02
117.02
114.12
113.91
112.66
112.42
77.48
77.16
76.85
21.25
4f
AcO
F
O
O
N
180
160
140
120
100
80
60
40
20
ppm
Current Data Parameters
NAME PVK 4-F QUNZ-MACTX
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date 20170124
Time 16.45
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 256
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 100.6238298 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 100.6127625 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Sample Name	PVK-4-F-QUNZ-OAC-M	**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-OAC-M.d	**ACQ Method**	Pondicherry Universi	**Comment**	PVK-MB-300.0672	**Acquired Time**	11-09-2017 12:23:26

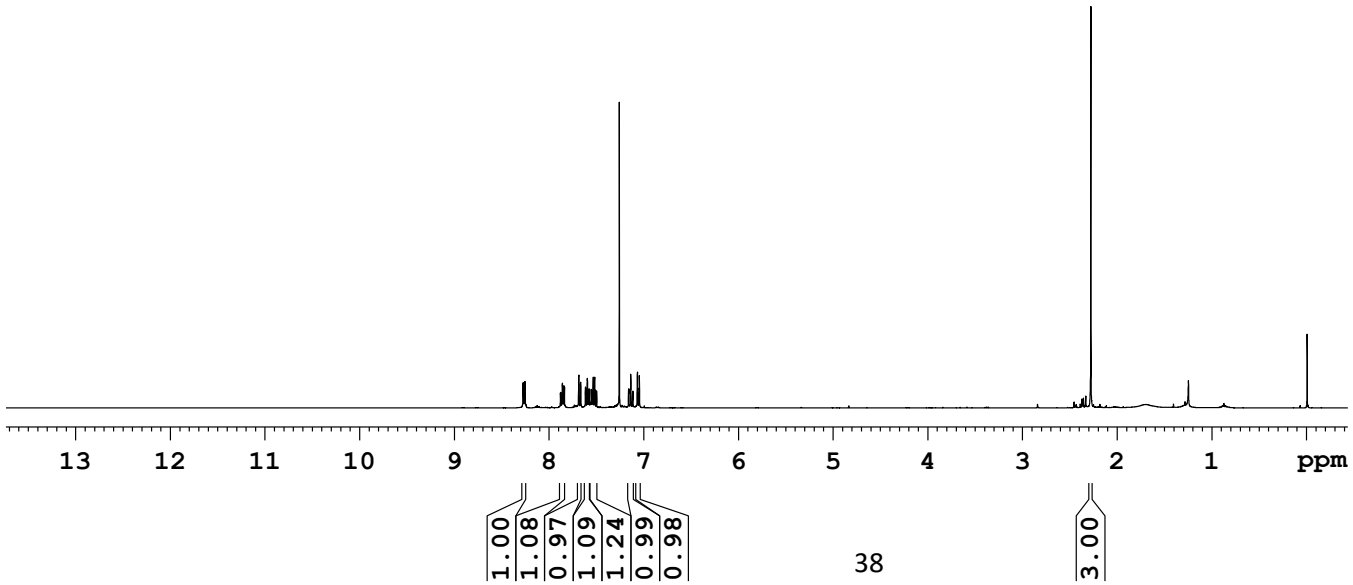


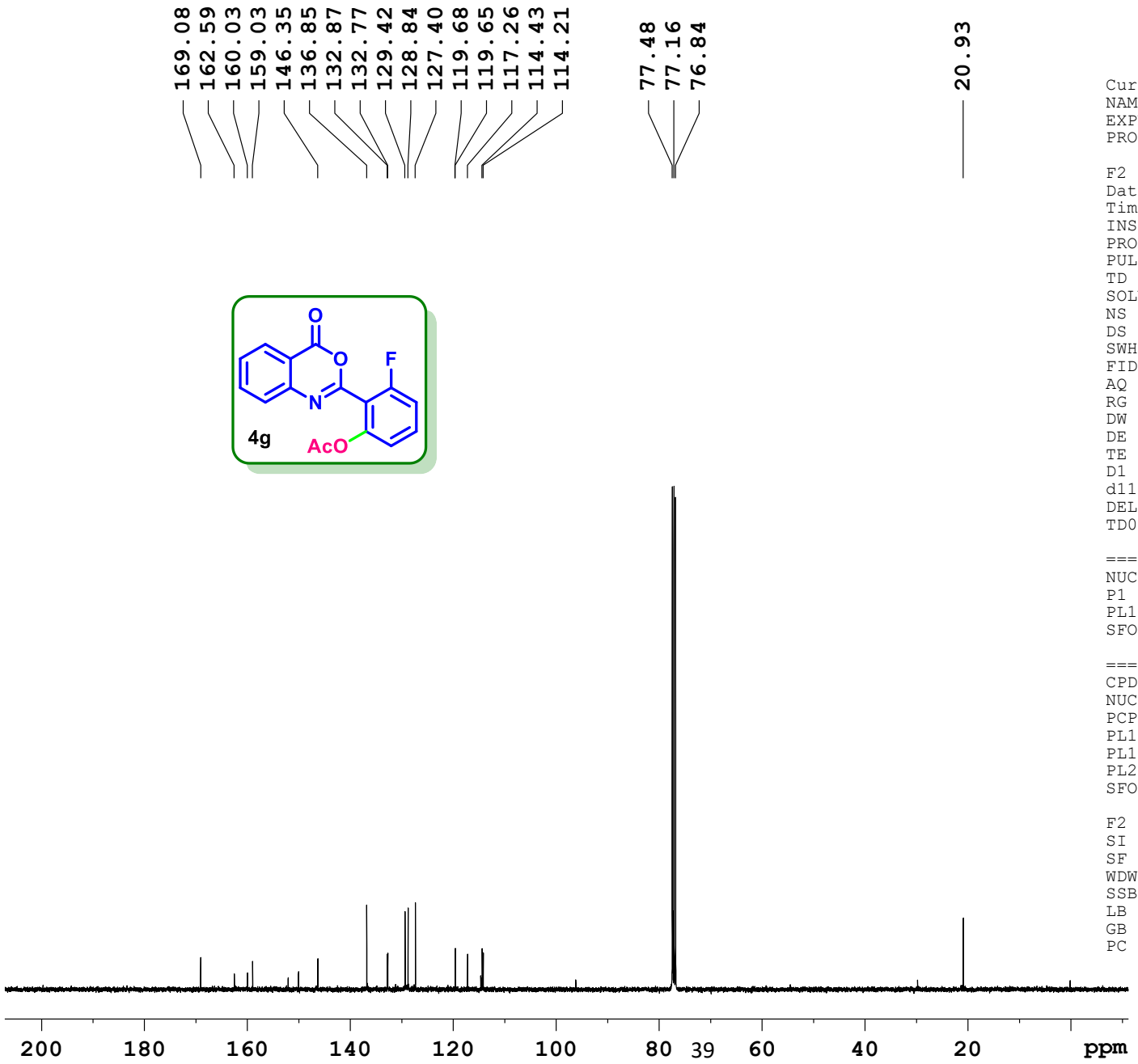
PROTON CDCl3 {D:\MB} KOPAL 1





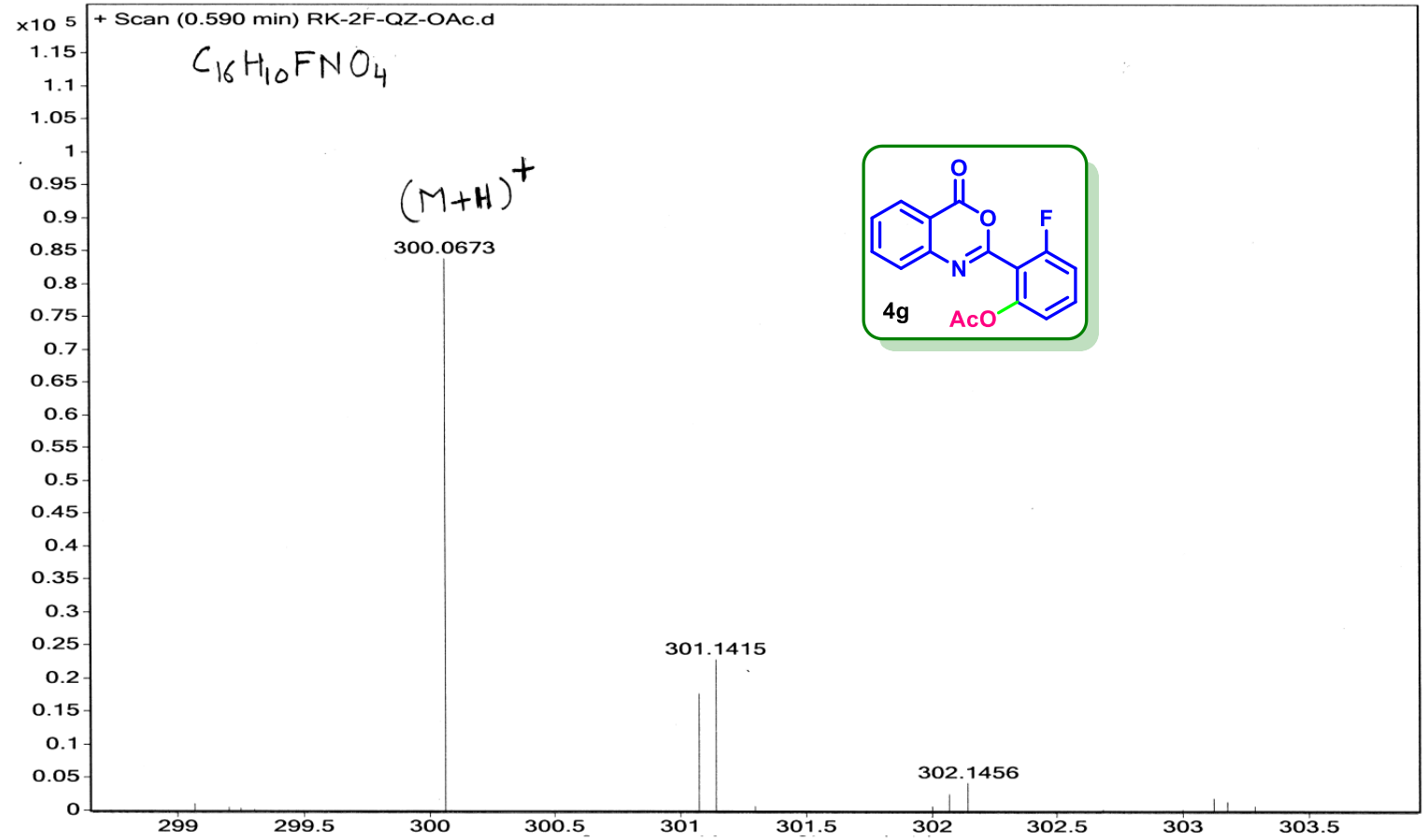

```
Current Data Parameters
NAME      RK-2-F-QUNZ-OAc
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_            20171101
Time                17.17
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                 293.2 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           400.1300051 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   1.00
```

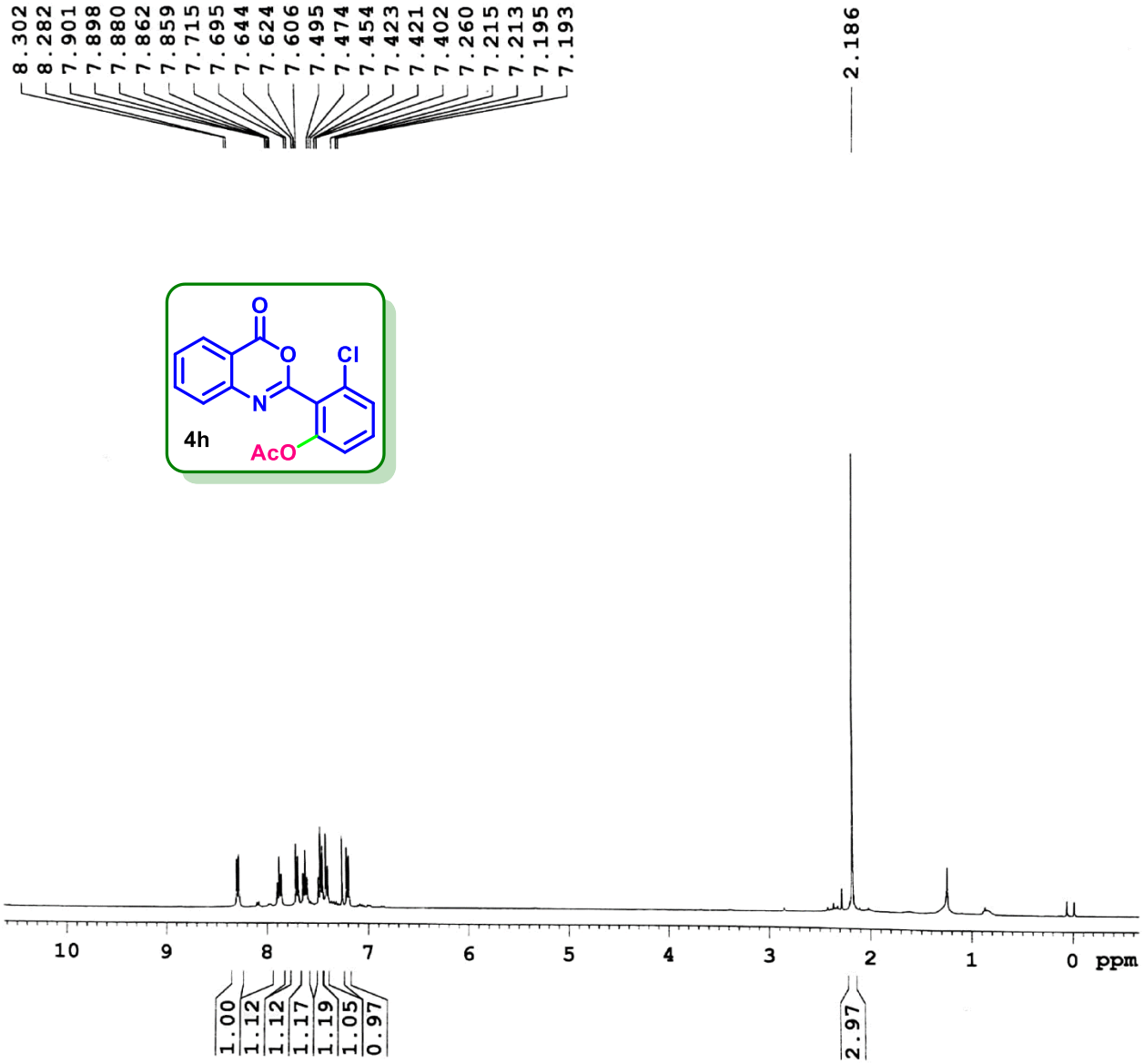




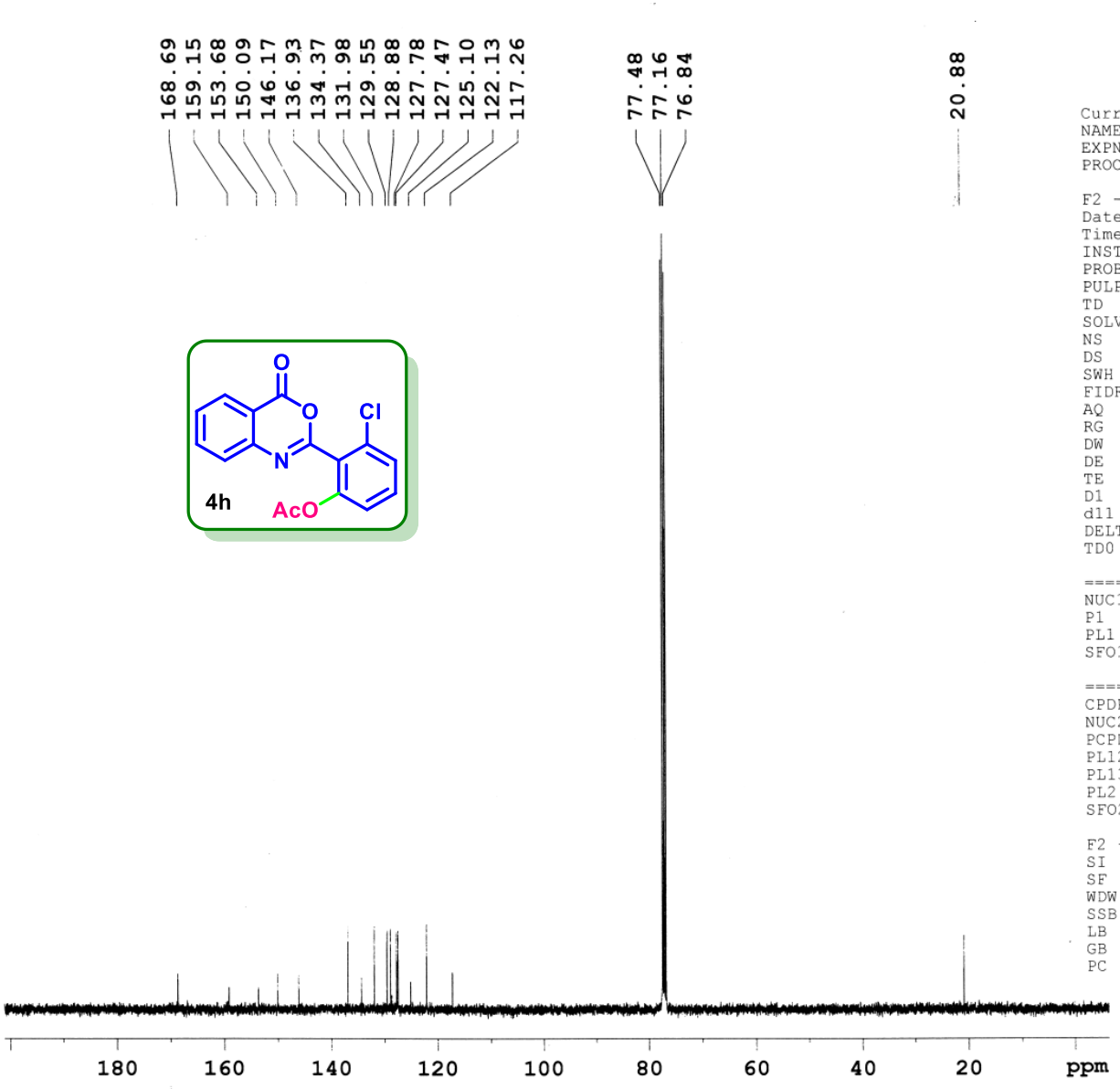

```
Current Data Parameters
NAME      RK-2-F-QUNZ-OAc
EXPNO                   2
PROCNO                  1

F2 - Acquisition Parameters
Date_           20171101
Time              18.00
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                293.9 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          100.6127553 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

Sample Name	RK-2F-QZ-OAc	**Position**		**Instrument Name**	Q-TOF	**User Name**	QTOF-PU\admin
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	RK-2F-QZ-OAc.d	**ACQ Method**	Pondicherry Universi	**Comment**	RK-MB-300.0667	**Acquired Time**	20-04-2018 14:54:29



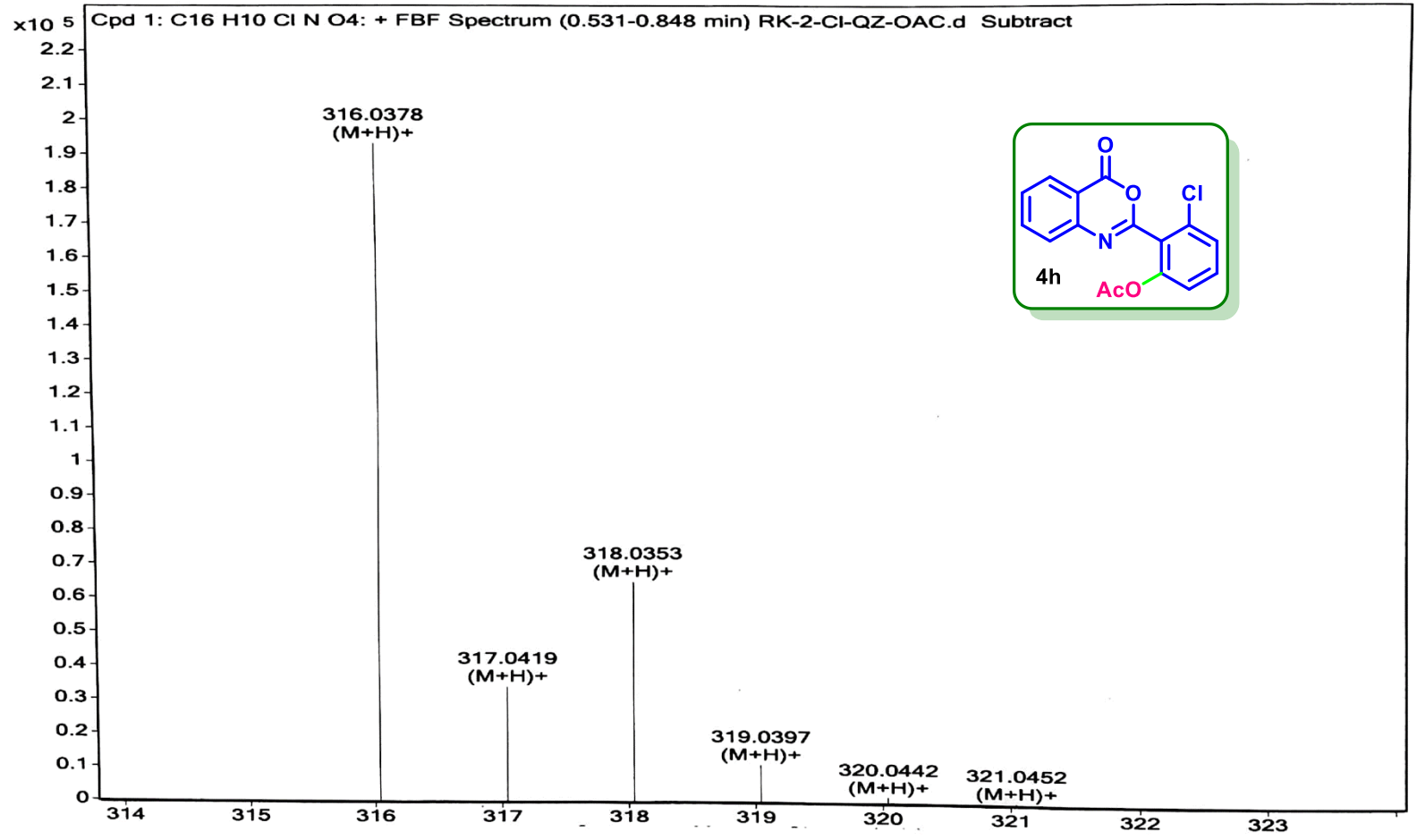



```
Current Data Parameters
NAME      RK-2-Cl-QZ-OAC
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20171223
Time               16.50
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           400.1300054 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```




```
Current Data Parameters
NAME      RK-2-Cl-QZ-OAC
EXPNO                  3
PROCNO                 1

F2 - Acquisition Parameters
Date_           20171223
Time              17.12
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                50.8
DW               20.800 usec
DE                6.00 usec
TE               293.6 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          100.6127553 MHz
WDW                EM
SSB                 0
LB                1.00 Hz
GB                  0
PC                1.40
```

ample Name	RK-2-Cl-QZ-OAC	**Position**		**Instrument Name**	Q-TOF	**User Name**	QTOF-PU\admin
ıj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
ata Filename	RK-2-Cl-QZ-OAC.d	**ACQ Method**	Pondicherry Universi	**Comment**	RK-MB-315.0298	**Acquired Time**	26-04-2018 13:42:38



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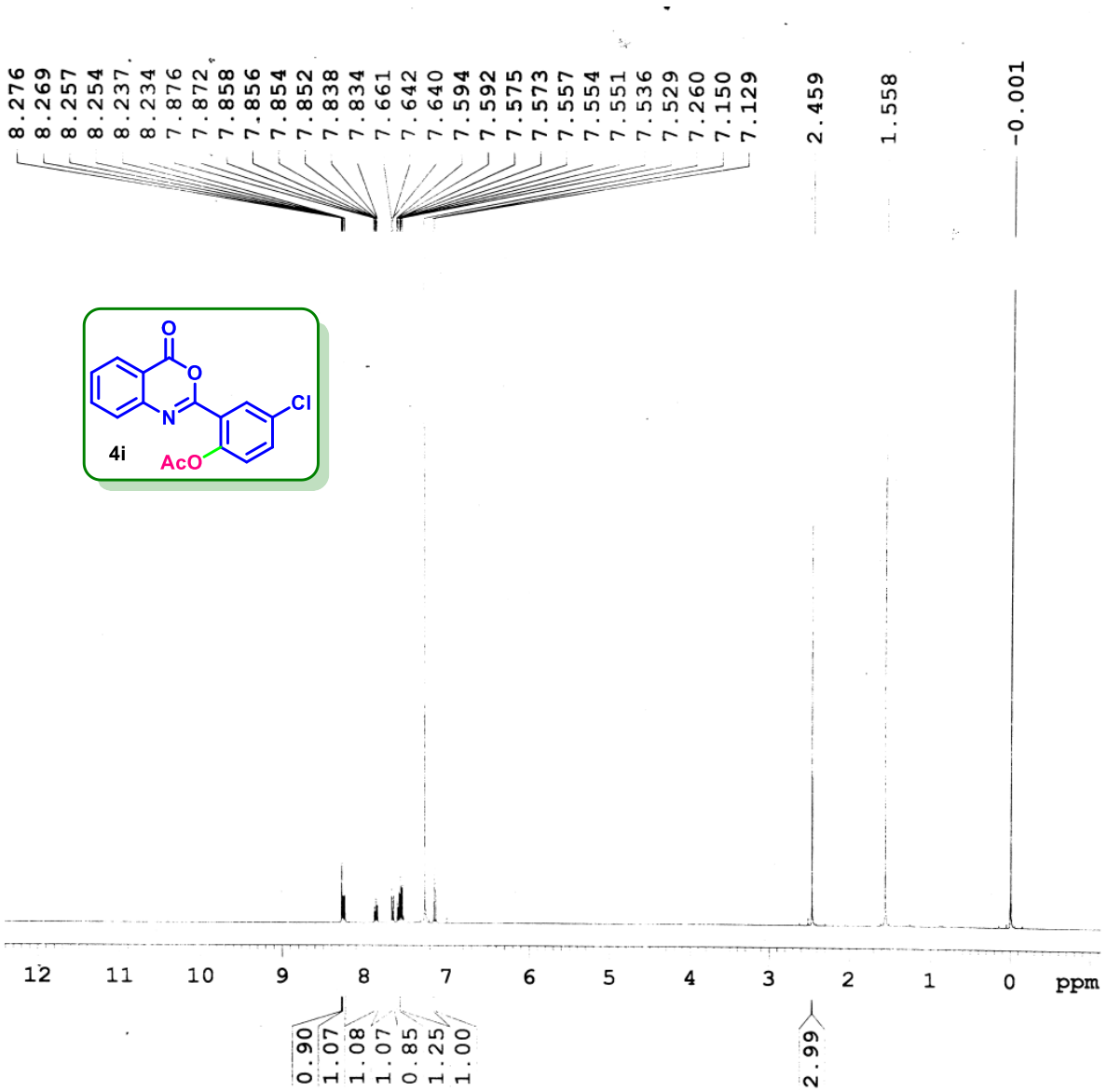
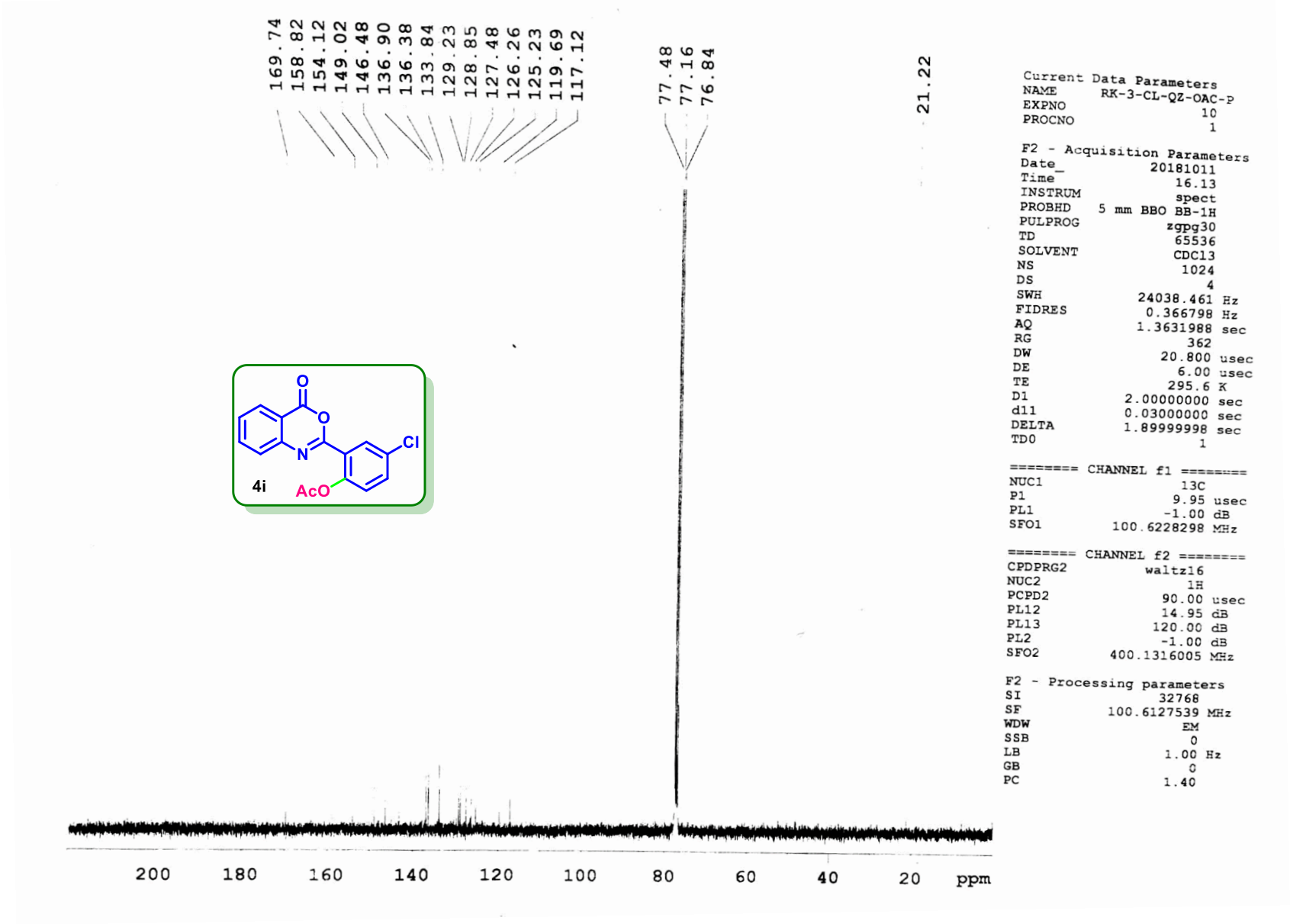
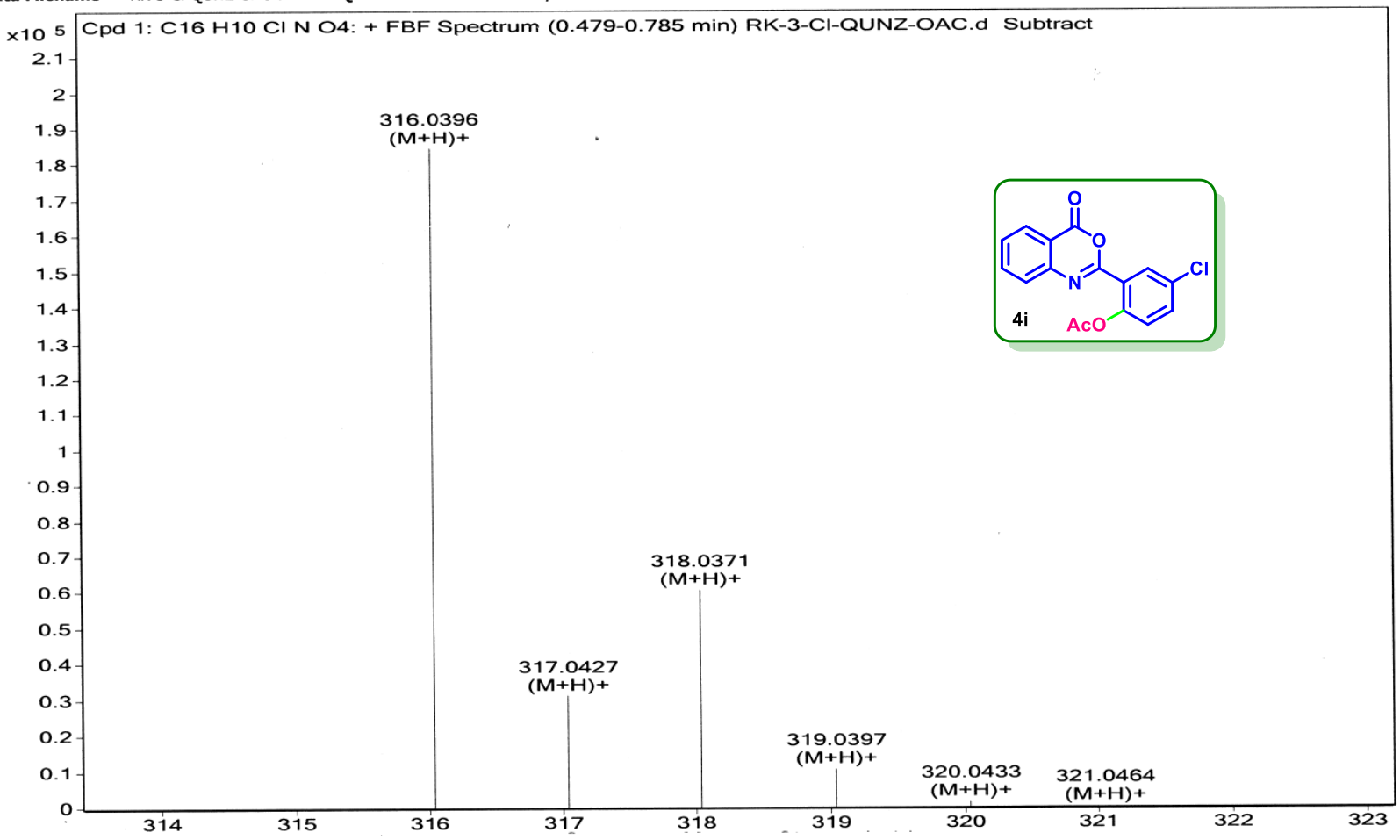
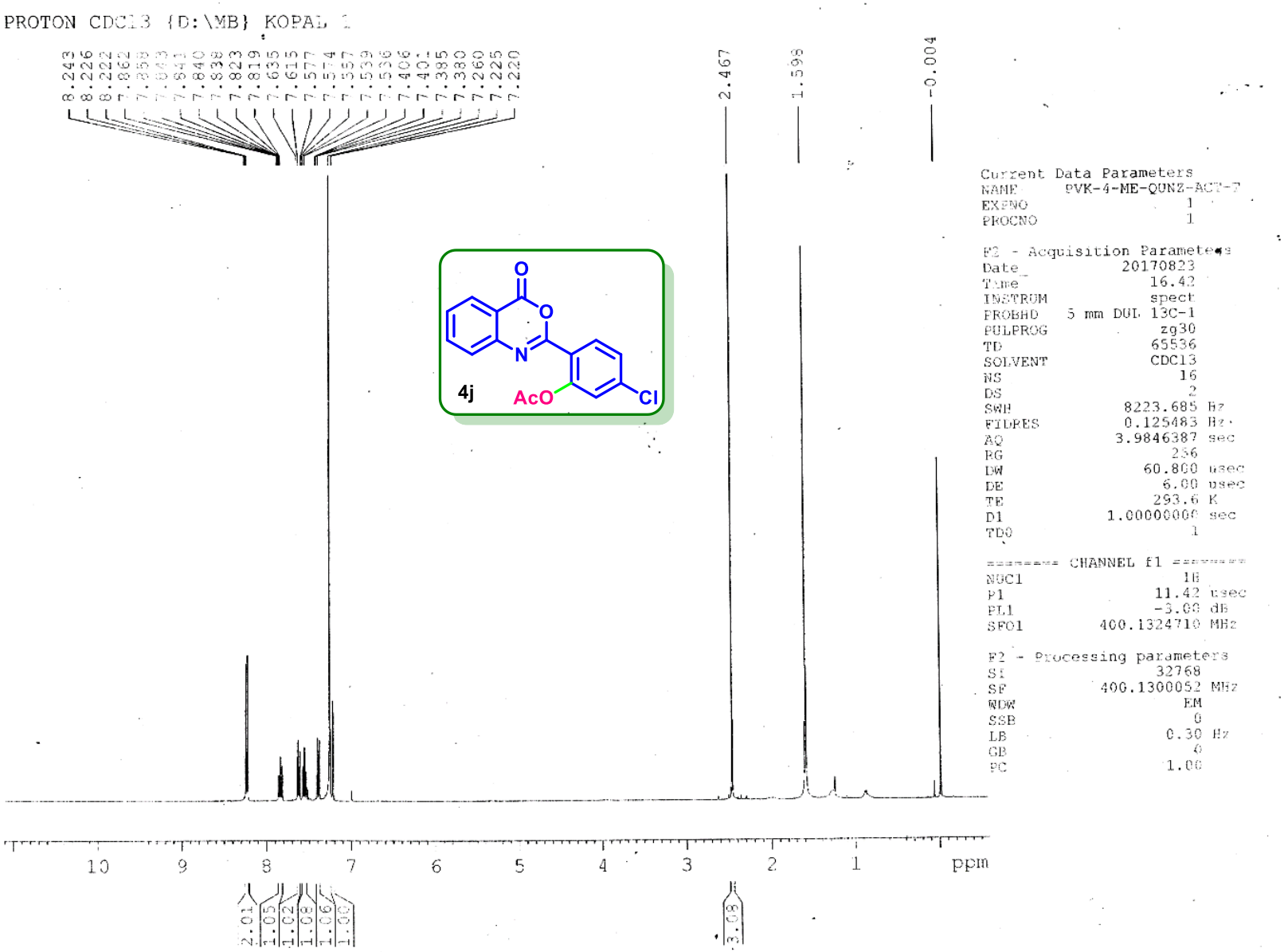


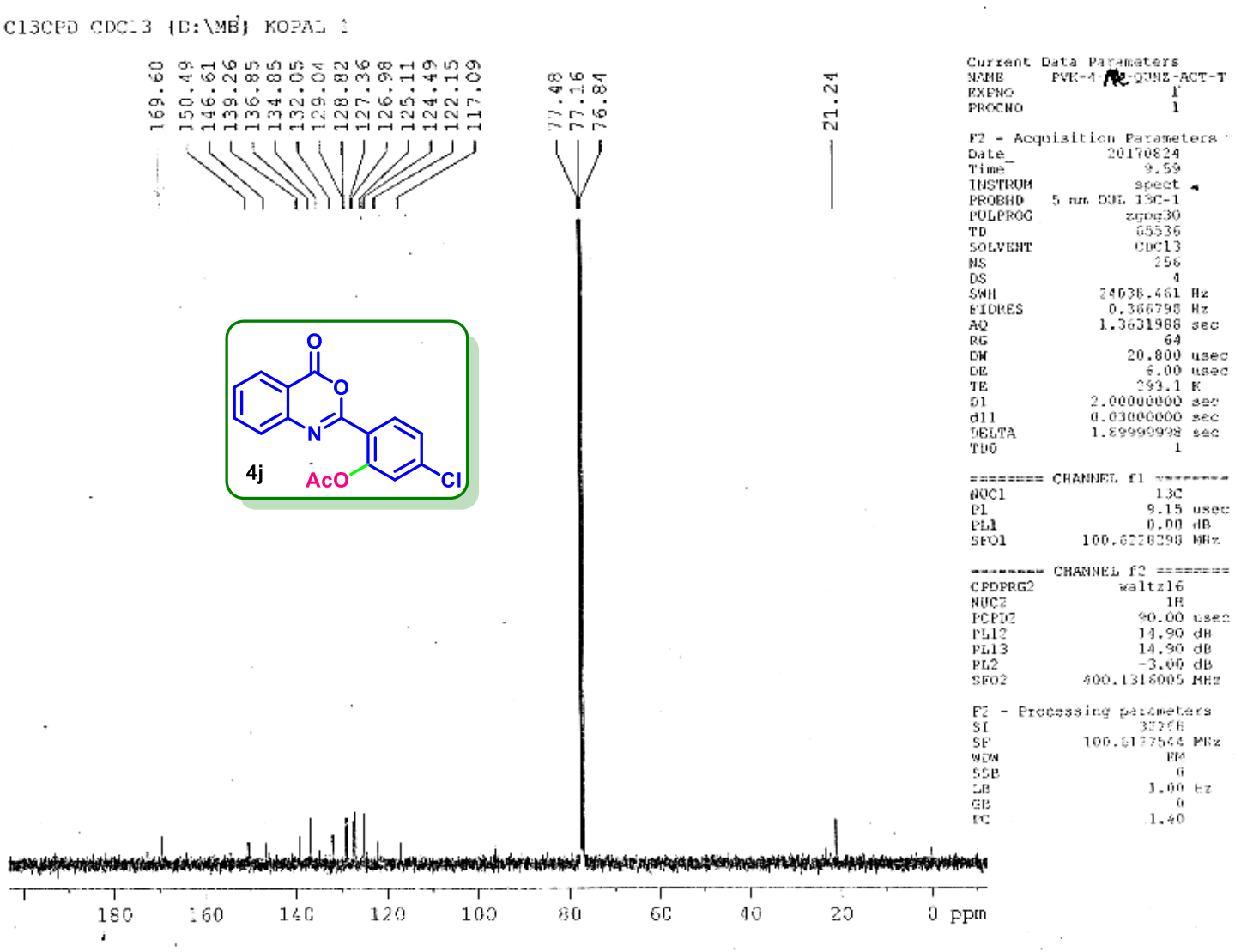

```
Current Data Parameters
NAME      RK-3-CL-QZ-OAC-P
EXPNO                    3
PROCNO                   1

F2 - Acquisition Parameters
Date_             20180914
Time                 10.18
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                    724
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             400.1300048 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   1.00
```


169.74
158.82
154.12
149.02
146.48
136.90
136.38
133.84
129.23
128.85
127.48
126.26
125.23
119.69
117.12
77.48
77.16
76.84
21.22
O
O
N
Cl
4i
AcO
200
180
160
140
120
100
80
60
40
20
ppm
Current Data Parameters
NAME RK-3-CL-QZ-OAC-P
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20181011
Time 16.13
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 295.6 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 100.6127539 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

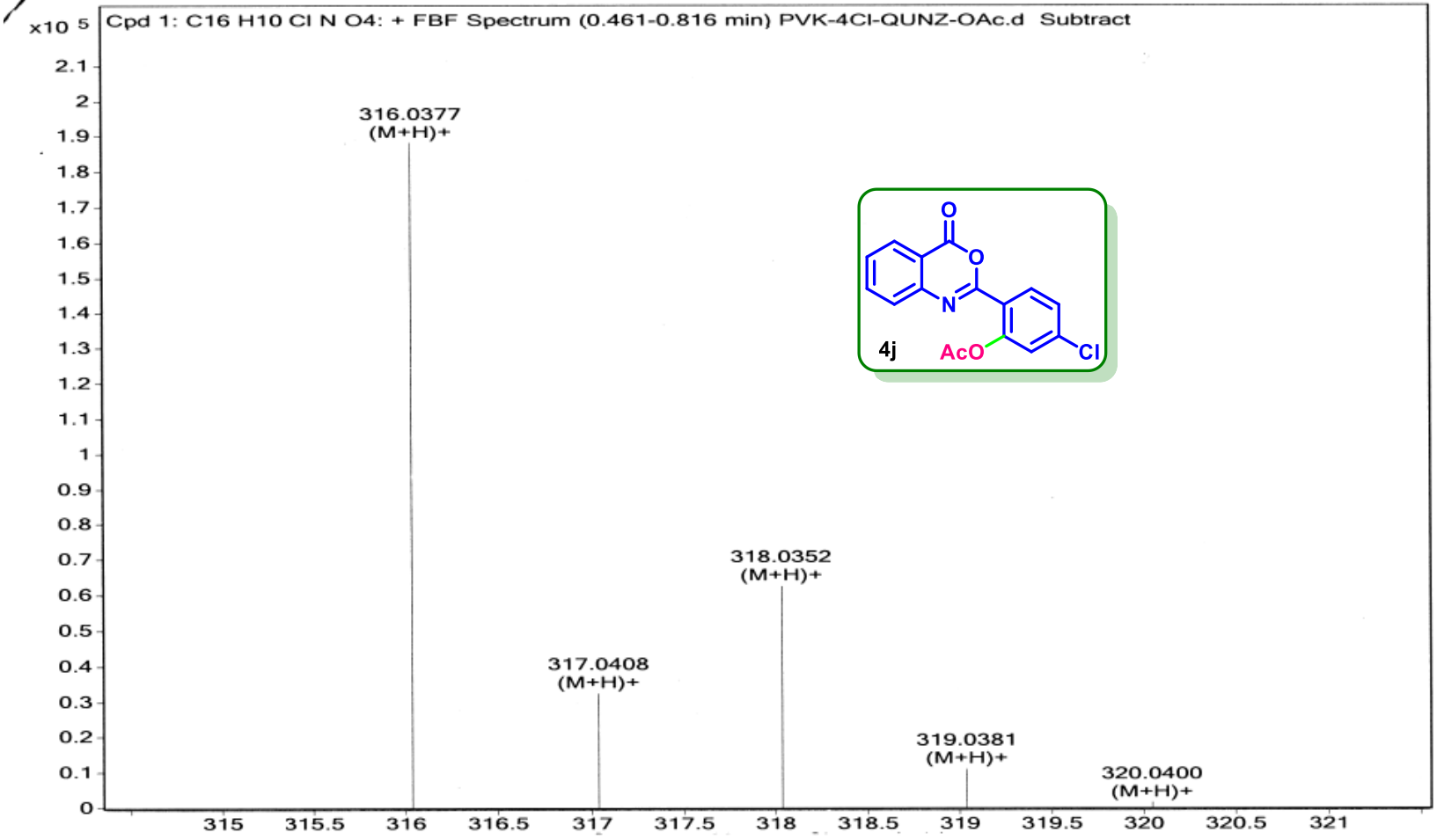
Sample Name	RK-3-Cl-QUNZ-OAC	**Position**		**Instrument Name**	Q-TOF	**User Name**	QTOF-PU\admin
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	RK-3-Cl-QUNZ-OAC.d	**ACQ Method**	Pondicherry Universi	**Comment**	RK-MB-316.0337	**Acquired Time**	23-04-2018 15:46:34

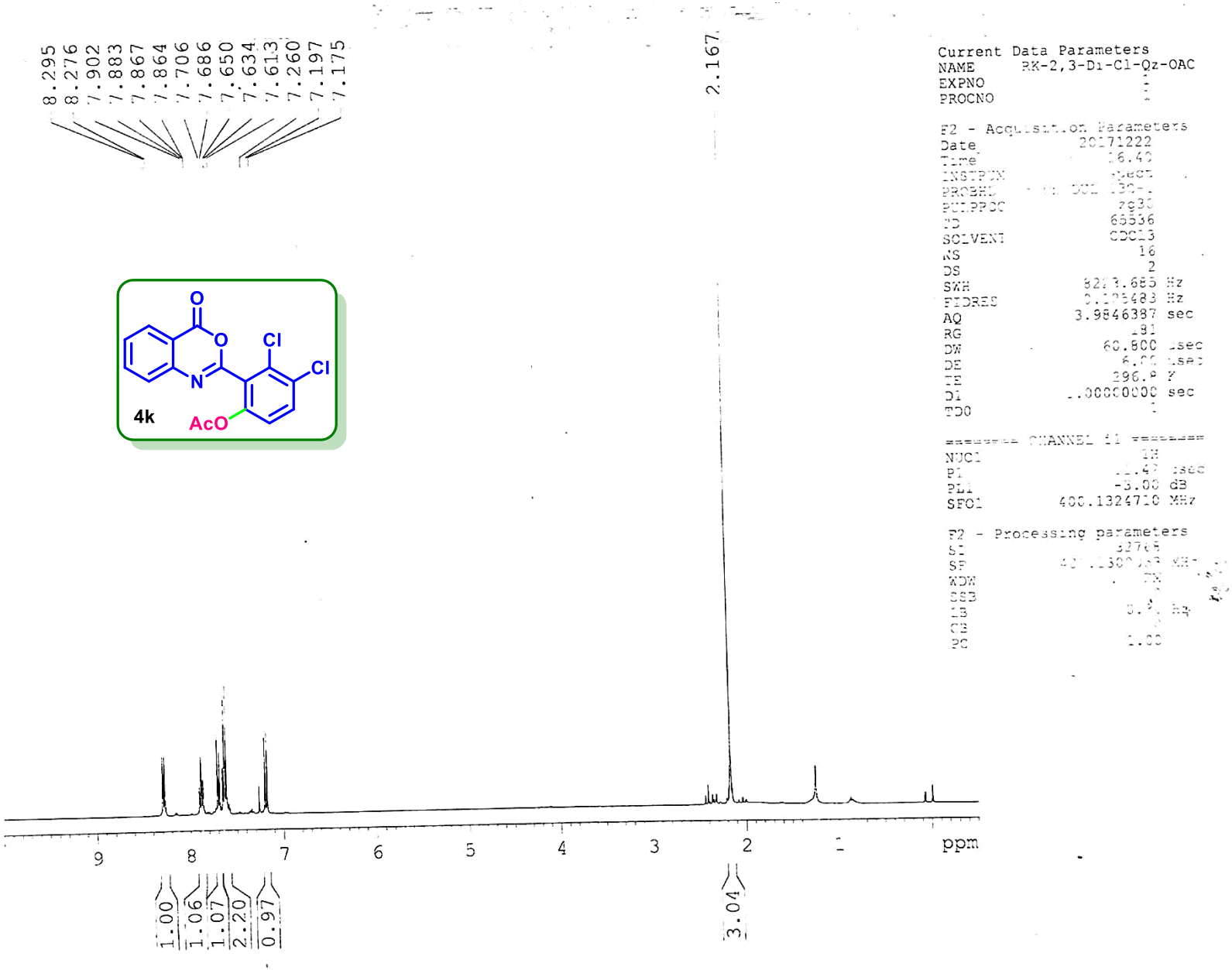


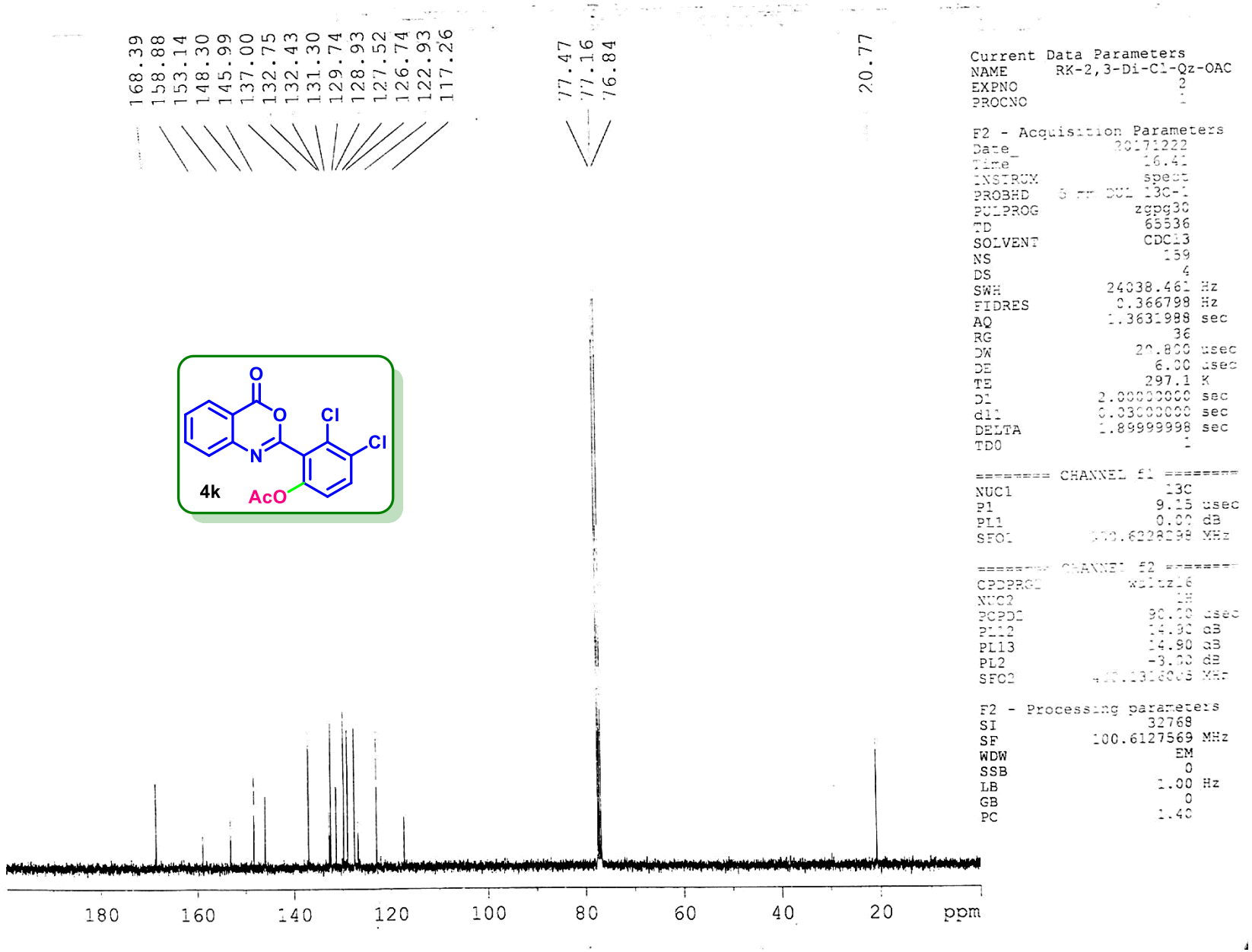

PROTON CDCl3 {D:\MB} KOPAL 1
8.243
8.226
8.222
7.853
7.840
7.838
7.823
7.819
7.635
7.615
7.577
7.574
7.557
7.539
7.536
7.406
7.401
7.385
7.380
7.260
7.225
7.220
2.467
1.598
-0.004
4j
AcO
Cl
O
O
N
Current Data Parameters
NAME PVK-4-ME-QUNZ-ACT-7
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170823
Time 16.42
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 293.6 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
10
9
8
7
6
5
4
3
2
1
ppm
2.01
1.05
1.02
1.08
1.06
1.00
3.08


C13CPD CDCl3 (D:\MB) KOPAL 1
169.60
150.49
146.61
139.26
136.85
134.85
132.05
129.04
128.82
127.36
126.98
125.11
124.49
122.15
117.09
77.48
77.16
76.84
21.24
4j
AcO
Cl
O
O
N
180
160
140
120
100
80
60
40
20
0 ppm
Current Data Parameters
NAME PVK-4-Me-QUNZ-ACT-T
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170824
Time 9.59
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 256
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 293.1 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 100.6127544 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

ame	PVK-4Cl-QUNZ-OAc	Position		Instrument Name	Q-TOF	User Name	QTOF-PU\admin
	-1	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Filename	PVK-4Cl-QUNZ-OAc.d	ACQ Method	Pondicherry Universi	Comment	PVK-MB-316.0377	Acquired Time	20-04-2018 15:03:06

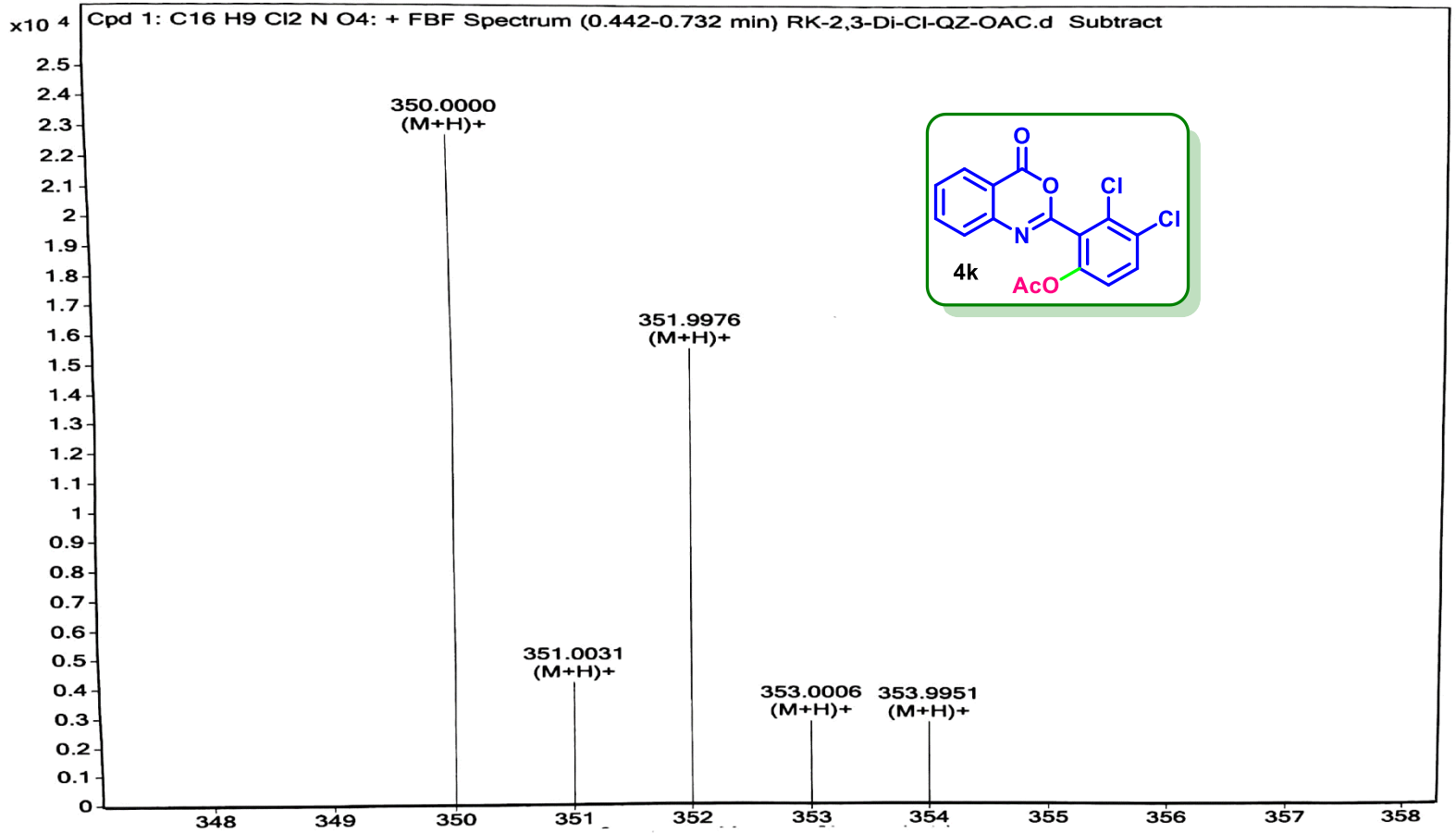


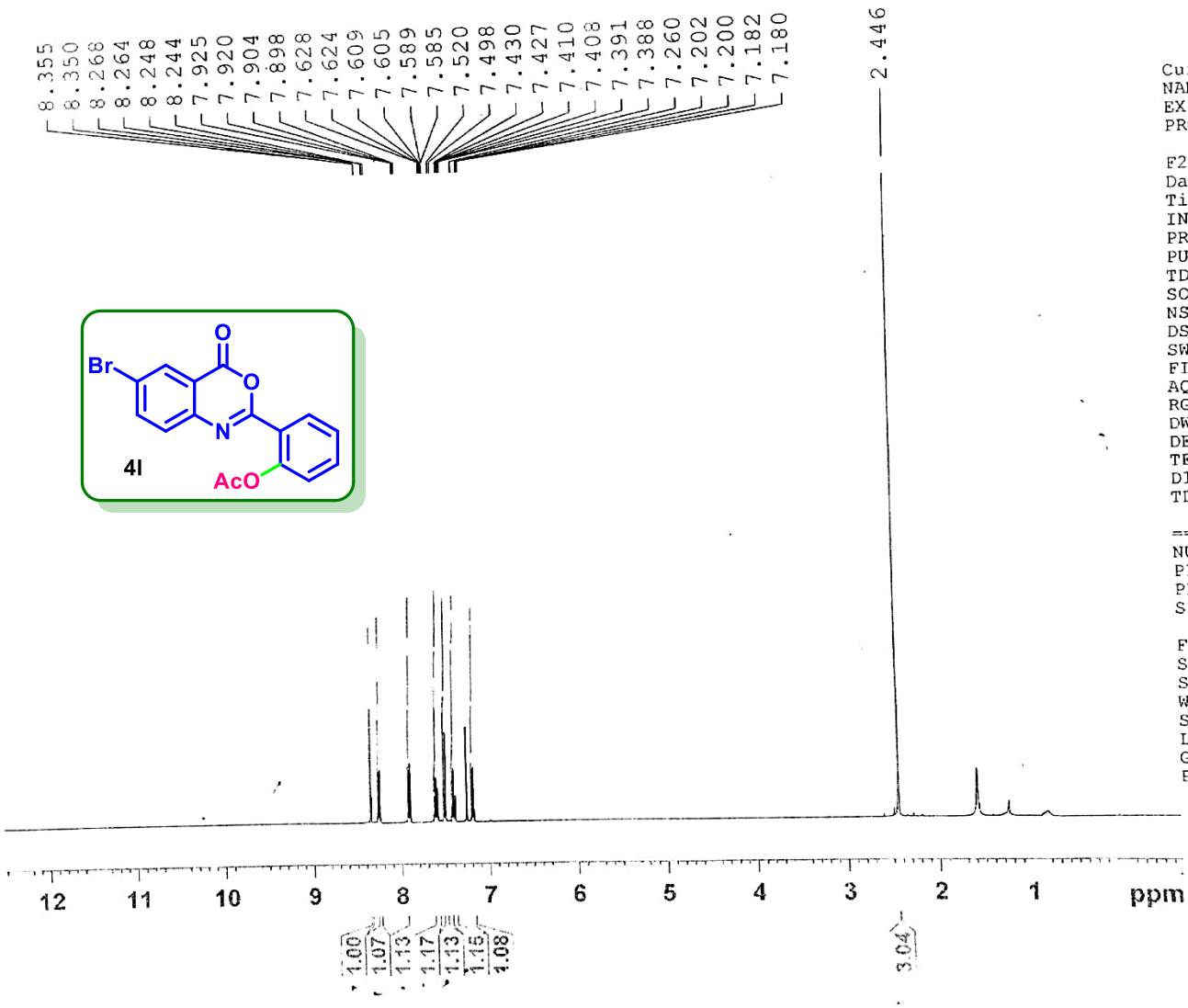

8.295
8.276
7.902
7.883
7.867
7.864
7.706
7.686
7.650
7.634
7.613
7.260
7.197
7.175
2.167
4k
AcO
Cl
Cl
O
O
N
Current Data Parameters
NAME RK-2,3-D1-Cl-Qz-OAC
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date 20171222
Time 16.40
INSTRM spect
PROBHD 5 mm DUL 13C-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8213.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 181
DW 60.800 usec
DE 6.00 usec
TE 296.8 K
D1 1.00000000 sec
TD0 1
CHANNEL f1
NUC1 1H
P1 15.40 usec
PL1 -3.00 dB
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
9
8
7
6
5
4
3
2
1
ppm
1.00
1.06
1.07
2.20
0.97
3.04



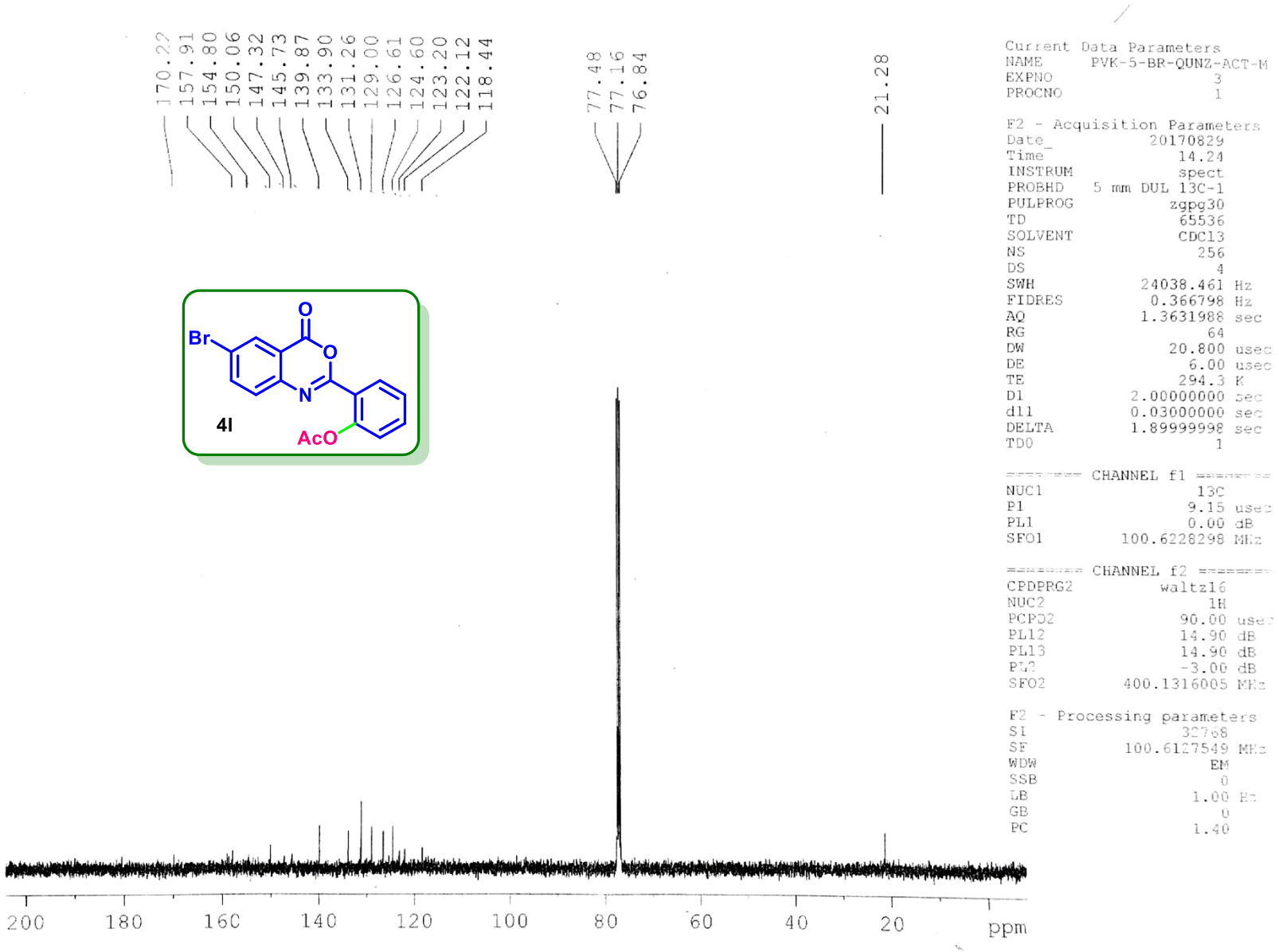

```
Current Data Parameters
NAME      RK-2,3-Di-Cl-Qz-OAC
EXPNO                       2
PROCNO                      1

F2 - Acquisition Parameters
Date_            20171222
Time                16.41
INSTRUM             spect
PROBHD   5 mm DUL 13C-1
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   159
DS                     4
SWH            24038.461 Hz
FIDRES         0.366798 Hz
AQ             1.3631988 sec
RG                    36
DW                20.800 usec
DE                 6.00 usec
TE                297.1 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          100.6127569 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

Sample Name	RK-2,3-Di-Cl-QZ-OAC	**Position**		**Instrument Name**	Q-TOF	**User Name**	QTOF-PU\admin
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	RK-2,3-Di-Cl-QZ-OAC.	**ACQ Method**	Pondicherry Universi	**Comment**	RK-MB-348.9909	**Acquired Time**	03-05-2018 12:45:32



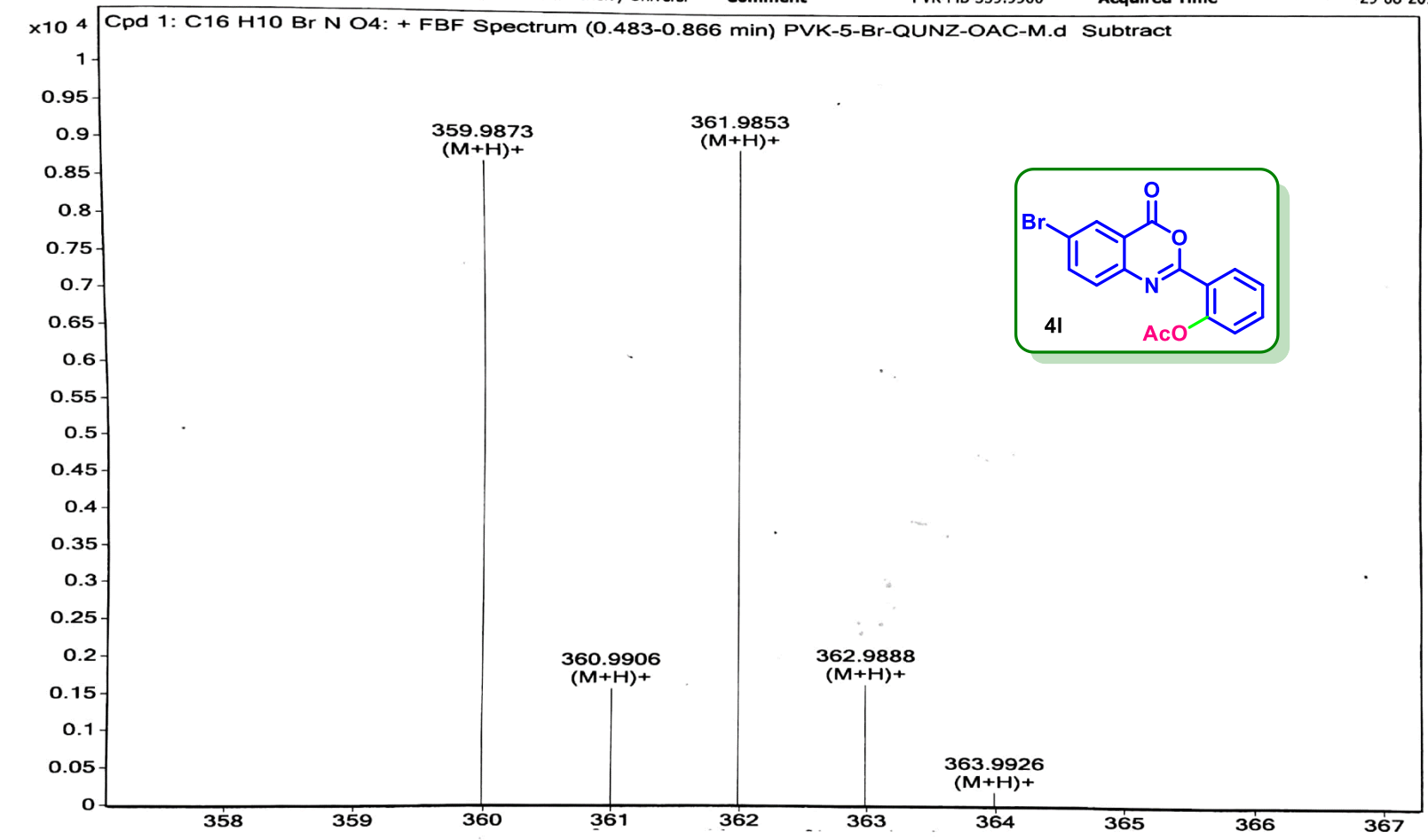


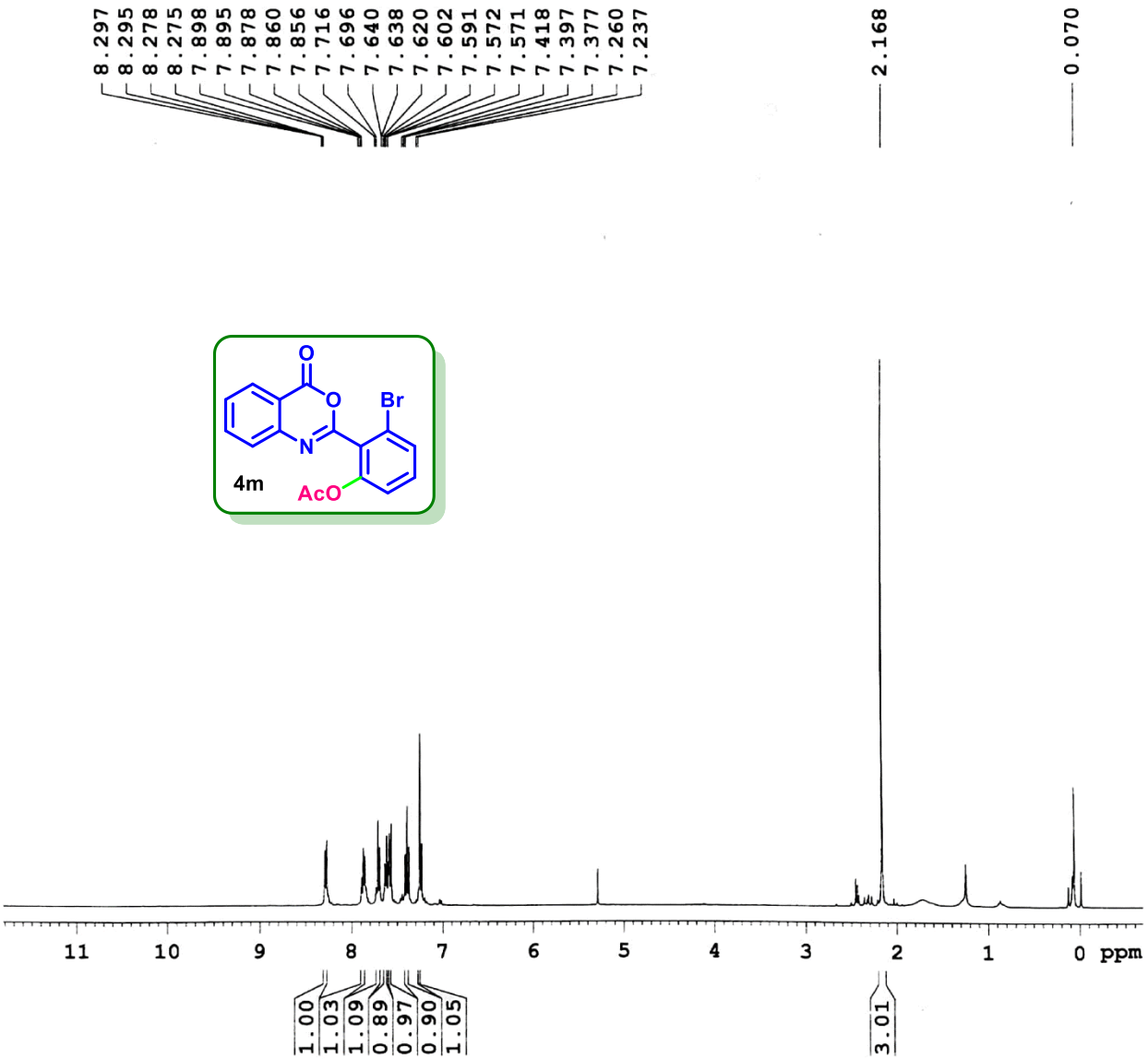

```
Current Data Parameters
NAME        PVK-5-BR-QUNZ-ACT-D
EXPNO                         1
PROCNO                        1

F2 - Acquisition Parameters
Date_                  20170828
Time                      15.13
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                      294.3 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
```



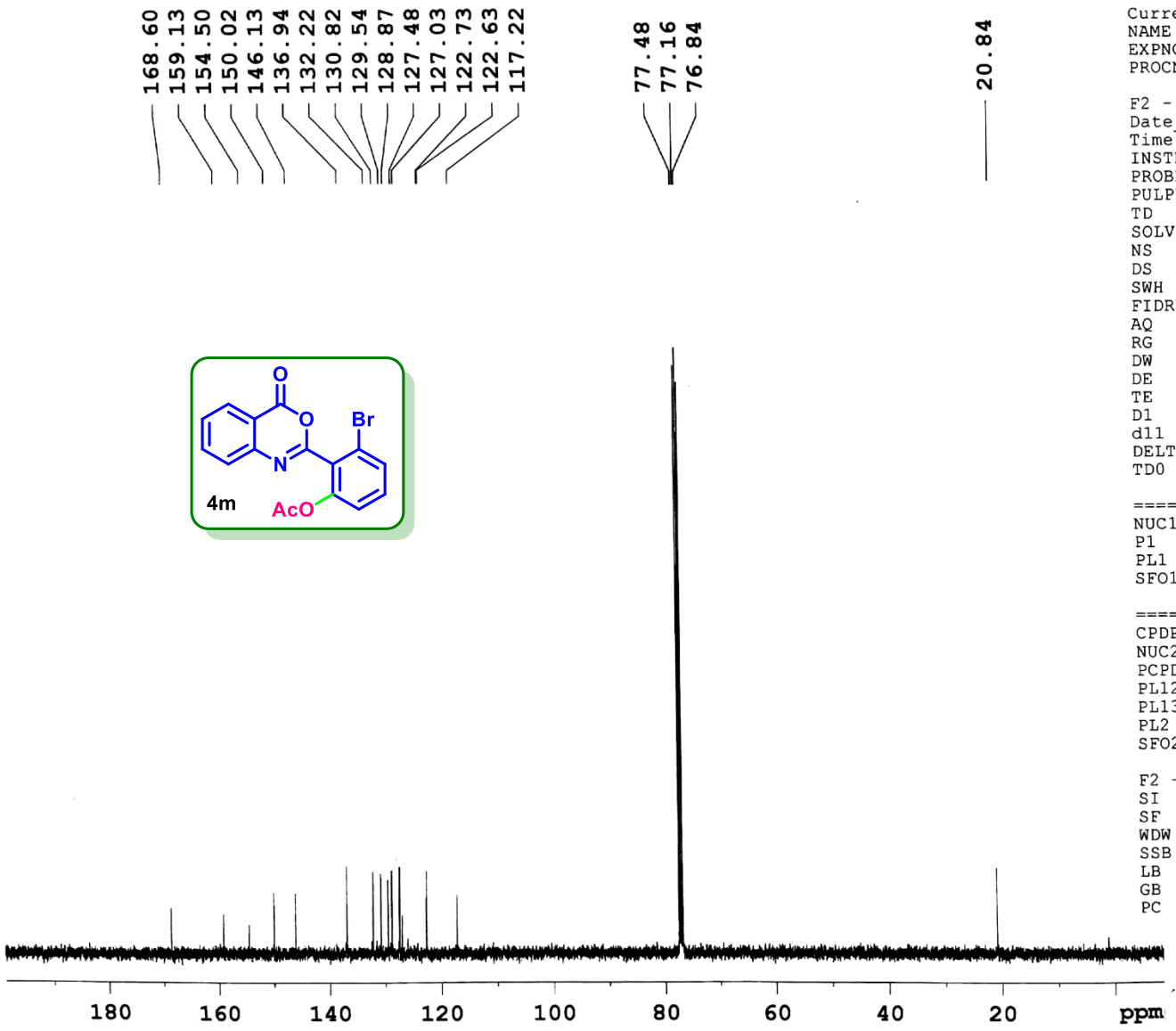

```
Current Data Parameters
NAME      PVK-5-BR-QUNZ-ACT-M
EXPNO                       3
PROCNO                      1

F2 - Acquisition Parameters
Date_              20170829
Time                 14.24
INSTRUM              spect
PROBHD   5 mm DUL 13C-1
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                     256
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                  294.3 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            100.6127549 MHz
WDW                      EM
SSB                       0
LB                     1.00 Hz
GB                        0
PC                     1.40
```

ample Name	PVK-5-Br-QUNZ-OAC-M	**Position**		**Instrument Name**	Q-TOF	**User Name**	QTOF-PU\admin
nj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	PVK-5-Br-QUNZ-OAC-M.	**ACQ Method**	Pondicherry Universi	**Comment**	PVK-MB-359.9900	**Acquired Time**	29-08-2017 11:31:28



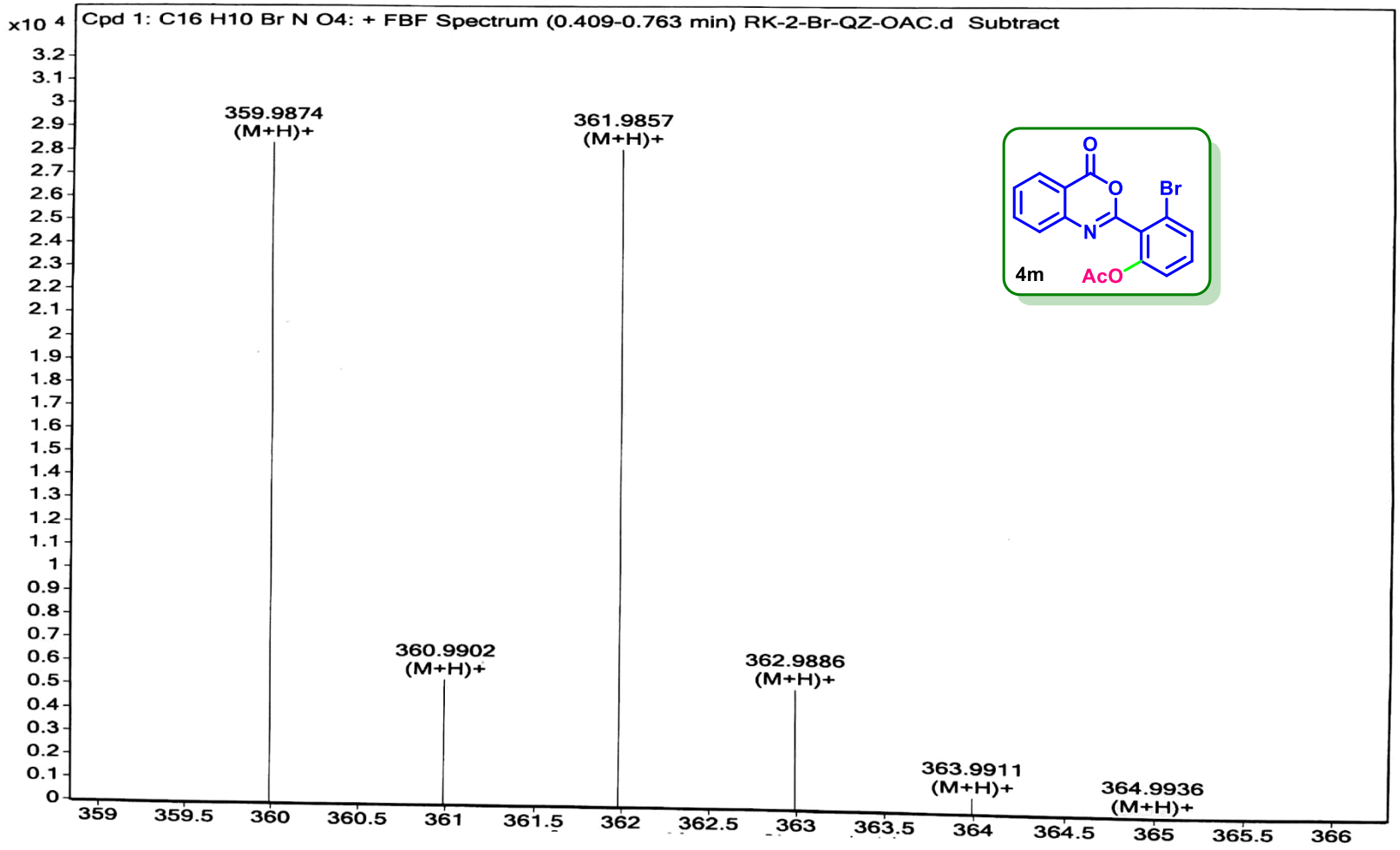



```
Current Data Parameters
NAME      RK-2-BR-42-OAC-D
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_            20180522
Time                16.36
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                    228
DW                 60.800 usec
DE                  6.00 usec
TE                 295.1 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            400.1300046 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   1.00
```

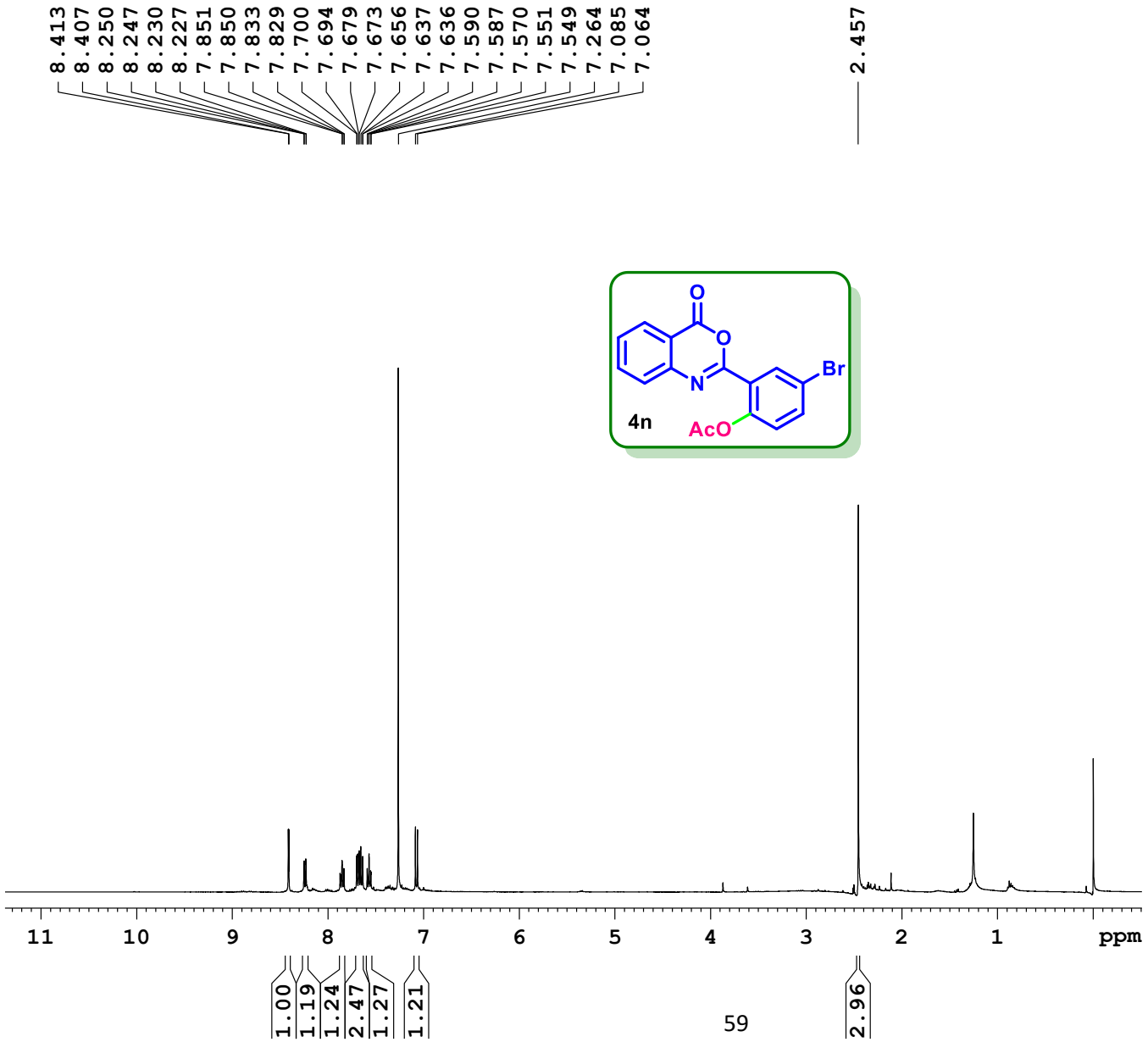



```
Current Data Parameters
NAME      RK-2-BR-42-OAC-D
EXPNO                    2
PROCNO                   1

F2 - Acquisition Parameters
Date_             20180522
Time                 16.51
INSTRUM              spect
PROBHD   5 mm BBO BB-1H
PULPROG              zgpg30
TD                    65536
SOLVENT               CDCl3
NS                      257
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            100.6127567 MHz
WDW                       EM
SSB                        0
LB                      1.00 Hz
GB                         0
PC                      1.40
```

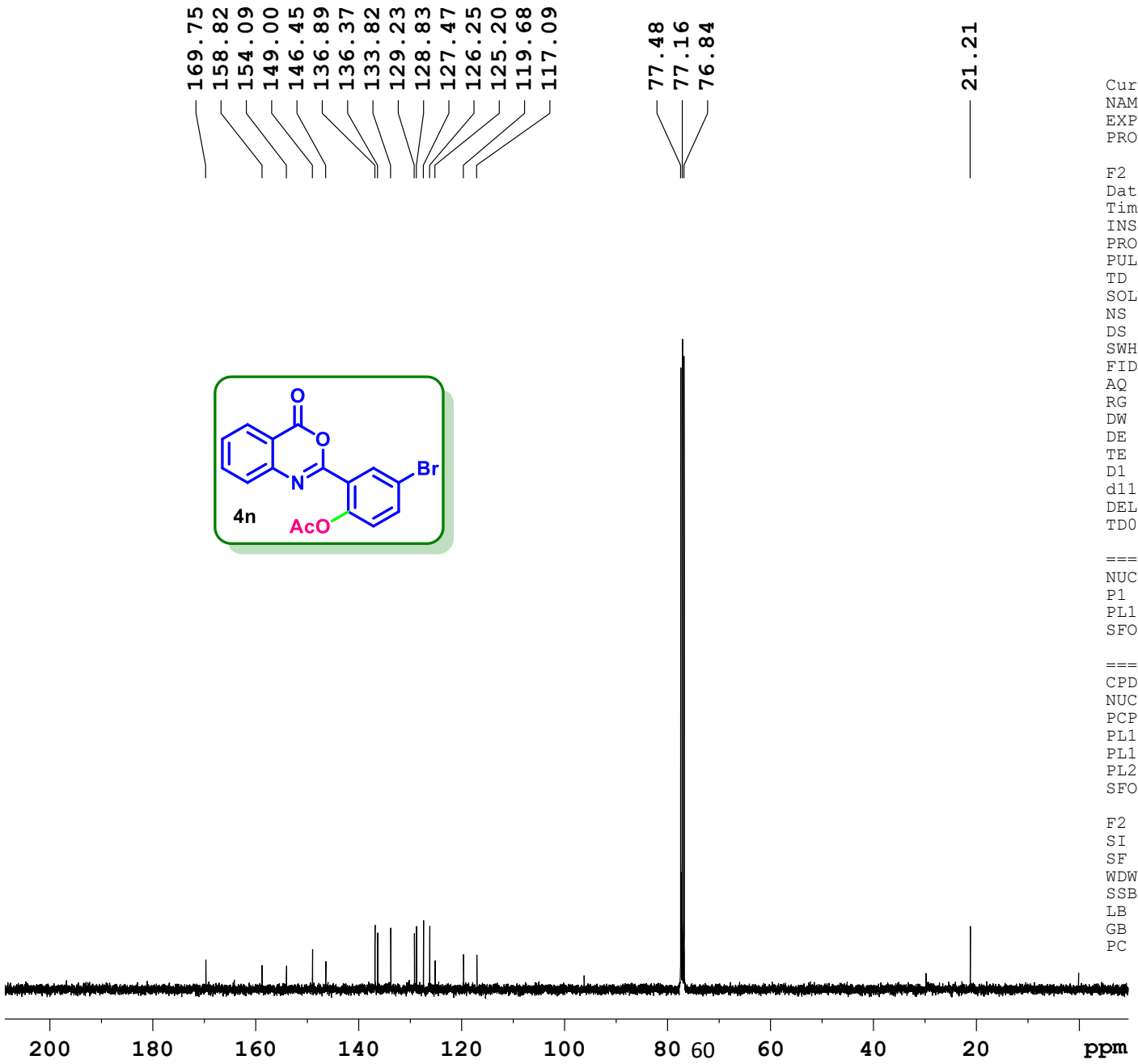
Sample Name	RK-2-Br-QZ-OAC	**Position**		**Instrument Name**	Q-TOF	**User Name**	QTOF-PU\admin
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	RK-2-Br-QZ-OAC.d	**ACQ Method**	Pondicherry Universi	**Comment**	RK-MB-358.9793	**Acquired Time**	23-05-2018 12:17:35



PROTON CDCl3 {D:\MB} KOPAL 1

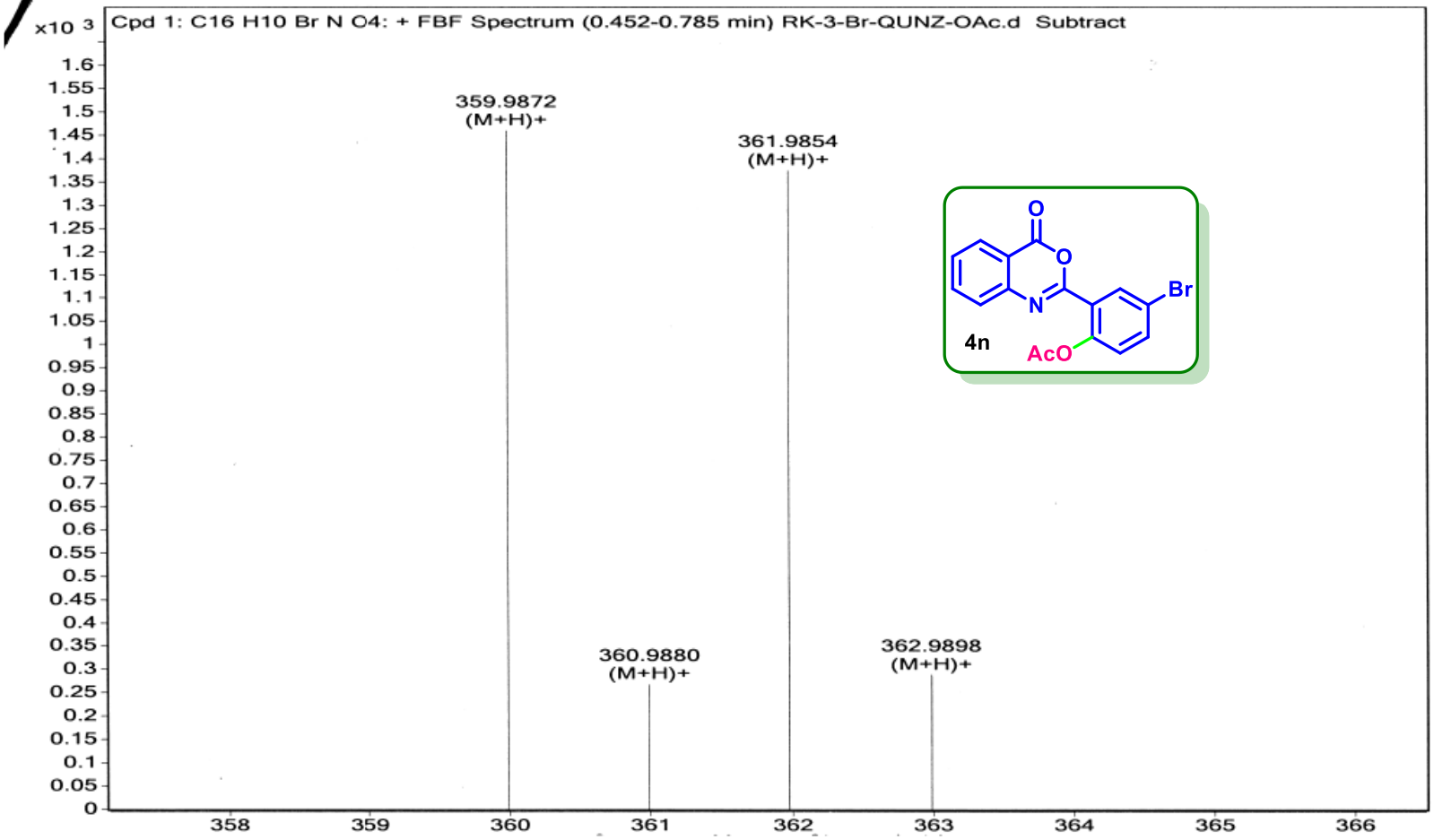



```
Current Data Parameters
NAME      RK-QUNZ-OAC-3-BR
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_           20171025
Time                11.57
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                    161
DW                 60.800 usec
DE                  6.00 usec
TE                 294.4 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           400.1300036 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   1.00
```

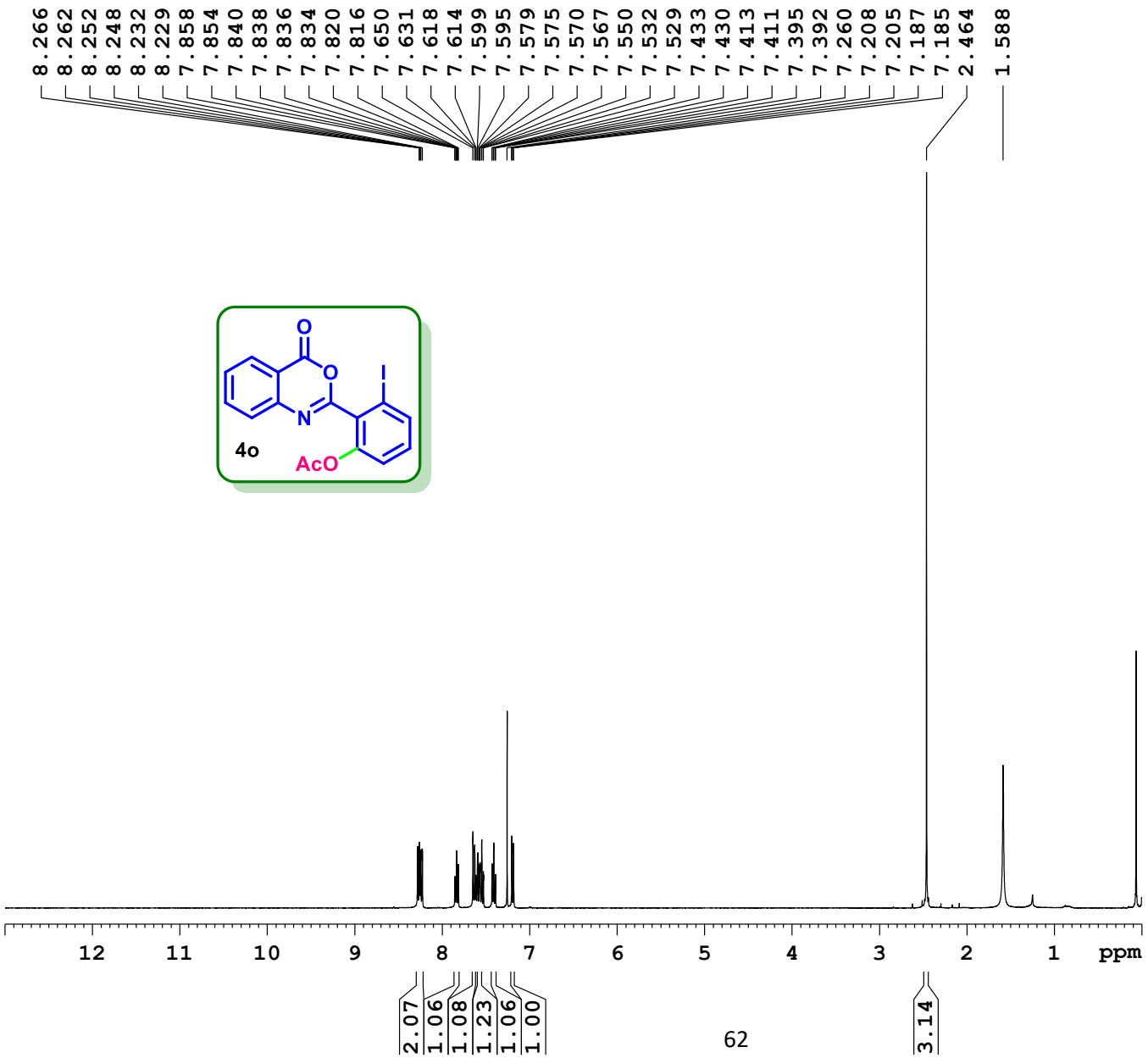



```
Current Data Parameters
NAME      RK-QUNZ-OAC-3-BR
EXPNO                    2
PROCNO                   1

F2 - Acquisition Parameters
Date_           20171025
Time              12.13
INSTRUM           spect
PROBHD   5 mm DUL 13C-1
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  256
DS                    4
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3631988 sec
RG                 45.2
DW               20.800 usec
DE                6.00 usec
TE               294.8 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          100.6127551 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

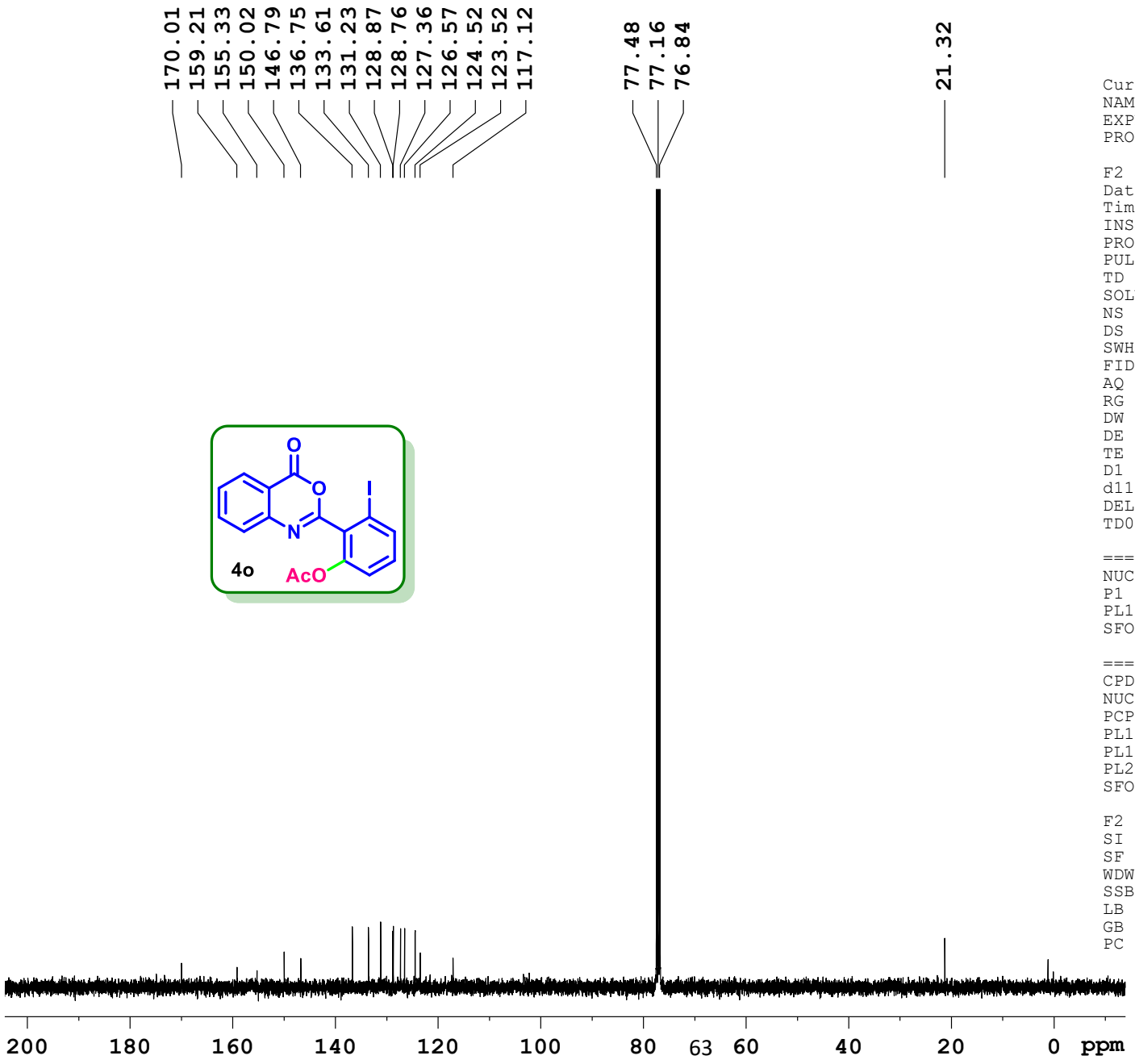
e Name	RK-3-Br-QUNZ-OAc	**Position**		**Instrument Name**	Q-TOF	**User Name**	QTOF-PU\admin
ol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
a Filename	RK-3-Br-QUNZ-OAc.d	**ACQ Method**	Pondicherry Universi	**Comment**	RK-MB-358.9919	**Acquired Time**	14-09-2017 12:30:07



PROTON CDCl3 {D:\MB} KOPAL 1

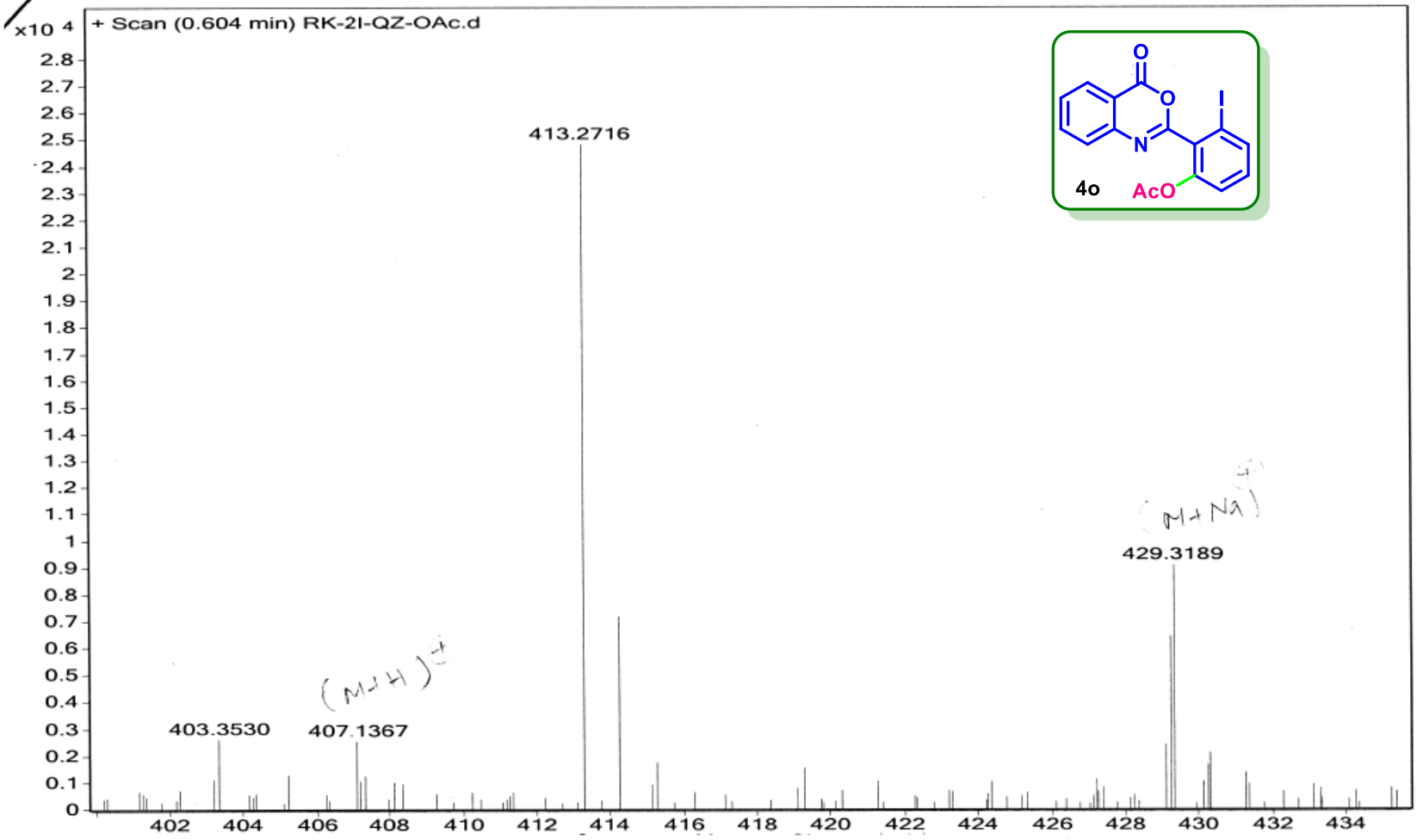


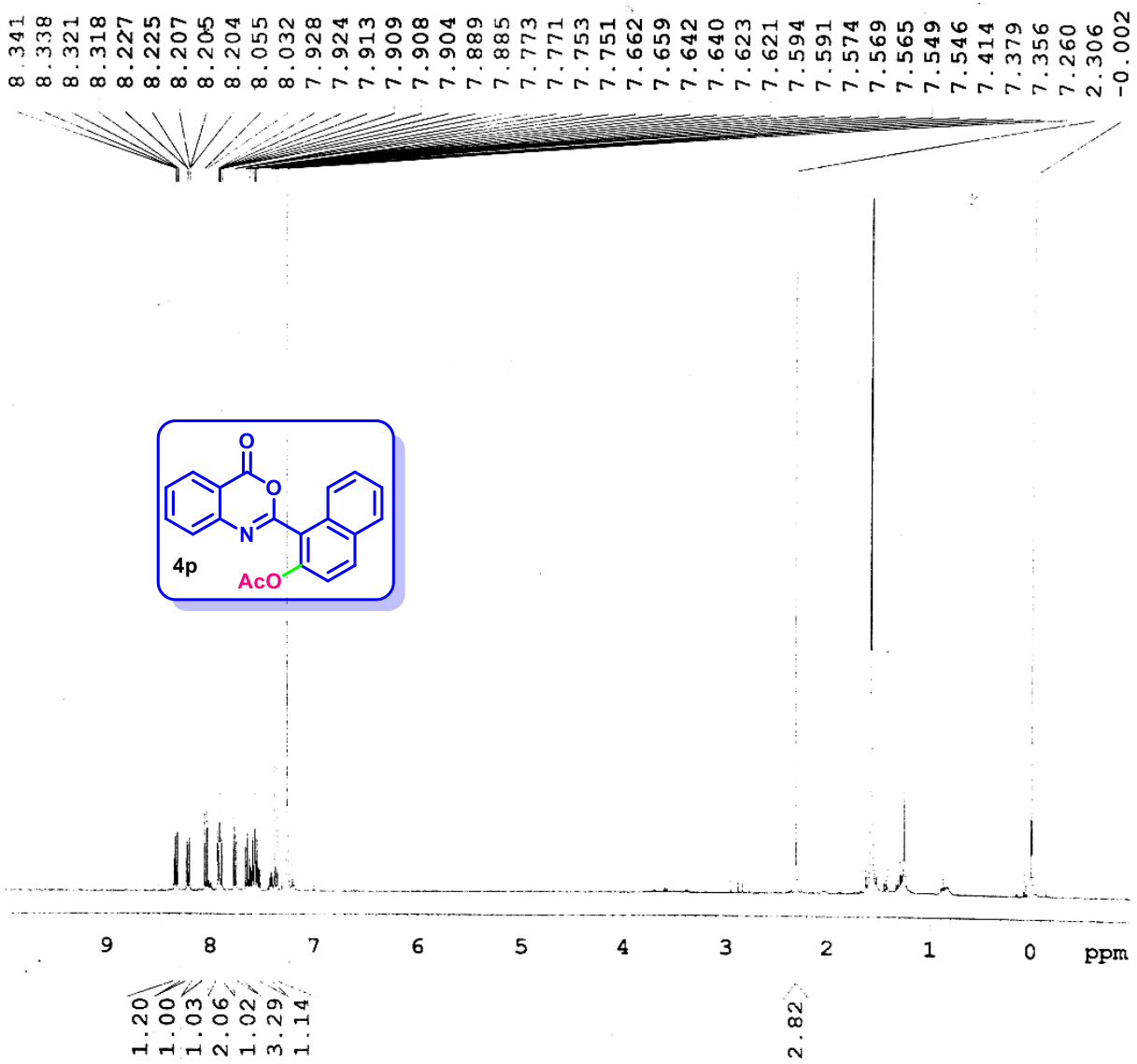

```
Current Data Parameters
NAME       RK-Z-I-QZ-OAC
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20180130
Time                12.16
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                    362
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          400.1300053 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```



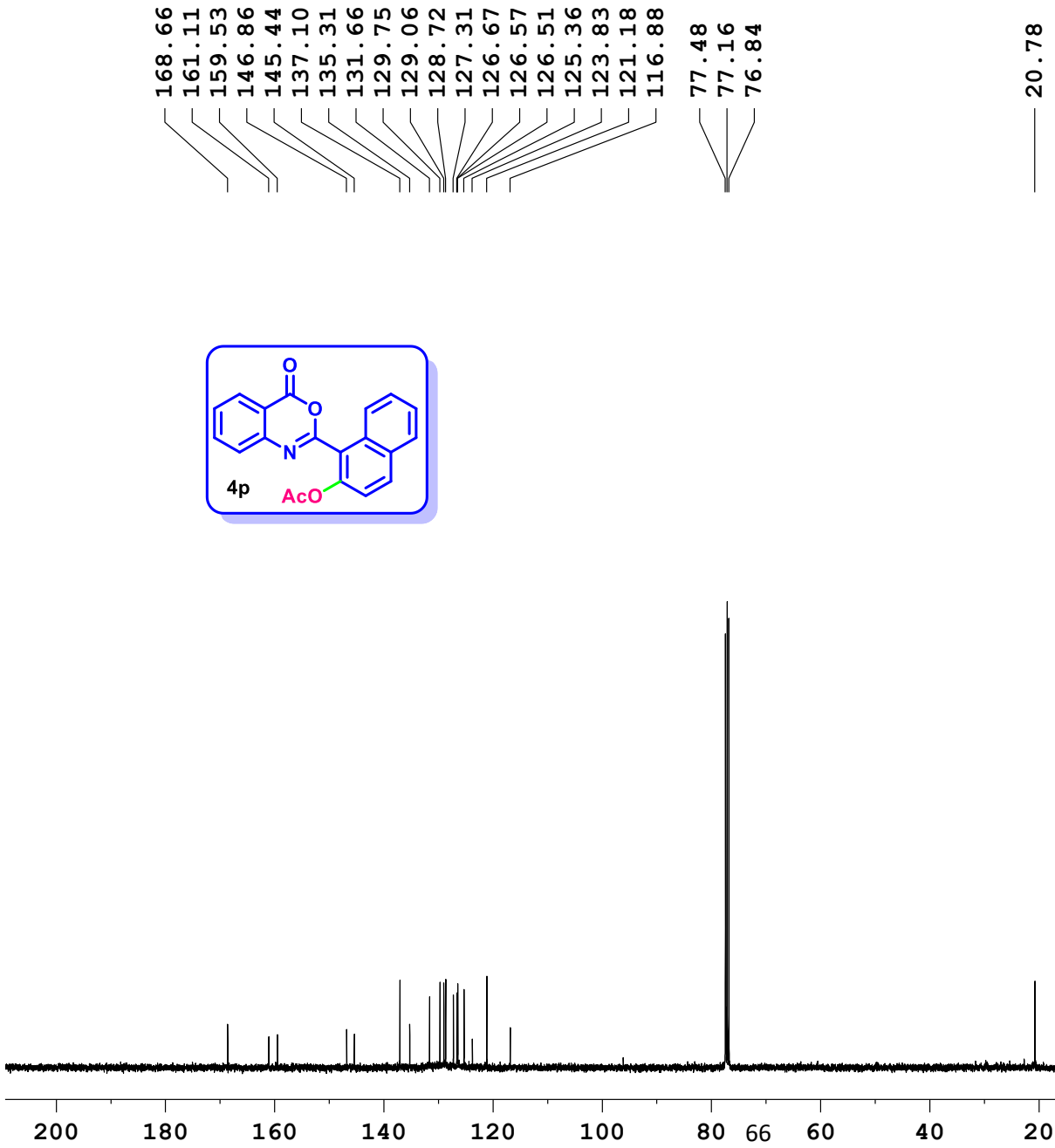

```
Current Data Parameters
NAME       RK-Z-I-QZ-OAC
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20180130
Time              12.31
INSTRUM           spect
PROBHD   5 mm DUL 13C-1
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  256
DS                    4
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3631988 sec
RG                 50.8
DW               20.800 usec
DE                6.00 usec
TE               293.9 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          100.6127544 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

me	RK-2I-QZ-OAc	**Position**		**Instrument Name**	Q-TOF	**User Name**	QTOF-PU\admin
	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Filename	RK-2I-QZ-OAc.d	**ACQ Method**	Pondicherry Universi	**Comment**	RK-MB-258.0761	**Acquired Time**	20-04-2018 14:49:39



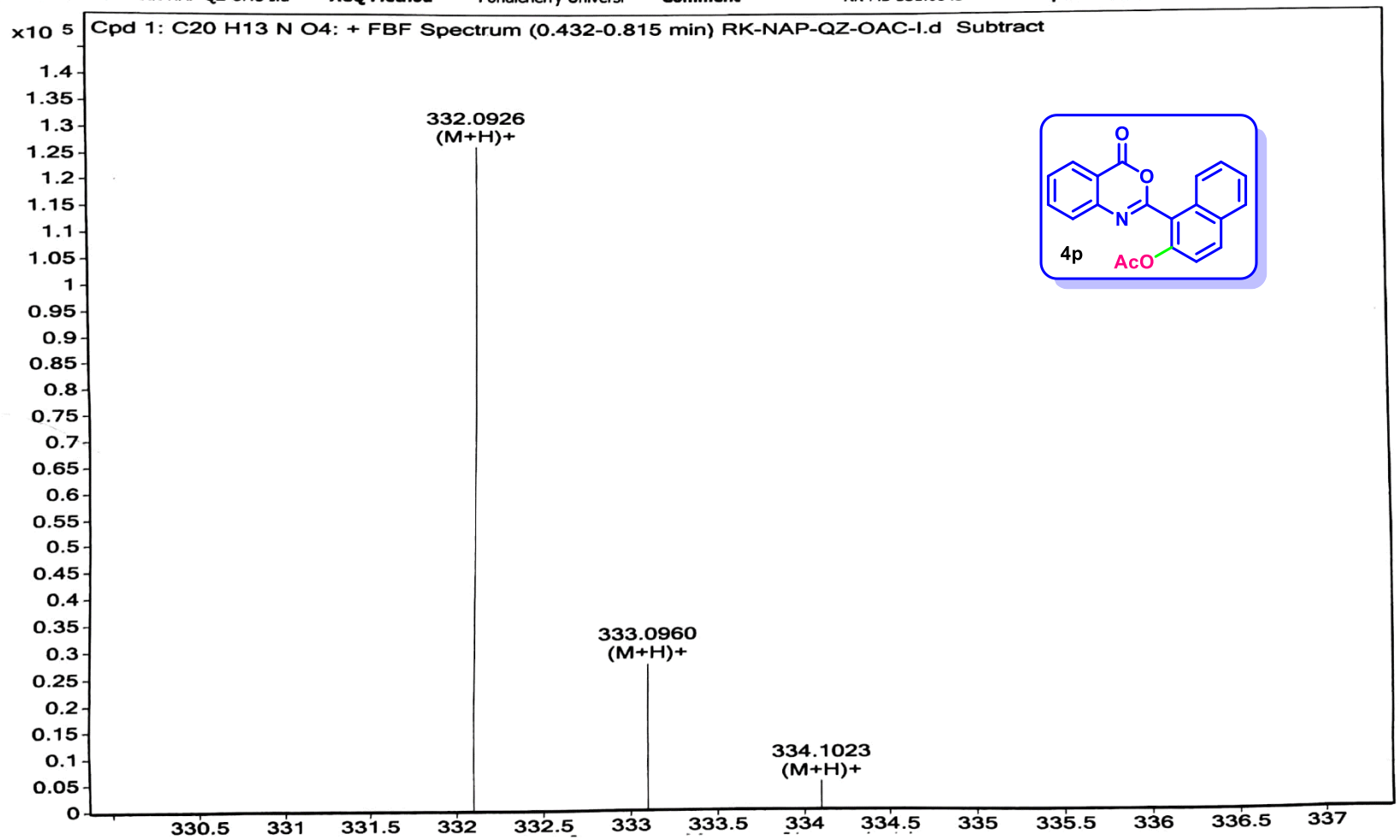


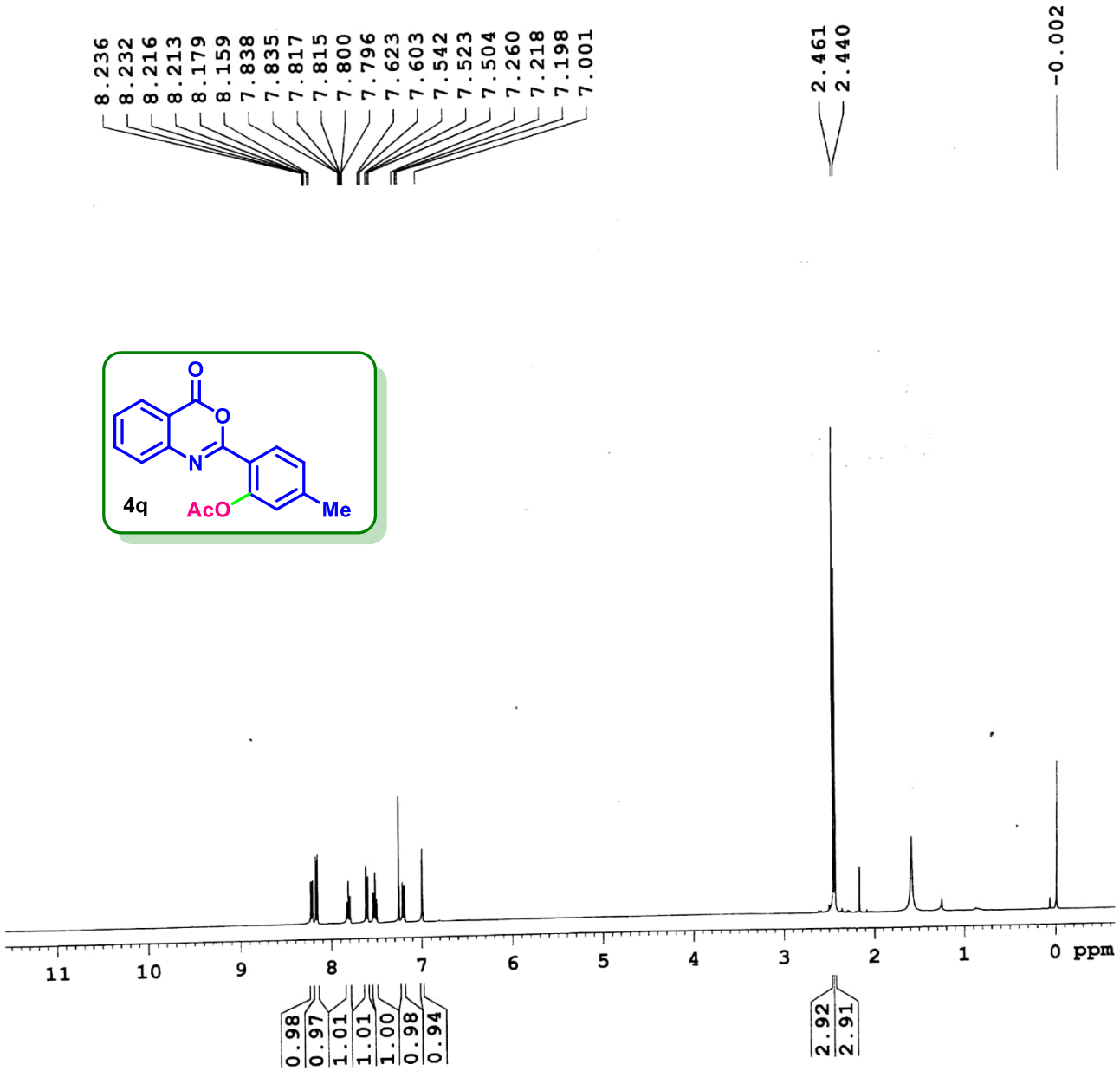

```
Current Data Parameters
NAME                  RK-Nap-QZ-OAC-P
EXPNO                               3
PROCNO                              1

F2 - Acquisition Parameters
Date_                        20180908
Time                             9.48
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                               645
DW                          60.800 usec
DE                           6.00 usec
TE                           294.1 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                    400.1300048 MHz
WDW                               EM
SSB                                0
LB                            0.30 Hz
GB                                 0
PC                              1.00
```



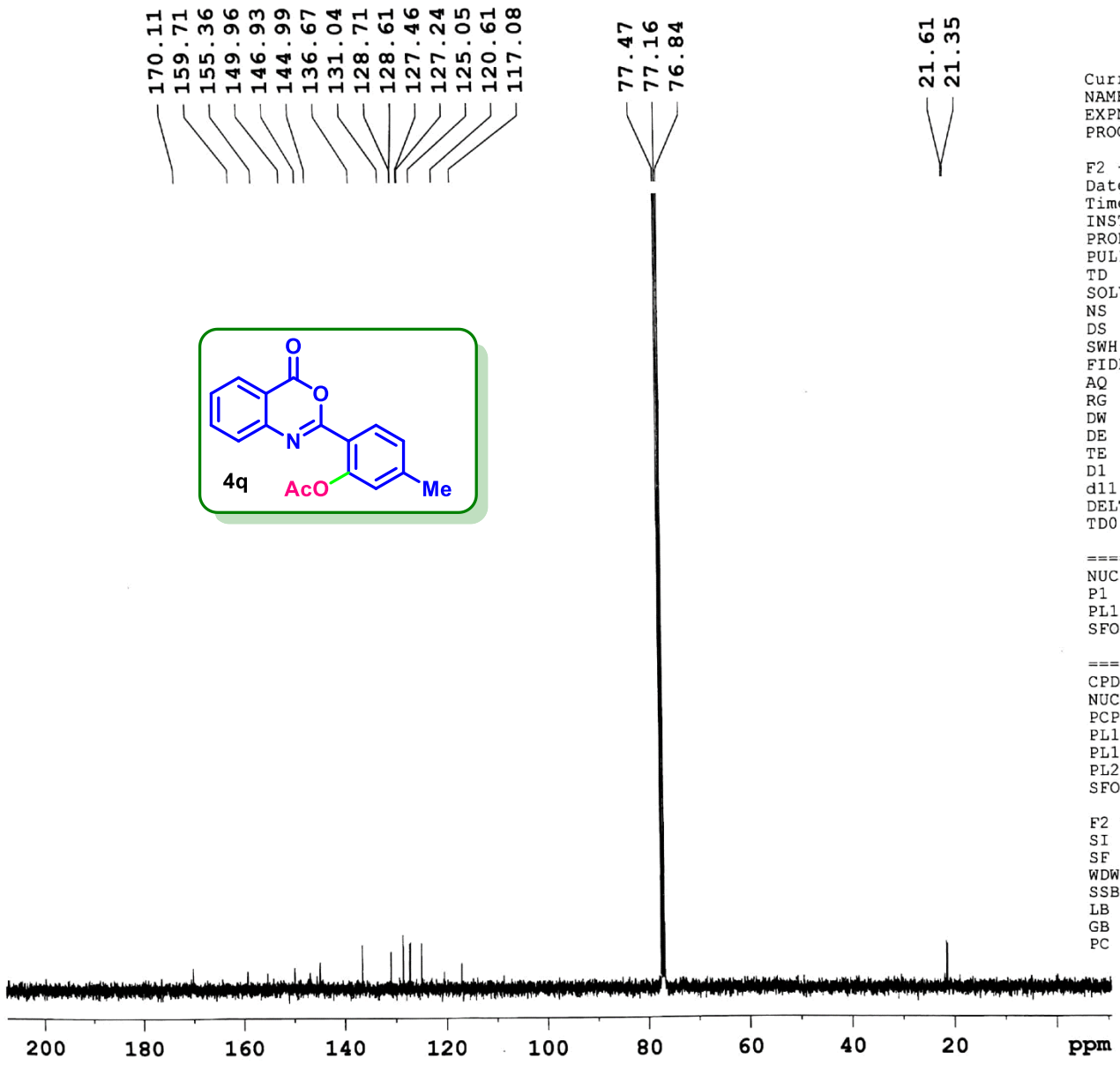

```
Current Data Parameters
NAME      RK-2-Nap-QUNZ-OAC
EXPNO                     3
PROCNO                    1

F2 - Acquisition Parameters
Date_           20171116
Time               12.21
INSTRUM            spect
PROBHD   5 mm DUL 13C-1
PULPROG          zgpg30
TD                65536
SOLVENT            CDCl3
NS                   256
DS                     4
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ             1.3631988 sec
RG                  50.8
DW                20.800 usec
DE                 6.00 usec
TE                295.7 K
D1             2.00000000 sec
d11            0.03000000 sec
DELTA          1.89999998 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                  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           100.6127590 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

Sample Name	RK-NAP-QZ-OAC-I	**Position**		**Instrument Name**	Q-TOF	**User Name**	QTOF-PU\admin
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	RK-NAP-QZ-OAC-I.d	**ACQ Method**	Pondicherry Universi	**Comment**	RK-MB-331.0845	**Acquired Time**	26-04-2018 13:46:10



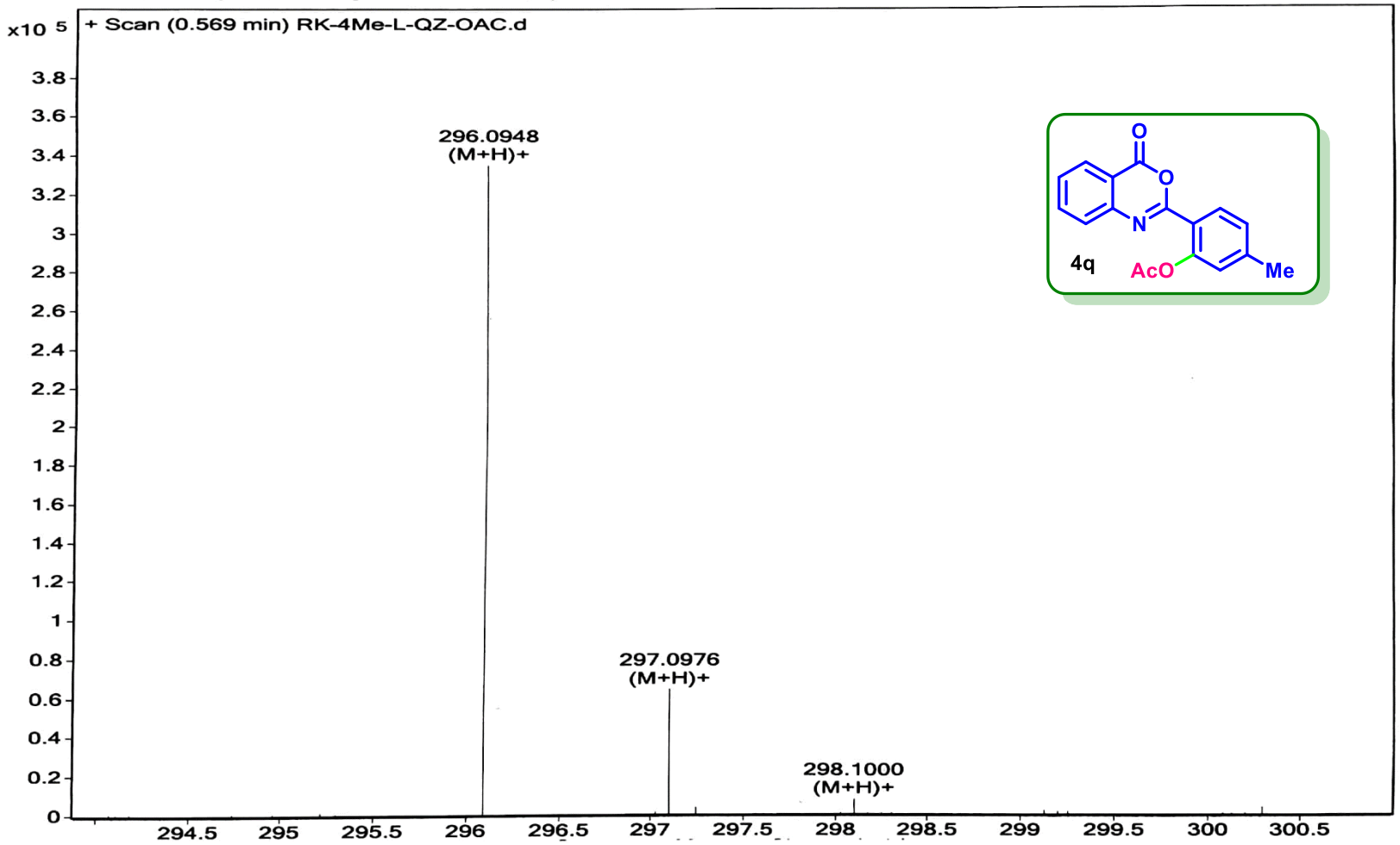


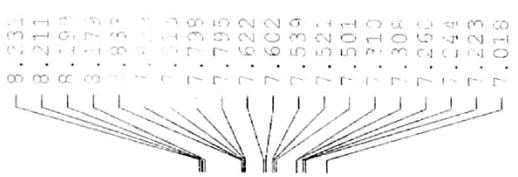

```
Current Data Parameters
NAME      RK-4MC-L-QZ-OAC-1
EXPNO                    3
PROCNO                   1

F2 - Acquisition Parameters
Date_              20180110
Time                 16.55
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                 295.6 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            400.1300054 MHz
WDW                    EM
SSB                     0
LB                 0.30 Hz
GB                      0
PC                   1.00
```

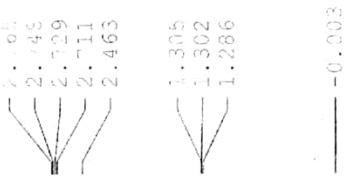


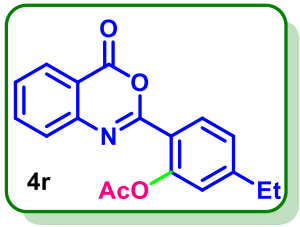

```
Current Data Parameters
NAME      RK-4MC-L-QZ-OAC-1
EXPNO                    4
PROCNO                   1

F2 - Acquisition Parameters
Date_             20180110
Time                 17.05
INSTRUM              spect
PROBHD   5 mm DUL 13C-1
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   166
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                296.2 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           100.6127539 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

Sample Name	RK-4Me-L-QZ-OAC	**Position**		**Instrument Name**	Q-TOF	**User Name**	QTOF-PU\admin
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	RK-4Me-L-QZ-OAC.d	**ACQ Method**	Pondicherry Universi	**Comment**	RK-MB-295.2940	**Acquired Time**	03-05-2018 13:00:09







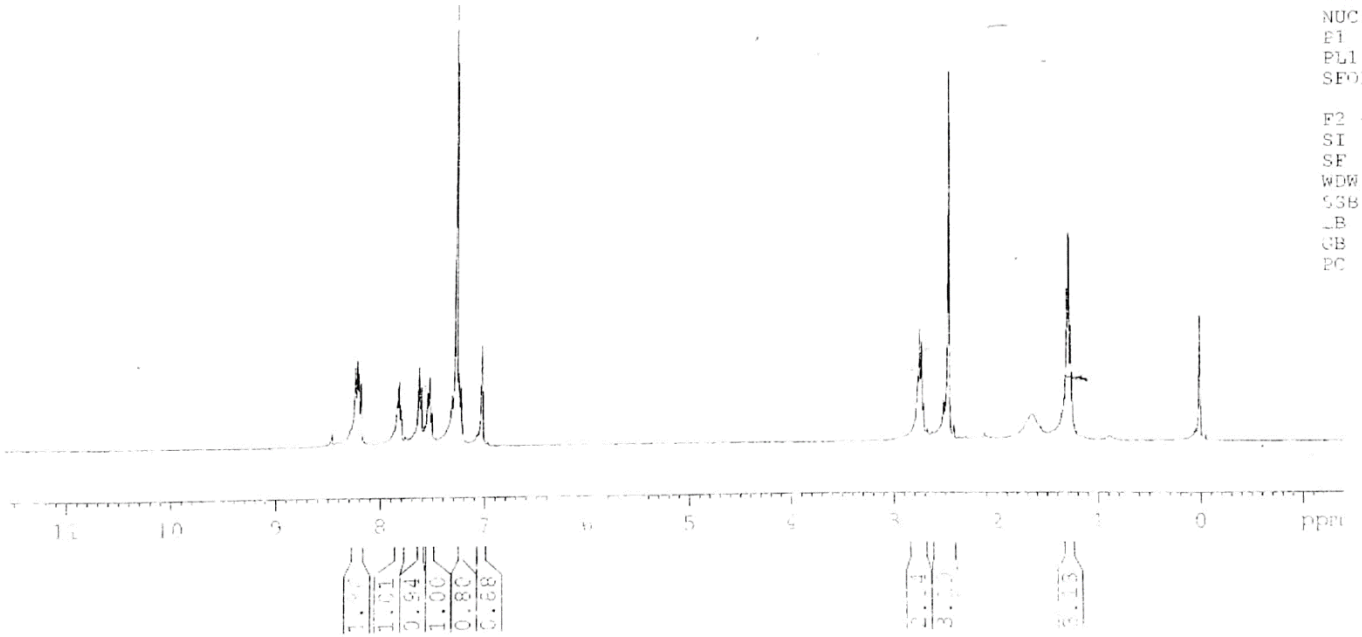


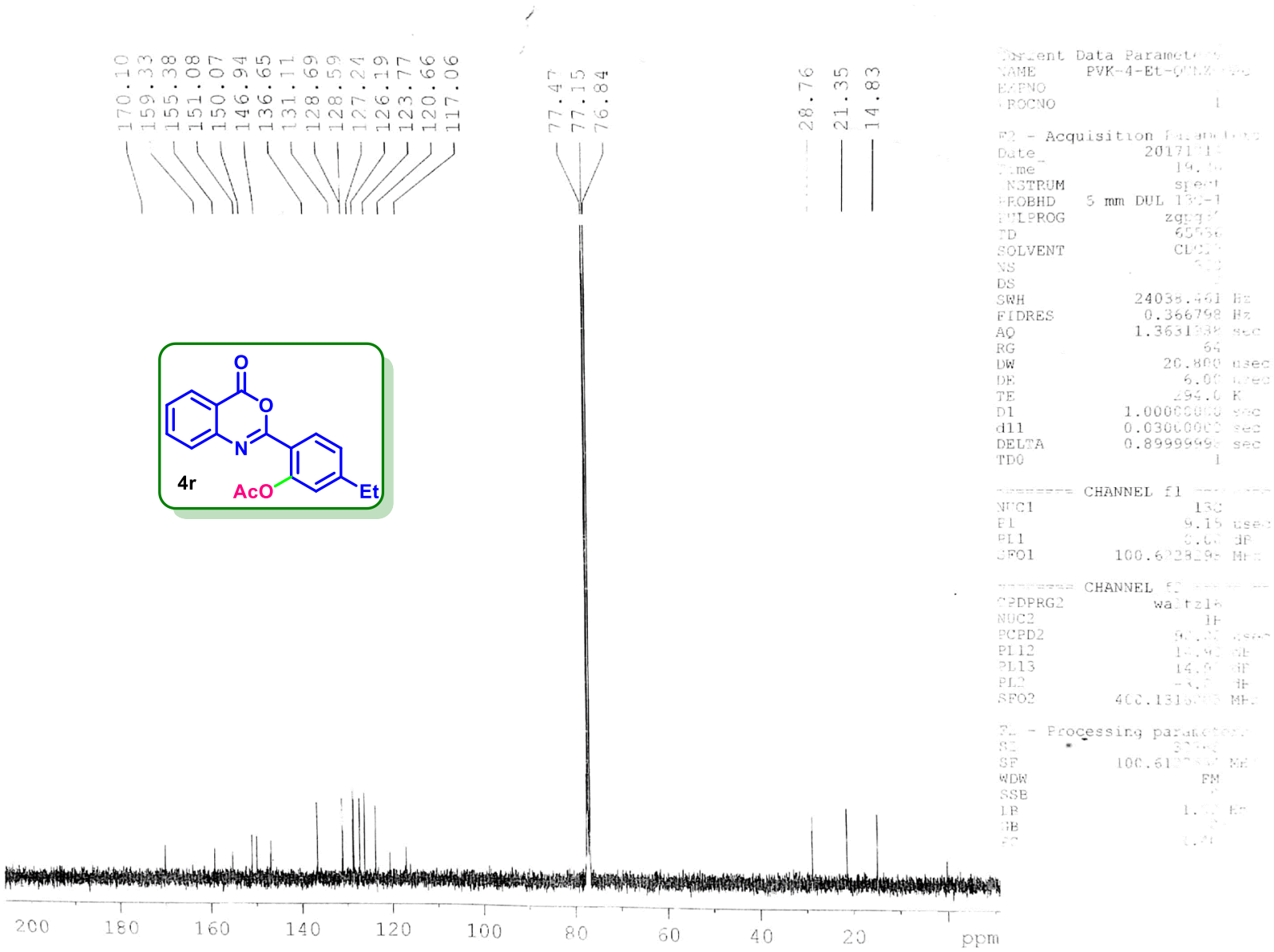
Current Data Parameters
NAME PVK-4-Et-QUNZ-OAc
EXPNO 1
PROCNO 1

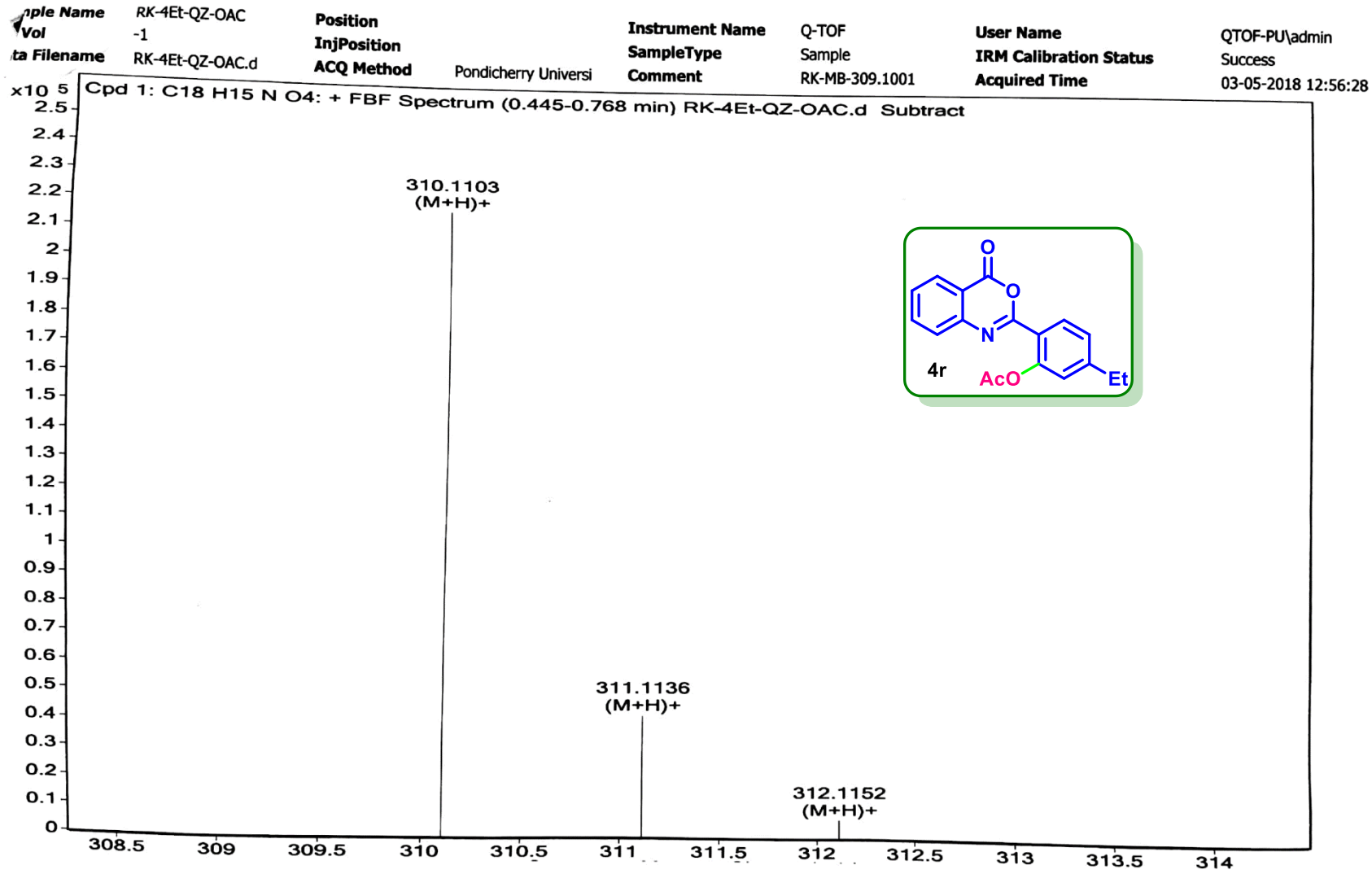
F2 - Acquisition Parameters
Date 20171014
Time 19.11
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8278.646 Hz
FIDRES 0.126346 Hz
AQ 3.9846287 sec
RG 203
DW 60.400 usec
DE 6.00 usec
TE 293.6 K
D1 1.00000000 sec
TD0 1

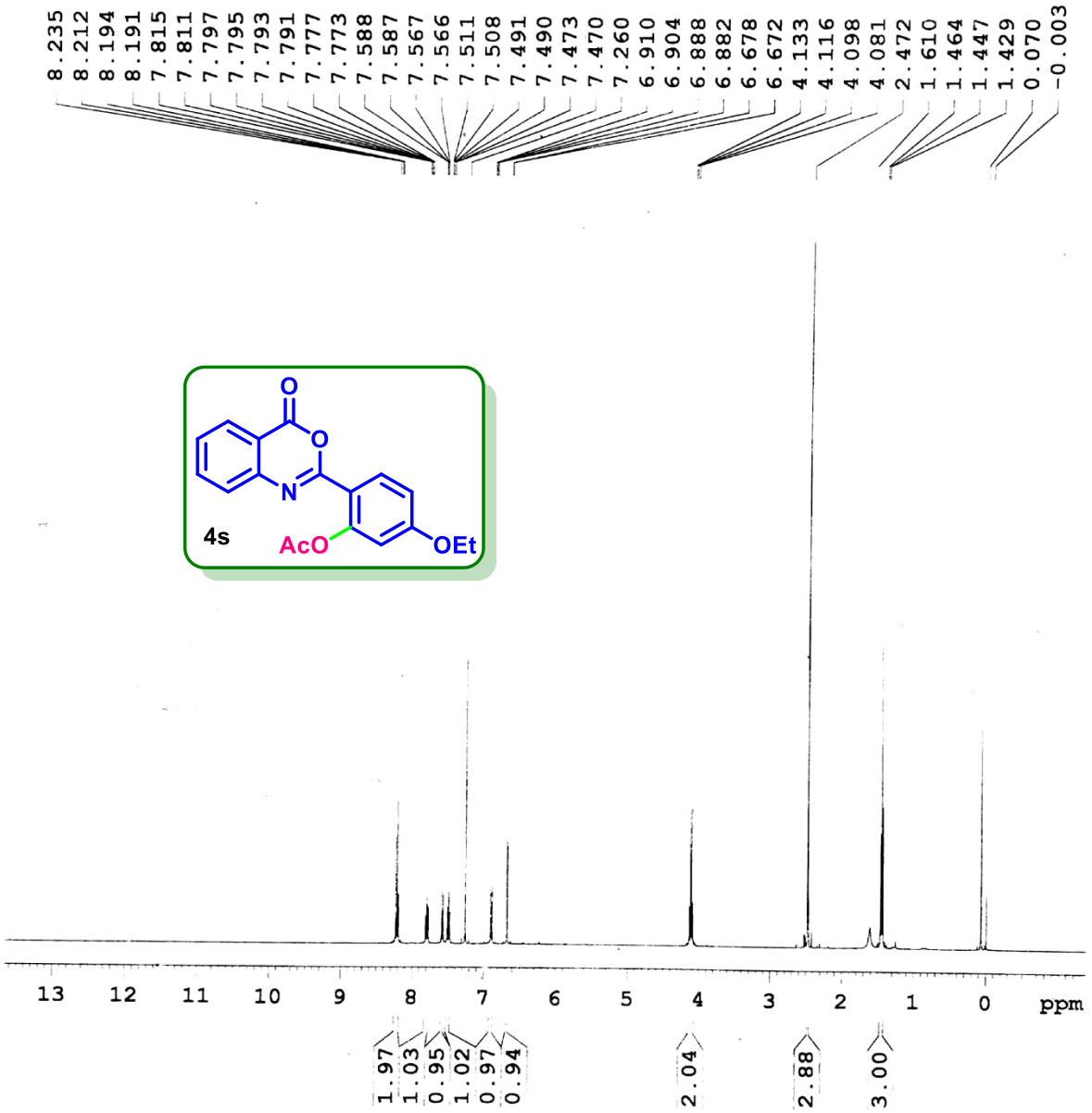
======== CHANNEL f1 ========
NUC1 1H
P1 11.40 usec
PL1 -3.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300036 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

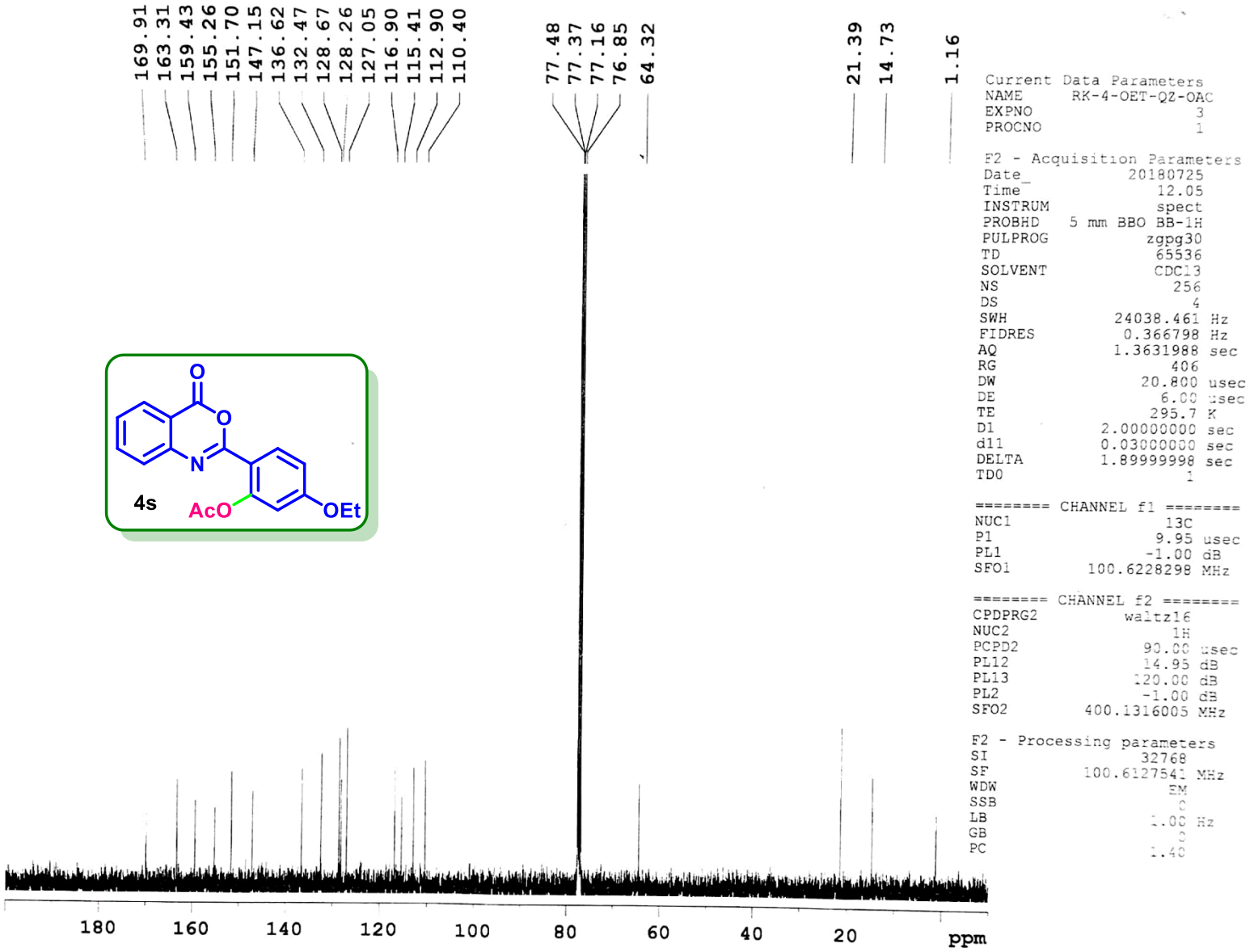



170.10
159.33
155.38
151.08
150.07
146.94
136.65
131.11
128.69
128.59
127.24
126.19
123.77
120.66
117.06
77.47
77.15
76.84
28.76
21.35
14.83
4r
AcO
Et
200
180
160
140
120
100
80
60
40
20
ppm

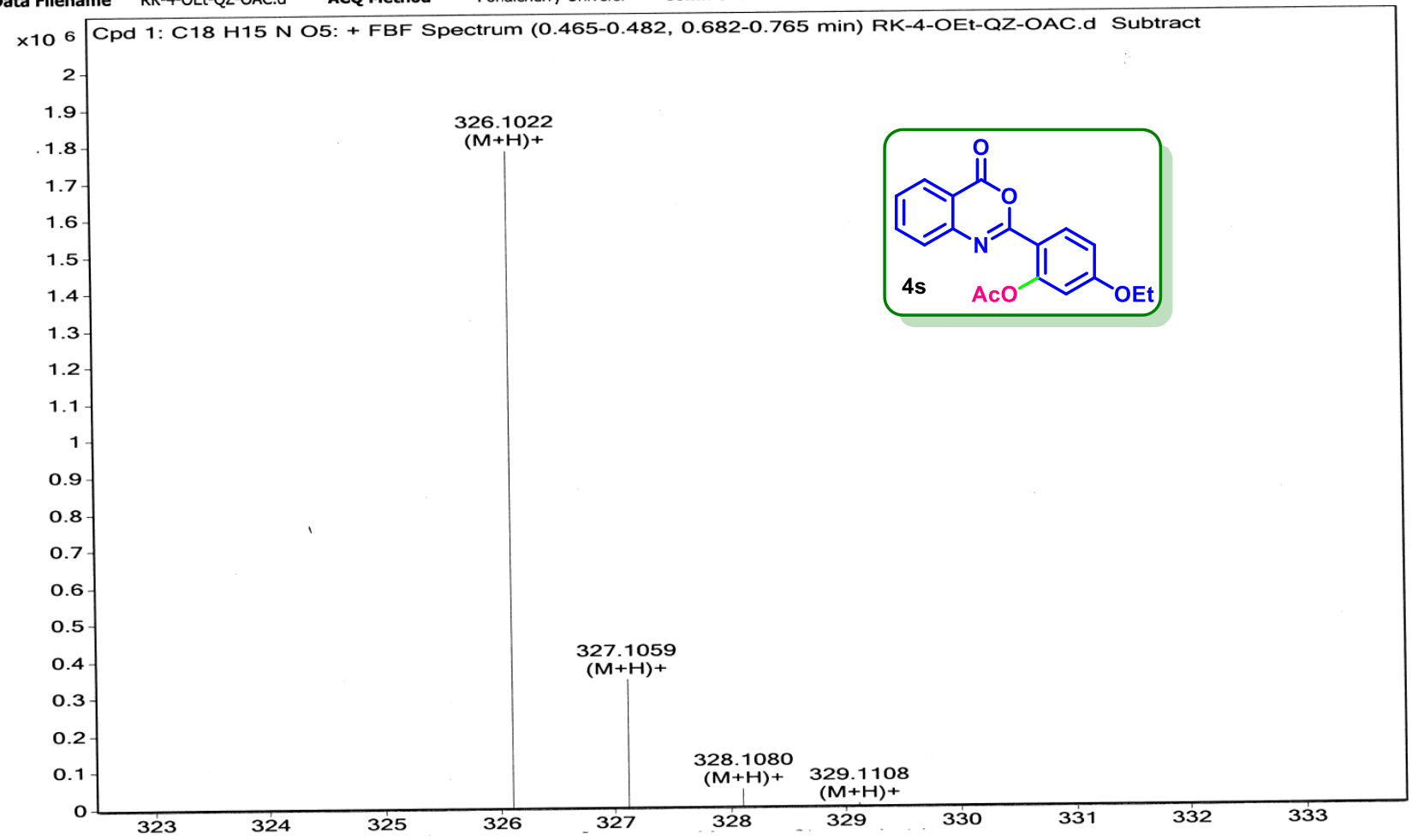

ple Name RK-4Et-QZ-OAC
Vol -1
ta Filename RK-4Et-QZ-OAC.d
Position
InjPosition
ACQ Method
Pondicherry Universi
Instrument Name Q-TOF
SampleType Sample
Comment RK-MB-309.1001
User Name QTOF-PU\admin
IRM Calibration Status Success
Acquired Time 03-05-2018 12:56:28
x10 5
Cpd 1: C18 H15 N O4: + FBF Spectrum (0.445-0.768 min) RK-4Et-QZ-OAC.d Subtract
310.1103
(M+H)+
311.1136
(M+H)+
312.1152
(M+H)+
4r
AcO
Et
O
O
N
2.5
2.4
2.3
2.2
2.1
2
1.9
1.8
1.7
1.6
1.5
1.4
1.3
1.2
1.1
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
308.5
309
309.5
310
310.5
311
311.5
312
312.5
313
313.5
314

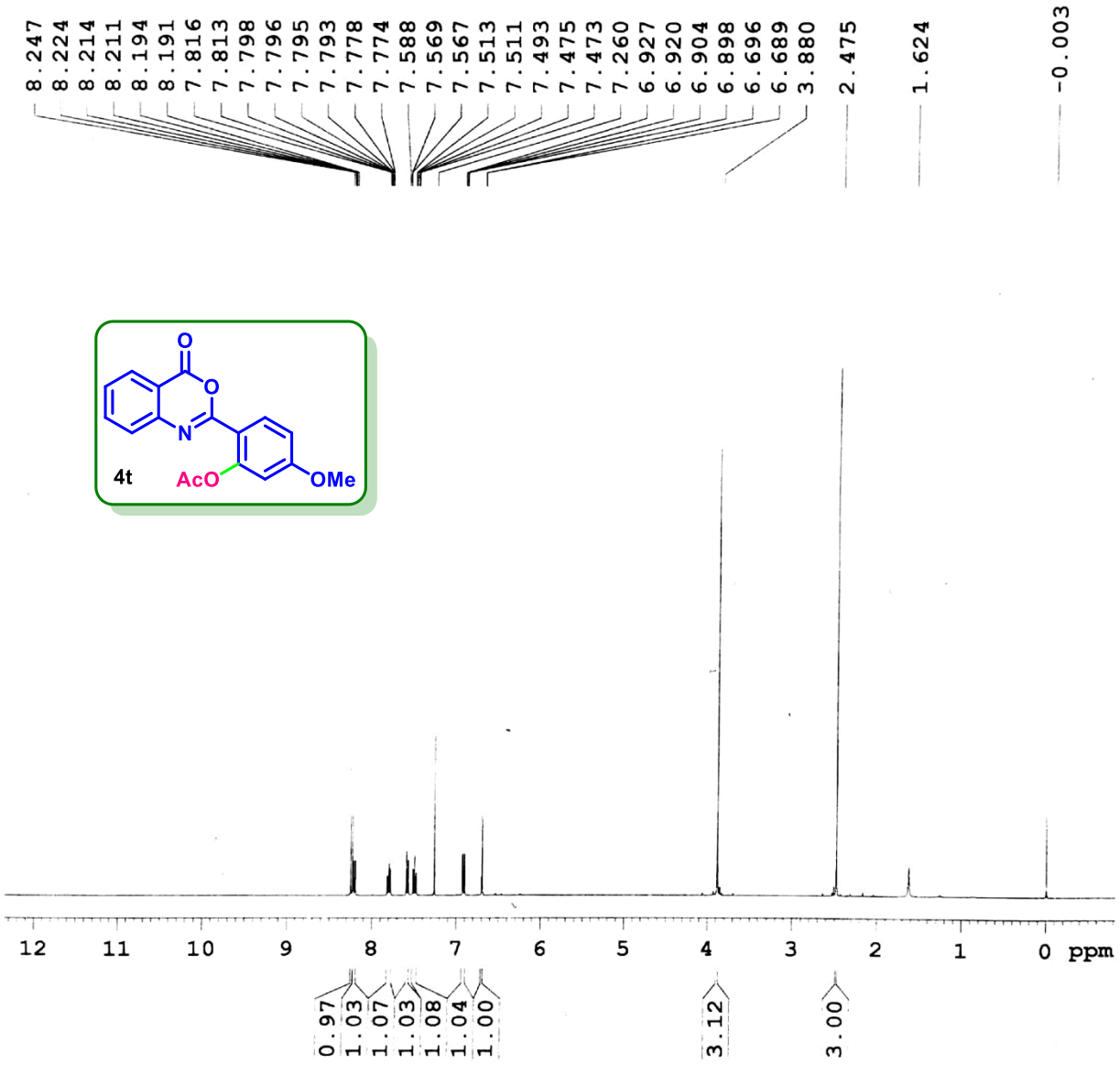



```
Current Data Parameters
NAME      RK-4-OET-QZ-OAC
EXPNO                   2
PROCNO                  1

F2 - Acquisition Parameters
Date_           20180725
Time               11.49
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               295.4 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
```

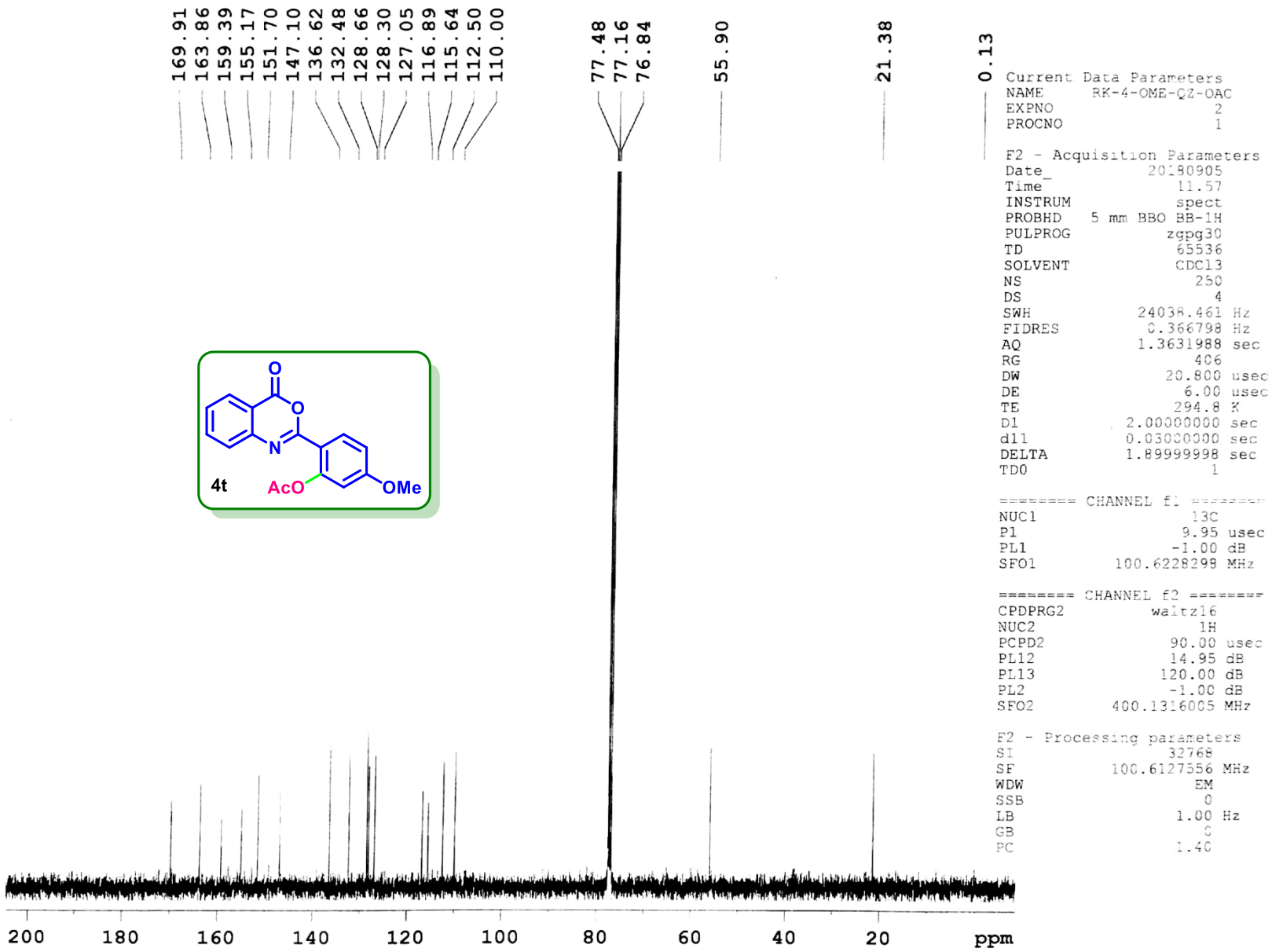

169.91
163.31
159.43
155.26
151.70
147.15
136.62
132.47
128.67
128.26
127.05
116.90
115.41
112.90
110.40
77.48
77.37
77.16
76.85
64.32
21.39
14.73
1.16
4s
AcO
OEt
180
160
140
120
100
80
60
40
20
ppm
Current Data Parameters
NAME RK-4-OET-QZ-OAC
EXPNO 3
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180725
Time 12.05
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 295.7 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 100.6127541 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Sample Name	RK-4-OEt-QZ-OAC	**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-OAC.d	**ACQ Method**	Pondicherry Universi	**Comment**	RK-MB-325.0950	**Acquired Time**	27-07-2018 14:10:31



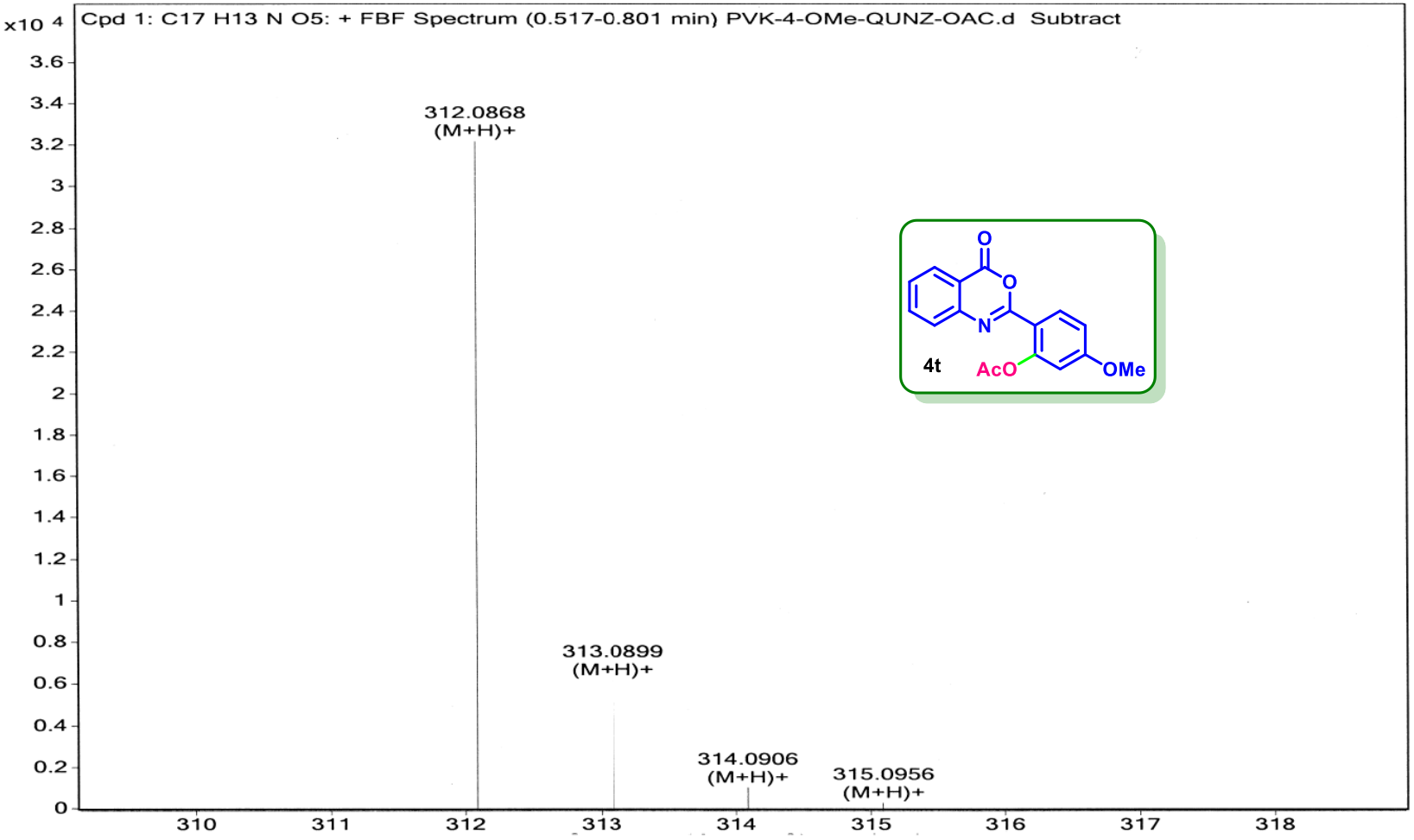


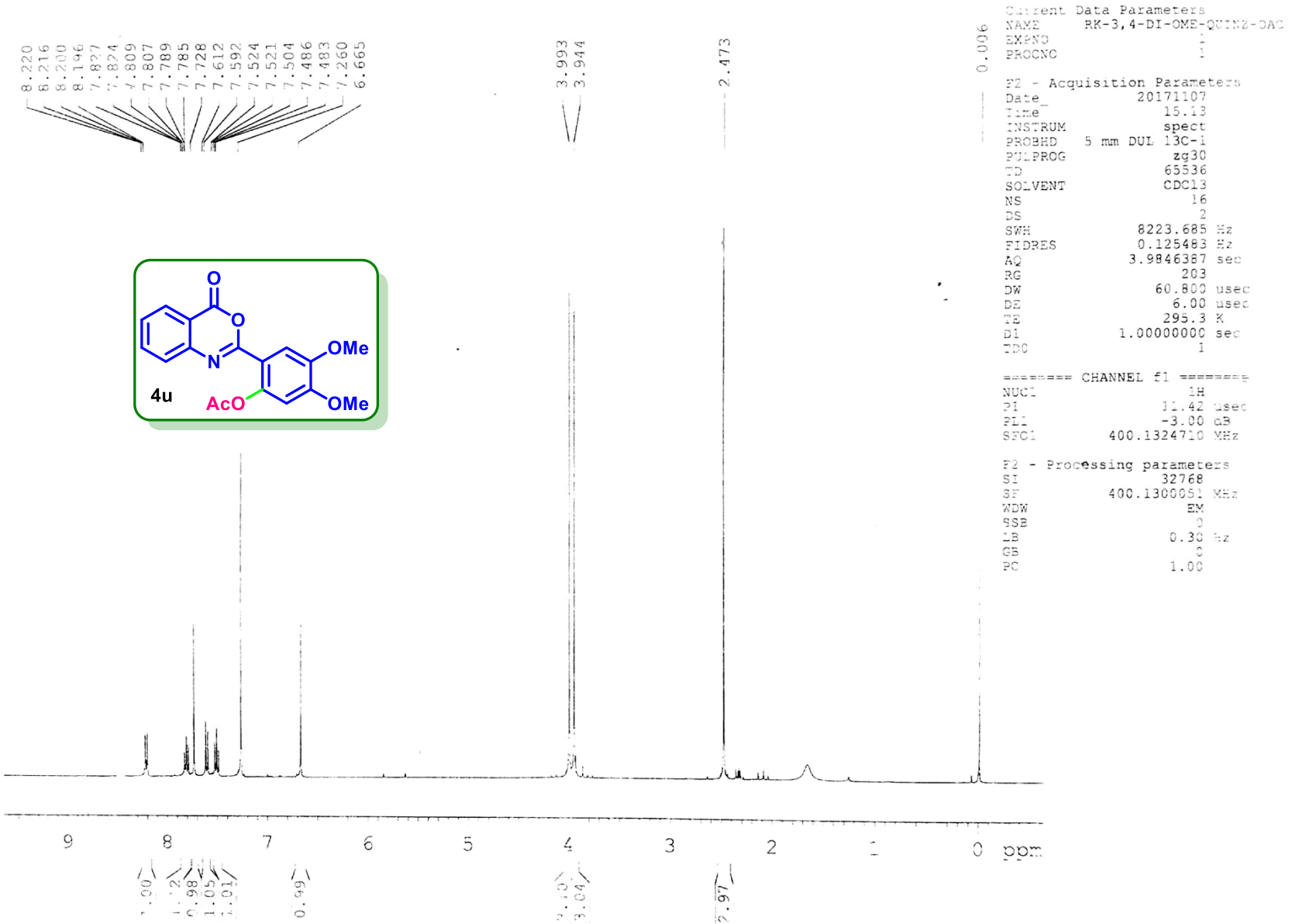

```
Current Data Parameters
NAME      RK-4-OME-QZ-OAC
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_            20180905
Time                11.45
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                    256
DW                 60.800 usec
DE                  6.00 usec
TE                 295.0 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-OME-QZ-OAC
EXPNO                   2
PROCNO                  1

F2 - Acquisition Parameters
Date_            20180905
Time               11.57
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  250
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                294.8 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          100.6127556 MHz
WDW                    EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

Sample Name	PVK-4-OMe-QUNZ-OAC	**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-OAC.d	**ACQ Method**	Pondicherry Universi	**Comment**	PVK-MB-312.0872	**Acquired Time**	25-10-2017 15:33:55



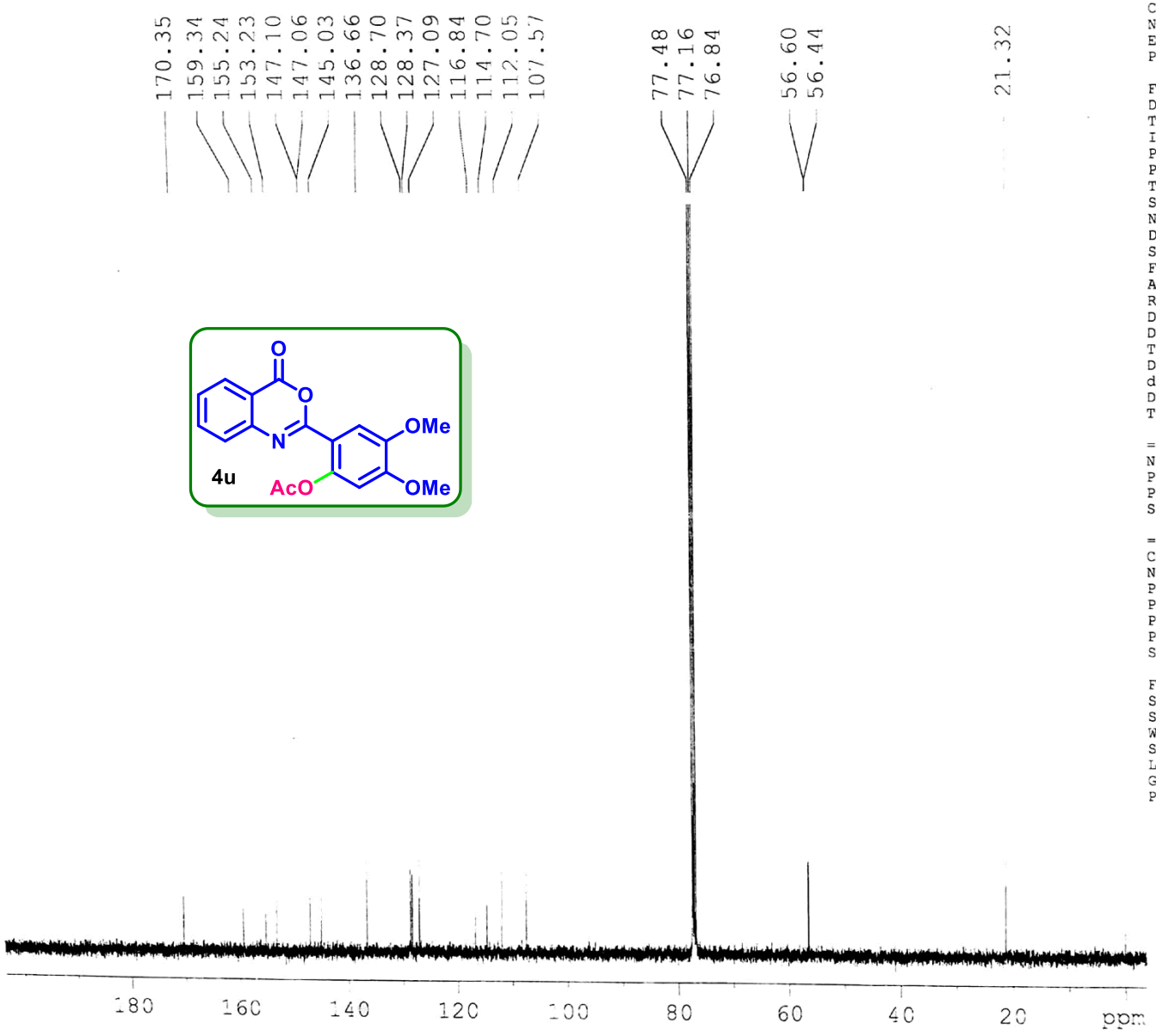


Current Data Parameters
NAME RK-3,4-DI-OME-QUINZ-OAC
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20171107
Time 15.13
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 295.3 K
D1 1.00000000 sec
TD0 1

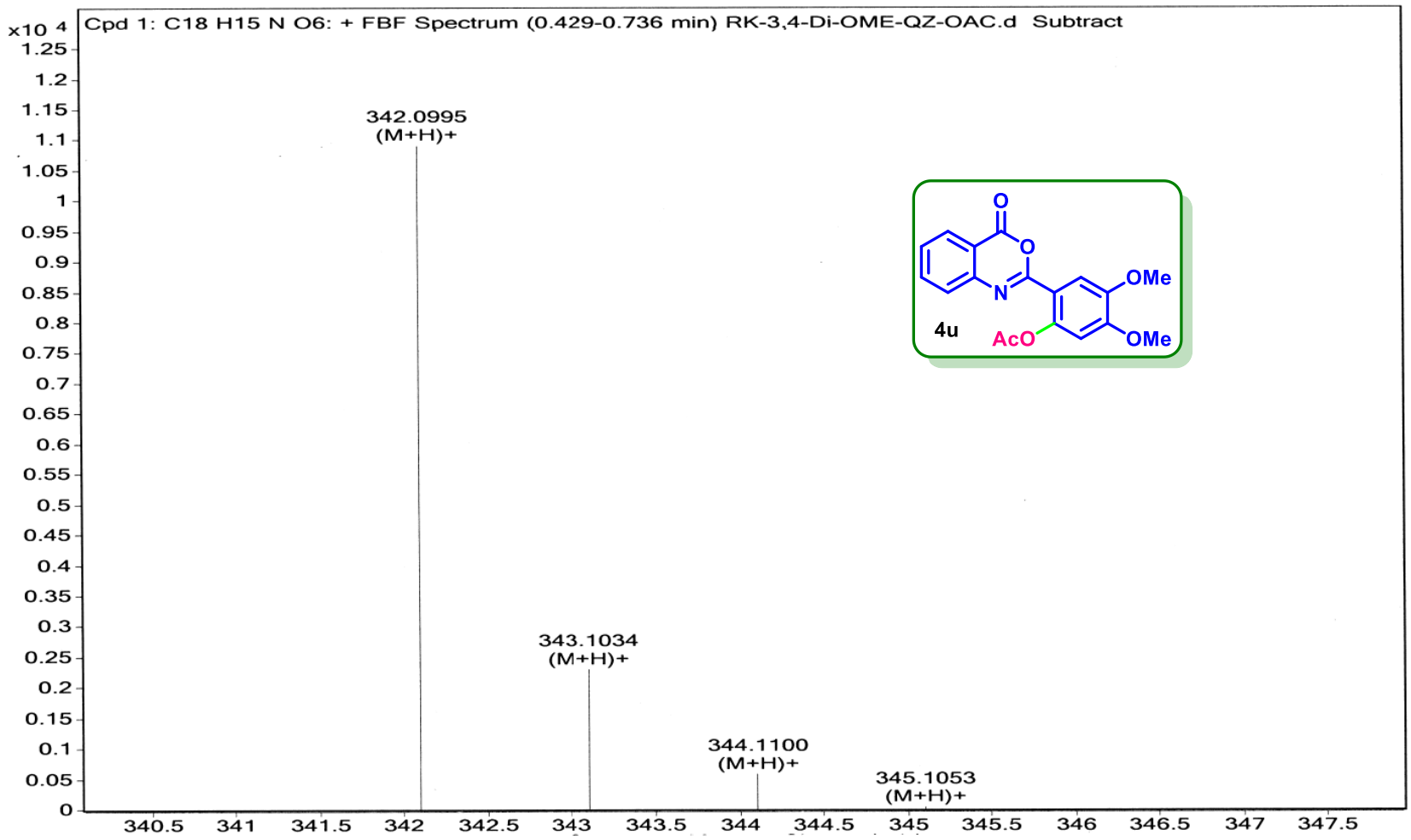
======== CHANNEL f1 ========
NUC1 1H
P1 11.42 usec
PL1 -3.00 dB
SFO1 400.1324710 MHz

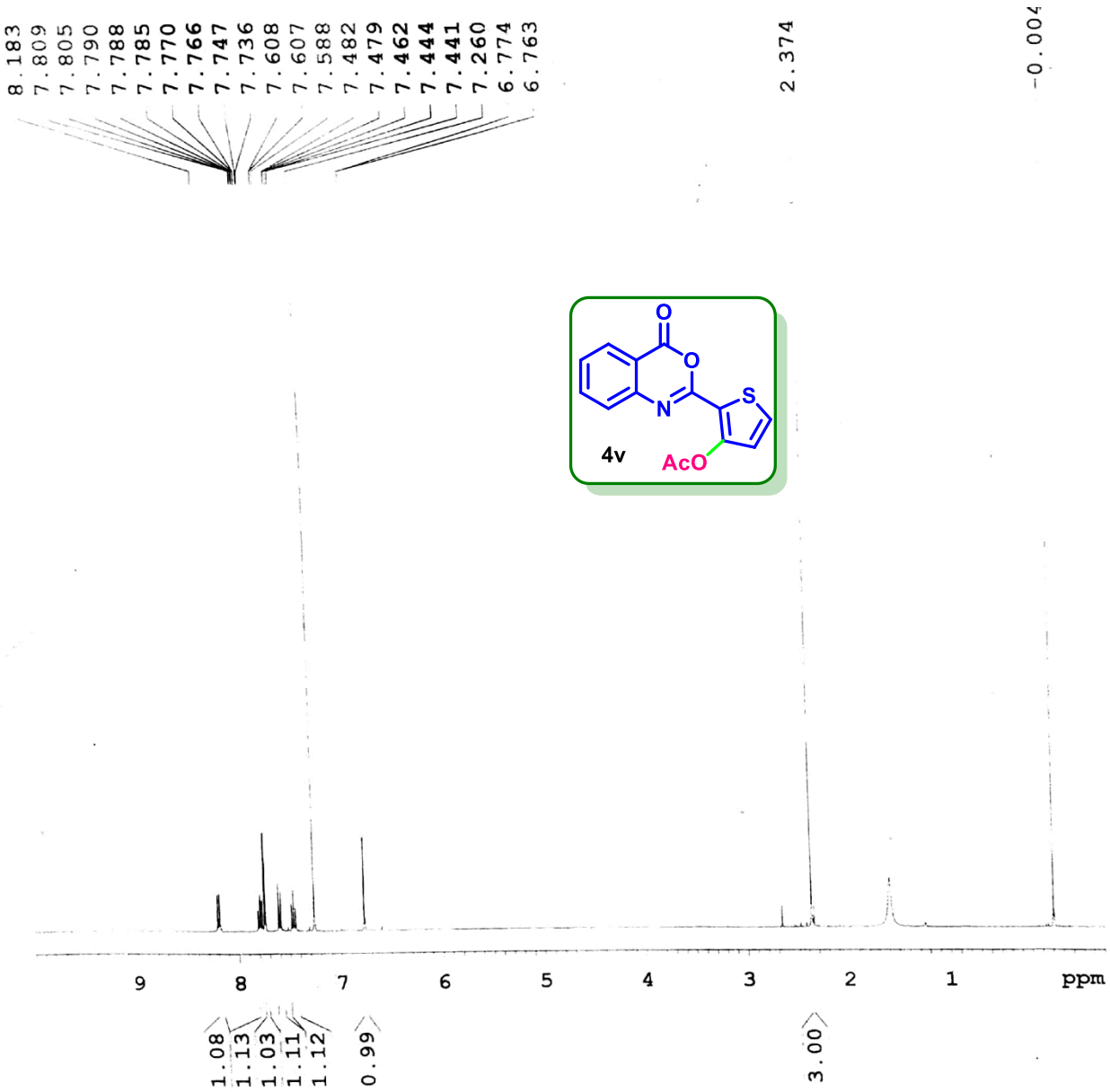
F2 - Processing parameters
SI 32768
SF 400.1300051 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00




```
Current Data Parameters
NAME      RK-3,4-DI-OME-QUINZ-OAC
EXPNO                           2
PROCNO                          1

F2 - Acquisition Parameters
Date_                    20171107
Time                        15.26
INSTRUM                     spect
PROBHD    5 mm DUL 13C-1
PULPROG                  zgpg30
TD                          65536
SOLVENT                     CDCl3
NS                            237
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                          295.9 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                  100.6127546 MHz
WDW                             EM
SSB                              0
LB                            1.00 Hz
GB                               0
PC                            1.40
```

ple Name	RK-3,4-Di-OME-QZ-OAC	**Position**		**Instrument Name**	Q-TOF	**User Name**	QTOF-PU\admin
Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
ata Filename	RK-3,4-Di-OME-QZ-OAC	**ACQ Method**	Pondicherry Universi	**Comment**	RK-MB-341.0899	**Acquired Time**	03-05-2018 12:52:50





Current Data Parameters

NAME	RK-THPN-Qz-OAc
EXPNO	1
PROCNO	1

F2 - Acquisition Parameters

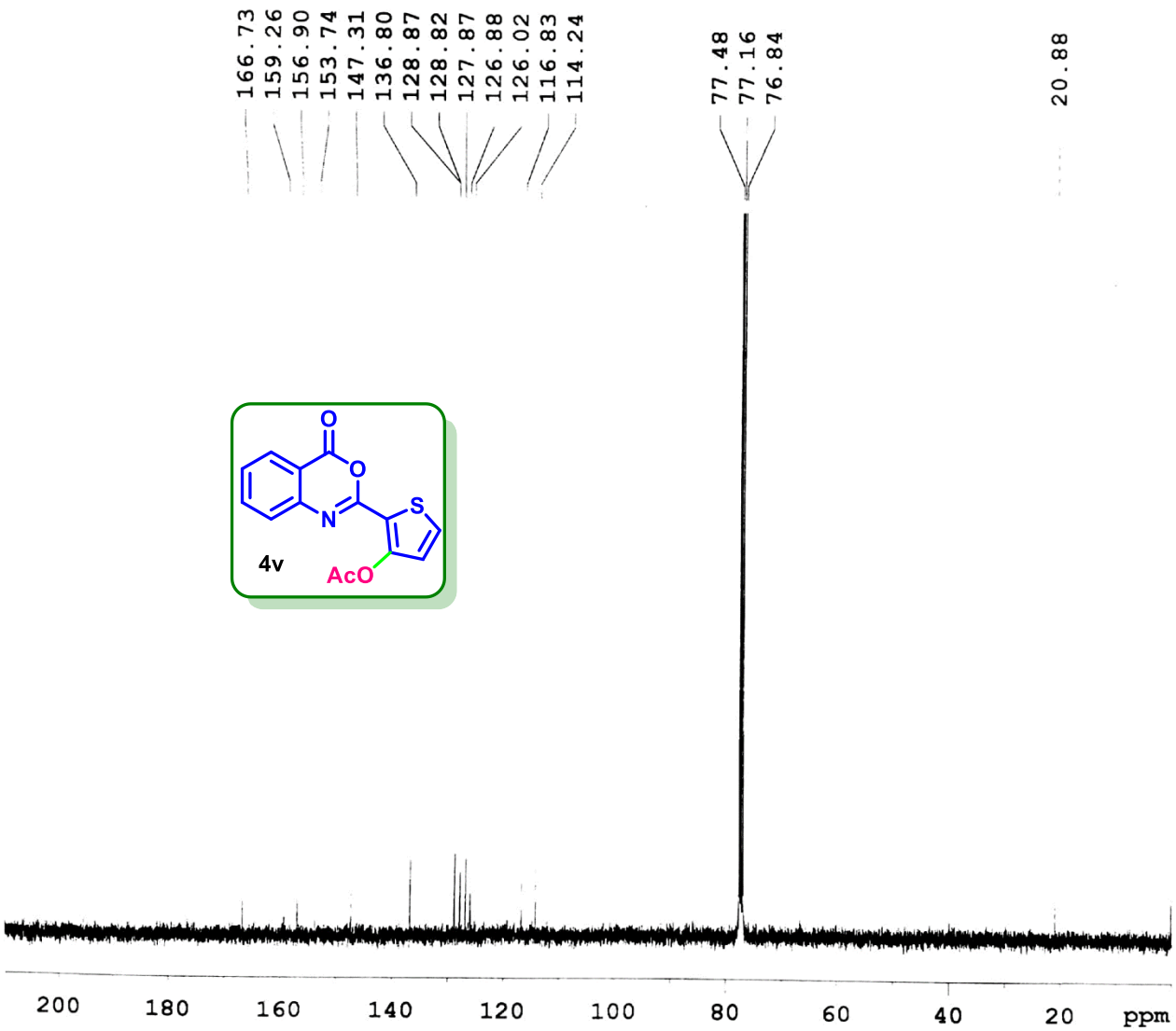
Date_	20180930
Time	10.09
INSTRUM	spect
PROBHD	5 mm BBO BB-1H
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	645
DW	60.800 usec
DE	6.00 usec
TE	293.5 K
D1	1.00000000 sec
TD0	1

======== CHANNEL f1 ========

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

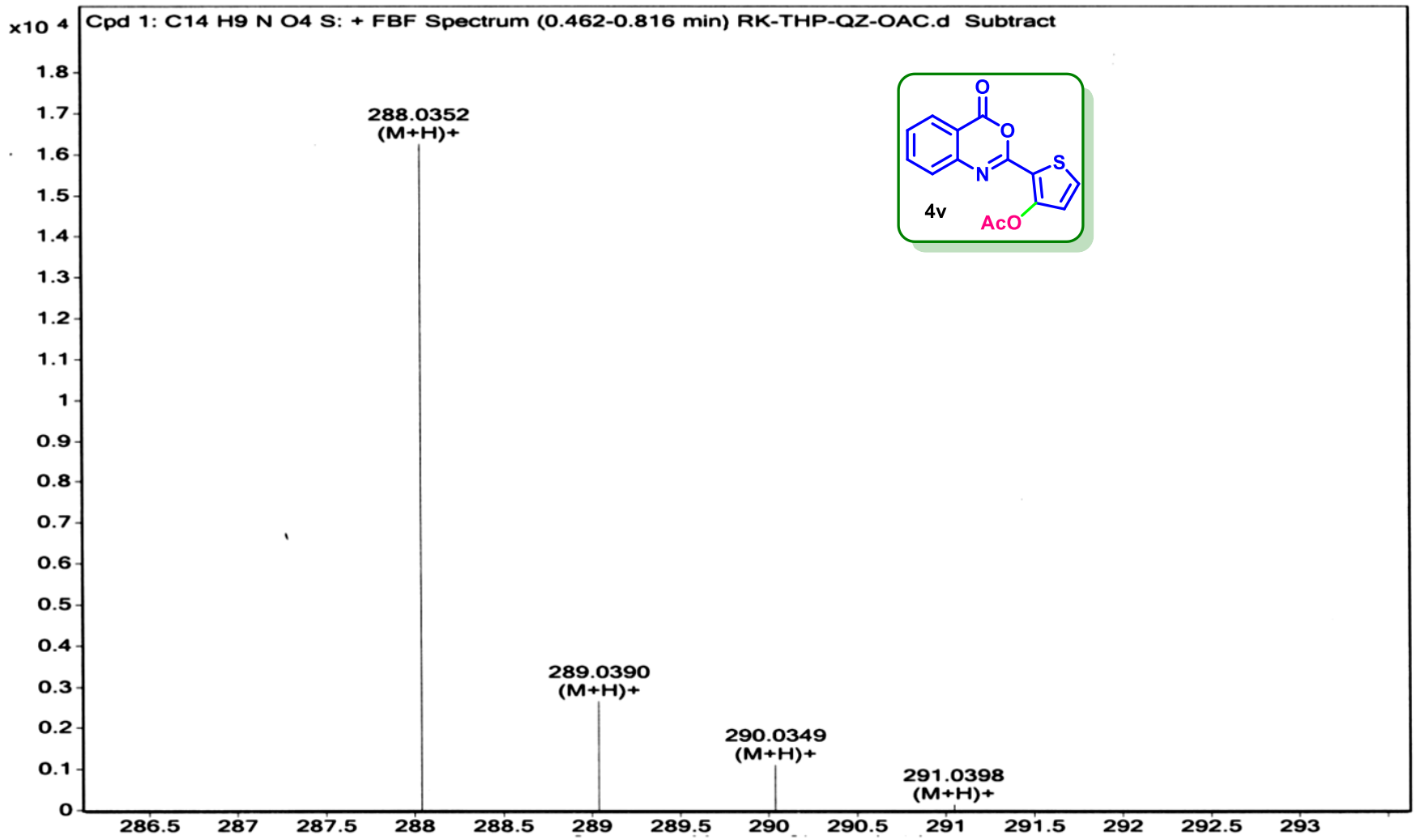
F2 - Processing parameters

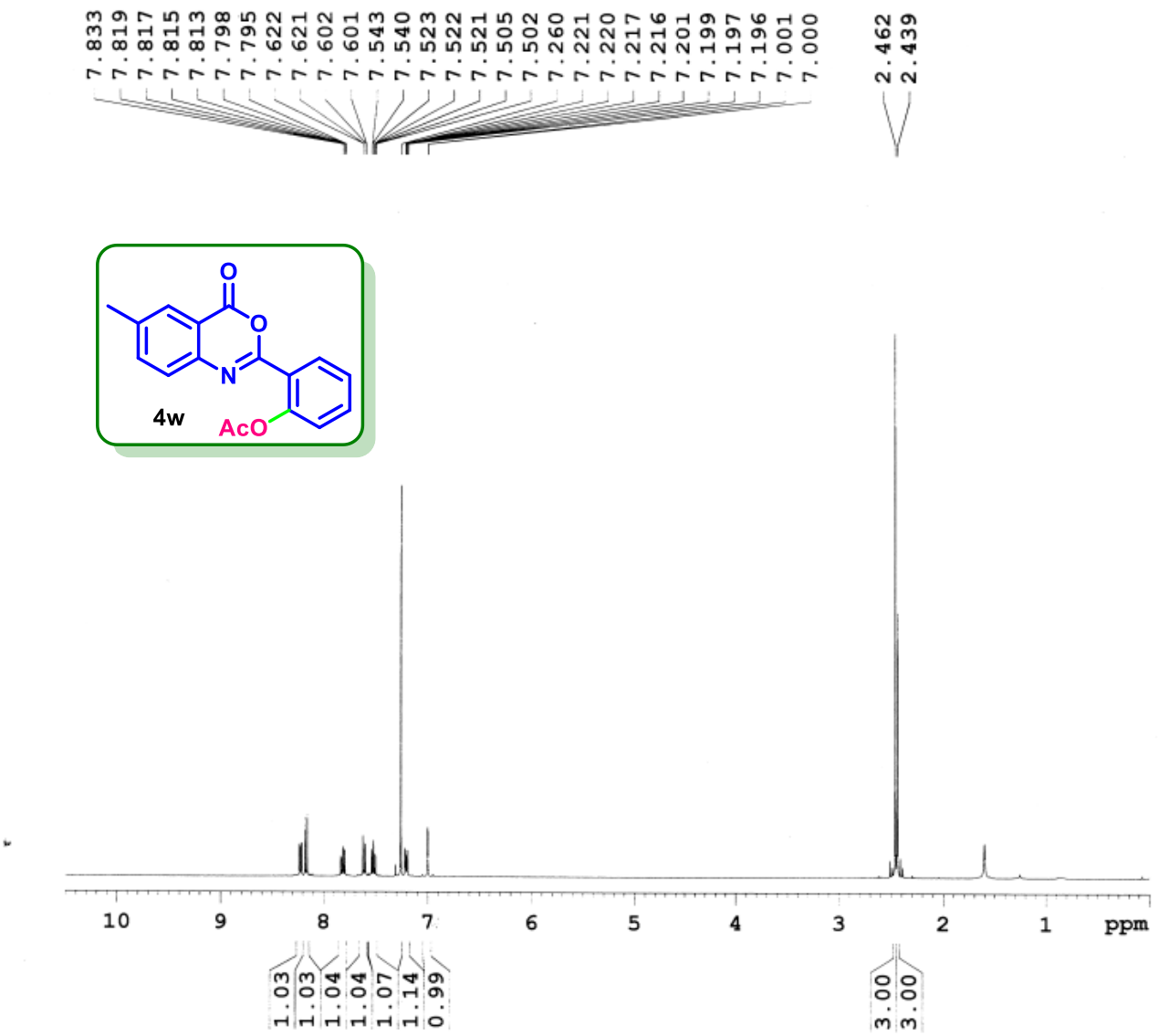
SI	32768
SF	400.1300048 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



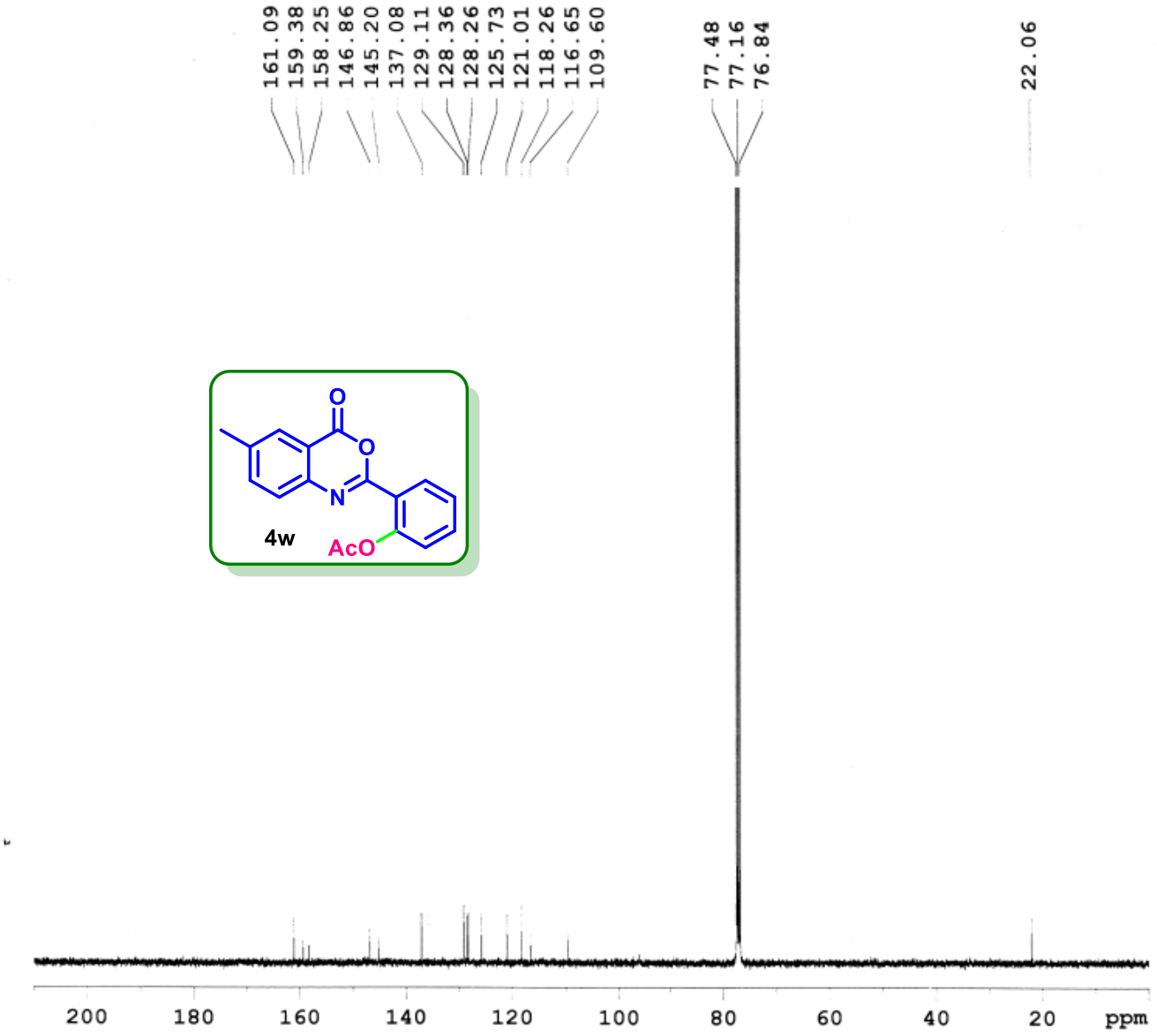

```
Current Data Parameters
NAME      RK-THPN-Qz-OAc
EXPNO                  3
PROCNO                 1

F2 - Acquisition Parameters
Date_           20181008
Time              13.38
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                 45.2
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                 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          100.6127540 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

Sample Name	RK-THP-QZ-OAC	**Position**		**Instrument Name**	Q-TOF	**User Name**	QTOF-PU\admin
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	RK-THP-QZ-OAC.d	**ACQ Method**	Pondicherry Universi	**Comment**	RK-MB-287.0252	**Acquired Time**	03-05-2018 13:04:41



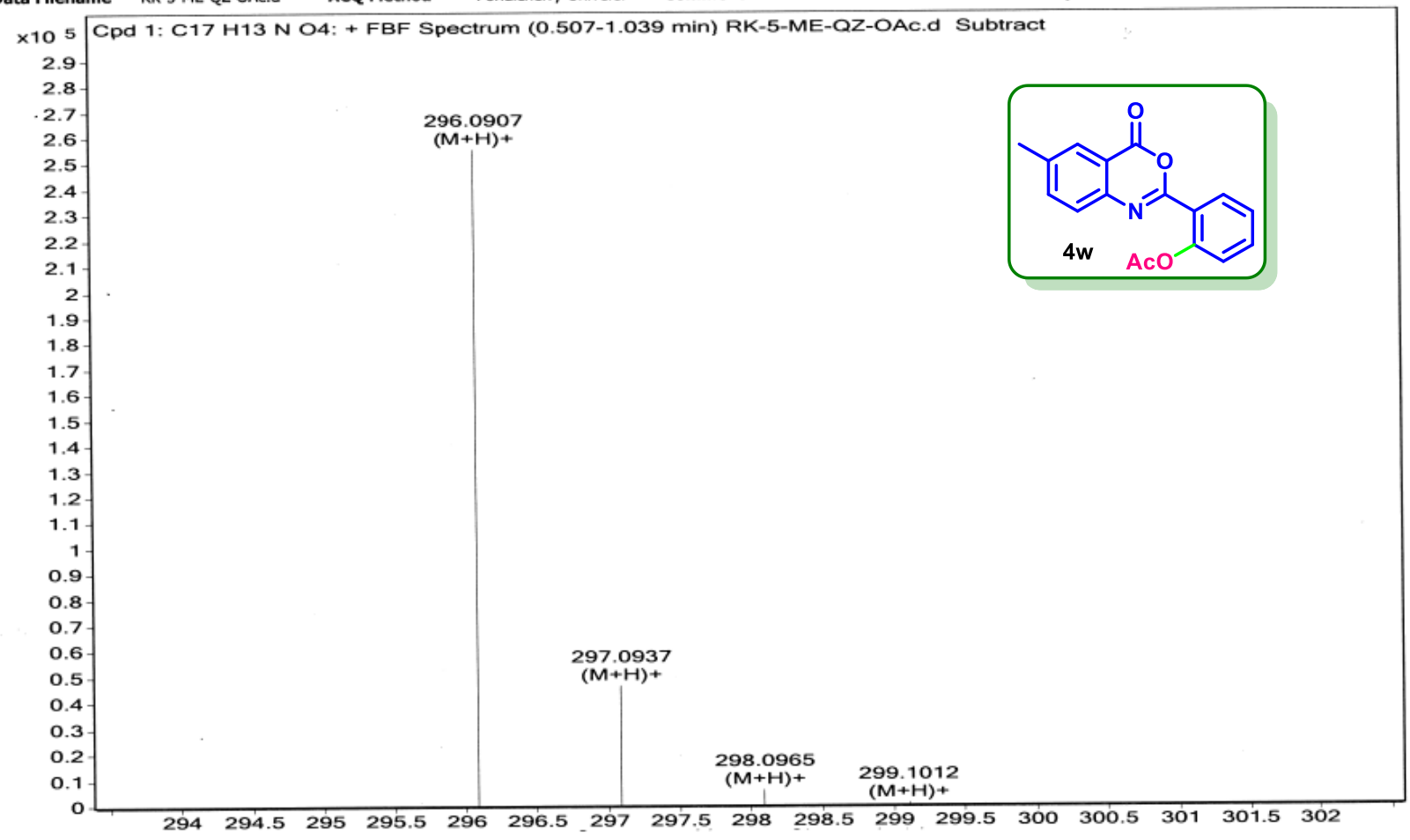


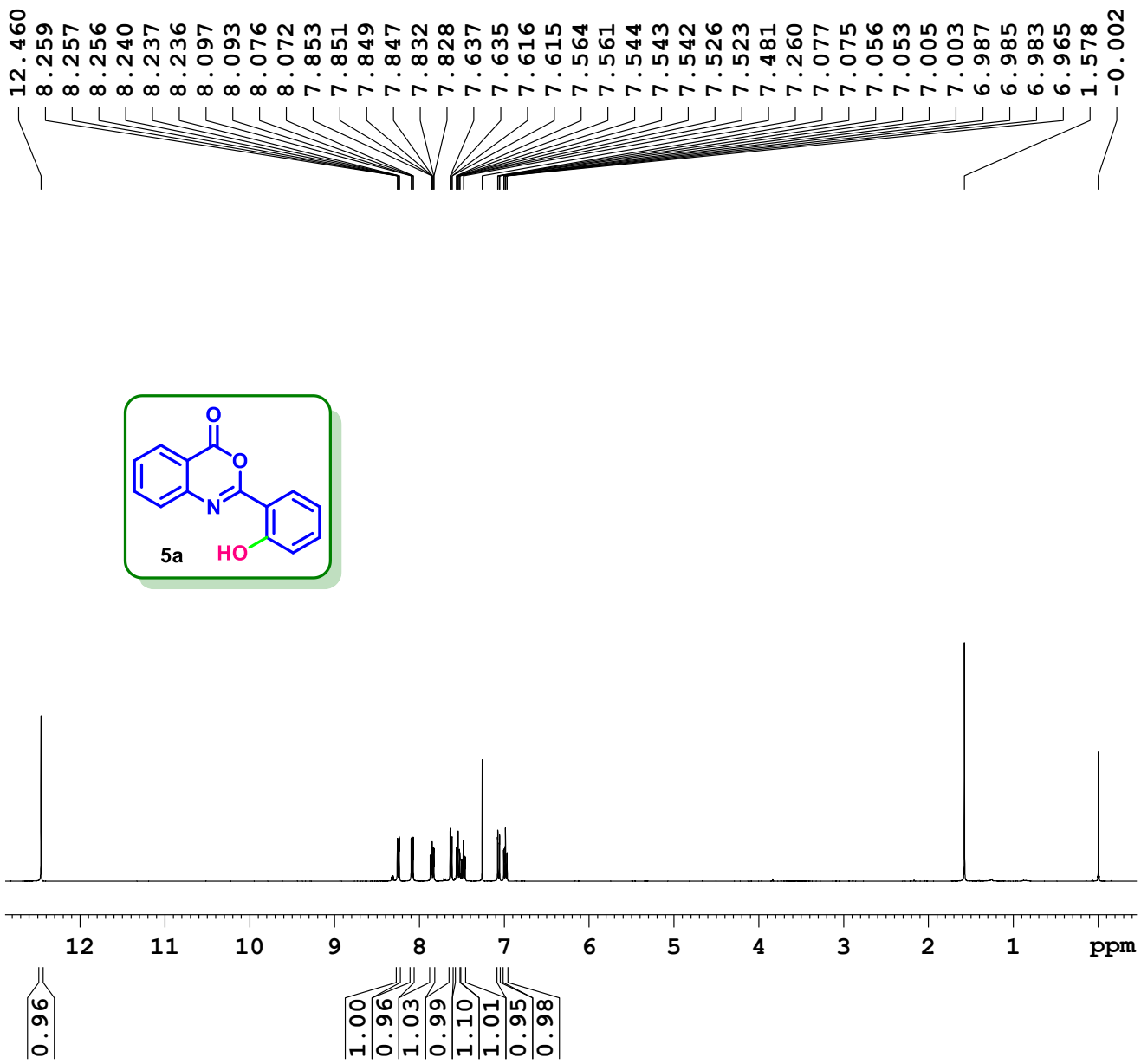

```
Current Data Parameters
NAME       RK-5ME-QZ-OAC
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20190408
Time               16.47
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                295.0 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
```



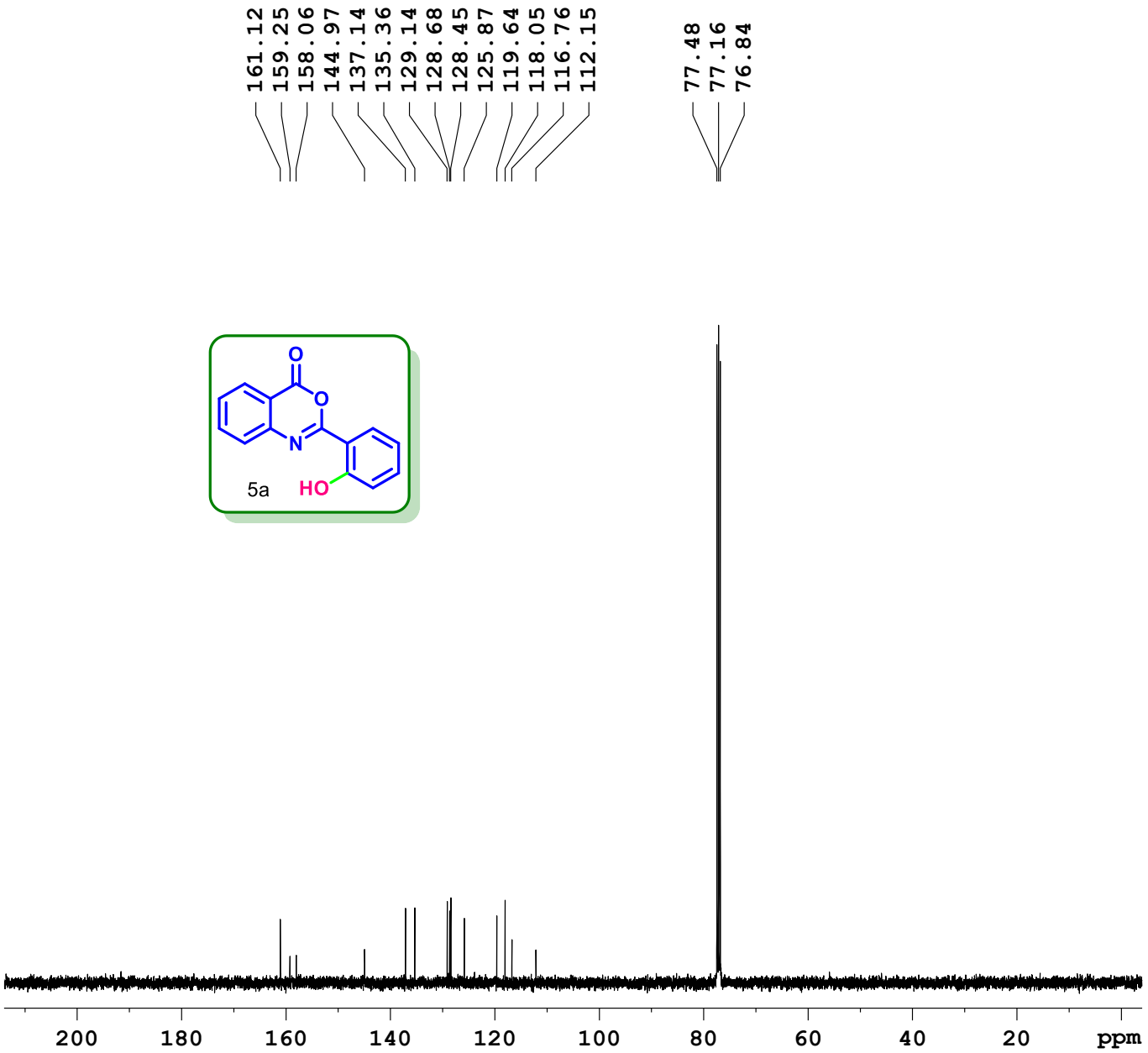

```
Current Data Parameters
NAME       RK-5-ME-QZ-OH
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20190408
Time              20.22
INSTRUM           spect
PROBHD   5 mm BBO BB-1H
PULPROG         zgpg30
TD               65536
SOLVENT          CDCl3
NS                1351
DS                   4
SWH          24038.461 Hz
FIDRES        0.366798 Hz
AQ           1.3631988 sec
RG                 575
DW              20.800 usec
DE               6.00 usec
TE              293.6 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          100.6127557 MHz
WDW                EM
SSB                 0
LB               1.00 Hz
GB                  0
PC               1.40
```

Sample Name	RK-5-ME-QZ-OAc	**Position**		**Instrument Name**	Q-TOF	**User Name**	QTOF-PU\admin
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	RK-5-ME-QZ-OAc.d	**ACQ Method**	Pondicherry Universi	**Comment**	RK-CRR-295.0845	**Acquired Time**	09-04-2019 12:30:47



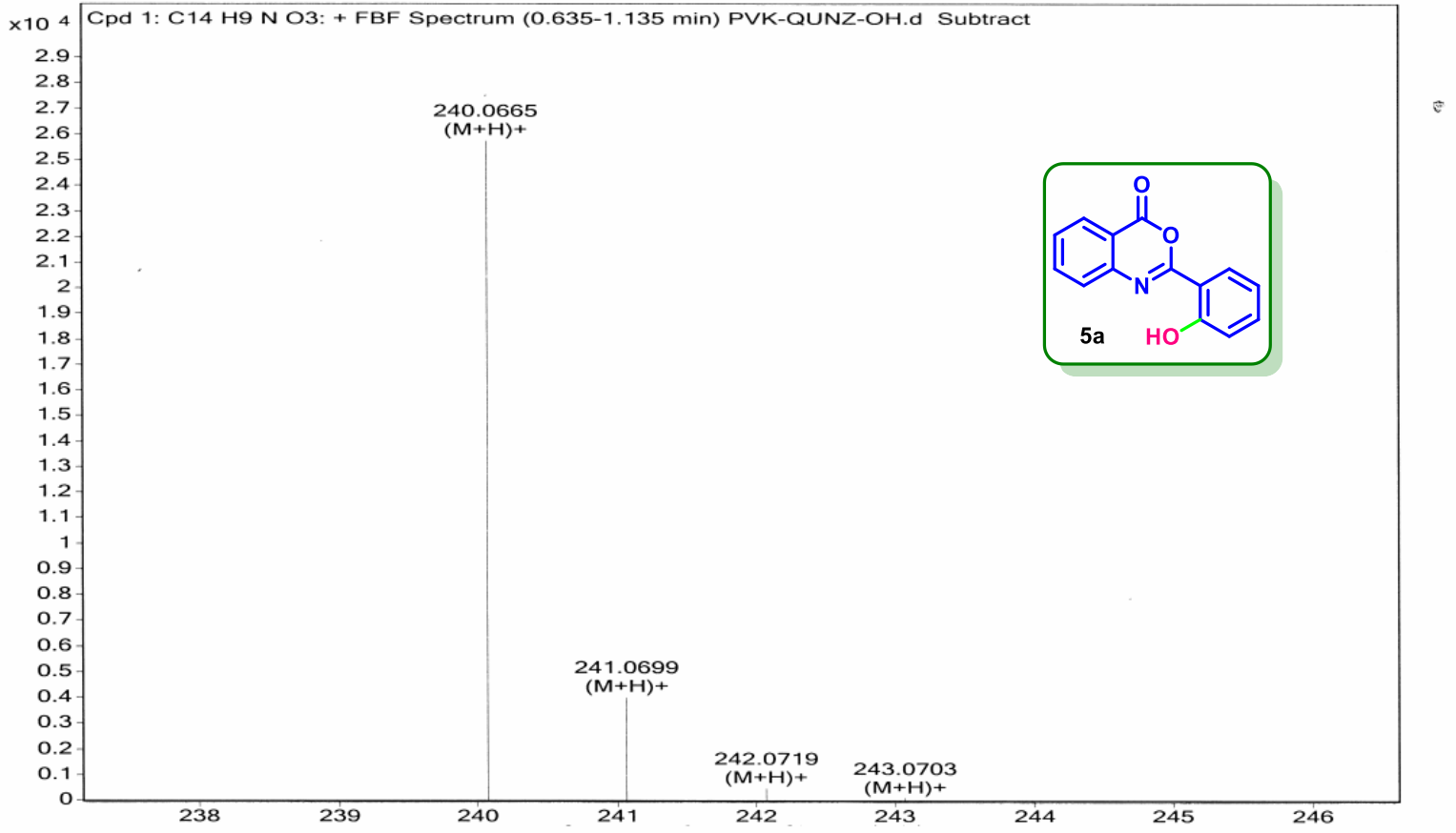


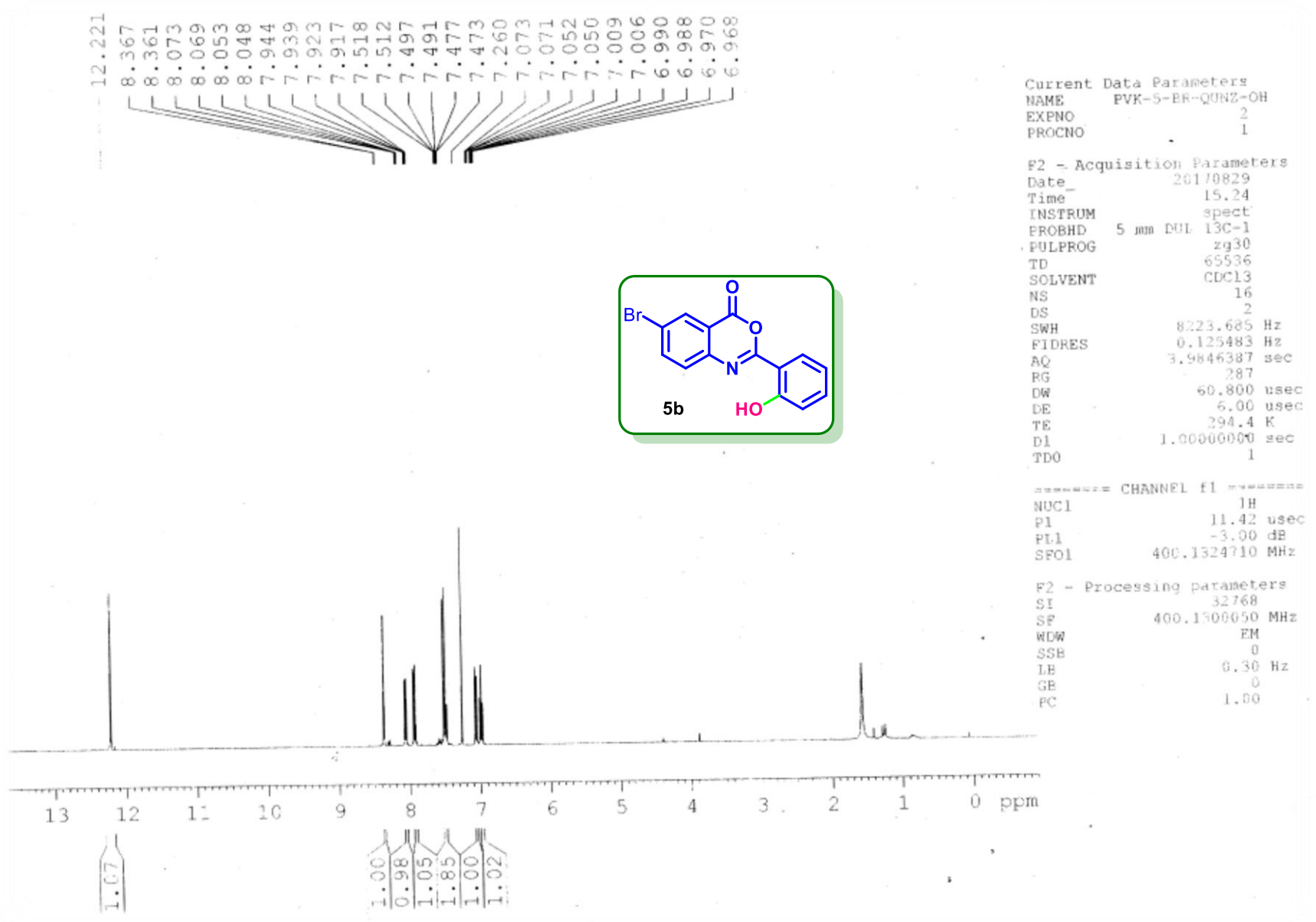

```
Current Data Parameters
NAME       PVK-QUNZ-DIAD
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20161206
Time               14.00
INSTRUM            spect
PROBHD   5 mm DUL 13C-1
PULPROG             zg30
TD                 65536
SOLVENT            CDC13
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                293.9 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
```

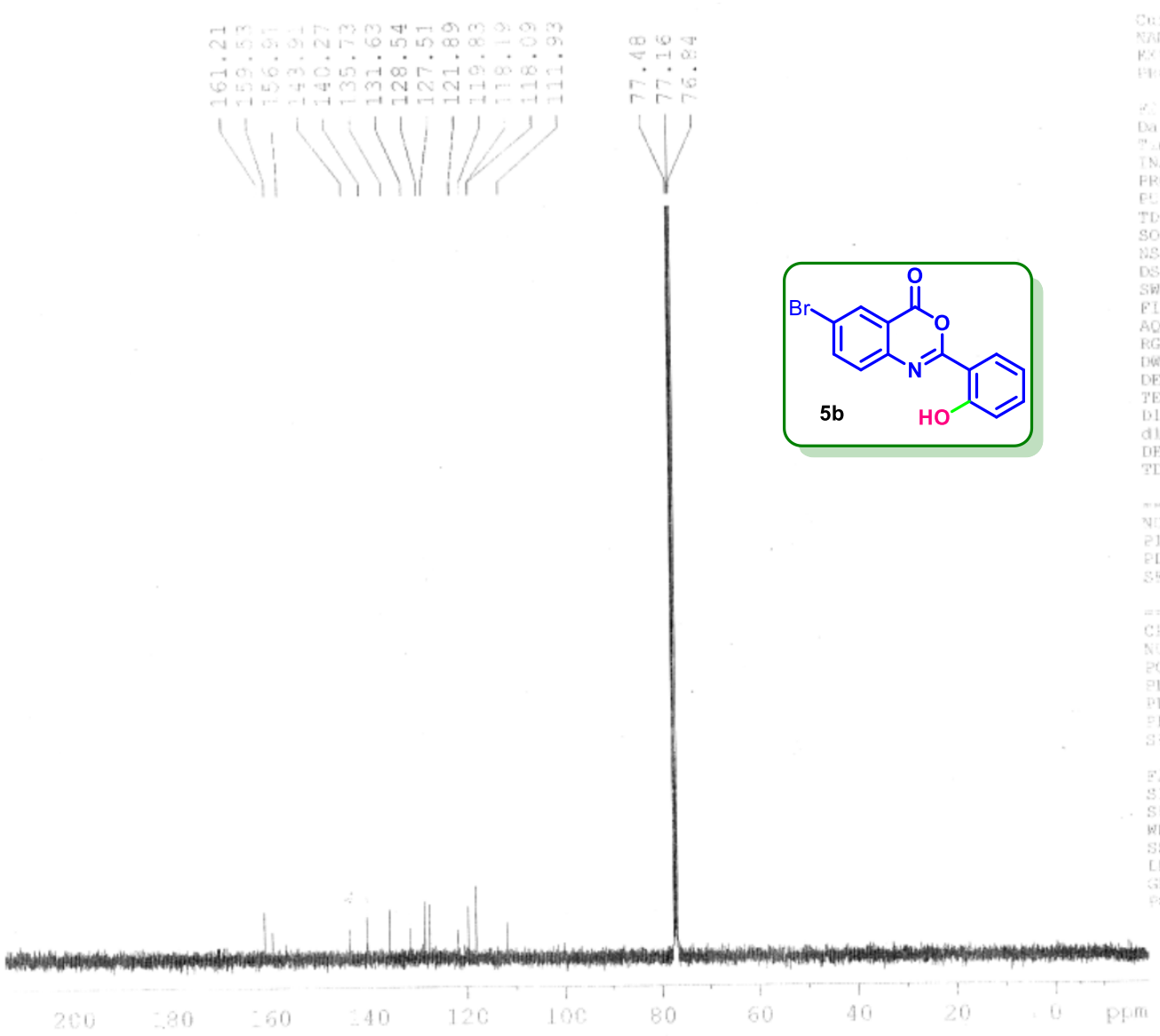



```
Current Data Parameters
NAME          RK-QZ-OH-M
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20180806
Time              10.47
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                  256
DW               20.800 usec
DE                6.00 usec
TE               292.5 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          100.6127556 MHz
WDW                 EM
SSB                  0
LB                1.00 Hz
GB                   0
PC                1.40
```

Sample Name	PVK-QUNZ-OH	**Position**		**Instrument Name**	Q-TOF	**User Name**	QTOF-PU\admin
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	PVK-QUNZ-OH.d	**ACQ Method**	Pondicherry Universi	**Comment**	PVK-MB-239.0582	**Acquired Time**	09-12-2016 12:34:51




12.221
8.367
8.361
8.073
8.069
8.053
8.048
7.944
7.939
7.923
7.917
7.518
7.512
7.497
7.491
7.477
7.473
7.260
7.073
7.071
7.052
7.050
7.009
7.006
6.990
6.988
6.970
6.968
Br
O
O
N
HO
5b
Current Data Parameters
NAME PVK-5-BR-QUNZ-OH
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170829
Time 15.24
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 294.4 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
13 12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
1.07
1.00
0.98
1.05
1.85
1.00
1.02



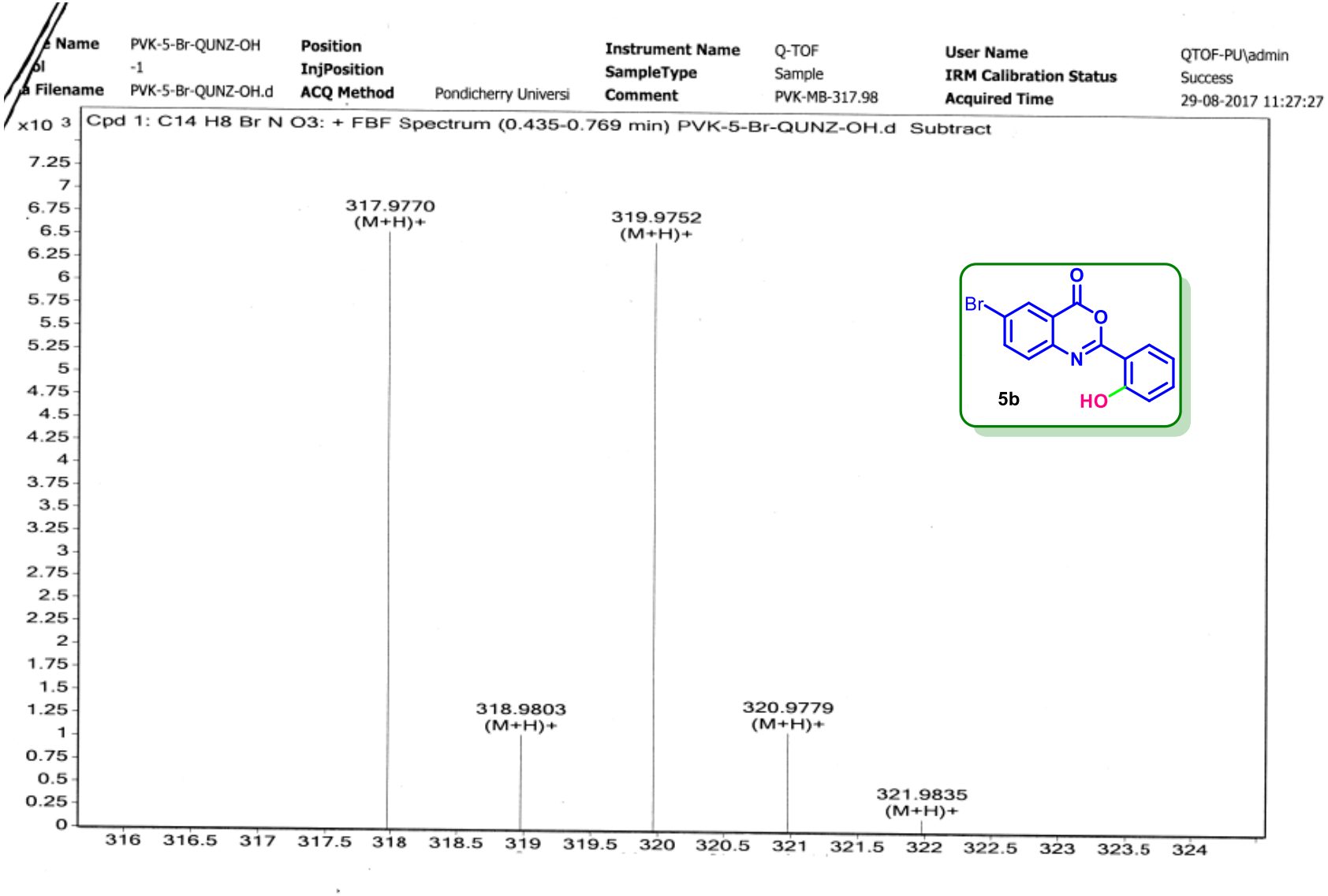
Current Data Parameters
NAME PVK-5-BR-QUNZ-OE
EXPNO 3
PROCNO 1

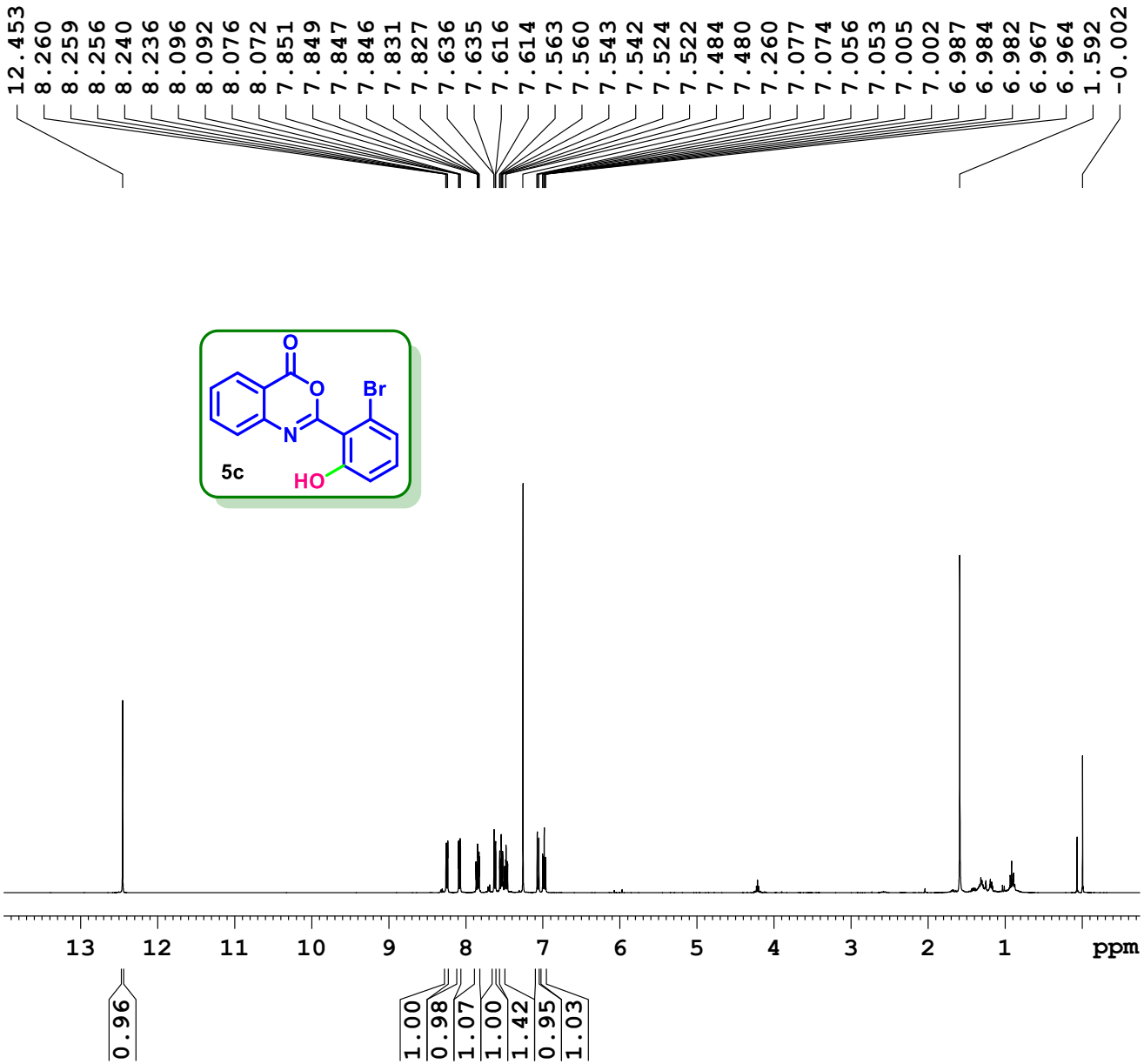
F2 - Acquisition Parameters
Date 20170831
Time 16.29
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631989 sec
RG 64
DW 20.800 usec
DE 6.00 usec
TE 294.4 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

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

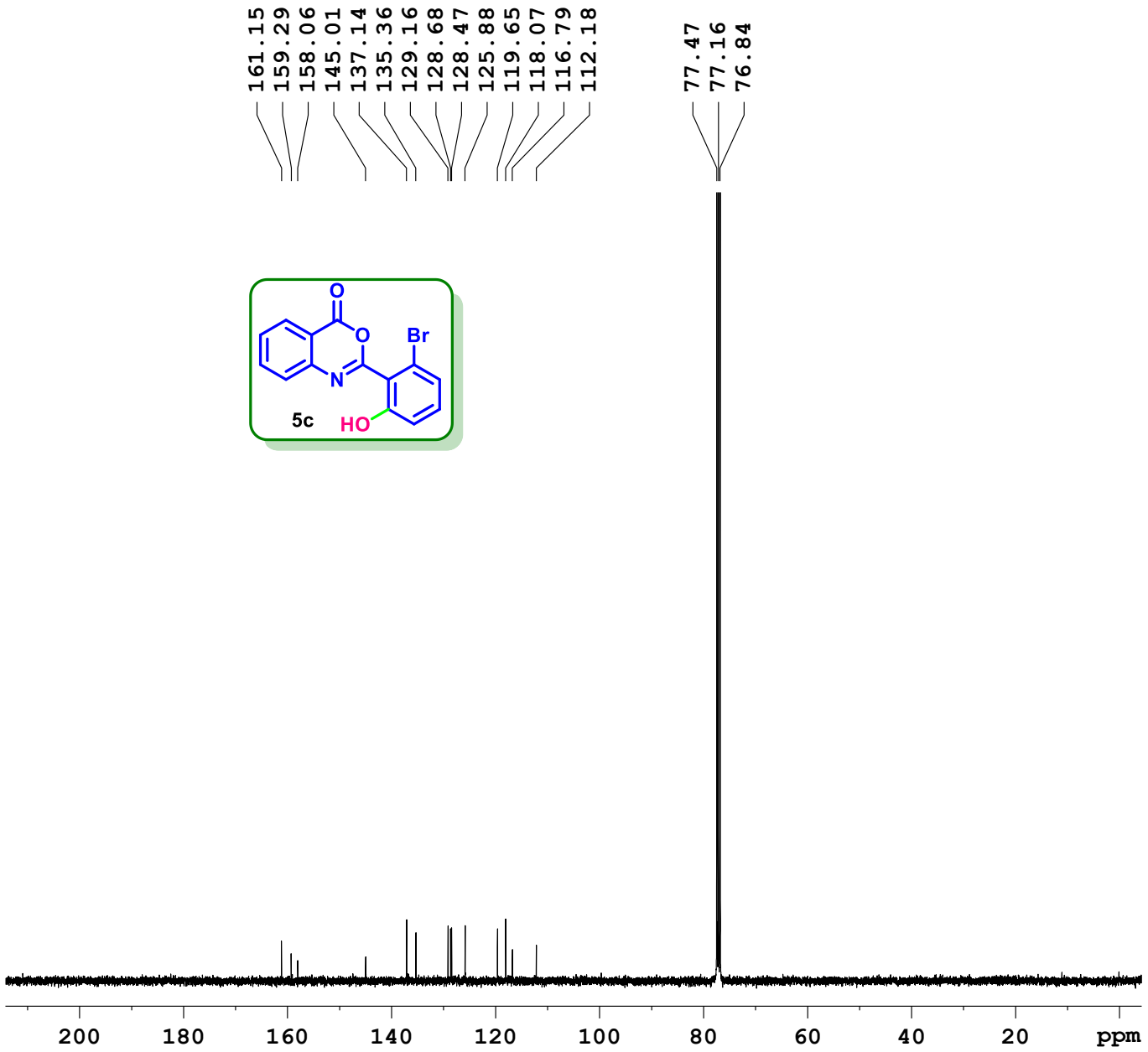
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL12 14.90 dB
PL13 14.90 dB
PL2 -3.00 dB
SFO2 400.1316005 MHz

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

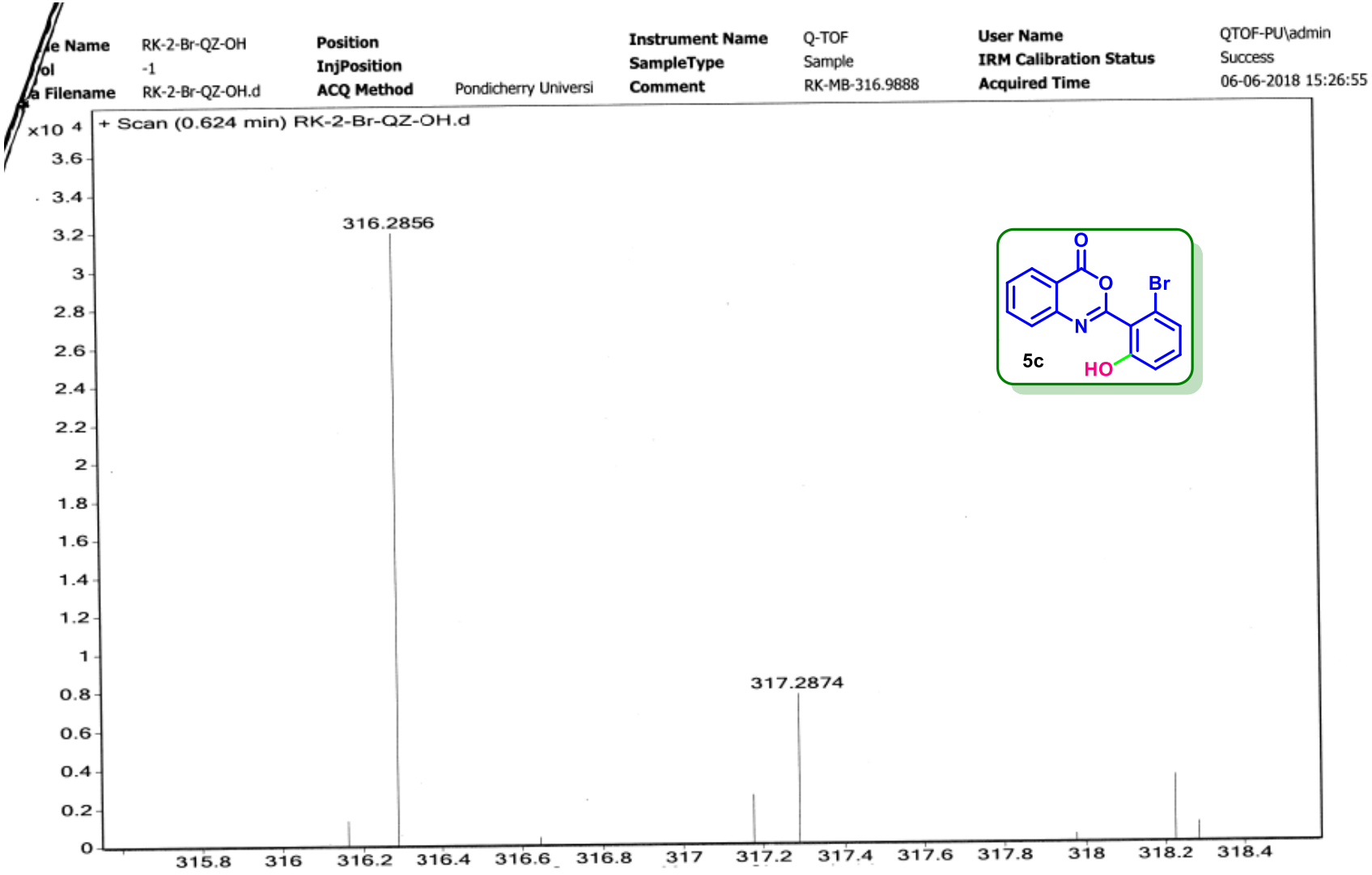

e Name PVK-5-Br-QUNZ-OH
ol -1
a Filename PVK-5-Br-QUNZ-OH.d
Position
InjPosition
ACQ Method
Pondicherry Universi
Instrument Name Q-TOF
SampleType Sample
Comment PVK-MB-317.98
User Name QTOF-PU\admin
IRM Calibration Status Success
Acquired Time 29-08-2017 11:27:27
x10 3
Cpd 1: C14 H8 Br N O3: + FBF Spectrum (0.435-0.769 min) PVK-5-Br-QUNZ-OH.d Subtract
317.9770 (M+H)+
319.9752 (M+H)+
318.9803 (M+H)+
320.9779 (M+H)+
321.9835 (M+H)+
Br
O
O
N
HO
5b

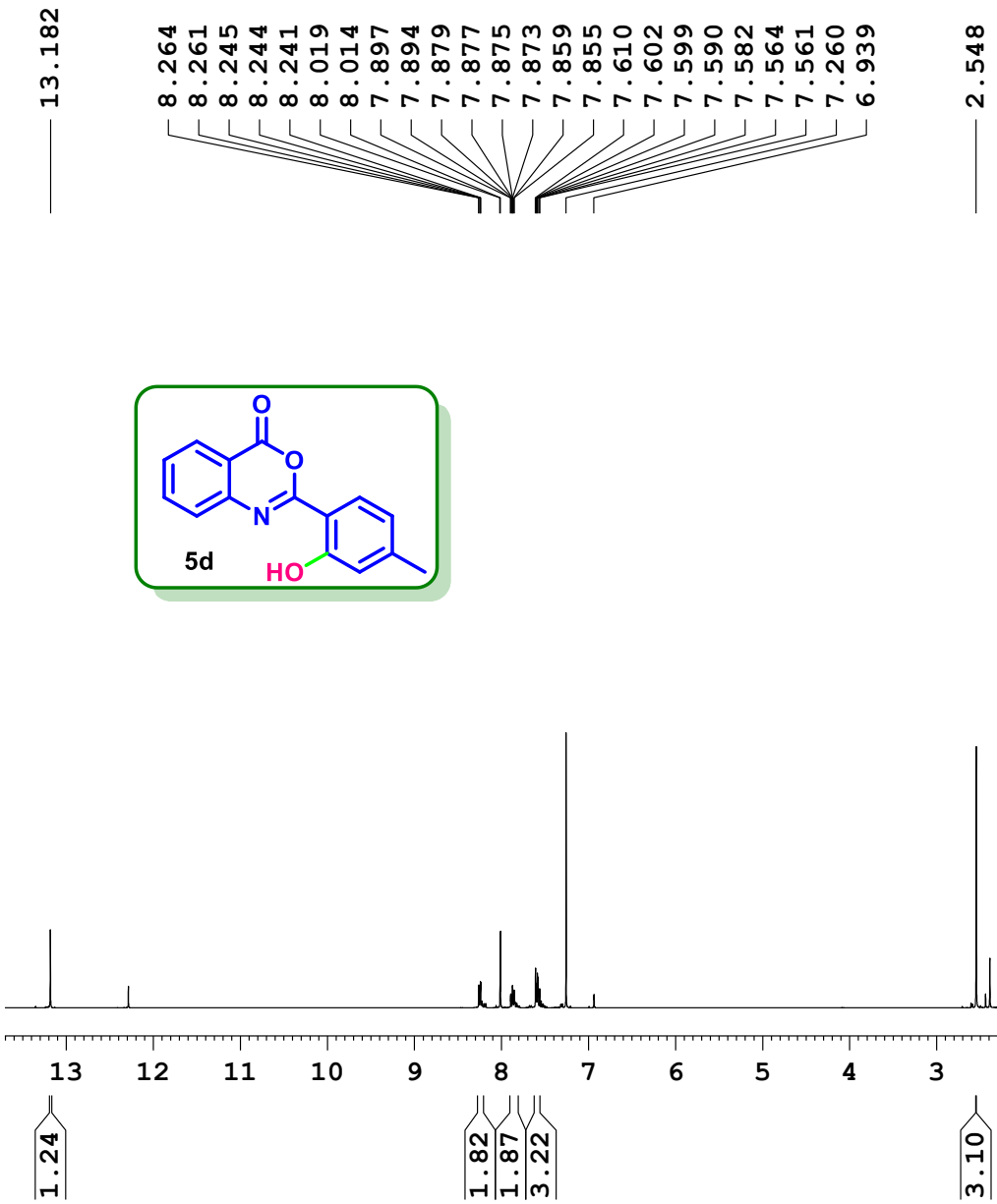



```
Current Data Parameters
NAME      PVK-2-BR-QZ-OH
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20180605
Time               12.41
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                296.0 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          400.1300047 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

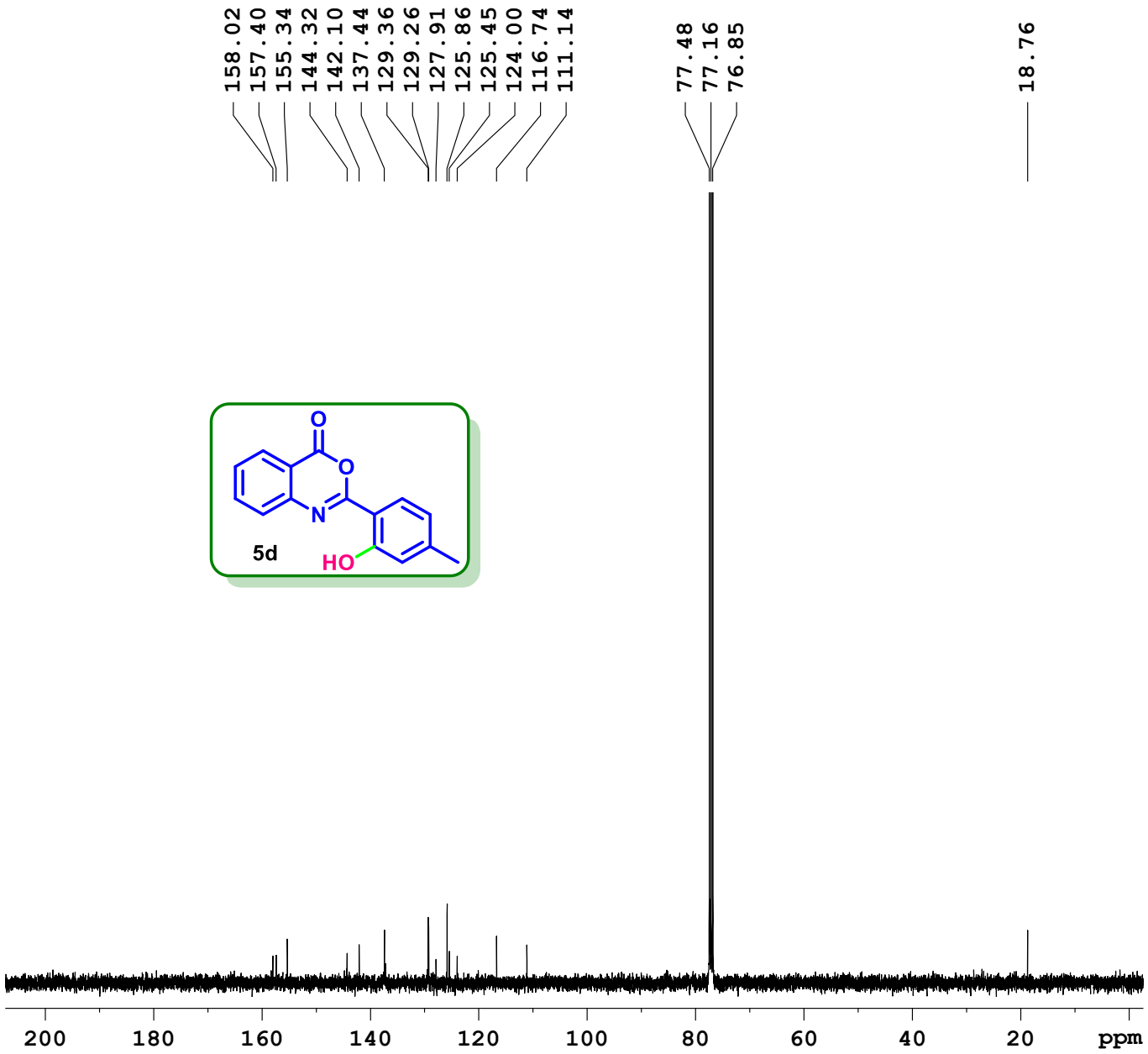



```
Current Data Parameters
NAME      PVK-2-BR-QZ-OH
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20180605
Time               13.13
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                  406
DW               20.800 usec
DE                6.00 usec
TE                296.2 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          100.6127539 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```


e Name RK-2-Br-QZ-OH
ol -1
a Filename RK-2-Br-QZ-OH.d
Position
InjPosition
ACQ Method Pondicherry Universi
Instrument Name Q-TOF
SampleType Sample
Comment RK-MB-316.9888
User Name QTOF-PU\admin
IRM Calibration Status Success
Acquired Time 06-06-2018 15:26:55
+ Scan (0.624 min) RK-2-Br-QZ-OH.d
x10 4
316.2856
317.2874
5c
O
O
N
Br
HO

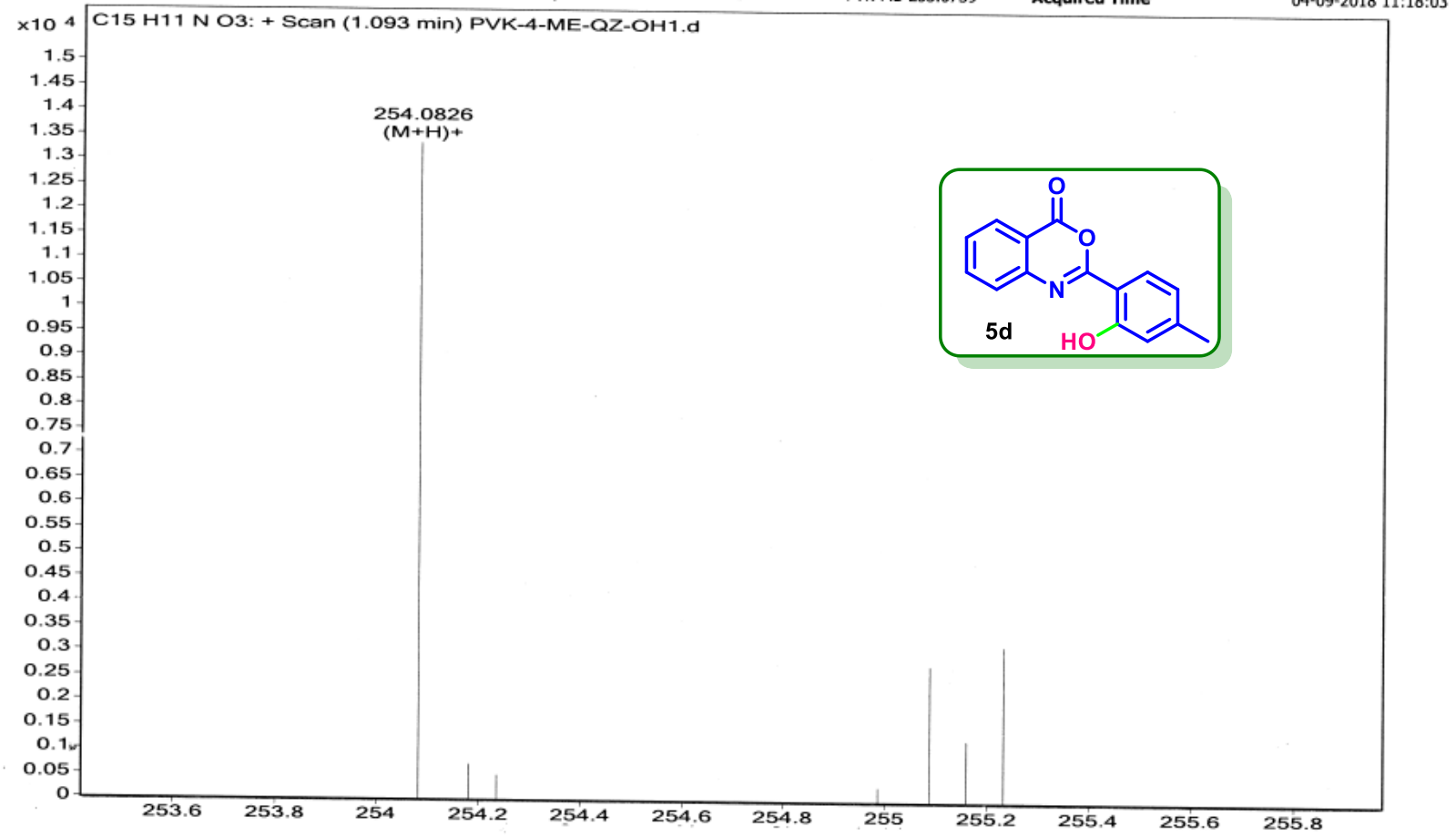


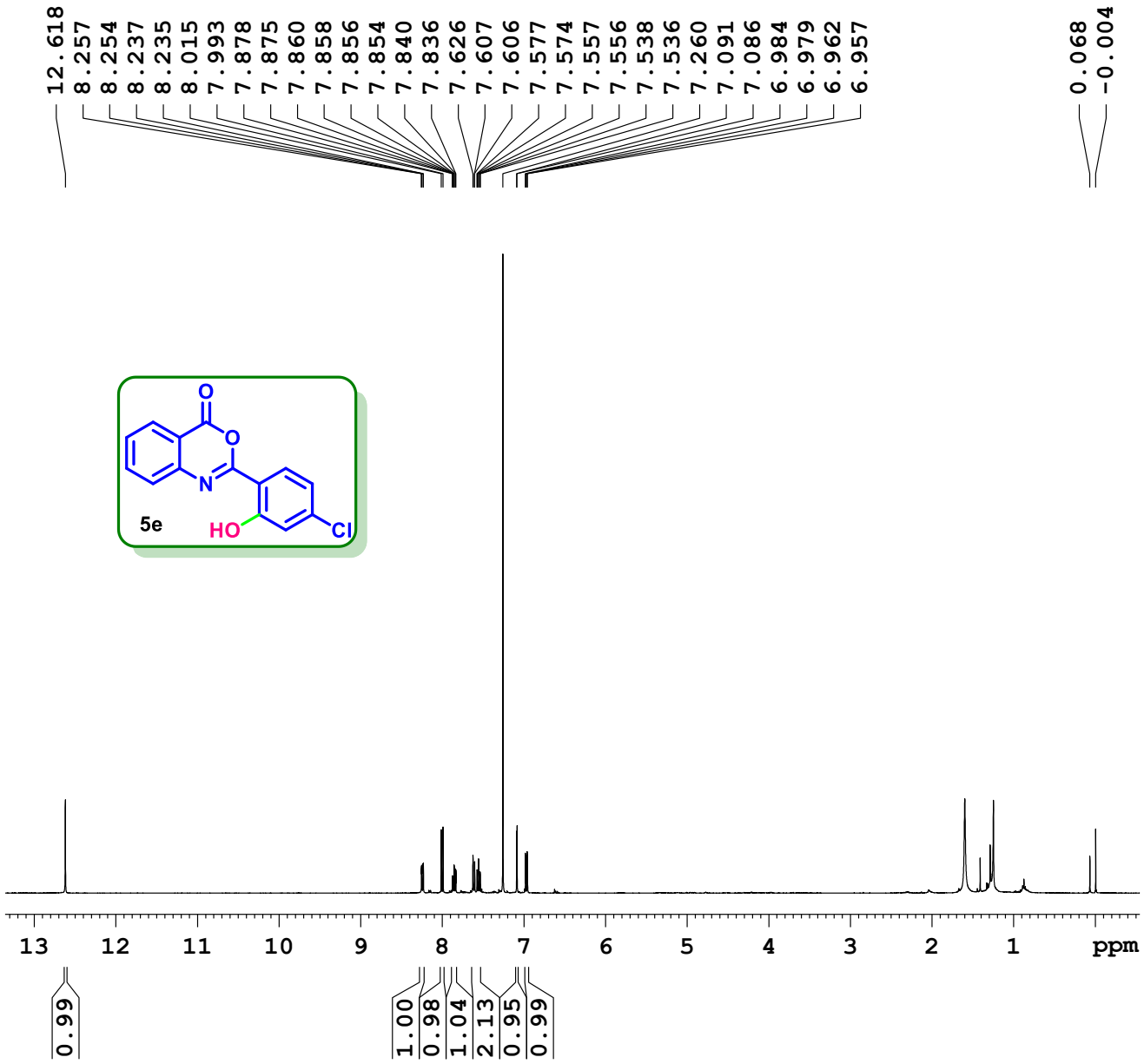

```
Current Data Parameters
NAME       RK-4-Me-Qz-OH
EXPNO                  4
PROCNO                 1

F2 - Acquisition Parameters
Date_           20180617
Time               17.30
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                290.5 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
```



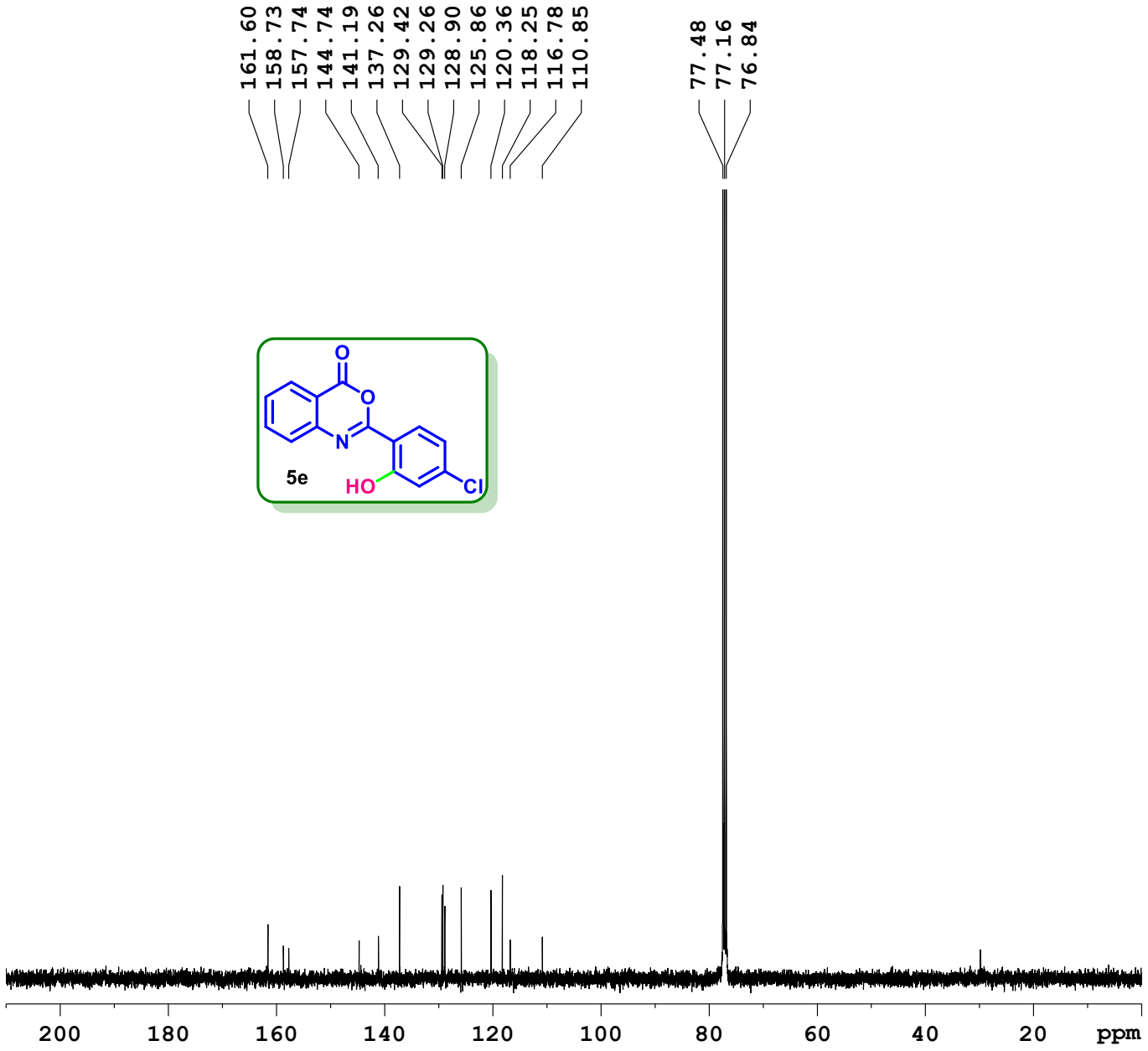

```
Current Data Parameters
NAME      RK-4-Me-Qz-OH
EXPNO                 5
PROCNO                1

F2 - Acquisition Parameters
Date_          20180617
Time              17.51
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                  406
DW               20.800 usec
DE                6.00 usec
TE                290.9 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          100.6127550 MHz
WDW                EM
SSB                 0
LB               1.00 Hz
GB                  0
PC               1.40
```

Sample Name	PVK-4-ME-QZ-OH	**Position**		**Instrument Name**	Q-TOF	**User Name**	QTOF-PU\admin
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	PVK-4-ME-QZ-OH1.d	**ACQ Method**	Pondicherry Universi	**Comment**	PVK-MB-253.0739	**Acquired Time**	04-09-2018 11:18:03



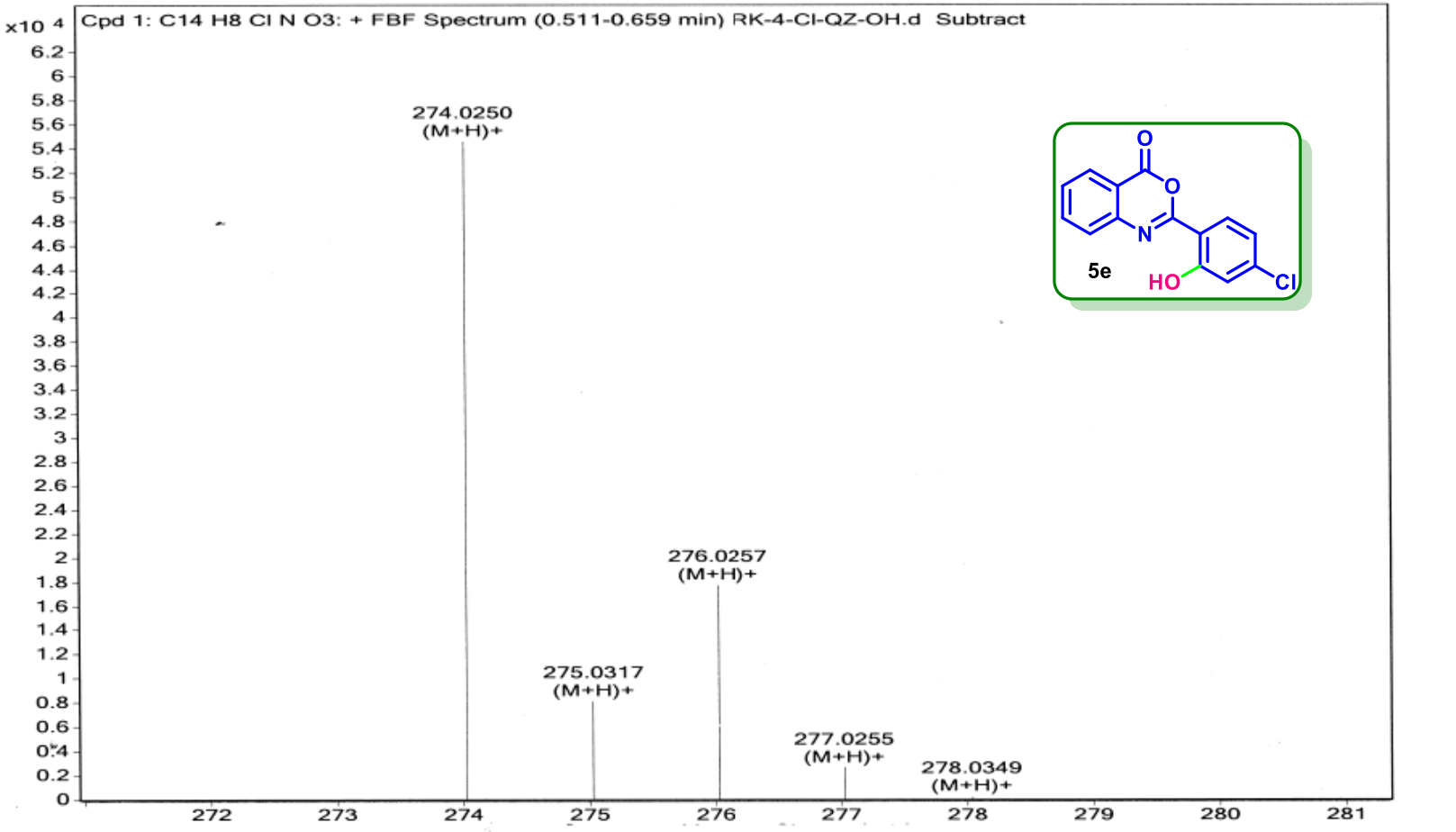


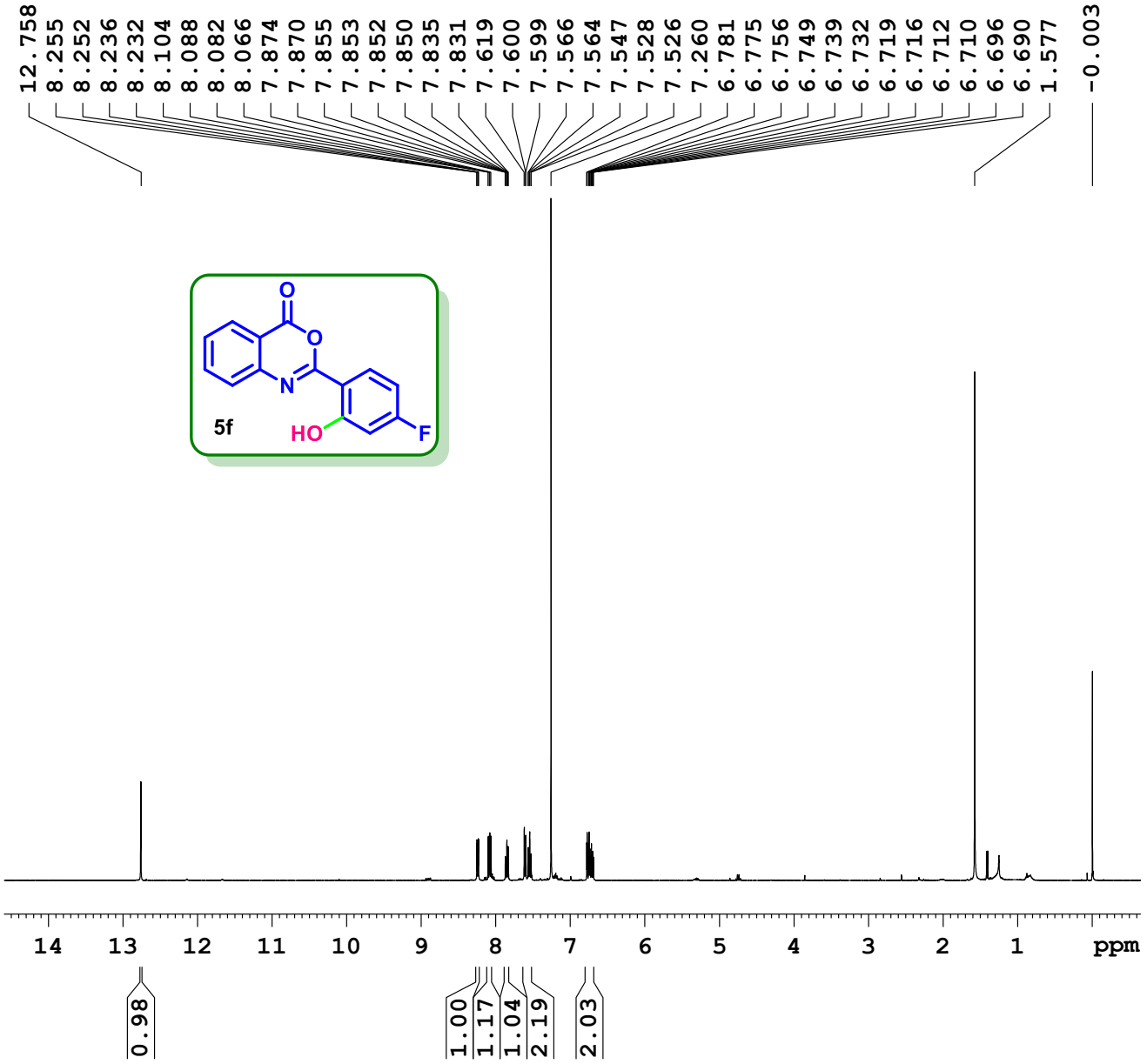

```
Current Data Parameters
NAME      PVK-4-Cl-Qz-OH
EXPNO                  3
PROCNO                 1

F2 - Acquisition Parameters
Date_           20181012
Time               11.43
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG             zg30
TD                 65536
SOLVENT            CDC13
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                295.3 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
```



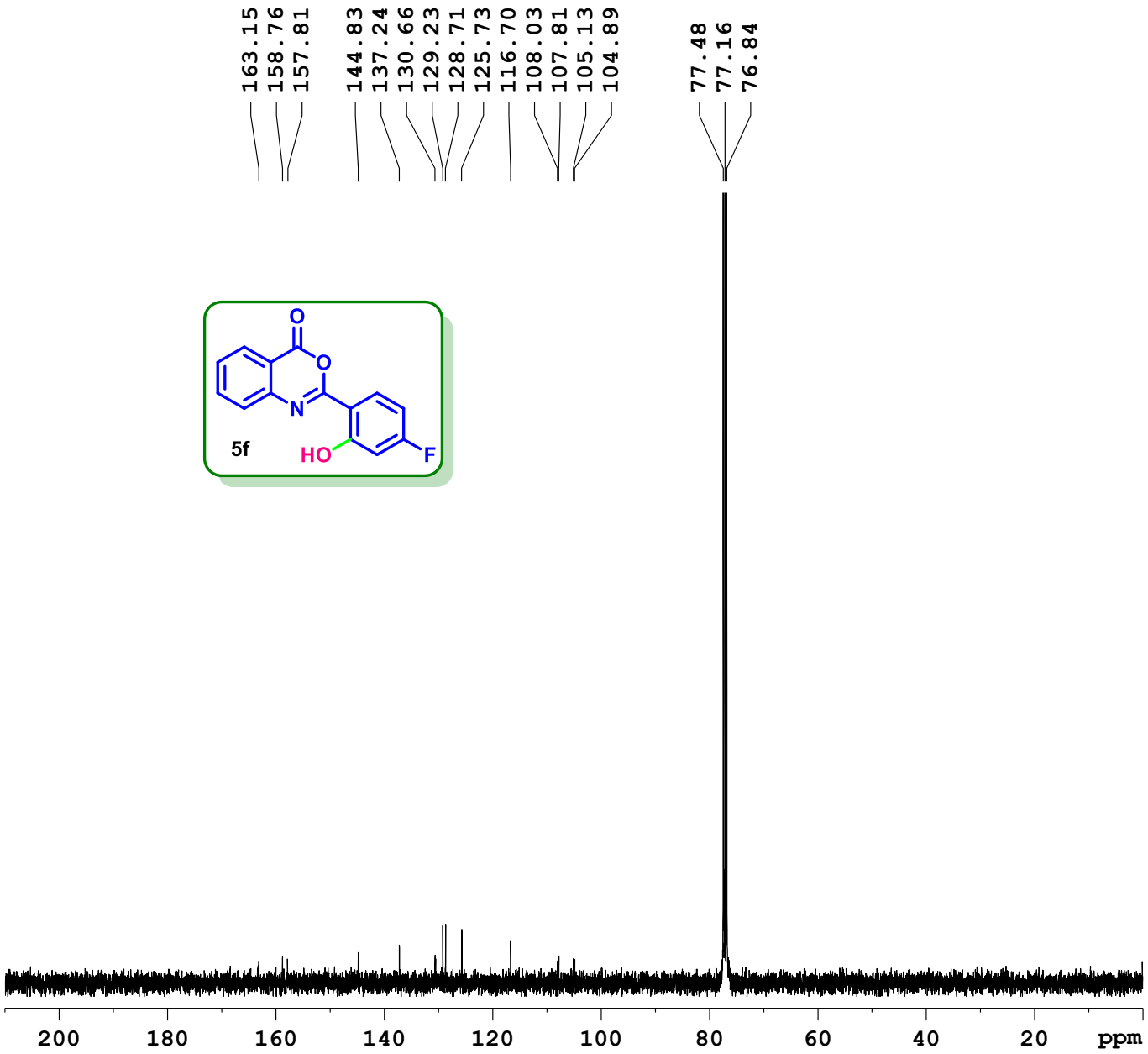

```
Current Data Parameters
NAME      PVK-4-Cl-Qz-OH
EXPNO                  4
PROCNO                 1

F2 - Acquisition Parameters
Date_           20181013
Time               10.23
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                 50.8
DW               20.800 usec
DE                6.00 usec
TE               295.5 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          100.6127538 MHz
WDW                   EM
SSB                    0
LB                1.00 Hz
GB                     0
PC                  1.40
```

ame	RK-4-Cl-QZ-OH	Position		Instrument Name	Q-TOF	User Name	QTOF-PU\admin
	-1	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Filename	RK-4-Cl-QZ-OH.d	ACQ Method	Pondicherry Universi	Comment	PVK-MB-273.0193	Acquired Time	22-10-2018 11:00:42



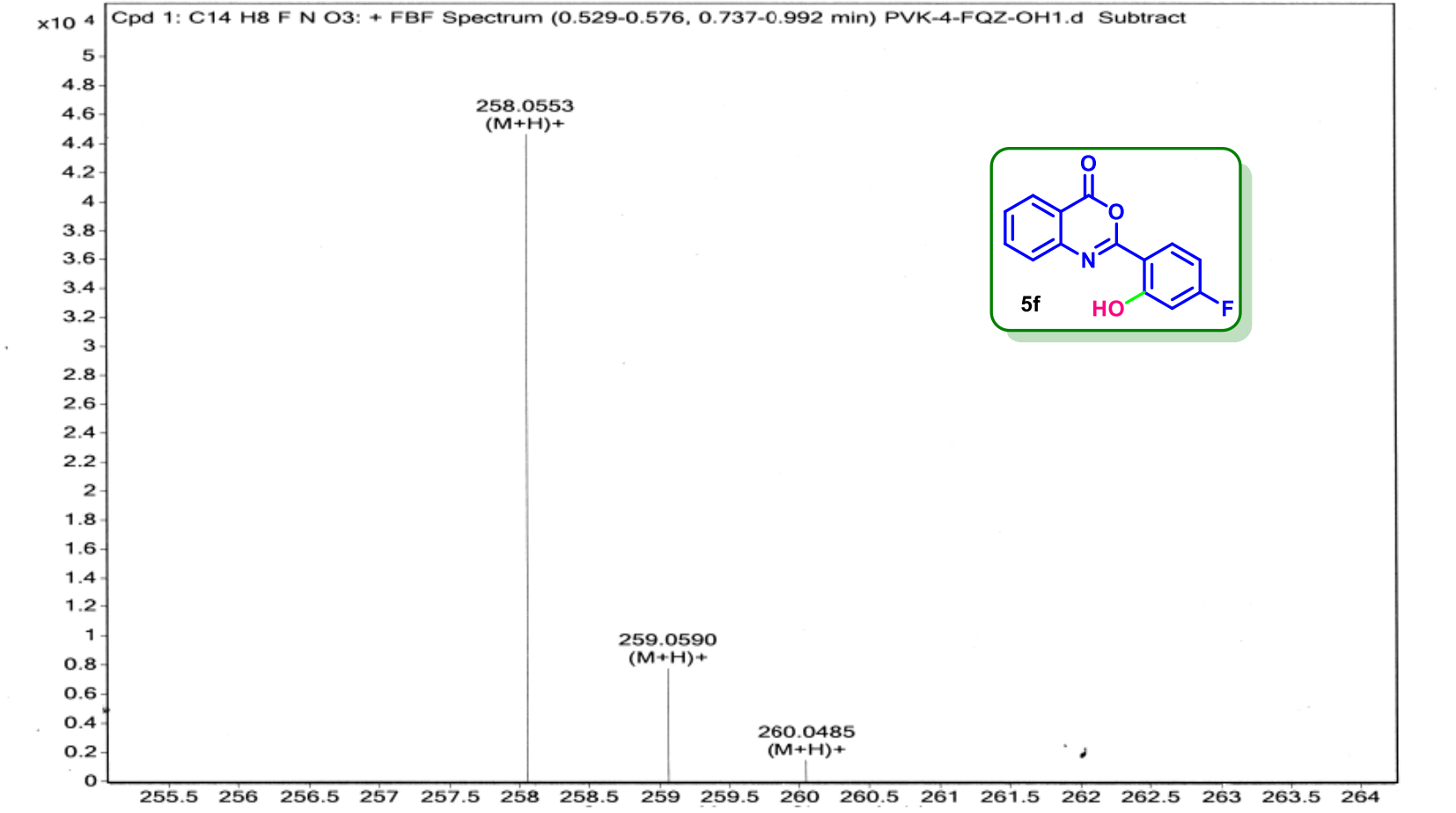


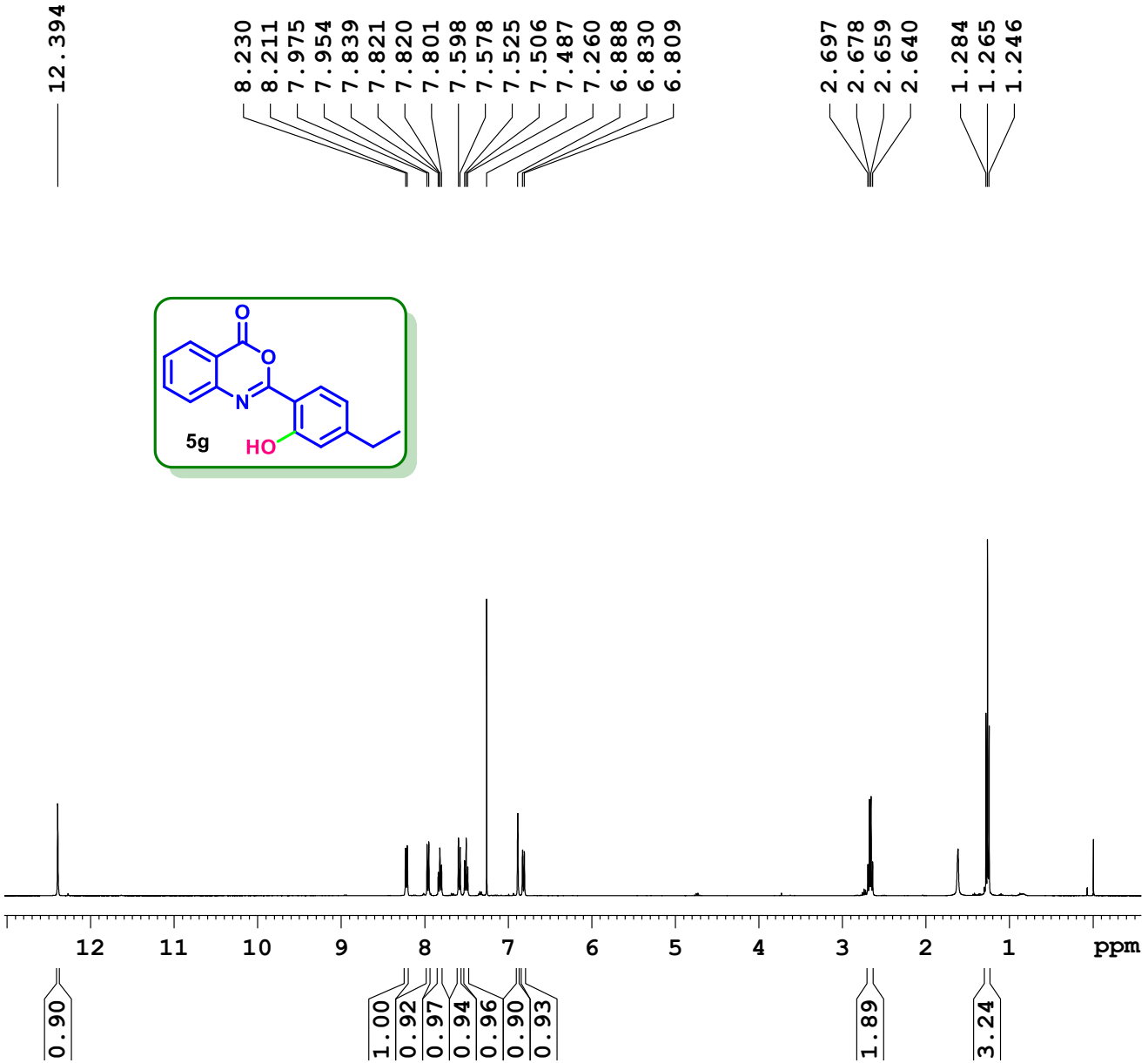

```
Current Data Parameters
NAME      PVK-4-FQZ-OH-R
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20190102
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                   645
DW                60.800 usec
DE                 6.00 usec
TE                294.1 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          400.1300048 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```



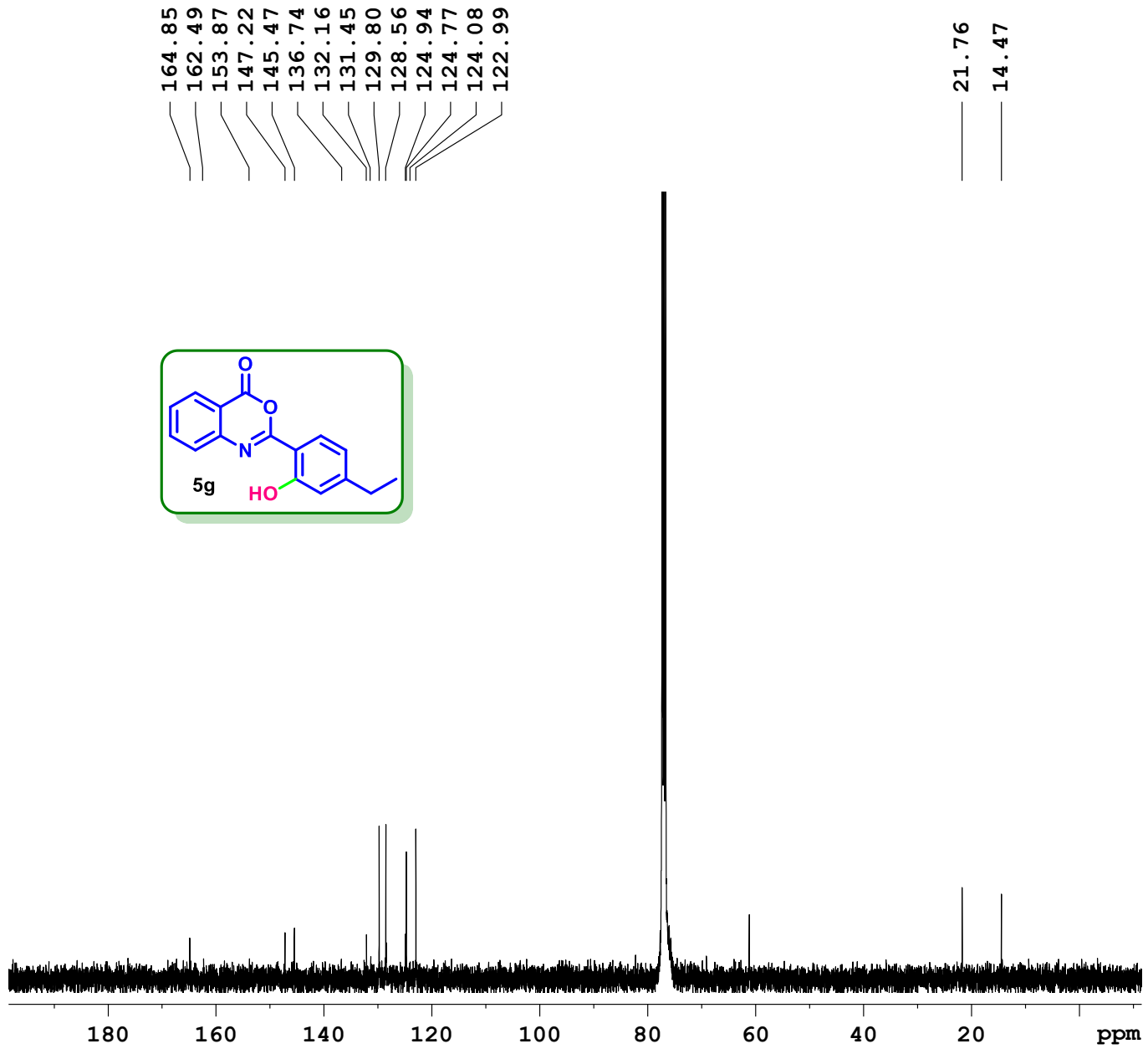

```
Current Data Parameters
NAME      PVK-4-F-QZ-OH-R
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_           20190103
Time              10.29
INSTRUM           spect
PROBHD   5 mm BBO BB-1H
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  736
DS                    4
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ             1.3631988 sec
RG                 45.2
DW                20.800 usec
DE                 6.00 usec
TE                293.9 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           100.6127543 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

Sample Name	PVK-4-FQZ-OH	**Position**		**Instrument Name**	Q-TOF	**User Name**	QTOF-PU\admin
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	PVK-4-FQZ-OH1.d	**ACQ Method**	Pondicherry Universi	**Comment**	PVK-MB-257.0488	**Acquired Time**	03-01-2019 12:19:09



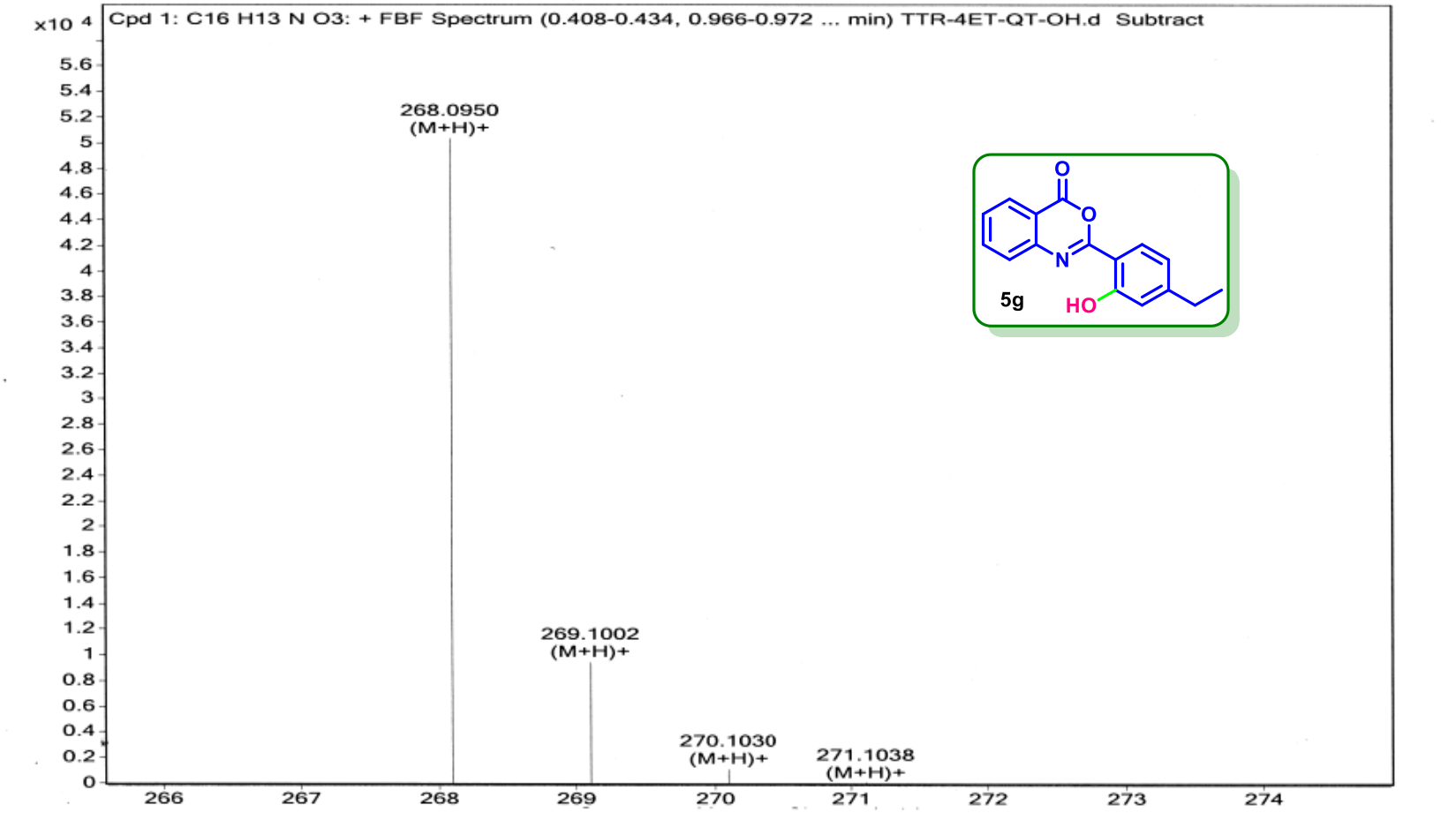


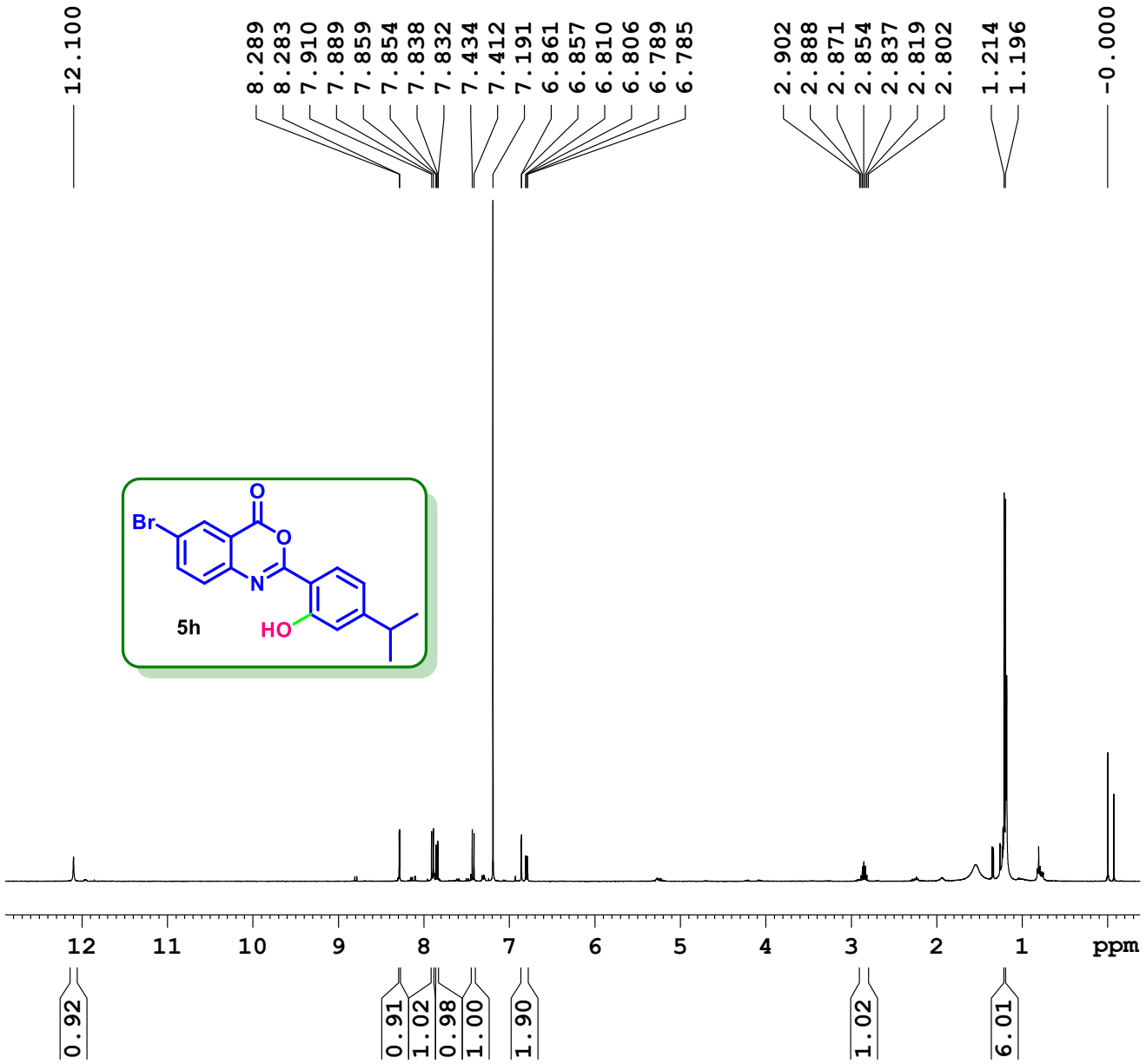

```
Current Data Parameters
NAME      TTR-4-ET-QZ-OH
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20181218
Time               15.08
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                   256
DW                60.800 usec
DE                 6.00 usec
TE                295.1 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          400.1300048 MHz
WDW                   EM
SSB                    0
LB                0.30 Hz
GB                     0
PC                1.00
```



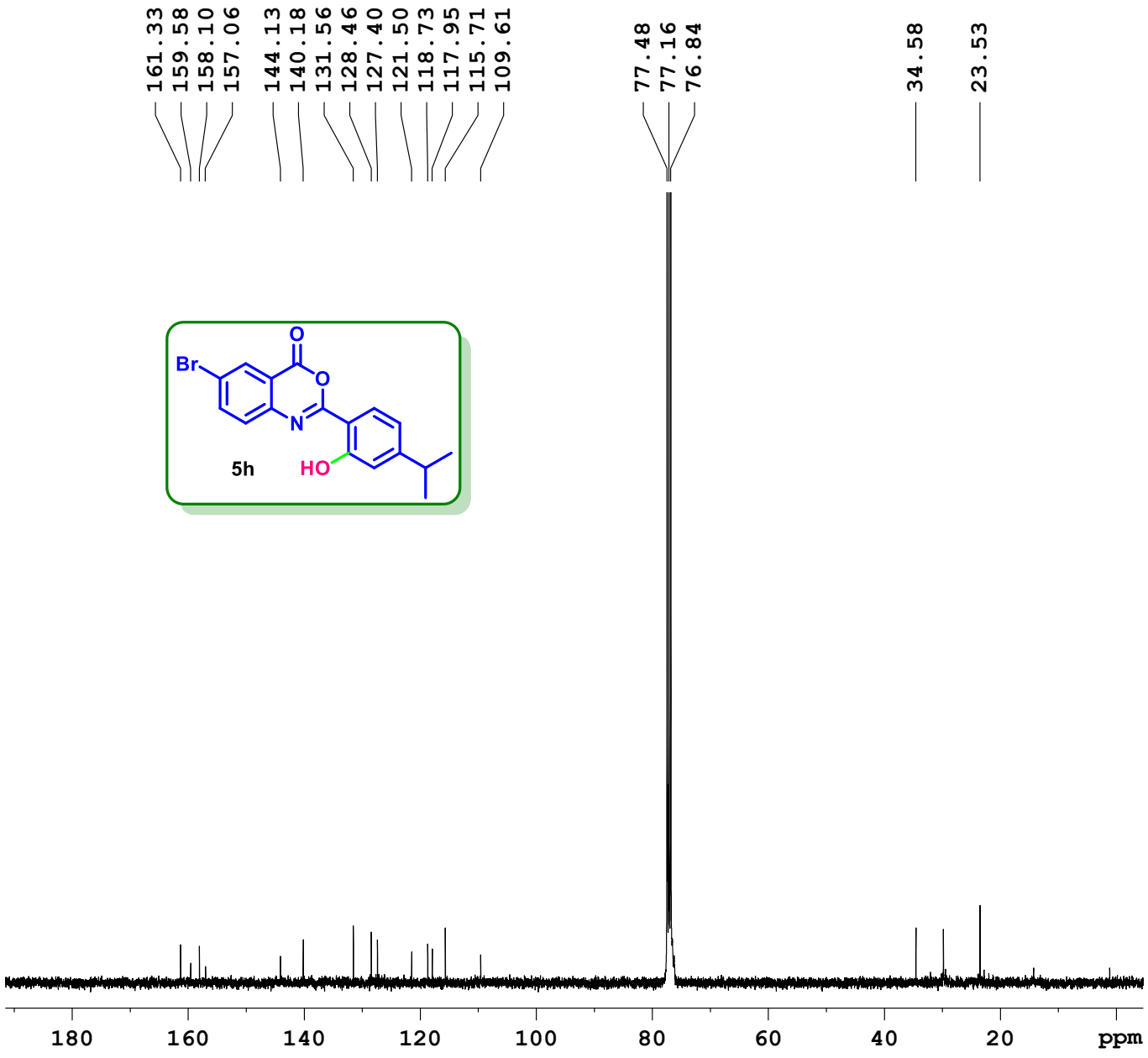

```
Current Data Parameters
NAME       TTR-4ET-QZ-OH
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20181230
Time                6.18
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG          zgpg30
TD                65536
SOLVENT            CDCl3
NS                 6500
DS                    4
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ             1.3631988 sec
RG                  512
DW                20.800 usec
DE                 6.00 usec
TE                290.6 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          100.6127690 MHz
WDW                   EM
SSB                    0
LB                 1.00 Hz
GB                     0
PC                 1.40
```

Sample Name	TTR-4ET-QT-OH	**Position**		**Instrument Name**	Q-TOF	**User Name**	QTOF-PU\admin
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	TTR-4ET-QT-OH.d	**ACQ Method**	Pondicherry Universi	**Comment**	TTR-MB-267.0895	**Acquired Time**	18-12-2018 15:09:35



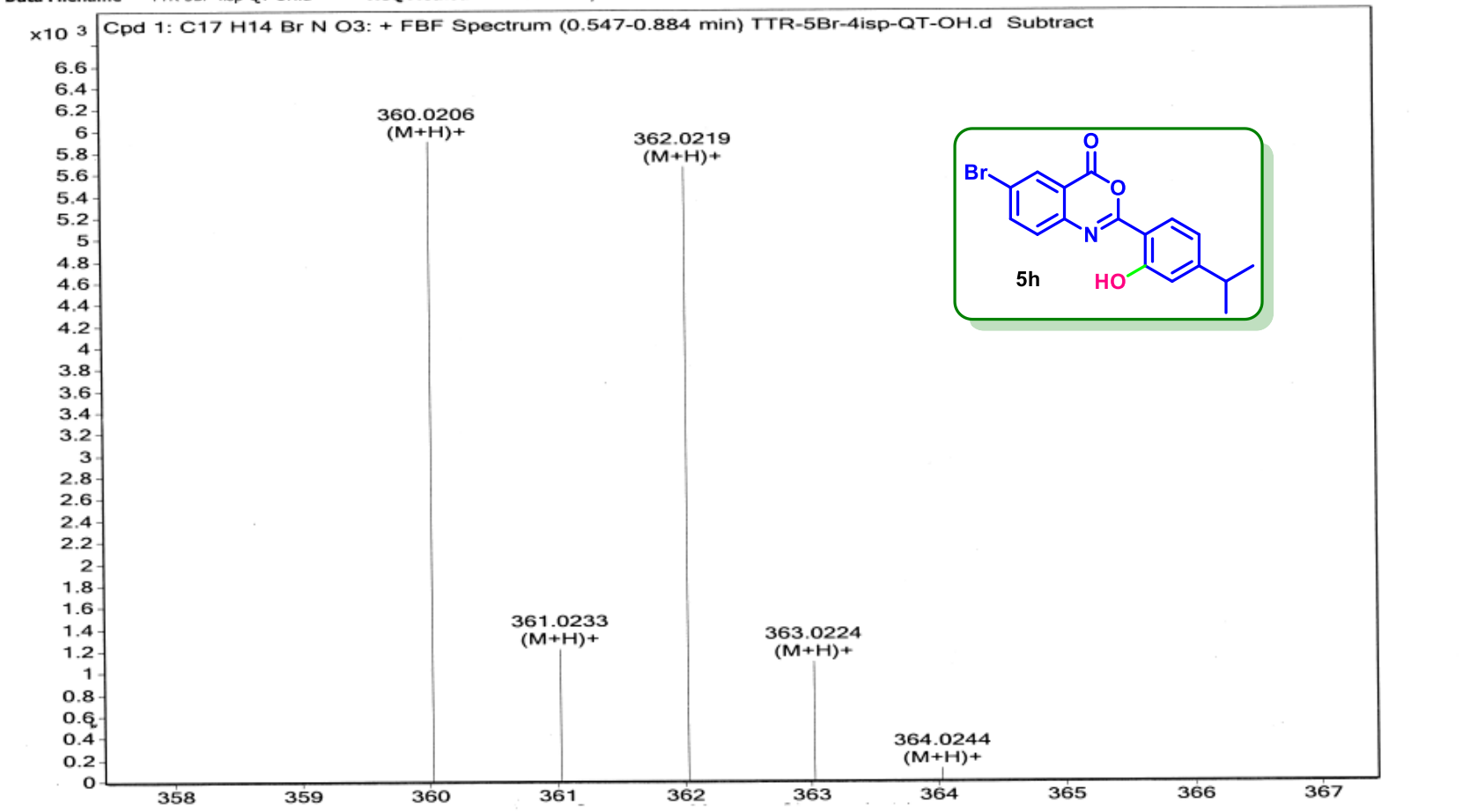


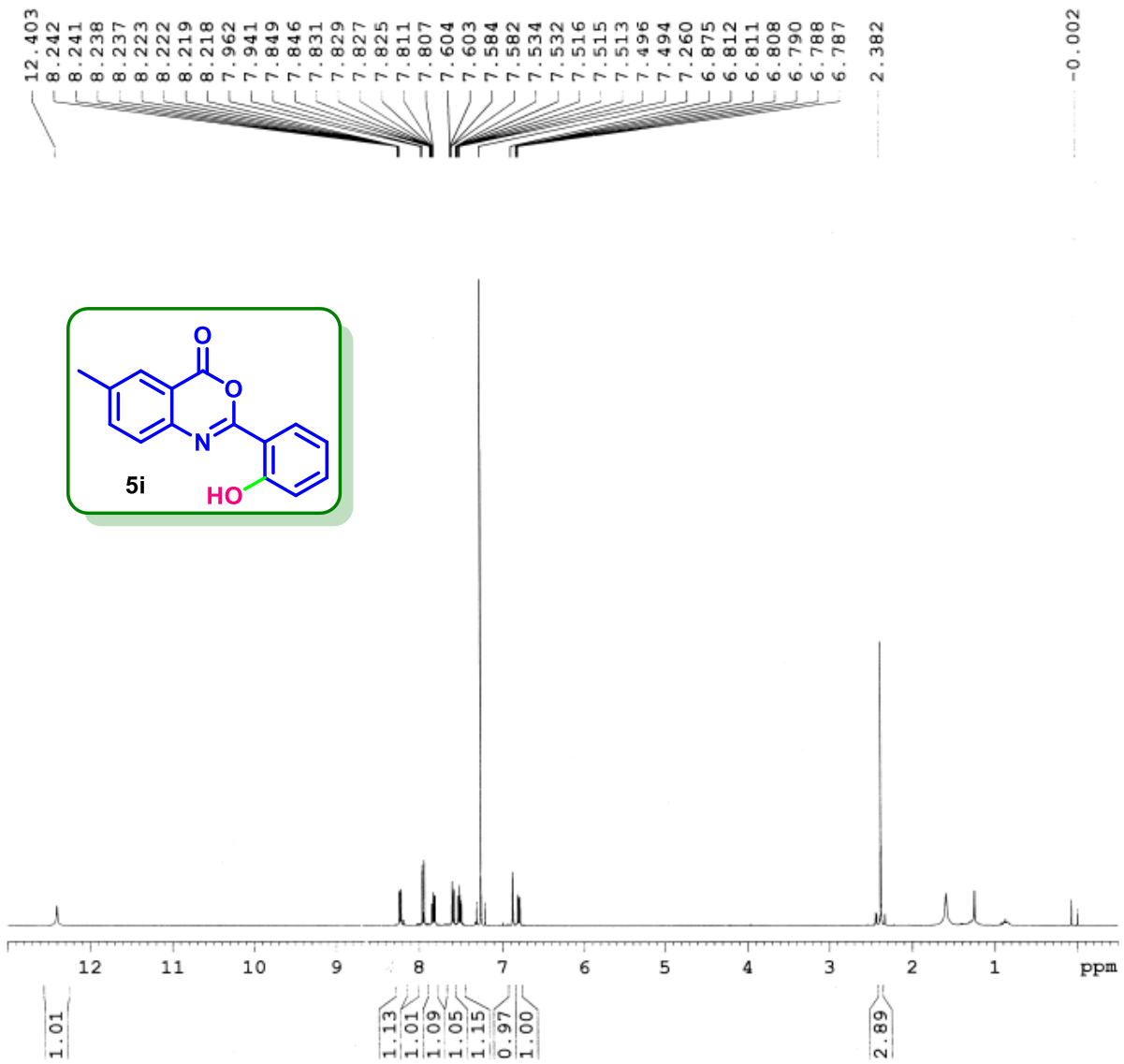

```
Current Data Parameters
NAME      PVK-5Br-4ISP-QZ-OH
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_             20181219
Time                 19.15
INSTRUM              spect
PROBHD    5 mm BBO BB-1H
PULPROG               zg30
TD                   65536
SOLVENT              CDC13
NS                      16
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                  295.0 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            400.1300323 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.00
```



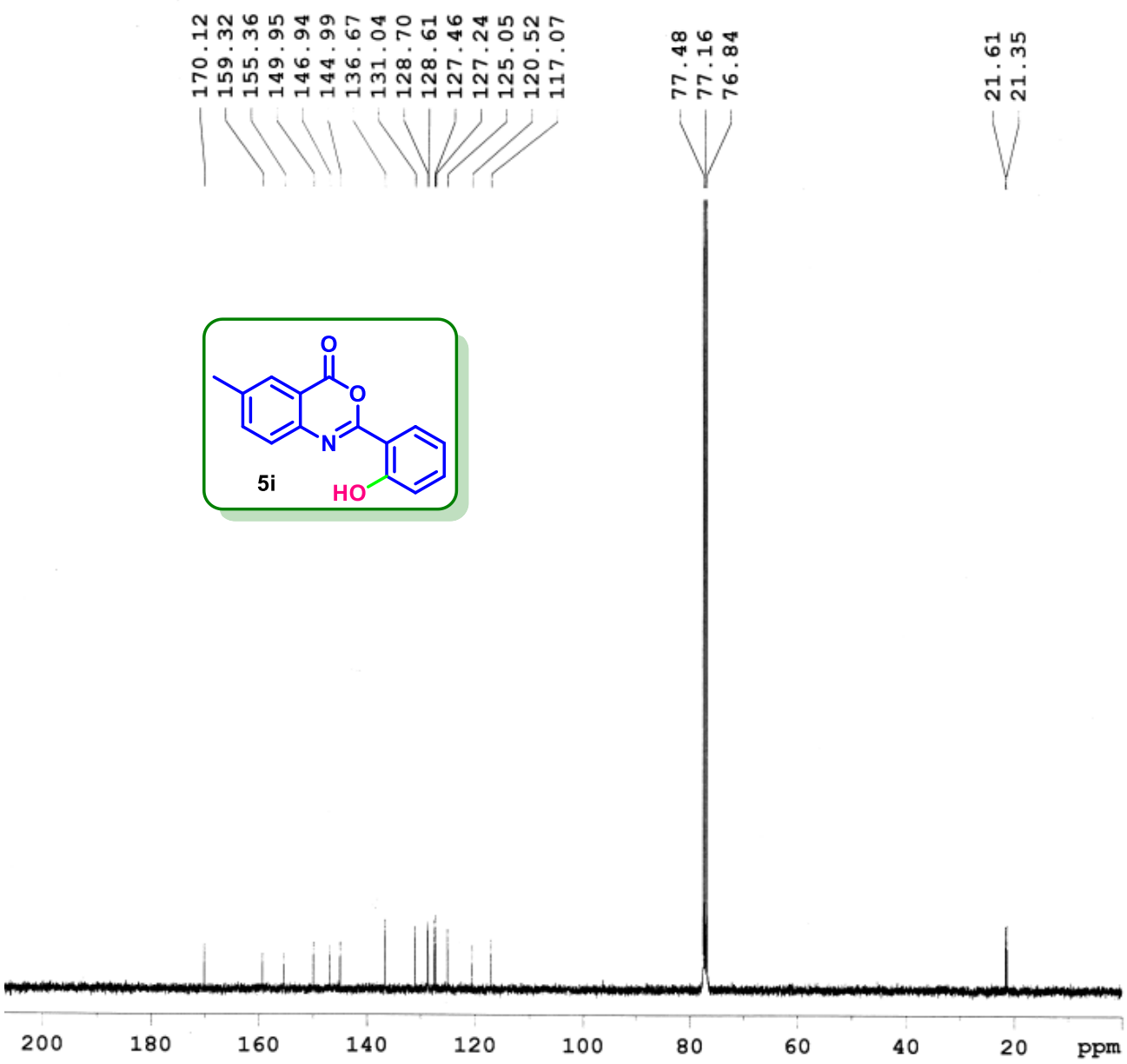

```
Current Data Parameters
NAME      PVK-5Br-4ISP-QZ-OH
EXPNO                      2
PROCNO                     1

F2 - Acquisition Parameters
Date_              20181220
Time                   2.53
INSTRUM               spect
PROBHD    5 mm BBO BB-1H
PULPROG              zgpg30
TD                    65536
SOLVENT               CDCl3
NS                     8000
DS                        4
SWH              24038.461 Hz
FIDRES            0.366798 Hz
AQ                1.3631988 sec
RG                     45.2
DW                   20.800 usec
DE                    6.00 usec
TE                   290.5 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            100.6127549 MHz
WDW                       EM
SSB                        0
LB                    1.00 Hz
GB                         0
PC                     1.40
```

. ample Name	TTR-5Br-4isp-QT-OH	**Position**		**Instrument Name**	Q-TOF	**User Name**	QTOF-PU\admin
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	TTR-5Br-4isp-QT-OH.d	**ACQ Method**	Pondicherry Universi	**Comment**	TTR-MB-359.0157	**Acquired Time**	18-12-2018 15:03:53



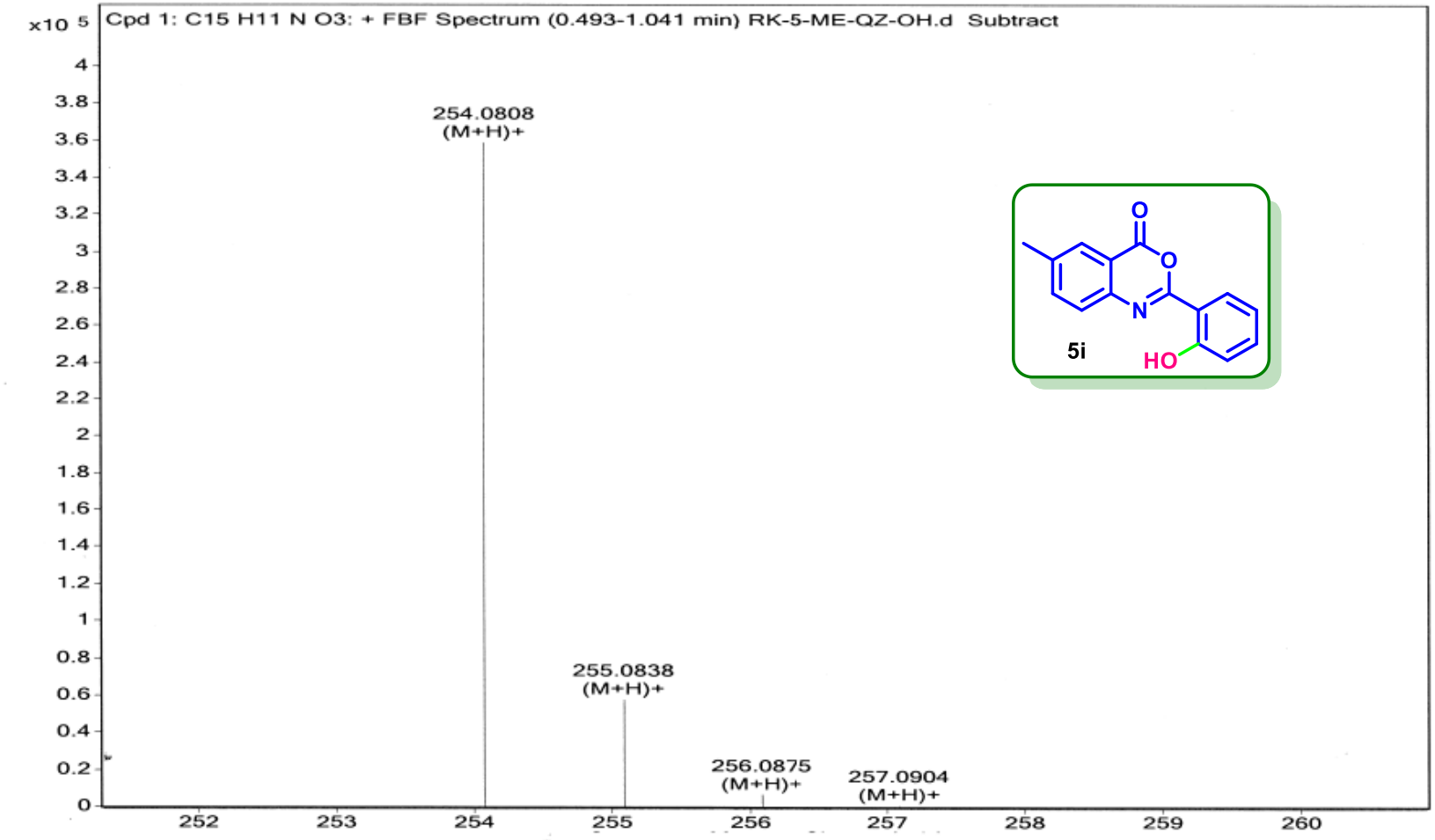


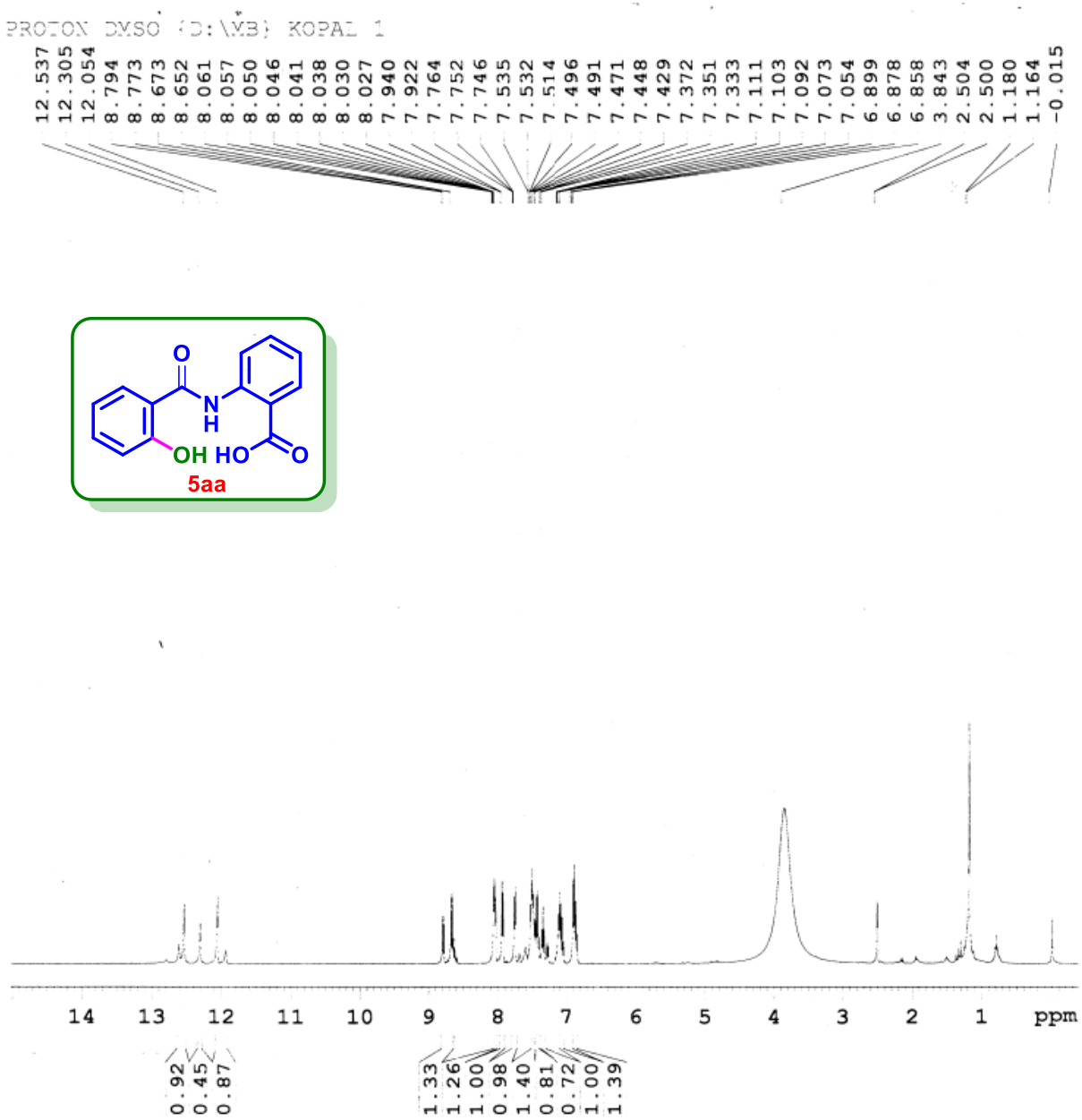

```
Current Data Parameters
NAME                  RK-5ME-QZ-OA
EXPNO                            1
PROCNO                           1

F2 - Acquisition Parameters
Date_                     20190408
Time                         16.43
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                          294.8 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                    400.1300094 MHz
WDW                             EM
SSB                              0
LB                            0.30 Hz
GB                               0
PC                            1.00
```



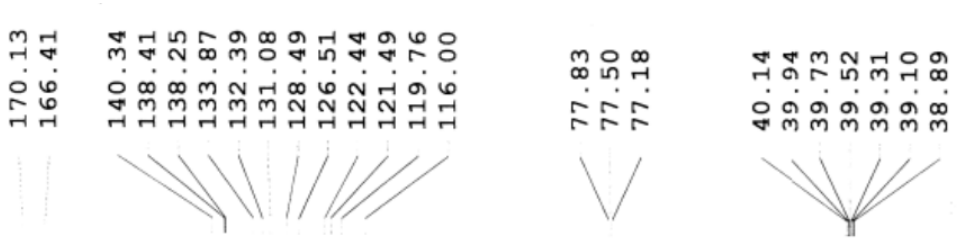

```
Current Data Parameters
NAME      RK-5-ME-QZ-OAC
EXPNO                  3
PROCNO                 1

F2 - Acquisition Parameters
Date_           20190408
Time              18.30
INSTRUM           spect
PROBHD   5 mm BBO BB-1H
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  765
DS                    4
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3631988 sec
RG                 45.2
DW                20.800 usec
DE                 6.00 usec
TE                295.0 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          100.6127557 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

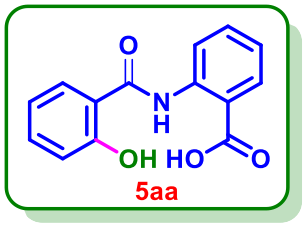
Sample Name	RK-5-ME-QZ-OH	**Position**		**Instrument Name**	Q-TOF	**User Name**	QTOF-PU\admin
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	RK-5-ME-QZ-OH.d	**ACQ Method**	Pondicherry Universi	**Comment**	RK-CRR-253.0739	**Acquired Time**	09-04-2019 12:27:01

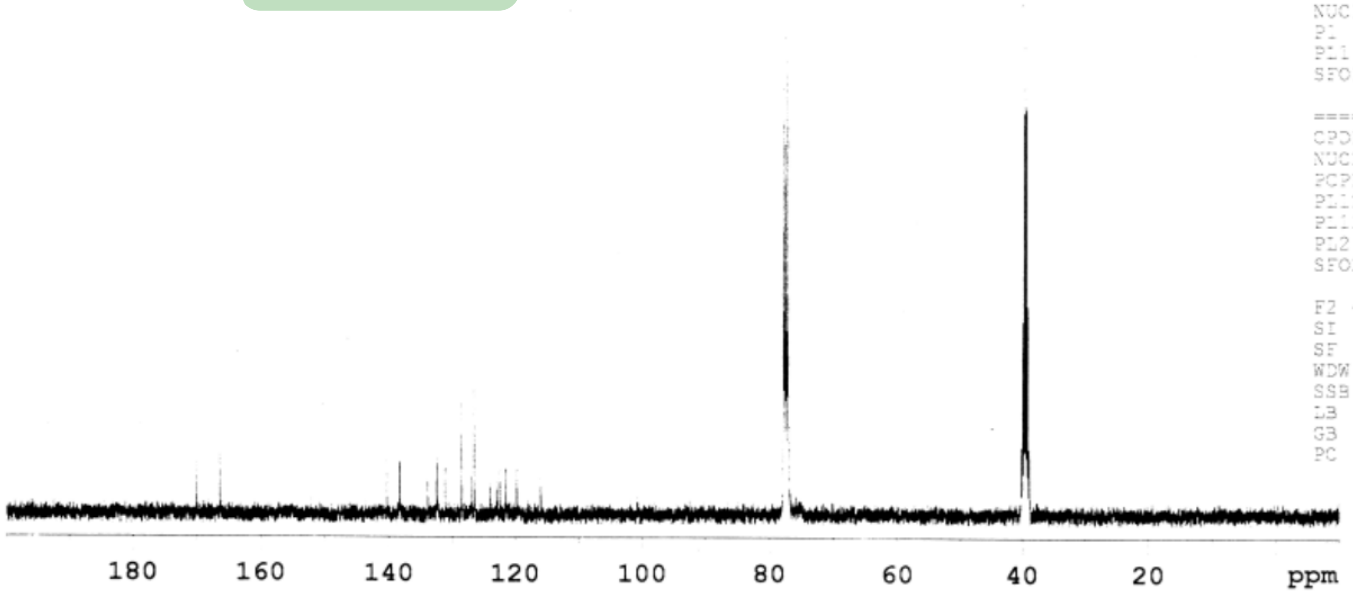





```
Current Data Parameters
NAME      PVK-QUNZ-OH-HYDL
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_           20180726
Time                11.29
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                   228
DW                  60.800 usec
DE                   6.00 usec
TE                  294.8 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           400.1299970 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```








```
Current Data Parameters
NAME      PVK-QUNZ-OH-HYDL
EXPNO                    4
PROCNO                   1

F2 - Acquisition Parameters
Date_             20180727
Time                 13.21
INSTRUM              spect
PROBHD   5 mm BBO BB-1H
PULPROG             zgpg30
TD                   65536
SOLVENT                DMSO
NS                     1024
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                   295.9 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            100.6128176 MHz
WDW                       EM
SSB                        0
LB                      1.00 Hz
GB                         0
PC                      1.40
```

Sample Name	QUNZ-OH-HYDL	**Position**		**Instrument Name**	Q-TOF	**User Name**	QTOF-PU\admin
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	QUNZ-OH-HYDL.d	**ACQ Method**	Pondicherry Universi	**Comment**	PVK-MB-257.0688	**Acquired Time**	27-07-2018 14:29:13